# Application of the Recurrence Relations Method to a Many Body Model for the Study of Irreversibility and Ergodicity

by

Eduardo Pestana Mariño

(Under the direction of M. Howard Lee)

## Abstract

In the context of linear response theory, by means of the Recurrence Relations Method, (RRM), we find exact solutions for the relaxation function and the memory function of an harmonic oscillator chain in thermal equilibrium with one end fixed. We study the analytical properties of these solutions and show that they can exhibit reversible-non-ergodic, irreversible-non-ergodic, and irreversible-ergodic behaviors.

Index words: Statistical Mechanics, Recurrence Relations Method, Harmonic Oscillators Chain, Linear Chain, Ergodic Hypotheses, Ergodicity, Relaxation function, Memory Function, Deltas Sequences

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# Chapter 1

## Introduction

In this work we consider an either, finite or infinite, linear chain of harmonic oscillators with one end fixed. The chain is in thermal equilibrium, and then an external time-dependent field is applied. Within the context of linear response theory we use the Recurrence Relations Method (RRM) to study the dynamics of the chain. We find *exact* closed solutions for the relaxation function, $a_0(t)$, for particular values of the parameters that describe the linear chain. We also find a closed general solution for the relaxation function $\tilde{a}_0(z)$ and for the memory function $b_1(t)$, both of them valid for any combination of values of the parameters of the chain. We study the relation between the singularities and analytical properties of these solutions and the dynamics of chain. We find that the chains can exhibit reversible-non-ergodic, irreversible-non-ergodic, and irreversible-ergodic behaviors.

We review M. Howard Lee's Recurrence Relations Method (RRM) in Chapter §2. In §2.2 we present the concept of the *realized space* of a dynamical variable. A key feature of the RRM is that the actual calculations are carried out in this model-dependent *realized space* of a dynamical variable of interest, rather than in some general abstract space. The ensuing simplifications have allowed the finding of *exact*[1] solutions to dynamical problems in statistical physics. The orthogonalization of this space and the definition of the Deltas, that constitute the basis of the Recurrence Relations Method, are presented in §2.3. The time evolution of the chosen dynamical variable and the resulting RR1 and RR2 calculation schemes are reviewed in §2.4. In §2.5 the concept of subspaces in the RRM is presented.

[1] Or *exact* in some limit or range of the parameters of the model

We review some previous applications of the Recurrence Relations Method. Chapter 3 is about the electron gas with $k \ll k_F$ in the ground state, except in §3.4, where an asymptotic expansion for the dynamic structure factor of the 3D electron gas, valid for $k \gg k_F$ is considered.

In Chapter 4 we review the work by M. Howard Lee, I. M. Kim and Raf Dekeyser on the spin-$\frac{1}{2}$ anisotropic Heisenberg model in infinite lattice dimensions [Lee, Kim & Dekeyser 1984]. This system is an instance (it is shown in Chap. 4 that it becomes the spin van der Waals model) of certain statistical mechanics models that are exactly solvable at some special limits, providing useful insight into the behavior of these models [Lee, Kim & Dekeyser 1984], [Baxter 1982].

The concept of *Dynamical Equivalence* (DE) is described in Chapter 5. Loosely put, if the relationships among the set of recurrants or Delta's of two physical systems are the same, the time evolutions of the systems will be identical aside from a time-scale factor. Thus, two totally different physical systems may share the same time dependence for a particular choice of the corresponding dynamic variables. As an example we review two dynamical equivalences between the one dimensional (1-D) spin-$\frac{1}{2}$ XY model and the spin van der Waals model.

In Chapter 6 we review a previous application of the RRM to harmonic oscillators chains. Following Lee, Florencio & Hong [1989], we show that the 2D electron gas model of §3.2 and the classical harmonic oscillator (HO) chain with a tagged mass are dynamically equivalent [see the previous paragraph and §5.1]. Unlike other dynamical equivalences mentioned so far, this is the first between a quantum system: The 2D electron gas, and a classical system: The harmonic oscillator chain.

Our model for the linear chain of harmonic oscillators (HOC) with an impurity mass at one end that is coupled to a fixed wall (ICFW) is presented in Chapter 7. The parameters and the Hamiltonian are defined in §7.1.

Another model, closely related to ours, is the homogeneous (HOC) with periodic boundary conditions (PBC) or with fixed-ends boundary conditions (FEBC) studied by

Florencio & Lee [1985]. We review this work in §7.2 and we do the delta's calculation for our model in §7.3.

In Chapter 8 we obtain a new exact closed solution for the relaxation function, $a_0(t)$, for a particular set of values of our model parameters. We also show that two previously known solutions of the HOC with PBC or FEBC [see §7.2 and the previous paragraph] are also solutions to our model.

We are able to obtain an exact closed solution for $\tilde{a}_0(z)$ valid for all values our model parameters in Chapter 9. We calculate explicitly this general solution of the relaxation function, $\tilde{a}_0(z)$, by means of the continued fraction representation of $\tilde{a}_0(z)$ provided by the Recurrence Relations Method. We also review some convergence issues and concepts about continued fractions in general.

Again using the continued fraction representation of $\tilde{a}_0(z)$ we obtain in Chapter 10 the general solution for the memory function $\tilde{b}_1(z)$, then by inversion we also obtain the general solution for $b_1(t)$.

The inversion of $\tilde{a}_0(z)$ to get the time-dependent relaxation function, $a_0(t)$ is carried out in Chapter 11 for a subset of the parameters of our model.

The long time behavior of the solutions is considered in Chapter 12. Here we show that the non-ergodic behavior of the chain can be reversible or irreversible, while the ergodic behavior is irreversible.

# Chapter 2

# The Recurrence Relations Method (RRM)

## 2.1 Introduction

To obtain the dynamical behavior of the linear chain of harmonic oscillators (or any other many body system) a Heisenberg type equation of motion for a relevant dynamic variable[1] must be solved [Balucani, Lee & Tognetti 2003]. Since this is an operator equation it is difficult to extract physical content out of the equation even when a model is already explicitly defined as in our case. Mori made significant advances in this problem around 1965. He was able to transform Heisenberg's equation of motion into a form that was more transparent and tractable that resembled Langevin's equation, a phenomenological equation famous as a model for Brownian motion. The resemblance was so strong that Mori's equation became known as the "generalized Langevin equation" (GLE) a somewhat unfortunate happenstance for the clarity of the physics involved. Mori's work was a big breakthrough, but his original derivation neither simple nor transparent requiring considerable formal analysis [Balucani, Lee & Tognetti 2003, §1.1.1, p 412; §3]. Essentially the derivation is based on an orthogonalization process, the Mori-Zwanzig (M–Z) projection operator formalism that basically is a Gram-Schmidt orthogonalization process in the theory of Hilbert spaces. In this approach a Hilbert space is introduced but it remains "unrealized" in the sense that the motion takes place in an abstract space [Balucani, Lee & Tognetti 2003, §3].

[1] If, for example, the system is perturbed by a time dependent field that couples to the physical variable $A$ the response of the system is proportional to $(A, A(t))$ where $(X, Y)$ denotes the Kubo scalar product defined below. Here the time dependence $A(t)$ of the physical variable $A$ is given by the its Heisenberg equation written with the unperturbed Hamiltonian of the system

The recurrence relations formalism was developed in the early 1980's to solve Heisenberg's equation of motion directly, it is an exact approach from which the GLE can also be obtained through a more simple and transparent derivation. The basis of the RRM is also an orthogonalization procedure. In contrast to Mori's approach the inner product depends on the model Hamiltonian and thus the space is "realized" and characterized by the model dependent dimensionality $d$ obtained from the orthogonalization procedure. Hence the evolution becomes model dependent from the outset. If $d$ as determined form the model is finite, the trajectory turns out to be closed and the motion is periodic. If $d$ is not finite, the trajectory is open, and the motion is non-periodic. In other words the time evolution of a Hermitian system is sensitive to $d$ and is determined by the shape of the realized space.

## 2.2 Realized space and physical interpretation of the time evolution of a dynamical variable

The inner product used in the recurrence relations formalism is the Kubo scalar product defined for a pair of arbitrary operators $X$ and $Y$ as

$$(X,Y) = \int_0^\beta \langle \mathrm{e}^{\lambda H} X^\dagger \mathrm{e}^{-\lambda H} Y \rangle \mathrm{d}\lambda - \beta \langle X^\dagger \rangle \langle Y \rangle \,, \tag{2.1}$$

where $\beta$ is the inverse temperature and the brackets are ensemble averages with the density matrix of a given Hamiltonian $H$ assumed to Hermitian, i.e.

$$\langle \quad \rangle \equiv \frac{\mathrm{Tr}(\quad \mathrm{e}^{-\beta H})}{\mathrm{Tr}(\mathrm{e}^{-\beta H})} \tag{2.2}$$

The realized space $\mathcal{S}$ of a dynamical variable $A$ is spanned by a set of $d$ vectors $f_0, f_1, \ldots, f_{d-1}$. These basis vectors must be linearly independent, i.e. complete, and orthogonal. The *basis vectors* $\{f_\nu\}$ and their associated *basis functions* $\{a_\nu(t)\}$ are defined through the fundamental expansion

$$A(t) = \sum_{\nu=0}^{d-1} a_\nu(t) f_\nu \tag{2.3}$$

of the solution of the Heisenberg equation for $A$

$$\frac{\mathrm{d}A(t)}{\mathrm{d}t} \equiv \dot{A}(t) = \frac{\mathrm{i}}{\hbar}[H, A(t)]. \tag{2.4}$$

Here, again, $H$ is a given Hamiltonian, for example in the context of linear response theory, $H$ would be the unperturbed Hamiltonian of the system. If both sets, the basis vectors $\{f_\nu\}$ and the associated basis functions $\{a_\nu(t)\}$ are known, the expansion (2.3) is in effect the solution of the Heisenberg equation of motion for $A$, Eq. (2.4). Below in §2.3 and §2.4 we will present a method, the RR1 and RR2 calculation schemes, to obtain the sets $\{f_\nu\}$ and $\{a_\nu(t)\}$.

The definition of the realized space of a dynamical variable allows the following physical interpretation of the time evolution spanned by its Heisenberg equation.

Let us assume the dynamical variable is $A$ and let's denote its realized space by $\mathcal{S}$. Then $A(t)$ is a vector in its realized space. It is easily shown that if the system is Hermitian the norm of $A(t)$, calculated with the inner product of $\mathcal{S}$ defined in (2.1) (Kubo's scalar product), is a constant of the motion

$$(A(t), A(t)) = (A, A). \tag{2.5}$$

Since the norm of $A(t)$ cannot change, $A(t)$ can only change its direction. As $t$ increases, on the hyper-surface of $\mathcal{S}$ the vector $A(t)$ delineates a trajectory that clearly depends on the shape of $\mathcal{S}$. Let $d$ be the dimension of $\mathcal{S}$ (we will show below that $d$ is model dependent and can be either finite or denumerably infinite). If $d$ is finite the trajectory traced by $A(t)$ on the hypersurface of $\mathcal{S}$ is closed otherwise it will be open. The detailed shape of $\mathcal{S}$ also, in general, depends on the temperature: Kubo's scalar product (2.1) depends on three ensemble averages.

## 2.3 Orthogonalization and the RR1 scheme

Let $\mathcal{S}$ be an inner product space realized by the Kubo's scalar product defined in (2.1). It can be shown [Lee 1982*b*] that the basis vectors $\{f_m\}$ that completely span $\mathcal{S}$ must satisfy the following *three-term recurrence relation*, that henceforth will be referred as RR1:

$$f_{\nu+1} = \dot{f}_\nu + \Delta_\nu f_{\nu-1}, \tag{2.6a}$$

for $\nu = 0, 1, \ldots, d-1$. Here $\dot{f} \equiv (\mathrm{i}/\hbar)[H, f]$, $d$ is the dimension of $\mathcal{S}$, the space spanned by the $f_\nu$, and

$$\Delta_\nu \equiv \begin{cases} 1 & \nu = 0, \\ (f_\nu, f_\nu)/(f_{\nu-1}, f_{\nu-1}) & \nu = 1, \ldots, d-1. \end{cases} \tag{2.6b}$$

To avoid ambiguities, since there are only $d$ basis vectors $f_0, f_1, \ldots, f_{d-1}$, we set $f_{-1} \equiv 0$ and $\Delta_0 \equiv 1$. The set $\{\Delta_m\}$ is known as the *recurrants*.

This three term recurrence relation can be obtained by considering a complete set

$$\mathcal{A} = \{A^{(0)}, A^{(1)}, A^{(2)}, \ldots, A^{(\nu)}, \ldots\}$$

in $\mathcal{S}$, where

$$A^{(\nu)} = (\frac{\mathrm{i}}{\hbar} L)^\nu A,$$

$LA \equiv [H, A]$, and $0 \leq \nu$. Then by applying an orthogonalization process on the set $\mathcal{A}$ the three term recurrence relation (2.6a) for the $\{f_\nu\}$, known as the RR1, is obtained [Lee 1982*b*].

Eq. (2.6a) is a set of $d$ difference equations that is hierarchic in the sense that each equation determines the next equation successively. The starting term is obtained by setting $\nu = 0$ in Eq. (2.6a):

$$f_1 = \dot{f}_0 = (\mathrm{i}/\hbar)[H, f_0]. \tag{2.7}$$

Hence if $f_0$ is known, $f_1$ is calculable for a given Hamiltonian $H$. Then we may calculate $\|f_1\|$ and obtain $\Delta_1 = \|f_1\|/\|f_0\|$. Setting $\nu = 1$ in Eq. (2.6a), we obtain the next equation in the hierarchy:

$$f_2 = \dot{f}_1 + \Delta_1 f_0. \tag{2.8}$$

Since $\Delta_1$, $f_0$ and $f_1$ are now known we can calculate $f_2$ and consequently $\Delta_2$, and go to the next step in the hierarchy. We may continue this process until, for some value of $\nu = M < \infty$ one finds that the basis vector $f_M = 0$. Eq. (2.6a) implies that $f_{M+1} = 0$, and so on. Hence the dimension of $\mathcal{S}$ is $d = M$. The value of $M$ will very much be model-dependent. It also may happen that no $f$'s vanish, signaling that $\mathcal{S}$ is an infinite dimensional space. In both cases the dimension $d$ is determined by the RR1 equations (2.6a).

## 2.4 The RR2 scheme

In this section we show that the basis functions can be generated through a three term recurrence relation known as RR2.

In §2.3 we saw that the RR1 scheme begins with some $f_0$ as a "seed". In any orthogonalization process there is always one degree of freedom we can exercise in choosing the basal or primary basis vector. We shall choose

$$f_0 = A(t=0) \equiv A, \tag{2.9}$$

termed the *canonical basis*. This is a natural choice since in most applications we also choose that $A(t)$ performs a trajectory starting at $t = 0$. The fundamental expansion (2.3) evaluated at $t = 0$ gives

$$A(0) = \sum_{\nu=0}^{d-1} a_\nu(0) f_\nu = A = f_0, \tag{2.10}$$

so, the canonical basis imposes the following important boundary condition for Eq. (2.3):

$$a_\nu(t=0) = \begin{cases} 1 & \text{if} \quad \nu = 0, \\ \\ 0 & \text{if} \quad \nu = 1, 2, \ldots, d-1 \ . \end{cases} \tag{2.11}$$

Also, taking the Kubo scalar product of both sides of the fundamental expansion (2.3) with $f_0 = A$, and using the orthogonality property of the $f$'s

$$(A, A(t)) = (A, \ \sum_{\nu=0}^{d-1} a_\nu(t) f_\nu \ ) = a_0(t) \ (A, A). \tag{2.12a}$$

Hence, the canonical basis also defines the primary basis function $a_0(t)$ as

$$a_0(t) = \frac{(A, A(t))}{(A, A)} \ , \tag{2.12b}$$

which coincides with the relaxation function of linear response theory. Note that if $d = 1$, then $f_1 = 0$ and Eq. (2.7) gives $[H, A] = 0$, which together with the boundary condition (2.11) implies that $a_0(t) = 1$ for $t \geqslant 0$. The time invariance (2.5) of the norm of $A(t)$ and the fundamental orthogonal expansion (2.3) imply Bessel Equality (BE):

$$\sum_{\nu=0}^{d-1} [a'_\nu(t)]^2 = 1 \, , \tag{2.13}$$

with $a'_0 \equiv a_0$, and $a'_\nu \equiv \sqrt{\Delta_1 \Delta_2 \ldots \Delta_\nu} a_\nu$. In contrast to the case $[H, A] = 0$, when $[H, A] \neq 0$ then $d > 1$ and Bessel equality implies that the magnitude of $a_0(t)$ cannot stay constant and equal to 1 and must change in time. Note also that the Schwartz Inequality

$$|(A, A(t)|^2 \leq (A(t), A(t))(A, A), \tag{2.14}$$

together with the time invariance of the norm of $A(t)$, Eq. (2.5), imply that

$$|a_0(t)|^2 \leq 1 \ . \tag{2.15}$$

For the fundamental orthogonal expansion (2.3) to constitute a general solution to Eq. (2.4) on $\mathcal{S}$ we still need to know the set $\{a_\nu\}$. It must be complete, linearly independent and satisfy the boundary condition (2.11). Requiring that the expansion (2.3) satisfies Heisenberg equation (2.4) for $A(t)$ on $\mathcal{S}$, and applying the RR1 (2.6a) on Eq. (2.3), we obtain a recurrence relation for the set $\{a_\nu\}$ called RR2:

$$\Delta_{\nu+1} a_{\nu+1}(t) = -\dot{a}_\nu(t) + a_{\nu-1}(t) \qquad\qquad \nu = 0, 1, \ldots, d-1 \tag{2.16}$$

with $a_{-1} \equiv 0$ and $\dot{a} \equiv \mathrm{d}a/\,\mathrm{d}t$. The RR2 relations are realized by the recurrants $\{\Delta_m\}$ obtained from RR1. Hence the realized RR2 scheme is also uniquely model-dependent.

As an example of a very general application of the RR2, its hierarchical structure implies that if $a_0(t)$ were known, all other $a$'s could be calculable given the recurrants $\{\Delta_\nu\}$, e.g. if $a_0(t) = \exp(-ct)$ with $c > 0$ it is found that the other basis functions implied by RR2 will not be linear independent neither complete. This argument rules out on very general grounds an *exact* exponential decay of the autocorrelation function. A related proof of the same statement follows from the Bessel Equality, Eq. (2.13), that is the same as saying $\|A(t)\| = \|A\|$, which an exponential law cannot satisfy [Lee 1983]. The structure of RR2 also rules out an expression the $\{a_\nu\}$ in terms of orthogonal polynomials [Balucani et al. 2003].

The RR2 also shed light on the dynamics of the system according to whether the dimension $d$ of the realized space $\mathcal{S}$ is finite or not finite. Let us denote by $\tilde{a}_m(z)$ the Laplace

transform of $a_m(t)$ with $\mathrm{Re}\, z > 0$. Then the Laplace transform of RR2, Eq. (2.16), is:

$$1 = z\tilde{a}_0 + \Delta_1 \tilde{a}_1(z)\,, \qquad \nu = 0\,, \tag{2.17a}$$

$$\tilde{a}_{\nu-1}(z) = z\tilde{a}_\nu(z) + \Delta_{\nu+1}\tilde{a}_{\nu+1}(z)\,, \qquad 1 \leqslant \nu \leqslant d-1\ , \tag{2.17b}$$

where the two cases: $\nu = 0$ and $1 \leqslant \nu \leqslant d-1$, stem from the boundary condition (2.11). This is an hierarchy of linear coupled equations for the $\tilde{a}_\nu(z)$. Suppose, for the moment that the hierarchy of equations is finite. This happens when the RR1 terminates at some $\nu$, say, $\nu = d-1$. Then the basis vectors are $\{f_0, f_1, \ldots, f_{\nu-1}\}$, the dimension of the spanned space is $d$, and the last non-null recurrant is $\Delta_{\nu-1}$. The last equation of the hierarchy would be the $\nu = d-1$ equation

$$\begin{aligned} \tilde{a}_{d-2}(z) &= z\tilde{a}_{d-1}(z) + \Delta_d \tilde{a}_d(z)\ , \\ &= z\tilde{a}_{d-1}(z)\ , \end{aligned} \tag{2.18}$$

since $\Delta_d = 0$. Substituting $\tilde{a}_{d-1}(z) = \tilde{a}_{d-2}(z)/z$ into the $\nu = d-2$ equation

$$z\tilde{a}_{d-2}(z) + \Delta_{d-1}\tilde{a}_{d-1}(z) = \tilde{a}_{d-3}(z)\ , \tag{2.19}$$

one gets

$$\tilde{a}_{d-2}(z) = \frac{\tilde{a}_{d-3}(z)}{z + \Delta_{d-1}/z}\ , \tag{2.20}$$

thus eliminating $\tilde{a}_{d-1}(z)$ from the hierarchy. Repeating this procedure until one arrives to the $\nu = 0$ equation, all the $\tilde{a}_\nu(z)$ but, $\tilde{a}_0(z)$, will have been eliminated. We obtain the continued fraction

$$\tilde{a}_0(z) = \cfrac{1}{z + \cfrac{\Delta_1}{z + \cfrac{\Delta_2}{z + \cdots + \cfrac{\Delta_{d-2}}{z + \cfrac{\Delta_{d-1}}{z}}}}}\ . \tag{2.21}$$

If $d$ is finite, the rhs of Eq. (2.21) is a quotient of polynomials of finite order, and as such, with a finite number of zeroes. In this case by an inverse Laplace transform we obtain $a_0(t)$ as periodic function. If on the other hand, $d \to \infty$, the rhs of Eq. (2.21) is clearly an infinite continued fraction. Thus, the origin of a continued fraction in the time evolution problem is clearly embedded in the RR2.

## 2.5 Subspaces

Once that a complete set of basis vectors $\{f_0, f_1, f_2, \ldots, f_{d-1}\}$ is obtained, we can construct *subspaces* of $\mathcal{S}$. We will show that this possibility is useful for a neat derivation of the generalized Langevin equation, and hence of memory function. Let us denote by $\mathcal{S}_1$ a space spanned by the basis vectors

$$\{f_1, f_2, \ldots, f_{d-1}\}. \tag{2.22}$$

Also let $B(t)$ a vector in $\mathcal{S}_1$, given the orthogonal expansion

$$B(t) = \sum_{\nu=1}^{d-1} b_\nu(t) f_\nu, \tag{2.23}$$

where $\{b_\nu\}$ is a complete and linearly independent set of basis functions in $\mathcal{S}_1$ analogous to $\{a_\nu\}$ in $\mathcal{S}$. Suppose that in $\mathcal{S}_1$ we impose on the $\{b_\nu\}$ a boundary condition, analogous to Eq. (2.11), on the $b$'s:

$$b_\nu(t=0) = \begin{cases} 1 & \text{if } \nu = 1, \\ 0 & \text{if } \nu = 2, 3, \ldots, d-1 \ . \end{cases} \tag{2.24}$$

as well as similar RR2 scheme:

$$\Delta_{\nu+1} b_{\nu+1}(t) = -\dot{b}_\nu(t) + b_{\nu-1}(t) \quad (\nu = 1, 2, \ldots, d-1) \tag{2.25}$$

with $b_0 \equiv 0$. Then $B(t=0) = b_1$ and by Eq. (2.7), $f_1 = \dot{f}_0 = \dot{A}$. Thus, by exactly the same arguments of §2.3 and §2.4, $B(t)$ is the time evolution of $\dot{A}$ on the subspace $\mathcal{S}_1$ as $A(t)$ is on the space $\mathcal{S}$. Although in different spaces, their time evolutions are related in the sense that the basis functions $\{b_\nu\}$ are not arbitrary but related to $\{a_\nu\}$.

The set of basis functions $\{b_\nu\}$ that satisfies the RR2 recurrence relations (2.25) on $\mathcal{S}_1$ and the boundary conditions (2.24) may be defined by a convolution integral with $\{a_\nu\}$:

$$a_\nu(t) = \int_0^t \mathrm{d}t'\, b_\nu(t') a_0(t-t'). \quad (\nu \geqslant 1). \tag{2.26}$$

Differentiating Eq (2.26), and using the boundary condition (2.11) on $a_0(t)$, we find:

$$\dot{a}_\nu(t) = b_\nu(t) + \int_0^t \mathrm{d}t'\, b_\nu(t') \dot{a}_0(t-t') \quad (\nu \geqslant 1). \tag{2.27}$$

Hence

$$b_\nu(t=0) = \dot{a}_\nu(t=0) \quad (\nu \geqslant 1). \tag{2.28}$$

Using the boundary condition (2.11) for the $a$'s and the RR2 (2.16) in Eq.(2.28) above, we find that the boundary conditions (2.24) for the $b$'s are verified. Also, integrating by parts the integral on the rhs of Eq. (2.27), and using again the RR2 (2.16) on $\mathcal{S}$, the RR2 relation (2.25) on $\mathcal{S}_1$ for the $b$'s is verified.

The Laplace transform of the convolution integral (2.26) definition of the $b$'s is

$$\tilde{a}_\nu(z) = \tilde{b}_\nu(z) \tilde{a}_0(z) \quad (1 \leqslant \nu \leqslant d-1)\ . \tag{2.29}$$

Using the above relation (2.29) with $\nu = 1$ in the Laplace transform of RR2 for $\nu = 0$, Eq. (2.17a), we find

$$\tilde{a}_0(z) = \frac{1}{z + \Delta_1 \tilde{b}_1(z)}\ . \tag{2.30}$$

The comparison of Eq. (2.30) with $\tilde{a}_0(z)$ expressed as a continued fraction in Eq. (2.21) shows that $\tilde{b}_1(z)$ is also a continued fraction:

$$\tilde{b}_1(z) = \cfrac{1}{z + \cfrac{\Delta_2}{z + \cfrac{\Delta_3}{z + \cdots + \cfrac{\Delta_{d-2}}{z + \cfrac{\Delta_{d-1}}{z}}}}}\ , \tag{2.31}$$

a result which can be also obtained in the same way that the continued fraction (2.21) for $\tilde{a}_0(z)$ was obtained; from the direct application of RR2 on $\mathcal{S}_1$ by using Eqs. (2.24) and (2.25).

The relationship between $a_0$ and $b_1$ is just what Kubo called the *second* fluctuation-dissipation theorem. In the formalism of this section, it denotes a relation [Balucani et al. 2003] between two spaces $\mathcal{S}$ and $\mathcal{S}_1$. This relation is fundamental to establishing the generalized Langevin equation in a simple and clear manner.

## 2.6 The Recurrence Relations Method and the Generalized Langevin Equation

In the search of a method to solve Heisenberg equation for dynamical variables of many body systems, Mori made a significant advance when he was able to reformulate Heisenberg equation as the (later so called) generalized Langevin equation. Some of the terminology he introduced is still in use today, e.g. the memory function.

Mori's work thus represented a big breakthrough [Balucani et al. 2003], in the sense that it obviated the need to introduce approximations from the outset as in the equation of motion methods. Unfortunately, no application of the GLE to any physical model has ever been solved without the eventual need for some kind of approximation that sometimes has been physically unwarranted and on occasion ultimately was proved wrong.

The reason for this is that Mori's approach is based on the Mori-Zwanzig (MZ) projection operator formalism. This is an orthogonalization process of abstract Hilbert space and it seems not to have been recognized [Lee 2000*a*] that the MZ formalism is a reinvention of the Gram-Schmidt process.

The MZ or Gram-Schmidt process is general, but the generality also diffuses the underlying physics (e.g., subspaces and dimensionality). The resultant analysis necessarily is heavily formal. It is no surprise that the GLE on occasion has been incorrectly approximated and even incorrectly applied [Lee 2000*a*].

The recurrence relations method is an exact approach developed by M. H. Lee to avoid the aforementioned difficulties and solve *directly* the Heisenberg equation in many body systems. In many instances it has been able to provide *exact* solutions for specific physical models. The RRM can also be used to rederive the GLE in a simple and transparent manner (Mori's original derivation was neither simple nor transparent) and also provides an interpretation of the GLE as a consequence of the relationship between a realized inner-product space and its subspaces [Lee 2000*a*].

To show this relationship, let's outline the derivation of the GLE using the RRM:

1. Take the time derivative of the orthogonal expansion of $A(t)$.

2. Remove the "dots" (the time derivatives) using the RR2.

3. Make the connection to the $\mathcal{S}_1$ space with the convolution definition of the $b$'s.

4. Use the convolution definition again to transform the expressions to make the expansion of $A(t)$ appear and indeed get an equation for $A(t)$. At this stage one would notice that to accomplish this goal an additional step would be needed: In step 1 one would have to split-off the first term of the summation.

The derivative of the fundamental orthogonal expansion, Eq. (2.3), with respect to the time is:

$$\dot{A}(t) = \dot{a}_0(t) f_0 + \sum_{\nu=1}^{d-1} \dot{a}_\nu(t) f_\nu \ , \tag{2.32}$$

where the rhs has been split into two terms on account of the boundary behavior (2.11). Substituting the $\nu = 0$ term of the RR2 (2.16):

$$\dot{a}_0(t) = -\Delta_1 a_1(t), \tag{2.33}$$

into the convolution definition (2.26) of the $b$'s, we get for the first term on the r.h.s:

$$\dot{a}_0(t) f_0 = -\Delta_1 \int_0^t \mathrm{d}t' \, b_1(t') a_0(t - t') f_0 \ . \tag{2.34}$$

Again using the $\nu = 0$ term of the RR2, Eq. (2.33), but this time in the time derivative (2.27) of the convolution definition of the $b$'s, we find for the second term on rhs

$$\sum_{\nu=1}^{d-1} \dot{a}_\nu(t) f_\nu = \sum_{\nu=1}^{d-1} b_\nu(t) f_\nu - \Delta_1 \sum_{\nu=1}^{d-1} \int_0^t \mathrm{d}t'\, b_\nu(t') a_1(t-t') f_\nu \ . \tag{2.35}$$

Collecting both results we find

$$\dot{A}(t) = -\Delta_1 \int_0^t \mathrm{d}t'\, b_1(t') a_0(t-t') f_0 + B(t) - \Delta_1 \sum_{\nu=1}^{d-1} \int_0^t \mathrm{d}t'\, b_\nu(t') a_1(t-t') f_\nu \ , \tag{2.36}$$

with $B(t) = \sum_{\nu=1}^{d-1} b_\nu(t) f_\nu$ .

The Laplace domain convolution definition (2.26) of the $b$'s for $\nu = 1$ is $\tilde{a}_1(z) = \tilde{b}_1(z)\tilde{a}_0(z)$. It also gives $\tilde{a}_1(z)\tilde{b}_\nu(z) = \tilde{b}_1(z)\tilde{a}_0(z)\tilde{b}_\nu(z) = \tilde{b}_1(z)\tilde{a}_\nu(z)$. In the time domain, then

$$\int_0^t \mathrm{d}t'\, b_\nu(t') a_1(t-t') = \int_0^t \mathrm{d}t'\, b_1(t') a_\nu(t-t') \ . \tag{2.37}$$

This allows us to group under one single summation sign the first term and the last term in the r.h.s of Eq. (2.36) to obtain

$$\dot{A}(t) = B(t) - \Delta_1 \sum_{\nu=0}^{d-1} \int_0^t \mathrm{d}t'\, b_1(t') a_\nu(t-t') f_\nu \tag{2.38}$$

$$= B(t) - \int_0^t \mathrm{d}t'\, M(t') A(t-t') \ , \tag{2.39}$$

where the memory function is $M(t) \equiv \Delta_1 b_1(t)$. Eq. (2.39) constitutes the generalized Langevin Equation.

To further illustrate the relationship between $\mathcal{S}$ and $\mathcal{S}_1$ we may remark that for Hermitian systems, the length of the vector $A(t)$ remains constant, Eq.(2.5). Consequently, $A(t)$ can change only its direction as time evolves. Hence $\dot{A}(t)$ has a component, in subspace $\mathcal{S}_1$, that remains orthogonal to $f_0 = A = A(t=0)$ always, which may be called a *normal* component of $\dot{A}(t)$. At $t = 0$, there is only the normal component. But as time evolves, there appears another component, in the full space $\mathcal{S}$, not orthogonal to $f_0$, which may be thus called an *induced* component of $\dot{A}(t)$.

The *scalar* GLE may also be derived by with the method sketched so far. Substitute the convolution definition of $b_1$ (Eq. (2.26) with $\nu = 1$) in the $\nu = 0$ term of the RR2, Eq. (2.33), to obtain

$$\dot{a}_0(t) = -\int_0^t \mathrm{d}t'\, M(t')a_0(t-t'). \tag{2.40}$$

An identical result is also obtained taking the scalar product of $A = f_0$ with both sides of the GLE, Eq.(2.39), dividing out the norm $(A, A)$ and using the fact that $(A = f_0, B(t))$=0.

# Chapter 3

## Applications of the Recurrence Relations Method

## I: Introduction

The recurrence relations method, RRM, has been applied to a variety of dynamical problems by Lee and his coworkers and others, and there now exists a large body of literature on the applications of the RRM, and also on the applications of the results obtained by the RRM (See: [Lee 2000*b*, §II, p3572], and the references cited therein).

In this chapter and the next two, we will illustrate the use of the recurrence relations method by reviewing previous applications [Lee, Hong & J. Florencio 1987] of the RRM to three well known physical models: (i) The electron gas, (ii) The spin van der Waals model, (iii) The one-dimensional spin chain.

Before going on to the specific examples, it is important to note that the RRM is used to calculate the time evolution of dynamical variables and that these calculations are carried out with the static properties of the physical system or model, fixed at some given value(s). For example, for the electron gas we will confine ourselves to $k \ll k_F$ at the ground state, here in Chapter 3, except in §3.4, where we will consider an asymptotic expansion for the dynamic structure factor of the 3D electron gas, valid for $k \gg k_F$. Once the static properties are defined, Eq. (2.6b) may be used to calculate the recurrants $\{\Delta_m\}$. They only depend on which dynamic variable we choose and the given static properties. At this point the RR1, Eq. (2.6a), and RR2, Eq. (2.16), schemes are realized and provide the exact dynamic evolution of the chosen variable. All the results quoted above, in the first paragraph, are *exact* in this sense, i.e., no approximation is ever made in the application of the RRM.

In the following sections we will illustrate in specific examples how the application of recurrence relations method, RRM, is carried out.

## 3.1 Homogeneous electron gas at $T = 0$

The electron gas model is at the basis of our understanding of metals and over the years a considerable amount of theoretical work has been done about it (See, for example, [Fetter & Walecka 2003, Chap. 4], [Mahan 2007, Chap. 5] and [Dickhoff & Neck 2008, §10.5]).

The homogeneous electron gas model may be defined [Lee & Hong 1985*b*] by the Hamiltonian

$$H = \sum_k \varepsilon_k a_k^\dagger a_k + \sum_k \upsilon_k \varrho_k \varrho_{-k} \equiv H_0 + V \,, \tag{3.1}$$

where $\varepsilon_k = k^2/2m$, and $a_k^\dagger$ and $a_k$ are, respectively, the fermion creation and annihilation operators at wave vector $k$. In the interaction term of the Hamiltonian, the two body interaction, with $k \neq 0$, is

$$\upsilon_k = \begin{cases} 2\pi e^2/k & 2-\mathrm{D}, \\ 4\pi e^2/k^2 & 3-\mathrm{D}, \end{cases} \tag{3.2}$$

and

$$\varrho_k \equiv \sum_p a_p^\dagger a_{p-k} \,, \tag{3.3}$$

is the density-fluctuation operator. The Hamiltonian given in Eq. (3.1), when restricted to $k \ll k_F$, and further transformed to become non-interacting in terms of plasma modes, constitutes the Sawada model. It accurately describes the electron-hole excitations near the Fermi surface [Mahan 2007].

## 3.2 Homogeneous 2-D electron gas at $T = 0$ and $k \ll k_F$

The two dimensional electron gas model is defined by the Hamiltonian of Eq. (3.1). Our system is under the influence of an external perturbing potential

$$H_{ext} = \sum_k \varrho_k(t) p_k \, \mathrm{e}^{\mathrm{i}\,\omega t}, \tag{3.4}$$

where $p_k$ is the Fourier component of the externally applied electric field, sufficiently small as to permit the use of linear- response theory, $\omega$ is the frequency of the applied field, and

$$\varrho_k(t) = \mathrm{e}^{\mathrm{i}\,Ht}\,\varrho_k\,\mathrm{e}^{-\mathrm{i}\,Ht}, \tag{3.5}$$

with $\varrho_k(0) = \varrho_k$, the density fluctuation operator defined in Eq. (3.3).

Our aim is to calculate the relaxation function, $(\varrho_k, \varrho_k(t))/(\varrho_k, \varrho_k)$, from which other physical quantities can be calculated via linear-response relations. Here the inner product means, the Hamiltonian dependent (thus model-dependent), Kubo scalar product defined in Eq. (2.1). To accomplish this goal we will use the recurrence relations method, RRM, and choose as dynamical variable the density fluctuations operator, that is $A(t) \equiv \varrho_k(t)$. Thus

$$A(0) = A \equiv f_0 \equiv \varrho_k. \tag{3.6}$$

Taking the scalar product with $f_0$ on both sides of the fundamental orthogonal expansion of Eq. (2.3) for $\varrho_k(t)$, we find

$$a_0(t) = (\varrho_k, \varrho_k(t), )/(\varrho_k, \varrho_k). \tag{3.7}$$

According to the RRM, at least two avenues are available to obtain the relaxation function. One may proceed to calculate $a_0(t)$ by solving the RR2 difference equations (2.16), directly in the time domain, or use the continued fraction expansion (2.21) for $\tilde{a}_0(z)$ and then use the inverse Laplace transform to get $a_0(t)$. In either case a full knowledge of the *recurrants* (2.6b) is required, as we shall see below. In fact the set $\{\Delta_m\}$ completely defines the RR1, Eqs. (2.6a), and the RR2, Eqs. (2.16), thus completely realizing the RRM.

### 3.2.1 Basis vectors and norms

With the choice made for $f_0$ in Eq. (3.6) we can directly [Lee & Hong 1985*b*] obtain from the RR1 all other basis vectors spanning $\mathcal{S}$:

$$f_0 = \varrho_k \,, \tag{3.8a}$$

$$f_1 = \dot{\varrho}_k \,, \tag{3.8b}$$

$$f_2 = \ddot{\varrho}_k + \Delta_1 \varrho_k \,, \tag{3.8c}$$

$$f_3 = \dddot{\varrho}_k + (\Delta_1 + \Delta_2)\dot{\varrho}_k \,, \tag{3.8d}$$

$$f_4 = \overset{(4)}{\varrho}_k + (\Delta_1 + \Delta_2 + \Delta_3)\ddot{\varrho}_k + \Delta_1\Delta_3\varrho_k \,, \tag{3.8e}$$

$$f_5 = \overset{(5)}{\varrho}_k + (\Delta_1 + \Delta_2 + \Delta_3 + \Delta_4)\dddot{\varrho}_k + (\Delta_1\Delta_3 + \Delta_1\Delta_4 + \Delta_2\Delta_4)\dot{\varrho}_k \,, \tag{3.8f}$$

etc., where the number of dots or the number above $\varrho_k$ is the number of times the commutator of $\varrho_k$ with $H$ is being nested, e.g,

$$\dddot{\varrho}_k = \mathrm{i}[H, \ddot{\varrho}_k] = \mathrm{i}^3[H, [H, [H, \varrho_k]]] = \overset{(3)}{\varrho}_k \,.$$

The norms of these vectors [Lee & Hong 1985*b*] are

$$(f_0, f_0) = (\varrho_k, \varrho_k) = \chi_k \,, \tag{3.9a}$$

$$(f_1, f_1) = (\dot{\varrho}_k, \dot{\varrho}_k) \,, \tag{3.9b}$$

$$(f_2, f_2) = (\ddot{\varrho}_k, \ddot{\varrho}_k) - \Delta_1(\dot{\varrho}_k, \dot{\varrho}_k) \,, \tag{3.9c}$$

$$(f_3, f_3) = (\dddot{\varrho}_k, \dddot{\varrho}_k) - (\Delta_1 + \Delta_2)(\ddot{\varrho}_k, \ddot{\varrho}_k) \,, \tag{3.9d}$$

$$(f_4, f_4) = (\overset{(4)}{\varrho}_k, \overset{(4)}{\varrho}_k) - (\Delta_1 + \Delta_2 + \Delta_3)(\dddot{\varrho}_k, \dddot{\varrho}_k) + \Delta_1\Delta_3(\ddot{\varrho}_k, \ddot{\varrho}_k) \,, \tag{3.9e}$$

$$\begin{aligned}(f_5, f_5) = {} & (\overset{(5)}{\varrho}_k, \overset{(5)}{\varrho}_k) - (\Delta_1 + \Delta_2 + \Delta_3 + \Delta_4)(\ddot{\dddot{\varrho}}_k, \ddot{\dddot{\varrho}}_k) \\ & + (\Delta_1\Delta_3 + \Delta_1\Delta_4 + \Delta_2\Delta_4)(\dddot{\varrho}_k, \dddot{\varrho}_k) \,,\end{aligned} \tag{3.9f}$$

etc., where we have used the identity

$$(\overset{(n)}{\varrho}, \overset{(m)}{\varrho}) = -(\overset{(n-1)}{\varrho}, \overset{(m+1)}{\varrho}) = -(\overset{(n+1)}{\varrho}, \overset{(m-1)}{\varrho}) \,,$$

$n$ or $m \geqslant 1$.

Observe that to calculate $f_\nu$ or its norm, we need to know the norms of $f_{\nu-1}, f_{\nu-2}, \ldots, f_0$. Thus if we calculate the norms successively starting with the basal vector $f_0$, we can obtain all the basis vectors and their norms explicitly. For the electron gas at long wavelengths, these norms can be obtained by working out the nested commutators of $\varrho_k$ and evaluating the inner products at $T = 0$. Observe also that

$$\dot{\varrho}_k = \mathrm{i}[H, \varrho_k] = \mathrm{i}[H_0, \varrho_k] = \dot{\varrho}_k^{(0)} \,,$$

where $H_0$ is the non-interacting or ideal Hamiltonian.

### 3.2.2 Basis vectors and norms: Non-interacting (Ideal) system

Here we express $k$ in units of $k_F$ such that $\varepsilon_F = 1/2m$, where $\varepsilon_F$ is the Fermi energy in two dimensions. In these units, the norms for the two-dimensional electron gas are [Lee & Hong 1985*b*]

$$(f_0, f_0)^{(0)} = \chi_k^{(0)} = m/\pi \,, \quad k \leqslant 2 \tag{3.10a}$$

$$(f_1, f_1)^{(0)} = k^2 \varepsilon_F \,, \tag{3.10b}$$

$$(f_2, f_2)^{(0)} = [k^4 + k^6]\varepsilon_F^3/\pi \,, \tag{3.10c}$$

$$(f_3, f_3)^{(0)} = [k^6 + k^8 + O(k^{10})]\varepsilon_F^5/\pi \,, \tag{3.10d}$$

$$(f_4, f_4)^{(0)} = [k^8 + 10k^{10} + O(k^{12})]\varepsilon_F^7/\pi \,, \tag{3.10e}$$

$$(f_5, f_5)^{(0)} = [k^{10} + 20k^{12} + O(k^{14})]\varepsilon_F^9/\pi \,, \tag{3.10f}$$

etc. We shall retain only the leading order in $k$ in the recurrants valid for the $k \ll 1$ regime. Then Eqs. (2.6b) gives

$$\Delta_1^{(0)} = 2k^2 \varepsilon_F^2 \,, \tag{3.11a}$$

$$\Delta_2^{(0)} = \Delta_3^{(0)} = \Delta_4^{(0)} = \cdots = k^2 \varepsilon_F^2 \equiv \Delta \,. \tag{3.11b}$$

Observe that the norms are finite and non-vanishing for $\nu$'s. Hence, for the two-dimensional ideal electron gas the dimensionality of the Hilbert space of $\varrho_k$ is infinite ($d = \infty$).

### 3.2.3 Basis vectors and norms: Interacting system

To leading order in $k$, for the static regime of small $k$, we find for the norms [Lee & Hong 1985*b*]

$$(f_0, f_0) = \chi_k^{(0)}(1 + \upsilon_k \chi_k^{(0)}) \,, \tag{3.12a}$$

$$(f_\nu, f_\nu) = (f_\nu, f_\nu)^{(0)}, \quad \nu \geqslant 1 \,. \tag{3.12b}$$

Hence, to leading order in $k$, Eqs. (2.6b) give

$$\Delta_1 = 2\Delta + \Gamma \,, \tag{3.13a}$$

$$\Delta_\nu = \Delta_\nu^0 = \Delta \,, \quad \nu \geqslant 1 \tag{3.13b}$$

with $\Gamma = (\omega_p^{class})^2 = 2\pi\rho e^2 k/m$, where $\rho$ is the number density. Again, we observe that the norms are finite and non-vanishing, hence for the two-dimensional interacting electron gas the dimensionality of the Hilbert space of $\varrho_k$ is also infinite ($d = \infty$).

Below we will show, first how to obtain the autocorrelation functions $a_\nu^{(0)}(t)$, directly in §3.2.4, from the RR2 difference equations (2.16) and then, in §3.2.6, how to use the continued fraction expansion (2.21) for $\tilde{a}_0(z)$ to obtain the relaxation function $a_0(t)$, for both the ideal and the interacting systems.

### 3.2.4 Direct RR2 difference equations approach for the ideal system

Defining

$$\Delta \equiv \frac{1}{4}\mu^2 \,, \tag{3.14}$$

and writing out explicitly the $m = 0$ term of the RR2 equations (2.16), we obtain

$$\frac{1}{2}\mu^2 a_1^{(0)}(t) = -\dot{a}_0^{(0)}(t) \,, \tag{3.15a}$$

$$\frac{1}{4}\mu^2 a_{\nu+1}^{(0)}(t) = -\dot{a}_\nu^{(0)}(t) + a_{\nu-1}^{(0)}(t) \,, \quad \nu \geqslant 1 \,. \tag{3.15b}$$

We will try to find a function that satisfies the above recurrence relations. We look up first among the known special functions of mathematical physics that satisfy a three term

recurrence relation similar to Eqs. (3.15a)–(3.15b). To this end, following [Lee & Hong 1985*b*], we write the $a$'s in terms of some $h$'s whose arguments and images are dimensionless

$$a_\nu^{(0)}(t) \equiv \lambda^{-\nu} U_\nu h_\nu(\lambda t)\,, \tag{3.16}$$

where $\lambda$ is a scale factor, $U_\nu$ is a coefficient and $h_\nu$ is a function, all to be determined. Up front, the boundary condition $a_{(0)}(t=0)=1$, Eq. (2.11), imposes that $U_0 = 1$ and $h_0(0) = 1$. Substituting the definition (3.16) into Eqs. (3.15a)–(3.15b), we obtain

$$\frac{1}{2}\mu^2\lambda^{-2} U_1 h_1 = -h_0'\ , \tag{3.17a}$$

$$\frac{1}{4}\mu^2\lambda^{-2}(U_{\nu+1}/U_{\nu-1})h_{\nu+1} = -(U_\nu/U_{\nu-1})h_\nu' + h_{\nu-1}\,, \qquad \nu \geqslant 1\ , \tag{3.17b}$$

where $h' \equiv \mathrm{d}h(x)/\,\mathrm{d}x$. Clearly, the scale factor is $\lambda = \mu$, which to some extent simplifies Eqs. (3.17a)–(3.17b) into

$$\frac{1}{2} U_1 h_1 = -h_0'\ , \tag{3.18a}$$

$$\frac{1}{4}(U_{\nu+1}/U_{\nu-1})h_{\nu+1} = -(U_\nu/U_{\nu-1})h_\nu' + h_{\nu-1}\,, \qquad \nu \geqslant 1\ . \tag{3.18b}$$

The above may now be compared [Lee & Hong 1985*b*] with the recurrence relation [Abramowitz & Stegun 1972] for the Bessel function $\mathrm{J}_\nu$

$$\mathrm{J}_1 = -\mathrm{J}_0'\ , \tag{3.19a}$$

$$\mathrm{J}_{\nu+1} = -2\mathrm{J}_\nu' + \mathrm{J}_{\nu-1}\,, \qquad \nu \geqslant 1\ . \tag{3.19b}$$

Setting $U_\nu = 2^\nu$, Eqs. (3.18a)–(3.18a) become identical to Eqs. (3.19a)–(3.19b). Hence

$$a_\nu^{(0)}(t) = 2^\nu \mu^{-\nu} \mathrm{J}_\nu(\mu t)\,, \qquad \nu \geqslant 0\ . \tag{3.20}$$

Note that the solution satisfies the remaining boundary conditions that $a_\nu^{(0)}(t=0) = 0$, $\nu \geqslant 1$. Thus, the RR2 realized by the recurrants (3.11a)–(3.11b) of the two-dimensional ideal electron gas is isomorphic to the recurrence relation for the integer Bessel functions. The solution satisfies the boundary condition $a_\nu^{(0)}(t)$ satisfies the boundary condition, Eq. (2.11),

and their short and long time behavior are given directly by the properties [Abramowitz & Stegun 1972] of the Bessel functions, e.g.

$$a_0(t) \sim t^{-1/2}\cos(\mu t - \pi/4) \qquad \text{as } t \to \infty\,. \tag{3.21}$$

The Laplace transform of the relaxation functions will be needed to calculate the $b$'s to obtain the memory function.

$$\begin{aligned}\tilde{a}_0^{(0)}(z) &= \mathcal{L}((a_0^{(0)}(t)) \\ &= 2^\nu \mu^{-2\nu}[(z^2+\mu^2)^{1/2} - z]^\nu/(z^2+\mu^2)^{1/2},\end{aligned} \tag{3.22}$$

where $\mathcal{L}$ is the Laplace transform operator. Using Eq. (2.29), the Laplace transform of the time convolution definition of the $b$'s, we obtain that, in general

$$\tilde{b}_\nu(z) = \tilde{a}_\nu(z)/\tilde{a}_0(z) \tag{3.23}$$

Then, for the ideal, non-interacting system, using Eq. (3.22), we find directly

$$\begin{aligned}\tilde{b}_\nu^{(0)}(z) &= \tilde{a}_\nu^{(0)}(z)/\tilde{a}_0^{(0)}(z) \\ &= 2^\nu \mu^{-2\nu}[(z^2+\mu^2)^{1/2} - z]^\nu\,, \quad \nu \geqslant 1\,.\end{aligned} \tag{3.24}$$

Hence [Abramowitz & Stegun 1972],

$$\begin{aligned}b_\nu^{(0)}(t) &= \mathcal{L}^{-1}\left(\tilde{b}_\nu^{(0)}(z)\right) \\ &= 2^\nu \mu^{1-\nu}\nu \mathrm{J}_\nu(\mu t)/\mu t\,, \quad \nu \geqslant 1\,.\end{aligned} \tag{3.25}$$

It is worth noting at this point that point that, as we will show below in §3.2.6, the $b$'s are the same for the ideal non-interacting and for the interacting homogeneous electron gas system. Now, the memory function for the ideal system can written as

$$\begin{aligned}M^{(0)}(t) &= \Delta_1^{(0)} b_1^{(0)}(t) = \mu^2 \mathrm{J}_1(\mu t)/\mu t \\ &= t^{-3/2}\cos(\mu t - 3\pi/4) \quad \text{as } t \to \infty\,.\end{aligned} \tag{3.26}$$

### 3.2.5 The response function, $\chi_k(\omega)$, and the dynamic structure factor, $S_k(\omega)$ for the ideal system

Many experimental techniques used to probe the intrinsic dynamics of a physical system are based on measuring [Balucani et al. 2003] either (i) the response of the system to an applied field or (ii) the scattering of some "particles" by the system. Thus the response function $\chi_k(\omega)$ and the dynamic structure factor, $S_k(\omega)$ are often readily accessible experimentally.

Using linear response theory (see, for example [Balucani et al. 2003], [Kubo, Toda & Hashitsume 1991], [Marshall & Lowde 1968]) it can be shown in general that both the response function, $\chi_k(\omega)$, and the dynamic structure factor, $S_k(\omega)$, can be obtained in terms of the relaxation function. Thus:

$$\tilde{\chi}(t) \equiv \chi(t)/\chi = -\frac{\partial}{\partial t} a_0(t) = \Delta_1 a_1(t), \qquad t \geqslant 0\,. \tag{3.27}$$

Hence,

$$\tilde{\chi}^{(0)}(t) = \mu \mathrm{J}_1(\mu t)\,, \tag{3.28}$$

and

$$\begin{aligned}
\tilde{\chi} &\equiv \left[\mathcal{L}\left(\chi^{(0)}(t)\right)\right]_{z=\mathrm{i}\,\omega} \\
&= 1 - \mathrm{i}\,\omega(\mu^2 - \omega^2)^{-1/2}\,, \quad 0 < \omega < \mu \qquad (3.29)\\
&= 1 - \omega(\omega^2 - \mu^2)^{-1/2}\,, \quad \mu < \omega < \infty\,. \qquad (3.30)
\end{aligned}$$

Also, since

$$\pi S(\omega) = -\mathrm{Im}\,\chi(z = \mathrm{i}\,\omega)\,, \tag{3.31}$$

we obtain directly

$$\begin{aligned}
\tilde{S}^{(0)}(\omega) &\equiv S^{(0)}(\omega)/\chi^{(0)} = \\
&= \frac{\omega}{\pi}(\mu^2 - \omega^2)^{-1/2}\,, \qquad 0 < \omega < \mu\,, \qquad (3.32)\\
&= 0\,, \qquad \mu < \omega < \infty\,. \qquad (3.33)
\end{aligned}$$

### 3.2.6 Continued fraction approach for the ideal and the interacting systems

It was shown in §2.4 that the Laplace transform $\tilde{a}_0(z)$ of the relaxation function $a_0(t)$ can be written as a continued fraction, Eq. (2.21), that only depends on the corresponding set of recurrants for the particular physical system or model under consideration. To leading order in $k$, comparing the recurrants for the ideal system, Eqs. (3.11a)–(3.11b), and the recurrants for the interacting system, Eqs. (3.13a)–(3.13b), one notes that both sets have an infinite number of terms and that the sets only differ in the first recurrant. Looking at the general continued fraction for $\tilde{a}_0(z)$, Eq. (2.21), and the continued fraction for $\tilde{b}_1(z)$, Eq. (2.31), one finds

$$\tilde{a}_0^{(0)}(z) = \frac{1}{z + \Delta_1^{(0)}\tilde{b}_1(z)} \,, \tag{3.34}$$

for the ideal system, and

$$\tilde{a}_0(z) = \frac{1}{z + \Delta_1\tilde{b}_1(z)} \,, \tag{3.35}$$

for the interacting system. In both cases, since

$$\Delta_\nu^{(0)} = \Delta_\nu = k^2\varepsilon_F^2 \equiv \Delta, \qquad \nu \geqslant 1 \,, \tag{3.36}$$

the $\tilde{b}_1(z)$ is given by

$$\tilde{b}_1(z) = \cfrac{1}{z + \cfrac{\Delta}{z + \cfrac{\Delta}{z + \cdots + \cfrac{\Delta_{d-2}}{z + \cfrac{\Delta_{d-1}}{z}}}}} \,, \tag{3.37}$$

where $\Delta_{d-2} = \Delta_{d-1} = \Delta$ and, the dimensionality, $d$, is infinite, $d \to \infty$. Thus $\tilde{b}_1(z)$ is an periodic infinite continued fraction which can be readily evaluated (see e.g. [Wall 1948]) as

$$\tilde{b}_1(z) = \frac{2}{z + \sqrt{z^2 + 4\Delta}} = 2\mu^{-2}[(z^2 + \mu^2)^{1/2} - z] \,, \tag{3.38}$$

with $\mu^2 \equiv 4\Delta$ (see Eq. (3.14)). Taking $\nu = 1$ in Eq. (3.24) one obtains also the above result.

Following M. Howard Lee and J. Hong, we may obtain the relaxation function, $a_0(t)$, for the interacting system as follows [Lee & Hong 1985*b*].

Substituting the result (3.38) for $\tilde{b}_1(z)$ into Eq. (3.35), we obtain

$$\tilde{a}_0(z)/s\mu = \frac{(z^2+\mu^2)+(1-s)z}{\mu^2+\alpha z^2}\,, \tag{3.39}$$

where

$$s \equiv \Delta_1^{(0)}/\Delta_1 = \mu^2/(\mu^2+2\Gamma)\,, \tag{3.40}$$

$$\alpha \equiv 1-(1-s)^2 = (x^2+\tfrac{1}{4})/(x^2+\tfrac{1}{2})^2\,, \tag{3.41}$$

with $x^2 \equiv \Gamma/\mu^2$. Note that

$$0 \leqslant s \leqslant 1\,, \tag{3.42}$$

and hence

$$0 \leqslant \alpha \leqslant 1\,. \tag{3.43}$$

In both cases, the upper bound is reached in the non-interacting ideal limit. Taking the inverse Laplace transform

$$a_0(t) = \frac{s\mu}{2\pi \mathrm{i}} \int_c \mathrm{d}z\ \mathrm{e}^{zt}\ \frac{(z^2+\mu^2)+(1-s)z}{\mu^2+\alpha z^2}\ , \tag{3.44}$$

where the contour $c$ runs along the imaginary axis. There are two classes of singularities on the imaginary axis. There is a cut from $z = -\mathrm{i}\mu$ to $z = \mathrm{i}\mu$. In addition, there are a pair of isolated poles

$$z = \pm\alpha^{-1/2}\mu \equiv \pm\,\mathrm{i}\,\omega_p\,, \tag{3.45}$$

that are outside the cut on account of the conditions (3.42) and (3.43) on the parameters $s$ and $\alpha$. The inverse transform can be carried out explicitly (see: Appendix A of [Lee & Hong 1985*b*]):

$$\begin{aligned} a_0(t) =& A_s \sum_{\nu=0}^{\infty} (-1)^\nu \left[\frac{\partial}{\partial(\mu t)}\right]^{2\nu} \left[\frac{\mathrm{J}_1(\mu t)}{\mu t}\right] \\ &+ A_p \cos(\omega_p t)\,, \end{aligned} \tag{3.46}$$

where

$$A_s = 1 - (1 - \alpha^{1/2})\,, \tag{3.47}$$

$$A_p = 2[(1-\alpha)^{1/2} - (1-\alpha)]/\alpha\ . \tag{3.48}$$

It can be shown [Lee & Hong 1985*b*] that this solution satisfies the appropriate boundary conditions, Eqs. (2.11). It can also be shown that in the ideal, non-interacting limit $\alpha = 1$, $a_0(t)$ is given by the $\nu = 0$ term of the ideal system solution Eq. (3.20) that is

$$a_0(t)|_{\alpha=1} = a_0^{(0)}(t) = \mathrm{J}_0(\mu t)\,. \tag{3.49}$$

### 3.2.7 The response function, $\chi_k(\omega)$, and the dynamic structure factor, $S_k(\omega)$ for the non-ideal interacting system

As remarked in §3.2.5 the response function, $\chi_k(\omega)$, and the dynamic structure factor, $S_k(\omega)$ are often readily accessible experimentally measuring the response of the system to the corresponding applied weak field or through the appropriate scattering experiment. They can be obtained from the relaxation function $a_0(t)$ using linear response theory (see §3.2.5).

For the non-ideal interacting 2-D electron gas the response function can be obtained [Lee & Hong 1985*b*] substituting the relaxation function $a_0(t)$ given by Eq. (3.46), into Eq (3.27). Thus, for $\tilde{\chi}_k(\omega) \equiv \chi_k(\omega)/\chi_k$ we find (again suppressing the k dependence)

$$\mathrm{Re}\tilde{\chi}(\omega) = 1 + \frac{A_s(1-\alpha)^{1/2}\omega^2}{\mu^2 - \alpha\omega^2}\,, \quad 0 < \omega < \mu \tag{3.50a}$$

$$= 1 + \frac{A_s(1-\alpha)^{1/2}(1-\mu^2\omega^2)^{1/2}\omega^2}{\mu^2 - \alpha\omega^2}\,, \quad \mu < \omega < \infty \tag{3.50b}$$

and

$$-\mathrm{Im}\tilde{\chi}(\omega) = \frac{A_s\omega(\mu^2 - \omega^2)^{1/2}}{\mu^2 - \alpha\omega^2}\,, \quad 0 < \omega < \mu \tag{3.51a}$$

$$= \tfrac{1}{2}\pi A_p\omega[\delta(\omega - \omega_p) + \delta(\omega + \omega_p)]\,, \quad \mu < \omega < \infty\ . \tag{3.51b}$$

The dynamic structure factor can be obtained from the relation $\pi S(\omega) = -\mathrm{Im}\chi(\omega)$. Hence, directly from Eqs. (3.51a)–(3.51b) we obtain

$$\tilde{S}(\omega) \equiv S(\omega)/\chi = \frac{A_s \omega(\mu^2 - \omega^2)^{1/2}}{\mu^2 - \alpha\omega^2}\,, \quad 0 < \omega < \mu \tag{3.52a}$$

$$= \tfrac{1}{2}\pi A_p \omega[\delta(\omega - \omega_p) + \delta(\omega + \omega_p)]\,, \quad \mu < \omega < \infty\,. \tag{3.52b}$$

## 3.3 Homogeneous 3-D electron gas at $T = 0$ and $k \ll k_F$

In the last section (§3.2) we reviewed an example of the application of the recurrence relations method (RRM) to the homogeneous electron gas in two dimensions. We considered the electron-hole excitations near the Fermi surface at $T = 0$, with $k \ll k_F$, by means of the Sawada model Hamiltonian, Eq. (3.1), that accurately describes that physical situation.

In this section we will show the results of the application of the RRM to the Sawada model in the 3-D case, again in the long wavelength limit.

For the electron gas in three dimensions, and in the same static regime of §3.2, (that is, $T = 0$ and $k \ll k_F$) M. Howard Lee and J. Hong showed that [Lee & Hong 1984]

$$\Delta_1 = u^2/3 + \Gamma \quad \text{and} \quad \Delta_\nu = u^2\nu^2/(4\nu^2 - 1)\,, \quad \nu \geqslant 2\,, \tag{3.53}$$

where $u = 2k\,\varepsilon_F$, $\Gamma = \omega_{pl}^2$ ($\omega_{pl}$ the classical plasma frequency). As in two dimensions, the interaction appears in $\Delta_1$ only. For the ideal system ($\Gamma = 0$), the RR-II is then realized by

$$\Delta_\nu^{(0)} = u^2\nu^2/(4\nu^2 - 1)\,, \quad \nu \geqslant 1\,. \tag{3.54}$$

Following a procedure similar to the one applied in §3.2.4, we observe that the realized RR-II, obtained from Eq. (2.16) with the above recurrants for the ideal (non-interacting) system, is congruent to the recurrence relation for the spherical Bessel functions $\mathrm{j}_\nu$. Hence,

$$a_\nu^{(0)}(t) = \frac{2^\nu(2\nu+1)!!}{u^\nu(2\nu)!!}\mathrm{j}_\nu(ut)\,. \tag{3.55}$$

The Delta's sequences or recurrants completely determine the dynamics of the system through the RR1 and RR2 recurrence schemes. In the last section, for the 2-D electron gas

the solutions were in terms of regular Bessel functions, with cylindrical symmetry, while for the 3-D case in this section the solutions turn out to be in terms of spherical Bessel functions. At this point, thus, it is important to note that also the dimensionality of the physical system is embedded in the Delta's.

To obtain the memory function, we use Eq. (2.30) to write

$$\Delta_1^{(0)}\tilde{b}_1^{(0)}(z) = \frac{1}{\tilde{a}_0^{(0)}(z)} - z\,. \tag{3.56}$$

This can be solved, since

$$\tilde{a}_0^{(0)}(z) = \mathcal{L}[\mathrm{j}_0(ut)] = \tan^{-1} u/z\,. \tag{3.57}$$

Now, by an application of the RR-II one can obtain the memory functions $\tilde{b}_\nu^{(0)}(z)$, and hence $b_\nu^{(0)}(t)$ by the inverse Laplace transform.

To obtain the relaxation and memory functions for the non-ideal system, one can use the fact that recurrants for the ideal and the interacting systems are identical except for the first one. Then, one may use the continued fraction representations of $\tilde{a}_0^{(0)}(z)$ and $\tilde{b}_1(z)$ to obtain the latter and $\tilde{a}_0(z)$, in a manner similar to the one used in §3.2.6.

## 3.4 Asymptotically exact, $k \gg k_F$, solution for the dynamic structure factor of an electron gas at $r_s \approx 3.5$

In this section we will review an asymptotically exact (i.e. $k \gg k_F$) solution for the dynamic structure factor of an electron gas at $r_s \approx 3.5$, developed by J. Hong and M. Howard Lee [Hong & Lee 1993].

The only free parameter in an electron gas is $r_s$. If we set the volume per electron to be $\frac{4}{3}\pi a^3$, then $r_s$ is defined [Gell-Mann & Brueckner 1957] as

$$r_s \equiv \frac{a}{r_{\mathrm{Bohr}}}\,, \tag{3.58}$$

where $r_{\mathrm{Bohr}}$ is the Bohr radius. Thus, $r_s$ is roughly the particle inter-spacing in units of the Bohr radius. Small values of $r_s$ correspond to high density and close packing of the electrons.

In this limit, the kinetic energy, KE, is considerable due to the strong curvature of the wave function because of the Pauli Principle, and dominates over the Coulomb repulsion energy. Therefore, the small $r_s$ limit corresponds to the non-interacting regime. On the other hand, big $r_s$ values correspond to the strongly interacting regime, since, due to very low curvature of the wave function, the KE is smaller than the Coulomb repulsion energy. Metallic densities lie in the range $r_s = 2$–$6$ . This fact precludes direct perturbative approaches in powers of $r_s$. The dynamic structure factor $S(k, \omega)$ of a 3D electron gas is not exactly known in [Hong & Lee 1993], [Mahan 2007] the metallic densities range, except possibly in the long wavelength limit.

We consider the standard homogeneous 3D electron gas model defined [Mahan 2007] by $H = H_0 + V$, where $H_0$ is the KE and $V$ is the Coulomb interaction energy $v(r) = e^2/r$. Therefore,

$$H = \sum_k \epsilon_k a_k^\dagger a_k + \sum_k \upsilon_k \rho_k \rho_{-k} \equiv H_0 + V \,, \tag{3.59}$$

where $\epsilon_k = k^2/2m$, and $a_k^\dagger$ and $a_k$ are, respectively, the fermion creation and annihilation operators at wave vector $k$. In the Coulomb interaction term of the Hamiltonian, the two body interaction, with $k \neq 0$, is

$$\upsilon_k = 4\pi e^2/k^2 \ , \tag{3.60}$$

and

$$\rho_k \equiv \sum_p a_p^\dagger a_{p-k} \ , \tag{3.61}$$

is the density operator.

The dynamic structure factor

$$S(k, \omega) = \frac{1}{N} \int_{-\infty}^{\infty} \mathrm{d}t \ \mathrm{e}^{\mathrm{i}\,\omega t} \langle \rho(k, t) \rho(-k, 0) \rangle \tag{3.62}$$

is related to physical quantities directly measurable through scattering experiments.

The dynamics of an electron gas have been most often studied via the frequency moments $c_n(k)$, which are related to $S(k, \omega)$ through the frequency–moment sum rules at $T = 0$

$$\tfrac{1}{2} c_n(k) = \int_0^{\infty} \mathrm{d}\omega S(k, \omega) \omega^{2n-1} \,, \quad n = 0, 1, 2, \dots \ , \tag{3.63}$$

that are (see [Mahan 2007, Chap. 5]) exact results. The moments of the density response function are calculable from

$$c_n(k) = (L^n\rho_k, L^n\rho_k) \ , \tag{3.64}$$

where

$$L\rho_k \equiv [H, \rho_k] \ , \tag{3.65}$$

$H$ is the Hamiltonian, Eq. (3.59), and the inner product means the Kubo scalar product defined in Eq. (2.1). From the $c_n(k)$ on can construct $S(k,\omega)$ by means of the recurrence relations method (RRM) described in §2.3 and §2.4. The density relaxation function

$$a_0(t) \equiv \frac{(\rho_k(t), \rho_k)}{(\rho_k, \rho_k)} \tag{3.66}$$

is connected to $S(k,\omega)$ as follows

$$\tilde{S}(k,\omega) \equiv S(k,\omega)/c_0(k) \tag{3.67}$$

$$= -\frac{1}{\pi}\mathrm{Im}[1 - z\tilde{a}_0(z)]_{z=\mathrm{i}\,\omega+\epsilon} \ , \tag{3.68}$$

where $\tilde{a}_0(z) \equiv \mathcal{L}a_0(t)$, and $\mathcal{L}$ is the Laplace transform operator.

Using the RR2 scheme we show in §2.4 in Eq. (2.21) that

$$\tilde{a}_0(z) = \cfrac{1}{z + \cfrac{\Delta_1}{z + \cfrac{\Delta_2}{z + \cdots + \cfrac{\Delta_{d-2}}{z + \cfrac{\Delta_{d-1}}{z}}}}} \ , \tag{3.69}$$

where the dimensionality, $d$, in this case is infinite, $d \to \infty$. Each recurrant $\Delta_n$ (see §2.3) can be expressed entirely [Hong & Lee 1993] in terms of the ratios

$$\lambda_{n-1}, \lambda_{n-2}, \ldots, \lambda_0 \ , \quad \text{where} \quad \lambda_n \equiv \frac{c_{n+1}}{c_n} \ . \tag{3.70}$$

Hence, $S(k,\omega)$ may be obtained, given $\{c_n\}$ or $\{\lambda_n\}$ independently. Thus, to obtain $S(k,\omega)$ the moments $c_n$'s given by the Kubo scalar product, Eq. (3.64), must be calculated using the Hamiltonian, Eq. (3.59). For $k \gg k_F$ ($k_F$ the Fermi wave vector), M. H. Lee and J. Hong find [Hong & Lee 1993] that the ratios of the successive moments can be given as

$$\lambda_n = P + nQ + \sum_{i=1}^{n} R_i + o(k^{-2}) \,, \quad n = 0, 1, 2, \ldots, \tag{3.71a}$$

$$P = k^4 - (4x/3)k^2 + \tfrac{16}{9}x^2 - \tfrac{16}{5}y + \tfrac{1}{3}\omega_p^2[1 + 2g(0)] \,, \tag{3.71b}$$

$$Q = (16x/3)k^2 - \tfrac{16}{9}x^2 + \tfrac{16}{5}y \,, \tag{3.71c}$$

$$R_\nu = -2^6/3(\nu-1)(2\nu-3)A - 2^7/9(\nu-1)B \,, \tag{3.71d}$$

$$A = x^2 - \tfrac{3}{5}y \,, \tag{3.72a}$$

$$B = x^2 - \tfrac{3}{16}\omega_p^2[1 - g(0)] \,, \tag{3.72b}$$

where $k$ is now expressed in units of $k_F$, $\hbar = 1$, $\omega_p$ is the plasma frequency expressed in units of $\epsilon_F$, the Fermi energy, and $g(0)$ is the pair correlation function at the origin; $x$ and $y$ are the average one particle KE and KE-squared, expressed in units of $\epsilon_F$ and $\epsilon_F^2$, respectively[1]. Evidently, $\lambda_n$ in Eq. (3.71a) depends on $r_s$ through $x$, $y$, $g(0)$, and $\omega_p$.

If $\lambda_n$ were independent of n, e.g. $\lambda_n = \lambda$, Eq. (3.71a) would be in the form of a 1D transfer matrix equation, $c_{n+1} = \lambda c_n$, in which $\lambda$ would act as an eigenvalue. But it is not; $\lambda_n$ is non-linearly dependent on $n$ through $R_n$. Therefore, a general solution even for large $k$ is probably precluded. To obtain a particular solution, M. H. Lee and J. Hong make the following assumption [Hong & Lee 1993] (to be justified):

$$\text{At} \quad r_s = r_s^* \,, \quad A = B = 0 \,. \tag{3.73}$$

Then, to order $k^0$, Eq. (3.71a) under the assumption becomes

$$\lambda_n(r_s = r_s^*) \equiv \lambda^* = P^* + nQ^* = (n+s)Q^*, \quad s \equiv P^*/Q^*, \tag{3.74}$$

[1]In this high-$k$ expansion, M. H. Lee and J. Hong retain [Hong & Lee 1993] terms to order $k^0$ and neglect those of order $k^{-2}$ and lower. The expansion for $n = 0, 1, 2$ may be obtained from [Raedt & Raedt 1978]

where an asterisk on a real quantity means that its density is set at $r_s = r_s^*$. Then, valid to this order of $k$,

$$\lambda_n^* - \lambda_{n-1}^* = Q^*, \tag{3.75}$$

i.e., the difference is now independent of $n$.

Since $\Delta_n$ is a function of the ratios $\lambda_{n-1}, \lambda_{n-2}, \ldots, \lambda_0$ (see Eq. (3.70)), the particular form of the primary asymptotic definition of $\lambda_n$, given in Eq. (3.71a), and Eq. (3.74) imply that $\{\Delta_n^*\}$ is composed of two families:

$$\Delta_{2n-1}^*(k) = (n - 1 + s)Q^*\,, \tag{3.76a}$$

$$\Delta_{2n}^*(k) = nQ^*\,, \tag{3.76b}$$

$n = 1, 2, \ldots$. Substituting Eqs. (3.76a)–(3.76b) in the continued fraction expansion of $\tilde{a}_0(z)$, Eq (3.69), M. H. Lee and J. Hong obtain [Hong & Lee 1993]:

$$\tilde{a}_0(z) = \frac{z}{Q^*\Gamma(s)} \int_0^\infty \frac{\mathrm{e}^{-u}\, u^{s-1}\, \mathrm{d}u}{u + z^2/Q^*}\,, \tag{3.77}$$

if Re$s > 0$ and[2] $z \neq \pm \mathrm{i}\,|\xi|$. Finally, substituting the closed result, Eq. (3.77), in Eq. (3.68) M. H. Lee and J. Hong also obtain [Hong & Lee 1993]

$$\tilde{S}^*(k, \omega) = \frac{\omega^{2s}}{(Q^*)^s \Gamma(s)}\,, \mathrm{e}^{-\omega^2/Q^*} \tag{3.78}$$

where the frequency $\omega$ is in units of $\epsilon_F$. Therefore, Eq. (3.78) is an asymptotically exact expression for the dynamic structure factor of the electron gas at $r_s = r_s^*$ *subject to the assumption* given in Eq. (3.73). Observe that $\tilde{S}^*(k, \omega)$ is smoothly peaked at $\omega = \overline{\omega}$ i.e. $(\partial/\partial\omega)\tilde{S}^*(k, \overline{\omega}) = 0,\ \overline{\omega} = (sQ^*)^{1/2}$, which may be interpreted as the recoil frequency (since, e.g. $\overline{\omega} \to \hbar k^2/2m$ as $k \to \infty$)[Hong & Lee 1993].

To justify the assumption $A^* = B^* = 0$ note that it asserts that there exist unique relationships between $x$, $y$, and $g(0)$ at $r_s = r_s^*$. These relationships cannot be determined from the frequency sum-rules (3.63). But if they exist one may be able to deduce them

[2]This is a continued fraction of Gauss. See [Wall 1948, p. 355]. By definition, $s > 0$. Since $s = (3/16x^*)k^2 + \cdots$, $s \to \infty$ smoothly as $k \to \infty$. Also, $z = \mathrm{i}\,\omega + \epsilon$, $\epsilon > 0$. Hence, $z \neq \pm \mathrm{i}\,|\xi|$.

from other general properties of dynamic structure factor. If, for example, $\mathcal{T}$ denotes the one-particle KE in 3D, its average at $T = 0$ is given by

$$\langle \mathcal{T}^n \rangle = \lim_{k\to\infty} \frac{2n+1}{(4\,\omega_r)^n} \int_0^\infty S(k,\omega)(\omega - \omega_r)^{2n}\,\mathrm{d}\omega\,, \quad n = 1, 2, \ldots, \tag{3.79}$$

where $\omega_r$ is the recoil frequency [Lee & Sindoni 1992, App. F, p. 3035]. Recall that $\langle \mathcal{T} \rangle = x$ and $\langle \mathcal{T}^2 \rangle = y$, where $x$ and $y$ are *parameters* of the moments. See Eqs. (3.71a)–(3.71d) and Eqs. (3.72a)–(3.72b). Since $S(k,\omega)$ is valid for large $k$, it may be used in Eq. (3.79) to calculate $\langle \mathcal{T}^n \rangle$ at $r_s = r_s^*$. Substituting Eq. (3.78) in Eq. (3.79), with $\omega_r = \omega_r^* = \overline{\omega}$, [Hong & Lee 1993] obtain, when $n = 1$ and $n = 2$,

$$\langle \mathcal{T} \rangle_{r_s^*} = x^*\,, \tag{3.80a}$$

$$\langle \mathcal{T}^2 \rangle_{r_s^*} = \tfrac{5}{3}(x^*)^2 = y^*\,. \tag{3.80b}$$

Eq. (3.80a) indicates that the average KE is given correctly by Eq. (3.78). It is a necessary condition for the validity of the expression (3.78) for $\tilde{S}^*(k,\omega)$, here obtained independently of the frequency moment sum rules (3.63). Equation (3.80b) indicates that $A^* = (x^*)^2 - \frac{3}{5}y^* = 0$, i.e. the first part of the assumption is satisfied.

Next, M. H. Lee and Hong use a relation due to [Kimball 1973], given as

$$\mu \equiv \lim_{k\to\infty} \{k^4[1 - S(k)]\} = \tfrac{1}{2}\omega_p^2\, g(0)\,, \tag{3.81}$$

which ties $g(0)$ to the large-$k$ form of the static structure factor $S(k)$ [Lee & Hong 1985*a*]. Since $S(k)$ may be obtained from $S(k,\omega)$ by

$$S(k) = \frac{1}{\rho}\int_0^\infty \mathrm{d}\omega\, S(k,\omega)\,, \tag{3.82}$$

where $\rho$ is the number density, Eq. (3.81) can be used to establish a connection between $g(0)$ and $x$ or $y$. Using Eq. (3.78), Eq. (3.81) and Eq. (3.71c), [Hong & Lee 1993] obtain (without using $A^* = 0$) the desired relationship

$$\tfrac{1}{6}(\omega_p^*)^2[1 - g^*(0)] = -\tfrac{10}{9}(x^*)^2 + \tfrac{6}{5}y^* \tag{3.83}$$

Then by Eq. (3.72b)

$$B^* = (x^*)^2 - \tfrac{3}{16}(\omega_p^*)^2[1 - g^*(0)] = \tfrac{9}{4}A^* \ . \tag{3.84}$$

Since $A^* = 0$ by Eq. (3.80b), $B^* = 0$ also. This shows that $A$ and $B$ vanish simultaneously at one unique value of $r_s$. Thus, Hong & Lee [1993] conclude that Eq. (3.78), is an asymptotically exact solution of the dynamic structure factor at $r_s = r_s^*$.

The possible usefulness of the asymptotic expression (3.78) hinges on the value of $r_s$. Since the one-body and two-body distribution functions are not analytically known, it is not possible to determine it exactly. Hong & Lee [1993] attempt to obtain it by numerical means. To do so it is necessary to know the values of $x$, $y$, and $g(0)$ for a range of $r_s$. They review approaches by several people. Although different methods yield somewhat different results, most seem to agree to two significant decimal places. M. H. Lee and J. Hong finally conclude that $r_s = 3.5 \pm 0.2$, and therefore also $\omega_p^* = 1.76 \pm 0.10$ using Lantto, Pietiläinen & Kallio [1982] results.

The fact that $r_s$ falls within the metallic density range makes the asymptotic solution (3.78) meaningful. The value of $r_s$ is in fact close to that of Li ($r_s = 3.25$). Fortunately there is an old measurement for Li at $k = 2.08k_F$ [Eisenberger, Platzman & Schmidt 1975]. This value of $k$ is probably large enough to permit a comparison with asymptotic result (3.78). In Fig.3.1 we reproduce Fig. 2 of [Hong & Lee 1993]. Shown there is the measured dynamic structure factor for Li against the theoretical one (3.78) with $k$ set at the experimental value. The position of the maximum $S(k, \omega)$ is nearly indistinguishable. Also shown is the RPA result at the same value of $k$ which is markedly different as is well known [Hong & Lee 1993].

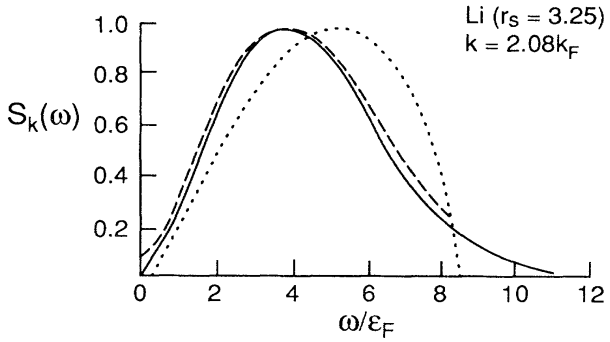



FIG. 2. $S(k,\omega)$ vs $\omega$. Experimental (dashed line), Ref. [12(a)]; Eq. (10) (solid line); RPA (dotted line). The vertical scale is arbitrary.

Figure 3.1: Reproduction of Fig. 2 taken from [Hong & Lee 1993]. Eq. (10) corresponds to the asymptotic expression for the dynamical structure factor, our Eq. (3.78), and [12(a)] is the experimental result for Li.

# Chapter 4

## Applications of the Recurrence Relations Method II: The Spin van der Waals Model

In this chapter we will review an application of the recurrence relations method (RRM) to a system whose static properties are —in marked contrast to the electron gas examples considered in Chapter 3— simple, in fact, mean-field like. It is well worth noting again that RRM is used to calculate *exactly* the time evolution of dynamical variables in terms of the recurrants (or Delta's) $\{\Delta_m\}$, and that they only depend on the given *static* properties of the system and the choice of the dynamic variable. This dependence is through the Kubo scalar product, KSP, which in turn depends on an ensemble average of a correlation function (see the KSP definition, Eq. (2.1)), that involves the model Hamiltonian and the chosen dynamical variable. Therefore, the specific features of the physical model, the statistical assumptions, and the temperature will be embedded in the $\{\Delta_m\}$. The RRM will then allow the comparison of the different dynamics that may arise according to the corresponding static regime of the system, picked by the particular choice of the parameters and/or the temperature.

The model system we will consider is the spin-$\frac{1}{2}$ anisotropic Heisenberg model, in infinite lattice dimensions, following the work by M. Howard Lee, I. M. Kim and Raf Dekeyser in [Lee, Kim & Dekeyser 1984].

This system is an instance (in the following it is shown that it becomes the spin van der Waals model) of certain statistical mechanics models that are exactly solvable at some special limits, providing useful insight into the behavior of these models [Lee, Kim & Dekeyser

1984],[Baxter 1982]. An example is the classical Heisenberg model, that when its spin dimensionality is made infinitely large, it becomes the spherical model [Stanley 1968], whose static behavior is well understood [Berlin & Kac 1952], and has been useful for understanding critical behaviors [Stanley 1968].

Consider the spin-$\frac{1}{2}$ nearest neighbor (nn) anisotropic[1] Heisenberg model on an hypercubic lattice of dimensionality $D$,

$$H = -\sum_{\alpha} \sum_{(i,j)} J_{ij}^{\alpha}(D) s_i^{\alpha} s_j^{\alpha} \ , \tag{4.1}$$

where $\alpha = x, y, z$. M. H. Lee and N. L. Sharma showed that an infinite-*lattice*-dimensional limit [Lee & Sharma n.d.] ($D \to \infty$) of Eq. (4.1) is the spin van Waals model. In the static regime this limit is uninteresting since the model should behave in a mean-field fashion. However, it may qualitatively describe the time-dependent behavior of the quantum model in finite lattice dimensions. Other than in $D = 1$ at $T = 0$ or $T \to \infty$, the time-dependent behavior of Eq. (4.1) is not exactly known presently.

Lee, Kim & Dekeyser [1984] tackle the $D \to \infty$ limit, i.e., the spin van der Waals model. Setting

$$J_{ij}^{x}(D) = J_{ij}^{y}(D) \equiv J/N \ , \tag{4.2}$$

and

$$J_{ij}^{z} \equiv J_z/N \ , \tag{4.3}$$

[1]The variable chosen for the study of its dynamical behavior is the total spin $S_\alpha$. If the system were isotropic, $[H, S_\alpha] = 0$, i.e., this variable would be a constant of the motion ($S_\alpha$ and $H$ are defined below).

in the Hamiltonian (4.1), where $J$ and $J_z$ are non-negative, they choose $f_0 = S_x$, i.e., $\alpha = x$, and using, Eq. (2.6a), the RR1 recurrence relation for the basis vectors, $f_\nu$'s , they obtain

$$f_1 = -2\omega S_z S_y \,, \tag{4.4a}$$

$$f_2 = -4\omega^2 S_z^2 S_x + \Delta_1 S_x \,, \tag{4.4b}$$

$$f_3 = 8\omega^3 S_z^3 S_y - 2(\Delta_2 + \Delta_1)\omega S_z S_y \,, \tag{4.4c}$$

$$f_4 = 16\omega^4 S_z^4 S_x - 4(\Delta_3 + \Delta_2 + \Delta_1)\omega^2 S_z^2 S_x + \Delta_3\Delta_1 S_x \,, \tag{4.4d}$$

etc., where $\hbar = 1$ and

$$\omega = (J - J_z)/N \,. \tag{4.5}$$

In Eqs. (4.4), for each $f_\nu$, only the terms that contribute to the leading order of $N$ when $(f_\nu, f_\nu)$ is evaluated, are retained.

To evaluate the norm $(f_\nu, f_\nu)$ of $f_\nu$ explicitly, one needs to know the ensemble averages that appear in the inner product[Lee 1982*c*]. Thus the evaluation depends on whether $J > J_z$ ($XY$ regime) or $J < J_z$ (Ising regime).

## 4.1 $XY$ REGIME

### 4.1.1 —FOR $T > T_c = J/2\mathrm{k}$

Kim & Lee [1981] have shown that

$$\langle S_z^{2\nu} S_x^2 \rangle = \langle S_z^{2\nu} \rangle \, \langle S_x^2 \rangle \,, \tag{4.6a}$$

$$\langle S_z^{2\nu} \rangle = (2\nu - 1)!! \langle S_z^2 \rangle^\nu \,, \qquad \nu = 1, 2, 3, \ldots, \tag{4.6b}$$

where

$$\langle S_z^2 \rangle = \tfrac{1}{2} N/(2 - \beta J_z) \,, \tag{4.6c}$$

and

$$\langle S_x^2 \rangle = \tfrac{1}{2} N/(2 - \beta J) \,. \tag{4.6d}$$

Using these results and retaining only the leading terms of $N$, Kim & Lee [1981] obtain

$$(f_\nu, f_\nu) = \langle S_x^2 \rangle \,. \tag{4.7}$$

Hence the $\nu$th recurrant is

$$\Delta_\nu = \nu \, (4\omega^2 \langle S_z^2 \rangle) \equiv \nu \Delta \;, \quad \nu \geqslant 1 \,. \tag{4.8}$$

The upper limit on $\nu$ [Lee, Kim & Dekeyser 1984] is unbounded. Therefore $d \to \infty$.

### 4.1.2 —For $T < T_c$

There exists an ordered phase, i.e. $\langle S_x \rangle = O(N)$ (See [Lee 1982*a*] [Pathria 1983]). Notwithstanding, Lee, Kim & Dekeyser [1984] obtain that the same form of the decoupling equations, Eqs. (4.6), is still valid provided that one uses Eq. (4.6d) for $\langle S_x^2 \rangle$; and, that one sets

$$\chi = (f_0, f_0) = \langle S_x^2 \rangle - \langle S_x \rangle^2 \;. \tag{4.9}$$

Therefore, the norm of $f_\nu$ for has the same form, and the structure of the recurrants is consequently identical whether $T$ is above or below $T_c$ for the $XY$ regime.

## 4.2 Ising regime

### 4.2.1 —For $T > T_c = J_z/2\mathrm{k}$

Lee, Kim & Dekeyser [1984] show that the Ising and $XY$ static properties are identical. Hence, the recurrants given by Eq. (4.8) are also valid for the high-temperature Ising regime.

### 4.2.2 —For $T < T_c = J_z/2\mathrm{k}$

The ordered phase is characterized by $\langle S_z \rangle = O(N)$. The first of the decoupling equations, Eq. (4.6a), remains valid but now (See, e.g., [Lee 1982*a*] [Pathria 1983]), instead of Eq. (4.6b) one has

$$\langle S_z^{2\nu} \rangle = \langle S_z \rangle^{2\nu} \,. \tag{4.10}$$

Using both equations Lee, Kim & Dekeyser [1984] find

$$(f_0, f_0) = \chi\,, \tag{4.11a}$$

$$(f_1, f_1) = 4\omega^2 \langle S_z \rangle^2 \chi\,, \tag{4.11b}$$

and thus

$$\Delta_1 = 4\omega^2 \langle S_z \rangle^2 \equiv \Omega^2\,. \tag{4.12}$$

Using these results, they also find $(f_2, f_2) = 0$ and therefore $\Delta_2 = 0$. A more careful [Lee, Kim & Dekeyser 1984] analysis shows that

$$(f_\nu, f_\nu) = O(N) \quad \nu = 0 \text{ and } 1\,, \tag{4.13}$$

$$= O(N^{-1}) \quad \nu \geqslant 2\,. \tag{4.14}$$

This behavior implies that the $d$-dimensional Hilbert space $\mathcal{S}_0^{(d)}$ becomes effectively reduced to a two dimensional space, i.e.,

$$\mathcal{S}_0^{(d)} = \mathcal{S}_0^{(2)} \otimes \mathcal{S}_2^{(d-2)}\,, \tag{4.15}$$

where $\mathcal{S}_0^{(d)}$ is a two-dimensional (2D) subspace spanned by $f_0$ and $f_1$, and $\mathcal{S}_2^{(d-2)}$ is a $(d-2)$-dimensional subspace spanned by $f_2, \ldots, f_{d-1}$. The time evolution of $S_x$ is confined to the 2D space $\mathcal{S}_0^{(2)}$ at all times. It does not extend into $\mathcal{S}_2^{(d-2)}$ [Lee, Kim & Dekeyser 1984].

In summary, using the RRM, Lee, Kim & Dekeyser [1984] found two distinct dynamical regimes.

—For the $XY$ and high-temperature Ising regimes the RR2 is

$$(\nu+1)\Delta\, a_{\nu+1}(t) = -\dot{a}_\nu(t) + a_{\nu-1}(t)\,, \qquad 0 \leqslant \nu \leqslant \infty\,, \tag{4.16}$$

where $\Delta$ is given by Eq. (4.8). The solution to this difference equation is

$$a_\nu(t) = (t^\nu/\nu!)\exp(-\tfrac{1}{2}\Delta\, t^2) \tag{4.17}$$

—For the low-temperature Ising regime, $d = 2$ and $\Delta_1 = \Omega^2$ only ($\Omega$ is given by Eq. (4.12)). Therefore, the RR2 is

$$\Omega^2 a_1(t) = -\dot{a}_0(t)\,, \tag{4.18a}$$

$$0 = -\dot{a}_1(t) + a_0(t)\,. \tag{4.18b}$$

Hence, $a_0(t) = \cos\Omega t$ and $a_1(t) = \sin\Omega t$.

In the $XY$ and high-temperature Ising regimes the trajectory traced out by the time evolution of $S_x$ is spiral-like, but with

$$(S_x(t), S_x(t)) = (S_x, S_x) = \text{const}\,, \tag{4.19}$$

since the system is hermitian. It starts from the basal vector $f_0$ winding towards to the highest vector $f_{d\to\infty}$. In the low-temperature Ising regime the trajectory only can only be rotacional, being confined to a two-dimensional space.

Remarkably [Lee 2009], a realization of the spin van der Waals model is found, not in a magnetic material but, in hydrogen absorbed in a lattice matrix of palladium. de Ribaupierre & Manchester [1974] report a finite discontinuity in the specific heat vs $T$ of this system. Such a discontinuity is characteristic [Lee 2009][Pathria 1983] of mean-field behavior. The forces between H atoms [Lee 2009] are long range and approximately constant due to its origin in compressional waves. These waves arise from the interstitial occupation by H atoms.

# Chapter 5

## Applications of the Recurrence Relations Method
## III: Quantum Spin Chains at T=$\infty$

### 5.1 Dynamical Equivalence (DE)

If we use the recurrence relations method (RRM) to investigate the time evolution of two dynamic variables corresponding to two different physical models, say, $A$ and $B$, then the sets of recurrants:

$$R_A \equiv \{\Delta_\nu^{(A)}\}\,, \quad \nu = 0, 1, \ldots, d_A - 1\ , \tag{5.1a}$$

and

$$R_B \equiv \{\Delta_\nu^{(B)}\}\,, \quad \nu = 0, 1, \ldots, d_B - 1\ . \tag{5.1b}$$

will be different[1]. But, even though different, the sets $R_A$ and $R_A$ may be *similar*, in the sense that the relationships among the $\{\Delta_\nu^{(A)}\}$, and among the $\{\Delta_\nu^{(B)}\}$ are the same, and that

$$d_A = d_B \equiv d. \tag{5.2a}$$

Then, one would have

$$\Delta_\nu^{(A)} = \kappa^2 \Delta_\nu^{(B)}\,, \quad \nu = 0, 1, \ldots, d - 1\ , \tag{5.2b}$$

with $\kappa^2 > 0$. If Eqs. (5.2) hold, the geometries of the realized spaces $\mathcal{S}_A$ and $\mathcal{S}_B$ are the same, and then, one may say that the systems $A$ and $B$ are *dynamically equivalent* for the particular choices of dynamic variables and corresponding model parameters. Since the

[1]The $\Delta$'s are model dependent and parameter dependent. See §2.3. One could think loosely about them as the characteristic system frequencies squared, but in fact, they define the shape of the realized (dynamical) Hilbert space.

recurrants uniquely determine the time evolution, aside from a constant time-scaling factor their time evolutions will be *identical*.

In this chapter we will review the application, by João Florencio, Jr. and M. Howard Lee, of the RRM to the one-dimensional (1–D) spin-$\frac{1}{2}$ XY model which may be defined by the Hamiltonian

$$H = 2\sum_{i}^{N}(J^x S_i^x S_{i+1}^x + J^y S_i^y S_{i+1}^y) - B\sum_{i}^{N} S_i^z \ , \tag{5.3}$$

where $S_i^\alpha$ are spin operators, $J^\alpha$ are the coupling constants, and $B$ is an external magnetic field. Periodic boundary conditions are imposed, that is, $S_{N+1}^\alpha = S_1^\alpha$ , where $N$ is the total number of spins and $\alpha = x, y,$ or $z$. João Florencio & Lee [1987] consider two particular cases of this Hamiltonian:

—The isotropic XY model which corresponds to

$$J^x = J^y = J, \quad B = 0\,. \tag{5.4}$$

—The transverse Ising TI model given by

$$J^x = J, \ J^y = 0\,, \quad B \neq 0\,. \tag{5.5}$$

Following [João Florencio & Lee 1987] we will show that in the high temperature limit, and for a particular choice of parameters[2], these two models are dynamically equivalent to the $d = \infty$ dynamic regime[3] of the spin van der Waals model reviewed in the last chapter.

The model defined by the Hamiltonian of Eq. (5.3), is an instance of a solvable many-body system (See, e.g., [Mattis 1994, *The Many-Body Problem: An Encyclopedia of Exactly Solved Models*] and the references therein). The equilibrium properties of these systems are well known [Mattis 1994], [Lieb, Schultz & Mattis 1961], [Katsura 1962], but their dynamical behavior is less understood. Non-equilibrium exact results are few. João Florencio & Lee [1987] cite as noteworthy the time-dependent longitudinal spin correlations functions at any temperature due to Niemeijer [1967], and the time-dependent transverse spin correlation

[2] $B = J$ for the TI model.

[3] That comprises the XY regime for $T$ above or below $T_c$, and the Ising regime with $T > T_c$.

functions at infinite temperature obtained by Brandt & Jacoby [1976], and also by Capel & Perk [1977].

It is pointed out by João Florencio & Lee [1987] that the time-dependent properties of simple spin chain models such as the XY and TI in 1–D have been first studied extensively by means of special or *ad-hoc* mathematical techniques [Lieb et al. 1961]. To their knowledge these techniques cannot be applied to study 1–D models of higher complexity, e.g., the XYZ model. They cannot be generalized to study the XY and TI models in two or higher dimensions and, perhaps, the most important limitation is that they cannot be used to obtain approximate solutions (See the last appendix of [João Florencio & Lee 1987]).

## 5.2 Isotropic XY model at $T = \infty$

The XY model is defined by Eq. (5.3) and Eq. (5.4). João Florencio & Lee [1987] pick $S_j^x$ as the dynamical variable of interest. The time evolution of $S_j^x$ is given, according to the RR2 of §2.4, as

$$S_j^x(t) = \sum_{\nu=0}^{d-1} a_\nu(t) f_\nu \ , \tag{5.6}$$

where $f_0 = S_j^x(0) = S_j^x$. Using the RR1 of §2.3, João Florencio & Lee [1987] obtain (setting $\hbar = 1$) the following basis vectors:

$$f_1 = 2J(S_{j-1}^y S_j^z + S_j^z S_{j+1}^y) \ , \tag{5.7a}$$

$$\begin{aligned} f_2 = -4J^2(&S_{j-2}^x S_{j-1}^z S_j^z - S_{j-1}^x S_j^y S_{j+1}^y + 2S_{j-1}^y S_j^x S_{j+1}^y \\ &- S_{j-1}^y S_j^y S_{j+1}^x + S_j^z S_{j+1}^z S_{j+2}^x) \ , \end{aligned} \tag{5.7b}$$

$$\begin{aligned} f_3 = 2J^3(&-4S_{j-3}^y S_{j-2}^z S_{j-1}^z S_j^z + 4S_{j-2}^y S_{j-1}^z S_j^y S_{j+1}^y - 8S_{j-2}^x S_{j-1}^z S_j^y S_{j+1}^x \\ &+ 12S_{j-2}^x S_{j-1}^z S_j^x S_{j+1}^y + 3S_{j-1}^y S_{j+1}^z + 3S_{j-1}^z S_{j+1}^y + 12S_{j-1}^y S_j^x S_{j+1}^z S_{j+2}^x \\ &- 8S_{j-1}^x S_j^y S_{j+1}^z S_{j+2}^x + 4S_{j-1}^y S_j^y S_{j+1}^z S_{j+2}^y - 4S_j^z S_{j+1}^z S_{j+2}^z S_{j+3}^y) \ , \end{aligned} \tag{5.7c}$$

etc.

Notwithstanding tediousness, it is a straightforward matter to obtain the expression for the basis vector of any desired order, say $f_\nu$, using the known expressions for the basis vectors

of lower orders $f_0, f_1, \ldots, f_{\nu-1}$ in the RR1 given by Eq. (2.6a) of §2.3. Note that as the order ($\nu$) increases, the basis vectors involve more and more spins which are farther and farther removed from the original lattice point $j$. This feature indicates that in the thermodynamic limit ($N \to \infty$) the dimension $d$ of the realized Hilbert space $\mathcal{S}$ will ultimately grow to infinity ($d \to \infty$).

In the high temperature limit ($T \to \infty$) the norms of the basis vectors of Eqs. (5.7) can be readily calculated. In this limit the Kubo scalar product defined in Eq. (2.1) of §2.2 becomes

$$(A, B) \equiv \frac{1}{Z}\mathrm{Tr}A^{\dagger}B \ , \tag{5.8}$$

with $Z = 2^N$: the partition function of the system in the same limit. Using Eq. (5.8), João Florencio & Lee [1987] find for $f_0$ that

$$(f_0, f_0) = \langle S_j^x S_j^x \rangle = \tfrac{1}{4} \ , \tag{5.9a}$$

and for $f_1$ ,

$$(f_1, f_1) = 4J^2\langle (S_{j-1}^y S_j^z + S_j^z S_{j+1}^y)(S_j^z S_{j-1}^y + S_{j+1}^y S_j^z)\rangle = \frac{J^2}{2} \ . \tag{5.9b}$$

Similarly, they obtain

$$(f_2, f_2) = 2J^4 \ , \tag{5.9c}$$

$$(f_3, f_3) = 16J^4 \ , \tag{5.9d}$$

$$(f_4, f_4) = 96J^4 \ , \tag{5.9e}$$

etc. These calculations were simplified by the fact that the crossed-product terms vanish since they always contain unpaired spins which are traceless. The norm of each basis vector is, therefore, given by a trace over the sum of the squares of each term of the basis vector being considered.

Substituting the values of the norms given in Eqs (5.9) into the recurrants definition, Eq. (2.6b) of §2.3, it is found immediately that

$$\Delta_\nu = \nu\,\Delta\,, \qquad \nu = 1, 2, 3, \ldots, \tag{5.10}$$

with $\Delta = 2J^2$ . Once the recurrants are known, the time evolution is uniquely defined. The basis functions $a_\nu(t)$ can be calculated —directly, using the RR2 scheme given by Eq. (2.16) of §2.4 (See §3.2.4 for an example of this approach), or —alternatively, using the continued fraction representation, Eq. (2.21), of $\tilde{a}_0(z)$ (the Laplace transform of $a_0(t)$) and then through the RR2 scheme and the inverse Laplace transform, calculate the other $a_\nu$'s. Let's see the latter. Substituting the deltas given by Eq. (5.10) into the continued fraction representation of $\tilde{a}_0(z)$, Eq. (2.21), we find:

$$\tilde{a}_0(z) = \cfrac{1}{z + \cfrac{\Delta}{z + \cfrac{2\Delta}{z + \cfrac{3\Delta}{z + \cdots}}}} \,, \tag{5.11a}$$

$$= \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \mathrm{d}s \, \frac{\mathrm{e}^{-s^2}}{z + \mathrm{i}\,(2\Delta)^{1/2} s} \,. \tag{5.11b}$$

The closed form, Eq. (5.11b), of the infinite continued fraction follows from [João Florencio & Lee 1987, Appendix A] and from the integral representation of [Wall 1948, p. 358] that, for $p > 0$ gives

$$\mathrm{e}^{p^2/2} \int_p^{\infty} \mathrm{d}u \; \mathrm{e}^{-u^2/2} = \cfrac{1}{p + \cfrac{1}{p + \cfrac{2}{p + \cfrac{3}{p + \cdots}}}} \,, \tag{5.12}$$

and the identity

$$\int_p^{\infty} \mathrm{d}u \; \mathrm{e}^{-u^2/2} = \frac{\mathrm{e}^{-p^2}}{2\sqrt{\pi}} \int_{-\infty}^{\infty} \mathrm{d}s \, \frac{\mathrm{e}^{-s^2}}{p + \mathrm{i}\, s} \,. \tag{5.13}$$

Taking the inverse Laplace transform of Eq. (5.11b)

$$a_0(t) = \frac{1}{2\pi\,\mathrm{i}} \int_C \mathrm{d}z\ \mathrm{e}^{zt}\, \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \mathrm{d}s\, \frac{\mathrm{e}^{-s^2}}{z + \mathrm{i}(2\Delta)^{1/2} s}\ , \tag{5.14}$$

where $C$ denotes a contour running along the right side of the imaginary axis. Exchanging the order of integration, it is readily obtained

$$a_0(t) = \mathrm{e}^{-\Delta\, t^2/2}\ . \tag{5.15}$$

Once $a_0(t)$ is know, the RR2 in the time domain, Eq. (2.16), may be used repeatedly to obtain the other $a_\nu$'s. E.g., the RR2 for $m = 0$ gives

$$\Delta_1 a_1(t) = -\dot{a}_0(t)\,, \tag{5.16}$$

therefore, using the $\Delta_\nu$'s definition, Eq. (5.10), we obtain immediately

$$a_1(t) = t\, \mathrm{e}^{-\Delta\, t^2/2}\ .$$

Proceeding in the same manner, the solution is obtained

$$a_\nu(t) = \frac{t^\nu}{\nu!}\, \mathrm{e}^{-\Delta\, t^2/2}\ . \tag{5.17}$$

Thus, for the $S_j^x$ variable in the isotropic XY model at $T = \infty$

$$\begin{aligned} a_0(t) &\equiv \frac{(S_j^x(t), S_j^x)}{(S_j^x, S_j^x)} = 4\langle S_j^x(t), S_j^x\rangle\,, \\ &= \exp(-J^2 t^2) \end{aligned} \tag{5.18}$$

## 5.3 Transverse Ising (TI) model at $T = \infty$

The TY model is defined by the Hamiltonian of Eq. (5.3), and the parameter conditions of Eq. (5.5). The time evolution of $S_j^x$ is given, according to the RR2 of §2.4, as

$$S_j^x(t) = \sum_{\nu=0}^{d-1} a'_\nu(t) f'_\nu\ , \tag{5.19}$$

where $f'_0 = S^x_j(0) = S^x_j$, and the primes in this case are used to distinguish the notation here from that of the XY model. Using the RR1 of §2.3, João Florencio & Lee [1987] obtain the following basis vectors:

$$f'_1 = BS^y_j \ , \tag{5.20a}$$

$$f'_2 = -2JB(S^x_{j-1}S^z_j + S^z_j S^x_{j+1}) \ , \tag{5.20b}$$

$$f'_3 = -2JB^2(S^y_{j-1}S^z_j + S^z_j S^y_{j+1}) - 8J^2 B S^x_{j-1}S^y_j S^x_{j+1} \ , \tag{5.20c}$$

$$\begin{aligned} f'_4 = -4J^2B^2(&S^x_{j-2}S^z_{j-1}S^z_j - 2S^x_{j-1}S^x_j S^x_{j+1} - 3S^x_{j-1}S^y_j S^y_{j+1} \ , \\ &- 3S^y_{j-1}S^y_j S^x_{j+1} + S^z_j S^z_{j+1}S^x_{j+2}) \ , \end{aligned} \tag{5.20d}$$

etc.

The basis vectors are simpler than those for the XY model as a consequence of the relatively simpler coupling in the transverse Ising (TI) model. Also, the Ising basis vectors contain [João Florencio & Lee 1987] one less spin operator in each term. This difference stems from the fact that $f'_1$ is bound to the original lattice site $j$, unlike $f_1$ that includes the sites $j \pm 1$. Again, as the order increases, the TI basis vectors also involve more and more spins which are farther and farther removed from the original lattice point.

The norms of the Ising basis vectors may be calculated directly. As in the calculations of the norms of the XY basis vectors, only the square of each term of $f'_\nu$ contributes to its norm. In a manner similar to that of Eqs. (5.8)–(5.9), João Florencio & Lee [1987] obtain

$$(f'_0, f'_0) = \langle S^x_j S^x_j \rangle = \tfrac{1}{4} \ , \tag{5.21a}$$

$$(f'_1, f'_1) = B^2 \langle S^y_j S^y_j \rangle = \frac{B^2}{4} \ , \tag{5.21b}$$

$$(f'_2, f'_2) = 4J^2B^2 \langle (S^x_{j-1}S^z_j + S^z_j S^x_{j+1})(S^z_j S^x_{j-1} + S^x_{j+1}S^z_j) \rangle = \frac{J^2B^2}{2} \ , \tag{5.21c}$$

etc. The Ising recurrants are

$$\Delta'_1 = B^2 \ , \tag{5.22a}$$

$$\Delta'_2 = 2J^2 \ , \tag{5.22b}$$

$$\Delta'_3 = 2J^2 + B^2 \ , \tag{5.22c}$$

$$\Delta'_4 = \frac{12J^2B^2}{2J^2 + B^2} \ . \tag{5.22d}$$

When $B = J$, these recurrants are thus given by

$$\Delta'_{nu} = \nu\,\Delta' \qquad \nu = 1, 2, 3, \ldots \quad , \tag{5.23}$$

where $\Delta' = J^2$. This linear relationship is the same one satisfied by the XY norms, differing only in the scaling factor. Therefore, the XY and the TI models are dynamically equivalent when $B = J$. This means that the basis functions $a'_\nu(t)$ have identically the same time-dependence as $a_\nu(t)$ with $\Delta = 2J^2$ replaced by $\Delta' = J^2$. For instance, for the TI model

$$\langle S^x_j(t) S^x_j \rangle = \tfrac{1}{4} \exp(-\tfrac{1}{2} J^2 t^2) \ . \tag{5.24}$$

If we review the results of Chapter 4, we see that the above dynamic equivalence has to be extended to include [João Florencio & Lee 1987] the $d = \infty$ dynamic regime[4] of the spin van der Waals model[5].

This is another example of different physical models that may share the same dynamics, an unexpected feature that nonetheless can be straight forward to investigate with the RRM, by calculating the corresponding sets of Delta's or recurrants.

[4]That comprises the XY regime for $T$ above or below $T_c$, and the Ising regime with $T > T_c$.

[5]Which is an infinite-lattice-dimensional, $D \to \infty$, limit [Lee & Sharma n.d.] of the spin-$\frac{1}{2}$ nearest neighbor, anisotropic Heisenberg model on an hypercubic lattice of dimensionality $D$. See Eq. (4.1)

# Chapter 6

## Applications of the Recurrence Relations Method IV: Dynamic equivalence of a 2D quantum electron gas and a classical harmonic oscillator chain with an impurity mass

In the last chapter we showed, by means of the recurrence relations method (RRM), that three seemingly unrelated physical models may share exactly the same time-dependence by being dynamically (See §5.1) equivalent (DE). Here, following Lee et al. [1989], we will do the same for the 2D electron gas model of §3.2 and the classical harmonic oscillator (HO) chain with a tagged mass. Unlike other dynamical equivalences reviewed so far, this is the first between a quantum system: The 2D electron gas, and a classical system: The harmonic oscillator chain.

According to the RRM (§2.3 and §2.4) the time *evolution* of a dynamical variable, say $A$, is through, only, the *time-dependence* of the basis functions $a_\nu(t)$. The basis functions are determined *uniquely* by a three term linear recurrence relation, Eq. (2.16) of §2.4, known as the Recurrence Relation II, or simply RR2. The RR2 *only* depends on the set $\{\Delta_\nu\}$ of the recurrants or Delta's. Therefore, in general, two different sets of Delta's imply differing time evolutions. But, if the sets are similar (in the sense of §5.1) they will give rise to exactly the same time evolution for the corresponding variables aside from a global constant factor and a constant time-scale factor[1].

This *concrete* example shows that the unifying, and at the same time defining feature of dynamics, is the shape of the *realized* Hilbert space. One could think of a catalogue of shapes as a catalogue of dynamics.

[1]The RR2 is linearly dependent on both the $a$'s and the Delta's, though, only homogeneously on the former.

Lee, Florencio & Hong [1989] show that at $T = 0$ , a 2D electron gas at long wavelengths, and a classical nearest-neighbor coupled harmonic oscillator chain, with one impurity mass, both belong to the same dynamical class, i.e., they are DE.

The time evolution in an HO chain has been studied by several authors, almost always relying on the standard, normal modes approach [Li 1986], [Fox 1983]. On the other hand, the recurrence relations analysis is carried out in the *original* lattice.[2] As a result, one can, for example follow the delocalisation of an initial excitation from site to site. Also, inhomogeneities are easier to handle. An impurity mass, for example, can greatly complicate the standard analysis and the ensuing algebra, while in the RRM the structure of the calculations is not changed: one only has to consider some additional steps in the difference equations.

We review in §3.2 a complete solution [Lee & Hong 1985*b*] for the time evolution of the density fluctuations operator, $\rho_k$, at long wavelengths, i.e., $k \ll 1$, where $k$ is the wavevector measured in units of the Fermi wavevector $k_F$. To order $k$, Lee, Florencio & Hong [1989] describe the realised Hilbert space of $\rho_k(t)$, as given by $d = \infty$ and the recurrants

$$\begin{aligned} \sigma &= (2s^{-1}\mu^2/4, \mu^2/4, \mu^2/4, \dots) , \\ &= (2s^{-1}, 1, 1, 1, 1, \dots\dots\dots) \times \tfrac{\mu^2}{4} , \end{aligned} \tag{6.1}$$

with $\mu = 2k\epsilon_F$, $\epsilon_F$ is the Fermi energy, $s^{-1} = 1+2\Gamma/\mu^2$, and $\Gamma = 2\pi\rho e^2/m$, which is essentially the electron-electron interaction in 2D (See Eqs. (3.13) and Eq. (3.40)). Other symbols have their usual meanings, e.g., $\rho$ is the electron number density. Since the interaction is repulsive, $1 \leqslant s \leqslant \infty$, where $s^{-1} = 1$, and $s^{-1} = \infty$ represent the ideal and non-ideal limits of the electron gas, respectively.

Lee, Florencio & Hong [1989] now consider a chain of $N$ HO's with periodic boundary conditions, where $N$ is an even number. Each spring has the same force constant $\kappa$, and each oscillator is only coupled to its two nearest-neighbors. They choose one oscillator to have mass $m_0$ (designated as a tagged mass) and all others to have an identical mass $m$. They

[2]In the normal modes analysis one solves canonical equations in one form or another.

introduce the parameter

$$\lambda = m/m_0\,, \tag{6.2}$$

where $\lambda = 0$ and $\lambda = \infty$ represent the heavy and light impurity mass limits, respectively. They choose $A = P_0$ the momentum of the tagged mass as the dynamical variable. They find for the realized space of $P_0(t)$ that

$$\begin{aligned}\sigma &= (2\lambda\kappa/m, \lambda\kappa/m, \lambda\kappa/m, \ldots, \lambda\kappa/m, 2\lambda\kappa/m)\,, \quad d = N+1 \\ &= (2\lambda, 1, 1, 1, \ldots\ldots, 1, 1, 2) \times \tfrac{\kappa}{m}\ .\end{aligned} \tag{6.3}$$

For $\lambda = 1$ (equal-mass limit) there is a front-end symmetry in $\sigma$. This symmetry is broken when $N \to \infty$; and this symmetry breaking gives rise to irreversibility [Lee, Florencio & Hong 1989].

In the limit $N \to \infty$, the Hilbert space of $P_0(t)$ becomes exactly the same as the Hilbert space of $\rho_k(t)$ up to some scale factors. Therefore the two systems are dynamically equivalent in the sense of Eqs. (5.2) of §5.1. If we make the following two replacements

$$\mu^2/4 \leftarrow \kappa/m\ , \tag{6.4}$$

$$s^{-1} \leftarrow \lambda\,. \tag{6.5}$$

Then, the time evolution of $P_0$ in the ($\lambda = 1$) equal-mass chain becomes identical to the time evolution of $\rho_k$ in the ideal 2d electron gas ($s^{-1} = 1$). Similarly, the light impurity regime of the HO chain ($\lambda > 1$) corresponds to the non-ideal or Coulomb electron gas (normal fermions). The heavy impurity regime ($\lambda < 1$) would correspond to an attractively interacting electron gas ('abnormal fermions'). If such an 'abnormal fermion' system existed, it would just become bound (see Eq.) at $\lambda = 0$. There are no time evolutions known for this novel system, but one can obtain them from the heavy impurity regime of the HO chain. Thus Lee, Florencio & Hong [1989] seek a general solution.

In the ideal limit of the electron gas or in the equal-mass limit of the HO chain ($s^{-1} = 1,\ \lambda = 1$), one has

$$\sigma = (2,1,1,1,1,1,\dots)\,, \tag{6.6a}$$

$$\sigma_1 = (1,1,1,1,1,\dots)\,, \tag{6.6b}$$

up to the scale factors that have been set to unity. The hypersurface $\sigma_1$ is obtained by removing the first entry (see §2.5) from the hypersurface $\sigma$. Using the RRM, it is shown in §3.2.4, that Eqs. (6.6), imply that

$$a_\nu(t) = 2^\nu \mu^{-\nu} \mathrm{J}_\nu(\mu t)\,, \qquad \nu \geqslant 0\,, \tag{6.7}$$

$$b_\nu(t) = 2^\nu \mu^{1-\nu} \mathrm{J}_\nu(\mu t)/\mu t\,, \qquad \nu \geqslant 1\,, \tag{6.8}$$

where $\mathrm{J}_\nu$ is the Bessel function of order $\nu$. The interaction or the impurity mass changes $\sigma$ but not $\sigma_1$ (see Eq. (6.1) and Eq. (6.3)). Hence, $a_\nu(t)$ changes but not $b_\nu(t)$. In §3.2.6 it is shown that

$$\tilde{a}_0(z) = (z + \Delta_1 \tilde{b}_1(z))^{-1} \tag{6.9}$$

(the tilde means Laplace transform). It is also shown how to use this relation and take advantage of the invariance of $\sigma_1$ to obtain the general solution. From (6.8), $\tilde{b}_1(z) = 2\mu^{-2}(\sqrt{z^2+\mu^2} - z)$. Therefore,

$$a_0(t) = \frac{1}{2\pi \mathrm{i}} \int_C \mathrm{d}z\ \mathrm{e}^{zt}\, \tilde{a}_0(z) = \frac{1}{2\pi \mathrm{i}\,\lambda} \int_C \mathrm{d}z\, \frac{\mathrm{e}^{zt}}{pz + \sqrt{z^2+\mu^2}}\ , \tag{6.10}$$

where

$$p \equiv \lambda^{-1} - 1\ . \tag{6.11}$$

Given $a_0(t)$ from Eq. (6.10) all other $a_\nu(t)$ can be obtained by the RR2. Therefore the time evolution can be completely described by this procedure[3].

It is seen in Eq. (6.10) that there is a branch cut and singularities in both branches. The physical branch is picked up by the requirement

$$\tilde{a}_0(z \to \infty) = \frac{1}{z}\ , \tag{6.12}$$

[3]The basis vectors $f_\nu$ can be obtained with the RR1, given that $f_0 = P_0$ or $\rho_k$. See §2.4.

so the boundary condition (See §2.4)

$$a_0(t=0) = 1 \ , \tag{6.13}$$

is fulfilled. This requirement is met by choosing the principal branch of the square root in Eq. (6.10). To obtain the singularities explicitly, [Lee et al. 1989], write the relevant part of Eq. (6.10) as

$$\frac{\sqrt{z^2+\mu^2} - pz}{\alpha(z^2 + \alpha^{-1} + \mu^2} \ , \tag{6.14}$$

where

$$\alpha = 1 - p^2 = (2\lambda - 1)/\lambda^2 \ . \tag{6.15}$$

Clearly, the locations of the isolated poles in a given branch depend on the sign and size of $\alpha^{-1}$. It is also seen from Eq. (6.14) that for the poles to be in the physical branch, $p$ has to be negative. Below, in Fig. 6.1 we reproduce Figure 1. of [Lee, Florencio & Hong 1989]. There, in (a), $\alpha^{-1}$ and $p$ are both plotted against $\lambda$.

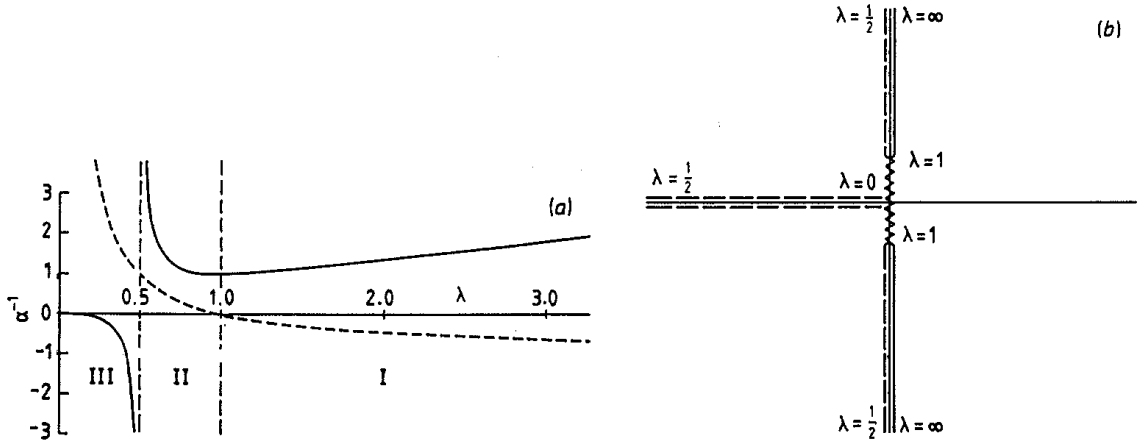



**Figure 1.** (*a*) **The solid curve is a plot of $\alpha^{-1}$ against $\lambda$. The function $p = \lambda^{-1} - 1$ is plotted as a broken curve.** (*b*) **Poles in the first branch (full lines), poles in the second branch (broken lines) and the branch cut (zigzag).**

Figure 6.1: Reproduction of Figure 1. Taken from [Lee, Florencio & Hong 1989].

There are three distinct regions. In region I we have, $1 < \lambda < \infty$, where $1 < \alpha^{-1}$ and $p < 0$ . There are a pair of poles on the imaginary axis beyond the branch points in the first

(principal) or physical sheet. In region II, $\frac{1}{2} < \lambda < 1$, where $1 < \alpha^{-1}$ and $0 < p$. There are also the same poles of region I, but on the second or non-physical sheet. In region III, $0 < \lambda < \frac{1}{2}$, where $\alpha^{-1} < 0$ and $0 < p$. There is one pole on the negative real axis, also on the non-physical sheet. In the reproduction of Figure 1(b), the behavior of the poles is illustrated as a function of $\lambda$ for a given branch.

Contributions to Eq. (6.10) from isolated poles are limited to those on the physical sheet, i.e., the poles of region I[4]. [Lee et al. 1989] obtain that the contributions from the branch cut are similar in each of the three regions depending only on $\alpha^{-1}$. They are identical in regions I and II since both regions have the same $\alpha^1$. Region III has to be subdivided into IIIA ($\alpha^{-1} < -1$) and IIIB ($-1 < \alpha^{-1}$). In subregion IIIA the solution of regions I and II applies with $-\alpha$. In subregion IIIB the solution is different.

In region I, the complete solution is

$$a_0(t) = \frac{2|p|}{1+|p|}\cos\Omega t + \sum_{n=0}^{\infty}(-\alpha)^n \left(\frac{\partial}{\partial \mu t}\right)^{2n} \frac{\mathrm{J}_1(\mu t)}{\mu t} \tag{6.16}$$

where $\Omega = (\alpha^{-1}\mu^2)^{1/2}$. The above solution without the cosine term is also the solution in regions II and IIIA as previously noted.

In subregion IIIB, the complete solution is

$$a_0(t) = (\pi\lambda|\alpha|)^{-1} \sum_{n=1}^{\infty} \beta^n \Gamma(n+\tfrac{1}{2})\mathrm{J}_n(\mu t)/(\mu t/2)^n \tag{6.17}$$

where $\beta = |\alpha|/(1+|\alpha|) = (1-2\lambda)/(1-\lambda)^2$. In region III, this parameter $\beta$ ranges from 0 to 1. Therefore, the above solution, Eq. (6.17), also applies to subregion IIIA. When $\beta = 1$, (6.17) is divergent except when $t = 0$, wherein $a_0(t=0) = 1$. Thus no expansion about $\lambda = 0$ is possible for an arbitrary time[5].

The correspondence of the solutions to the physical behavior of the two systems as $\lambda$ varies from $\infty$ to 0 is outlined by Lee, Florencio & Hong [1989] as follows. When $\lambda = \infty$

[4]For the electron gas these are just the plasma poles, with the branch cut representing the single-particle excitations.

[5]An expansion solution is possible [Lee et al. 1989] only under some special conditions, e.g., $\lambda t < 1$. In contrast, (6.16) is a general expansion about $\lambda^{-1} = 0$ and converges even at $\alpha = 1$.

($m = \infty,\ m_0 < \infty$), one gets $a_0(t) = \cos\Omega_\infty t$, $\Omega_\infty = (2\kappa/m_0)^{1/2}$, i.e., the tagged mass is bound to two stationary walls. In the electron gas it is exactly the condition in which single-particle motions are either frozen or completely overwhelmed by the plasma oscillation (strong-coupling limit). As $\lambda \to 1$, the initial simple oscillatory motion becomes perturbed by the 'moving walls'. In the equal mass limit it disappears entirely as when the electrons no longer interact. But in this limit, the motion of the tagged mass is indistinguishable from the motions of other masses in the chain. Therefore it is more nearly in phase and its autocorrelation function decays more slowly, i.e., $a_0(t \to \infty) \sim t^{-1/2}\cos(\mu t - \pi/4)$. It is just the behavior of long-lived electron-hole pair excitations, existing very near the Fermi surface in the weak-coupling limit [Mahan 2007].

As $\lambda \to 0$, the motion of the tagged mass begins to go out of phase. For the electrons (now abnormal fermions) the excitations tend to be localised owing to an attractive interaction, thus precluding any formation of plasma-like collective modes. For $0 < \lambda < 1$, the motions of the tagged mass represent the scattering states of the abnormal fermions, which therefore cannot be continuously changed into the state of $\lambda = 0$, a bound state. The time evolutions evidently are asymmetric in the mass difference $m - m_0$ about $m = m_0$, which is equivalent to the electron-electron interaction[6].

Finally, a one-impurity HO chain has a subspace $\mathcal{S}_1$ independent of $\lambda$. This is just the condition that the generalized RPA theory of an electron gas [Li 1986] is exactly valid. Hence, selectively adding more impurity masses to the chain is similar to systematically correcting the RPA. One particular limit of a homogeneous multi-impurity chain is a diatomic chain. This limiting process, in effect, forms new branch cuts by extending the isolated poles of a one-impurity chain. The two chains differ in time evolution to the extent of this difference in the analytic structure [Yu & Lee n.d.]

[6]The HO chain is not dynamically equivalent to the electron gas in $D = 1$ and $D = 3$. If $D = 1$, then [Lee, Hong & Sharma 1984] $d = 2$. If $D = 3$, $d = \infty$, but $\sigma = (4s^{-1}/3, \frac{16}{15}, \frac{36}{35}, \ldots, 4\nu^2/(4\nu^2 - 1), \ldots)$ in units of $\mu^2/4 = 1$. See §3.3.

# Chapter 7

## The harmonic oscillator chain (HOC) with one end-impurity coupled to a fixed wall (ICFW)

In previous chapters we reviewed the recurrence relations method and some of its applications to several different physical models. In this chapter and the ensuing, we will consider an harmonic oscillator chain (HO) with an impurity mass at one end that is coupled to a fixed wall.

Interacting HO models have very long been used to study lattice vibrations. Their equilibrium and static properties have been the focus [Florencio & Lee 1985] of investigation and exact results for dispersion relations, normal modes, and thermodynamical quantities are available [Montroll 1947], [Rosenstock & Newell 1953], [Maraudin, Montroll, Weiss & Ipatova 1971], [Mahan 2007].

The non-equilibrium properties of these models have not been so extensively studied. On the contrary, there are just a few papers on the dynamics of these systems and, most of them, for one-dimensional models. Florencio & Lee [1985] cite as noteworthy Ford, Kac & Mazur's [1965] statistical mechanics of assemblies of coupled oscillators, and Fox's [1983] study of long time tails and diffusion. We add [Cukier & Mazur 1971] and [Cukier 1972] studies of the dynamic and ergodic properties of an impurity in a harmonic oscillator chain, Jhon & Dahler's [1977] velocity correlation functions for HO chains, Hong's [1989] exact time evolution of a quantum HO chain, and Florencio & Lee's [1985] exact time evolution of a classical HO chain.

We will use the RRM to study the dynamics of the HO chain with one end-impurity coupled to a fixed wall and to show that it is possible to find closed exact solutions of the relaxation function $a_0(t)$ for particular (see Chapter 8) values of the parameters (see §7.1, below). We also find a closed general solution for the relaxation function $\tilde{a}_0(z)$ and for the memory function $b_1(t)$, both of them valid (Chapters 9–10) for any values[1] in the parameter space of the model. The inversion of $\tilde{a}_0(z)$

[1] Except at some singular points.

into the time-domain is carried out in Chapter 11. This allows us to investigate the time-dependent features of the relaxation function $a_0(t)$, e.g., the long-time behavior.

M. Howard Lee has shown using the RRM that there are stringent restrictions [Lee 2001] on the allowed functional forms of $a_0(t)$. In fact, e.g., a long-time exponential decay is not [Lee 1983] permitted (see also §2.4). The long-time behavior of the solutions is studied in Chapter 12 and we show that our $a_0(t)$ satisfies the aforementioned restrictions. We also show that the irreversible behavior can be ergodic or non-ergodic, thus providing an example of irreversibility *not* being a *sufficient* condition for ergodicity as shown by Lee [2007*c*]. The chain can also present reversible behavior. The Hamiltonian is defined in the next section and the Delta's calculation is presented in §7.3.

## 7.1 The model

We consider a linear chain of $N$ classical harmonic oscillators, labeled $0, 1, 2, \ldots, N-1$. The first oscillator has mass equal to $m_0$, and it is coupled to a fixed wall with a spring of elastic constant $k_0$ and to the next oscillator with a spring of elastic constant $k$. All other oscillators $(1, 2, \ldots, N-1)$ have the same mass $m$ and are coupled only to their nearest neighbors with the same elastic constant $k$. Their coordinates, measured from the equilibrium positions, are $q_0, q_1, \ldots, q_{N-1}$, and their momenta are $p_0, p_1, \ldots, p_{N-1}$. Therefore, the Hamiltonian for the harmonic oscillators chain (HOC) with one end impurity coupled to a fixed wall (ICFW), is

$$H = \frac{p_0^2}{2m_0} + \tfrac{1}{2}k_0 q_0^2 + \sum_{\nu=1}^{N-1}\left[\frac{p_\nu^2}{2m} + \tfrac{1}{2}k(q_\nu - q_{\nu-1})^2\right]. \tag{7.1}$$

This Hamiltonian only has three independent parameters, one of which is $N$. To define the only mass ratio in our model, we chose the parameter $\lambda$ that was employed by Lee, Florencio & Hong [1989] to define the same mass ratio in an HOC with an impurity mass and periodic boundary conditions (PBC) (See Chapter 6). Thus, for reference purposes we define right away the following two parameters:

$$\kappa \equiv \frac{k_0}{k}\,, \tag{7.2}$$

and

$$\lambda \equiv \frac{m}{m_0}\,, \tag{7.3}$$

with $k$, $k_0$, $m$, and $m_0$ defined in the preceding paragraph.

Another model, closely related to ours, is the homogeneous HOC with PBC or with fixed-ends boundary conditions (FEBC) studied by [Florencio & Lee 1985]. In our model, there is no available choice: the boundary conditions (variable coupling to a fixed wall and a free end) are imposed by the definition of the model. Therefore, before going on with the actual delta's calculation we will review in the next section the aforementioned work.

## 7.2 The homogeneous HOC with periodic boundary conditions (PBC) or with fixed-end boundary conditions (FEBC)

J. Florencio and M. Howard Lee study an homogeneous HOC with PBC or FEBC with the aim of investigating the role of the boundary conditions in this model [Florencio & Lee 1985]. They are particularly interested in clarifying the physical meaning of a finite diffusion constant $D$ obtained by Fox [1983], and a diverging mean square displacement, $\langle q^2 \rangle$, obtained by Ford et al. [1965]. Both results are the outcome of investigations of the dynamics of classical linearly-coupled harmonic-oscillator chains obeying periodic boundary conditions (PBC).

The diffusion constant may be defined by means of the Green-Kubo formula [Green 1954], [Kubo 1966]

$$D = \int_0^\infty \mathrm{d}t \, \langle \, v_j(t) v_j(0) \, \rangle \, , \tag{7.4}$$

or more fundamentally [Kubo 1966], [Kubo, Toda & Hashitsume 1991, p. 8] as

$$D = \lim_{t \to \infty} \left[ \frac{1}{2t} \langle \, [q_j(t) - q_j(0)]^2 \, \rangle \right] , \tag{7.5}$$

with $\langle \ldots \rangle \equiv \mathrm{Tr}[\ldots \mathrm{e}^{-\beta H}]/Z$, and $Z \equiv \mathrm{Tr}[\mathrm{e}^{-\beta H}]$. Here, $v_j$ is the velocity and $q_j$ is the coordinate (respect the equilibrium position) of the oscillator at site $j$ in the chain. In a context of periodic boundary conditions (PBC), there should be translation invariance (the chains are homogeneous) and therefore both integrands have to be independent of $j$. Fox [1983] finds

$$D = \int_0^\infty \mathrm{d}t \, \langle \, v_j(t) v_j(0) \, \rangle \; = \int_0^\infty \mathrm{d}t \; \frac{\mathrm{k_B}\, T}{m} \, \mathrm{J}_0(2\omega t) = \frac{\mathrm{k_B}\, T}{2m\, \omega} \; , \tag{7.6}$$

where all the symbols have their usual meanings. As argued by Fox [1983] "That the diffusion constant vanishes makes sense because there cannot be real diffusion in a fixed, oscillating lattice.

That $D \neq 0$ in one dimension is a kind of fluke". For a lattice, one would expect the mean square displacement (contained in the fundamental definition (7.5) of $D$) to be finite and, therefore, $D = 0$. On the other hand, Florencio & Lee [1985] point out that [Montroll 1956] obtained a finite value for the mean square displacement by using fixed-end boundary conditions (FEBC).

Florencio & Lee [1985] found that the source of these unexpected results was a zero frequency mode, which is the mode with full translational symmetry. To show this, they calculated $D$ and $\langle q^2 \rangle$ in terms of the velocity autocorrelation function, $\langle v_j(t) v_j(0) \rangle$, and the displacement autocorrelation function, $\langle q_j(t) q_j(0) \rangle$, first for the case of PBC and afterwards for the case of FEBC.

The Hamiltonian for the homogeneous HOC in the PBC case is:

$$H = \sum_{j=-N/2}^{N/2-1} p_j^2/2m + \sum_{j=-N/2}^{N/2-1} (k/2)(q_{j+1} - q_j)^2, \tag{7.7}$$

where, without loss of generality, $N$ is taken as an even number, only nearest neighbor couplings are taken into account, and $k = m\omega^2$ is the coupling constant. PBC are imposed, such that

$$q_{j+N} = q_j \,, \tag{7.8a}$$

$$p_{j+N} = p_j \,. \tag{7.8b}$$

This is the model system studied by Ford, Kac & Mazur [1965] and by Fox [1983]. The Hamiltonian (7.7) can be diagonalized by the introduction of normal mode coordinates $Q_\mu$ and $P_\mu$ through the transformations

$$q_j = \frac{1}{\sqrt{Nm}} \sum_{\mu=-N/2}^{N/2-1} \mathrm{e}^{\mathrm{i}(2\pi j/N)\mu} \, Q_\mu \tag{7.9a}$$

and

$$p_j = \left(\frac{m}{N}\right)^{1/2} \sum_{\mu=-N/2}^{N/2-1} \mathrm{e}^{\mathrm{i}(2\pi j/N)\mu} \, P_\mu \,. \tag{7.9b}$$

Notice that the PBC (7.8) are indeed satisfied, and that the set $\{\frac{1}{\sqrt{N}} \, \mathrm{e}^{\mathrm{i}(2\pi j/N)\mu}\} \quad -N/2 \leqslant \mu \leqslant N/2 - 1$, is complete and orthogonal in a periodic domain of the oscillator labels $j$. Also, since $q_j$ and $p_j$ are real,

$$Q_\mu^* = Q_{-\mu} \,, \tag{7.10a}$$

$$P_\mu^* = P_{-\mu} \,. \tag{7.10b}$$

In terms of the normal modes coordinates, the Hamiltonian (7.7) now reads

$$H = \tfrac{1}{2} \sum_{\mu=-N/2}^{N/2-1} \left(P_\mu^* P_\mu + \Omega_\mu^2 Q_\mu^* Q_\mu\right), \tag{7.11}$$

where

$$\Omega_\mu^2 = 4\omega^2 \sin^2 \frac{\pi\mu}{N} \quad -N/2 \leqslant \mu \leqslant N/2 - 1\,, \tag{7.12}$$

and $\Omega_\mu$ are the normal-mode frequencies.

Any time dependence in this problem can be written in terms of normal mode coordinates time evolution, in particular, $\langle v_j(t) v_j(0)\rangle$ and $\langle q_j(t) q_j(0)\rangle$. Florencio & Lee [1985] now use the recurrence relations method (RRM) to obtain the time evolution of the normal mode coordinates $Q_\mu$ and $P_\mu$. The RRM was described in detail in Chapter 2 and is summarized for the classical case at the beginning of the next section. It's application hinges on the Kubo scalar product defined in Eq. (2.1). For a classical system it is defined in (7.37), it reads $(X, Y) = \beta\left[\langle X^\dagger Y\rangle - \langle X^\dagger\rangle\langle Y\rangle\right]$. Since it only appears in the quotients of norms in the recurrants definition, any constant factor may be dropped off. Also, the mean value of all the dynamical variables is these systems is zero. Therefore

$$(X, Y) = \langle X^\dagger Y\rangle = \langle X^* Y\rangle \tag{7.13a}$$

$$= \frac{1}{Z}\mathrm{Tr}[\mathrm{e}^{-\beta H}\, X^* Y] = \frac{1}{Z}\int \mathrm{d}^N x\ \mathrm{e}^{-\beta H}\, X^* Y\,, \tag{7.13b}$$

where $\beta$ is the inverse temperature, $Z \equiv \int \mathrm{d}^N x\ \mathrm{e}^{-\beta H}$ is the classical partition function, and

$$\mathrm{d}^N x \equiv \prod_{i=1}^{N} \mathrm{d}q_i\, \mathrm{d}p_i \tag{7.13c}$$

Using the transformations (7.9), Eq. (7.13a), and Eqs. (7.10), Florencio & Lee [1985] find

$$\langle v_j(t) v_j(0)\rangle = \frac{1}{Nm} \sum_{\mu,\mu'} \mathrm{e}^{-\,\mathrm{i}(2\pi/N)(\mu-\mu')} (P_\mu(t), P_{\mu'}) \tag{7.14}$$

and

$$\langle q_j(t) q_j(0)\rangle = \frac{1}{Nm} \sum_{\mu,\mu'} \mathrm{e}^{-\,\mathrm{i}(2\pi/N)(\mu-\mu')} (Q_\mu(t), Q_{\mu'})\,. \tag{7.15}$$

The normal mode coordinate $P_\mu$ time dependence is expanded as

$$P_\mu(t) = \sum_{\nu=0}^{d-1} a_\nu(t) f_\nu\,. \tag{7.16}$$

Using the RR1, Eq. (7.36a), with the basis vector chosen as

$$f_0 = P_\mu(t=0) \equiv P_\mu \ , \tag{7.17a}$$

then the next basis vector is

$$f_1 = LP_\mu = -\Omega_\mu^2 Q_{-\mu} \ . \tag{7.17b}$$

Here the Liouville operator, Eq. (7.36b), is given by

$$L = \sum_{\mu=-N/2}^{N/2-1} \left[ P_{-\mu} \frac{\partial}{\partial Q_\mu} - \Omega_\mu^2 Q_{-\mu} \frac{\partial}{\partial P_\mu} \right] . \tag{7.18}$$

It is found that $(f_0, f_0) = 1/\beta$, $(f_1, f_1) = \Omega_\mu^2/\beta$, and $\Delta_1 = (f_1, f_1)/(f_0, f_0) = \Omega_\mu^2$. Taking these results into RR1 gives $f_2 = 0$, $\Delta_2 = 0$ and, therefore, $f_\nu = 0$ for $\nu \geqslant 2$. Thus, the Hilbert space for $P_\mu(t)$ is two dimensional, $d = 2$, with basis vectors $f_0$ and $f_1$ given by Eqs. (7.17).

The above results and the RR2, Eq. (2.16), give the equations for $a_\nu(t)$,

$$\Omega_\mu^2 a_1(t) = -\dot{a}_0(t) \ , \tag{7.19a}$$

and

$$0 = -\dot{a}_1(t) + a_0(t) \ , \tag{7.19b}$$

with initial conditions $a_0(0) = 1$ and $a_1(0) = 0$. The solutions of these equations are

$$a_0(t) = \cos(\Omega_\mu t) \tag{7.20a}$$

and

$$a_1(t) = \frac{1}{\Omega_\mu} \sin(\Omega_\mu t) \tag{7.20b}$$

Therefore, the time evolution of $P_\mu(t)$ is determined to be

$$P_\mu(t) = \cos(\Omega_\mu t) P_\mu - \Omega_\mu \sin(\Omega_\mu t) Q_{-\mu} \ . \tag{7.21}$$

The following scalar products are obtained

$$(P_\mu(t), P_{\mu'}) = \frac{\delta_{\mu,\mu'}}{\beta} \cos(\Omega_\mu t) \tag{7.22a}$$

and

$$(P_\mu(t), Q_{\mu'}) = 0 \ . \tag{7.22b}$$

Using the above results in Eq. (7.14), the velocity autocorrelation function is then

$$\langle v_j(t)v_j(0)\rangle = \frac{\mathrm{k_B}\,T}{Nm}\sum_{\mu=-N/2}^{N/2-1}\cos(\Omega_\mu t)\ . \tag{7.23}$$

To determine the displacement autocorrelation function, Eq. (7.15), a similar procedure is followed to obtain $Q_\mu(t)$. Using the RR1, Eqs. (7.36), it is found that the dynamical Hilbert space of $Q_\mu(t)$ also has two dimensions, with basis vectors

$$f_0 = Q_\mu \tag{7.24a}$$

and

$$f_1 = P_{-\mu}\ . \tag{7.24b}$$

Therefore, the only nontrivial $\Delta_\nu$ is $\Delta_1 = \Omega_\mu^2$, which, using the RR2, Eq. (2.16), gives a system of equations for the basis functions identical to Eqs. (7.19). Thus

$$Q_\mu(t) = \cos(\Omega_\mu t)Q_\mu + \frac{1}{\Omega_\mu}\sin(\Omega_\mu t)P_{-\mu}\ , \tag{7.25}$$

and the following scalar product is obtained

$$(Q_\mu(t), Q_{\mu'}) = \frac{\delta_{\mu,\mu'}}{\beta\Omega_\mu^2}\cos(\Omega_\mu t)\ , \tag{7.26}$$

which substituted into Eq. (7.15), gives the displacement autocorrelation function

$$\langle q_j(t)q_j(0)\rangle = \frac{\mathrm{k_B}\,T}{Nm}\sum_{\mu=-N/2}^{N/2-1}\frac{\cos(\Omega_\mu t)}{\Omega_\mu^2}\ . \tag{7.27}$$

Equations (7.23) and (7.27) were first obtained by Ford, Kac & Mazur [1965] using another method.

In the thermodynamic limit $N \to \infty$, Eq. (7.23) and Eq. (7.27) become

$$\langle v_j(t)v_j(0)\rangle = \frac{\mathrm{k_B}\,T}{m}\int_{-1/2}^{1/2}\mathrm{d}x\ \cos[\Omega(x)t] \tag{7.28}$$

and

$$\langle q_j(t)q_j(0)\rangle = \frac{\mathrm{k_B}\,T}{m}\int_{-1/2}^{1/2}\mathrm{d}x\ \frac{\cos[\Omega(x)t]}{\Omega^2(x)}\ , \tag{7.29}$$

where

$$\Omega^2(x) = 4\omega^2\sin^2(\pi x) \tag{7.30}$$

Notice that these correlation functions do not depend on the oscillator label $j$, reflecting the translational invariance of the system. Equation (7.28) can be written as

$$\langle v_j(t)v_j(0)\rangle = \frac{\mathrm{k_B}\,T}{m}\frac{2}{\pi}\int_0^{\pi/2}\mathrm{d}y\,\cos(2\omega t\sin y) = \frac{\mathrm{k_B}\,T}{m}\mathrm{J}_0(2\omega t)\ , \tag{7.31}$$

where $\mathrm{J}_0$ is the Bessel function of order zero. This expression was first derived by [Fox 1983]. It leads immediately to the unexpected result of Equation (7.6). In order to clarify this result Florencio & Lee [1985] substitute the displacement autocorrelation function before the themodynamic limit is taken, Eq. (7.27), into the fundamental definition of the diffusion constant $D$ in terms of the mean square displacement, Eq. (7.5), to obtain

$$D = \lim_{t\to\infty}\left[\frac{1}{t}\frac{2\mathrm{k_B}\,T}{Nm}\sum_{\mu=-N/2}^{N/2-1}\frac{\sin^2(\Omega_\mu t/2)}{\Omega_\mu^2}\right]\ . \tag{7.32}$$

Florencio & Lee [1985] take the thermodynamic limit first

$$\begin{aligned} D &= \lim_{t\to\infty}\left[\frac{1}{t}\frac{2\mathrm{k_B}\,T}{m}\int_{-1/2}^{1/2}\mathrm{d}x\ \frac{\sin^2[\Omega(x)t/2]}{\Omega^2(x)}\right] \\ &= \frac{\pi\mathrm{k_B}\,T}{2m}\int_{-1/2}^{1/2}\mathrm{d}x\left(\lim_{t\to\infty}\frac{\sin^2[\Omega(x)t/2]}{\pi t[\Omega(x)/2]^2}\right) \\ &= \frac{\pi\mathrm{k_B}\,T}{2m}\int_{-1/2}^{1/2}\mathrm{d}x\ \delta\left[\frac{\Omega(x)}{2}\right], \end{aligned} \tag{7.33}$$

where $\delta$ is the Dirac $\delta$ function. Thus, the above expression can be written

$$D = \frac{\mathrm{k_B}\,T}{m}\sum_i\int_{-1/2}^{1/2}\mathrm{d}x\,\frac{\delta(x-x_i)}{\left|\frac{\mathrm{d}\Omega(x)}{\mathrm{d}x}\right|_{x=x_i}}\ , \tag{7.34}$$

where $x_i$ are the zeros of $\Omega(x)$. In this case

$$x_i = 0, \pm 1, \pm 2, \ldots$$

Notice that only $x_i = 0$ contributes to the integral. This corresponds to the mode with zero frequency, which is the mode with full translational symmetry (see the normal mode transformation Eqs. (7.9)). This contribution from the zero-frequency mode gives the finite diffusion constant,

$$D = \frac{\pi\mathrm{k_B}\,T}{m}\int_{-1/2}^{1/2}\mathrm{d}x\,\frac{\delta(x)}{2\pi\omega} = \frac{\mathrm{k_B}\,T}{2m\omega}\ . \tag{7.35}$$

This is exactly the unexpected result, first obtained by [Fox 1983], that we had referred in Eq. (7.6) and in the discussion that follows. For the HOC with FEBC, Florencio & Lee [1985] carry out a

similar calculation. They find, that indeed, the zero frequency mode is missing due to the FEBC and the ensuing lack of full translational symmetry. They use again the RRM to analyse the dynamics of the system. They obtain, for example, that the mean square displacement of an oscillator is proportional to its position on the chain. This is the result that Florencio & Lee [1985] had pointed out that was first obtained by [Montroll 1956] and that led to a zero diffusion constant.

## 7.3 Delta sequences calculation for the HOC with one end ICFW

The dynamical variable we will investigate is the momentum of the mass next to the fixed wall, $p_0$. As already explained in Chapter 2, the time dependence is through the *basis functions* $a_m(t)$ which are uniquely determined by the recurrence relations II (RR2) of §2.4. The RR2 *only* depend on the set $\{\Delta_\nu\}$ defined in Eq. (2.6b) in terms of the ratios of the norms of the *basis vectors* $f_\nu$. These basis vectors are given by the recurrence relation I (RR1), Eq. (2.6a).

The RR1 depends on the time derivative of $f$, that for a quantum system is calculated using the commutator $(1/\,\mathrm{i}\,\hbar)[f,H]=\dot{f}$. Here we are concerned with a classical system and then the time derivative is given by the Poisson bracket $\{f,H\}=\dot{f}$. For convenience, we reproduce below the RR1 and the $\Delta_\nu$ definitions:

$$f_{\nu+1}=\{f_\nu,H\}+\Delta_\nu f_{\nu-1}\,,\qquad \nu=0,1,\ldots,d-1, \tag{7.36a}$$

with

$$\{f_\nu,H\}\equiv Lf_\nu=\sum_i\left[\frac{\partial f_\nu}{\partial q_i}\frac{\partial H}{\partial p_i}-\frac{\partial f_\nu}{\partial p_i}\frac{\partial H}{\partial q_i}\right], \tag{7.36b}$$

where $L$ is the Liouville operator, $d$ is the dimension of the realized space $\mathcal{S}$ spanned by the $f_\nu$, and

$$\Delta_\nu\equiv\begin{cases}1 & \nu=0,\\ (f_\nu,f_\nu)/(f_{\nu-1},f_{\nu-1}) & \nu=1,\ldots,d-1.\end{cases} \tag{7.36c}$$

To avoid ambiguities, since there are only $d$ basis vectors $f_0,f_1,\ldots,f_{d-1}$, we set $f_{-1}\equiv 0$ and $\Delta_0\equiv 1$.

The RR1 are used recursively. Once $f_0$ is chosen, one can obtain any $f_{\nu+1}$ from $f_\nu$ and $f_{\nu-1}$ using the RR1, Eq. (7.36a) above, repeatedly. We set $f_0\equiv p_0$. In this recursive process, it may happen that at some step, $\nu=\nu_F-1$, the next calculated basis vector $f_{\nu_F}=0$. Then, by the

equations above, the sequence terminates, i.e., $f_\nu = 0$ for $\nu \geqslant \nu_F$. In this case, the dimensionality of the set of the basis vectors is finite and given by $d = \nu_F$. Otherwise, if this does not happen, the sequence does not terminate and $d \to \infty$. For this model, the HOC with one end ICFW, we will show that $d = 2N$.

To implement the recursive process described in the above paragraph, one still needs to calculate the norms of the basis vectors in Eq. (7.36c). It was shown in §2.3, that the scalar product involved is the Kubo scalar product (KSP), defined in Eq. (2.1) for a quantum system as $(X, Y) = \int_0^\beta \langle \mathrm{e}^{\lambda H} X^\dagger \mathrm{e}^{-\lambda H} Y \rangle \mathrm{d}\lambda - \beta \langle X^\dagger \rangle \langle Y \rangle$. For a classical system, (or more generally, if $X$ or $Y$ commutes with the Hamiltonian $H$) then

$$(X, Y) = \beta \left[ \langle X^\dagger Y \rangle - \langle X^\dagger \rangle \langle Y \rangle \right], \tag{7.37}$$

where $\langle \ldots \rangle \equiv \mathrm{Tr}[\ldots \mathrm{e}^{-\beta H}]/Z$, and $Z \equiv \mathrm{Tr}[\mathrm{e}^{-\beta H}]$. In the recurrants $\Delta_\nu$ definition, Eq. (7.36c), the KSP *only appears in the quotient of norms of basis vectors* consequently, any constant multiplicative term may be dropped off in the Delta sequences calculations. Also, the mean value of either the displacement or velocity or momentum variables in this problem is zero. Additionally, in a classical system the variables are ordinary functions, ($\dagger \to *$), and the trace is an integral over the full phase space, thus, from here through §7.4 and §7.5 to the end of this chapter, in the Deltas calculations we omit the $\beta$ factor from the KSP definition in Eq. (7.37), and set

$$\begin{aligned} (X, Y) &= \langle X^\dagger Y \rangle = \langle X^* Y \rangle \\ &= \frac{1}{Z} \mathrm{Tr}[\mathrm{e}^{-\beta H} X^* Y] = \frac{1}{Z} \int \mathrm{d}^N x \; \mathrm{e}^{-\beta H} X^* Y \,, \end{aligned} \tag{7.38a}$$

where $\beta$ is the inverse temperature, $Z \equiv \int \mathrm{d}^N x \; \mathrm{e}^{-\beta H}$ is the classical partition function, and

$$\mathrm{d}^N x \equiv \prod_{i=0}^{N-1} \mathrm{d}q_i \, \mathrm{d}p_i \; . \tag{7.38b}$$

Using the definition of the parameter $\lambda$, Eq. (7.3),

$$\frac{p_0^2}{2m_0} = \frac{p_0^2}{\frac{2m_0}{m} m} = \lambda \frac{p_0^2}{2m} \; , \tag{7.39}$$

and the definition of the parameter $\kappa$, Eq. (7.2), we may write the Hamiltonian of our model as

$$\begin{aligned} H =& \tfrac{1}{2m}(\lambda p_0^2 + p_1^2 + \ldots + p_{N-1}^2) \\ &+ \tfrac{1}{2}k[\kappa q_0^2 + q_{01}^2 + \ldots + (q_{N-2} - q_{N-1})^2] \,, \qquad (7.40a) \\ \equiv& K(p) + U(q) \,. \qquad (7.40b) \end{aligned}$$

Any Poisson bracket, Eq. (7.36b), in this problem can be written in terms of $\{q_\nu, H\} = \dot{q}_\nu$ and $\{p_\nu, H\} = -\dot{p}_\nu$. The Poisson bracket definition (7.36b) gives

$$\begin{aligned} \{q_\nu, H\} = \quad \frac{\partial K}{\partial p_\nu} &= \lambda \frac{p_0}{m} \,, & \nu = 0 \,, \qquad (7.41a) \\ = \quad \frac{p_\nu}{m} \,, & & 1 \leqslant \nu \leqslant N-1 \,, \qquad (7.41b) \end{aligned}$$

for the displacements, and

$$\begin{aligned} \{p_\nu, H\} = -\frac{\partial U}{\partial q_\nu} = \quad & k[q_1 - (\kappa+1)q_0] \,, & \nu = 0 \,, \qquad (7.41c) \\ = \quad & k[q_{\nu-1} + q_{\nu+1} - 2q_\nu] \,, & 1 \leqslant \nu \leqslant N-2 \,, \qquad (7.41d) \\ = \quad & k[q_{N-2} - q_{N-1}] \,, & \nu = N-1 \,, \qquad (7.41e) \end{aligned}$$

for the momenta.

## 7.4 N=2 HOC with one end ICFW $\{\Delta_\nu\}$ calculation

Let us do now the $N = 2$ case. The dynamical variable we have chosen to investigate is $p_0$, so, $f_0 = p_0$. We will need the norm $(f_0, f_0)$. Using Eqs. (7.38) and the formulas of Appendix A, we find

$$(f_0, f_0) = \langle p_0^2 \rangle = \tfrac{1}{2}\frac{2m}{\lambda\beta} = \frac{m}{\lambda\beta} \,. \qquad (7.42)$$

Using the RR1, Eq. (7.36a), and Eq. (7.41c)

$$\begin{aligned} f_1 = \{p_0, H\} + \Delta_0 f_{-1} &= k[q_1 - (\kappa+1)q_0] + 1 \times 0 \\ &= k[q_1 - (\kappa+1)q_0] \\ &= -k(\kappa+1)\left[q_0 - \frac{q_1}{\kappa+1}\right] \,. \qquad (7.43) \end{aligned}$$

We need $(f_1, f_1)$ to obtain $\Delta_1$ to calculate $f_2$. Using Eqs. (7.38) and App. A

$$(f_1, f_1) = k^2(\kappa+1)^2 \, \tfrac{1}{2} \, \frac{2}{\beta k(\kappa+1)} = \frac{k(\kappa+1)}{\beta} \,, \qquad (7.44)$$

and therefore the first recurrant $\Delta_1$ is

$$\Delta_1 = \frac{(f_1, f_1)}{(f_0, f_0)} = \frac{k(\kappa+1)}{\beta}\,\frac{\lambda\beta}{m} = (\kappa+1)\lambda\,\frac{k}{m}\ . \tag{7.45}$$

Now, we can calculate $f_2$ using the RR1, Eq. (7.36a), Eqs. (7.41a)–(7.41b), and the $f_1$ obtained above

$$\begin{aligned} f_2 = \{f_1, H\} + \Delta_1 f_0 &= k\{q_1 - (\kappa+1)q_0, H\} + (\kappa+1)\lambda\,\frac{k}{m}\,p_0 \\ &= k\left[\frac{p_1}{m} - (\kappa+1)\lambda\frac{p_0}{m}\right] + (\kappa+1)\lambda\,\frac{k}{m}\,p_0 \\ &= \frac{k}{m}\,p_1\ . \end{aligned} \tag{7.46}$$

The norm of $f_2$ is

$$(f_2, f_2) = \frac{k^2}{m^2}\langle p_1^2\rangle = \frac{k^2}{m^2}\,\tfrac{1}{2}\,\frac{2m}{\beta} = \frac{k^2}{m\beta}\ , \tag{7.47}$$

and thus,

$$\Delta_2 = \frac{(f_2, f_2)}{(f_1, f_1)} = \frac{k^2}{m\beta}\,\frac{\beta}{k(\kappa+1)} = \frac{1}{\kappa+1}\,\frac{k}{m}\ . \tag{7.48}$$

We can now calculate $f_3$, again using the RR1, Eq. (7.36a), Eq. (7.41e) and the $f_2$ obtained above. It will turn out that this is the last non-null basis vector.

$$\begin{aligned} f_3 = \{f_2, H\} + \Delta_2 f_1 &= \frac{k}{m}\{p_1, H\} + \frac{1}{\kappa+1}\,\frac{k}{m}k[q_1 - (\kappa+1)q_0] \\ &= \frac{k^2}{m}\left[q_0 - q_1 + \frac{q_1}{\kappa+1} - q_0\right] \\ &= -\frac{\kappa}{\kappa+1}\frac{k^2}{m}\,q_1\ . \end{aligned} \tag{7.49}$$

Then

$$(f_3, f_3) = \frac{\kappa^2}{(\kappa+1)^2}\frac{k^4}{m^2}\langle q_1^2\rangle = \frac{\kappa^2}{(\kappa+1)^2}\frac{k^4}{m^2}\,\tfrac{1}{2}\,\frac{2}{\beta k}\,\frac{\kappa+1}{\kappa} = \frac{\kappa}{\kappa+1}\,\frac{k^3}{m^2\beta}\ , \tag{7.50}$$

and

$$\Delta_3 = \frac{(f_3, f_3)}{(f_2, f_2)} = \frac{\kappa}{\kappa+1}\,\frac{k^3}{m^2\beta}\,\frac{m\beta}{k^2} = \frac{\kappa}{\kappa+1}\,\frac{k}{m}\ . \tag{7.51}$$

Using the RR1, Eq. (7.36a), Eq. (7.41b) and the $f_3$ obtained above

$$f_4 = \{f_3, H\} + \Delta_3 f_2 = -\frac{\kappa}{\kappa+1}\frac{k^2}{m}\frac{p_1}{m} + \frac{\kappa}{\kappa+1}\,\frac{k}{m}\,\frac{k}{m}\,p_1 = 0\ , \tag{7.52}$$

and since $\Delta_4$ is zero, it is seen from the RR1, Eq. (7.36a) that $f_\nu = 0$ for $\nu \geqslant 4$. The non-null basis vectors are $\{f_0, f_1, f_2, f_3\}$ and the dimension of the realized space of $p_0(t)$ is $d = 4$ when $N = 2$. We will see that this is a general feature of this model, i.e., $d = 2N$.

## 7.5 N>2, HOC with one end ICFW $\{\Delta_\nu\}$ calculation

A direct application of the RRM shows that for $N = 3$ the basis vectors $\{f_0, f_1, f_2\}$ are the *same* as in the case of $N = 2$. This is because we chose to carry out the RRM in the actual physical lattice due to the lack of translational symmetry. Florencio & Lee [1985] showed that for an homogeneous (no impurity mass) chain with either PBC or FEBC, the Hamiltonian can be diagonalized with a transformation into the normal mode space, whereas in our model there is one fixed wall, an impurity mass and one free or open end.

The details of the application of RRM in the real lattice are dictated by the Poisson brackets, Eqs. (7.41), of the actual displacements and momenta with the Hamiltonian (written in the physical lattice) that appear in the RR1, Eq. (7.36a). For example, for $N = 2$, $f_2 \propto p_1$ and consequently $f_3$ will be special because the Poisson bracket $\{f_1, H\}$ involves the end of the chain, through Eq. (7.41e). On the other hand, for $N \geqslant 3$, $f_3$ will be the same in every case. This is the reason why the $f_\nu$ sequence terminates.

Let's see now when $N > 2$. As already explained above, $\{f_0, f_1, f_2\}$ are the same as in $N = 2$, and the $f_3$ below will be the same for all $N > 2$, (cf. (7.49))

$$\begin{aligned} f_3 = \{f_2, H\} + \Delta_2 f_1 &= \frac{k}{m}\{p_1, H\} + \frac{1}{\kappa+1}\,\frac{k}{m}k[q_1 - (\kappa+1)q_0] \\ &= \frac{k^2}{m}\left[q_0 - q_1 + q_2 - q_1 + \frac{q_1}{\kappa+1} - q_0\right] \\ &= \frac{k^2}{m}\left[q_2 - \frac{2\kappa+1}{\kappa+1}q_1\right] = -\frac{2\kappa+1}{\kappa+1}\frac{k^2}{m}\left[q_1 - \frac{\kappa+1}{2\kappa+1}q_2\right], \end{aligned} \tag{7.53}$$

the norm

$$(f_3, f_3) = \frac{(2\kappa+1)^2}{(\kappa+1)^2}\frac{k^4}{m^2}\,\tfrac{1}{2}\,\frac{2(\kappa+1)}{\beta k(2\kappa+1)} = \frac{2\kappa+1}{\kappa+1}\frac{k^3}{m^2\beta}\,, \tag{7.54}$$

and

$$\Delta_3 = \frac{2\kappa+1}{\kappa+1}\frac{k^3}{m^2\beta}\frac{m\beta}{k^2} = \frac{2\kappa+1}{\kappa+1}\frac{k}{m}\,. \tag{7.55}$$

Then $f_4$ below will also be the same for all $N > 2$

$$\begin{aligned} f_4 = \{f_3, H\} + \Delta_3 f_2 &= \frac{k^2}{m^2}\left[p_2 - \frac{2\kappa+1}{\kappa+1}p_1\right] + \frac{2\kappa+1}{\kappa+1}\frac{k}{m}\,\frac{k}{m}p_1 \\ &= \frac{k^2}{m^2}\,p_2\,, \end{aligned} \tag{7.56}$$

the norm

$$(f_4, f_4) = \frac{k^4}{m^4}\,\frac{1}{2}\,\frac{2m}{\beta} = \frac{k^4}{m^3\beta}\ , \tag{7.57}$$

and

$$\Delta_4 = \frac{k^4}{m^3\beta}\frac{\kappa+1}{2\kappa+1}\frac{m^2\beta}{k^3} = \frac{\kappa+1}{2\kappa+1}\,\frac{k}{m}\ . \tag{7.58}$$

Now, if among the $N > 2$ we are at $N = 3$, then the $f_5$ and $\Delta_5$ would be specially calculated (Eq. (7.41e)) for $N = 3$, and $f_6 = 0$ and $\Delta_6 = 0$ for this case. Otherwise, if among the $N > 2$ we are at $N > 3$, then $\{f_0, f_1, f_2, f_3, f_4\}$ are the same for all $N > 3$.

—In general, for a chain of particular length $N_p$, the set $\{f_0, f_1, \ldots, f_{2N_p-2}\}$ will be the same for all chains with $N > N_p$. The particular $N_p$-long chain will have a special $f_{2N_p-1}$ *last* basis vector and $f_{2N_p} = 0$, so that its dimension is $d = 2N_p$.

In the next table (Table 7.1), we show the $\{\Delta_\nu\}$ sequences for chains of length from $N = 2$ to $N = 6$. The relationships among them, e.g., an odd-Delta and the next even-Delta as well as the general formula of any Delta for any $\nu$, in particular, the end-Deltas in the sequences, are all apparent in the table. Recall that $\Delta_0 \equiv 1$.

Table 7.1: Delta sequence $\sigma = (\Delta_1, \Delta_2, \ldots, \Delta_{d-1})$, in units of $k/m$, for independent chains of harmonic oscillators with the left end anchored to a wall. The number of masses in the chain is $N$. All the spring constants and the masses are equal, except for the oscillator next to the wall. Here, $\lambda = m/m_0$ and $\kappa = k_0/k$, where the 0 subscript refers to the oscillator next to the wall.

| | $\sigma =$ | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| $N$ | $(\Delta_1$ | $\Delta_2$ | $\Delta_3$ | $\Delta_4$ | $\Delta_5$ | $\Delta_6$ | $\Delta_7$ | $\Delta_8$ | $\Delta_9$ | $\Delta_{10}$ | $\Delta_{11})$ |
| 2 | $\left(\ \frac{\lambda(1+\kappa)}{}\right.$ | $\frac{1}{\kappa+1}$ | $\left.\frac{\kappa}{\kappa+1}\ \right)$ | | | | | | | | |
| 3 | $\left(\ \frac{\lambda(1+\kappa)}{}\right.$ | $\frac{1}{\kappa+1}$ | $\frac{2\kappa+1}{\kappa+1}$ | $\frac{\kappa+1}{2\kappa+1}$ | $\left.\frac{\kappa}{2\kappa+1}\ \right)$ | | | | | | |
| 4 | $\left(\ \frac{\lambda(1+\kappa)}{}\right.$ | $\frac{1}{\kappa+1}$ | $\frac{2\kappa+1}{\kappa+1}$ | $\frac{\kappa+1}{2\kappa+1}$ | $\frac{3\kappa+1}{2\kappa+1}$ | $\frac{2\kappa+1}{3\kappa+1}$ | $\left.\frac{\kappa}{3\kappa+1}\ \right)$ | | | | |
| 5 | $\left(\ \frac{\lambda(1+\kappa)}{}\right.$ | $\frac{1}{\kappa+1}$ | $\frac{2\kappa+1}{\kappa+1}$ | $\frac{\kappa+1}{2\kappa+1}$ | $\frac{3\kappa+1}{2\kappa+1}$ | $\frac{2\kappa+1}{3\kappa+1}$ | $\frac{4\kappa+1}{3\kappa+1}$ | $\frac{3\kappa+1}{4\kappa+1}$ | $\left.\frac{\kappa}{4\kappa+1}\ \right)$ | | |
| 6 | $\left(\ \frac{\lambda(1+\kappa)}{}\right.$ | $\frac{1}{\kappa+1}$ | $\frac{2\kappa+1}{\kappa+1}$ | $\frac{\kappa+1}{2\kappa+1}$ | $\frac{3\kappa+1}{2\kappa+1}$ | $\frac{2\kappa+1}{3\kappa+1}$ | $\frac{4\kappa+1}{3\kappa+1}$ | $\frac{3\kappa+1}{4\kappa+1}$ | $\frac{5\kappa+1}{4\kappa+1}$ | $\frac{4\kappa+1}{5\kappa+1}$ | $\left.\frac{\kappa}{5\kappa+1}\ \right)$ |

The general form of the $f_\nu$ is as follows. If $\nu$ is odd, i.e., $\nu = 2n + 1$

$$f_{2n+1} = \frac{k^{n+1}}{m^n}\left[q_{n+1} - \frac{(n+1)\kappa+1}{n\kappa+1}q_n\right]\ . \tag{7.59a}$$

If $\nu$ is even, i.e., $\nu = 2n$

$$f_{2n} = \frac{k^n}{m^n} p_n \ , \tag{7.59b}$$

except when $\nu = 2N$, in which case $f_{2N} = 0$.

In Table 7.2 we show, for reference purposes, the same $\{\Delta_\nu\}$ sequences as Table 7.1, but in terms of the parameter $\alpha \equiv k/k_0$.

Table 7.2: Delta sequence $\sigma = (\Delta_1, \Delta_2, \ldots, \Delta_{d-1})$, in units of $k/m$, for independent chains of harmonic oscillators with the left end anchored to a wall. The number of masses in the chain is $N$. All the spring constants and the masses are equal, except for the oscillator next to the wall. Here, $\lambda = m/m_0$ and $\alpha = k/k_0$, where the 0 subscript refers to the oscillator next to the wall.

| | $\sigma =$ | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| $N$ | $(\Delta_1$ | $\Delta_2$ | $\Delta_3$ | $\Delta_4$ | $\Delta_5$ | $\Delta_6$ | $\Delta_7$ | $\Delta_8$ | $\Delta_9$ | $\Delta_{10}$ | $\Delta_{11})$ |
| 2 | $(\ \lambda\frac{\alpha+1}{\alpha}$ | $\frac{\alpha}{\alpha+1}$ | $\frac{1}{\alpha+1}\ )$ | | | | | | | | |
| 3 | $(\ \lambda\frac{\alpha+1}{\alpha}$ | $\frac{\alpha}{\alpha+1}$ | $\frac{\alpha+2}{\alpha+1}$ | $\frac{\alpha+1}{\alpha+2}$ | $\frac{1}{\alpha+2}\ )$ | | | | | | |
| 4 | $(\ \lambda\frac{\alpha+1}{\alpha}$ | $\frac{\alpha}{\alpha+1}$ | $\frac{\alpha+2}{\alpha+1}$ | $\frac{\alpha+1}{\alpha+2}$ | $\frac{\alpha+3}{\alpha+2}$ | $\frac{\alpha+2}{\alpha+3}$ | $\frac{1}{\alpha+3}\ )$ | | | | |
| 5 | $(\ \lambda\frac{\alpha+1}{\alpha}$ | $\frac{\alpha}{\alpha+1}$ | $\frac{\alpha+2}{\alpha+1}$ | $\frac{\alpha+1}{\alpha+2}$ | $\frac{\alpha+3}{\alpha+2}$ | $\frac{\alpha+2}{\alpha+3}$ | $\frac{\alpha+4}{\alpha+3}$ | $\frac{\alpha+3}{\alpha+4}$ | $\frac{1}{\alpha+4}\ )$ | | |
| 6 | $(\ \lambda\frac{\alpha+1}{\alpha}$ | $\frac{\alpha}{\alpha+1}$ | $\frac{\alpha+2}{\alpha+1}$ | $\frac{\alpha+1}{\alpha+2}$ | $\frac{\alpha+3}{\alpha+2}$ | $\frac{\alpha+2}{\alpha+3}$ | $\frac{\alpha+4}{\alpha+3}$ | $\frac{\alpha+3}{\alpha+4}$ | $\frac{\alpha+5}{\alpha+4}$ | $\frac{\alpha+4}{\alpha+5}$ | $\frac{1}{\alpha+5}\ )$ |

# Chapter 8

## Closed exact solutions of the relaxation function $a_0(t)$ for particular values of the parameters

In the recurrence relations method, once we pick the dynamical variable whose time evolution will be studied, say $A$, this choice fixes the basal vector as $f_0 = A$, and consequently, through the RR1, Eq. (7.36a), all the other basis vectors of the orthogonal set $\{f_\nu\}$. The successive quotients of the norms of these basis vectors constitute the set $\{\Delta_\nu\}$, Eq. (2.6b), of the recurrants, which in turn, determines the time evolution of $A$ through the fundamental expansion, Eq. (2.3) (reproduced below),

$$A(t) = \sum_{\nu=0}^{d-1} a_\nu(t) f_\nu \ . \tag{8.1}$$

The basis functions $a_\nu(t)$ in this expansion, are completely defined by the three term recurrence relation known as the recurrence relation II or RR2, Eq. (2.16), that for convenience, we reproduce and also reference again:

$$\Delta_{\nu+1} a_{\nu+1}(t) = -\dot{a}_\nu(t) + a_{\nu-1}(t)\,, \qquad (\nu = 0, 1, \ldots, d-1)\,, \tag{8.2}$$

with $a_{-1} \equiv 0$. This relation depends *exclusively* on the aforementioned set $\{\Delta_\nu\}$ of the recurrants.

In this chapter we will exploit the fact that for many mathematical (elementary, and advanced or special) functions, such three term recurrence relations are known [Abramowitz & Stegun 1972]. We have already reviewed some examples of this approach in the previous chapters, e.g., the ideal 2D electron gas in §3.2.4, and Eqs. (6.6)–(6.7).

The basis functions $a_\nu$ are time dependent and, from the fundamental expansion, Eq. (8.1), and the RR1, Eq. (7.36a), it is seen that the physical "dimension"[1] of $a_\nu(t)$ is

$$[a_\nu(t)] = \text{time}^\nu \ . \tag{8.3}$$

[1]The use of the singular should be noted. See, e.g., [Barenblatt 1996, §1.1.3].

In other words, $a_\nu(t)$ can be measured in units of, say, second$^\nu$. So, the first step in identifying a solution, directly, by means of the recurrence relation it obeys, is to rewrite the RR2 as a dimensionless relationship among a sequence of "pure mathematical" (i.e. non-dimensional domain and image) functions. To this end we set

$$a_\nu(t) \equiv \mu^{-\nu}\, U_\nu\, h_\nu(\mu t)\ , \tag{8.4}$$

where $\mu$ is a scale factor, $U_\nu$ is a $\nu$-dependent coefficient, and $h_\nu(x)$ is a set of "pure mathematical" functions; all of them to be determined. This is the notation used by M. Howard Lee and J. Hong in their study of the 2D electron gas at long wavelengths [Lee & Hong 1985*b*], that we reviewed in §3.2.4.

The $\mu^{-\nu}$ factor is introduced to account for the time derivative in the RR2 and make the $\nu$-dependence of the $U_\nu$ coefficients, the simplest possible. Thus, the $a_\nu(t)$ definition in Eq. (8.4) above is the simplest allowed. Another possibility (that we will explore) would be a (finite?) linear combination of $h$ like functions.

Using the definition of the $a_\nu(t)$ in terms of the $h_\nu(x)$, Eq. (8.4), the RR2 becomes

$$\Delta_{\nu+1}\mu^{-2}\, U_{\nu+1}\, h_{\nu+1}(\mu t) = -U_\nu\, h'_\nu(\mu t) + U_{\nu-1}\, h_{\nu-1}(\mu t)\ , \tag{8.5a}$$

where $h'_\nu$ denotes derivative respect to the "natural" argument of the function, in this case $x$, and $h_{-1} \equiv 0$. Now, it is seen, that if all the $\Delta_\nu$ have a common frequency-squared factor, say $\Omega^2$, then $\mu = \Omega$, or better,

$$\mu = c\,\Omega\,, \tag{8.5b}$$

to maybe allow for a simpler or more canonical definition of the coefficients $U_\nu$ and the functions $h_\nu$.

Before going on with the actual calculations we will show in the next section that it is possible to obtain a particular solution to our model, the HOC with an impurity mass coupled to a fixed wall (IMCFW), just by comparing our $\{\Delta_\nu\}$ to previously considered Delta's sequences that may turn out to be similar to ours and exploiting the ensuing dynamic equivalence.

## 8.1 Dynamical equivalence between the HOC with an impurity mass and periodic boundary conditions (PBC) and the HOC with an ICFW

We reviewed in Chapter 6 the dynamic equivalence of 2D quantum electron gas and an HOC with an impurity mass and PBC studied by Lee, Florencio & Hong [1989].

There, the set $\{\Delta_\nu\}$ is designated as the $\sigma$ hypersurface, thus emphasizing the fact the norm of the time-evolving dynamic variable being considered is constant in an hermitian system. We adopted the same terminology in the tables we presented for the $\{\Delta_\nu\}$ at the end of Chapter 7.

We will now compare Table 7.1 with the Delta's sequence obtained by [Lee, Florencio & Hong 1989]

$$\begin{aligned}\sigma &= (2\lambda k/m, \lambda k/m, \lambda k/m, \ldots, \lambda k/m, 2\lambda k/m)\,, \quad d = N+1 \\ &= (2\lambda, 1, 1, 1, \ldots\ldots, 1, 1, 2) \times \tfrac{k}{m}\ . \end{aligned} \tag{8.6}$$

The parameter $\lambda$ above is the same as ours, defined in Eq. (7.3). In both systems, the closed HOC with PBC and the HOC with an ICFW, the role of the $\lambda$ parameter is similar, it only appears in the first non trivial recurrant, $\Delta_1$. In [Lee et al. 1989], $\Delta_1 = 2\lambda$, while in our case, from Table 7.1, we have that $\Delta_1 = \lambda(1+\kappa)$ ($\kappa$ is defined as $k_0/k$ in Eq. (7.2), where $k_0$ is the coupling to the wall and $k$ is the coupling between n.n. oscillators). As to the other recurrants, at first sight from Table 7.1 they look $\kappa$ dependent and therefore not constant but, in fact, if $\kappa$ is set to zero, all the other recurrants become one or zero. Bellow, in Table 8.1, we reproduce Table 7.1 with $\kappa = 0$, which means that the impurity mass $m_0$ next to the wall is uncoupled from the wall.

With this choice our system is now a free open-ended (at both sides) HOC with an impurity mass at one end. It is seen immediately that the sigmas for both systems are quite similar, but not exactly equal: there is a factor of 2 at both ends of the $\sigma$ for the closed chain with PBC and, its dimension is $d = N+1$ (which means the last non-null recurrant is $\Delta_N = 2\,k/m$). For the HOC with an ICFW, the factors of 2 are missing at both ends of its $\sigma$ and, the dimension is $d = 2N-1$.

Lee, Florencio & Hong [1989] showed that the $N \to \infty$, HOC with an impurity mass and PBC is dynamically equivalent to a zero-temperature 2D interacting electron gas [Lee & Hong 1985*b*] at long wavelengths. In particular, the non-interacting limit of the electron gas and the homogeneous case when the impurity mass is equal to the other masses in the chain, both have recurrants $\{\Delta_\nu\}$

Table 8.1: Delta sequence $\sigma = (\Delta_1, \Delta_2, \ldots, \Delta_{d-1})$, in units of $k/m$, for independent chains of harmonic oscillators with the left end coupled to a wall. The number of masses in the chain is $N$. All the spring constants and the masses are equal, except for the oscillator next to the wall. Here, $\lambda = m/m_0$ and $\kappa = k_0/k$, where the 0 subscript refers to the oscillator next to the wall. In this table we have set $k_0 = 0$, i.e., the impurity mass $m_0$ is uncoupled from the wall.

| | $\sigma =$ | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| $N$ | $(\Delta_1$ | $\Delta_2$ | $\Delta_3$ | $\Delta_4$ | $\Delta_5$ | $\Delta_6$ | $\Delta_7$ | $\Delta_8$ | $\Delta_9$ | $\Delta_{10}$ | $\Delta_{11})$ |
| 2 | ( $\lambda$ | 1 | 0 ) | | | | | | | | |
| 3 | ( $\lambda$ | 1 | 1 | 1 | 0 ) | | | | | | |
| 4 | ( $\lambda$ | 1 | 1 | 1 | 1 | 1 | 0 ) | | | | |
| 5 | ( $\lambda$ | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 0 ) | | |
| 6 | ( $\lambda$ | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 0 ) |

sets that are *similar* (see Eqs. (6.6) and §3.2.4) to $(2, 1, 1, 1, \ldots)$, in the sense of Eqs. (5.2) of §5.1 and, therefore are dynamically equivalent (DE). We reviewed in Chapter 6 how [Lee et al. 1989] use this DE to write the solution for the equal-mass (homogeneous) limit of the HOC with an impurity mass and PBC. We can do similarly noting that the recurrants $\{\Delta_\nu\}$ set of our model, the HOC with an ICFW becomes *similar* (in the aforementioned sense) to $(2, 1, 1, 1, \ldots)$ when: $\kappa = 0$ (impurity uncoupled to the wall, see Table 8.1), in the $N \to \infty$ *and*, with $\lambda = 2$, that is, the impurity mass is half of the mass of each of the other oscillators. Thus, for this set of parameters ($\lambda = 2$, $\kappa = 0$, and $N \to \infty$) our model is DE to the other two mentioned above. The solution is worked out by Lee & Hong [1985*b*]. We will reproduce this solution below, with additional detail about how to pick the most convenient time-scale factor.

The recurrants sets $\{\Delta_\nu\}$ for the three models mentioned above have the form

$$\Delta_1 = 2\Omega^2 \,, \tag{8.7a}$$

$$\Delta_\nu = \ \Omega^2 \,, \qquad\qquad \nu \geqslant 1 \ , \tag{8.7b}$$

where $\Omega$ is a model dependent frequency. Using Eq. (8.5a) with the above expressions for the recurrants, and writing separately the special $\nu = 0$ case of Eq. (8.5a)

$$2c^{-2}\frac{U_1}{U_0}h_1 = -h_0' \ , \tag{8.8a}$$

$$c^{-2}\frac{U_{\nu+1}}{U_{\nu-1}}h_{\nu+1} = -\frac{U_\nu}{U_{\nu-1}}h_\nu' + h_{\nu-1} \ , \qquad \nu \geqslant 1 \ , \tag{8.8b}$$

where we have used Eq. (8.5b) to write the time-scale $\mu$. The $h_\nu$ definition, Eq. (8.4), together with the boundary condition $a_0(0) = 1$ (see Eq. (2.11)) gives that $h_0(0) = 1$, $U_0 = 1$, and suggests that

$$U_\nu = \mathrm{e}^{D\nu} \ , \tag{8.9}$$

where $D$ is a constant. Thus,

$$2c^{-2}\,\mathrm{e}^{D}\,h_1 = -h_0' \ , \tag{8.10a}$$

$$c^{-2}\,\mathrm{e}^{2D}\,h_{\nu+1} = -\,\mathrm{e}^{D}\,h_\nu' + h_{\nu-1} \ , \qquad \nu \geqslant 1 \ . \tag{8.10b}$$

Now, the above may be compared with the recurrence relation for the Bessel functions $\mathrm{J}_\nu$ [Abramowitz & Stegun 1972]

$$\mathrm{J}_1 = -\mathrm{J}_0' \ , \tag{8.11a}$$

$$\mathrm{J}_{\nu+1} = -2\mathrm{J}_\nu' + \mathrm{J}_{\nu-1} \ , \qquad \nu \geqslant 1 \ . \tag{8.11b}$$

The comparison gives that, if we choose $\mathrm{e}^D = 2$ and $c^2 = 4$, then the recurrence relation for the $h_\nu$, Eqs. (8.10), becomes identical to the recurrence relation for the Bessel functions $\mathrm{J}_\nu$ above. Then, the coefficient is $U_\nu = 2^\nu$ and, the scale factor is $\mu = c\,\Omega = 2\Omega$. Therefore, we have just shown that for $\sigma = (2, 1, 1, 1, \ldots) \times \Omega^2$ the basis functions are

$$\begin{aligned} a_\nu(t) &\equiv \mu^{-\nu} U_\nu \mathrm{J}_\nu(\mu t) \ , \\ &= \mu^{-\nu} 2^\nu \mathrm{J}_\nu(\mu t) \ , \end{aligned} \tag{8.12a}$$

or, in particular, substituting $\mu = 2\Omega$

$$= \Omega^{-\nu} \mathrm{J}_\nu(2\Omega t) \ . \tag{8.12b}$$

This is the solution for our model with ($\lambda = 2$, $\kappa = 0$, and $N \to \infty$), it corresponds to the $N \to \infty$, equal-mass (homogeneous, $\lambda = 1$) case of Lee, Florencio & Hong's [1989] model of the HOC with

an impurity and PBC. [Lee et al. 1989] also obtained the solution for $\lambda \neq 1$ in which case the $\sigma$ hypersurface is

$$\sigma = (2\lambda, 1, 1, 1, \dots) \times \tfrac{k}{m} \ . \tag{8.13}$$

We can take advantage again of the DE idea, noting, from Table 8.1, that in the $\kappa = 0$, $N \to \infty$, case, we may rewrite our $\sigma$ hypersurface as

$$\sigma = (2\,\tfrac{\lambda}{2}\,, 1, 1, 1, \dots) \times \tfrac{k}{m} \ , \tag{8.14}$$

to make it similar to the one above. Therefore, the solution for our model in the $N \to \infty$, $\kappa = 0$, and, *any* $\lambda$ case, is obtained by making the replacement

$$\lambda \leftarrow \frac{\lambda}{2} \ , \tag{8.15}$$

in the [Lee et al. 1989] solution for the $N \to \infty$, HOC with an impurity and PBC.

## 8.2 The $\mathrm{J}_0 - \mathrm{J}_n$ solutions

We will now investigate the possibility of finding particular solutions to our model in the form of simple linear combinations of known solutions of models similar to ours, e.g., like those reviewed in §8.1. We shall define such a linear combination and then try to satisfy the RR2, Eq. (8.2), and the boundary condition Eq. (2.11), by choosing appropriate values of the linear combination parameters and/or the model parameters. Let's start with the following choice that already satisfies the boundary condition $a_0(0) = 1$ ,

$$a_0(t) = \mathrm{J}_0(\Omega_1 t) - B\mathrm{J}_n(\Omega_2 t) \ , \tag{8.16}$$

where $\mathrm{J}_0$ and $\mathrm{J}_n$ are Bessel functions. Here $B$, $n$, $\Omega_1$ and $\Omega_2$ are to be determined. On account of

$$a_0(t) = a_0(-t) \ , \tag{8.17}$$

and the properties of the Bessel functions, $n$ has to be even. Now, we intend to successively determine $a_1(t), a_2(t), \dots$ using the RR2, Eq. (8.2), and to use the boundary condition, Eq. (2.11), to fix the values of $B$, $n$, $\Omega_1$ and $\Omega_2$. If this can be done, we will have found a solution(s).

Let us for the moment designate the recurrants of our model as

$$\Delta_\nu \equiv \delta_\nu \Omega^2 \,, \tag{8.18}$$

where $\Omega^2 = k/m$ , and for reference purposes we write

$$\Omega \equiv \sqrt{k/m} \,, \tag{8.19}$$

with $k$ and $m$ defined in Eq. (7.3) on page 60.

Using the RR2, Eq. (8.2), for $\nu = 1$: $\Delta_1 a_1(t) = -\dot{a}_0(t)$

$$\Omega^2 \delta_1 a_1(t) = \Omega_1 \mathrm{J}_1(\Omega_1 t) + \frac{B}{2}\Omega_2[\mathrm{J}_{n-1}(\Omega_2 t) - \mathrm{J}_{n+1}(\Omega_2 t)] \;, \tag{8.20}$$

and

$$a_1(t) = \frac{\Omega_1}{\Omega^2 \delta_1}\mathrm{J}_1(\Omega_1 t) + \frac{B}{2}\frac{\Omega_2}{\Omega^2 \delta_1}[\mathrm{J}_{n-1}(\Omega_2 t) - \mathrm{J}_{n+1}(\Omega_2 t)] \;. \tag{8.21}$$

The boundary condition, Eq. (2.11), $a_1(0) = 0$ is satisfied since $n$ is even and greater than zero. The RR2 for $\nu = 2$, $\Delta_2 a_2(t) = -\dot{a}_1(t) + a_0$, gives

$$\begin{aligned} \Omega^2 \delta_2 a_2(t) = &- \frac{\Omega_1^2}{\Omega^2 \delta_1}\frac{1}{2}[\mathrm{J}_0(\Omega_1 t) - \mathrm{J}_2(\Omega_2 t)] \\ &- \frac{B}{2}\frac{\Omega_2^2}{\Omega^2 \delta_1}\frac{1}{2}[\mathrm{J}_{n-2}(\Omega_2 t) - \mathrm{J}_n(\Omega_2 t) - \mathrm{J}_n(\Omega_2 t) + \mathrm{J}_{n+2}(\Omega_2 t)] \\ &+ \mathrm{J}_0(\Omega_1 t) - B\mathrm{J}_n(\Omega_2 t) \;. \end{aligned} \tag{8.22}$$

The above expression, evaluated at $t = 0$ is

$$\Omega^2 \delta_2 a_2(t=0) = -\frac{\Omega_1^2}{2\Omega^2 \delta_1} - \frac{B\Omega_2^2}{4\Omega^2 \delta_1}\mathrm{J}_{n-2}(0) + 1 \;. \tag{8.23}$$

The boundary condition, Eq. (2.11), requires that $a_2(0) = 0$ . Therefore, due to the presence of Bessel function $\mathrm{J}_{n-2}(0)$, we have to consider two cases for the above expression to meet this requirement, $n > 2$ and $n = 2$ . The $n > 2$, actually is not such a range. We will show below that $n \not> 4$ and, then only $n = 4$ is allowed. In both cases, it can be shown [Gianvittorio & Pestana n.d.] that to obtain a solution by the process outlined after Eq. (8.16), first, the constant $B$ has to be related to the time-scales as follows

$$B = \frac{\Omega_2}{l\Omega_1} \;, \tag{8.24}$$

where $l$ is an integer and, second, that both time scales, $\Omega_1$ and $\Omega_2$, of the two Bessel functions that appear in the original trial solution, Eq. (8.16), have to be equal among them, that is

$$\Omega_1 = \Omega_2 \equiv \Omega_B \,, \tag{8.25}$$

so, the above equation with the boundary condition $a_2(0) = 0$ imposed, now reads

$$\Omega^2 \delta_2 a_2(t=0) = -\frac{\Omega_B^2}{2\Omega^2\delta_1} - \frac{\Omega_B^2}{4l\Omega^2\delta_1} \mathrm{J}_{n-2}(0) + 1 = 0 \,. \tag{8.26}$$

## 8.3 The $\mathrm{J}_0 - \mathrm{J}_4$ particular solution

We now tackle the first case (mentioned just after Eq. (8.23)) of the two that have to be considered for the $a_2(0) = 0$ boundary condition requirement in Eq. (8.26).

For $n > 2$, then $\mathrm{J}_{n-2}(0) = 0$ in Eq. (8.26) above, and

$$\Omega_B^2 = 2\Omega^2\delta_1 \,. \tag{8.27}$$

To satisfy the $a_4(0) = 0$ boundary condition it is found [Gianvittorio & Pestana n.d.] that then $n$ cannot be greater than 4, thus, $n = 4$ is the only possible value for the case $n > 2$. We also find that $l = 1$ and, that $\lambda = 1$ and $\kappa = 1$ so, from Table 7.1 we have

$$\begin{aligned} \delta_1 \equiv \frac{\Delta_1}{\Omega^2} &= \lambda(1+\kappa) \,, \\ &= 2 \,, \end{aligned} \tag{8.28}$$

and then, from Eq. (8.27) above, that

$$\Omega_B = 2\Omega \equiv (k/m)^{1/2} \,, \tag{8.29}$$

is the common time-scale for all the Bessel functions.

The solution we have found is, thus

$$a_0(t) = \mathrm{J}_0(2\Omega t) - \mathrm{J}_4(2\Omega t) \,. \tag{8.30}$$

A similar solution had been found by [Florencio & Lee 1985] in their study of the homogeneous harmonic oscillators chain (HOC) with either periodic boundary conditions (PBC) or fixed ends (FEBC) boundary conditions. We reviewed in §7.2 Florencio & Lee's [1985] application of the

recurrence relations method (RRM) to the study of the dynamics of this system. Using a normal–mode[2] transformation and the RRM, they found for the FEBC case,

$$q_0 = q_{N+1} = 0 \ , \tag{8.31}$$

$$p_0 = p_{N+1} = 0 \ , \tag{8.32}$$

and in the thermodynamic limit, the velocity autocorrelation function is given by

$$\langle v_j(t)v_j(0)\rangle = \frac{\mathrm{k_B}T}{2m}[\mathrm{J}_0(2\Omega t) - \mathrm{J}_{4j}(2\Omega t)] \, , \qquad\qquad j = 1, 2, 3, 4, \ldots \ . \tag{8.33}$$

We thus see that for the oscillator next to the fixed wall, $j = 1$, this solution is identical to ours, Eq. (8.30). Note that in our model the site zero refers to the $m_0$ mass (with displacement $q_0$ and momentum $p_0$) coupled to wall by the spring of elastic constant $k_0$. Since $\lambda \equiv m/m_0$ and $\kappa \equiv m_0/m$, our solution, Eq. (8.30), is for $m_0 = m$ and $k_0 = k$, i.e., the homogeneous case of our model. The dynamical variable we chose was $p_0$ so,

$$a_0(t) = \frac{\langle p_0(t)p_0(0)\rangle}{\langle p_0(0)p_0(0)\rangle} = \frac{\langle p_0(t)p_0\rangle}{\langle p_0p_0\rangle} \tag{8.34}$$

is the momentum autocorrelation function. Therefore, Florencio & Lee's [1985] solution and ours are, not only identical, but also, they refer to exactly the same physical situation. The last sentence withstanding, note that Florencio & Lee's [1985] set of recurrants and ours, are different. Theirs is an infinite number of two-dimensional sets of $\Delta_\nu$, corresponding to the fact that they transformed the infinite, nearest–neighbor interacting, homogeneous, harmonic oscillator chain into an infinite set of non-interacting harmonic oscillators through the use of a normal-mode transformation, while ours is one infinite set of $\Delta_\nu$. The dynamical equivalence of the two models was established *without* using the similarity of the delta sets involved. Note that this equivalence can only be done in the thermodynamic limit of both systems, where the Bessel functions difference $\mathrm{J}_0 - \mathrm{J}_4$ solution appears. In Table 8.2 we show the $\{\Delta_\nu\}$ set for the first few values of $N$, the number of masses in our model chain, with $\lambda = 1$ and $\kappa = 1$. In the thermodynamic limit, $N \to \infty$, it corresponds to the $\mathrm{J}_0 - \mathrm{J}_4$ solution.

[2]The inhomogeneity of our system, the mass next to the wall is $m_0$ and its coupling to the wall is $k_0$, precludes us from using the normal–mode approach.

Table 8.2: $\lambda = 1$ and $\kappa = 1$ Delta sequence $\sigma = (\Delta_1, \Delta_2, \ldots, \Delta_{d-1})$, in units of $k/m$, for independent chains of harmonic oscillators with the left end coupled to a wall. The number of masses in the chain is $N$. All the spring constants and the masses are equal, except for the oscillator next to the wall. Here, $\lambda = m/m_0$ and $\kappa = k_0/k$, where the 0 subscript refers to the oscillator next to the wall. In the thermodynamic limit, $N \to \infty$, it corresponds to the $\mathrm{J}_0 - \mathrm{J}_4$ solution.

| | $\sigma =$ | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| $N$ | $(\Delta_1$ | $\Delta_2$ | $\Delta_3$ | $\Delta_4$ | $\Delta_5$ | $\Delta_6$ | $\Delta_7$ | $\Delta_8$ | $\Delta_9$ | $\Delta_{10}$ | $\Delta_{11})$ |
| 2 | ( 2 | $\frac{1}{2}$ | $\frac{1}{2}$ ) | | | | | | | | |
| 3 | ( 2 | $\frac{1}{2}$ | $\frac{3}{2}$ | $\frac{2}{3}$ | $\frac{1}{3}$ ) | | | | | | |
| 4 | ( 2 | $\frac{1}{2}$ | $\frac{3}{2}$ | $\frac{2}{3}$ | $\frac{4}{3}$ | $\frac{3}{4}$ | $\frac{1}{4}$ ) | | | | |
| 5 | ( 2 | $\frac{1}{2}$ | $\frac{3}{2}$ | $\frac{2}{3}$ | $\frac{4}{3}$ | $\frac{3}{4}$ | $\frac{5}{4}$ | $\frac{4}{5}$ | $\frac{1}{5}$ ) | | |
| 6 | ( 2 | $\frac{1}{2}$ | $\frac{3}{2}$ | $\frac{2}{3}$ | $\frac{4}{3}$ | $\frac{3}{4}$ | $\frac{5}{4}$ | $\frac{4}{5}$ | $\frac{6}{5}$ | $\frac{5}{6}$ | $\frac{1}{6}$ ) |

The $a_0(t)$ we found, is the first basis function of the fundamental expansion, Eq. (8.1) that, in this case, reads

$$p_0(t) = \sum_{\nu=0}^{\infty} a_\nu(t) f_\nu \,, \tag{8.35}$$

with the $f_\nu$ given by Eqs. (7.59) of §7.5. The other basis functions can be calculated using the RR2, Eq. (8.2), with the $\Delta_\nu$ given by Table 8.2, where $\lambda = 1$ and $\kappa = 1$. The first few are

$$a_1(t) = \tfrac{1}{\Omega}[\mathrm{J}_1(2\Omega t) + \tfrac{1}{2}\mathrm{J}_3(2\Omega t) - \tfrac{1}{2}\mathrm{J}_5(2\Omega t)] \,, \tag{8.36a}$$

$$a_2(t) = \tfrac{1}{\Omega^2}[\mathrm{J}_2(2\Omega t) - \mathrm{J}_6(2\Omega t)] \,, \tag{8.36b}$$

$$a_3(t) = \tfrac{1}{\Omega^3}[\mathrm{J}_3(2\Omega t) + \tfrac{1}{3}\mathrm{J}_5(2\Omega t) - \tfrac{2}{3}\mathrm{J}_7(2\Omega t)] \,, \tag{8.36c}$$

$$a_4(t) = \tfrac{1}{\Omega^4}[\mathrm{J}_4(2\Omega t) - \mathrm{J}_8(2\Omega t)] \,, \tag{8.36d}$$

$$a_5(t) = \tfrac{1}{\Omega^5}[\mathrm{J}_5(2\Omega t) + \tfrac{1}{4}\mathrm{J}_7(2\Omega t) - \tfrac{3}{4}\mathrm{J}_9(2\Omega t)] \,, \tag{8.36e}$$

$$a_6(t) = \tfrac{1}{\Omega^6}[\mathrm{J}_6(2\Omega t) - \mathrm{J}_{10}(2\Omega t)] \,, \tag{8.36f}$$

$$a_7(t) = \tfrac{1}{\Omega^7}[\mathrm{J}_7(2\Omega t) + \tfrac{1}{5}\mathrm{J}_9(2\Omega t) - \tfrac{4}{5}\mathrm{J}_{11}(2\Omega t)] \,. \tag{8.36g}$$

The general terms are

$$a_{2\nu-1}(t) = \tfrac{1}{\Omega^{2\nu-1}}[\mathrm{J}_{2\nu-1}(2\Omega t) + \tfrac{1}{\nu+1}\mathrm{J}_{2\nu+1}(2\Omega t) - \tfrac{\nu}{\nu+1}\mathrm{J}_{2\nu+3}(2\Omega t)]\,, \tag{8.37a}$$

$$a_{2\nu}(t) = \tfrac{1}{\Omega^{2\nu}}[\mathrm{J}_{2\nu}(2\Omega t) - \mathrm{J}_{2\nu+4}(2\Omega t)]\,, \tag{8.37b}$$

where $\nu = 1, 2, 3, 4, \ldots$ .

## 8.4 The $\mathrm{J}_0 - \mathrm{J}_2$ particular solution

We now tackle the second case (mentioned just after Eq. (8.23)) of the two that have to be considered for the $a_2(0) = 0$ boundary requirement in Eq. (8.26).

For $n = 2$, then $\mathrm{J}_{n-2}(0) = \mathrm{J}_0(0) = 1$ in Eq. (8.26) above, which now reads

$$-\frac{\Omega_B^2}{2\Omega^2\delta_1} - \frac{\Omega_B^2}{4l\Omega^2\delta_1} + 1 = 0\ . \tag{8.38}$$

Then,

$$\Omega_B^2 = \frac{4l}{2l+1}\delta_1\Omega^2\ . \tag{8.39}$$

This relation has to be substituted back into $a_1(t)$ and $a_2(t)$, given by Eqs. (8.21)–(8.22). Now the remaining parameters are chosen so that the boundary condition $a_2(0) = 0$ is fulfilled by the $a_3, a_4, \ldots$, successively generated by the RR2, Eq. (8.2). We find [Gianvittorio & Pestana n.d.] that $l = 1$, $\lambda = 1$ and $\kappa = 2$. From Table 7.1 and Eq. (8.18)

$$\delta_1 = \frac{\Delta_1}{\Omega^2} = \lambda(1+\kappa) = 3\ , \tag{8.40}$$

and thus

$$\Omega_B^2 = 4\Omega^2 = 4\frac{k}{m}\ . \tag{8.41}$$

From Eq. (8.25), $\Omega_1 = \Omega_2 = \Omega_B = 2\Omega$, and from Eq. (8.24), $B = \Omega_2/l\Omega_1 = 1$, thus all the parameters of the linear combination of Bessel functions trial solution for $a_0(t)$, Eq. (8.16), have been determined and the full set $\{a_0(t), a_1(t), a_2(t), \ldots\}$ satisfies the RR2 and the corresponding boundary conditions, consequently, now we can state simply that

$$a_0(t) = \mathrm{J}_0(2\Omega t) - \mathrm{J}_2(2\Omega t) \tag{8.42}$$

and the other $a_\nu$ generated by the RR2, constitute the solution for the basis wavefunctions that appear in the fundamental expansion, Eq. (8.35), of $p_0(t)$ when $\lambda = 1$, $\kappa = 2$ in our model.

The first few $a_\nu(t)$ are

$$a_1(t) = \tfrac{1}{\Omega}[\mathrm{J}_1(2\Omega t) - \tfrac{1}{3}\mathrm{J}_3(2\Omega t)]\,, \tag{8.43a}$$

$$a_2(t) = \tfrac{1}{\Omega^2}[\mathrm{J}_2(2\Omega t) - \mathrm{J}_4(2\Omega t)]\,, \tag{8.43b}$$

$$a_3(t) = \tfrac{1}{\Omega^3}[\mathrm{J}_3(2\Omega t) - \tfrac{3}{5}\mathrm{J}_5(2\Omega t)]\,, \tag{8.43c}$$

$$a_4(t) = \tfrac{1}{\Omega^4}[\mathrm{J}_4(2\Omega t) - \mathrm{J}_6(2\Omega t)]\,. \tag{8.43d}$$

The general terms are

$$a_{2\nu}(t) = \tfrac{1}{\Omega^{2\nu}}[\mathrm{J}_{2\nu}(2\Omega t) - \mathrm{J}_{2\nu+2}(2\Omega t)]\,, \tag{8.44a}$$

$$a_{2\nu+1}(t) = \tfrac{1}{\Omega^{2\nu+1}}[\mathrm{J}_{2\nu+1}(2\Omega t) - \tfrac{2\nu+1}{2\nu+3}\mathrm{J}_{2\nu+3}(2\Omega t)]\,. \tag{8.44b}$$

To our knowledge this solution is new. In Table 8.3 we show how the $\Delta_\nu$ set attains the thermodynamic limit, $N \to \infty$, for $\lambda = 1$ and $\kappa = 2$ in our model, which corresponds to the $\mathrm{J}_0 - \mathrm{J}_2$ solution.

Table 8.3: $\lambda = 1$ and $\kappa = 2$ Delta sequence $\sigma = (\Delta_1, \Delta_2, \ldots, \Delta_{d-1})$, in units of $k/m$, for independent chains of harmonic oscillators with the left end coupled to a wall. The number of masses in the chain is $N$. All the spring constants and the masses are equal, except for the oscillator next to the wall. Here, $\lambda = m/m_0$ and $\kappa = k_0/k$, where the 0 subscript refers to the oscillator next to the wall. In the thermodynamic limit, $N \to \infty$, it corresponds to the $\mathrm{J}_0 - \mathrm{J}_2$ solution.

| | $\sigma =$ | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| $N$ | $(\Delta_1$ | $\Delta_2$ | $\Delta_3$ | $\Delta_4$ | $\Delta_5$ | $\Delta_6$ | $\Delta_7$ | $\Delta_8$ | $\Delta_9$ | $\Delta_{10}$ | $\Delta_{11})$ |
| 2 | ( 3 | $\frac{1}{3}$ | $\frac{2}{3}$ ) | | | | | | | | |
| 3 | ( 3 | $\frac{1}{3}$ | $\frac{5}{3}$ | $\frac{3}{5}$ | $\frac{2}{5}$ ) | | | | | | |
| 4 | ( 3 | $\frac{1}{3}$ | $\frac{5}{3}$ | $\frac{3}{5}$ | $\frac{7}{5}$ | $\frac{5}{7}$ | $\frac{2}{7}$ ) | | | | |
| 5 | ( 3 | $\frac{1}{3}$ | $\frac{5}{3}$ | $\frac{3}{5}$ | $\frac{7}{5}$ | $\frac{5}{7}$ | $\frac{9}{7}$ | $\frac{7}{9}$ | $\frac{2}{9}$ ) | | |
| 6 | ( 3 | $\frac{1}{3}$ | $\frac{5}{3}$ | $\frac{3}{5}$ | $\frac{7}{5}$ | $\frac{5}{7}$ | $\frac{9}{7}$ | $\frac{7}{9}$ | $\frac{11}{9}$ | $\frac{9}{11}$ | $\frac{2}{11}$ ) |

## 8.5 The $2J_1/t$ solution

This last exact solution was not obtained by dynamical equivalence[3], like it was done in §8.1 for the $J_0$ solution. Neither by testing trial functions and combinations of parameters for consistency against the RR2, Eq. (8.2), as described in §§8.2–8.4 for the $J_0 - J_n$ solutions.

In Chapter 9 we will obtain for our model a general exact solution for the Laplace transform of $\tilde{a}_0(z)$ of the relaxation function $a_0(t)$. This will be done by "summing" the continued fraction expansion of $\tilde{a}_0(z)$.

This solution, given by Eq. (9.15), is valid for any value of the $\kappa$ and $\lambda$ parameters in the thermodynamical limit $N \to \infty$. We note in §9.5 in page 107, that all the examples of exact solutions, the $J_0$, the $J_0 - J_4$, and the $J_0 - J_2$ do not have singularities (more precisely, the singularities are either at the edge of the branch-cut or at infinity), and we argue that this suggests where to look for possible exact solutions, i.e., points in $(\kappa, \lambda)$ space with the above characteristic. Inspecting Figure 9.1 and Figure 9.2, we find that one more such point is $(0, 1)$, that is, $\kappa = 0$ and $\lambda = 1$, and from Eq. (9.15), we obtain

$$\begin{aligned} \tilde{a}_0(z)|_{\kappa=0,\,\lambda=1} &= \frac{2z}{z^2 + z\sqrt{z^2+\mu^2}} = \frac{2}{z + \sqrt{z^2+\mu^2}} \ , \\ &= \frac{2}{\mu}(z - \sqrt{z^2+\mu^2}) \ . \end{aligned} \tag{8.45}$$

Here, all the square roots mean the first or principal branch (see Eq. (9.15)p. 92). This can be inverse Laplace transformed (see, e.g., [Abramowitz & Stegun 1972, p. 1025, Eq. 29.3.58]) to get

$$a_0(t)|_{\kappa=0,\,\lambda=1} = 2J_1(\mu t)/t \ . \tag{8.46}$$

This corresponds to the $\lambda_{Lee} = 1/2$ solution of the last footnote of page L334 of [Lee, Florencio & Hong 1989]. Their model can be related to ours along the $\kappa = 0$ line where the coupling of the impurity to the fixed wall is zero. See Eq.(8.15) of §8.1 p. 79 where we show the dynamical equivalence between our model and theirs with the substitution

$$\lambda_{Lee} = \tfrac{1}{2}\lambda_{us} \ . \tag{8.47}$$

[3]Between the model described by Lee, Florencio & Hong [1989], the harmonic oscillator chain (HOC) with an impurity and periodic boundary conditions; and our model, the (HOC) with an impurity coupled to a fixed wall (ICFW).

Here, $\lambda_{Lee}$ and $\lambda_{us}$ have the same meaning. Both represent the quotient, $m/m_0$, with $m$ being any mass in the chains and $m_0$ being the mass of impurity.

# Chapter 9

## General solution of the relaxation function $\tilde{a}_0(z)$

Once the RR1 have been carried out, the basis vectors $\{f_\nu\}$ and the recurrants $\{\Delta_\nu\}$ are known. This step was done on Chapter 7. The dynamics of the chosen variable, $f_0 \equiv p_0$, are given by the basis functions $\{a_\nu(t)\}$, to be determined from the RR2, Eq. (8.2). We succeeded four times in doing so, in Chapter 8, for particular values of the parameters of our model. The first two by exploiting the similarity (see the idea of dynamic equivalence (DE) in §5.1) of our delta sequences to those of Lee, Florencio & Hong [1989] in their study of the DE of a 2D quantum electron gas to a classical HOC with an impurity mass. The others by finding two combinations of Bessel functions that satisfied the RR2 and the corresponding boundary conditions, Eq. (2.11). In this chapter we will show that it is possible to find, for all values of the parameters (in the thermodynamic limit), a closed general solution for the relaxation function, $\tilde{a}_0(z) = \mathcal{L}[a_0(t)]$, the Laplace transform of $a_0(t)$.

### 9.1 Continued fraction expansion and solution for the relaxation function $\tilde{a}_0(z)$

The Laplace transform of the recurrence relations II (RR2), Eq. (2.16), is given by Eq. (2.17), that we reproduce here, below, for convenience.

$$z\tilde{a}_0 + \Delta_1\tilde{a}_1(z) = 1\,, \qquad \nu = 0\,, \tag{9.1a}$$

$$z\tilde{a}_\nu(z) + \Delta_{\nu+1}\tilde{a}_{\nu+1}(z) = \tilde{a}_{\nu-1}(z)\ , \qquad 1 \leqslant \nu \leqslant d-1\,, \tag{9.1b}$$

where, $\tilde{a}_\nu(z) = \mathcal{L}[a_\nu(t)]$, is the Laplace transform of $a_\nu(t)$. This is an hierarchy of linear coupled equations for the $\tilde{a}_\nu(z)$, whose three-term nature immediately begets a continued fraction when one attempts to solve it. Suppose, for the moment that the hierarchy of equations is finite. This happens when the RR1 terminates at some $\nu$, say, $\nu = d-1$. Then the basis vectors are $\{f_0, f_1, \ldots, f_{\nu-1}\}$,

the dimension of the spanned space is $d$, and the last non-null recurrant is $\Delta_{\nu-1}$. The last equation of the hierarchy would be the $\nu = d-1$ equation

$$\begin{aligned} \tilde{a}_{d-2}(z) &= z\tilde{a}_{d-1}(z) + \Delta_d \tilde{a}_d(z) \ , \\ &= z\tilde{a}_{d-1}(z) \ , \end{aligned} \tag{9.2}$$

since $\Delta_d = 0$. Substituting $\tilde{a}_{d-1}(z) = \tilde{a}_{d-2}(z)/z$ into the $\nu = d-2$ equation

$$z\tilde{a}_{d-2}(z) + \Delta_{d-1}\tilde{a}_{d-1}(z) = \tilde{a}_{d-3}(z) \ , \tag{9.3}$$

one gets

$$\tilde{a}_{d-2}(z) = \frac{\tilde{a}_{d-3}(z)}{z + \Delta_{d-1}/z} \ , \tag{9.4}$$

thus eliminating $\tilde{a}_{d-1}(z)$ from the hierarchy. Repeating this procedure until one arrives to the $\nu = 0$ equation, all the $\tilde{a}_\nu(z)$ but, $\tilde{a}_0(z)$, will have been eliminated. Let's see an example. Suppose that $d = 4$. Suppressing the $z$-dependence for clarity,

$$\begin{aligned} z\tilde{a}_0 + \Delta_1\tilde{a}_1 &= 1 && \nu = 0 \\ z\tilde{a}_1 + \Delta_2\tilde{a}_2 &= \tilde{a}_0 && \nu = 1 \\ z\tilde{a}_2 + \Delta_3\tilde{a}_3 &= \tilde{a}_1 && \nu = 2 \\ z\tilde{a}_3 &= \tilde{a}_2 && \nu = 3 \end{aligned}$$

One starts substituting, from the last equation, up towards the $\nu = 0$ equation. Then $\tilde{a}_3 = \tilde{a}_2/z$, and substituting into the $\nu = 2$ equation

$$z\tilde{a}_2 + \Delta_3(\frac{\tilde{a}_2}{z}) = (z + \frac{\Delta_3}{z})\tilde{a}_2 = \tilde{a}_1 \ ,$$

$$\tilde{a}_2 = \frac{\tilde{a}_1}{z + \dfrac{\Delta_3}{z}} \ .$$

Substituting $\tilde{a}_2$ into the $\nu = 1$ equation, one gets

$$\tilde{a}_1 = \frac{\tilde{a}_0}{z + \dfrac{\Delta_2}{z + \dfrac{\Delta_3}{z}}} \ .$$

Putting this last result in the first, $\nu = 0$, equation all the $\tilde{a}_\nu$ have been eliminated, save for $\tilde{a}_0$. Then, for $d = 4$

$$\tilde{a}_0 = \cfrac{1}{z + \cfrac{\Delta_1}{z + \cfrac{\Delta_2}{z + \cfrac{\Delta_3}{z}}}} \, .$$

Similarly, for arbitrary, finite dimension $d$ we obtain the finite continued fraction

$$\tilde{a}_0(z) = \cfrac{1}{z + \cfrac{\Delta_1}{z + \cfrac{\Delta_2}{z + \cdots + \cfrac{\vdots}{z + \cfrac{\Delta_{d-2}}{z + \cfrac{\Delta_{d-1}}{z}}}}}} \, . \tag{9.5}$$

If, on the other hand $d \to \infty$, then the rhs of Eq. (9.5) is an *infinite* continued fraction.

The above is a totally general representation of the relaxation function of any Hermitian physical system in terms of the corresponding recurrants for the dynamical variable being considered.

Our aim in this chapter is to find a closed form, in the context of our model, the harmonic oscillator chain (HOC) with an impurity mass coupled to a fixed wall (ICFW), for the infinite case of the continued fraction above. One would expect the recurrants set to have a pattern or to be regular, in some sense, for this to be possible. Looking at Table 7.1 of Chapter 7 we see that the recurrants sequence in our model indeed is regular, except, for the *first* and the *last* terms of the sequence. The first term,

$$\Delta_1 = \lambda(\kappa + 1) \, , \tag{9.6a}$$

(where $\kappa \equiv k_0/k$, see Eq. (7.2)) is special due to the presence of parameter $\lambda \equiv m/m_0$, defined in Eq. (7.3). The last term,

$$\Delta_{2N-1} = \frac{\kappa}{(N-1)\kappa + 1} \, , \tag{9.6b}$$

where $N$ is the number of oscillators in the chain, is special simply because it deviates from the pattern in the sequence. The $\nu = 2N-1$ index of the last recurrant or Delta, indicates a dimension $d = 2N$ of the realized space $\mathcal{S}$ spanned by the $f_\nu$ (see Eqs. (2.6) or Eqs. (7.36), and Table 7.1).

In the thermodynamic limit, $N \to \infty$, we do not have to worry about the last recurrant, Eq. (9.6b), breaking the pattern of the sequence. The presence of the special $\Delta_1$ suggests considering instead of the full continued fraction, to consider instead, the continued fraction starting (and including) from the second partial quotient ($\equiv \Delta_2/z$), that is

$$\cfrac{1}{z+\cfrac{\Delta_2}{z+\cfrac{\Delta_3}{z+\cdots+\cfrac{\vdots}{z+\cfrac{\Delta_{d-2}}{z+\cfrac{\Delta_{d-1}}{z}}}}}} , \tag{9.7}$$

with $d = 2N$, and $N \to \infty$. This immediately suggests introducing the subspace $\mathcal{S}_1$, exactly analogous to $\mathcal{S}$, but spanned by the basis vectors $\{f_1, f_2, \ldots, f_{d-1}\}$ and with a recurrants set $\{\Delta_2, \Delta_3, \Delta_4, \ldots, \Delta_{d-1}\}$. In §2.5 it is shown that the corresponding basis functions $\{b_1(t), b_2(t), \ldots, b_{d-1}(t)\}$ can be defined, with an exactly analogous RR2 and, an exactly analogous boundary condition (BC) to the RR2 and the BC for the $a_\nu$. In §2.5 it is also shown that the $b_\nu$ are related to the $a_\nu$ through the convolution definition in the $z$-domain, Eq. (2.29),

$$\tilde{a}_\nu(z) = \tilde{b}_\nu(z)\tilde{a}_0(z) , \qquad 1 \leqslant \nu \leqslant d-1 . \tag{9.8}$$

Substituting the above definition for $\tilde{b}_1(z)$

$$\tilde{a}_1(z) = \tilde{b}_1(z)\tilde{a}_0(z) , \tag{9.9}$$

into the $\nu = 0$ RR2 for $\tilde{a}_0(z)$ one obtains

$$\tilde{a}_0(z) = \frac{1}{z + \Delta_1\tilde{b}_1(z)} . \tag{9.10}$$

Comparing the $\tilde{a}_0(z)$ continued fraction expansion, Eq. (9.5), with the above relationship, Eq. (9.10), one sees that the continued fraction (9.7) is in fact $\tilde{b}_1(z)$, that is

$$\tilde{b}_1(z) = \cfrac{1}{z + \cfrac{\Delta_2}{z + \cfrac{\Delta_3}{z + \cfrac{\vdots}{z + \cdots + \cfrac{\Delta_{d-2}}{z + \cfrac{\Delta_{d-1}}{z}}}}}} \,, \tag{9.11}$$

where $d = 2N$. We show in §10.6 that a closed solution, in the context of our model, can be found for the above continued fraction in the thermodynamic limit, $N \to \infty$. The solution is

$$\begin{aligned} \Delta_1 \, \tilde{b}_1(z) &= \lambda(\kappa+1)\frac{\Omega^2}{z} + \frac{\lambda}{2}\sqrt{z^2+4\Omega^2} - \frac{\lambda}{2}z - \lambda\frac{\Omega^2}{z} \,, \\ &= \kappa\lambda\frac{\Omega^2}{z} + \frac{\lambda}{2}\sqrt{z^2+4\Omega^2} - \frac{\lambda}{2}z \,. \end{aligned} \tag{9.12}$$

It is given by Eq. (10.32) in page 126 in §10.6. In the square root the first or principal branch has to be taken in order that $\tilde{b}_1(z)$ be positive when $z > 0$, as explained just before Eq. (10.32).

Substituting into Eq. (9.10), we obtain

$$\begin{aligned} \tilde{a}_0(z) &= \frac{1}{z + \Delta_1 \tilde{b}_1(z)} = \frac{1}{z + \kappa\lambda\frac{\Omega^2}{z} + \frac{\lambda}{2}\sqrt{z^2+4\Omega^2} - \frac{\lambda}{2}z} \,, \\ &= \frac{2z}{2z^2 + 2\kappa\lambda\Omega^2 + \lambda z\sqrt{z^2+4\Omega^2} - \lambda z^2} \,, \\ &= \frac{2z}{(2-\lambda)z^2 + 2\kappa\lambda\Omega^2 + \lambda z\sqrt{z^2+4\Omega^2}} \,. \end{aligned} \tag{9.13}$$

Introducing the parameter

$$\mu \equiv 2\Omega \,, \tag{9.14}$$

with $\Omega = \sqrt{k/m}$ already defined in Eq. (8.19) on page 80, the relaxation function becomes

$$\tilde{a}_0(z) = \frac{2z}{(2-\lambda)z^2 + \kappa\lambda\mu^2/2 + \lambda z\sqrt{z^2+\mu^2}} \,. \tag{9.15}$$

The parameters $\kappa \equiv k_0/k$, $\lambda \equiv m/m_0$ together with $k$, $k_0$, $m$ and $m_0$ were defined in Eqs. (7.2)-(7.3) on page 60. The boundary condition $a_0(t=0)=1$ imposes that when $|z| \to \infty$, then $\tilde{a}_0(z) = 1/z$. This condition is indeed satisfied when the first or principal sheet of $\sqrt{z^2+\mu^2}$ is chosen as explained above. This is the physical sheet of $\tilde{a}_0(z)$.

## 9.2 Singularities of $\tilde{a}_0(z)$

According to Eq. (9.5), $\tilde{a}_0(z)$ is expanded as a continued fraction. Before taking the thermodynamic limit, the continued fraction is finite, and consequently, it is the quotient of two polynomials. Thus the only singularities are poles.

After the thermodynamic limit, $N \to \infty$, is taken, $\tilde{a}_0(z)$ is given by Eq. (9.15). The main feature of the singularities is that some of the poles (at most two) remain isolated, while the others merge and give rise to a branch cut on the imaginary axis that is signaled by the presence of the square root $\sqrt{z^2+\mu^2}$ in Eq. (9.15). The branch-cut is the only non-isolated singularity of $\tilde{a}_0(z)$ in the thermodynamic limit, and we will show in §11.1 that the branch-cut corresponds to $[-\mathrm{i}\mu, +\mathrm{i}\mu]$.

To obtain the poles of $\tilde{a}_0(z)$ explicitly, we rewrite Eq. (9.15) as

$$\tilde{a}_0(z) = 2z \frac{(2-\lambda)z^2 + \kappa\lambda\mu^2/2 - \lambda z\sqrt{z^2+\mu^2}}{4(1-\lambda)z^4 - (\kappa\lambda+\lambda-2\kappa)\lambda\mu^2 z^2 + \kappa^2\lambda^2\mu^4/4}, \tag{9.16}$$

then we set the denominator equal to zero and solving for $z$ we find

$$z_{\substack{1\\2}} = \pm\sqrt{s_1}\ , \tag{9.17a}$$

for the *sometimes-physical* (SP) *poles*, and

$$z_{\substack{3\\4}} = \pm\sqrt{s_2}\ , \tag{9.17b}$$

for the *never-physical* (NP) *poles*. Here,

$$s_{\substack{1\\2}} = \frac{\lambda^2\mu^2}{8(1-\lambda)}[r \pm Q]\ , \tag{9.18a}$$

$$= \frac{\kappa^2\mu^2}{2}\frac{1}{r \mp Q}\ , \tag{9.18b}$$

where

$$r \equiv \kappa + 1 - \frac{2\kappa}{\lambda}\ , \tag{9.19a}$$

and

$$Q \equiv \sqrt{(\kappa+1)^2 - \frac{4\kappa}{\lambda}} = \sqrt{r^2 + \frac{4\kappa^2}{\lambda^2}(\lambda - 1)}\ . \tag{9.19b}$$

In the definition of $Q$ the principal (or the first) branch of the square root has to be taken.

By never-physical (NP), we mean the pair of poles that *never* are on the physical sheet, no matter what values of the parameters are chosen. Next, we will show that for certain values of the parameters the sometimes-physical (SP) poles, $z_1$ and $z_2$, are located in the physical sheet, i.e., the SP poles, for some values of the parameters can be located on the non-physical sheet.

## 9.3 $(\kappa, \lambda)$ PARAMETERS SPACE OF THE POLES OF $\tilde{a}_0(z)$

Figure 9.1 shows how the location of the SP poles depends upon the parameters $\lambda$ and $\kappa$.

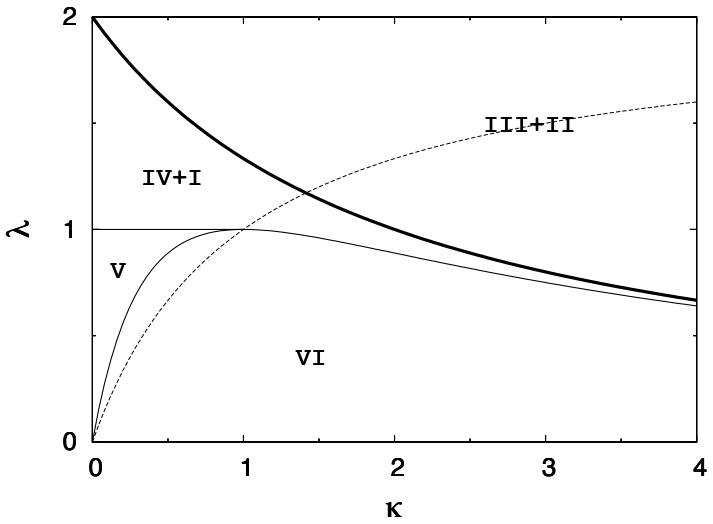



Figure 9.1: Features of the sometimes-physical (SP) poles of $\tilde{a}_0(z) = \frac{2z}{(2-\lambda)z^2+\kappa\lambda\mu^2/2+\lambda z\sqrt{z^2+\mu^2}}$ , in terms of the parameters $\kappa \equiv k_0/k$ and $\lambda \equiv m/m_0$.
Zone III+II: $z_1$ and $z_2$ symmetrically on the imaginary axis in the physical sheet.
Zone IV+I: $z_1$ and $z_2$ symmetrically on the imaginary axis in the non-physical sheet (NPS).
Zone VI: $z_1$ and $z_2$ are complex (conjugates) in the NPS.
Zone V: $z_1$ and $z_2$ symmetrically on the real axis in the NPS.

Figure 9.2 is the same but for the NP poles.

We are interested in getting a grasp of all the poles behavior in the $(\lambda, \kappa)$ space. From Eqs. (9.17) *and* Equation (9.18) it is seen that all poles depend on just two ($\lambda$ and $\kappa$ dependent) quantities $r(\lambda, \kappa)$ and $Q(\lambda, \kappa)$, through their difference and their sum, $r \mp Q$. Therefore, just their relative size

and sign; and nature, whether real or complex, can characterize a pole. One may think of the $(\lambda, \kappa)$ space in terms of the two regions determined by the $r = 0$ line and the two regions determined by $Q = 0$ line. The quantity $r$, given by Eq. (9.19a), is real (positive, negative or zero), and $Q$, given by Eq. (9.19b), is either real and positive or purely imaginary on the upper complex plane. From these definitions it is seen that the line $|r| = Q$, also relevant to the poles behavior, is just the $\lambda = 1$ line.

There are three lines that are common to both figures: the dashed line that corresponds to $r = 0$, the continuous line ($Q^2 = 0$) at the bottom that sets apart the Zone VI where $Q^2 < 0$, and the $|r| = Q$, i.e., $\lambda = 1$ line. In both figures

(a) Above (below) the dashed line $\lambda = \lambda_d$, $r$ is positive (negative).

$$\lambda_d = \frac{2\kappa}{\kappa + 1} \tag{9.20}$$

It is obtained setting $r = 0$ and solving for $\lambda$.

(b) Outside Zone VI and below $\lambda = 1$, $Q < |r|$

(c) Above $\lambda = 1$, $Q > |r|$.

(d) Inside Zone VI, $Q^2 < 0$ and consequently $z_1, z_2, z_3, z_4$ are all complex: they are located neither on the real nor on the imaginary axis.

(e) The line that bounds Zone VI is $\lambda = \lambda_0$ with

$$\lambda_0 = \frac{4\kappa}{(\kappa + 1)^2}. \tag{9.21}$$

It is obtained setting $Q^2 = 0$ and solving for $\lambda$.

From the above observations it can be seen, for example, that in Figure 9.1 outside Zones V and VI, $s_1$ is always negative and consequently $z_1$ and $z_2$ are located symmetrically in the imaginary axis. About $s_2$ it can be concluded that, in Figure 9.2, outside Zones VI and II+I, $0 < s_2$ and then $z_3$ and $z_4$ are located on the real axis also on a symmetrical manner.

The physical poles have to be complex conjugate pairs, located symmetrically *over* the imaginary axis. They can only enter or leave the physical sheet through the "point at infinity" or through

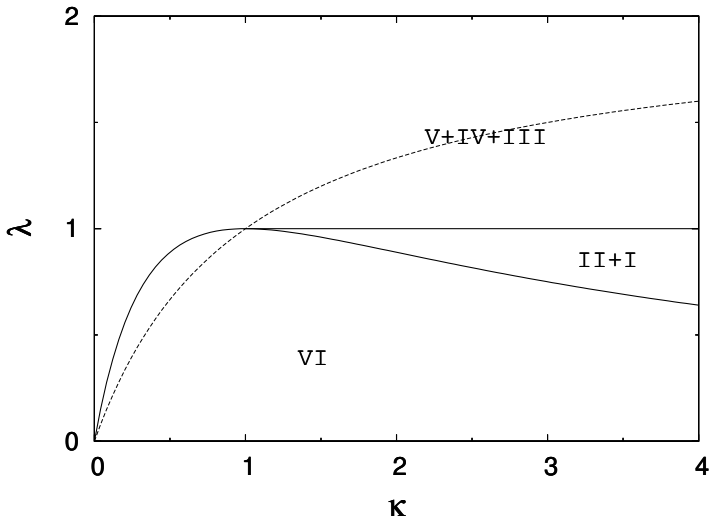



Figure 9.2: Features of the never-physical (NP) poles of $\tilde{a}_0(z) = \frac{2z}{(2-\lambda)z^2+\kappa\lambda\mu^2/2+\lambda z\sqrt{z^2+\mu^2}}$ in terms of the parameters $\kappa \equiv k_0/k$ and $\lambda \equiv m/m_0$.
Zone V+IV+III: $z_3$ and $z_4$ are located symmetrically on the real axis.
Zone II+I: $z_3$ and $z_4$ are located symmetrically on the imaginary axis.
Zone VI: $z_3$ and $z_4$ are complex.

the branch cut edges without ever leaving the imaginary axis in the physical sheet. In the latter case when a physical pole is at the branch cut edge, $z_p = \pm\,\mathrm{i}\,\mu$. Setting to zero the denominator of the original expression (9.15) for the relaxation function, putting $z^2 = -\mu^2$, and solving for $\lambda$, we obtain

$$\lambda_c = \frac{4}{2+\kappa}\ . \tag{9.22}$$

At $\lambda = \lambda_c$, as expected, $s_1$ (see Eq. (9.18)) attains its maximum algebraic value, $-\mu^2$ (the least modulus negative value), i.e., has a local extremum: Since a physical pole, e.g., $z_1$ (see Eq. (9.17a)) cannot move out of the imaginary axis, it can *only* turn back either along the same imaginary axis, staying in the physical sheet or, move out of the physical sheet through the corner of the cut, and turn back along the imaginary axis of the non-physical sheet.

Therefore, in Figure 9.1 that refers to the SP poles, along the (bold) line $\lambda = \lambda_c$, the physical poles $z_1$ and $z_2$ are both at the edges of the branch cut of $\tilde{a}_0(z)$, that is $z_{\frac{1}{2}} = \pm i\mu$. *Only* above this

line there are physical poles ($z_1$ and $z_2$), that is, poles on the physical sheet of of expression (9.15) for $\tilde{a}_0(z)$.

The four lines, $r = 0$, $Q = 0$, $|r| = Q$ (i.e. $\lambda = 1$), and $\lambda = \lambda_c$, mentioned above also allow one to understand, for example, how a pole would move among the physical and non-physical sheets if the parameters vary. We illustrate this in §9.4.

## 9.4 Poles trajectories in the two-sheets complex plane for simple variations of the parameters

In this section we will show some examples of pole trajectories in the two-sheets complex plane when one parameter is varied.

In Figure 9.3, the parameter $\kappa$ is held fixed and we show how the first SP pole, $z_1$ (see

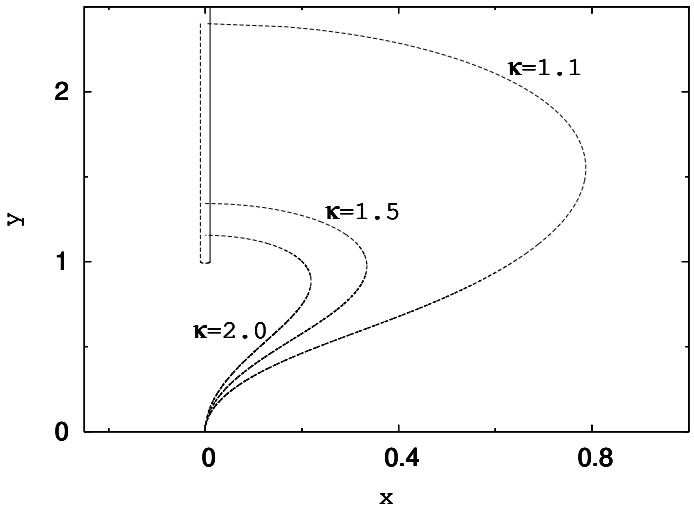



Figure 9.3: Path on the complex plane of the sometimes-physical (SP) pole $z_1$ of $\tilde{a}_0(z) = \frac{2z}{(2-\lambda)z^2+\kappa\lambda\mu^2/2+\lambda z\sqrt{z^2+\mu^2}}$ when $1 < \kappa$ is held constant ($\kappa = 1.1$, $\kappa = 1.5$, $\kappa = 2.0$) and $\lambda$ is varied from $\infty$ to 0. The continuous line corresponds to the trajectory of the pole on the physical-sheet (PS), that always is along the imaginary axis. The dashed line corresponds to the trajectory of the pole on the non-physical sheet (NPS).

Eq. (9.17a)) moves when $\lambda$ is varied from $\infty$ to zero. Above the line $\lambda = 1$, $Q$ is real and $Q > |r|$, so from Eq. (9.18) it is seen that $s_1$ is always negative. When $\lambda \to \infty$, it is seen from the definitions

of $Q$ and $r$, Eqs. (9.19), that $s_1 \propto (-\lambda)$ and $z_1 \propto \mathrm{i}\,\lambda^{1/2}$. In fact,

$$\tfrac{1}{\mu} z_1(\kappa,\lambda) = \frac{1}{2}\,\mathrm{i}\,\sqrt{\kappa+1}\,\sqrt{\lambda} + \frac{\mathrm{i}}{4(\kappa+1)^{3/2}\sqrt{\lambda}} + O\left[\frac{1}{\lambda}\right]^{3/2}, \qquad \lambda \to \infty\,. \tag{9.23}$$

Also, from the Figure 9.1 it is seen that $r - Q$ is always negative above the $\lambda = \lambda_c$ line, then from Eq. (9.17a), $z_1$ is always purely imaginary and thus, at $\lambda = \infty$, $z_1$ starts at $\infty$ in the upper imaginary axis and moves down as $\lambda$ is diminished, always along the imaginary axis, until $\lambda$ reaches the bold line $\lambda = \lambda_c$. At this point, $z_1$ is at the edge $\mathrm{i}\,\mu$ of the branch-cut.

This part of the trajectory of the pole, $\lambda : (\infty, \lambda_c]$, corresponds to the Zone III+II in the $(\kappa, \lambda)$ space of Figure 9.1, and takes place in the physical sheet. It is plotted in Fig. 9.3 with a continuous line offset a little bit to the right of the imaginary axis so it is possible to distinguish it from the next part of the plot that also proceeds along the imaginary axis but on the non-physical sheet, as we shall see below.

The trajectories of this SP (sometimes-physical) pole $z_1$ in the non-physical sheet are plotted with dashed lines. Thus at $\lambda = \lambda_c$, $z_1$ leaves the physical sheet through the top edge $+\mathrm{i}\,\mu$ of the branch cut. At this point also, $s_1$ reaches its algebraic maximum, $-\mu^2$ (its least modulus negative value).

The next part of the plot $\lambda : [\lambda_c, \lambda_0]$ in Zone IV+I of Fig. 9.1, proceeds along the imaginary axis of Fig. 9.3 again, but on the non-physical sheet, this time going up until $\lambda = \lambda_0$, at which point $Q = 0$. This corresponds to the edge of the of the Zone VI of Fig. 9.1. The value $\lambda_0$ is $\kappa$-dependent, it is given by Eq. (9.21). In Fig. 9.3 we show this point for three values of $\kappa$: $\kappa = 1.1$, $\kappa = 1.5$ and $\kappa = 2.0$. It is where the corresponding trajectory branches out to the right of the imaginary axis.

Beyond this point in the last part of the trajectory, $\lambda : [\lambda_0(\kappa), 0]$ is inside Zone VI of Fig. 9.1, where $Q^2 < 0$ and thus $s_1$ is complex and also the SP pole $z_1$ is complex, therefore moving away from the imaginary axis. This occurs first (lower in the imaginary axis) for the $\kappa = 2.0$ trajectory and last for the $\kappa = 1.1$ trajectory, as shown in Fig. 9.3. From Eq. (9.17a), we find

$$\tfrac{1}{\mu} z_1(\kappa,\lambda) = \frac{1}{2}\,\mathrm{i}\,\sqrt{\kappa}\,\sqrt{\lambda} + \frac{\lambda}{4} + O[\lambda]^{3/2}, \qquad \lambda \to 0\,. \tag{9.24}$$

Thus, the three trajectories end in the origin of Fig. 9.3, when $\lambda$ reaches the value $\lambda = 0$ at the bottom Fig. 9.1 in Zone VI of $(\kappa, \lambda)$ space at the corresponding abscissa $\kappa = 1.1$, $\kappa = 1.5$ or $\kappa = 2.0$.

The next figure, Figure 9.4 is the same as Fig. 9.3, except that the fixed $\kappa$ values along which we plot the path of the SP pole $z_1$ for $\lambda : (\infty, 0]$ are now chosen to be less than 1, that is $\kappa < 1$. The parts of the plot are as follows.

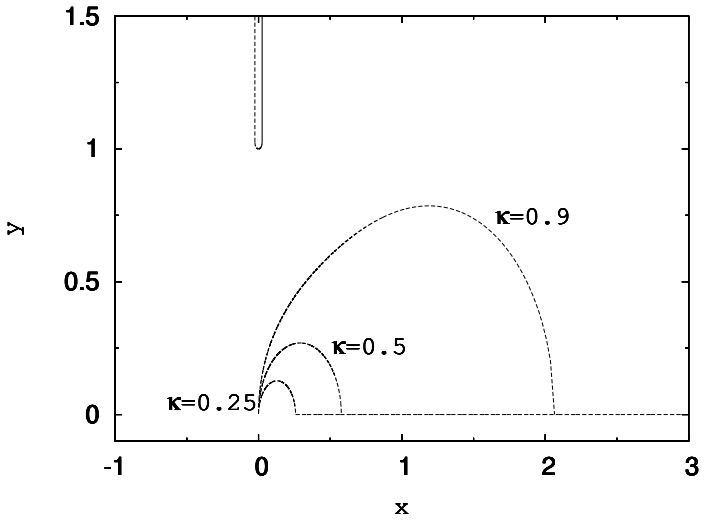



Figure 9.4: Path on the complex plane of the sometimes-physical (SP) pole $z_1$ of $\tilde{a}_0(z) = \frac{2z}{(2-\lambda)z^2+\kappa\lambda\mu^2/2+\lambda z\sqrt{z^2+\mu^2}}$, when $\kappa < 1$ is held constant ($\kappa = 0.9$, $\kappa = 0.5$, $\kappa = 0.25$) and $\lambda$ is varied from $\infty$ to 0. The full line corresponds to the trajectory of the pole on the physical sheet (PS). As expected the pole on the PS is always on the imaginary axis. The dashed line corresponds to the trajectory of the pole on the non-physical sheet (NPS).

$\lambda : (\infty, \lambda_c]$ is in the Zone III+II of $(\kappa, \lambda)$ space of Fig. 9.1. In this part of the plot the SP pole $z_1$ is on the physical sheet, i.e., is a physical pole, and from Eq. (9.23), it is seen that it moves from $\infty$ in the upper imaginary axis of down to the $\mathrm{i}\,\mu$ edge of the cut. In Fig. 9.4 this part is plotted with a solid line to indicate it is on the physical sheet (PS).

$\lambda : [\lambda_c, 1^+)$ is in the Zone IV+I of $(\kappa, \lambda)$ space of Fig. 9.1. In this leg of the plot the SP pole $z_1$ is in the non-physical sheet and moves up the imaginary axis of Fig. 9.4 back to $\infty$ as $\lambda \to 1^+$. This is plotted with a dashed line to indicate the non-physical sheet. At $\lambda = 1$, $r - Q = 0$ (see Eq. (9.18)),then changes sign, thus At $\lambda = 1^-$, $z_1$ jumps "at $\infty$", from the upper imaginary axis to the rhs real axis.

$\lambda : (1^-, \lambda_0(\kappa))$ is in the Zone V of $(\kappa, \lambda)$ space of Fig. 9.1. In this part of the plot, the SP $z_1$ pole moves from $\infty$ in the real axis of Fig. 9.4 rhs to the left towards the origin until the point where $\lambda = \lambda_0(\kappa)$ where $Q = 0$ at the edge of Zone VI in Fig. 9.1. Beyond this point $Q^2 < 0$, $s_1$ is

complex and thus $z_1$ leaves the real axis. This is shown in Fig. 9.4 for three values of $\kappa$, $\kappa = 0.9$, $\kappa = 0.5$ and $\kappa = 0.25$

$\lambda : [\lambda_0(\kappa), 0]$ is in the Zone VI of $(\kappa, \lambda)$ space of Fig. 9.1 where all the poles are complex. In particular $z_1$ moves in a curved, inflexion-less trajectory in the first quadrant of the complex plane in Fig. 9.4. Three different trajectories, corresponding to the three fixed values of $\kappa$ mentioned above, are shown. From Eq. (9.24) all the trajectories end in the origin of the complex plane at the $\lambda = 0$ value. All are plotted with dashed lines to indicate they take place in the non-physical sheet.

The next two figures also show the path of the SP pole $z_1$ but this time the parameter $\lambda$ is held fixed and $\kappa$ is varied from $\infty$ to zero. From Eq. (9.17a) we find,

$$\tfrac{1}{\mu} z_1(\kappa, \lambda) = \frac{1}{2}\,\mathrm{i}\,\sqrt{\lambda}\,\sqrt{\kappa} + \frac{1}{4}\,\mathrm{i}\,\sqrt{\lambda}\,\sqrt{\frac{1}{\kappa}} + O\left[\frac{1}{\kappa}\right]^{3/2}, \qquad \kappa \to \infty\,. \tag{9.25}$$

Therefore, $z_1$ comes down from infinity in the upper imaginary axis in both figures.

–In Figure 9.5 we show, for fixed $\lambda > 1$ values: $\lambda = 1.2$, $\lambda = 1.4$ and $\lambda = 1.8$, the corresponding trajectories of $z_1$ in the complex plane.

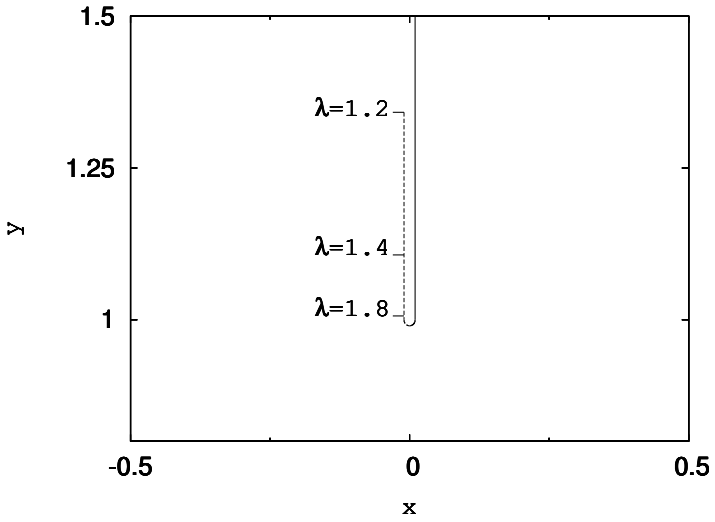



Figure 9.5: Path on the complex plane of the sometimes-physical (SP) pole $z_1$ of $\tilde{a}_0(z) = \frac{2z}{(2-\lambda)z^2+\kappa\lambda\mu^2/2+\lambda z\sqrt{z^2+\mu^2}}$, when $\lambda > 1$ is held constant ($\lambda = 1.2$, $\lambda = 1.4$, $\lambda = 1.8$) and $\kappa$ is varied from $\infty$ to $0$. The continuous line corresponds to the trajectory of $z_1$ in physical-sheet part, always along the imaginary axis. The dashed line is the trajectory of $z_1$ in the non-physical sheet (NPS).

In parameter space $(\lambda, \kappa)$, this corresponds to three horizontal lines above the $\lambda = 1$ line of Fig. 9.1. The three lines only intersect the $\lambda = \lambda_c$ bold line where a physical pole leaves the physical

sheet (Zone III+II), and moves back (reverses its trajectory) along the imaginary axis, in the $y > 0$ direction. From Eq. (9.17a) we find, when $\kappa \to 0$, with $\lambda > 1$

$$\tfrac{1}{\mu} z_1(\kappa, \lambda) = \frac{\mathrm{i}\,\lambda}{2\sqrt{\lambda - 1}} + \frac{\mathrm{i}(\lambda - 2)\kappa}{4\sqrt{\lambda - 1}} + O[\kappa]^2\,, \qquad \kappa \to 0\,,\ \lambda > 1\,. \tag{9.26}$$

Consequently the trajectory goes up to a $\lambda$-dependent final height at $\kappa = 0$, but this time in non-physical sheet, so this part of the trajectory is plotted with a dashed line in Fig. 9.5. The three trajectories coincide up to the $\kappa = 0$ point with $\lambda = 1.8$. Also, if the fixed $\lambda$ value line is above the $\lambda = 1$ line of Fig. 9.1, i.e., does not intersect the $\lambda = \lambda_c$ bold line, the whole trajectory $\kappa : (\infty, 0]$ of $z_1$ is in the imaginary axis of the physical sheet of Fig. 9.5.

–In Figure 9.6 we show the path of the first SP pole, $z_1$, also for fixed values of $\lambda$, with $\kappa : (\infty, 0]$. This figure is similar to Figure 9.5, except that fixed $\lambda$ values are now chosen to be less than 1, that is $\lambda < 1$. The three values we chose, $\lambda = 0.95$, $\lambda = 0.8$, $\lambda = 0.5$, are represented in the $(\lambda, \kappa)$

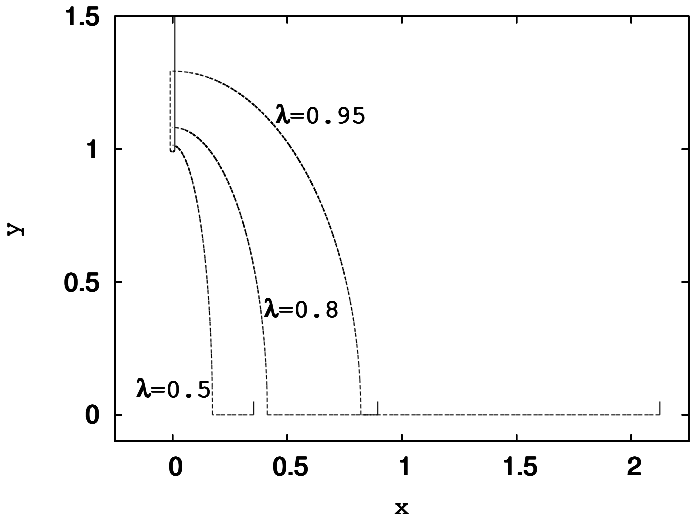



Figure 9.6: Path on the complex plane of the sometimes-physical (SP) pole $z_1$ of $\tilde{a}_0(z) = \frac{2z}{(2-\lambda)z^2 + \kappa\lambda\mu^2/2 + \lambda z\sqrt{z^2+\mu^2}}$, when $\lambda < 1$ is held constant ($\lambda = 0.95$, $\lambda = 0.8$, $\lambda = 0.5$) and $\kappa$ is varied from $\infty$ to 0. The solid line is the trajectory of of $z_1$ in the physical sheet, always on the imaginary axis. The dashed line is the trajectory of $z_1$ in the non-physical sheet (NPS).

space of Fig. 9.1 by three horizontal lines, that, like in the case of Fig. 9.5, come from $\infty$ in the rhs of the horizontal axis, inside the physical Zone III+II, and then intersect the $\lambda = \lambda_c$ and enter the non-physical Zone IV+I, just as $z_1$ leaves the physical sheet through the edge of the cut and begins to move up the imaginary axis of the non-physical sheet (dashed line).

Fig. 9.5 and Fig. 9.6 coincide till now. But in the former $z_1$ does not leave the imaginary axis since the $\lambda =$ constant lines remain in the Zone IV+I, where $s_1$ keeps being negative and thus $z_1$ is purely imaginary (see Eqs. (9.17a) and (9.18)). In the latter, the three lines $\lambda =$ constant that represent the trajectories of $z_1$ the $(\lambda, \kappa)$ space go into Zone VI in Fig. 9.1, where $Q^2$ is negative, $s_1$ is complex and thus, $z_1$ is complex too (see Eqs. (9.17a) and (9.18)). In Zone VI the trajectories of $z_1$ are the curved down dashed lines in the first quadrant of the complex plane of Fig. (9.6) outside the imaginary and the real axes in the non-physical sheet.

As the three $\lambda =$ constant lines leave Zone VI, $Q^2$ and $Q$ are both real and positive again, but this time $r - Q$ is positive, instead of negative, since $Q < |r|$ when $\lambda < 1$, e.g., in Zone V. Thus $z_1$ is real and positive. From Eq. (9.17a), we find that when $\kappa \to 0$ with $\lambda < 1$

$$\tfrac{1}{\mu} z_1(\kappa, \lambda) = \frac{\lambda}{2\sqrt{1-\lambda}} + \frac{(\lambda-2)\kappa}{4\sqrt{1-\lambda}} + O[\kappa]^2 \,, \qquad \kappa \to 0 \,,\ \lambda < 1 \,. \tag{9.27}$$

Therefore, the $\lambda = 0.95$ trajectory is the one that reaches farthest in the real axe of the non-physical sheet of Fig. (9.6), as indicated with a small vertical line at $x \approx 2.1$ . The $\lambda = 0.5$ trajectory is the one that reaches less to the right on the real axe, up to $x \approx 0.4$ .

As our last example we show in Figure 9.7 the trajectory of the never-physical pole $z_3$ of the

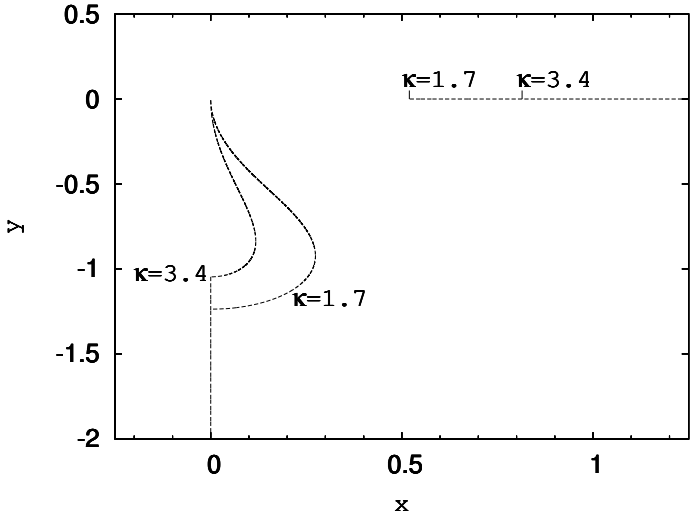



Figure 9.7: Path on the complex plane of the never-physical (NP) pole $z_3$ of $\tilde{a}_0(z) = \frac{2z}{(2-\lambda)z^2+\kappa\lambda\mu^2/2+\lambda z\sqrt{z^2+\mu^2}}$ when $\kappa > 1$ is held constant ($\kappa = 1.7$, $\kappa = 3.4$) and $\lambda$ is varied from $\infty$ to 0. The whole trajectory is plotted with dashed lines to indicate that it takes place only in the non-physical sheet. At $\lambda = \infty$ the pole starts on the real axis at $z_3(\kappa, \infty) = \mu \frac{\kappa}{2\sqrt{\kappa+1}}$ .

relaxation function $\tilde{a}_0(z)$ (see Eq. (9.15)), when $\kappa > 1$ is held constant ($\kappa = 1.7$, $\kappa = 3.4$) while $\lambda$ is varied from $\infty$ to zero, i.e., $\lambda : (\infty, 0]$. In the $(\kappa, \lambda)$ space of Figure 9.2, this corresponds to a vertical line that comes down from $\infty$ in Zone V+IV+III. The "never-physical" qualifier refers to the fact that $z_3$ (see Eq. (9.17b)) is never on the physical sheet of $\tilde{a}_0(z)$.

From Eq. (9.17b) we find that when $\lambda \to \infty$,

$$\tfrac{1}{\mu} z_3(\kappa, \lambda) = \frac{\kappa}{2\sqrt{\kappa+1}} + \frac{\kappa^2(2+\kappa)}{4(\kappa+1)^{5/2}\lambda} + O\left[\frac{1}{\lambda}\right]^2 . \tag{9.28}$$

Thus, the trajectory of $z_3(\kappa, \lambda)$ starts on the real axis of Fig. 9.7 at $z_3(\kappa, \infty) = \mu \frac{\kappa}{2\sqrt{\kappa+1}}$, and moves out towards $\infty$ along rhs of the aforementioned real axis. The first part, $\lambda : (\infty, 1^+]$, corresponds to Zone V+IV+III of the $(\kappa, \lambda)$ space of Fig. 9.2 of §9.3.

At $\lambda = 1$, it is seen from Eqs. (9.17b) and (9.18), that $z_3$ jumps "at infinity" from the positive real axis to the negative imaginary axis. The next part, $\lambda : [1^-, \lambda_0]$ proceeds up the imaginary axis till the $\lambda = \lambda_0$ point where $Q$ becomes imaginary, $s_2$ and $z_3$ become complex, thus $z_3$ leaves negative imaginary axis to follow the curved trajectories of Fig. 9.7.

From Eq. (9.17b) we find that when $\lambda \to 0$,

$$\tfrac{1}{\mu} z_3(\kappa, \lambda) = \frac{\lambda}{4} - \frac{1}{2}\,\mathrm{i}\,\sqrt{\kappa}\,\sqrt{\lambda} + O[\lambda]^{3/2} . \tag{9.29}$$

Therefore, at $\lambda = 0$, both trajectories end up in the origin of Fig. 9.7.

## 9.5 Collective modes (CMs), and why exponentially decaying CMs are not possible

It is possible to observe, under suitable conditions [see Appendix D], dynamic evolutions of physical variables with constant amplitude *proportional* to the applied or driving field. It is found that they have fixed denumerable frequencies and are known as collective modes.

In Chapter 6 we reviewed the dynamic equivalence described by [Lee, Florencio & Hong 1989] between an harmonic oscillator chain and a two dimensional electron gas. The collective modes are discussed in p. 58 and in Figure 6.1 which is a reproduction of Fig.1 of [Lee, Florencio & Hong 1989].

A first approximation to this physical situation is to assume that the applied is sufficiently weak as to permit the application of linear response theory, whose essence is, precisely, to keep everything in the calculation only up to linear terms in the applied field.

One finds that the response of the system is proportional to the applied field, which is the same as saying that the "proportionality entity" that accompanies the applied field is independent[1] of the applied field. The "proportionality entity" is known as the response function. It is the minus time derivative of the relaxation function, only depends on the unperturbed Hamiltonian and thus, it is an intrinsic property of the system.

The distinctive feature of the collective modes in relation to the relaxation function $a_0(t)$ is that their contribution to $a_0(t)$ does not decay with time. They are termed modes because each one of them has a characteristic frequency $\omega_p$.

The Laplace transform is particularly convenient for initial value, time evolution problems such as obtaining the autocorrelation function $a_0(t)$ and, the Recurrence Relations Method furnishes $\tilde{a}_0(z)$ directly in terms of the recurrants $\{\Delta_\nu\}$. Thus, to check for collective modes in $a_0(t)$ we just have to look for isolated singularities $z_p$, i.e. poles in $\tilde{a}_0(z)$. Each pole $z_p$ yields the corresponding characteristic frequency $\omega_p$ of its associated collective mode.

For our model the harmonic oscillator chain (HOC) with an impurity coupled to a fixed wall (ICFW), we described in §9.2 the effect of the thermodynamic limit on the nature of the singularities and we also obtained the explicit formulas for the poles of $\tilde{a}_0(z)$.

These formulas give, not only the physical poles that must come in complex conjugate pairs on the imaginary axis for their contributions to $a_0(t)$ to be real and not time decaying but, also give non-physical poles depending on the values of the parameters. Recall that the physical sheet of $\tilde{a}_0(z)$ is fixed by the boundary condition $a_0(t=0)=1$, that requires $\tilde{a}_0(z\to\infty)=1/z$. It also may be fixed by noting that $\tilde{b}_1(z)$ has to be positive when $z>0$. See the full discussion in p. 92 of §9.1.

Once the thermodynamic limit, $N\to\infty$ was taken, in §9.3 we subdivided the $(\kappa,\lambda)$ parameter space in regions according to presence or not of poles, their nature, and whether or not on the physical sheet of $\tilde{a}_0(z)$.

To get a grasp of the poles dependence on the parameters, in §9.4 we plotted some trajectories of the poles, in the two sheet complex plane, for simple variations of the parameters $\kappa$ and $\lambda$.

[1] Otherwise the response would not be linear.

One still may ask, stepping aside from the factual point of view, if it is possible to have poles outside the imaginary axis, i.e., complex poles. These would correspond to "exponentially time decaying collective modes". The question also has practical relevance since exponential functions are frequently used to represent decaying processes.

M. Howard Lee has shown using the RRM that a long-time exponential decay is not [Lee 1983] allowed. In fact, there are stringent restrictions [Lee 2001] on the functional forms of $a_0(t)$. The gist of the argument (see §2.4, pp. 8–9) is that if $a_0(t) \propto \mathrm{e}^{-\gamma t}$, the other $a_\nu(t)$ are known through the RR2 (2.16), and then $A(t) = \sum_\nu a_\nu(t) f_\nu$ cannot satisfy the constancy of the norm, $(A(t), A(t)) = (A, A)$, that holds for Hermitian systems.

Indeed, the part of the trajectory of the sometimes-physical (SP) $z_1$ pole that is on the physical sheet is always along the imaginary axis. This is indicated by the solid line in the first four figures of §9.4 that depict the path on the two branched complex plane of the SP $z_1$ pole for some simple variations of the parameters.

In Figure 9.8 we plot the imaginary part of the sometimes physical (SP) pole $z_1$ as a function of the parameters $\kappa$ and $\lambda$.

The $\mathrm{Im}(z_1)/\mu$ is depicted only where $z_1$ is in the physical sheet of $\tilde{a}_0(z)$. This region corresponds to Zone III+II of $(\kappa, \lambda)$ space in Figure 9.1 of §9.3p. 94.

Despite the complicated analytical form of Eq. (9.17a), the figure shows that the $z_1$ pole location (in the physical sheet) on the upper imaginary axis is a smooth, monotonically increasing function of both the $\kappa$ and $\lambda$ parameters. The behavior of the complex conjugate $z_2$ pole companion of $z_1$ is similar (smooth monotonically decreasing function of both the $\kappa$ and $\lambda$ parameters) but on the negative imaginary axis.

This regular behavior of $z_1$ and $z_2$ brings to mind their noted absence in particular situations. Neither of the four exact solutions for $a_0(t)$ (in terms of one or two Bessel functions) that we reviewed in Chapter 8, the previously known

- $\kappa = 0$, $\lambda = 2$: $\mathrm{J}_0(\mu t)$,
- $\kappa = 1$, $\lambda = 1$: $\mathrm{J}_0(\mu t) - \mathrm{J}_4(\mu t)$,
- $\kappa = 0$, $\lambda = 1$: $\mathrm{J}_1(\mu t)/t$;

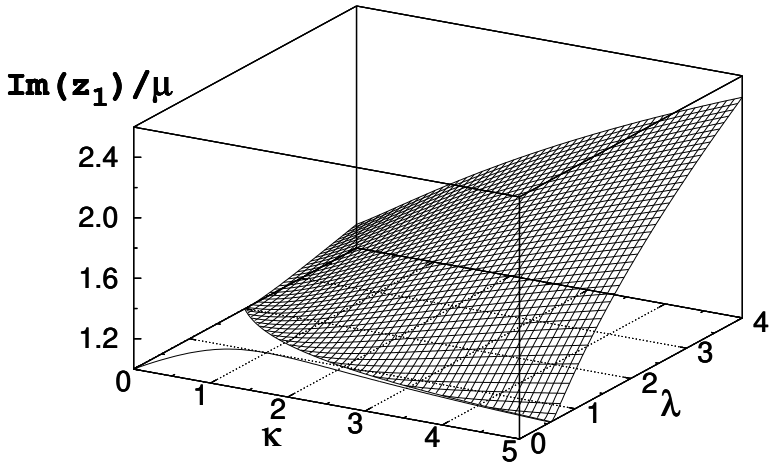



Figure 9.8: Plot of the imaginary part of the sometimes-physical (SP) $z_1$ pole versus $\kappa$ and $\lambda$. The "floor" of the plot corresponds to the plane $z = 1$. The surface is depicted only in the region of $(\kappa, \lambda)$ space where the $z_1$ pole is in the physical sheet of $\tilde{a}_0(z)$. This zone corresponds to Zone III+II of Fig. 9.1 in §9.3p. 94. In this region the real part of $z_1$ is zero. The solid line at which the surface ends on the $z = 1$ plane corresponds to the bold line in Fig. 9.1. It is the $\lambda = \lambda_c$ equation (9.22) of §9.3p. 96. Along this line, $z_1$ is at the upper edge $z = \mathrm{i}\,\mu$, of the branch-cut. The other solid line that starts at the origin corresponds to the $\lambda = \lambda_0$ line of Fig. 9.1 (see Eq. (9.21) of §9.3p. 95). Between $\lambda = 0$ and $\lambda = \lambda_0$ corresponds to Zone VI of Fig. 9.1 where $z_1$ would be complex and in the non-physical sheet. In the z-axis label, $\mu = 2\Omega$ with $\Omega = (k/m)^{1/2}$.

or the new one,

- $\kappa = 2$, $\lambda = 1$: $\mathrm{J}_0(\mu t) - \mathrm{J}_2(\mu t)$

has collective modes, since evidently, each of their Laplace transforms does not have isolated singularities in the complex plane. Thus, our general $\tilde{a}_0(z)$ solution has the feature that

> At *every* (finite) point in the $(\kappa, \lambda)$ space, $\tilde{a}_0(z)$ has <u>*two*</u> pairs of poles (at most one pair can be on the physical sheet[2], in this case they are on the imaginary[3] axis and are

[2]We term them the sometimes-physical (SP) poles. The other pair are the never-physical (NP) poles. The four poles are given in Eq. (9.17).

[3]See p. 105.

complex conjugates); *except* at some special lines or curves, or points where the poles either —move to the edges of the branch-cut or, —move out to infinity.

For example, at the line $\lambda = 2$, we find from Eq. (9.17) that the sometimes-physical (SP) poles $z_{\substack{1\\2}}(\kappa, \lambda)$ are given by

$$z_{\substack{1\\2}}(\kappa, \lambda = 2) = \pm \frac{\mathrm{i}}{\sqrt{2}} \mu \sqrt{1 + \sqrt{1 + \kappa^2}} \ , \tag{9.30}$$

and the never-physical (NP) poles $z_{\substack{3\\4}}(\kappa, \lambda)$ by

$$z_{\substack{3\\4}}(\kappa, \lambda = 2) = \pm \frac{1}{\sqrt{2}} \mu \sqrt{-1 + \sqrt{1 + \kappa^2}} \ . \tag{9.31}$$

If the parameter $\kappa$ moves over its allowed range, $0 \leqslant \kappa < \infty$, the SP pole $z_1$ in this case moves monotonically from the branch-cut edge out to infinity along the positive imaginary axis in the physical sheet. Its complex conjugate, $z_2$, moves correspondingly over the negative imaginary axis. The NP pole $z_3$ moves from the origin out to infinity along the real axis of the non-physical sheet. Its companion, $z_4$, moves similarly along the negative real axis.

Thus, looking for the *particular* combinations of parameters for which our general $\tilde{a}_0(z)$ is without *finite* poles may yield[4] simple exact solutions similar to the four already found. Aside from these particular combinations of parameters, the *four poles presence everywhere and their splitting into two distinct classes, the never-physical (NP) poles and the sometimes-physical (SP) poles*, suggests it should be possible to factor the denominator of the general solution (Eq. (9.15)) for $\tilde{a}_0(z)$ into two corresponding terms, —one that can never have singularities in the physical sheet of the complex plane, —other whose singularities can sometimes be on the physical sheet, for certain (see Fig. 9.1) sets of values of the parameters $\kappa$ and $\lambda$.

We will now obtain the

## 9.6 General solution for $\tilde{a}_0(z)$ with the denominator factored into physical and non-physical singularities related terms

Our general solution for $\tilde{a}_0(z)$ is given in Eq. (9.15) and reproduced below for convenience

$$\tilde{a}_0(z) = \frac{2z}{(2-\lambda)z^2 + \kappa\lambda\mu^2/2 + \lambda z\sqrt{z^2 + \mu^2}} \ . \tag{9.32}$$

[4]This possibility will be further explored in later work.

To find its poles, Eqs. (9.17), we removed the square root by multiplying by an appropriate "rationalizing" factor the denominator and the numerator, see Eq. (9.16), and then obtained the roots of the resulting polynomial in the denominator. Each root was then tested against the original denominator to ascertain whether it was on the physical sheet of the complex plane or not —a rather lengthy process: It had to be done for the full range of allowed values of the parameters $\kappa$ and $\lambda$. The results were presented in Figure 9.1 and Figure 9.2 of §9.3.

A much shorter —and enlightening— route to these results is available by directly factoring the original denominator in Eq. (9.32). This is possible *due to the z factor that multiplies the square root*.

Indeed, the coefficients $a$, $c$ and $g$ can be determined by equating similar order terms in

$$(az + g\sqrt{z^2+\mu^2})(cz + g\sqrt{z^2+\mu^2}) = (2-\lambda)z^2 + \kappa\lambda\mu^2/2 + \lambda z\sqrt{z^2+\mu^2}\,, \tag{9.33}$$

so that the above expression holds as an identity. Using this result we find

$$\tilde{a}_0(z) = \frac{(4\kappa/\lambda)z}{\left[(1-Q)z + \kappa\sqrt{z^2+\mu^2}\right]\left[(1+Q)z + \kappa\sqrt{z^2+\mu^2}\right]}\,, \tag{9.34}$$

where

$$Q \equiv \sqrt{(1+\kappa)^2 - 4\kappa/\lambda}\,, \tag{9.35}$$

is the same $Q$ already defined in Eq. (9.19b). In the definition of $Q$ the first or principal branch of the square root has to be taken. In fact, *in every square root* written in this work, the *first or principal branch is to be taken*.

The first factor, with the $(1-Q)$ coefficient yields the sometimes-physical (SP) poles and the second factor yields the never-physical poles. Note that $Q$ is always either —real, and greater or equal zero or —pure imaginary, with positive imaginary part. Then the results presented in Fig. 9.1 and Fig. 9.2 follow consequently.

For instance, if $|z| \gg \mu$, $\Longrightarrow$ $\sqrt{z^2+\mu^2} \sim z$. If additionally $z$ is not on the imaginary axis, neither the first nor the second factor can vanish if we stay in the physical branch, i.e. the first or principal branch of the $z$-dependent square root but, —on the second (non-physical) branch, *either* factor can vanish.

Now, suppose we have a pole $(1-Q)z_p + \kappa\sqrt{z_p^2+\mu^2} = 0$ and that it is outside the cut on the imaginary axis, $z_p = \pm\,\mathrm{i}\alpha\mu = \mathrm{e}^{\pm\,\mathrm{i}\,\pi/2}\alpha\mu$, with $1 < \alpha < \infty$. Then

$$\sqrt{z_p^2+\mu^2} = \sqrt{z_p - \mathrm{i}\mu}\sqrt{z_p + \mathrm{i}\mu} = \sqrt{\mathrm{e}^{\pm\,\mathrm{i}\,\pi/2}(\alpha \mp 1)\mu}\sqrt{\mathrm{e}^{\pm\,\mathrm{i}\,\pi/2}(\alpha \pm 1)\mu} =$$
$$\mathrm{e}^{\pm\,\mathrm{i}\,\pi/4}\sqrt{\mu}|\alpha \mp 1|^{1/2}\,\mathrm{e}^{\pm\,\mathrm{i}\,\pi/4}\sqrt{\mu}|\alpha \pm 1|^{1/2} = \pm\,\mathrm{i}\mu\sqrt{\alpha^2-1}\,. \tag{9.36}$$

Thus,

$$(1-Q)(\pm\,\mathrm{i}\alpha\mu) \pm \mathrm{i}\kappa\mu\sqrt{\alpha^2-1} = 0\,,$$
$$\alpha - Q\alpha + \kappa\sqrt{\alpha^2-1} = 0\,,$$

and

$$Q = 1 + \kappa\sqrt{1-1/\alpha^2}\,. \tag{9.37}$$

Therefore,

$$1 < \alpha < \infty\,, \Longrightarrow 1 < Q < 1+\kappa\,, \tag{9.38}$$

$\Longrightarrow$ Pole $z_p = z_{\frac{1}{2}} = \pm\,\mathrm{i}\alpha\mu$ in the imaginary axis of the physical sheet due to the first factor. Also, for the second factor to have a pole on the imaginary axis of the physical sheet, we would need

$$1 < \alpha < \infty\,, \Longrightarrow 1 < -Q < 1+\kappa\,, \tag{9.39}$$

which is clearly not possible.

The minimum allowed value of $Q$ in the inequality (9.38) corresponds to the sometimes-physical poles $z_1$ and $z_2$ being at the edges of the branch cut. Setting $Q$ equal to this value, i.e., $Q = 1$ and solving for $\lambda$

$$(\kappa+1)^2 - \frac{4\kappa}{\lambda} = 1\,,$$
$$\kappa^2 + 2\kappa = \frac{4\kappa}{\lambda}\,, \tag{9.40}$$

we obtain ($\kappa \neq 0$)

$$\lambda = \frac{4}{\kappa+2}\,. \tag{9.41}$$

This value is depicted, as a function of $\kappa$, by the bold line in Fig. 9.1 on page 94. Above this line: Zone III+II in Fig. 9.1, the pair of sometimes-physical poles $z_1$ and $z_2$ are on the imaginary axis

of the physical sheet. The function given by Eq. (9.41) had already being obtained by a different approach as $\lambda_c(\kappa)$ in Eq. (9.22) of §9.3. Similarly, all other results and features presented in Fig. 9.1 and Fig. 9.2 of §9.3, follow suite.

Another useful result can be obtained from the general solution for $\tilde{a}_0(z)$ with its denominator factored into physical and non-physical singularities terms given in Eq. (9.34). In Chapter 11 we calculate the inverse Laplace transform of the general solution $\tilde{a}_0(z)$ to obtain the autocorrelation function $a_0(t)$. There we will need to take apart $\tilde{a}_0(z)$ in simple fractions. Using Eq. (9.34) to write

$$\begin{aligned}\tilde{a}_0(z) &= \frac{(4\kappa/\lambda)z}{\left[(1-Q)z+\kappa\sqrt{z^2+\mu^2}\right]\left[(1+Q)z+\kappa\sqrt{z^2+\mu^2}\right]}\,,\\ &= \frac{c_1}{(1-Q)z+\kappa\sqrt{z^2+\mu^2}}+\frac{c_2}{(1+Q)z+\kappa\sqrt{z^2+\mu^2}}\,,\end{aligned} \tag{9.42}$$

the coefficients $c_1$ and $c_2$ can be determined and we obtain

$$\tilde{a}_0(z) = \frac{2\kappa}{\lambda Q}\left[\frac{1}{(1-Q)z+\kappa\sqrt{z^2+\mu^2}}-\frac{1}{(1+Q)z+\kappa\sqrt{z^2+\mu^2}}\right]. \tag{9.43}$$

Had it not been possible the factorization in Eq. (9.34), we would had been forced to first remove the $z$-dependent square root in the denominator by multiplying the denominator and numerator by an appropriate "rationalizing factor" to obtain a fourth order polynomial in the denominator —that also would had to be factored. The resulting partial fractions expansion would had been much more complex.

# Chapter 10

## General solution for the memory functions $\tilde{b}_1(z)$ and $b_1(t)$

### 10.1 Continued fraction expansion for $\tilde{b}_1(z)$

We showed in §9.1, page 90, that the continued fraction expansion (9.5) of the relaxation function

$$\tilde{a}_0(z) = \cfrac{1}{z + \cfrac{\Delta_1}{z + \cfrac{\Delta_2}{z + \cdots + \cfrac{}{z + \cfrac{\Delta_{d-2}}{z + \cfrac{\Delta_{d-1}}{z}}}}}}, \tag{10.1}$$

has a regular pattern if the first and the last recurrants, Eqs. (9.6a)–(9.6b), are excluded (see the paragraph above Eqs. (9.6) in page 90). Here $d = 2N$, with $N$ being the number of oscillators. This led us to consider the continued fraction expansion (9.11) of the function $\tilde{b}_1(z)$,

$$\tilde{b}_1(z) = \cfrac{1}{z + \cfrac{\Delta_2}{z + \cfrac{\Delta_3}{z + \cdots + \cfrac{}{z + \cfrac{\Delta_{d-2}}{z + \cfrac{\Delta_{d-1}}{z}}}}}}, \tag{10.2}$$

—related to first subspace $\mathcal{S}_1$ that does not contain the first delta— in terms of which the relaxation function is written as (see Eq. (9.10)):

$$\tilde{a}_0(z) = \frac{1}{z + \Delta_1 \tilde{b}_1(z)} \ . \tag{10.3}$$

In the thermodynamic limit, $N \to \infty$, we do not have to worry about the last delta

$$\Delta_{d-1} = \Delta_{2N-1} = \frac{\kappa}{(N-1)\kappa + 1} \ , \tag{10.4}$$

breaking the pattern of the sequence. See the paragraph above Eq. (9.7) in page 91.

## 10.2 Deltas pattern of $\tilde{b}_1(z)$

Our aim in this chapter is then, first to find a closed solution for the infinite continued fraction

$$\tilde{b}_1(z) = \cfrac{1}{z + \cfrac{\Delta_2}{z + \cfrac{\Delta_3}{z + \ddots}}} \ , \tag{10.5}$$

and afterwards calculate its Laplace transform to obtain $b_1(t)$.

The part of the Delta's sequence that appears in $\tilde{b}_1(z)$ does not include $\Delta_1$, starts at $\Delta_2$, and looking at Table 7.1 on page 72 of §7.5 –that we reproduce below for convenience– one sees that

Table 10.1: Delta sequence $\sigma = (\Delta_1, \Delta_2, \ldots, \Delta_{d-1})$, in units of $k/m$

| | $\sigma =$ | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| $N$ | $(\Delta_1$ | $\Delta_2$ | $\Delta_3$ | $\Delta_4$ | $\Delta_5$ | $\Delta_6$ | $\Delta_7$ | $\Delta_8$ | $\Delta_9$ | $\Delta_{10}$ | $\Delta_{11})$ |
| 2 | $\left(\ \frac{\lambda(1+\kappa)}{}\right.$ | $\frac{1}{\kappa+1}$ | $\left.\frac{\kappa}{\kappa+1}\ \right)$ | | | | | | | | |
| 3 | $\left(\ \frac{\lambda(1+\kappa)}{}\right.$ | $\frac{1}{\kappa+1}$ | $\frac{2\kappa+1}{\kappa+1}$ | $\frac{\kappa+1}{2\kappa+1}$ | $\left.\frac{\kappa}{2\kappa+1}\ \right)$ | | | | | | |
| 4 | $\left(\ \frac{\lambda(1+\kappa)}{}\right.$ | $\frac{1}{\kappa+1}$ | $\frac{2\kappa+1}{\kappa+1}$ | $\frac{\kappa+1}{2\kappa+1}$ | $\frac{3\kappa+1}{2\kappa+1}$ | $\frac{2\kappa+1}{3\kappa+1}$ | $\left.\frac{\kappa}{3\kappa+1}\ \right)$ | | | | |
| 5 | $\left(\ \frac{\lambda(1+\kappa)}{}\right.$ | $\frac{1}{\kappa+1}$ | $\frac{2\kappa+1}{\kappa+1}$ | $\frac{\kappa+1}{2\kappa+1}$ | $\frac{3\kappa+1}{2\kappa+1}$ | $\frac{2\kappa+1}{3\kappa+1}$ | $\frac{4\kappa+1}{3\kappa+1}$ | $\frac{3\kappa+1}{4\kappa+1}$ | $\left.\frac{\kappa}{4\kappa+1}\ \right)$ | | |
| 6 | $\left(\ \frac{\lambda(1+\kappa)}{}\right.$ | $\frac{1}{\kappa+1}$ | $\frac{2\kappa+1}{\kappa+1}$ | $\frac{\kappa+1}{2\kappa+1}$ | $\frac{3\kappa+1}{2\kappa+1}$ | $\frac{2\kappa+1}{3\kappa+1}$ | $\frac{4\kappa+1}{3\kappa+1}$ | $\frac{3\kappa+1}{4\kappa+1}$ | $\frac{5\kappa+1}{4\kappa+1}$ | $\frac{4\kappa+1}{5\kappa+1}$ | $\left.\frac{\kappa}{5\kappa+1}\ \right)$ |

in the thermodynamic limit, $N \to \infty$, it is completely regular since then we do not have to worry about the special value (10.4) of the end-Delta breaking the sequence.

This sequence, although completely regular, oscillates about the value 1 , in units of $\Omega^2 \equiv k/m$. The odd Deltas

$$\Delta_{2\nu-1} = \frac{\nu\kappa + 1}{(\nu-1)\kappa + 1} \ , \qquad \nu = 2, 3, 4, \ldots \tag{10.6a}$$

constitute an uniformly decreasing sequence towards the limit value 1, while the even Deltas

$$\Delta_{2\nu} = \frac{(\nu-1)\kappa + 1}{\nu\kappa + 1} \ , \qquad \nu = 2, 3, 4, \ldots \tag{10.6b}$$

form an uniformly increasing sequence toward the value 1 . These sequences are not independent, the table shows that

$$\Delta_{2\nu} = \frac{\Omega^4}{\Delta_{2\nu-1}} \ , \qquad \nu = 2, 3, 4, \ldots \tag{10.6c}$$

or, in units of $\Omega^2$

$$\Delta_{2\nu} = \frac{1}{\Delta_{2\nu-1}} \ , \qquad \nu = 2, 3, 4, \ldots \tag{10.6d}$$

Note that $\Delta_2$ would have satisfied this relation if $\Delta_1$ had not been special because of the $\lambda$ factor.

The above being said, how does one go about summing the infinite continued fraction expansion of $\tilde{b}_1(z)$? In our case, the sequences are different from any previous sequences that have been analyzed. In earlier problems that we have reviewed it is the specificity of the Delta sequences –they are realized, model dependent– that has allowed them to be successfully studied.

The oscillatory nature of the Deltas as a whole, together with their regularity when separated in even and odd terms, as described in Eqs. (10.6), should be reflected in the sequence of approximants of the continued fraction (10.2).

This suggests to look separately at the even terms and at the odd terms of the sequence of *approximants*. To proceed we need to define the concept of *approximant* of a continued fraction and some additional terminology. We will follow the definitions given by Wall [1948, p. 14].

## 10.3 The Even–Odd decomposition of a general continued fraction

Let $Cf$ be a *finite* continued fraction

$$Cf = \beta_0 + \cfrac{\alpha_1}{\beta_1 + \cfrac{\alpha_2}{\beta_2 + \cfrac{\alpha_3}{\beta_3 + \cfrac{\alpha_4}{\beta_4 + \cdots \cfrac{\vdots}{\beta_{M-2} + \cfrac{\alpha_{M-1}}{\beta_{M-1} + \cfrac{\alpha_M}{\beta_M}}}}}}} \,. \tag{10.7}$$

Here $\alpha_p$ is the $p$th *partial numerator*, $\beta_p$ is the $p$th *partial denominator* and then $\alpha_p/\beta_p$ is called the $p$th *partial quotient*. $M$ is the order of the continued fraction. We will need to look at the sequence of approximants of various kinds of continued fractions. An approximant is simply the continued fraction written up to the required order, that is, the finite quantity $[\![Cf]\!]_{(n)}$, defined below

$$\beta_0 + \cfrac{\alpha_1}{\beta_1 + \cfrac{\alpha_2}{\beta_2 + \cdots + \cfrac{\vdots}{\beta_{n-2} + \cfrac{\alpha_{n-1}}{\beta_{n-1} + \cfrac{\alpha_n}{\beta_n}}}}} \equiv [\![Cf]\!]_{(n)} \equiv \frac{A_n}{B_n} \tag{10.8a}$$

is called the $n$th approximant, with $A_0 \equiv \beta_0$ and $B_0 \equiv 1$. If $n$ is even, we say that $[\![Cf]\!]_{(n)}$ is an even approximant. Similarly, if $n$ is odd, we say that $[\![Cf]\!]_{(n)}$ is an odd approximant. We call $A_n$ the $n$th *numerator* and $B_n$ the $n$th *denominator*. Thus, $[\![Cf]\!]_{(0)} = A_0/B_0 = \beta_0$ is the 0th approximant. The first approximant is

$$[\![Cf]\!]_{(1)} = \beta_0 + \frac{\alpha_1}{\beta_1} = \frac{\alpha_1 + \beta_0\beta_1}{\beta_1} \equiv \frac{A_1}{B_1} \,. \tag{10.8b}$$

The second approximant is

$$[\![Cf]\!]_{(2)} = \beta_0 + \cfrac{\alpha_1}{\beta_1 + \cfrac{\alpha_2}{\beta_2}} = \beta_0 + \frac{\alpha_1\beta_2}{\alpha_2 + \beta_1\beta_2} = \frac{\alpha_2\beta_0 + \alpha_1\beta_2 + \beta_0\beta_1\beta_2}{\alpha_2 + \beta_1\beta_2} \equiv \frac{A_2}{B_2}\,, \tag{10.8c}$$

etc.

Returning to the idea of looking separately at the even-$n$ terms, and at the odd-$n$ terms of the sequence of approximants (10.8a), there is procedure that allows one to obtain, from the original continued fraction, two more continued fractions. The first one with the property that its approximants constitute the even terms of the original continued fraction approximants sequence. The second with the exactly analogous property that its approximants constitute the odd terms of the original continued fraction approximants sequence.

This procedure is known as the *even–odd decomposition* of a continued fraction. The first continued fraction is known as the *even part* of the original continued fraction and the second continued fraction is known is known as the *odd part* of the original continued fraction. Any outcome is possible, both parts may converge (to equal or different limits), or neither one, or only one.

The even–odd decomposition formulas are simpler for a continued fraction whose partial denominators are set to unity (PDSU). The general continued fraction (10.7) can be written in terms of such a continued fraction with the partial denominators set to unity (PDSU) as follows

$$\begin{aligned} Cf &= \beta_0 + \alpha_1\beta_1^{-1}\cfrac{1}{1+\cfrac{\alpha_2\beta_1^{-1}\beta_2^{-1}}{1+\cfrac{\alpha_3\beta_2^{-1}\beta_3^{-1}}{1+\cfrac{\alpha_4\beta_3^{-1}\beta_4^{-1}}{1+\cdots\cfrac{\vdots}{1+\cfrac{\alpha_{M-1}\beta_{M-2}^{-1}\beta_{M-1}^{-1}}{1+\cfrac{\alpha_M\beta_{M-1}^{-1}\beta_M^{-1}}{1}}}}}}}\,, \\ &\equiv \beta_0 + \alpha_1\beta_1^{-1}\,\mathrm{PDSU}(Cf)\,. \end{aligned} \tag{10.9}$$

This is a particular case of an equivalence transformation[1]. Here,

$$\mathrm{PDSU}(Cf) \equiv \cfrac{1}{1+\cfrac{u_2}{1+\cfrac{u_3}{1+\cfrac{u_4}{1+\cdots\cfrac{\vdots}{1+\cfrac{u_{M-1}}{1+\cfrac{u_M}{1}}}}}}}\,. \tag{10.10}$$

The approximants of any continued fraction are calculated using Eq. (10.8a). Thus, the first few terms of the sequence of approximants of $\mathrm{PDSU}(Cf)$ are

$$[\![\mathrm{PDSU}(Cf)]\!]_{(1)} = 0 + \frac{1}{1} = \frac{A_1}{B_1} = 1, \tag{10.11a}$$

$$[\![\mathrm{PDSU}(Cf)]\!]_{(2)} = 0 + \cfrac{1}{1+\cfrac{u_2}{1}} = \frac{A_2}{B_2} = \frac{1}{1+u_2}\,, \tag{10.11b}$$

$$[\![\mathrm{PDSU}(Cf)]\!]_{(3)} = 0 + \cfrac{1}{1+\cfrac{u_2}{1+\cfrac{u_3}{1}}} = \frac{A_3}{B_3} = \frac{1+u_3}{1+u_2+u_3}\,, \tag{10.11c}$$

[1] An equivalence transformation is simply to multiply by the same factor the numerator and the denominator of any partial fraction of the continued fraction. Evidently, this does not change the continued fraction. This maybe done to *any* subset (one, two, all, etc) of the partial fractions, each one with its own factor. For example, here the first partial fraction gets the factor $r_1$ and the second partial fraction gets the factor $r_2$

$$\beta_0 + \cfrac{\alpha_1}{\beta_1+\cfrac{\alpha_2}{\beta_2+\cfrac{\alpha_3}{\beta_3+\ddots}}} = \beta_0 + \cfrac{r_1\alpha_1}{r_1\beta_1+\cfrac{r_2r_1\alpha_2}{r_2\beta_2+\cfrac{r_2\alpha_3}{\beta_3+\ddots}}}\,.$$

Note carefully the overlapped factors $r_2r_1$ on the second partial numerator.

$$[\![\mathrm{PDSU}(Cf)]\!]_{(4)} = 0 + \cfrac{1}{1 + \cfrac{u_2}{1 + \cfrac{u_3}{1 + \cfrac{u_4}{1}}}} = \frac{A_4}{B_4} = \frac{1 + u_3 + u_4}{1 + u_3 + u_4 + u_2(1 + u_4)} \ , \tag{10.11d}$$

$$[\![\mathrm{PDSU}(Cf)]\!]_{(5)} = 0 + \cfrac{1}{1 + \cfrac{u_2}{1 + \cfrac{u_3}{1 + \cfrac{u_4}{1 + \cfrac{u_5}{1}}}}} =$$

$$\frac{A_5}{B_5} = \frac{1 + u_4 + u_5 + u_3(1 + u_5)}{1 + u_4 + u_5 + u_3(1 + u_5) + u_2(1 + u_4 + u_5)} \ , \tag{10.11e}$$

$$[\![\mathrm{PDSU}(Cf)]\!]_{(6)} = 0 + \cfrac{1}{1 + \cfrac{u_2}{1 + \cfrac{u_3}{1 + \cfrac{u_4}{1 + \cfrac{u_5}{1 + \cfrac{u_6}{1}}}}}} =$$

$$\frac{A_6}{B_6} = \frac{1 + u_5 + u_6 + u_4(1 + u_6) + u_3(1 + u_5 + u_6)}{1 + u_4 + u_5 + u_6 + u_4u_6 + u_3(1 + u_5 + u_6) + u_2(1 + u_5 + u_6 + u_4(1 + u_6))} \ . \tag{10.11f}$$

Note that $[\![\mathrm{PDSU}(Cf)]\!]_{(0)} = 0$ in this case. Each successive term in the sequence of approximants is obtained by adding an additional partial quotient step to the continued fraction, switching the parity from even to odd or vice-verse. Thus, if one could contract or condense two steps into one, it would be possible to obtain *separately* the sequence of even terms and the sequence of odd terms.

This is indeed possible. We show in page 186 of Appendix B, that the sequence of approximants of the following continued fraction is equal to the sequence of odd approximants of the original

PDSU($Cf$) (We will work out explicitly the first few terms below). In other words, we obtain the odd part of Eq. (10.10) as

$$\text{ODD}(\text{PDSU}(Cf)) =$$

$$1 - \cfrac{u_2}{1 + u_2 + u_3 - \cfrac{u_3 u_4}{1 + u_4 + u_5 - \cfrac{u_5 u_6}{1 + u_6 + u_7 - \cdots \cfrac{\vdots}{1 + u_{M^*-2} + u_{M^*-1} - \cfrac{u_{M^*-1} u_{M^*}}{1 + u_{M^*} + \varsigma\, u_{M^*+1}}}}}}} . \tag{10.12}$$

Similarly, we also show in page 187 Appendix B, that the sequence of approximants of the continued fraction below is equal to the sequence of even approximants of the original PDSU($Cf$). Put in another way, the even part of Eq. (10.10) is

$$\text{EVEN}(\text{PDSU}(Cf)) =$$

$$\cfrac{1}{1 + u_2 - \cfrac{u_2 u_3}{1 + u_3 + u_4 - \cfrac{u_4 u_5}{1 + u_5 + u_6 - \cdots \cfrac{\vdots}{1 + u_{M^*-3} + u_{M^*-2} - \cfrac{u_{M^*-2} u_{M^*-1}}{1 + u_{M^*-1} + u_{M^*} - \varsigma\, \cfrac{u_{M^*}\, u_{M^*+1}}{1 + u_{M^*+1}}}}}}} . \tag{10.13}$$

In both formulas above, Eq. (10.12) and Eq. (10.13), $M^* = M - \varsigma$, with $M$ being the order of the original PDSU($Cf$), Eq. (10.10), and $\varsigma =\ \mod (M, 2)$.

As an example, we will now write the first few terms of the sequence of approximants of the even-part EVEN(PDSU($Cf$)), Eq. (10.13), and the odd-part ODD(PDSU($Cf$)), Eq. (10.12).

Each term of the respective sequence of approximants is calculated using the general definition of $[\![\ \ ]\!]_{(n)}$, given in Eq. (10.8a). In other words, $[\![\ \ ]\!]_{(n)}$ is the operator that gives the $n$th approximant of any continued fraction.

–For the even-part EVEN(PDSU($Cf$)), Eq. (10.13), of the continued fraction PDSU($Cf$), Eq. (10.10), the first three approximants are:

$$[\![\mathrm{EVEN}(\mathrm{PDSU}(Cf))]\!]_{(1)} = 0 + \frac{1}{1+u_2} = \frac{A_1^{(Even)}}{B_1^{(Even)}} = \frac{1}{1+u_2}\ , \tag{10.14a}$$

$$[\![\mathrm{EVEN}(\mathrm{PDSU}(Cf))]\!]_{(2)} = 0 + \cfrac{1}{1+u_2-\cfrac{u_2u_3}{1+u_3+u_4}} = \frac{A_2^{(Even)}}{B_2^{(Even)}} = \frac{1+u_3+u_4}{1+u_3+u_4+u_2(1+u_4)}\ , \tag{10.14b}$$

$$[\![\mathrm{EVEN}(\mathrm{PDSU}(Cf))]\!]_{(3)} = 0 + \cfrac{1}{1+u_2-\cfrac{u_2u_3}{1+u_3+u_4-\cfrac{u_4u_5}{1+u_5+u_6}}} =$$

$$\frac{A_3^{(Even)}}{B_3^{(Even)}} = \frac{1+u_5+u_6+u_4(1+u_6)+u_3(1+u_5+u_6)}{1+u_4+u_5+u_6+u_4u_6+u_3(1+u_5+u_6)+u_2(1+u_5+u_6+u_4(1+u_6))}\ . \tag{10.14c}$$

–For the odd-part ODD(PDSU($Cf$)), Eq. (10.12), of the continued fraction PDSU($Cf$), Eq. (10.10), we show the first two approximants (only these two are needed for this example):

$$[\![\mathrm{ODD}(\mathrm{PDSU}(Cf))]\!]_{(1)} = 1 - \frac{u_2}{1+u_2+u_3} = \frac{A_1^{(Odd)}}{B_1^{(Odd)}} = \frac{1+u_3}{1+u_2+u_3}\ , \tag{10.15a}$$

$$[\![\mathrm{ODD}(\mathrm{PDSU}(Cf))]\!]_{(2)} = 1 - \cfrac{u_2}{1+u_2+u_3-\cfrac{u_3u_4}{1+u_4+u_5}} =$$

$$\frac{A_2^{(Odd)}}{B_2^{(Odd)}} = \frac{1+u_4+u_5+u_3(1+u_5)}{1+u_4+u_5+u_3(1+u_5)+u_2(1+u_4+u_5)}\ . \tag{10.15b}$$

The definition of the even part, and the definition of the odd part of a continued fraction make good on their pledge. Looking at Eqs. (10.11), the first three approximants of the even-part are equal to the second, fourth and sixth approximants, respectively, of the continued fraction (10.10).

On the other hand, the first two approximants of the odd-part are equal to the third and fifth approximants, respectively, of the continued fraction (10.10).

## 10.4 Even-part and Odd-part of the $\tilde{b}_1(z)$ continued fraction expansion

The continued fraction expansion (10.2) of $\tilde{b}_1(z)$ was shown in §9.1 to have a completely regular pattern in thermodynamic limit, $N \to \infty$, and its relationship to the $\tilde{a}_0(z)$ relaxation function was reviewed in §10.1.

We will first assume that the order $d$ of the continued fraction expansion of $\tilde{b}_1(z)$ is *finite* to apply the even-odd decomposition formulas obtained in the previous section and afterwards we will take the thermodynamic limit to obtain a closed solution for $\tilde{b}_1(z)$ in the next section.

In the previous section we explain the meaning of the even-odd decomposition of a general finite continued fraction. The corresponding formulas are more compact and simpler to derive (see Appendix B p. 182) for a continued fraction whose partial denominators have been set to unity (PDSU).

Thus, we use an equivalence transformation, with all the factors set to $1/z$ (see [1] p. 116) to convert the partial denominators of $\tilde{b}_1(z)$, Eq. (10.2), into 1's, thus casting it into the simple form (10.10). We get

$$\tilde{b}_1(z) = \cfrac{1/z}{1+\cfrac{\Delta_2/z^2}{1+\cfrac{\Delta_3/z^2}{1+\cdots+\cfrac{\vdots}{1+\cfrac{\Delta_{d-2}/z^2}{1+\cfrac{\Delta_{d-1}/z^2}{1}}}}}}\,, \tag{10.16}$$

and then

$$z\tilde{b}_1(z) = \cfrac{1}{1+\cfrac{\Delta_2/z^2}{1+\cfrac{\Delta_3/z^2}{1+\cdots+\cfrac{\vdots}{1+\cfrac{\Delta_{d-2}/z^2}{1+\cfrac{\Delta_{d-1}/z^2}{1}}}}}} \equiv \mathrm{PDSU}(z\tilde{b}_1(z)) \ . \tag{10.17}$$

Note that $\mathrm{PDSU}(z\tilde{b}_1(z))$ is exactly in the required (10.10) form, with all its partial denominators set to unity (PDSU), and also, with the first numerator set to unity.

Before using (10.13)–(10.12) to obtain the even–odd decomposition of Eq. (10.17), note that the even-part (EP) of a given continued fraction is just the *same* continued fraction transformed so the sequence of approximants of the EP is the sequence of the even approximants of the original continued fraction. Similarly the odd-part (OP) of a given continued fraction is just the *same* continued fraction transformed so the sequence of approximants of the OP is the sequence of the odd approximants of the original continued fraction. Thus, if the EP and OP approximants are alternated one obtains the sequence of approximants of the original continued fraction as if no decomposition had been carried out.

The above is illustrated by the detailed examples we provide at the end of the previous section. In Eqs. (10.11)p. 116 we show the first six approximants of the continued fraction $\mathrm{PDSU}(Cf)$, in Eqs. (10.14)p. 119 we show the first three approximants of the continued fraction $\mathrm{EVEN}(\mathrm{PDSU}(Cf))$ and in Eqs. (10.15)p. 119 we show the first two approximants of the continued fraction $\mathrm{ODD}(\mathrm{PDSU}(Cf))$. One verifies that *indeed*:

$$[\![\mathrm{EVEN}(\mathrm{PDSU}(Cf))]\!]_{(1)} = [\![\mathrm{PDSU}(Cf)]\!]_{(2)} \ , \tag{10.18a}$$

$$[\![\mathrm{ODD}(\mathrm{PDSU}(Cf))]\!]_{(1)} = [\![\mathrm{PDSU}(Cf)]\!]_{(3)} \ , \tag{10.18b}$$

$$[\![\mathrm{EVEN}(\mathrm{PDSU}(Cf))]\!]_{(2)} = [\![\mathrm{PDSU}(Cf)]\!]_{(4)} \ , \tag{10.18c}$$

$$[\![\mathrm{ODD}(\mathrm{PDSU}(Cf))]\!]_{(2)} = [\![\mathrm{PDSU}(Cf)]\!]_{(5)} \ , \tag{10.18d}$$

$$[\![\mathrm{EVEN}(\mathrm{PDSU}(Cf))]\!]_{(3)} = [\![\mathrm{PDSU}(Cf)]\!]_{(6)} \ . \tag{10.18e}$$

Let's return to our problem. We will now assume that the order $d$ of the continued fraction expansion of $\tilde{b}_1(z)$ besides being *finite* is also *big*, say $d > 15$, so that we don't have to worry about writing the special values of the final partial quotients in the even–odd decomposition formulas Eq. (10.13) and Eq. (10.12).

Using the formula (10.13) to calculate the even part of (10.17), we find the *finite* continued fraction

$$\mathrm{EVEN}(\mathrm{PDSU}(z\tilde{b}_1(z))) = \cfrac{1}{1+\Delta_2/z^2-\cfrac{\Delta_2\Delta_3/z^4}{1+(\Delta_3+\Delta_4)/z^2-\cfrac{\Delta_4\Delta_5/z^4}{1+(\Delta_5+\Delta_6)/z^2-\cfrac{\Delta_6\Delta_7/z^4}{1+(\Delta_7+\Delta_8)/z^2-\ddots}}}}. \tag{10.19}$$

Similarly, using the formula (10.12) to calculate the odd-part of (10.17), we find the *finite* continued fraction

$$\mathrm{ODD}(\mathrm{PDSU}(z\tilde{b}_1(z))) = 1 - \cfrac{\Delta_2/z^2}{1+(\Delta_2+\Delta_3)/z^2-\cfrac{\Delta_3\Delta_4/z^4}{1+(\Delta_4+\Delta_5)/z^2-\cfrac{\Delta_5\Delta_6/z^4}{1+(\Delta_6+\Delta_7)/z^2-\cfrac{\Delta_7\Delta_8/z^4}{1+(\Delta_8+\Delta_9)/z^2-\ddots}}}}. \tag{10.20}$$

Looking at the Table 10.1 on page 112 we find the following simple relations among the Deltas of our model:

$$\begin{aligned}
\Delta_2 + \Delta_3 &= 2\Omega^2, \quad \Delta_3\Delta_4 = \Omega^4, \\
\Delta_4 + \Delta_5 &= 2\Omega^2, \quad \Delta_5\Delta_6 = \Omega^4, \\
\Delta_6 + \Delta_7 &= 2\Omega^2, \quad \Delta_7\Delta_8 = \Omega^4, \\
&\vdots \qquad\quad \vdots \qquad .
\end{aligned} \tag{10.21}$$

This immediately gives that all the partial numerators of the finite continued fraction

$$\mathrm{ODD}(\mathrm{PDSU}(z\tilde{b}_1(z))),$$

*except* the first, are all equal among themselves. Also all the partial denominators are equal among themselves. Therefore, for our model, the regularity of the finite continued fraction,

$$\mathrm{ODD}(\mathrm{PDSU}(z\tilde{b}_1(z))),$$

makes it readily summable in the thermodynamic limit, as we will show in the next section.

The analogous relations for the continued fraction $\mathrm{EVEN}(\mathrm{PDSU}(z\tilde{b}_1(z)))$ are neither constant nor simple.

Substituting the relations among the deltas given by Eq. (10.21), into $\mathrm{ODD}(\mathrm{PDSU}(z\tilde{b}_1(z)))$, Eq. (10.20), above, we find the finite continued fraction

$$\begin{aligned}\mathrm{ODD}(\mathrm{PDSU}(z\tilde{b}_1(z))) =& 1 - \cfrac{\frac{\Omega^2/z^2}{\kappa+1}}{1+2\Omega^2/z^2 - \cfrac{\Omega^4/z^4}{1+2\Omega^2/z^2 - \cfrac{\Omega^4/z^4}{1+2\Omega^2/z^2 - \cfrac{\Omega^4/z^4}{1+2\Omega^2/z^2 - \ddots}}}}, \\ =& 1 - \cfrac{\frac{1}{\kappa+1}\frac{\Omega^2}{z^2}}{\frac{z^2+2\Omega^2}{z^2} - \cfrac{\frac{\Omega^4}{z^4}}{\frac{z^2+2\Omega^2}{z^2} - \cfrac{\frac{\Omega^4}{z^4}}{\frac{z^2+2\Omega^2}{z^2} - \cfrac{\frac{\Omega^4}{z^4}}{\frac{z^2+2\Omega^2}{z^2} - \ddots}}}}. \end{aligned} \tag{10.22}$$

It is convenient to do another equivalence transformation with all the factors (see [1] in page 116) set to $z^2/\Omega^2$ to convert the $\Omega^4/z^4$ partial numerators into 1's. We get the finite continued fraction

$$\mathrm{ODD}(\mathrm{PDSU}(z\tilde{b}_1(z))) = 1 - \cfrac{\frac{1}{\kappa+1}}{\frac{z^2+2\Omega^2}{\Omega^2} - \cfrac{1}{\frac{z^2+2\Omega^2}{\Omega^2} - \cfrac{1}{\frac{z^2+2\Omega^2}{\Omega^2} - \cfrac{1}{\frac{z^2+2\Omega^2}{\Omega^2} - \ddots}}}}. \tag{10.23}$$

## 10.5 Absolute convergence of the continued fraction representation of $\tilde{b}_1(z)$

In Appendix C, p. 188 we review the classical concept of convergence for continued fractions [Wall 1948, p. 16] and the same concept in the modern ([Cuyt, Petersen, Verdonk, Waadeland & Jones 2008, p. 12], [Borwein & Crandall 2004, p. 288]) context.

We provide an introduction to the concept of absolute convergence [Lane & Wall 1949, p. 369], [Jones & Thron 1980, p. 126] of continued fractions and we show that the continued fraction representation of $\tilde{b}_1(z)$ for our model is *absolutely convergent* for all values of $z$ outside the cut $[-\mathrm{i}\,2\Omega, +\mathrm{i}\,2\Omega]$ on the imaginary axis. As pointed out by Borwein & Crandall [2004, p. 289], and by Lorentzen & Waadeland [1992, p. 128], if a continued fraction converges absolutely, then it converges to a finite limit. This means that *all* the approximants, the *even* and the *odd*, converge to the same finite limit. Therefore, in this case we may set the original continued fraction *equal* to either its even part or its odd part, whichever turns out the easiest to evaluate.

The aforementioned absolute convergence of the continued fraction representation of $\tilde{b}_1(z)$ allows us to set

$$z\tilde{b}_1(z) \leftarrow \mathrm{ODD}(\mathrm{PDSU}(z\tilde{b}_1(z))) \ , \tag{10.24}$$

and then

$$z\,\tilde{b}_1(z) = 1 - \cfrac{\frac{1}{\kappa+1}}{\frac{z^2+2\Omega^2}{\Omega^2} - \cfrac{1}{\frac{z^2+2\Omega^2}{\Omega^2} - \cfrac{1}{\frac{z^2+2\Omega^2}{\Omega^2} - \cfrac{1}{\frac{z^2+2\Omega^2}{\Omega^2} - \ddots}}}} \ . \tag{10.25}$$

It is evident that this continued fraction is summable in the thermodynamic limit.

## 10.6 General solution for $\tilde{b}_1(z)$ in the thermodynamic limit

In the thermodynamic limit, the order $d$ of $\mathrm{PDSU}(z\tilde{b}_1(z))$, Eq. (10.17), becomes infinite. Also, $z\tilde{b}_1(z) = \mathrm{ODD}(\mathrm{PDSU}(z\tilde{b}_1(z)))$, given in (10.25), becomes an *infinite* continued fraction, with all

its partial denominators equal to $z^2/\Omega^2 + 2$, and all its partial numerators, but the first, equal to $-1$ .

Let's define an infinite continued fraction $Cf_{all\ equal} \equiv Cf_{ae}$ with all the partial numerators equal to $-1$, and all the partial denominators equal to a given variable, say $\zeta$, as

$$Cf_{ae}(\zeta) = \cfrac{1}{\zeta - \cfrac{1}{\zeta - \cfrac{1}{\zeta - \ddots}}} . \tag{10.26}$$

Then, the function $z\tilde{b}_1(z)$ may be written as:

$$z\tilde{b}_1(z) = 1 - \frac{1}{\kappa+1}\, Cf_{ae}(w) \ , \qquad\qquad w \equiv \frac{z^2 + 2\Omega^2}{\Omega^2} \ . \tag{10.27}$$

To evaluate the continued fraction $C_{ae}(\zeta)$, note that it must satisfy

$$Cf_{ae}(\zeta) = \frac{1}{\zeta - Cf_{ae}(\zeta)} \ . \tag{10.28}$$

Solving this equation and making the substitution $\zeta \leftarrow w$, we find

$$\begin{aligned} Cf_{ae}(w) &= \tfrac{1}{2}\frac{z^2}{\Omega^2} + 1 \pm \tfrac{1}{2}\frac{z}{\Omega^2}\sqrt{z^2+4\Omega^2} \ , \\ &= 1 - \frac{z}{2\Omega^2}(\mp\sqrt{z^2+4\Omega^2} - z) \ , \\ &= 1 - \frac{2z}{\mp\sqrt{z^2+4\Omega^2}+z} = \frac{\mp\sqrt{z^2+4\Omega^2}-z}{\mp\sqrt{z^2+4\Omega^2}+z} \ , \qquad w \equiv \frac{z^2+2\Omega^2}{\Omega^2} \ . \end{aligned} \tag{10.29}$$

From Eq. (10.16) we see that $\tilde{b}_1(z)$ is real and positive when $z > 0$ . Consequently, assuming that the first or principal branch of the square root is used, we have to pick the second choice of sign in the expressions (10.29) for $Cf_{ae}(w)$, to ensure this condition and also to have $\tilde{b}_1(z \to \infty) = 1/z$.

Now, we can write the $\tilde{b}_1(z)$ function in a closed finite form. This solution is also general. Although it was obtained in thermodynamic limit, $N \to \infty$, it is valid for any choice of the remaining parameters of the system. Substituting the above expression (10.29) for $Cf_{ae}(w)$, into $z\tilde{b}_1(z)$ given by (10.27), we obtain

$$\begin{aligned} z\tilde{b}_1(z) &= 1 - \frac{1}{\kappa+1}\left[1 - \frac{z}{2\Omega^2}(\sqrt{z^2+4\Omega^2} - z)\right] \ , \\ &= 1 - \frac{1}{\kappa+1}\,\frac{\sqrt{z^2+4\Omega^2}-z}{\sqrt{z^2+4\Omega^2}+z} \ . \end{aligned} \tag{10.30}$$

We will now evaluate $\Delta_1\tilde{b}_1(z)$. This function is related to the first dynamical subspace of $\mathcal{S}$, $\mathcal{S}_1$ (see §2.5), and is needed to obtain the Laplace transform of the relaxation function $\tilde{a}_0(z)$ that we seek in §9.1. The relationship among the two, given by Eq. (10.3), was reviewed in §9.1, p. 91. The function[2] $\Delta_1\tilde{b}_1(z)$ is also known as the "memory function". From Table 10.1 on page 112, we have $\Delta_1 = \lambda(\kappa+1)\Omega^2$ and with Eq. (10.30) we find

$$\begin{aligned} z\,\Delta_1\,\tilde{b}_1(z) &= \lambda(\kappa+1)\Omega^2 - \lambda\Omega^2 + \frac{\lambda}{2}z\sqrt{z^2+4\Omega^2} - \frac{\lambda}{2}z^2\ , \\ &= \kappa\lambda\Omega^2 + \frac{\lambda}{2}z\sqrt{z^2+4\Omega^2} - \frac{\lambda}{2}z^2\ , \end{aligned} \tag{10.31}$$

and then

$$\Delta_1\,\tilde{b}_1(z) = \kappa\lambda\frac{\Omega^2}{z} - \frac{\lambda}{2}z + \frac{\lambda}{2}\sqrt{z^2+4\Omega^2}\ . \tag{10.32}$$

With this expression we can now also obtain a closed and finite solution for the relaxation function $\tilde{a}_0(z)$ by substituting it into (9.10), i.e., $\tilde{a}_0(z) = 1/(z+\Delta_1\,\tilde{b}_1(z))$.

## 10.7 General solution for $b_1(t)$ in the thermodynamic limit

In this section we will obtain $b_1(t)$ by means of the inverse Laplace transform of the general solution (in the thermodynamic limit) for $\tilde{b}_1(z)$ that we obtained in the previous section.

We first rewrite Eq. (10.30) as

$$\begin{aligned} z\tilde{b}_1(z) &= 1 - \frac{1}{\kappa+1} + \frac{1}{\kappa+1}\,\frac{z}{2\Omega^2}(\sqrt{z^2+4\Omega^2}-z)\ , \\ &= \frac{1}{\kappa+1}\,\left[\kappa + \frac{z}{2\Omega^2}(\sqrt{z^2+4\Omega^2}-z)\right]\ , \end{aligned} \tag{10.33}$$

and then

$$\begin{aligned} \tilde{b}_1(z) &= \frac{\kappa}{\kappa+1}\,\frac{1}{z} + \frac{1}{(\kappa+1)2\Omega^2}(\sqrt{z^2+4\Omega^2}-z)\ , \\ &= \frac{\kappa}{\kappa+1}\,\frac{1}{z} + \frac{2}{(\kappa+1)\mu^2}(\sqrt{z^2+\mu^2}-z)\ , \end{aligned} \tag{10.34}$$

with $\mu \equiv 2\Omega$. In [Abramowitz & Stegun 1972, p. 1025, Eq. 29.3.58] we find that

$$\mathcal{L}^{-1}\{(\sqrt{z^2+\mu^2}-z)^k\} = \frac{k\mu^k}{t}\mathrm{J}_k(\mu t)\,, \tag{10.35}$$

[2]This is the Laplace transform of the "memory function" $\Delta_1 b_1(t)$ of Eq. (2.39) in §2.6.

and, since $\mathcal{L}^{-1}\{1/z\} = 1$, we obtain

$$b_1(t) = \frac{1}{\kappa+1}\left[\kappa + 2\frac{\mathrm{J}_1(\mu t)}{\mu t}\right] . \tag{10.36}$$

By picking the second choice of sign in Eq. (10.29) we had already ensured that $\tilde{b}_1(z \to \infty) = 1/z$ in Eqs. (10.33)–(10.34). Let's now check the $t$-space corresponding boundary condition,

$$b_1(t \to 0) = 1\,, \tag{10.37}$$

for the $b_1(t)$ we just obtained in Eq. (10.36). Keeping only the first term in the series

$$\mathrm{J}_\nu(\zeta) = (\tfrac{1}{2}\zeta)^\nu \sum_{k=0}^{\infty} \frac{(-\frac{1}{4}\zeta^2)^k}{k!\,\Gamma(\nu+k+1)} , \tag{10.38}$$

given in Abramowitz & Stegun [1972, p. 360, Eq. 9.1.10], it is found that

$$\mathrm{J}_\nu(\zeta \to 0) = \frac{(\zeta/2)^\nu}{\Gamma(\nu+1)} , \tag{10.39}$$

so $\mathrm{J}_1(\zeta \to 0) = \zeta/2$ and then the boundary condition (10.37) is indeed satisfied by the $b_1(t)$ we obtained in (10.36).

# Chapter 11

## The relaxation function $a_0(t)$

In this chapter we will use Laplace's inversion formula or Bromwich's integral (see, e.g., [Mathews & Walker 1970, p. 107, §4-3], [Abramowitz & Stegun 1972, p. 1020, Eq. 29.2.2]):

$$a_0(t) = \frac{1}{2\pi \mathrm{i}} \int_{c-\mathrm{i}\infty}^{c+\mathrm{i}\infty} \tilde{a}_0(z)\, \mathrm{e}^{zt}\, \mathrm{d}z\,, \tag{11.1}$$

to calculate $a_0(t)$ from the general solution (9.15) for $\tilde{a}_0(z)$ —*in the thermodynamic limit*— we found in Chapter 9. We were able to obtain a series solution for a *certain* region of the $(\kappa, \lambda)$ parameters phase-space.

A closed solution (i.e. *not* in terms of a series) for $a_0(t)$ was attained only for particular values of the parameters $\kappa$ and $\lambda$ that correspond to the closed exact solutions of the relaxation function $a_0(t)$ already obtained in Chapter 8 through their recurrence relations.

We obtained the general solution for the relaxation function $\tilde{a}_0(z)$ in three forms (that we will reproduce below for reference convenience). First, it was calculated in §9.1 by summing its continued fraction representation, yielding Eq. (9.15) on page 92, that is:

$$\tilde{a}_0(z) = \frac{2z}{(2-\lambda)z^2 + \kappa\lambda\mu^2/2 + \lambda z\sqrt{z^2+\mu^2}}\,, \tag{11.2}$$

where $\kappa \equiv k_0/k$, $\lambda \equiv m/m_0$, together with $k$, $k_0$, $m$ and $m_0$ were defined in Eqs. (7.2)-(7.3) on page 60, and $\mu \equiv 2\Omega$, with $\Omega \equiv \sqrt{k/m}$ in Eq. (9.14). Due to the $z$ factor multiplying the square root above, we showed in §9.6 that the denominator in Eq. (11.2) factors into two terms, the first one related to the *sometimes-physical* singularities, and the other related to the *never-physical* singularities, allowing us to obtain the alternate form, Eq. (9.34) on page 108, for the relaxation function, i.e.,

$$\tilde{a}_0(z) = \frac{(4\kappa/\lambda)z}{\left[(1-Q)z + \kappa\sqrt{z^2+\mu^2}\right]\left[(1+Q)z + \kappa\sqrt{z^2+\mu^2}\right]}\,, \tag{11.3}$$

where

$$Q \equiv \sqrt{(1+\kappa)^2 - 4\kappa/\lambda}\,, \tag{11.4}$$

is the same $Q$ already defined in Eq. (9.19b) on page 94. The two factors in the denominator of Eq. (11.3) immediately suggested writing this expression for $\tilde{a}_0(z)$ in partial fractions in Eq. (9.43) of §9.6 on page 110:

$$\tilde{a}_0(z) = \frac{2\kappa}{\lambda Q}\left[\frac{1}{(1-Q)z + \kappa\sqrt{z^2+\mu^2}} - \frac{1}{(1+Q)z + \kappa\sqrt{z^2+\mu^2}}\right]. \tag{11.5}$$

To evaluate Laplace's inversion formula or Bromwich's integral, Eq. (11.1), the vertical integration path ($c - \mathrm{i}\infty \to c + \mathrm{i}\infty$) has to be chosen to the *right* of all the singularities of $\tilde{a}_0(z)$ [Mathews & Walker 1970, p. 107, §4-3].

## 11.1 Review of the singularities of $\tilde{a}_0(z)$ and choice of the appropriate branch-cut path in the thermodynamic limit

The Recurrence Relations Method furnishes a continued-fraction general representation for the auto-correlation function $\tilde{a}_0(z)$. It was written in §9.1, Eq. (9.10), as

$$\tilde{a}_0(z) = \frac{1}{z + \Delta_1 \tilde{b}_1(z)}\,, \tag{11.6}$$

where $\tilde{b}_1(z)$ is the simple continued fraction

$$\tilde{b}_1(z) = \cfrac{1}{z + \cfrac{\Delta_2}{z + \cfrac{\Delta_3}{z + \cdots + \cfrac{\vdots}{z + \cfrac{\Delta_{d-2}}{z + \cfrac{\Delta_{d-1}}{z}}}}}}\,, \tag{11.7}$$

of order $d-1$, with $\{\Delta_1, \Delta_2, \ldots, \Delta_{d-1}\}$ being the model dependent *recurrants* and $d$ being the dimension of its realized space $\mathcal{S}$ as defined in §2.3. The recurrants and $d$ for our model are calculated

in §§7.3–7.5 and reported in Table 7.1. It is shown that $d = 2N - 1$, with $N$ being the length of the harmonic oscillators chain.

Thus, $\tilde{b}_1(z)$ and $\tilde{a}_0(z)$ are the quotient of two polynomials in $z$. In the case of $\tilde{b}_1(z)$, both the numerator and denominator are of order $N$, while for $\tilde{a}_0(z)$ the numerator is also of order $N$ but the denominator's order is one degree higher, i.e., $N + 1$. Consequently, *for finite* $N$, the only possible singularities of $\tilde{a}_0(z)$ are poles, that have to come in conjugated pairs on the imaginary axis, as explained in §9.5, each pair corresponding to a collective mode .

In the thermodynamic limit[1] $N \to \infty$ —using the results of Appendix C— the continued fraction representation of $\tilde{a}_0(z)$ was summed up in §9.1, obtaining Eq. (9.15) reproduced for convenience in Eq. (11.2) in the present chapter. When the limit $N \to \infty$ is taken, the ensuing infinite number of poles merge[2] into a continuous structure that is signaled to be a branch-cut by the presence of the square root $\sqrt{z^2 + \mu^2}$ in $\tilde{a}_0(z)$ given by either of Eqs. (11.2), (11.3) or (11.5). The square root is to be understood[3] as

$$\sqrt{z^2 + \mu^2} = \sqrt{z + \mathrm{i}\mu}\,\sqrt{z - \mathrm{i}\mu}\,. \tag{11.8}$$

The first factor gives rise to a branch-point at $z = -\,\mathrm{i}\mu$, while the second gives rise to the $z = \mathrm{i}\mu$ branch-point. In Figure 11.1 we show four possible choices of branch-cuts, that preclude a simple loop around either[4] of the branch-points, thus assuring single-valuedness of the product of the two square root factors.

A branch-cut severs the complex plane along a line that extends from the corresponding branch-point either to "infinity" or to another branch-point. The path[5] is arbitrary as long as it precludes

[1] In this limit the *particular pattern of our model recurrants* allows the summation of the continued fraction representation (11.7) of $\tilde{b}_1(z)$, as explained in §§10.5–10.6.

[2] At most only a pair of conjugated poles remain isolated, according to the values of the parameters $\kappa$ and $\lambda$ as explained in §9.2 and §9.5.

[3] $\sqrt{(z-a)(z-b)} = \sqrt{z-a}\,\sqrt{z-b}$ is the *only* consistent way of interpreting such a complex function. See [Mathews & Walker 1970, p. 475, §A-1].

[4] A simple loop around *both* branch-points of $\sqrt{z-a}\,\sqrt{z-b}$ is allowed [Mathews & Walker 1970, p. 476, §A-1] for any finite complex values of $a$ and $b$. Thus a simple loop around both branch-points of $\sqrt{z+\mathrm{i}\mu}\,\sqrt{z-\mathrm{i}\mu}$ is also allowed. It is *not* necessary for $a$ and $b$ to be symmetrically placed about the origin.

[5] Along this path the "sheets" ($\geqslant 2$) of a multiple valued function are joined. See, e.g., [Mathews & Walker 1970, pp. 473-474, §A-1] or [Markushevich 1977, Vol. 1, Chap. 11, pp. 212-239].

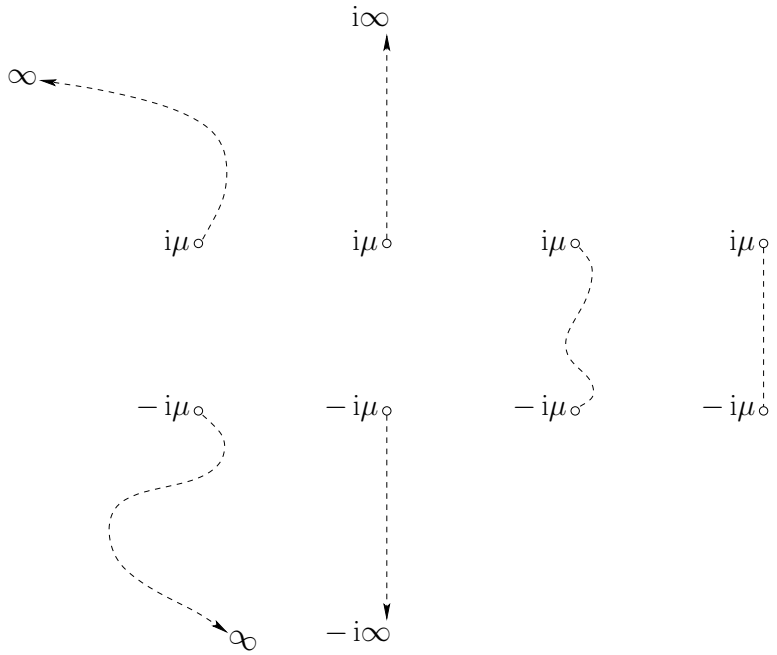



Figure 11.1: Four possible choices of branch-cuts for the function $\sqrt{z^2+\mu^2} = \sqrt{z+\mathrm{i}\mu}\,\sqrt{z-\mathrm{i}\mu}$, that appears in $\tilde{a}_0(z)$ when the thermodynamic limit is taken. There are two branch-points, $z = \mp\,\mathrm{i}\mu$, that arise from the first factor and second factor respectively. Only the last choice is appropriate for our model, as explained bellow Eq. (11.8).

the possibility of completing a simple closed loop[6] around the branch-point, and its actual shape is determined by additional mathematical or physical requirements:

- There cannot result an infinite number of collective modes with non-finite excitation energies, when the thermodynamic limit $N \to \infty$ is taken. This rules out the first and second choices in Figure 11.1.

- The poles —whether isolated or not— cannot be outside the imaginary axis. This is related to the fact that "long-time exponentially decaying modes" are not possible, a result M. Howard Lee [1983] obtained using the Recurrence Relations Method (RRM) as explained in §9.5 p. 105. Thus, the third choice in Figure 11.1, and again the first one are excluded.

[6]By simple closed loop we mean a loop —that staying within the current sheet— returns to the same spot in the same sheet.

Therefore, only the last branch-cut choice in Figure 11.1 is appropriate for our model, i.e., a cut $[-\mathrm{i}\mu, \mathrm{i}\mu]$ that merely joins the branch-points along a straight line in the imaginary axis.

A mathematical requirement also points to this choice. We obtained in §C.11, p. 203, a sufficient condition for the absolute convergence[7] of the continued fraction representation (11.6) of $\tilde{a}_0(z)$:

$$z \in \{\mathbb{C} - [-\mathrm{i}\,2\Omega,\, +\mathrm{i}\,2\Omega]\}\,, \tag{11.9a}$$

or

$$z \notin [-\mathrm{i}\,2\Omega,\, +\mathrm{i}\,2\Omega]\,, \tag{11.9b}$$

i.e. the complex plane has to be cut exactly as the last choice of Figure 11.1, that is, $[-\mathrm{i}\mu, \mathrm{i}\mu]$, the same that was pinpointed by the physical requirements above.

Once the branch-cut is fixed, we can deal with the multivalued behavior of $\tilde{a}_0(z)$. The multivaluedness is manifested only when the branch-cut is trespassed. Two interpretations are possible:

1. Go through the branch-cut *into the next sheet*. This way the function *behaves continuously*.
2. Breach the branch-cut and *stay in the same sheet*. In this case the function *behaves discontinuously*.

Thus, a multivalued function when considered wholly within the current sheet is discontinuous[8] along the branch-cut(s). In this chapter, we have to choose this (the second) alternative.

In our case, the presence of $\sqrt{z^2+\mu^2}$ in the general solution for $\tilde{a}_0(z)$ given by either of Eqs. (11.2), (11.3) or (11.5), makes $\tilde{a}_0(z)$ a double valued function of $z$ and to have physical consistency we have to pick the first or principal branch of the square root, as explained at the end of §9.1. We call it the physical sheet. The second sheet —the non-physical sheet— may be accessed through the branch-cut $[-\mathrm{i}\mu, \mathrm{i}\mu]$ as explained in the first interpretation above. The cut $[-\mathrm{i}\mu, \mathrm{i}\mu]$ is the *only non-isolated singularity* of the general solution for $\tilde{a}_0(z)$.

There can be at most two isolated singularities: a pair of conjugated poles. It is shown in §9.2 and §9.5 that according to the values of the parameters $\kappa$ and $\lambda$ three cases are possible:

[7] This *absolute convergence* ensures the proper summation, in the thermodynamic limit, of the continued fraction representation of $\tilde{b}_1(z)$ that was carried out in §§10.5–10.6.

[8] This is why the branch-cut has to be secluded out in the application of Cauchy's residue theorem in §11.3.

1. No poles are present. This happens only at special values or lines on the $(\kappa, \lambda)$ phase diagram.

2. The pair of conjugated poles are on the non-physical sheet.

3. The pair of conjugated poles are on the physical sheet

For the purpose of calculating $a_0(t)$ using Bromwich's integral, Eq. (11.1), the isolated pair of conjugated poles only has to be taken in account when they are present in the physical sheet. In this case the are *always* in the imaginary axis. This is related to the fact that "long-time exponentially decaying modes" are not possible, a result [Lee 1983] obtained by M. Howard Lee using the Recurrence Relations Method (RRM) as explained in §9.5 p. 105.

## 11.2 Cauchy's residue theorem applied to Bromwich's inversion integral

"Cauchy's residue theorem" or simply the "residue theorem" states [Mathews & Walker 1970, p. 65, §3-3] that if a function $\tilde{f}(z)$ is regular in a region bounded by a closed contour $C$, except for a finite number of poles and/or isolated essential singularities in the interior of $C$, then the integral of $\tilde{f}(z)$ along the contour $C$ is

$$\oint_C \tilde{f}(z)\,\mathrm{d}z = 2\pi\mathrm{i}\sum \text{Residues of } \tilde{f}(z)\,, \tag{11.10}$$

where the sum is over all the poles and essential singularities of $\tilde{f}(z)$ that are inside $C$.

To evaluate the inverse Laplace transform given by Bromwich's integral[9] (see, e.g., [Mathews & Walker 1970, p. 107, §4-3], [Abramowitz & Stegun 1972, p. 1020, Eq. 29.2.2] and references therein):

$$f(t) = \frac{1}{2\pi\mathrm{i}}\int_{c-\mathrm{i}\infty}^{c+\mathrm{i}\infty} \tilde{f}(z)\,\mathrm{e}^{zt}\,\mathrm{d}z\,. \tag{11.11}$$

using the residue theorem, Bromwich's contour must be closed by the addition of a supplementary path to the above integral. To be possible that $\tilde{f}(z)\,\mathrm{e}^{zt}\,\mathrm{d}z$ integrated along this supplementary path to be zero, the supplementary contour has to be at "infinity" to the right (left) real axis if $t < 0$ ($t > 0$), due to the $\mathrm{e}^{zt}$ factor in the integrand. This can also be seen from Jordan's lemma [Hildebrand 1962, p. 555, §10.14].

[9] The real positive finite constant $c$ is to be chosen to the *right* of all the singularities of $\tilde{f}(z)$.

We remind ourselves that in formula (11.11) directly above, in tables of Laplace transforms pairs, and in the direct Laplace transform definition [Mathews & Walker 1970, p. 107, §4-3]

$$\tilde{f}(z) = \mathcal{L}\{f(t)\} = \int_0^\infty \mathrm{e}^{-zt}\, f(t)\, \mathrm{d}t\,, \tag{11.12}$$

the Heavyside unit step function

$$H(t) = \begin{cases} 0 & : \quad t < 0 \\ 1/2 & : \quad t = 0 \\ 1 & : \quad t > 0 \end{cases} \tag{11.13}$$

is [Abramowitz & Stegun 1972, p. 1020, Eq. 29.1.3],[Mathews & Walker 1970, p. 107, §4-3] *always* to be understood as multiplying the original $f(t)$. Consequently, when $t < 0$, Bromwich's integral (11.11) for $f(t)$ must be identically zero. Closing Bromwich's contour with a supplementary path at "infinity" to the right, say a semi-circle, as shown in Figure 11.2, the residue theorem yields

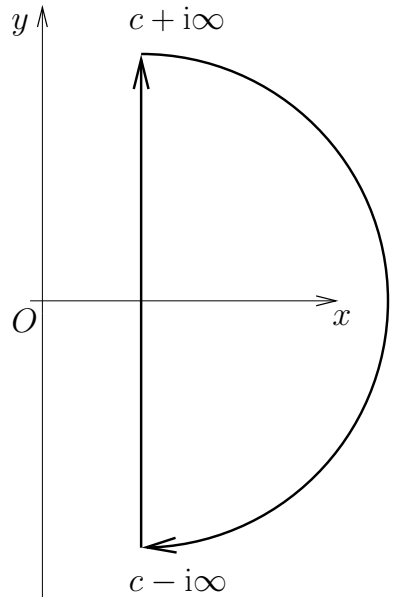



Figure 11.2: Bromwich's contour $(c - \mathrm{i}\infty, c + \mathrm{i}\infty)$ closed to the right at "infinity" when $t < 0$ for *any* $\tilde{f}(z)$. No singularities are shown since $\tilde{f}(z)$ is analytic and single valued in the right-hand half-plane $\mathrm{Re}\, z > c$. See Eq. (11.15b).

$$\int_{c-\mathrm{i}\infty}^{c+\mathrm{i}\infty} \mathrm{e}^{zt}\, \tilde{f}(z)\, \mathrm{d}z + \int_{\curvearrowright} \mathrm{e}^{zt}\, \tilde{f}(z)\, \mathrm{d}z = -2\pi\mathrm{i} \sum \text{Residues of } \mathrm{e}^{zt}\, \tilde{f}(z)\,,$$

or

$$\int_{c-\mathrm{i}\infty}^{c+\mathrm{i}\infty} \mathrm{e}^{zt}\,\tilde{f}(z)\,\mathrm{d}z = -2\pi\mathrm{i}\sum \text{Residues of } \mathrm{e}^{zt}\,\tilde{f}(z) - \int_{\circlearrowleft} \mathrm{e}^{zt}\,\tilde{f}(z)\,\mathrm{d}z\,. \tag{11.14}$$

By hypotheses [see Eq. (11.11)], the real positive constant $c$ is chosen to the *right* of all the singularities of $\tilde{f}(z)$ and therefore the $\sum$Residues term on the right-hand side of Eq. (11.14) above, is zero. Indeed, *if* the following integral

$$\lim_{\substack{A\to 0\\ B\to\infty}} \int_A^B \mathrm{e}^{-c\,t}\,f(t)\,\mathrm{d}t \tag{11.15a}$$

exists for a particular real positive finite constant $c$, then

1. The direct Laplace transform

$$\tilde{f}(z) = \mathcal{L}\{f(t)\} = \int_0^\infty \mathrm{e}^{-zt}\,f(t)\,\mathrm{d}t\,, \tag{11.15b}$$

converges for *every* $\mathrm{Re}\,z > c$, and the image function $\tilde{f}(z)$ above, is a *single valued analytic* function of $z$ in the half-plane $\mathrm{Re}\,z > c$. See [Abramowitz & Stegun 1972, p. 1020, Eq. 29.1.1] and [Markushevich 1977, Vol. 1, p. 421, Theor. 17.21].

2. Moreover, the image function $\tilde{f}(z)$ tends to zero as $z \to \infty$, that is:

$$\lim_{z\to\infty} \tilde{f}(z) = 0\,, \tag{11.15c}$$

along any ray whose argument $\in (-\pi/2, \pi/2)$, i.e., any ray that points to right half plane. See [Doetsch 1974, p. 141, Theor. 23.2]. This result, together with Jordan's lemma [Hildebrand 1962, p. 555, §10.14], assures that the integral of $\mathrm{e}^{zt}\,\tilde{f}(z)\,\mathrm{d}z$ along the semi-circle at "infinity" of Figure 11.2, i.e., the second term on the right-hand side of Eq. (11.14), is zero.

In summary, the relatively weak condition (11.15a) on $f(t)$ yields the two strong results (11.15b) and (11.15c) for $\tilde{f}(z)$ in the right-hand half-plane $\mathrm{Re}\,z > c$, which allow —*when $t < 0$*— a completely general[10] and simple application of Cauchy's residue theorem to Bromwich's inversion formula.

When $t > 0$, to apply the residue theorem to Bromwich's inversion formula (11.11), the $(c - \mathrm{i}\infty, c + \mathrm{i}\infty)$ path must again be closed with a supplementary contour. To be possible that

[10] It is always assumed $f(t < 0) \equiv 0$ for any function $f(t)$ which is to be Laplace transformed. See Eq. (11.13).

$\int \tilde{f}(z)\,\mathrm{e}^{zt}\,\mathrm{d}z$ along the supplementary contour to be zero, the $\mathrm{e}^{zt}$ factor in the integrand and Jordan's lemma [Hildebrand 1962, p. 555, §10.14] tell us that the additional path has to be at "infinity" to the left in the 2nd and 3rd quadrants. Equations (11.15a) and (11.15b) assure that $\tilde{f}(z)$ is *single valued analytic* to the right of Bromwich's path, $(c-\mathrm{i}\infty, c+\mathrm{i}\infty)$, therefore this resulting closed "on the left" contour will encompass <u>all</u> the singularities of $\tilde{f}(z)$. Only the *residues* at the isolated (poles and essential) singularities contribute directly to the residue theorem. Other kinds of singularities (e.g. branch cuts when $\tilde{f}(z)$ is not single-valued) also contribute indirectly: the closed contour must be deformed to exclude them.[11]

## 11.3 Bromwich's inversion integral applied to the general solution for $\tilde{a}_0(z)$ in the thermodynamic limit.

We reviewed in §11.1 that $\tilde{a}_0(z)$ has a branch-cut $[-\mathrm{i}\mu, \mathrm{i}\mu]$, and *at most* a pair of conjugated simple poles that only have to be taken into account if they are present in the physical-sheet. When this happens —depending on the values of the parameters $\kappa$ and $\lambda$— the poles are always situated on the imaginary axis. Using the ideas of the previous section, §11.2, two examples of appropriate closed contours for Bromwich's inversion integral with $t > 0$, applied to $\tilde{a}_0(z)$ using the residue theorem, are depicted in Figure 11.3.

Call $C_L$ the *closed* contour that would be obtained by joining Bromwich's $(c-\mathrm{i}\infty, c+\mathrm{i}\infty)$ path, with a semi-circular path $C_{\circlearrowleft}$ to the left, i.e.

$$C_L = (c-\mathrm{i}\infty, c+\mathrm{i}\infty) \cup C_{\circlearrowleft} \,. \tag{11.16}$$

To apply the residue theorem to $C_L$, the <u>branch-cut has to excluded from the interior of $C_L$</u> (see the last paragraph of §11.2 and p. 132 in §11.5 above). This is done by means of parallel paths that join the nicked $C_L$:

—Bromwich's $(c-\mathrm{i}\infty, c+\mathrm{i}\infty)$ path in the first example, the semi-circle in the second example— to the (also nicked) contour that rounds the cut in clockwise-sense. The parallel paths form a "tube" that connects (through both nicks) the space *outside* $C_L$ to the inside of the clockwise contour (call

[11] "Cauchy's residue theorem" or simply the "residue theorem" requires [Mathews & Walker 1970, p. 65, §3-3] the function $\tilde{f}(z)$ to be regular in a region bounded by a closed contour $C$, except for a finite number of poles and/or isolated essential singularities in the interior of $C$.

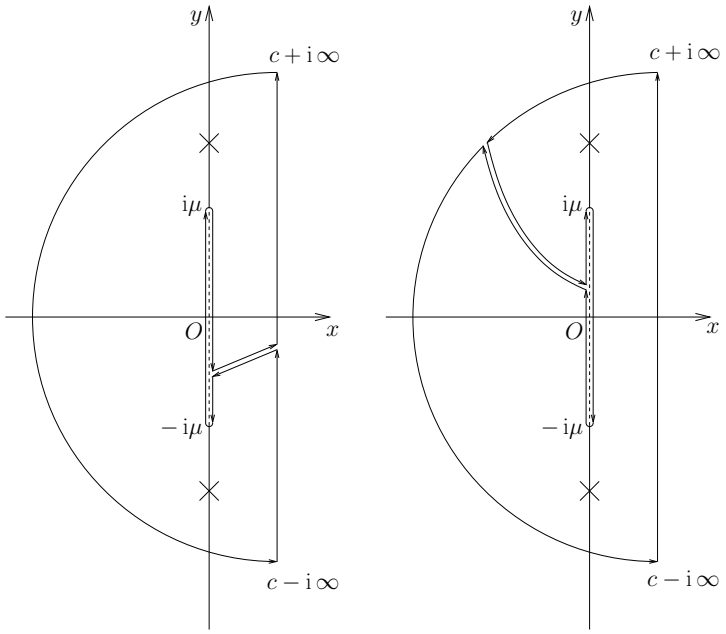
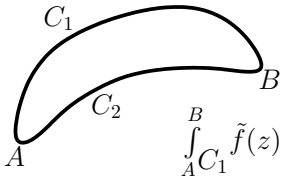



Figure 11.3: Two examples of a closed possible contour (called $C_L$ in §11.3) for the evaluation, when $t > 0$, of Bromwich's inversion integral for $\tilde{a}_0(z)$ using Cauchy's residue theorem. For the case $t > 0$, the $e^{zt}$ factor in the integrand together with Jordan's lemma requires Bromwich's contour $(c - i\infty, c + i\infty)$ to be closed with a supplementary path to the *left* at "infinity" (see the last paragraph of §11.2). The singularities of $\tilde{a}_0(z)$ are shown: a branch-cut $[-i\mu, i\mu]$ (dashed line), that is always present, and two conjugated poles (at the x-like crossed lines), that —when present, depending on the values of the parameters $\kappa$ and $\lambda$— are always on the imaginary axis. See §11.1. The residue theorem requires (see the last paragraph of §11.2) the branch-cut to be excluded from the closed contour. In the first example, Bromwich's contour $(c - i\infty, c + i\infty)$ is modified to exclude the branch-cut, while in the second example, it is the supplementary path that is modified to exclude the branch-cut. In both cases a detour $C_{BC}$ encloses the only branch-cut –and no other singularity– in clock-wise sense. The final result does not depend on the shape of the detour. See §11.3.

it $C_{BC}$) that encloses the branch-cut. The argument summarized in Figure 11.4, applied repeatedly, allows the adjustment of contour $C_{BC}$ so that the whole branch-cut and no singularity, other than the branch-cut itself, is contained in $C_{BC}$. Since the conjugated poles, if present, are always on the imaginary axis *outside* the cut, any $C_{BC}$ with the bottom edge at $-i\mu$ and the top edge at $i\mu$ (e.g. a circle of radius $\mu$ centered at the origin, a rectangle of height $2\mu$, etc) would have been




If the function $\tilde{f}(z)$ is regular, i.e., does not have singularities inside $C_1 \cup C_2$, Cauchy's residue theorem gives:

$$\int_A^B C_1 \tilde{f}(z)\,\mathrm{d}z + \int_B^A C_2 \tilde{f}(z)\,\mathrm{d}z = 0, \text{ thus} \qquad \int_A^B C_1 \tilde{f}(z)\,\mathrm{d}z = \int_A^B C_2 \tilde{f}(z)\,\mathrm{d}z\,.$$

Figure 11.4: The integral of $\tilde{f}(z)$ along a path, say $C_1$ between two points does not change when the path $C_1$ is deformed into another path $C_2$ as long as there are no singularities between the two paths. This is a consequence of Cauchy's residue theorem.

appropriate, and the result would also be the same. The simplest choice is the rod shaped path shown in Figure 11.3.

In the limit that the parallel paths are made infinitely close, the "tubes" and the nicks disappear, resulting the same $C_L$ traversed counter-clockwise *and* the same $C_{BC}$ traversed clockwise from both examples. Thus the residue theorem, Eq. (11.10), for $\int \tilde{a}_0(z)\,\mathrm{e}^{zt}\,\mathrm{d}z$ (with $t > 0$), along the limiting form of the contours of Figure 11.3 reads:

$$\int_{c-\mathrm{i}\infty}^{c+\mathrm{i}\infty} \tilde{a}_0(z)\,\mathrm{e}^{zt}\,\mathrm{d}z + \int_{\subsetneq} \tilde{a}_0(z)\,\mathrm{e}^{zt}\,\mathrm{d}z + \int_{\substack{\text{around the}\\ \text{branch-cut}}\uparrow\downarrow} \tilde{a}_0(z)\,\mathrm{e}^{zt}\,\mathrm{d}z$$
$$= 2\pi\mathrm{i}\sum \text{Residues of}\left[\tilde{a}_0(z)\,\mathrm{e}^{zt}\right]. \tag{11.17}$$

The boundary condition $a_0(t = 0) = 1$ imposes that when $|z| \to \infty$, then $\tilde{a}_0(z) = 1/z$. This condition is indeed satisfied by $\tilde{a}_0(z)$ given in either of Eqs. (11.2), (11.3) or (11.5), when the first or principal sheet of $\sqrt{z^2+\mu^2}$ is chosen in this expressions[12], as explained in §9.1 above Eq. (9.15). This is the *physical sheet* of $\tilde{a}_0(z)$. Thus, the second term on the left-hand side of Eq. (11.17) above is zero on account of Jordan's lemma [Hildebrand 1962, p. 555, §10.14] and then, for $\int \tilde{a}_0(z)\,\mathrm{e}^{zt}\,\mathrm{d}z$ (with $t > 0$) along Bromwich's path, we obtain

$$\int_{c-\mathrm{i}\infty}^{c+\mathrm{i}\infty} \tilde{a}_0(z)\,\mathrm{e}^{zt}\,\mathrm{d}z = \int_{\substack{\text{around the}\\ \text{branch-cut}}\downarrow\uparrow} \tilde{a}_0(z)\,\mathrm{e}^{zt}\,\mathrm{d}z + 2\pi\mathrm{i}\sum \text{Residues of}\left[\tilde{a}_0(z)\,\mathrm{e}^{zt}\right], \tag{11.18}$$

[12]Though, it is specially clear in Eq. (11.2).

and therefore for $a_0(t)$ given by Bromwich's integral, Eq. (11.11), of $\tilde{a}_0(z)$ we get

$$\begin{aligned} a_0(t) &= \frac{1}{2\pi\mathrm{i}} \int_{c-\mathrm{i}\infty}^{c+\mathrm{i}\infty} \tilde{a}_0(z)\, \mathrm{e}^{zt}\, \mathrm{d}z\,, \\ &= \frac{1}{2\pi\mathrm{i}} \int_{\substack{\text{around the} \\ \text{branch-cut}\ \downarrow\uparrow}} \tilde{a}_0(z)\, \mathrm{e}^{zt}\, \mathrm{d}z + \sum \text{Residues of } \left[\tilde{a}_0(z)\, \mathrm{e}^{zt}\right]. \end{aligned} \tag{11.19}$$

## 11.4 Parity of a two-branch-points function $\sqrt{(z-z_1)(z-z_2)}$

To obtain $a_0(t)$ from Eq. (11.19) above, the integral of $\tilde{a}_0(z)$ around its branch-cut must be performed. The behavior of $\tilde{a}_0(z)$ in the neighborhood of the cut is dictated by the two-branch-points function $\sqrt{z^2+\mu^2} = \sqrt{(z+\mathrm{i}\mu)(z-\mathrm{i}\mu)}$ (see Eq. (11.8)).

A function like our $\sqrt{(z+\mathrm{i}\mu)(z-\mathrm{i}\mu)}$, say $sQ_2(z) \equiv \sqrt{(z-z_1)(z-z_2)}$, is to be understood (see [3] on page 130) as

$$sQ_2(z) = \sqrt{(z-z_1)(z-z_2)} = \sqrt{z-z_1}\,\sqrt{z-z_2}\,. \tag{11.20}$$

Introduce, the arithmetic mean $z_m \equiv (z_1+z_2)/2$, and the half difference $\delta \equiv (z_2-z_1)/2$ of the branch-points $z_1$ and $z_2$, to write

$$sQ_2(z) = \sqrt{z-z_m+\delta}\,\sqrt{z-z_m-\delta}\,, \tag{11.21}$$

with $z_{\substack{1\\2}} = z_m \mp \delta$. A shift, $z \leftarrow z+z_m$ —shown in Figure 11.5— gives

$$sQ_2(z+z_m) = \sqrt{z+\delta}\,\sqrt{z-\delta}\,, \tag{11.22}$$

and, under a change of sign:

$$sQ_2(-z+z_m) = \sqrt{-z+\delta}\,\sqrt{-z-\delta} = \sqrt{\mathrm{e}^{\mathrm{i}\pi}(z-\delta)}\,\sqrt{\mathrm{e}^{\mathrm{i}\pi}(z+\delta)}\,, \tag{11.23a}$$

$$= \mathrm{e}^{\mathrm{i}\pi/2}\sqrt{z-\delta}\ \ \mathrm{e}^{\mathrm{i}\pi/2}\sqrt{z+\delta} = \mathrm{e}^{\mathrm{i}\pi}\sqrt{z-\delta}\,\sqrt{z+\delta}\,, \tag{11.23b}$$

$$= -sQ_2(z+z_m)\,. \tag{11.23c}$$

Therefore, if $z_m = (z_1+z_2)/2 = 0$

$$sQ_2(-z) = -sQ_2(z)\,, \tag{11.24}$$

i.e., $sQ_2(z)$ is an odd-function of $z$ when $z_1$ and $z_2$ are located symmetrically about the origin.

This is illustrated in Figure 11.5. Before the shift by $z_m = (z_1 + z_2)/2$ is done, there is no simple symmetry among the four sides of the left diagram with solid lines, except that the four complex numbers $z_2 - z,\ -z - z_2,\ z_1 - (-z),\ z - z_1$ form an irregular quadrilateral. The shift $z \leftarrow z + z_m$ turns the quadrilateral into a parallelogram —the dashed lines diagram— with sides

$$\text{lower:} \qquad -z + z_m - z_1 \qquad = -z + \delta\,, \tag{11.25a}$$

$$\text{left:} \qquad -z + z_m - z_2 \qquad = -z - \delta\,, \tag{11.25b}$$

$$\text{right:} \qquad z + z_m - z_1 \qquad = \quad z + \delta\,, \tag{11.25c}$$

$$\text{upper:} \qquad z + z_m - z_2 \qquad = \quad z - \delta\,. \tag{11.25d}$$

In the dashed figure, the square root of the lower [(11.25a)] side, and the square root of the left

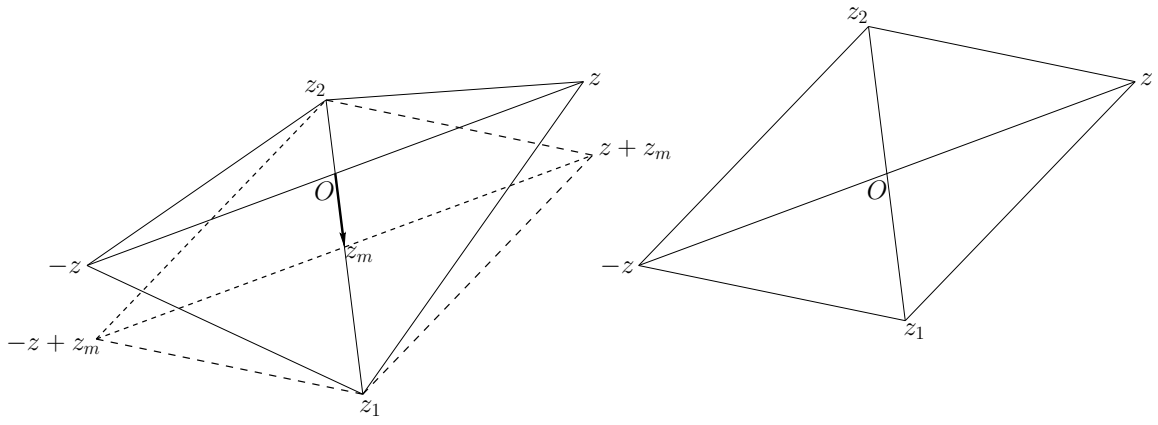



Figure 11.5: Graphical representation of the factors $\pm z - z_1$ and $\pm z - z_2$ involved in the calculation of $sQ_2(\pm z) = \sqrt{\pm z - z_1}\,\sqrt{\pm z - z_2}$ to illustrate the parity of $sQ_2(z)$. In the first diagram, the branch points $z_1$ and $z_2$ are not located symmetrically about the origin $O$ of the complex plane. A shift by $z_m = (z_1 + z_2)/2$ restores the symmetry. In the second diagram, the relative position $\delta = (z_2 - z_1)/2$ of one branch-point to the other is the same as in the first diagram, but now $z_1$ and $z_2$ are located symmetrically respect the origin. In both diagrams the same representative point $z$ is used.

[(11.25b)] side, correspond to the first two factors in Eq. (11.23a) of the calculation of $sQ_2(-z+z_m)$. After a phase factor or $\mathrm{e}^{\mathrm{i}\pi}$ is pulled out of each of them, they become parallel to the square root of the upper [(11.25d)] side, and to the square root of the right [(11.25c)] side —the terms that appear in Eq. (11.23b)—. We get a phase factor of $\mathrm{e}^{\mathrm{i}\pi/2}$ from the square root of each of the above terms, and a global phase factor of $\mathrm{e}^{\mathrm{i}\pi/2} \times \mathrm{e}^{\mathrm{i}\pi/2} = \mathrm{e}^{\mathrm{i}\pi}$. In the diagram on the right, the branch-points are

symmetrically placed about the origin and the figure has the same symmetry of the dashed lines diagram, without the need for the shift by $z_m$.

Let's call, for reference convenience, $q(z)$ the two-branch-points function for our case (see Eq. (11.8)):

$$q(z) = \sqrt{z^2+\mu^2} = \sqrt{z+\mathrm{i}\mu}\,\sqrt{z-\mathrm{i}\mu}\,. \tag{11.26}$$

The first branch-point, $-\mathrm{i}\mu$, and the second branch-point, $+\mathrm{i}\mu$, are located symmetrically about the origin on the imaginary axis, therefore the above results give that

$$q(-z) = -q(z)\,. \tag{11.27}$$

## 11.5 The integral of $\tilde{a}_0(z)\,\mathrm{e}^{zt}$ around its branch-cut $[-\mathrm{i}\mu, \mathrm{i}\mu]$

In the actual calculation of $a_0(t)$ from expression (11.19) on page 139 (reproduced below)

$$\begin{aligned} a_0(t) &= \frac{1}{2\pi\mathrm{i}}\int_{c-\mathrm{i}\infty}^{c+\mathrm{i}\infty} \tilde{a}_0(z)\,\mathrm{e}^{zt}\,\mathrm{d}z\,, \text{ (Bromwich's Integral)} \\ &= \frac{1}{2\pi\mathrm{i}}\int_{\substack{\text{around the}\\ \text{branch-cut}\,\downarrow\uparrow}} \tilde{a}_0(z)\,\mathrm{e}^{zt}\,\mathrm{d}z + \sum \text{Residues of } \left[\tilde{a}_0(z)\,\mathrm{e}^{zt}\right], \end{aligned} \tag{11.28}$$

the only involved part is the integral of $\tilde{a}_0(z)\,\mathrm{e}^{zt}$ around its branch-cut. Here, $\tilde{a}_0(z)$ is given by either of Eqs. (11.2), (11.3) or (11.5).

The branch-cut of $\tilde{a}_0(z)$ arises from taking the thermodynamic limit: We reviewed in §11.1 on page 130, how in the limit $N \to \infty$, the ensuing infinite number of poles of the continued fraction representation of $\tilde{a}_0(z)$ merge into a continuous structure signaled to be a branch-cut by the presence in $\tilde{a}_0(z)$ of the —two branch points, $\mp\mathrm{i}\mu$— function $q(z)$, reproduced in Eq. (11.26) on this page. We also showed in §11.1 that, in this case, the *only appropriate choice for the branch-cut path* is the last one of Figure 11.1 on page 131, i.e., the straight line $[-\mathrm{i}\mu, \mathrm{i}\mu]$ along the imaginary axis.

The result for $a_0(t)$ given by Eq. (11.28) on this page was obtained by the application Cauchy's residue theorem (11.10), to Bromwich's inversion formula (11.11). The first term on the rhs is the integral around the branch-cut. This term stems from the requirement that the branch-cut is excluded from the interior of the contour to which Cauchy's residue theorem is applied, as explained in §11.3 on page 136, in the paragraph just below Eq. (11.16).

In the same paragraph we discussed the shape of the contour $C_{BC}$ around the branch-cut and we showed that *any contour that only encloses the branch-cut and no other singularity* would suffice. Therefore, we picked the simplest possible contour for the integral around the branch-cut in Eq. (11.28) on the preceding page, that is, the *rod-shaped path* —in the limit of vanishing width that "hugs the cut"— shown[13] in Figure 11.3. This path is made up of the following four parts, and the choice of vanishing width requires to the limit $\epsilon \to 0^+$ to be taken in the four parts that follow:

1. The "going up" leg at the rhs of the cut, along $\mathrm{Re}z = \epsilon$, from $z = \epsilon - \mathrm{i}\mu$ to $z = \epsilon + \mathrm{i}\mu$.

2. The top semi-circumference convex upwards of radius $\epsilon$ with center at the upper branch-point $+\mathrm{i}\mu$, from $z = \epsilon + \mathrm{i}\mu$ to $z = -\epsilon + \mathrm{i}\mu$.

3. The "going down" leg at the lhs of the cut, along $\mathrm{Re}z = -\epsilon$, from $z = -\epsilon + \mathrm{i}\mu$ to $z = -\epsilon - \mathrm{i}\mu$.

4. The bottom semi-circumference convex downwards of radius $\epsilon$ with center at the lower branch-point $-\mathrm{i}\mu$, from $z = -\epsilon - \mathrm{i}\mu$ to $z = +\epsilon - \mathrm{i}\mu$.

From the expressions for $\tilde{a}_0(z)$ given in Equations (11.2), (11.3) and (11.5) at the beginning of Chapter 11 on page 128, it is readily seen that $\tilde{a}_0(z)$ evaluated at any of the branch-points, i.e., $\tilde{a}_0(\mp\,\mathrm{i}\mu)$ remains finite. Therefore, the integral of $\tilde{a}_0(z)\,\mathrm{e}^{zt}$ around each of the semi-circumferences, parts 1 and 4 above, vanishes in the limit $\epsilon \to 0^+$.

Any continuous complex function of $z$ yields zero when evaluated in the limit $\epsilon \to 0^+$ along the path "part 1 + part 3". In our case $\tilde{a}_0(z)\,\mathrm{e}^{zt}$ is discontinuous across the cut *only* because it contains the function $\sqrt{z^2+\mu^2}$ —named $q(z)$ in Eq. (11.26) on the preceding page— and $q(z)$ jumps across the cut, as explained in the paragraph that follows Equations (11.9) of §11.1 on page 132. Therefore, we have to pick from $\tilde{a}_0(z)$ the terms proportional to $q(z) \equiv \sqrt{z^2+\mu^2}$ and, to this end, we have to remove the $q(z)$'s from the denominators of $\tilde{a}_0(z)$.

[13] Note that in Eq. (11.28), the rod shaped path is traversed counter-clockwise, while in Figure 11.3 same path is traversed clockwise.

From Eq. (11.5) on page 129

$$\begin{aligned}\tilde{a}_0(z) &= \frac{2\kappa}{\lambda Q}\left[\frac{1}{(1-Q)z+\kappa\, q(z)} - \frac{1}{(1+Q)z+\kappa\, q(z)}\right], \\ &= \frac{2\kappa}{\lambda Q}\left[\frac{(1-Q)z-\kappa\, q(z)}{(1-Q)^2z^2-\kappa^2\, q^2(z)} - \frac{(1+Q)z-\kappa\, q(z)}{(1+Q)^2z^2-\kappa^2\, q^2(z)}\right], \end{aligned} \tag{11.29}$$

with the parameter $Q$ being the same given in Eq. (11.4), i.e.,

$$Q \equiv \sqrt{(1+\kappa)^2 - 4\kappa/\lambda} = \sqrt{r^2 + 4(\lambda-1)\kappa^2/\lambda^2} \tag{11.30}$$

and the parameter $r$ being quoted below in Eq. (11.33).

The zeros of the denominators above correspond to the poles of $\tilde{a}_0(z)$. We rewrite both denominators to make the zeros explicit:

$$(1\mp Q)^2z^2 - \kappa^2\, q^2(z) = (1\mp Q)^2z^2 - \kappa^2(z^2+\mu^2) = [(1\mp Q)^2 - \kappa^2]z^2 - \kappa^2\mu^2\,. \tag{11.31}$$

But,

$$\begin{aligned}(1\mp Q)^2 - \kappa^2 &= 1 + (1+\kappa)^2 - 4\kappa/\lambda \mp 2Q - \kappa^2\,, \\ &= 2 + 2\kappa - 4\kappa/\lambda \mp 2Q\,, \\ &= 2\,(\kappa + 1 - 2\kappa/\lambda \mp Q) = 2(r\mp Q)\,, \end{aligned} \tag{11.32}$$

the parameter $r$ being the same that was defined in Eq. (9.19a) on page 93. It is:

$$r \equiv \kappa + 1 - 2\kappa/\lambda\,. \tag{11.33}$$

Using Eq. (11.32) and Eq. (11.31) in Eq. (11.29) above, we get

$$\begin{aligned}\tilde{a}_0(z) &= \frac{2\kappa}{\lambda Q}\left[\frac{(1-Q)z-\kappa\, q(z)}{2(r-Q)z^2-\kappa^2\mu^2} - \frac{(1+Q)z-\kappa\, q(z)}{2(r+Q)z^2-\kappa^2\mu^2}\right], \\ &= \frac{2\kappa}{\lambda Q}\frac{1}{\kappa^2\mu^2}\left[\frac{\kappa^2\mu^2}{2(r-Q)}\frac{(1-Q)z-\kappa\, q(z)}{z^2-\frac{\kappa^2\mu^2}{2(r-Q)}} - \frac{\kappa^2\mu^2}{2(r+Q)}\frac{(1+Q)z-\kappa\, q(z)}{z^2-\frac{\kappa^2\mu^2}{2(r+Q)}}\right], \\ &= \frac{2}{\kappa\lambda\mu^2 Q}\left[s_1\,\frac{(1-Q)z-\kappa\, q(z)}{z^2-s_1} - s_2\,\frac{(1+Q)z-\kappa\, q(z)}{z^2-s_2}\right]. \end{aligned} \tag{11.34}$$

Here, $q(z) \equiv \sqrt{z^2+\mu^2}$ was named in Eq. (11.26) and its symmetries and parity were studied §11.4. The quantities $s_1$ and $s_2$ are the same given in Equations (9.18), i.e.

$$s_{\frac{1}{2}} = \frac{\kappa^2\mu^2}{2(r\mp Q)}\,, \tag{11.35a}$$

$$= \frac{\lambda^2\mu^2}{8(1-\lambda)}(r\pm Q)\,; \tag{11.35b}$$

they are the *squares* of the *sometimes-physical* poles and of the *never-physical* poles, respectively. All the poles are given in terms of $s_1$ and $s_2$ in Equations (9.17) on page 93 of §9.2. The parameters $Q$ and $r$ are quoted and reproduced in Eq. (11.30) and Eq. (11.33).

Thus, the part of $\tilde{a}_0(z)$ that "jumps" across the cut, i.e., is discontinuous across the cut, is given by the terms of Eq. (11.34) that are proportional to $q(z) = \sqrt{z^2+\mu^2}$, that is

$$\tilde{a}_0(z)|_{\text{jumps}} = \frac{2}{\lambda\mu^2 Q}\left[\frac{s_2}{z^2-s_2} - \frac{s_1}{z^2-s_1}\right] q(z) \equiv g(z)q(z)\,. \tag{11.36}$$

Here, the function $g(z)$ is defined for conciseness in the argument that follows. It is *continuous* across the branch-cut.

The function $\tilde{a}_0(z)\,\mathrm{e}^{zt}$ has to be integrated around the cut and *only* the part that "jumps" across the cut, $g(z)q(z)$, yields a non-vanishing result. We explain on page 142 the choice the rod-shaped path described and we show also that only the straight parts of the path, part 1 and part 3, are different from zero in the limit that the width of the rod-shaped path vanishes. Thus

$$\int_{\substack{\text{around the}\\ \text{branch-cut}\downarrow\uparrow}} \tilde{a}_0(z)\,\mathrm{e}^{zt}\,\mathrm{d}z = \int_{\substack{\text{part1+part3}\\ \text{vanishing width}}} g(z)q(z)\,\mathrm{e}^{zt}\,\mathrm{d}z = \tag{11.37a}$$

$$= \lim_{\epsilon\to 0^+}\left[\int_{-\mu}^{\mu} g(\epsilon+\mathrm{i}\,y)q(\epsilon+\mathrm{i}\,y)\,\mathrm{e}^{(\epsilon+\mathrm{i}\,y)t}\,\mathrm{i}\,\mathrm{d}y + \int_{\mu}^{-\mu} g(-\epsilon+\mathrm{i}\,y)q(-\epsilon+\mathrm{i}\,y)\,\mathrm{e}^{(-\epsilon+\mathrm{i}\,y)t}\,\mathrm{i}\,\mathrm{d}y\right], \tag{11.37b}$$

we make the dummy integration variable change $y \leftarrow -y$ in the second integral:

$$= \lim_{\epsilon\to 0^+}\left[\int_{-\mu}^{\mu} g(\epsilon+\mathrm{i}\,y)q(\epsilon+\mathrm{i}\,y)\,\mathrm{e}^{(\epsilon+\mathrm{i}\,y)t}\,\mathrm{i}\,\mathrm{d}y + \int_{-\mu}^{\mu} g(-\epsilon-\mathrm{i}\,y)[-q(-\epsilon-\mathrm{i}\,y)]\,\mathrm{e}^{(-\epsilon-\mathrm{i}\,y)t}\,\mathrm{i}\,\mathrm{d}y\right], \tag{11.37c}$$

*only* q(z) is discontinuous across the cut:

$$= \int_{-\mu}^{\mu} g(\mathrm{i}\,y)q(0^+ + \mathrm{i}\,y)\,\mathrm{e}^{\mathrm{i}yt}\,\mathrm{i}\,\mathrm{d}y + \int_{-\mu}^{\mu} g(-\mathrm{i}\,y)[-q(0^- - \mathrm{i}\,y)]\,\mathrm{e}^{-\mathrm{i}yt}\,\mathrm{i}\,\mathrm{d}y\,, \tag{11.37d}$$

and we use Eq. (11.27) on page 141, i.e., $-q(-z) = q(z)$

$$= \int_{-\mu}^{\mu} g(\mathrm{i}\,y)q(0^+ + \mathrm{i}\,y)\,\mathrm{e}^{\mathrm{i}yt}\,\mathrm{i}\,\mathrm{d}y + \int_{-\mu}^{\mu} g(-\mathrm{i}\,y)q(0^+ + \mathrm{i}\,y)\,\mathrm{e}^{-\mathrm{i}yt}\,\mathrm{i}\,\mathrm{d}y\,, \tag{11.37e}$$

but, $g(z)$ defined in Eq. (11.36) on the current page is even in $z$ and the integration interval $[-\mu,\mu]$ is also even, so we may write $\mathrm{e}^{\pm\,\mathrm{i}\,yt}$ indifferently in either of the two previous integrals

$$\int_{\substack{\text{part1+part3}\\ \text{vanishing width}}} g(z)q(z)\,\mathrm{e}^{zt}\,\mathrm{d}z = 2\int_{-\mu}^{\mu} g(\mathrm{i}\,y)q(0^+ + \mathrm{i}\,y)\,\mathrm{e}^{\mathrm{i}yt}\,\mathrm{i}\,\mathrm{d}y\,. \tag{11.37f}$$

One has to keep the $0^+$ in the argument of $q(z) \equiv \sqrt{z^2+\mu^2}$ to keep track of the physical sheet near the branch-cut. For example, if $|y| < \mu$

$$q(0^+ + \mathrm{i}\, y) = + \left|\sqrt{\mu^2 - y^2}\right| , \tag{11.38a}$$

while

$$q(0^- + \mathrm{i}\, y) = - \left|\sqrt{\mu^2 - y^2}\right| . \tag{11.38b}$$

If $\mu < |y|$, the jump does not happen. All this follows from the results of §11.1 and §11.4. The —continuous across the branch-cut— function $g(z)$ is given in Eq. (11.36) on the preceding page and the integral of $\tilde{a}_0(z)\, \mathrm{e}^{zt}$ around the cut, written out explicitly is

$$\int_{\substack{\text{around the}\\ \text{branch-cut}\downarrow\uparrow}} \tilde{a}_0(z)\, \mathrm{e}^{zt}\, \mathrm{d}z = \frac{4\,\mathrm{i}}{\lambda\mu^2 Q} \int_{-\mu}^{\mu} \left[\frac{s_1}{y^2+s_1} - \frac{s_2}{y^2+s_2}\right] \sqrt{\mu^2-y^2}\; \mathrm{e}^{\mathrm{i}yt}\, \mathrm{d}y\,, \tag{11.39}$$

with $s_1$ and $s_2$ being the squares of the *sometimes-physical* and *never-physical* poles, respectively. They scale with $\mu^2$, i.e., are proportional to $\mu^2$ and depend on the parameters $\kappa$ and $\lambda$ as shown in Eqs. (11.35). $Q$ is quoted in Eq. (11.30).

This expression, Eq. (11.39) above, is useful whenever the poles are present, that is, at *most points*[14] of the $(\kappa, \lambda)$ phase diagram of the poles. (See Figs. 9.1-9.2 on pages 94 and 96 in §9.3). We have not been able to find a general closed expression for this integral, however, an integral representation of the Bessel function $\mathrm{J}_\nu(\zeta)$ [Abramowitz & Stegun 1972, p. 360, Eq. 9.1.20], [Watson 1944, Chapter 6, p. 160]

$$\mathrm{J}_\nu(\zeta) = \frac{(\frac{1}{2}\zeta)^\nu}{\pi^{1/2}\Gamma(\nu+\frac{1}{2})} \int_{-1}^{1} (1-\eta^2)^{\nu-\frac{1}{2}}\, \mathrm{e}^{\mathrm{i}\zeta\eta}\, \mathrm{d}\eta\,, \quad \mathrm{Re}\,\nu > -\tfrac{1}{2}\,, \tag{11.40}$$

has allowed us to evaluate Eq. (11.39) above for certain sets of the $(\kappa, \lambda)$ parameters, after each of the two fractions in the square brackets is expanded in a series of positive powers of the variable $y$. Both series have to be convergent[15] over the whole range $[-\mu, \mu]$ of the integration variable $y$.

[14] Only at certain points, lines or curves the poles "disappear": they either move to the edge of the branch-cut, or out to infinity, as explained in §9.3.

[15] To be able to integrate both series term by term, as we will need later, *uniform convergence* is enough. If we want change the order of the terms or operate on them with another series, e.g., multiply by another series, we also need *absolute convergence*.The *uniform convergence* of a series in a domain does not require its *absolute convergence* at any points of the domain, nor conversely. See, especially, [Whittaker & Watson 1927, §3.3, p. 48]

We have achieved this[16] in regions of the $(\kappa, \lambda)$ phase diagram of the poles such that, each $s_1$ and $s_2$, satisfies *either one* of the following conditions. In what follows $s$ will designate either one of $s_1$ and $s_2$.

- $\mu^2 < |s|$. This condition allows us to write

$$\frac{s}{y^2+s} = \frac{1}{1+y^2/s} = \sum_{k=0}^{\infty}(-1)^k \left(\frac{y^2}{s}\right)^k . \tag{11.41}$$

  Since $-\mu < y < \mu \,, \implies y^2 < \mu^2 < |s| \,, \implies$ the series is *absolutely convergent*.

- $\mu^2 < |\mu^2 + s|$. In this case, the condition allows us to write

$$\frac{s}{y^2+s} = \frac{s}{s+\mu^2-(\mu^2-y^2)} = \frac{s/(s+\mu^2)}{1-\frac{\mu^2-y^2}{s+\mu^2}} = \frac{s}{s+\mu^2}\sum_{k=0}^{\infty}\left(\frac{\mu^2-y^2}{s+\mu^2}\right)^k . \tag{11.42}$$

  Again, since $-\mu < y < \mu \,, \implies 0 < \mu^2 - y^2 < \mu^2 < |\mu^2 + s| \,, \implies$ this series is *absolutely convergent*.

To evaluate the integral in Eq. (11.39) we need to integrate term by term both series above, thus, they must be *uniformly convergent*. The so called *M*-test, devised by [Weierstrass 1886, p. 70], is a *sufficient* though *not necessary* [Whittaker & Watson 1927, p. 49, §3.34] condition for *uniform convergence*. It is enunciated below by

> [Whittaker & Watson 1927, p. 49, §3.34]: If, for all values of $z$ within a domain, the moduli of the terms of a series
>
> $$S = u_1(z) + u_2(z) + u_3(z) + \ldots \tag{11.43a}$$
>
> are respectively less than the corresponding terms in a convergent series of positive terms
>
> $$T = M_1 + M_2 + M_3 + \ldots \tag{11.43b}$$
>
> where $M_n$ is *independent* of $z$, then the series $S$ is *uniformly convergent* and also is *absolutely convergent* by the *Comparison Theorem* [Whittaker & Watson 1927, §2.34, p. 20].

[16] In fact, each of the following conditions is *sufficient* to guarantee *absolute convergence*, as we shall see below.

The range of integration variable $y$ is $-\mu < y < \mu$ for both series Eqs. (11.41)–(11.42). Then the absolute value of the general term of the first series, Eq. (11.41), satisfies

$$\left|\frac{y^2}{s}\right|^k = \left(\frac{y^2}{|s|}\right)^k < \left(\frac{\mu^2}{|s|}\right)^k = M_k^{(1)}. \tag{11.44}$$

The series $\sum_{k=0}^{\infty} M_k^{(1)}$ is convergent by the $\mu^2 < |s|$ condition and therefore the first series, Eq. (11.41) on the previous page, is *uniformly convergent* by the $M$-test, Eqs. (11.43).

For the second series, the absolute value of its general term fulfills

$$\left|\frac{\mu^2 - y^2}{s + \mu^2}\right|^k < \left|\frac{\mu^2}{s + \mu^2}\right|^k = M_k^{(2)}. \tag{11.45}$$

The series $\sum_{k=0}^{\infty} M_k^{(2)}$ is convergent by the $\mu^2 < |\mu^2 + s|$ condition, $\Longrightarrow$ the second series, Eq. (11.42) on the preceding page, is also *uniformly convergent* by the $M$-test, Eqs. (11.43).

In the next section we provide an example of the application of the two series expansions, Eqs. (11.41)–(11.42) to a representative zone of the $(\kappa, \lambda)$ phase diagram of the poles.

## 11.6 An example of the power series expansion of the integral of $\tilde{a}_0(z)\, \mathrm{e}^{zt}$ around its branch-cut $[-\mathrm{i}\mu, \mathrm{i}\mu]$

To illustrate the power series expansions, Eqs. (11.41)–(11.42), we obtained in the previous section in order to perform the integral of $\tilde{a}_0(z)\, \mathrm{e}^{zt}$ around its branch-cut, Eq. (11.39) on page 145, we chose a region such that the two conditions below were satisfied

- The squares of the *sometimes-physical* (SP) poles $s_1$ are real and

$$s_1 < -\mu^2, \tag{11.46}$$

  in other words, the SP poles are located symmetrically in the imaginary axis outside the branch-cut $[-\mu, \mu]$. The parameter $\mu = 2\Omega = 2\sqrt{k/m}$ was defined in Eq. (9.14) on page 92.

- The squares of the *never-physical* (NP) poles are real and positive

$$0 < s_2\,, \tag{11.47}$$

  the same as saying that the NP poles are located symmetrically in the real axis.

In §9.3 we described the behavior of the isolated singularities (poles) of $\tilde{a}_0(z)$ in terms of the parameters $\kappa$ and $\lambda$ (defined in Eqs. (7.2)-(7.3) on page 60), and the squares of the SP and NP poles, i.e., $s_1$ and $s_2$ respectively, are quoted in Eqs. (11.35).

According to the phase-diagram of the SP poles, Figure 9.1 of §9.3, the SP poles are *located symmetrically in the imaginary axis* in $\{\text{Zone IV+I}\}^{(1)}$ *and* in $\{\text{Zone III+II}\}^{(1)}$ of this first diagram. In $\{\text{Zone III+II}\}^{(1)}$ the SP poles are on the *physical* sheet, whilst in $\{\text{Zone IV+I}\}^{(1)}$ they are on the *non-physical* sheet. So,

$$s_1 < -\mu^2 \;\; \underline{\text{when}} \;\; (\kappa, \lambda) \in \{\text{Zone IV+I}\}^{(1)} \cup \{\text{Zone III+II}\}^{(1)}. \tag{11.48a}$$

In the case of the NP poles their phase-diagram, Figure 9.2, shows that

$$0 < s_2 \;\; \underline{\text{when}} \;\; (\kappa, \lambda) \in \{\text{Zone V+IV+III}\}^{(2)} \tag{11.48b}$$

of this second figure. Inspection of both figures reveals that the intersection the regions addressed in Equations (11.48) above is simply $\lambda > 1$. In summary

$$s_1 < -\mu^2 \;\; \underline{\text{and}} \;\; 0 < s_2\,, \;\; \underline{\text{when}} \;\; \lambda > 1\,. \tag{11.49}$$

We have thus shown that in the $\lambda > 1$ region, $s_1$ and $s_2$ comply with either of the conditions that we obtained in (11.41)-(11.42) in the last section as prerequisites to be able to expand in series the partial fractions that appear in the square bracket factor of Eq. (11.39). Now, we proceed to apply the expansions (11.41)-(11.42) to our example.

For the first partial fraction inside the square brackets of Eq. (11.39), we write

$$\frac{s_1}{y^2 + s_1} = \frac{1}{1 + y^2/s_1} = \sum_{k=0}^{\infty} (-1)^k (y^2/s_1)^k = \sum_{k=0}^{\infty} (y^2/|s_1|)^k\,. \tag{11.50}$$

Eq. (11.39) states that $-\mu < y < \mu$; this, together with Eq. (11.49) gives $y^2 < \mu^2 < |s_1|\,, \Longrightarrow$ the series above is *absolutely convergent*. This series is a particular instance of Eq. (11.41) and consequently by Eq. (11.44), and the $M$-test, Eqs. (11.43), it is also *uniformly convergent*.

In Eq. (11.39), it is convenient to make the integration variable change

$$y \leftarrow \mu\,\eta\,, \tag{11.51}$$

and the substitution

$$s_{\frac{1}{2}} = \mu^2 \sigma_{\frac{1}{2}}\,, \tag{11.52}$$

to write

$$\int_{\substack{\text{around the}\\ \text{branch-cut}\downarrow\uparrow}} \tilde{a}_0(z)\,\mathrm{e}^{zt}\,\mathrm{d}z = \frac{4\,\mathrm{i}}{\lambda Q}\int_{-1}^{1}\left[\frac{\sigma_1}{\eta^2+\sigma_1} - \frac{\sigma_2}{\eta^2+\sigma_2}\right]\sqrt{1-\eta^2}\;\mathrm{e}^{\mathrm{i}\mu t\eta}\,\mathrm{d}\eta\,. \tag{11.53}$$

Making the substitutions (11.51)-(11.52) into the series expansion (11.50), it reads

$$\frac{s_1}{y^2+s_1} = \frac{\sigma_1}{\eta^2+\sigma_1} = \frac{1}{1+\eta^2/\sigma_1} = \sum_{k=0}^{\infty}(-1)^k(\eta^2/\sigma_1)^k = \sum_{k=0}^{\infty}(\eta^2/|\sigma_1|)^k\,. \tag{11.54}$$

We now introduce this series expansion, into the first term on the right of Eq. (11.53) above. The uniform convergence of this series allows us to exchange the summation and integration signs to get

$$\frac{4\,\mathrm{i}}{\lambda Q}\int_{-1}^{1}\frac{\sigma_1}{\eta^2+\sigma_1}\sqrt{1-\eta^2}\;\mathrm{e}^{\mathrm{i}\mu t\eta}\,\mathrm{d}\eta = \frac{4\,\mathrm{i}}{\lambda Q}\sum_{k=0}^{\infty}\int_{-1}^{1}\left(\frac{\eta^2}{|\sigma_1|}\right)^k\sqrt{1-\eta^2}\;\mathrm{e}^{\mathrm{i}\mu t\eta}\,\mathrm{d}\eta\,. \tag{11.55}$$

To use the integral representation of the Bessel functions, Eq. (11.40) on page 145, we have to leave inside the integral above only the square root $\sqrt{1-\eta^2}$, and the exponential $\mathrm{e}^{\mathrm{i}\mu t\eta}$. Note that

$$\left(\frac{\eta^2}{|\sigma_1|}\right)^k \mathrm{e}^{\mathrm{i}\mu t\eta} = \left(\frac{-\partial^2}{|\sigma_1|\partial(\mu t)^2}\right)^k \mathrm{e}^{\mathrm{i}\mu t\eta}\,, \tag{11.56}$$

allowing us then to take the factor $(\eta^2/|\sigma_1|)^k$ out of the integral:

$$\begin{aligned}
&\frac{4\,\mathrm{i}}{\lambda Q}\int_{-1}^{1}\frac{\sigma_1}{\eta^2+\sigma_1}\sqrt{1-\eta^2}\;\mathrm{e}^{\mathrm{i}\mu t\eta}\,\mathrm{d}\eta\\
&= \frac{4\,\mathrm{i}}{\lambda Q}\sum_{k=0}^{\infty}\left(\frac{-\partial^2}{|\sigma_1|\partial(\mu t)^2}\right)^k\int_{-1}^{1}\sqrt{1-\eta^2}\;\mathrm{e}^{\mathrm{i}\mu t\eta}\,\mathrm{d}\eta\,,\\
&= \frac{4\,\mathrm{i}}{\lambda Q}\sum_{k=0}^{\infty}\left(\frac{-\partial^2}{|\sigma_1|\partial(\mu t)^2}\right)^k\left\{\frac{\pi^{1/2}\Gamma(1+\frac{1}{2})}{(\frac{1}{2}\mu t)^1}\left[\frac{(\frac{1}{2}\mu t)^1}{\pi^{1/2}\Gamma(1+\frac{1}{2})}\int_{-1}^{1}(1-\eta^2)^{1-1/2}\;\mathrm{e}^{\mathrm{i}\mu t\eta}\,\mathrm{d}\eta\right]\right\}.
\end{aligned} \tag{11.57}$$

Comparing the above expression with the integral representation of the Bessel functions, Eq. (11.40), we see that the term inside the square brackets is just $\mathrm{J}_1(\mu t)$. Also, from [Abramowitz & Stegun 1972, §6.1, p. 255], $\Gamma(\frac{1}{2}) = \pi^{1/2}$ and $\Gamma(z+1) = z\,\Gamma(z), \Longrightarrow \Gamma(\frac{1}{2}+1) = \frac{1}{2}\pi^{1/2}$. Thus

$$\frac{4\,\mathrm{i}}{\lambda Q}\int_{-1}^{1}\frac{\sigma_1}{\eta^2+\sigma_1}\sqrt{1-\eta^2}\;\mathrm{e}^{\mathrm{i}\mu t\eta}\,\mathrm{d}\eta = \frac{4\pi\mathrm{i}}{\lambda Q}\sum_{k=0}^{\infty}\left(\frac{-\partial^2}{|\sigma_1|\partial(\mu t)^2}\right)^k\frac{\mathrm{J}_1(\mu t)}{\mu t}\,. \tag{11.58}$$

For the second partial fraction inside the square brackets of Eq. (11.39), we write

$$\frac{s_2}{y^2+s_2} = \frac{s_2}{s_2+\mu^2-(\mu^2-y^2)} = \frac{s_2/(s_2+\mu^2)}{1-\frac{\mu^2-y^2}{s_2+\mu^2}} = \frac{s_2}{s_2+\mu^2}\sum_{k=0}^{\infty}\left(\frac{\mu^2-y^2}{s_2+\mu^2}\right)^k. \tag{11.59}$$

Again, Eq. (11.39) states that $-\mu < y < \mu$, this, together with Eq. (11.49) on page 148 gives $0 < \mu^2 - y^2 < \mu^2 < s_2 + \mu^2$, $\Longrightarrow$ the series above is *absolutely convergent*. This series is a special instance of Eq. (11.42) on page 146 of the last section, consequently, by Eq. (11.45) and the $M$-test, Eqs. (11.43), this series is also *uniformly convergent*.

We made the substitutions, Eqs. (11.51)–(11.52), into Eq. (11.39) to get Eq. (11.53). Making the same substitutions into the series above

$$\frac{s_2}{y^2+s_2} = \frac{\sigma_2}{\eta^2+\sigma_2} = \frac{\sigma_2}{\sigma_2+1}\sum_{k=0}^{\infty}\left(\frac{1-\eta^2}{\sigma_2+1}\right)^k. \tag{11.60}$$

We introduce this series into the second term on the r.h.s of Eq. (11.53) and exchange the summation and integration signs on account of the *uniform convergence* of this series

$$\begin{aligned}
&\frac{4\,\mathrm{i}}{\lambda Q}\int_{-1}^{1}\frac{\sigma_2}{\eta^2+\sigma_2}\sqrt{1-\eta^2}\;\mathrm{e}^{\mathrm{i}\mu t\eta}\,\mathrm{d}\eta \\
&= \frac{4\,\mathrm{i}}{\lambda Q}\frac{\sigma_2}{\sigma_2+1}\sum_{k=0}^{\infty}\int_{-1}^{1}\left(\frac{1-\eta^2}{\sigma_2+1}\right)^k\sqrt{1-\eta^2}\;\mathrm{e}^{\mathrm{i}\mu t\eta}\,\mathrm{d}\eta\,, \\
&= \frac{4\,\mathrm{i}\,\sigma_2}{\lambda Q}\sum_{k=0}^{\infty}\frac{\pi^{1/2}\Gamma(k+3/2)}{(\sigma_2+1)^{k+1}(\tfrac{1}{2}\mu t)^{k+1}}\left[\frac{(\frac{1}{2}\mu t)^{k+1}}{\pi^{1/2}\Gamma(k+1+\frac{1}{2})}\int_{-1}^{1}(1-\eta^2)^{k+1-1/2}\;\mathrm{e}^{\mathrm{i}\mu t\eta}\,\mathrm{d}\eta\right].
\end{aligned} \tag{11.61}$$

Again, comparing the above expression with the integral representation of the Bessel functions, Eq. (11.40), we see that the term inside the square brackets is just $\mathrm{J}_{k+1}(\mu t)$, therefore

$$\frac{4\,\mathrm{i}}{\lambda Q}\int_{-1}^{1}\frac{\sigma_2}{\eta^2+\sigma_2}\sqrt{1-\eta^2}\;\mathrm{e}^{\mathrm{i}\mu t\eta}\,\mathrm{d}\eta = \frac{4\pi^{1/2}\,\mathrm{i}\,\sigma_2}{\lambda Q}\sum_{k=0}^{\infty}\frac{2^{k+1}\Gamma(k+3/2)}{(\sigma_2+1)^{k+1}}\,\frac{\mathrm{J}_{k+1}(\mu t)}{(\mu t)^{k+1}} \tag{11.62}$$

Collecting the results of Eq. (11.58) and Eq. (11.62) we obtain

$$\begin{aligned}
&\int_{\substack{\text{around the}\\ \text{branch-cut}}\downharpoonleft\upharpoonright}\tilde{a}_0(z)\,\mathrm{e}^{zt}\,\mathrm{d}z \\
&= \frac{4\pi\mathrm{i}}{\lambda Q}\sum_{k=0}^{\infty}\left(\frac{-\partial^2}{|\sigma_1|\partial(\mu t)^2}\right)^k\frac{\mathrm{J}_1(\mu t)}{\mu t} - \frac{4\pi^{1/2}\,\mathrm{i}\,\sigma_2}{\lambda Q}\sum_{k=0}^{\infty}\frac{2^{k+1}\Gamma(k+3/2)}{(\sigma_2+1)^{k+1}}\,\frac{\mathrm{J}_{k+1}(\mu t)}{(\mu t)^{k+1}}\,,
\end{aligned} \tag{11.63}$$

or

$$\begin{aligned}
&\frac{\lambda Q}{4\pi\mathrm{i}}\int_{\substack{\text{around the}\\ \text{branch-cut}}\downharpoonleft\upharpoonright}\tilde{a}_0(z)\,\mathrm{e}^{zt}\,\mathrm{d}z \\
&\qquad = \sum_{k=0}^{\infty}\left[\left(\frac{-\partial^2}{|\sigma_1|\partial(\mu t)^2}\right)^k\frac{\mathrm{J}_1(\mu t)}{\mu t} - \frac{\sigma_2}{\pi^{1/2}}\,\frac{2^{k+1}\Gamma(k+3/2)}{(\sigma_2+1)^{k+1}}\,\frac{\mathrm{J}_{k+1}(\mu t)}{(\mu t)^{k+1}}\right].
\end{aligned} \tag{11.64}$$

We remind ourselves that this expression is valid only when $\lambda > 1$ (See Eq. (11.49)).

## 11.7 The sum of the residues of $\tilde{a}_0(z)\,\mathrm{e}^{zt}$

To obtain $a_0(t)$ from the expression (11.19) on page 139 (reproduced below for convenience)

$$\begin{aligned} a_0(t) &= \frac{1}{2\pi\mathrm{i}}\int_{c-\mathrm{i}\infty}^{c+\mathrm{i}\infty}\tilde{a}_0(z)\,\mathrm{e}^{zt}\,\mathrm{d}z\,, \text{ (Bromwich's Integral)} \\ &= \frac{1}{2\pi\mathrm{i}}\int_{\substack{\text{around the}\\ \text{branch-cut}\downarrow\uparrow}}\tilde{a}_0(z)\,\mathrm{e}^{zt}\,\mathrm{d}z + \sum \text{Residues of}\left[\tilde{a}_0(z)\,\mathrm{e}^{zt}\right], \end{aligned} \tag{11.65}$$

we still need to calculate the $\sum$ Residues of $\left[\tilde{a}_0(z)\,\mathrm{e}^{zt}\right]$ term. The integral around the branch-cut was calculated in the example of the last section for the region $\lambda > 1$.

In §9.3 we obtained the isolated singularities (only poles) of $\tilde{a}_0(z)$ in Equations (9.17) on page 93, and described their behavior of in terms of the parameters $\kappa$ and $\lambda$ (defined in Eqs. (7.2)-(7.3) on page 60). They are the *sometimes-physical* (SP) poles:

$$z_{\substack{1\\2}} = \pm\sqrt{s_1}\,, \tag{11.66}$$

and the *never-physical* (NP) poles:

$$z_{\substack{3\\4}} = \pm\sqrt{s_2}\,, \tag{11.67}$$

with $s_{\substack{1\\2}}$ defined in Eq. (9.18) and quoted in Eq. (11.35) on page 143.

The $\sum$ Residues of $\left[\tilde{a}_0(z)\,\mathrm{e}^{zt}\right]$ term, only contributes for the *sometimes-physical* (SP) poles when these are on the *physical-sheet*. According to the phase-diagram of the SP poles, Fig. 9.1 on page 94, this happens only when

$$(\kappa,\lambda) \in \{\text{Zone III+II}\} \tag{11.68a}$$

of this diagram. In this zone

$$s_1 < -\mu^2 \tag{11.68b}$$

and $z_1$ and $z_2$ are located symmetrically on the imaginary axis of the physical sheet, outside the branch-cut[17] $[-\mu,\mu]$. The parameter $\mu = 2\sqrt{k/m} = 2\Omega$ was defined in Eq. (9.14) on page 92.

To calculate the residues the most convenient form of $\tilde{a}_0(z)$ is that given in Eq. (11.34), which we reproduce below for convenience

$$\tilde{a}_0(z) = \frac{2}{\kappa\lambda\mu^2 Q}\left[s_1\,\frac{(1-Q)z - \kappa\,q(z)}{z^2 - s_1} - s_2\,\frac{(1+Q)z - \kappa\,q(z)}{z^2 - s_2}\right]. \tag{11.69}$$

[17] $[-\mu,\mu]$ is the only possible and consistent choice for the branch-cut. See §11.1.

$Q$ is quoted in Eq. (11.30) and $q(z) = \sqrt{z^2+\mu^2}$ was defined in Eq. (11.26). Only the first term above contributes to the residues of $\tilde{a}_0(z)\,\mathrm{e}^{zt}$ at the SP poles. At $z = z_1$

$$\begin{aligned}\mathrm{Res}\big[\tilde{a}_0(z)\,\mathrm{e}^{zt}\big]_{z=z_1} &= \lim_{z\to z_1}(z-z_1)\tilde{a}_0(z)\,\mathrm{e}^{zt} = \lim_{z\to z_1}(z-z_1)\frac{2}{\kappa\lambda\mu^2 Q}z_1^2\frac{(1-Q)z-\kappa\,q(z)}{z^2-z_1^2}\,\mathrm{e}^{zt}\,,\\ &= \lim_{z\to z_1}\frac{2}{\kappa\lambda\mu^2 Q}z_1^2\frac{(1-Q)z-\kappa\,q(z)}{(z+z_1)}\,\mathrm{e}^{zt}\,,\\ &= \frac{z_1}{\kappa\lambda\mu^2 Q}\left[(1-Q)z_1-\kappa\,q(z_1)\right]\mathrm{e}^{z_1 t}\,. \end{aligned} \tag{11.70a}$$

For the residue at $z = z_2 = -z_1$

$$\begin{aligned}\mathrm{Res}\big[\tilde{a}_0(z)\,\mathrm{e}^{zt}\big]_{z=-z_1} &= \frac{-z_1}{\kappa\lambda\mu^2 Q}\left[(1-Q)(-z_1)-\kappa\,q(-z_1)\right]\mathrm{e}^{-z_1 t}\,,\\ &= \frac{z_1}{\kappa\lambda\mu^2 Q}\left[(1-Q)z_1-\kappa\,q(z_1)\right]\mathrm{e}^{-z_1 t}\,. \end{aligned} \tag{11.70b}$$

In the last line of Eq. (11.70b) above, we used the fact that $q(z)$ is an odd function of $z$, i.e.

$$q(-z) = -q(z)\,. \tag{11.71}$$

This was obtained in Eq. (11.27) on page 141 of §11.4.

The expression for $\tilde{a}_0(z)$ decomposed in two partial fractions in which the $q(z) = \sqrt{z^2+\mu^2}$ has <u>not</u> been removed from the denominators, Eq. (11.5) on page 129 (that we reproduce below for reference convenience)

$$\tilde{a}_0(z) = \frac{2\kappa}{\lambda Q}\left[\frac{1}{(1-Q)z+\kappa\sqrt{z^2+\mu^2}} - \frac{1}{(1+Q)z+\kappa\sqrt{z^2+\mu^2}}\right]. \tag{11.72}$$

permits us to enlighten the results of Eqs. (11.70). The derivation of Eq. (11.69), which is given in Eq. (11.34), shows that the denominator of the first term of Eq. (11.72) vanishes at $z = z_{\frac{1}{2}} = \pm z_1$

$$(1-Q)z_{\frac{1}{2}} + \kappa\sqrt{z_{\frac{1}{2}}^2+\mu^2} = 0\,, \tag{11.73a}$$

thus

$$(1-Q)z_{\frac{1}{2}} = -\kappa\sqrt{z_{\frac{1}{2}}^2+\mu^2} = -\kappa\,q(z_{\frac{1}{2}})\,. \tag{11.73b}$$

In Eqs. (11.73) above we used again Eq. (11.71) on the current page, i.e., $q(-z) = -q(z)$. This allows us to write for the residues we obtained in Eqs. (11.70)

$$\mathrm{Res}\big[\tilde{a}_0(z)\,\mathrm{e}^{zt}\big]_{z=\pm z_1} = \frac{-2}{\lambda\mu^2 Q}\,z_1\,q(z_1)\;\mathrm{e}^{\pm z_1 t}\,, \tag{11.74}$$

and the sum of the residues as

$$\sum \text{Residues of } \left[\tilde{a}_0(z)\,\mathrm{e}^{zt}\right] = \frac{-2}{\lambda\mu^2 Q}\, z_1\, q(z_1)\,(\mathrm{e}^{z_1 t} + \mathrm{e}^{-z_1 t})\,. \tag{11.75}$$

We remind ourselves that the residues only need to be calculated, Eqs. (11.68) on page 151, when the SP poles are on the physical sheet. Then $s_1 < -\mu^2$, and $z_1$ given in Eq. (11.66) is

$$z_1 = \sqrt{s_1} = \mathrm{i}\sqrt{-s_1} = \mathrm{i}\sqrt{|s_1|} = \mathrm{i}\,\omega_1\,, \tag{11.76}$$

with

$$\omega_1 \equiv \sqrt{|s_1|}\,. \tag{11.77}$$

Using the results of §11.4

$$\begin{aligned} q(z_1) &= \sqrt{z_1^2 + \mu^2} = \sqrt{s_1 + \mu^2} = \mathrm{i}\sqrt{-s_1 - \mu^2} = \mathrm{i}\sqrt{|s_1| - \mu^2}\,, \\ &= \mathrm{i}\sqrt{\omega_1^2 - \mu^2}\,. \end{aligned} \tag{11.78}$$

Here, $s_1 < -\mu^2 \Longrightarrow \omega_1^2 > \mu^2$. The sum of the residues, Eq. (11.75) above, may be written then as

$$\begin{aligned} \sum \text{Residues of } \left[\tilde{a}_0(z)\,\mathrm{e}^{zt}\right] &= \frac{-2}{\lambda\mu^2 Q}\;\mathrm{i}\,\omega_1\;\mathrm{i}\sqrt{\omega_1^2 - \mu^2}\,(\mathrm{e}^{\mathrm{i}\,\omega_1 t} + \mathrm{e}^{-\mathrm{i}\,\omega_1 t})\,, \\ &= \frac{4}{\lambda\mu^2 Q}\,\omega_1\sqrt{\omega_1^2 - \mu^2}\,\cos\omega_1 t\,. \end{aligned} \tag{11.79}$$

Collecting the results of Eq. (11.64) on page 150 and Eq. (11.79) above, we obtain for $a_0(t)$ given in the expression (11.19) on page 139

$$\begin{aligned} a_0(t) &= \frac{1}{2\pi\mathrm{i}}\int_{c-\mathrm{i}\infty}^{c+\mathrm{i}\infty} \tilde{a}_0(z)\,\mathrm{e}^{zt}\,\mathrm{d}z\,,\ \text{(Bromwich's Integral)} \\ &= \frac{1}{2\pi\mathrm{i}}\int_{\substack{\text{around the}\\ \text{branch-cut}\downarrow\uparrow}} \tilde{a}_0(z)\,\mathrm{e}^{zt}\,\mathrm{d}z + \sum \text{Residues of } \left[\tilde{a}_0(z)\,\mathrm{e}^{zt}\right], \\ &= \frac{2}{\lambda Q}\left\{\sum_{k=0}^{\infty}\left[\left(\frac{-\partial^2}{|\sigma_1|\partial(\mu t)^2}\right)^k \frac{\mathrm{J}_1(\mu t)}{\mu t} - \frac{\sigma_2}{\pi^{1/2}}\,\frac{2^{k+1}\Gamma(k+3/2)}{(\sigma_2+1)^{k+1}}\,\frac{\mathrm{J}_{k+1}(\mu t)}{(\mu t)^{k+1}}\right]\right. \\ &\qquad \left. + \frac{2\omega_1}{\mu^2}\sqrt{\omega_1^2 - \mu^2}\,\cos\omega_1 t\right\}. \end{aligned} \tag{11.80}$$

The series expansion in this last example is valid only when $\lambda > 1$, and the last term only has to be taken into account for the poles in the physical sheet: See Eqs. (11.68) on page 151.

# Chapter 12

## Irreversibility and ergodicity of the harmonic oscillator chain (HOC) with one end-impurity coupled to a fixed wall (ICFW)

We have been able to obtain in Chapter 9 an *exact* and *general* (valid for all values the system parameters) solution for $\tilde{a}_0(z)$, i.e., the Laplace transform of the autocorrelation function

$$a_0(t) = \frac{(p_0, p_0(t))}{(p_0, p_0)}\,, \tag{12.1}$$

first defined in Eq. (2.12) on page 8 in §2.4. Here, $p_0$ is the momentum of the mass next to the fixed wall and $(\ ,\ )$ is the Kubo scalar product defined in Eq. (2.1) and Eqs. (7.37)–(7.38).

The solution was obtained by means of M. Howard Lee's Recurrence Relations Method (RRM) [reviewed in §§2.1-2.4] as a continued fraction that —in the thermodynamic limit— we were also able to sum and thus attain a closed form. This exact solution opens the possibility of analysing whether the system presents reversible or irreversible behavior and also allows testing the system for ergodicity.

The present state of the research related to the ergodic hypotheses (EH) is most clearly summarized by M. Howard Lee in

> [Lee 2007*b*, §1, pp. 1837-1838] ... Statistical mechanics is built on two important foundations: Gibbs' ensemble theory and Boltzmann's ergodic hypotheses. The ensemble theory is used almost exclusively in statistical mechanical calculations, so that its validity is beyond question. The *ergodic hypotheses* (EH) is generally assumed to be valid but it rests on much less firm ground. In many places one reads that it is not universally valid [Landsberg 1990, p. 139]. There have been shown that in certain models it actually fails based on the arguments of inequalities [Mazur 1969], [Suzuki 1971]. These uncertainties make it all the more necessary that we need to put the study of the validity of EH in the forefront of our attention.

> The difficulty of proving or disproving EH in a many body system in thermal equilibrium is well known [ter Haar 1960, p. 333]. One would need to know how to solve the equations of motion e.g. Heisenberg equation. One must still face an infinite time integral which may not be easy to handle. For these reasons the study of EH has not been undertaken until very recent times ...

Very crudely put, ergodicity says that the time averages and the ensemble averages of dynamic functions are the same. Most approaches to this subject are set [Lee 2001, p. 250601-1] in highly abstract terms like in [Farquhar 1964], [Halmos 1956], that make it difficult to pinpoint the specific physical properties that make a many-body model ergodic. On the other hand, Khinchin's approach [Khinchin 1949] is to use correlation functions from quantum many-body problems, such as those that have been studied by [Kubo 1957]. We want to consider the EH in this context. First, in classical ergodic theory the EH reads

$$\langle \mathcal{Q}_t \rangle_{time} = \langle \mathcal{Q} \rangle_{ens} \,, \tag{12.2}$$

where $\mathcal{Q}$ is a phase space function. Taking the ensemble average on both sides of the previous equation

$$\langle \langle \mathcal{Q}_t \rangle_{time} \rangle_{ens} = \langle \langle \mathcal{Q} \rangle_{ens} \rangle_{ens} = \langle \mathcal{Q} \rangle_{ens} \,. \tag{12.3}$$

Since

$$\langle \langle \mathcal{Q}_t \rangle_{time} \rangle_{ens} = \langle \langle \mathcal{Q}_t \rangle_{ens} \rangle_{time} \,, \tag{12.4}$$

[Lee 2001, fn. [5]], [Farquhar 1964, p. 123], then

$$\langle \langle \mathcal{Q}_t \rangle_{ens} \rangle_{time} = \langle \mathcal{Q} \rangle_{ens} \,. \tag{12.5}$$

In the analogous quantum relation, the phase space function $\mathcal{Q}$ is to be replaced [Lee 2001, fn. [5]] by the corresponding operator $\hat{\mathcal{Q}}$

$$\langle \langle \hat{\mathcal{Q}}_t \rangle_{ens} \rangle_{time} = \langle \hat{\mathcal{Q}} \rangle_{ens} \,. \tag{12.6}$$

Thus, the statement of the EH for a dynamical quantity or variable $A(t)$, with the time average written explicitly, reads

$$\lim_{T \to \infty} \frac{1}{2T} \int_{-T}^{T} \langle A(t) \rangle \, \mathrm{d}t = \langle A \rangle \,, \tag{12.7}$$

(where: $\langle\ \rangle$ denotes *ensemble average*, $A = A(0)$) and immediately brings to mind having to solve equations of motion for a many body problem and doing the ensuing infinite integral —the hurdles mentioned in the last paragraph of M. H. Lee's text quoted above— with both tasks to be done *exactly* or, if this were not possible, within controlled approximations.

The lhs of the EH definition, Eq. (12.7) on the previous page, is the time average of the dynamical quantity or variable $A(t)$ that —according to the EH— one would expect to relax into the ensemble equilibrium value on the rhs.

Some kind of non-equilibrium situation has to be set up for the relaxation to occur. M. Howard Lee has suggested to perturb the system by inelastic scattering, thus, the energy absorbed by the system would delocalize in some manner [Lee 2007*b*, §2, p. 1838] —a relaxation process— that would entail a time evolution.

To test the EH, the analysis of this dynamical evolution must be feasible. To ease this task M. Howard Lee has proposed to consider the applied field, that gives rise to the inelastic scattering process (ISP), to be sufficiently weak so that linear response theory (LRT) [Kubo 1957] is applicable[1]. This task is further facilitated by M. Howard Lee's Recurrence Relations Method (RRM), that does not require the equations of motion to be formulated in the mathematical space of the many body problem, but instead, in the *"realized space"* (see §§2.1-2.2) of any physically relevant dynamical quantity or variable of the many body problem that we deem choosing. We review the RRM in Chapter 2 and we show how it is used in Chapters 3 to 6 where we consider some applications.

M. Howard Lee's approach to the EH by means of LRT and the RRM (that we summarized in the previous paragraph) is the most important advance in the study of the validity of EH [Marconi, Puglisi, Rondoni & Vulpiani 2008, §3.4.1, p 130-131]. It is described in [Lee 2001], [Lee 2002], [Lee 2006], [Lee 2007*a*], [Lee 2007*c*], [Lee 2007*b*]. In a general application of this strategy one would look —among all the system dynamical functions that couple to the chosen scattering field— for a particular one that plays a significant role in the ISP being considered [Lee 2007*b*, §2, p. 1838].

In our case, we have chosen the momentum of the mass next to the fixed wall, $p_0(t)$ (see §7.1 and §7.3), as the particular dynamical function and we assume that it couples to an —unspecified—

[1]It could be argued there is loss of generality by using LRT, the tradeoff is that it becomes feasible to obtain *exact* results by means of the RRM as we shall see below.

applied field that scatters the system inelastically and weakly so that LRT can be used. In the next section we review the application of the RRM and LRT to a weak ISP and show the preeminent role that the autocorrelation function $\tilde{a}_0(z)$, Eq. (12.1), plays in the analysis of the EH in this context.

## 12.1 Linear Response Theory (LRT), the Ergodic Hypotheses (EH), and the Recurrence Relations Method (RRM)

Following the ideas presented in the previous section, we now consider the *particular situation* of a quantum many body system (MBS) with Hamiltonian $H$, that is perturbed by a weak applied field $h(t)$ that we *turn on* at a remote past $t = -T$, $T \to \infty$. We will also assume below, later, that the applied field $h(t)$ *attains a constant value*.

The applied field $h(t)$ *couples* to the MBS observable variable $B$, giving rise to a time dependent potential

$$\mathcal{V}(t) = -h(t)B\,, \tag{12.8}$$

so that the total energy at time $t$ is given by the Hamiltonian $H'$

$$H'(t) = H + \mathcal{V}(t) = H - h(t)B\,. \tag{12.9}$$

We wish to calculate both sides of the ergodic hypotheses (EH) definition, Eq. (12.7) on page 155, within the framework of linear response theory (LRT), that is, up to linear order in the applied field. In Eq. (12.7) the angular brackets $\langle\ \ \rangle$ denoted ensemble average and it was understood that the full perturbed Hamiltonian was used. In this section we have to distinguish and keep track of whether the ensemble average is made for the perturbed system or the unperturbed system. For the former, the ensemble average will be denoted by $\langle \dots \rangle_{H'}$, that is

$$\langle \dots \rangle_{H'} \equiv \frac{\mathrm{Tr}(\dots \mathrm{e}^{-\beta H'})}{\mathrm{Tr}(\mathrm{e}^{-\beta H'})}\ . \tag{12.10}$$

Since we are using LRT all the results eventually are given in terms of expectation values in the unperturbed system, thus, we will keep the *plain* angular brackets to also denote the ensemble average for the *unperturbed* system:

$$\langle \dots \rangle_{H} \equiv \frac{\mathrm{Tr}(\dots \mathrm{e}^{-\beta H})}{\mathrm{Tr}(\mathrm{e}^{-\beta H})} \equiv \langle \dots \rangle\ . \tag{12.11}$$

The EH definition, Eq. (12.7) on page 155, for the MBS dynamic variable $A$ now reads

$$\lim_{T\to\infty}\frac{1}{2T}\int_{-T}^{T}\langle A(t)\rangle_{H'}\,\mathrm{d}t=\langle A\rangle_{H'}\ . \tag{12.12}$$

In Appendix D, Eq. (D.21) on page 207 we show that the *time dependent* ensemble-expectation-value inside the integral in Eq. (12.12) above is

$$\langle A(t)\rangle_{H'(t)}=\langle A(t)\rangle_{H}+\int_{-T}^{t}h(t')\,\frac{\mathrm{i}}{\hbar}\langle[A(t),B(t')]\rangle\,\mathrm{d}t'\,, \tag{12.13a}$$

$$\equiv\langle A\rangle+\int_{-T}^{t}h(t')\,C_{AB}(t-t')\,\mathrm{d}t'\,. \tag{12.13b}$$

The integrand in the second term in the rhs of Eq. (12.13a) contains the terms $\langle A(t)B(t')\rangle$ and $\langle B(t')A(t)\rangle$. Each one is a *time correlation function* (TCF) of the kind defined in App. D, §D.7, p. 219, Eqs. (D.94).

The hermiticity and time independence of $H$ imply the stationarity [Eq. (D.95) on page 219] of the TCFs

$$\langle X(0)Y(t)\rangle=\langle X(\tau)Y(t+\tau)\rangle\,,\quad\text{for arbitrary }\tau. \tag{12.14}$$

We can write, for example, $\langle A(t)B(t')\rangle=\langle A(t-t')B(t'-t')\rangle=\langle A(t-t'),B\rangle$. This allows us to write the second of Eqs. (12.13) above, where

$$C_{AB}(t-t')=\begin{cases}(\mathrm{i}/\hbar)\langle[A(t),B(t')]\rangle=(\mathrm{i}/\hbar)\langle[A(t-t'),B]\rangle & t>t'\\ 0 & t\leqslant t'\end{cases} \tag{12.15}$$

is the so called *response function* [Balucani, Lee & Tognetti 2003, §1.3.1, p. 420]. We see that the response $\langle A(t)\rangle_{H'(t)}-\langle A(t)\rangle_{H}$ is indeed linear in the applied field $h(t)$. In the case $B=A$ —the applied field $h(t)$ coupling variable is the same dynamic variable we chose to observe— the response function [Marshall & Lowde 1968, §2.6, p. 713]

$$C_{AA}(t-t')=\begin{cases}(\mathrm{i}/\hbar)\langle[A(t),A(t')]\rangle=(\mathrm{i}/\hbar)\langle[A(t-t'),A]\rangle & t>t'\\ 0 & t\leqslant t'\end{cases} \tag{12.16}$$

is also known as the *time dependent susceptibility* $\chi_A(t-t')$, or simply $\chi(t-t')$ [Lee 2007*b*, §2, p. 1839].

Following [Lee 2007*c*, §3], to simplify the time average (TA)

$$I_{TA} \equiv \lim_{T\to\infty} \frac{1}{2T} \int_{-T}^{T} \langle A(t)\rangle_{H'} \, \mathrm{d}t \tag{12.17}$$

on the lhs of Eq. (12.12) on the preceding page, we assume that the applied field is a constant

$$h(t) = h \,, \tag{12.18}$$

and we also only consider the $B = A$ case. The only time dependence stems from the switching-on of the applied field and we obtain

$$I_{TA} = \langle A\rangle + h \lim_{T\to\infty} \frac{1}{2T} \int_{-T}^{T} \mathrm{d}t \int_{-T}^{t} \mathrm{d}t' \, \chi_A(t-t') \,. \tag{12.19}$$

To calculate the time independent ensemble-average on the rhs of Eq. (12.12) note that after —the now assumed constant— applied field $h$ is turned on, the perturbed Hamiltonian $H'$ of the MBS is also a constant

$$H' = H + V \,, \quad \text{with} \quad V = -hB \,. \tag{12.20}$$

Again using LRT, we show in Appendix D, §D.2, Eq. (D.50) on page 211, that the *static response* $\langle A\rangle_{H'} - \langle A\rangle$ of the MBS is

$$\langle A\rangle_{H'} - \langle A\rangle = h\,(B^\dagger, A) \,, \tag{12.21}$$

in terms of the *Kubo scalar product* [Eq. (2.1) on page 5]:

$$(X, Y) = \int_0^\beta \langle \mathrm{e}^{\lambda H} X^\dagger \mathrm{e}^{-\lambda H} Y\rangle \mathrm{d}\lambda - \beta \langle X^\dagger\rangle\langle Y\rangle \,.$$

The *static response* is also written as either of

$$\langle A\rangle_{H'} - \langle A\rangle = h\,\{B, A\} \,, \tag{12.22a}$$

$$= h\, R_{AB}(t=0) \,. \tag{12.22b}$$

In Eqs. (12.22) above, $\{B, A\}$ is the *relaxation function* defined in [Marshall & Lowde 1968, p. 710, Eq. (18)], and $R_{AB}(t)$ is the *Kubo relaxation function* [Balucani et al. 2003, p. 415]. Both can be written in terms of the *Kubo scalar product*:

$$\{B, A\} \equiv (B^\dagger, A) \,, \tag{12.23}$$

$$R_{AB}(t) \equiv (B^\dagger, A(t)) \,. \tag{12.24}$$

Following [Lee 2007*c*, §3], we choose to observe the coupling variable, i.e. we set $B = A$, and we write

$$\langle A \rangle_{H'} = \langle A \rangle + h\,\chi_A\,. \tag{12.25}$$

Here, $\chi_A$ is the *static response function* or *time-independent susceptibility*

$$\chi_A \equiv R_A(t=0)\,, \tag{12.26}$$

and $R_A(t)$ is the *autocorrelation function* [Lee 2007*c*, §3, Eq. (10)]:

$$\begin{aligned} R_A(t) \equiv R_{AA}(t) &= (A^\dagger, A(t))\,, \\ &= (A(t)^\dagger, A) = (A^\dagger(t), A)\,. \end{aligned} \tag{12.27}$$

In the last line we used $(X, Y) = (Y^\dagger, X^\dagger)$ [App. D, Eq. (D.89) on page 218], and the time independence and hermiticity of $H$ that $\Rightarrow\ A(t)^\dagger = A^\dagger(t)$. See App. D, Eq. (D.106) on page 221.

Introducing Eq. (12.25) and Eq. (12.19) into the EH definition given in Eq. (12.12), we obtain

$$\begin{aligned} \langle A \rangle + h \lim_{T\to\infty} \frac{1}{2T} \int_{-T}^{T} \mathrm{d}t \int_{-T}^{t} \mathrm{d}t'\, \chi_A(t-t') &= \langle A \rangle + h\,\chi_A\,, \\ \lim_{T\to\infty} \frac{1}{2T} \int_{-T}^{T} \mathrm{d}t \int_{-T}^{t} \mathrm{d}t'\, \chi_A(t-t') &= \chi_A\,. \end{aligned} \tag{12.28}$$

This is the EH written in terms of the *time-dependent response function* and the *static response functions*, within the context of LRT. *This expression for the EH is written totally in terms of intrinsic properties of the MBS*: The <u>constant</u> applied field $h$ cancels out in both sides of Eq. (12.28). Also note that the prevailing notation can be somewhat misleading: The *time dependent response function*, $\chi_A(t-t')$ [Eq. (12.16)], evaluated at $t - t' = 0$ is <u>not</u> equal to the *static response function*, Eq. (12.26)

$$\chi_A(0) \neq \chi_A\,. \tag{12.29}$$

The time average on the lhs of Eq. (12.28) is performed in Appendix D. Following Lee [2007*b*, §§3-4] we obtain

$$\lim_{T\to\infty} \frac{1}{T-b} \int_{b}^{T} \mathrm{d}t \int_{b}^{t} \mathrm{d}t'\, \chi_A(t-t') = \tilde{\chi}_A(0) + \lim_{T\to\infty} \Big[ R_A(T) - \frac{1}{T-b} \tilde{R}_A(0) \Big]\,. \tag{12.30}$$

Here $\tilde{\chi}_A(z)$ and $\tilde{R}_A(z)$ are the Laplace transforms of the *time-dependent response function* [Eq. (12.16)] and the *autocorrelation function* [Eq. (12.27)], respectively. The letter $b$ in the lower limit of both integrals in Eq. (12.30) designates the "beginning" time at which the applied (constant) [See Eq. (12.18)] field is switched on. Setting the beginning time to $-\infty$, i.e., $b = -T$, with $T \to \infty$

$$\lim_{T\to\infty} \frac{1}{2T} \int_{-T}^{T} \mathrm{d}t \int_{-T}^{t} \mathrm{d}t' \, \chi_A(t-t') = \tilde{\chi}_A(0) + \lim_{T\to\infty} \left[ R_A(T) - \frac{1}{2T} \tilde{R}_A(0) \right] . \tag{12.31}$$

Using the above result, the EH [Eq. (12.28)] reads

$$\tilde{\chi}_A(0) + R_A(T) - \frac{1}{2T} \tilde{R}_A(0) = \chi_A \, , \quad \text{with} \quad T \to \infty \, . \tag{12.32}$$

Up to now what we have done is just cast the EH into a convenient form, Eq. (12.32) above, to be able to proceed to the next step: find a suitable condition for the validity of the EH as stated by the Equation (12.32) and in the particular context of Eq. (12.32): —within LRT— a dynamical variable $A$ of the system under consideration couples to an applied weak inelastic scattering field. We will show below that the condition for the validity of the EH [Eq. (12.32)] is just that the Laplace transform of the *autocorrelation function* $R_A(t)$ [Eq. (12.27)] has to be finite and non-null [Lee 2007*c*, §2], i.e.,

$$0 < \tilde{R}_A(z=0) < \infty \, . \tag{12.33}$$

To arrive here, the following fundamental properties [Eqs. (12.34) below] of the *autocorrelation function* were needed. All three were used to write the time average [Eq. (12.31)] in the lhs of the final form of the EH given in Eq. (12.32). The definitive *ergodicity condition* [Eq. (12.33)] is also given in terms of the *autocorrelation function*. To obtain this condition we will follow Lee [2007*b*, §4] and we will use the last two properties below.

(a) Although the domain of $R_A(t)$ is $0 \leqslant t$, it can be extended to $t < 0$ by means of the definition (12.27) in terms of the Kubo scalar product. We show in App. D, §D.3 that $R_A(t)$ is <u>*even*</u> [Eq. (D.54) on page 212]:

$$R_A(-t) = R_A(t) \, . \tag{12.34a}$$

(b) Relation to the *time-independent susceptibility* or *static response function* $\chi_A$. See Eq. (12.26) on page 160:

$$R_A(t=0) = \chi_A \,. \tag{12.34b}$$

(c) Relation to the *time dependent susceptibility* $\chi_A(t-t')$ defined in Eq. (12.16). In App. D, §D.4 on page 212, we first calculate the time derivative of the Kubo relaxation function $R_{AB}(t)$. [See Eqs. (D.67)-(D.68) on page 214.] We then set $B \leftarrow A$ to obtain

$$\frac{\mathrm{d}R_A(t)}{\mathrm{d}t} = -\chi_A(t) \,. \tag{12.34c}$$

The EH as stated in Eq. (12.32) is written in terms of the functions $\tilde{\chi}_A(z)$, $R_A(t)$, and $\chi_A$. To test its validity, we need a similar relation obtained independently. To this end [Lee 2007*b*, §4, p. 1841] we take the Laplace transform of Relation (c) above

$$-R_A(t=0) + z\tilde{R}_A(z) = -\tilde{\chi}_A(z) \,,$$

and use Relation (b) to obtain

$$\begin{aligned} -\chi_A + z\tilde{R}_A(z) &= -\tilde{\chi}_A(z) \,, \\ \tilde{\chi}_A(z) + z\tilde{R}_A(z) &= \chi_A \,. \end{aligned} \tag{12.35}$$

We now compare the EH stated in Eq. (12.32) with the <u>*exact*</u> relation in Eq. (12.35) above, in the limit $z \to 0$. Let's write them together

$$\tilde{\chi}_A(0) + R_A(T) - \frac{1}{2T}\tilde{R}_A(0) \qquad = \chi_A \,, \quad \text{with} \quad T \to \infty \,. \tag{12.36a}$$

$$\tilde{\chi}_A(0) \qquad\qquad + \; z\,\tilde{R}_A(z)\Big|_{z\to 0} = \chi_A \,. \tag{12.36b}$$

The conclusion is most clearly stated by M. H. Lee in

> [Lee 2007*b*, §4, p. 1841] We at once see that they do not agree. One must conclude the EH cannot generally be valid!
>
> But can it be valid in some special situations?

Looking at both equations [Eqs. (12.36) on the preceding page] one sees that for them to agree it would suffice $\tilde{R}_A(z=0) = \int_0^\infty R_A(t)\,\mathrm{d}t$ to be finite, since this requires[2] —when the dimension $d_A$ of the realized space spanned by the dynamic variable $A$ is infinite— that

$$\lim_{t\to\infty} R_A(t) = 0\,. \tag{12.38}$$

It could also happen that $\tilde{R}_A(0)$ is identically zero. This possibility must be removed since it would make the first (the EH) of Eqs. (12.36) on the previous page independent of $T$ as $T \to \infty$. Therefore, we obtain the condition already stated in Eq. (12.33)

$$0 < \tilde{R}_A(z=0) < \infty\,. \tag{12.39}$$

Recall that $R_A(t) = (A^\dagger, A)\, a_0(t)$ [§2.4 on page 8]. If $R_A(0) = (A^\dagger, A)$ is finite, the ergodicity condition [Eq. (12.39) above] may be written as

$$0 < \tilde{a}_0(z=0) < \infty\,. \tag{12.40}$$

Using the RRM we showed [§2.4, Eq. (2.21) on page 10] that $\tilde{a}_0(z)$ can be expressed as a continued fraction that evaluated at $z = 0$ yields —*after* the limit $d_A \to \infty$ (see [2] on the current page) is taken—

$$\tilde{a}_0(z=0) = \frac{\Delta_2\,\Delta_4\,\Delta_6\,\Delta_8\ldots}{\Delta_1\,\Delta_3\,\Delta_5\,\Delta_7\ldots}\,. \tag{12.41}$$

M. H. Lee in [Lee 2007*b*, §4, p. 1841] defines

$$W \equiv \tilde{a}_0(0) \tag{12.42}$$

[2]Here, it is understood that the dimension of the realized space of the dynamic variable $A$ *is infinite*, i.e.

$$d_A = \infty\,. \tag{12.37}$$

The continued fraction representation of $\tilde{a}_0(z)$ [§2.4, Eq. (2.21) on page 10] shows that $\tilde{R}_A(z) = (A^\dagger, A)\tilde{a}_0(z)$ is the quotient of two polynomials in $z$, the numerator of degree $d_A - 1$ and the denominator of degree $d_A$. Consequently, if $d_A$ were finite, the only possible singularities of $\tilde{R}_A(z)$ would be poles, in fact [§9.5, p. 105], pairs of complex conjugated poles on imaginary axis (if $d_A$ is odd $z = 0$ is always a pole). Then, $R_A(t)$ would be just a sum of oscillatory functions of time (sines) and therefore the condition given in Eq. (12.38) could not ever be fulfilled, notwithstanding, $\tilde{a}_0(z=0) = 0$ *always*, if $d_A$ is finite and even (if $d_A$ is odd, then $\tilde{a}_0(z=0) = \infty$). See [§2.4, Eq. (2.21) on page 10]. Thus, following [Lee 2007*b*, §5, p. 1842] we exclude the cases when $d_A$ is finite in the considerations that follow right below Eq. (12.38). When $d_A = \infty$ the poles *can* coalesce into a branch cut (or cuts). See §11.1, p. 129.

after the English mathematician J. Wallis who studied infinite products[3] in 1655, and thus the condition [Eq. (12.40) on the preceding page] that insures the validity of the EH given in Eq. (12.36a), p. 162 becomes

$$0 < W < \infty \,. \tag{12.44}$$

The ergodicity condition [Eq. (12.44) above] and equations (12.36a) and (12.36b) that gave rise to it, involve the related concept of *irreversibility* by requiring (see [2] on the preceding page, again) that

$$\lim_{T\to\infty} R_A(T) = 0 \,, \tag{12.45}$$

for Eqs. (12.36) on page 162 to agree: the term $2\lim_{T\to\infty} R_A(T)$ is present in Eq. (12.36a) (the EH) but not in the *exact* Eq. (12.36b) (the Laplace transform of the time derivative of the auto-correlation function $R_A(t)$), thus it must be null. But, this condition *is not enough*. We still need that $\lim_{T\to\infty}(-2/T)\tilde{R}_A(0)$ in Eq. (12.36a), and $\lim_{z\to 0} z\tilde{R}_A(z)$ in Eq. (12.36b) both to vanish. We have already shown in the paragraph above Eq. (12.38) that $\tilde{R}_A(z=0) = \int_0^\infty R_A(t)\,\mathrm{d}t$ to be finite and non-zero would suffice. The *irreversibility condition*, Eq. (12.45) is again, *necessary* but not enough for this to happen. Thus, following M. Howard Lee in [Lee 2007*b*, §§3-5] we have shown that *irreversibility is a necessary, though not sufficient condition for ergodicity* [Lee 2007*c*].

In the next section we test the exact solution for $\tilde{a}_0(z)$ that we have obtained in Chapter 9 against these ideas.

[3] In his book *Arithmetica Infinitorium* (1655), Wallis obtained the infinite product

$$\frac{\pi}{2} = \frac{2\cdot 2}{1\cdot 3}\,\frac{4\cdot 4}{3\cdot 5}\,\frac{6\cdot 6}{5\cdot 7}\cdots = \prod_{n=1}^{\infty}\Big[\frac{(2n)^2}{(2n-1)(2n+1)}\Big] \,. \tag{12.43}$$

Also, he was the first mathematician to systematically study continued fractions. The term *continued fraction*, and the formula to obtain the continued fraction *approximants* or *convergents* as a sequence of *linear transformations* are due to him: *Opera Mathematica* (1695).

## 12.2 Exact results about the irreversibility and ergodicity of an harmonic oscillator chain (HOC) in thermal equilibrium with one end-impurity coupled to fixed wall (ICFW)

The Recurrence Relations Method (RRM) furnishes a continued-fraction *general* representation for the auto-correlation function $\tilde{a}_0(z)$. Using the Recurrence Relations II (RR2) we showed [§2.4, Eq. (2.21) on page 10] that $\tilde{a}_0(z)$ can be expressed as the, order $d$, continued fraction

$$\tilde{a}_0(z) = \cfrac{1}{z + \cfrac{\Delta_1}{z + \cfrac{\Delta_2}{z + \cdots + \cfrac{\Delta_{d-2}}{z + \cfrac{\Delta_{d-1}}{z}}}}}\,, \tag{12.46}$$

where $d$ is the model dependent —and choice of dynamic variable dependent— dimension of the realized space $\mathcal{S}$ as defined in §2.3, and $\{\Delta_1, \Delta_2, \ldots, \Delta_{d-1}\}$ are the *recurrants* spanned [See §2.3] by $\mathcal{S}$.

We have chosen the *momentum of the mass next to the wall* as the dynamic variable to be investigated in our model of an harmonic oscillator chain (HOC) in thermal equilibrium with one end-impurity coupled to fixed wall (ICFW). Thus, the auto-correlation function $\tilde{a}_0(z)$ [Eq. (12.46)] is the Laplace transform of

$$a_0(t) = \frac{(p_0, p_0(t))}{(p_0, p_0)}\,, \tag{12.47}$$

first defined in Eq. (2.12) on page 8 in §2.4. Here, $p_0$ is the momentum of the mass next to the fixed wall and $(\ ,\ )$ is the Kubo scalar product defined in Eq. (2.1) and Eqs. (7.37)–(7.38).

The corresponding recurrants and $d$ are calculated in §§7.3-7.5 and reported in Table 7.1, that we reproduce below for convenience. It is shown that $d = 2N - 1$, with $N$ being the length of the harmonic oscillators chain.

It is in this context: A physical model and a choice of dynamical variable that we speak of the *system* irreversibility and ergodicity.

Table 12.1: Delta sequence $\sigma = (\Delta_1, \Delta_2, \ldots, \Delta_{d-1})$, in units of $\Omega^2 \equiv k/m$. The quantity $\Omega$ was defined in Eq. (8.19) on page 80. The parameters $\kappa \equiv k_0/k$ and $\lambda \equiv m_0/m$ were defined in Eqs. (7.2)-(7.3) on page 60: $k_0$ is the coupling of the first harmonic oscillator mass $m_0$ to the fixed wall, $k$ is the coupling of all the other harmonic oscillators masses ($= m$) in the chain.

| $N$ | $\sigma =$ $(\Delta_1$ | $\Delta_2$ | $\Delta_3$ | $\Delta_4$ | $\Delta_5$ | $\Delta_6$ | $\Delta_7$ | $\Delta_8$ | $\Delta_9$ | $\Delta_{10}$ | $\Delta_{11})$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 2 | $\left(\ \frac{\lambda(1+\kappa)}{}\right.$ | $\frac{1}{\kappa+1}$ | $\left.\frac{\kappa}{\kappa+1}\ \right)$ | | | | | | | | |
| 3 | $\left(\ \frac{\lambda(1+\kappa)}{}\right.$ | $\frac{1}{\kappa+1}$ | $\frac{2\kappa+1}{\kappa+1}$ | $\frac{\kappa+1}{2\kappa+1}$ | $\left.\frac{\kappa}{2\kappa+1}\ \right)$ | | | | | | |
| 4 | $\left(\ \frac{\lambda(1+\kappa)}{}\right.$ | $\frac{1}{\kappa+1}$ | $\frac{2\kappa+1}{\kappa+1}$ | $\frac{\kappa+1}{2\kappa+1}$ | $\frac{3\kappa+1}{2\kappa+1}$ | $\frac{2\kappa+1}{3\kappa+1}$ | $\left.\frac{\kappa}{3\kappa+1}\ \right)$ | | | | |
| 5 | $\left(\ \frac{\lambda(1+\kappa)}{}\right.$ | $\frac{1}{\kappa+1}$ | $\frac{2\kappa+1}{\kappa+1}$ | $\frac{\kappa+1}{2\kappa+1}$ | $\frac{3\kappa+1}{2\kappa+1}$ | $\frac{2\kappa+1}{3\kappa+1}$ | $\frac{4\kappa+1}{3\kappa+1}$ | $\frac{3\kappa+1}{4\kappa+1}$ | $\left.\frac{\kappa}{4\kappa+1}\ \right)$ | | |
| 6 | $\left(\ \frac{\lambda(1+\kappa)}{}\right.$ | $\frac{1}{\kappa+1}$ | $\frac{2\kappa+1}{\kappa+1}$ | $\frac{\kappa+1}{2\kappa+1}$ | $\frac{3\kappa+1}{2\kappa+1}$ | $\frac{2\kappa+1}{3\kappa+1}$ | $\frac{4\kappa+1}{3\kappa+1}$ | $\frac{3\kappa+1}{4\kappa+1}$ | $\frac{5\kappa+1}{4\kappa+1}$ | $\frac{4\kappa+1}{5\kappa+1}$ | $\left.\frac{\kappa}{5\kappa+1}\ \right)$ |

If the length $N$ of the chain is finite, $d$ is also finite, the only singularities of $\tilde{a}_0(z)$ [the continued fraction in Eq. (12.46) on the preceding page] are isolated conjugated poles on the imaginary axis, thus [See [2] on page 163] $a_0(t)$ is reversible and therefore the system is not ergodic.

For an infinite chain the quantity $W \equiv \tilde{a}_0(0)$ [Eq. (12.42)] determines whether it is ergodic or not, $0 < W < \infty$ being the condition for ergodicity [see Eq. (12.44) on page 164]. We first calculate $W$ directly from the continued fraction representation of $\tilde{a}_0(z)$ in the limit $z \to 0$ by means of Eq. (12.41) on page 163 reproduced below for convenience

$$\tilde{a}_0(z=0) = \frac{\Delta_2\,\Delta_4\,\Delta_6\,\Delta_8\ldots}{\Delta_1\,\Delta_3\,\Delta_5\,\Delta_7\ldots}\,. \tag{12.48}$$

The recurrants are given in the Table 12.1 above in units of $\Omega^2$ [Eq. (8.19) on page 80], thus we write

$$\Delta_i \equiv \delta_i \Omega^2\,, \tag{12.49}$$

and then

$$\tilde{a}_0(z=0) = \frac{\delta_2\Omega^2\ \delta_4\Omega^2\ \delta_6\Omega^2\ \delta_8\Omega^2\ldots}{\delta_1\Omega^2\ \delta_3\Omega^2\ \delta_5\Omega^2\ \delta_7\Omega^2\ldots}\ , \tag{12.50a}$$

$$= \frac{\delta_2\,\delta_4\,\delta_6\,\delta_8\ldots}{\delta_1\,\delta_3\,\delta_5\,\delta_7\ldots} \times \frac{\Omega^2\,\Omega^2\,\Omega^2\,\Omega^2\ldots}{\Omega^2\,\Omega^2\,\Omega^2\,\Omega^2\ldots}\ . \tag{12.50b}$$

The second fraction on the rhs of Eq. (12.50b) above is an indeterminate factor *unless* $\Omega^2 = 1$. Otherwise, it is either

a) Of the form $\infty/\infty$, if $\Omega^2 > 1$.

b) Of the form $0/0$, if $\Omega^2 < 1$.

This indeterminacy cannot be removed merely by simplifying the corresponding $\Omega^2$ factors in the numerator and denominator of Eq. (12.50a), since this would lead to incorrect physical units: a dimensionless $\tilde{a}_0(z=0)$.

The $\Omega^2$ factors may be removed by rewriting —*before* the $z \to 0$ limit is taken— the continued fraction expansion [Eq. (12.46) on page 165] of $\tilde{a}_0(z)$ in terms of the dimensionless $\delta$'s by means of an equivalence transformation (see [1], §10.3, p. 116), as follows

$$\tilde{a}_0(z) = \cfrac{1/\Omega}{z/\Omega + \cfrac{\Delta_1/\Omega^2}{z/\Omega + \cfrac{\Delta_2/\Omega^2}{z/\Omega + \cfrac{\Delta_3/\Omega^2}{z/\Omega + \cfrac{\Delta_4/\Omega^2}{z/\Omega + \ddots}}}}}\ ,$$

$$= \frac{1}{\Omega} \times \cfrac{1}{z/\Omega + \cfrac{\delta_1}{z/\Omega + \cfrac{\delta_2}{z/\Omega + \cfrac{\delta_3}{z/\Omega + \cfrac{\delta_4}{z/\Omega + \ddots}}}}}\ . \tag{12.51}$$

Now, we again take the limit $z \to 0$ in Eq. (12.51) on the preceding page to get

$$\tilde{a}_0(z=0) = \frac{1}{\Omega} \times \frac{\delta_2\,\delta_4\,\delta_6\,\delta_8\ldots}{\delta_1\,\delta_3\,\delta_5\,\delta_7\ldots}\ , \tag{12.52}$$

which now has the correct physical units. Substituting the values of the $\delta$'s from Table 12.1 on page 166 we obtain the following infinite product

$$\tilde{a}_0(z=0) = \frac{1}{\Omega} \times \frac{1}{(\kappa+1)\lambda}\,\frac{1}{\kappa+1}\,\frac{\kappa+1}{2\kappa+1}\,\frac{\kappa+1}{2\kappa+1}\,\frac{2\kappa+1}{3\kappa+1}\,\frac{2\kappa+1}{3\kappa+1}\,\frac{3\kappa+1}{4\kappa+1}\,\frac{3\kappa+1}{4\kappa+1}\,\frac{4\kappa+1}{5\kappa+1}\,\frac{4\kappa+1}{5\kappa+1}\ldots \tag{12.53}$$

We only have written the first ten terms of the infinite product in Eq. (12.53) above. The value of $\tilde{a}_0(z=0)$ with just these ten terms is

$$\tilde{a}_0(z=0)\Big|_{(\text{ten terms})} = \frac{1}{\Omega}\,\frac{1}{\lambda}\,\frac{1}{(5\kappa+1)^2}\ . \tag{12.54}$$

With nine terms the value of $\tilde{a}_0(z=0)$ would have been

$$\tilde{a}_0(z=0)\Big|_{(\text{nine terms})} = \frac{1}{\Omega}\,\frac{1}{\lambda}\,\frac{1}{(4\kappa+1)(5\kappa+1)}\ . \tag{12.55}$$

Both results, for $n \geqslant 1$, can be generalized to

$$\tilde{a}_0(z=0)\Big|_{(2n\ \text{terms})} = \frac{1}{\Omega}\,\frac{1}{\lambda}\,\frac{1}{(n\kappa+1)^2}\ , \tag{12.56a}$$

and

$$\tilde{a}_0(z=0)\Big|_{[(2n-1)\,\text{terms}]} = \frac{1}{\Omega}\,\frac{1}{\lambda}\,\frac{1}{[(n-1)\kappa+1](n\kappa+1)}\ . \tag{12.56b}$$

In the limit $n \to \infty$, Eq. (12.56a) and Eq. (12.56b) above become equivalent and

$$\tilde{a}_0(z=0) = \begin{cases} \infty & \text{if}\ \ \lambda = 0\ \ \text{and/or}\ \ \Omega = 0\,, \\ & \text{else} \\ \frac{1}{\Omega}\,\frac{1}{\lambda} & \text{if}\ \ \kappa = 0\,, \\ & \text{else} \\ 0 & \text{if}\ \ \kappa \neq 0\,. \end{cases} \tag{12.57}$$

Thus, with $W \equiv \tilde{a}_0(z=0)$ [Eq. (12.42)], the condition $0 < W < \infty$ [Eq. (12.44) on page 164] tells us that the system can only be ergodic when the chain is uncoupled from the fixed wall, i.e., when the parameter $\kappa \equiv k_0/k$ [Eq. (7.2) on page 60] is zero.

Now we will obtain $W$ from the closed general solution for $\tilde{a}_0(z)$ [Eq. (9.15) on page 92] that we calculated in §9.1 by summing its continued fraction representation, yielding

$$\tilde{a}_0(z) = \frac{2z}{(2-\lambda)z^2 + \kappa\lambda\mu^2/2 + \lambda z\sqrt{z^2+\mu^2}} \,, \tag{12.58}$$

where $\kappa \equiv k_0/k$, $\lambda \equiv m/m_0$, together with $k$, $k_0$, $m$ and $m_0$ were defined in Eqs. (7.2)-(7.3) on page 60: $k_0$ is the coupling of the first harmonic oscillator mass, $m_0$, to the fixed wall and $k$ is the coupling among all the other masses ($= m$) of harmonic oscillator chain. The quantity $\mu \equiv 2\Omega$, with $\Omega \equiv \sqrt{k/m}$ was defined in Eq. (9.14).

Let's check out the value of $\tilde{a}_0(z \to 0)$ that is obtained from the general solution, Eq. (12.58) above.

1. If $\lambda = 0$:

$$\tilde{a}_0(z) = \frac{2z}{2z^2} = \frac{1}{z} \,, \tag{12.59a}$$

and then

$$\tilde{a}_0(z \to 0) = \infty \,. \tag{12.59b}$$

2. If $\mu = 2\Omega = 0$, first we remind ourselves that $\sqrt{z^2 - z_b^2}$ is an odd function of $z$ for *any* value of the complex parameter $z_b$ [§11.4 on page 139], thus, $q(z) \equiv \sqrt{z^2+\mu^2}$ is an <u>odd</u> function of $z$, i.e., $q(-z) = -q(z)$ [<u>See</u> §11.4, Eqs. (11.26)-(11.27) on page 141] and consequently

$$\lim_{\mu \to 0} \sqrt{z^2+\mu^2} = z \,. \tag{12.59c}$$

Thus, if $\mu = 0$

$$\tilde{a}_0(z) = \frac{2z}{(2-\lambda)z^2 + \lambda\, z\, z} = \frac{2z}{2z^2} = \frac{1}{z} \,, \tag{12.59d}$$

and then, when $z \to 0$

$$\tilde{a}_0(z \to 0) = \infty \,. \tag{12.59e}$$

We obtain again that: If $\lambda = 0$ and/or $\mu = 2\Omega = 0$, then $\tilde{a}_0(z \to 0) = \infty$.

3. If $\kappa = 0$ :

$$\tilde{a}_0(z) = \frac{2z}{(2-\lambda)z^2 + \lambda z\sqrt{z^2+\mu^2}} = \frac{2}{(2-\lambda)z + \lambda\sqrt{z^2+\mu^2}}\,, \tag{12.59f}$$

thus, when $z \to 0$

$$\tilde{a}_0(z \to 0) = \frac{2}{\lambda\,\mu} = \frac{1}{\lambda\,\Omega}\,. \tag{12.59g}$$

4. If $\kappa \neq 0$ then $\tilde{a}_0(z \to 0) = 0$ .

As expected, the results for $W \equiv \tilde{a}_0(z = 0)$ from the infinite product expansion [Eq. (12.57) on page 168] and from the general solution [Eqs. (12.59) on the preceding page] are the same. Also note that the behavior at $z \to \infty$ [Eq. (12.59a), Eq. (12.59d), Eq. (12.59f)] is $\sim 1/z$ as required by the $a_0(t = 0) = 1$ [§2.4, Eq. (2.11) on page 8] boundary condition.

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# Appendix A

## Gaussian integrals formulas and identities

Define

$$I \equiv \int_{-\infty}^{\infty} \mathrm{e}^{-\lambda x^2}\,\mathrm{d}x = \pi^{1/2}\lambda^{-1/2}\,. \tag{A.1}$$

Then

$$\overline{x^2} = \frac{1}{I}\int_{-\infty}^{\infty} x^2\,\mathrm{e}^{-\lambda x^2}\,\mathrm{d}x\,. \tag{A.2a}$$

But

$$-\frac{\mathrm{d}I}{\mathrm{d}\lambda} = \int_{-\infty}^{\infty} x^2\,\mathrm{e}^{-\lambda x^2}\,\mathrm{d}x\,, \tag{A.2b}$$

therefore

$$\overline{x^2} = -\frac{1}{I}\frac{\mathrm{d}I}{\mathrm{d}\lambda} = -\frac{\mathrm{d}\ln I}{\mathrm{d}\lambda} = \frac{1}{2\lambda}\,. \tag{A.2c}$$

Now consider

$$\begin{aligned}
b\,(x_1-x_2)^2 + c\,(x_2-x_3)^2 &\equiv bx_{12}^2 + cx_{23}^2\\
&= (b+c)x_2^2 - 2(bx_1+cx_3)x_2 + bx_1^2 + cx_3^2\\
&= (b+c)\left[\Big(x_2 - \frac{bx_1+cx_3}{b+c}\Big)^2 - \Big(\frac{bx_1+cx_3}{b+c}\Big)^2 + \frac{bx_1^2+cx_3^2}{b+c}\right]\\
&= (b+c)\left[\Big(x_2 - \frac{bx_1+cx_3}{b+c}\Big)^2 + \frac{(bx_1^2+cx_3^2)(b+c) - (bx_1+cx_3)^2}{(b+c)^2}\right]\\
&= (b+c)\Big(x_2 - \frac{bx_1+cx_3}{b+c}\Big)^2 + \frac{(bx_1^2+cx_3^2)(b+c) - (bx_1+cx_3)^2}{b+c}\\
&= (b+c)\Big(x_2 - \frac{bx_1+cx_3}{b+c}\Big)^2 + \frac{bcx_1^2 + cbx_3^2 - 2bcx_1x_3}{b+c}\\
&= (b+c)\Big(x_2 - \frac{bx_1+cx_3}{b+c}\Big)^2 + \frac{bc}{b+c}(x_1-x_3)^2\,. \quad \square
\end{aligned} \tag{A.3a}$$

Also, setting $x_1 \equiv 0$

$$\begin{aligned} bx_2^2 + c\,(x_2 - x_3)^2 &\equiv bx_2^2 + cx_{23}^2 \\ &= (b+c)\Big(x_2 - \frac{cx_3}{b+c}\Big)^2 + \frac{bc}{b+c}x_3^2\,. \end{aligned} \tag{A.3b}$$

These allow us to write

$$\int \mathrm{e}^{-bx_{12}^2 - cx_{23}^2}\,\mathrm{d}x_2 = \Big(\frac{\pi}{b+c}\Big)^{1/2}\,\mathrm{e}^{-\frac{bc}{b+c}x_{13}^2}\,, \tag{A.4}$$

and

$$\int \mathrm{e}^{-bx_2^2 - cx_{23}^2}\,\mathrm{d}x_2 = \Big(\frac{\pi}{b+c}\Big)^{1/2}\,\mathrm{e}^{-\frac{bc}{b+c}x_3^2}\,. \tag{A.5}$$

As an example, consider

$$\begin{aligned} &\int \mathrm{d}x_0\,\mathrm{d}x_1\,\mathrm{d}x_2\,\mathrm{e}^{-ax_0^2 - bx_{01}^2 - cx_{12}^2} \\ &\quad= \Big(\frac{\pi}{b+c}\Big)^{1/2}\int \mathrm{d}x_0\,\mathrm{d}x_2\,\mathrm{e}^{-ax_0^2 - \frac{bc}{b+c}x_{02}^2} \\ &\quad= \Big(\frac{\pi}{b+c}\Big)^{1/2}\Big(\frac{\pi}{a+\frac{bc}{b+c}}\Big)^{1/2}\int \mathrm{d}x_2\,\exp\Big[-\frac{a\,bc/(b+c)}{a+\frac{bc}{b+c}}x_2^2\Big] \\ &\quad= \Big(\frac{\pi}{b+c}\Big)^{1/2}\Big(\pi\frac{b+c}{ab+ac+bc}\Big)^{1/2}\int \mathrm{d}x_2\,\exp\Big[-\frac{abc}{ab+ac+bc}x_2^2\Big] \\ &\quad= \Big(\frac{\pi}{b+c}\Big)^{1/2}\Big(\pi\frac{b+c}{ab+ac+bc}\Big)^{1/2}\Big(\pi\frac{ab+ac+bc}{abc}\Big)^{1/2} \\ &\quad= \Big(\frac{\pi^3}{abc}\Big)^{1/2}. \end{aligned} \tag{A.6}$$

Similarly

$$\begin{aligned} &\int \mathrm{d}x_0\,\mathrm{d}x_1\,\mathrm{d}x_2\ldots\mathrm{d}x_{N-1}\,\exp[-a_0x_0^2 - a_1x_{01}^2 - a_2x_{12}^2\cdots - a_{N-1}x_{N-2,N-1}^2] \\ &\qquad= \Big(\frac{\pi^N}{a_0a_1a_2\ldots a_{N-1}}\Big)^{1/2}. \end{aligned} \tag{A.7}$$

We will finish this appendix with the calculation of the norm of $f_1(q) = -k(\kappa{+}1)[q_0 - q_1/(\kappa{+}1)]$ [See Eq. (7.43), p. 69] for an $N = 2$ chain. According to Eqs. (7.38)

$$\begin{aligned} (f_1, f_1) &= \frac{1}{Z}\int \mathrm{e}^{-\beta H}\,f_1^2(q)\,\mathrm{d}p\,\mathrm{d}q \\ &= \frac{1}{Z}\int \mathrm{e}^{-\beta[K(p)+U(q)]}\,k^2(\kappa+1)^2\big(q_0 - \frac{q_1}{\kappa+1}\big)^2\,\mathrm{d}p\,\mathrm{d}q \\ &= k^2(\kappa+1)^2\frac{1}{Z_U}\int \mathrm{e}^{-\beta\,U(q)}\,\big(q_0 - \frac{q_1}{\kappa+1}\big)^2\,\mathrm{d}q\,. \end{aligned} \tag{A.8}$$

Here, $Z_U = \int \mathrm{e}^{-\beta\, U(q)}\, \mathrm{d}q$ , with $U(q) = \frac{1}{2}k(\kappa q_0^2 + q_{01}^2)$ [See Eqs. (7.40), p. 69]. Using Eqs. (A.3)

$$U(q) = \frac{1}{2}k\Big[(\kappa+1)\big(q_0 - \frac{q_1}{\kappa+1}\big)^2 + \frac{\kappa}{\kappa+1}q_1^2\Big]\,. \tag{A.9}$$

The partition function $Z_U$ now reads

$$Z_U = \int \mathrm{d}q_1\, \exp\Big[-\frac{\beta k}{2}\frac{\kappa}{\kappa+1}q_1^2\Big] \times \int \mathrm{d}q_0\, \exp\Big[-\frac{\beta k}{2}(\kappa+1)\big(q_0 - \frac{q_1}{\kappa+1}\big)^2\Big] \tag{A.10}$$

and the norm $(f_1, f_1)$ becomes

$$\begin{aligned}(f_1, f_1) = k^2(\kappa+1)^2\frac{1}{Z_U}\int \mathrm{d}q_1\, \exp\Big[-\frac{\beta k}{2}\frac{\kappa}{\kappa+1}q_1^2\Big] \\ \times \int \mathrm{d}q_0\, \big(q_0 - \frac{q_1}{\kappa+1}\big)^2 \exp\Big[-\frac{\beta k}{2}(\kappa+1)\big(q_0 - \frac{q_1}{\kappa+1}\big)^2\Big]\end{aligned} \tag{A.11}$$

Comparing the last two equations and using Eqs. (A.2)

$$\begin{aligned}(f_1, f_1) &= k^2(\kappa+1)^2\overline{\big(q_0 - \frac{q_1}{\kappa+1}\big)^2} \\ &= k^2(\kappa+1)^2\,\frac{1}{2}\,\frac{2}{\beta k\,(\kappa+1)} \\ &= \frac{k\,(\kappa+1)}{\beta}\,.\end{aligned} \tag{A.12}$$

# Appendix B

## Even-odd parts of a continued fraction whose all its partial denominators are set to unity: $\mathrm{K}(u_n/1)$

Consider the sequence, Eqs. (10.11) in page 116, of approximants of PDSU($Cf$). Each term is calculated using the approximant definition, Eq. (10.8a), applied to PDSU($Cf$), Eq. (10.10). For convenience, we will reproduce here below the first few terms.

$$[\![\mathrm{PDSU}(Cf)]\!]_{(1)} = 0 + \frac{1}{1} = \frac{A_1}{B_1} = 1, \tag{B.1a}$$

$$[\![\mathrm{PDSU}(Cf)]\!]_{(2)} = 0 + \cfrac{1}{1 + \cfrac{u_2}{1}} = \frac{A_2}{B_2} = \frac{1}{1+u_2}\ , \tag{B.1b}$$

$$[\![\mathrm{PDSU}(Cf)]\!]_{(3)} = 0 + \cfrac{1}{1 + \cfrac{u_2}{1 + \cfrac{u_3}{1}}} = \frac{A_3}{B_3} = \frac{1+u_3}{1+u_2+u_3}\ , \tag{B.1c}$$

$$[\![\mathrm{PDSU}(Cf)]\!]_{(4)} = 0 + \cfrac{1}{1 + \cfrac{u_2}{1 + \cfrac{u_3}{1 + \cfrac{u_4}{1}}}} = \frac{A_4}{B_4} = \frac{1+u_3+u_4}{1+u_3+u_4+u_2(1+u_4)}\ , \tag{B.1d}$$

$$[\![\mathrm{PDSU}(Cf)]\!]_{(5)} = 0 + \cfrac{1}{1 + \cfrac{u_2}{1 + \cfrac{u_3}{1 + \cfrac{u_4}{1 + \cfrac{u_5}{1}}}}} =$$

$$\frac{A_5}{B_5} = \frac{1 + u_4 + u_5 + u_3(1 + u_5)}{1 + u_4 + u_5 + u_3(1 + u_5) + u_2(1 + u_4 + u_5)} \,, \quad \text{(B.1e)}$$

$$[\![\mathrm{PDSU}(Cf)]\!]_{(6)} = 0 + \cfrac{1}{1 + \cfrac{u_2}{1 + \cfrac{u_3}{1 + \cfrac{u_4}{1 + \cfrac{u_5}{1 + \cfrac{u_6}{1}}}}}} =$$

$$\frac{A_6}{B_6} = \frac{1 + u_5 + u_6 + u_4(1 + u_6) + u_3(1 + u_5 + u_6)}{1 + u_4 + u_5 + u_6 + u_4u_6 + u_3(1 + u_5 + u_6) + u_2(1 + u_5 + u_6 + u_4(1 + u_6))} \,. \quad \text{(B.1f)}$$

Note that $[\![\mathrm{PDSU}(Cf)]\!]_{(0)} = 0$ in this case. Each successive term in the sequence of approximants is obtained by adding an additional partial quotient step to the continued fraction, switching the parity from even to odd or vice-verse. Thus, if one could contract or condense two steps into one, it would be possible to obtain *separately* the sequence of even terms and the sequence of odd terms.

To represent the steps define the transformation

$$\tau_p(w) \equiv \frac{1}{1 + w} \,, \qquad p = 1, \quad \text{(B.2a)}$$

$$\equiv \frac{u_p}{1 + w} \,. \qquad p \geqslant 2 \quad \text{(B.2b)}$$

Composing successively the transformation one can represent any approximant, for example,

$$\begin{aligned}
[\![\mathrm{PDSU}(Cf)]\!]_{(1)} = \tau_1(w=0) &= \frac{1}{1+w|_{=0}} &&= 1\,,\\
[\![\mathrm{PDSU}(Cf)]\!]_{(2)} = \tau_1\tau_2(w=0) &= \cfrac{1}{1+\cfrac{u_2}{1+w|_{=0}}} &&= \frac{1}{1+u_2}\,,\\
[\![\mathrm{PDSU}(Cf)]\!]_{(3)} = \tau_1\tau_2\tau_3(w=0) &= \cfrac{1}{1+\cfrac{u_2}{1+\cfrac{u_3}{1+w|_{=0}}}} &&= \frac{1+u_3}{1+u_2+u_3}\,,
\end{aligned}$$

etc. In general, for the $n$th approximant we have

$$[\![\mathrm{PDSU}(Cf)]\!]_{(n)} = \tau_1 \ldots \tau_n(w=0), \tag{B.3a}$$

$$= \tau_1 \ldots \tau_n\tau_{n+1}(w=\infty). \tag{B.3b}$$

Let's condense a pair of steps into a two-step

$$t_\nu(w) \equiv \tau_\nu\tau_{\nu+1}(w) = \cfrac{u_\nu}{1+\cfrac{u_{\nu+1}}{1+w}} = \frac{u_\nu + u_\nu w}{1+u_{\nu+1}+w}\,. \tag{B.4}$$

At first sight, it seems that we won't be able to compose two-steps as we did single steps because of the presence of $w$ in the numerator and denominator, but a two-step can be rewritten as

$$\begin{aligned}
t_\nu(w) \equiv \tau_\nu\tau_{\nu+1}(w) &= u_\nu + \frac{u_\nu + u_\nu w}{1+u_{\nu+1}+w} - u_\nu\,,\\
&= u_\nu - \frac{u_\nu u_{\nu+1}}{1+u_{\nu+1}+w}\,.
\end{aligned} \tag{B.5}$$

Therefore, similarly to single steps, two-steps can be composed and a different kind of continued fraction is generated:

$$t_\nu t_{\nu+2}(w) = u_\nu - \cfrac{u_\nu u_{\nu+1}}{1+u_{\nu+1}+u_{\nu+2}-\cfrac{u_{\nu+2}u_{\nu+3}}{1+u_{\nu+3}+w}}\,. \tag{B.6}$$

The partial numerators will be the product of the corresponding single-step numerators. The partial denominators will be the sum of the old partial denominator: unity, plus the foremost numerator of the two-step, in this case the $u_{\nu+1}$, *plus* the forward neighbor numerator $u_{\nu+2}$.

Bearing the above in mind, the two-step sequence (assuming that $M$, the order of PDSU($Cf$) is big but finite, say, bigger than 12, to avoid worrying about the end-term)

$$\overbrace{\tau_1\,\tau_2}\,\overbrace{\tau_3\,\tau_4}\,\overbrace{\tau_5\,\tau_6}\,\overbrace{\tau_7\,\tau_8}\ldots \tag{B.7}$$

will yield the *odd* approximants of the original continued fraction: The first two-step, $t_1 = \tau_1\tau_2$

$$t_1(w) = u_1 - \frac{u_1 u_2}{1 + u_2 + w}\ , \tag{B.8}$$

$$= 1 - \frac{u_2}{1 + u_2 + w} \tag{B.9}$$

involves $u_2$ and, *also* $u_3$, which is grabbed by $w$ from the next two-step. Looking at Eqs. (10.11), this corresponds to the third original approximant. Notice that in the first one-step, Eqs. (B.2a) the first partial numerator $u_1$ is set to unity.

The grouping of one-steps indicated in Eq. (B.7) is

$$t_1\, t_3\, t_5\, t_7\, t_9\ \ldots\ , \tag{B.10}$$

in terms of two-steps. Writing the two-steps and composing them, we obtain the continued fraction whose successive approximants will be the odd approximants of the original PDSU($Cf$). In other words we obtain (again assuming that $M$ is big but finite, to avoid worrying about the end-partial-quotient) the odd part of Eq. (10.10) as

$$\mathrm{ODD}(\mathrm{PDSU}(Cf)) = 1 - \cfrac{u_2}{1 + u_2 + u_3 - \cfrac{u_3 u_4}{1 + u_4 + u_5 - \cfrac{u_5 u_6}{1 + u_6 + u_7 - \cfrac{u_7 u_8}{1 + u_8 + u_9 - \ddots}}}}\ , \tag{B.11}$$

Writing explicitly the end-partial-quotient, the above becomes

$$\mathrm{ODD}(\mathrm{PDSU}(Cf)) =$$

$$1 - \cfrac{u_2}{1 + u_2 + u_3 - \cfrac{u_3 u_4}{1 + u_4 + u_5 - \cfrac{u_5 u_6}{1 + u_6 + u_7 - \cdots \cfrac{\vdots}{1 + u_{M^*-2} + u_{M^*-1} - \cfrac{u_{M^*-1} u_{M^*}}{1 + u_{M^*} + \varsigma\, u_{M^*+1}}}}}} \,. \tag{B.12}$$

Here, $M^* = M - \varsigma$, with $M$ being the order of the original $\mathrm{PDSU}(Cf)$, Eq. (10.10), and $\varsigma = \mathrm{mod}\,(M, 2)$.

Now, we will turn our attention to the only other possible grouping of the original one-steps into two-steps (again assuming $M$ is big but finite, say, $M > 12$)

$$\tau_1 \overbrace{\tau_2\, \tau_3} \overbrace{\tau_4\, \tau_5} \overbrace{\tau_6\, \tau_7} \overbrace{\tau_8\, \tau_9} \ldots \tag{B.13}$$

Writing this in terms of two-steps we have

$$\tau_1\, t_2\, t_4\, t_6\, t_8\, t_{10} \ldots \tag{B.14}$$

This sequence will yield the even approximants: It starts with the first one-step $\tau_1$, that grabs the $u_2$ from the next two-step. Looking at Eqs. (10.11), this corresponds to the second approximant of the original continued fraction.

Writing $\tau_1$, the two-steps that follow, and composing them we obtain the continued fraction whose successive approximants will be the even approximants of the original $\mathrm{PDSU}(Cf)$. In other words we have obtained the even part of Eq. (10.10) as

$$\mathrm{EVEN}(\mathrm{PDSU}(Cf)) = \cfrac{1}{1 + u_2 - \cfrac{u_2 u_3}{1 + u_3 + u_4 - \cfrac{u_4 u_5}{1 + u_5 + u_6 - \cfrac{u_6 u_7}{1 + u_7 + u_8 - \ddots}}}} \,. \tag{B.15}$$

Taking care of the end-partial-quotient, the above becomes Eq. (10.10) is

$$\mathrm{EVEN}(\mathrm{PDSU}(Cf)) =$$

$$\cfrac{1}{1+u_2-\cfrac{u_2u_3}{1+u_3+u_4-\cfrac{u_4u_5}{1+u_5+u_6-\cdots\cfrac{\vdots}{1+u_{M^*-3}+u_{M^*-2}-\cfrac{u_{M^*-2}u_{M^*-1}}{1+u_{M^*-1}+u_{M^*}-\varsigma\,\cfrac{u_{M^*}\,u_{M^*+1}}{1+u_{M^*+1}}}}}}}. \tag{B.16}$$

Here, $M^*$ and $\varsigma$ have the same meanings as in Eq. (B.12).

The even part and the odd part of (10.10) are given in [Wall 1948, §4, p. 21]. The even–odd decomposition of a general continued fraction is given in [Jones & Thron 1980, §2.4.2-3]. More general contraction and extension formulas can be found in [Perron 1950, pages 197-205].

# Appendix C

## Convergence of the continued fraction representation of $\tilde{b}_1(z)$

### C.1 Summary

We will prove that, in the thermodynamic limit, the continued fraction representation of $\tilde{b}_1(z)$ for our model is *absolutely convergent* for $z \notin [-\mathrm{i}\,2\Omega,\, +\mathrm{i}\,2\Omega]$, and consequently, *all* its approximants (see the definition (C.6a) in §C.2 below)

$$\{[\![\tilde{b}_1(z)]\!]_{(1)}, [\![\tilde{b}_1(z)]\!]_{(2)}, [\![\tilde{b}_1(z)]\!]_{(3)}, [\![\tilde{b}_1(z)]\!]_{(4)}, [\![\tilde{b}_1(z)]\!]_{(5)}, \dots\} \ , \tag{C.1}$$

and <u>*any infinite subset*</u> of its approximants converge to a finite and unique limit. For example, the sequence of the $5th$-order approximant, the $10th$-order approximant, the $15th$-order approximant, ...

$$\{[\![\tilde{b}_1(z)]\!]_{(5)}, [\![\tilde{b}_1(z)]\!]_{(10)}, [\![\tilde{b}_1(z)]\!]_{(15)}, [\![\tilde{b}_1(z)]\!]_{(20)}, [\![\tilde{b}_1(z)]\!]_{(25)}, \dots\} \ , \tag{C.2a}$$

as well as the other four related sequences

$$\{[\![\tilde{b}_1(z)]\!]_{(4)}, [\![\tilde{b}_1(z)]\!]_{(9)}, [\![\tilde{b}_1(z)]\!]_{(14)}, [\![\tilde{b}_1(z)]\!]_{(19)}, [\![\tilde{b}_1(z)]\!]_{(24)}, \dots\} \ , \tag{C.2b}$$

$$\{[\![\tilde{b}_1(z)]\!]_{(3)}, [\![\tilde{b}_1(z)]\!]_{(8)}, [\![\tilde{b}_1(z)]\!]_{(13)}, [\![\tilde{b}_1(z)]\!]_{(18)}, [\![\tilde{b}_1(z)]\!]_{(23)}, \dots\} \ , \tag{C.2c}$$

$$\{[\![\tilde{b}_1(z)]\!]_{(2)}, [\![\tilde{b}_1(z)]\!]_{(7)}, [\![\tilde{b}_1(z)]\!]_{(12)}, [\![\tilde{b}_1(z)]\!]_{(17)}, [\![\tilde{b}_1(z)]\!]_{(22)}, \dots\} \ , \tag{C.2d}$$

$$\{[\![\tilde{b}_1(z)]\!]_{(1)}, [\![\tilde{b}_1(z)]\!]_{(6)}, [\![\tilde{b}_1(z)]\!]_{(11)}, [\![\tilde{b}_1(z)]\!]_{(16)}, [\![\tilde{b}_1(z)]\!]_{(21)}, \dots\} \ , \tag{C.2e}$$

*all* of them converge to the same limit as the full sequence of approximants (C.1), that contains all orders.

Similarly to the case above in which we pick each fifth approximant, we could have picked each *third* (three resulting sequences), or each *seventh* (seven resulting sequences), ..., or we could have picked the *prime* or the *non-prime* aproximants, etc. For all these infinite subsets of approximants, each resulting sequence has the *same* limit as the full sequence of approximants (C.1).

From *any* given continued fraction, one may obtain by a well known procedure[1] another continued fraction that *yields directly any desired subset of approximants*. This is known as a *contraction*. Absolute convergence of the original given continued fraction guarantees (we prove it is an —*if and only if*— relationship) that *all possible obtained contractions are equivalent*.

If we pick each *second* approximant we obtain the sequences

$$\{[\![\tilde{b}_1(z)]\!]_{(2)}, [\![\tilde{b}_1(z)]\!]_{(4)}, [\![\tilde{b}_1(z)]\!]_{(6)}, [\![\tilde{b}_1(z)]\!]_{(8)}, [\![\tilde{b}_1(z)]\!]_{(10)}, \dots\} \ , \tag{C.3a}$$

$$\{[\![\tilde{b}_1(z)]\!]_{(3)}, [\![\tilde{b}_1(z)]\!]_{(5)}, [\![\tilde{b}_1(z)]\!]_{(7)}, [\![\tilde{b}_1(z)]\!]_{(9)}, [\![\tilde{b}_1(z)]\!]_{(11)}, \dots\} \ . \tag{C.3b}$$

The first sequence is constituted by the even order approximants, while the second sequence is made up of the odd order approximants. The corresponding contractions are known[2] —somewhat misleadingly— as the even-part and the odd-part of $\tilde{b}_1(z)$. For the latter, all the partial numerators and denominators are equal among themselves (see §10.4) making it easily summable (see §10.6). The aforementioned *absolute convergence* of $\tilde{b}_1(z)$ for our model allows us to set the original continued fraction representation of $\tilde{b}_1(z)$ equal to any of its contractions —the odd part— in this case.

Thus, for our model it turned out to be mathematically convenient to deal directly and formally with the convergence properties of the continued fraction representation of $\tilde{b}_1(z)$ instead of the particular even and odd contractions. This was due to the simpler structure of the former.

We first review some needed definitions (§C.2) and the modern concept of convergence (§C.3) of a continued fraction. Then we prove that a continued fraction converges to a finite limit[3], if and only if, it converges absolutely.

We show that the convergence properties of a continued fraction are equivalent to those of any of its infinite tail parts in §C.4. We define $\mathfrak{T}_M(z)$ to be the infinite $M$th-tail part of the continued fraction representation of $\tilde{b}_1(z)$.

For reference convenience we state without proof (in §C.6) two theorems about absolute convergence, due to Borwein & Crandall [2004, pp. 291-292]. In §C.8 we show that $\tilde{b}_1(z)$ and any of

[1] Due to [Stieltjes 1894, Stieltjes 1895]. See [Jones & Thron 1980, §2.4.1].

[2] See §B and [Wall 1948, §4, p. 21]. The even-contraction and the odd-contraction of a general continued fraction are given in [Jones & Thron 1980, §2.4.2-3].

[3] And consequently any infinite subset of its approximants also.

its infinite $\mathfrak{T}_M(z)$ belong to the $\gamma$-class (defined in §C.5) of continued fractions to which the two theorems apply.

Both theorems provide *sufficient* though *not necessary* conditions for absolute convergence. The resulting regions of the complex plane are worked out in §C.9 and §C.10 for the first and the second theorems, respectively. Finally, in §C.11 we show that the *biggest* region of the complex plane in which *at least one* of the theorems holds is the complex plane cut from $-\mathrm{i}\,2\Omega$ to $+\mathrm{i}\,2\Omega$, i.e. $z \notin [-\mathrm{i}\,2\Omega, +\mathrm{i}\,2\Omega]$.

## C.2 Definitions. Approximants

Let $Cf$ be a *finite* continued fraction

$$Cf = \beta_0 + \cfrac{\alpha_1}{\beta_1 + \cfrac{\alpha_2}{\beta_2 + \cfrac{\alpha_3}{\beta_3 + \cfrac{\alpha_4}{\beta_4 + \cdots \cfrac{\vdots}{\beta_{N-2} + \cfrac{\alpha_{N-1}}{\beta_{N-1} + \cfrac{\alpha_N}{\beta_N}}}}}}} \equiv \beta_0 + \mathop{\mathrm{K}}_{i=1}^{N}(\alpha_i/\beta_i)\ . \tag{C.4}$$

Here $\alpha_p$ is the $p$th *partial numerator*, $\beta_p$ is the $p$th *partial denominator* and then $\alpha_p/\beta_p$ is called the $p$th *partial quotient*. $N$ is the order of the continued fraction. As long as $N$ *is finite*, this continued fraction is *always* well defined. The order $N$ can be as big as we want, without *ever* the need to consider convergence issues. Even the pathological cases can be handled if we agree to accept that the values assumed by the continued fraction belong to the extended complex field $\hat{\mathbb{C}}$ defined as

$$\hat{\mathbb{C}} = \mathbb{C} \cup \{\infty\}, \tag{C.5a}$$

where $\mathbb{C}$ is the usual complex field. Arithmetic operations involving the additional element $\infty$ are defined (see e.g. [Jones & Thron 1980, p. 21]) as follows: For all $z, z' \in \mathbb{C}$ with $z \neq 0$

$$z \cdot \infty = \infty, \qquad \frac{z}{\infty} = 0, \qquad \frac{z}{0} = \infty, \qquad \text{and} \quad z' + \infty = \infty. \tag{C.5b}$$

We will see below that this agreement is most convenient.

We need to be concerned about convergence *only* when the limit $N \to \infty$ is actually taken. Then, we will need to look at the sequence of approximants of the continued fraction (We already met the concept of approximant in §10.3: "The even–odd decomposition of a general continued fraction", p. 114).

Before going on, note that in all that follows when we refer to the continued fraction $Cf$ we will assume the limit $N \to \infty$ is taken.

An *approximant* is simply the continued fraction written up to the required order. That is, the finite quantity $[\![Cf]\!]_{(n)}$, defined below

$$\beta_0 + \cfrac{\alpha_1}{\beta_1 + \cfrac{\alpha_2}{\beta_2 + \cdots + \cfrac{\vdots}{\beta_{n-2} + \cfrac{\alpha_{n-1}}{\beta_{n-1} + \cfrac{\alpha_n}{\beta_n}}}}} = \beta_0 + \mathop{\mathrm{K}}_{i=1}^{n}(\alpha_i/\beta_i)$$

$$\equiv [\![Cf]\!]_{(n)} \equiv \frac{A_n}{B_n} \ , \quad n \geqslant 1 \ , \tag{C.6a}$$

is called the $n$th approximant, with $A_0 \equiv \beta_0$ and $B_0 \equiv 1$. If $n$ is even, we say that $[\![Cf]\!]_{(n)}$ is an even approximant. Similarly, if $n$ is odd, we say that $[\![Cf]\!]_{(n)}$ is an odd approximant. We call $A_n$ the $n$th *numerator* and $B_n$ the $n$th *denominator*. Thus, $[\![Cf]\!]_{(0)} = A_0/B_0 = \beta_0$ is the 0th approximant. The first approximant is

$$[\![Cf]\!]_{(1)} = \beta_0 + \mathop{\mathrm{K}}_{i=1}^{1}(\alpha_i/\beta_i) = \beta_0 + \frac{\alpha_1}{\beta_1} = \frac{\alpha_1 + \beta_0\beta_1}{\beta_1} \equiv \frac{A_1}{B_1} \ . \tag{C.6b}$$

The second approximant is

$$[\![Cf]\!]_{(2)} = \beta_0 + \mathop{\mathrm{K}}_{i=1}^{2}(\alpha_i/\beta_i) = \beta_0 + \cfrac{\alpha_1}{\beta_1 + \cfrac{\alpha_2}{\beta_2}}$$

$$= \beta_0 + \frac{\alpha_1\beta_2}{\alpha_2 + \beta_1\beta_2} = \frac{\alpha_2\beta_0 + \alpha_1\beta_2 + \beta_0\beta_1\beta_2}{\alpha_2 + \beta_1\beta_2} \equiv \frac{A_2}{B_2} \ , \tag{C.6c}$$

etc. We will denote the (infinite) sequence of approximants by $\{[\![Cf]\!]_{(n)}\}$. We are now prepared to state the following definition

## C.3 Convergence of a continued fraction

We say (see [Cuyt et al. 2008, p. 12], [Jones & Thron 1980, p. 19]) that an infinite continued fraction converges if its sequence of approximants has a unique limit (converges to a unique point) in $\hat{\mathbb{C}}$. Here, $\hat{\mathbb{C}}$ is the extended complex field defined in Eqs. (C.5). In the classical definition (e.g. [Wall 1948], [Perron 1950]) the limit is instead in $\mathbb{C}$, the usual complex field.

This modern definition conveniently handles [Borwein & Crandall 2004, p. 288] situations as the following. First note that the continued fraction $Cf$ may be written as

$$Cf = \beta_0 + \frac{\alpha_1}{\beta_1 + \underset{i=2}{\overset{\infty}{\mathrm{K}}}(\alpha_i/\beta_i)} \,. \tag{C.7}$$

It may happen that the infinite continued fraction $\underset{i=2}{\overset{\infty}{\mathrm{K}}}(\alpha_i/\beta_i)$ converges to $(-\beta_1) \in \mathbb{C}$, an instance which, under the old definition, would correspond to *no convergence* for $Cf$, while in the modern definition $Cf = \infty$ is a legit result (see Eqs. (C.5)!), whence $Cf$ converges in $\hat{\mathbb{C}}$. This example also illustrates that in the modern definition, divergence—maybe we should better say non-convergence or absence of convergence—must be oscillatory, say bifurcated or chaotic. [Borwein & Crandall 2004] and [Borwein, Borwein, Crandall & Mayer 2007] exhibit examples of such non-convergence scenarios.

If a continued fraction $Cf$ converges, the limit is customarily denoted with the same symbol $Cf$ and constitutes the value of the said continued fraction.

To analyze the convergence of the continued fraction representation of $\tilde{b}_1(z)$ we will use two theorems due to [Borwein & Crandall 2004] that hinge on the related concept of *absolute convergence of a continued fraction.*

## C.4 Absolute convergence of a continued fraction and proof that a continued fraction converges to a finite limit, if and only if, it converges absolutely

We say that a continued fraction $Cf$ converges absolutely (see [Borwein & Crandall 2004, p. 289], [Lorentzen & Waadeland 1992, p. 128] and [Jones & Thron 1980, p. 126]) if

$$\sum_{n=1}^{\infty} \left| \, [\![Cf]\!]_{(n)} - [\![Cf]\!]_{(n-1)} \, \right| = \sum_{n=1}^{\infty} \left| \frac{A_n}{B_n} - \frac{A_{n-1}}{B_{n-1}} \right| < \infty \,. \tag{C.8}$$

Here, $[\![Cf]\!]_{(n)} \equiv A_n/B_n$ is the $n$th approximant (defined in Eq. (C.6)). And —*if and only if* a continued fraction $Cf$ is *absolutely convergent*, then its sequence of approximants $\{[\![Cf]\!]_{(n)}\}$ *converges to a finite limit*. For conciseness, set

$$\mathfrak{A}_n \equiv [\![Cf]\!]_{(n)} - [\![Cf]\!]_{(n-1)} \ . \tag{C.9}$$

Suppose now that the sequence of approximants *does not converge to a finite limit*, that is

$$\lim_{n\to\infty} \big|\, [\![Cf]\!]_{(n)} \,\big| = \infty \ . \tag{C.10}$$

Then,

$$\lim_{n\to\infty} |\mathfrak{A}_n| \geqslant \lim_{n\to\infty} \big( \big|[\![Cf]\!]_{(n)}\big| - \big|[\![Cf]\!]_{(n-1)}\big| \big) >\neq 0 \ . \tag{C.11}$$

Consequently, by the well known result[4] ([Whittaker & Watson 1927, p. 15], [Cauchy 1821, p. 125]) that a *necessary* though not sufficient condition for the convergence of a series $\sum_{n=1}^{\infty} g_n$ is that $\lim_{n\to\infty} g_n = 0$, we have therefore

$$\text{The series} \quad \sum_{n=1}^{\infty} |\mathfrak{A}_n| \quad \text{is divergent.}$$

We now seek to prove the converse of the above proposition, i.e. if the sequence of approximants $\{[\![Cf]\!]\}$ has a finite limit then the continued fraction $Cf$ is absolutely convergent. We will need the following theorem due to

> [Cauchy 1821]: The necessary and sufficient condition for the existence of a limiting value of a sequence of numbers $z_1, z_2, z_3 \ldots$ is that *corresponding to any given positive number $\epsilon$, however small, it shall be possible to find a number $n$ such that*
>
> $$|z_{n+p} - z_n| < \epsilon \tag{C.12}$$
>
> *for all positive integral values of $p$.* This result [Whittaker & Watson 1927, p. 13] " . . . is one of the most important and fundamental theorems of analysis. It is sometimes called the *Principle of Convergence"*[Whittaker & Watson 1927].

[4]The lack of convergence of the series $\sum_{n=1}^{\infty} 1/n$ was noticed by Leibniz in 1673.

For conciseness set $\mathfrak{f}_n \equiv [\![Cf]\!]_{(n)}$. Define

$$S_k \equiv \sum_{i=1}^{k} |\mathfrak{f}_i - \mathfrak{f}_{i-1}| \ . \tag{C.13}$$

The sequence $\{S_k\}$, *has to satisfy Cauchy's theorem* in order to be convergent. Thus we need to show that corresponding to any given positive number $\epsilon$, however small, it is possible to find a number $k$ such that

$$\begin{aligned} |S_{k+p} - S_k| &= \left| \sum_{i=1}^{k+p} |\mathfrak{f}_i - \mathfrak{f}_{i-1}| \ - \sum_{i=1}^{k} |\mathfrak{f}_i - \mathfrak{f}_{i-1}| \right| < \epsilon \ , \\ &= \left| \sum_{i=k+1}^{k+p} |\mathfrak{f}_i - \mathfrak{f}_{i-1}| \right| = \sum_{i=k+1}^{k+p} |\mathfrak{f}_i - \mathfrak{f}_{i-1}| < \epsilon \ , \\ &= |\mathfrak{f}_{k+1} - \mathfrak{f}_k| + |\mathfrak{f}_{k+2} - \mathfrak{f}_{k+1}| + |\mathfrak{f}_{k+3} - \mathfrak{f}_{k+2}| + \cdots + |\mathfrak{f}_{k+p} - \mathfrak{f}_{k+p-1}| \ < \epsilon \ , \end{aligned} \tag{C.14}$$

for all positive integral values of $p$.

According to the hypotheses, Cauchy's theorem holds for the sequence $\{\mathfrak{f}_n\}$. Therefore, corresponding to any given $\epsilon$, however small, we can always find $\rho$ such that

$$|\mathfrak{f}_\rho - \mathfrak{f}_{\rho-1}| < \epsilon/p \ . \tag{C.15}$$

Now, choose $k = \rho$ and then each of the $p$ terms in the last sum above will be smaller than $\epsilon/p$ and the inequality (C.14) will be satisfied. □

## C.5 $\gamma$-FRACTIONS: A CLASS OF CONTINUED FRACTIONS

The two aforementioned (just before §C.4) theorems by Borwein & Crandall [2004] were designed by them only for a special kind of infinite continued fraction of the form

$$\gamma Cf = \cfrac{\gamma_1}{1 + \cfrac{\gamma_2}{1 + \cfrac{\gamma_3}{1 + \ddots}}} \ , \tag{C.16a}$$

and such that the $\gamma$-elements approach a *finite* complex limit, say

$$\gamma_n \to c \in \mathbb{C} \ . \tag{C.16b}$$

They designated this class of infinite continued fraction as a $\gamma$-fraction.

We note that for a general continued fraction the requirements are

> *A general continued fraction belongs to the class of $\gamma$-Fractions if all its partial denominators $\beta_n$ are different from zero and the sequence $\{\alpha_n\beta_{n-1}^{-1}\beta_n^{-1}\}$ approaches a finite complex limit. Here, $\alpha_n$ are the partial numerators.*

since then, an equivalence transformation (see §§10.3–10.4) to set all the partial denominators equal to unity (PDSU) can be performed. $\{\alpha_n\beta_{n-1}^{-1}\beta_n^{-1}\}$ is the sequence of resulting partial numerators if the PDSU equivalence transformation is performed.

## C.6 Two theorems due to J. Borwein & R. Crandall on the Absolute Convergence of $\gamma$-fractions

Both theorems are *sufficient, though, no necessary* conditions for the absolute convergence of a $\gamma$-fraction. For convenience we reproduce them below.

The first one is referred to as "Theorem 4.3" in [Borwein & Crandall 2004, p. 291], and reads: Assume

$$|c| < 1/4 \tag{C.17a}$$

and set

$$\varepsilon = 1/4 - |c| \ . \tag{C.17b}$$

If in the $\gamma$-fraction $\gamma Cf$ given in Definintion (C.16) we have

$$|\gamma_n - c| < \varepsilon/2 \ , \quad \underline{\text{for all}}\ n \, , \tag{C.17c}$$

then $\gamma Cf$ is absolutely convergent, with

$$\left| \, [\![\gamma Cf]\!]_{(n)} - [\![\gamma Cf]\!]_{(n-1)} \, \right| < \frac{2}{(1+2\varepsilon)^{2n}} \ . \tag{C.17d}$$

The proof is based on the Śleszyński-Pringsheim [Lorentzen & Waadeland 1992, p. 31] theorem, and uses the relationship we proved in §C.4 between convergence to a finite value and absolute convergence. See [Borwein & Crandall 2004, p. 291] for the proof.

The second [Borwein & Crandall 2004, Theorem 4.4, p. 292]: Assume

$$\theta = |\arg(c)| < \pi \tag{C.18a}$$

and that for the $\gamma$-fraction $\gamma Cf$ given in Definition (C.16) we have that

$$|\gamma_n - c| < h = \frac{2}{9}\cos^2(\theta/2)\ . \tag{C.18b}$$

Then $\gamma Cf$ is absolutely convergent, with

$$\left|\, [\![\gamma Cf]\!]_{(n)} - [\![\gamma Cf]\!]_{(n-1)} \,\right| < \frac{1}{\sqrt{h}}\frac{|c|+h}{[1+h/(|c|+h)]^{n-1}}\ . \tag{C.18c}$$

The proof follows [Borwein & Crandall 2004, p. 292] from the parabola-sequence theorem [Lorentzen & Waadeland 1992, Theorem 21, pages 136-137], with the multipliers assignment $g_k \leftarrow 1/3$.

To use the above theorems, the continued fraction representation of $\tilde{b}_1(z)$ has to be cast into the required form (this was done in §10.4) with all the partial denominators set unity (PDSU). We also need to introduce the introduce the *finite part* and the *infinite part* of the resulting continued fraction.

## C.7 The continued fraction representation of $\tilde{b}_1(z)$ and its infinite $M$th-tail part $\mathfrak{T}_M(z)$: Equivalent convergence or non–convergence behavior of both

The continued fraction representation of $\tilde{b}_1(z)$ was described in §9.1 and obtained in Eq. (9.11). We showed in §§10.1–10.2, that in the thermodynamic limit, $\tilde{b}_1(z)$ is given by the *infinite* continued fraction (10.5), that we reproduce below for convenience

$$\tilde{b}_1(z) = \cfrac{1}{z + \cfrac{\Delta_2}{z + \cfrac{\Delta_3}{z + \cfrac{\Delta_4}{z + \ddots}}}}\ . \tag{C.19}$$

By means of an equivalence transformation (see §§10.3–10.4) this continued fraction was cast (see Eq. (10.16)) into the following form, with all the partial denominators set to unity (PDSU)

$$\tilde{b}_1(z) = \cfrac{1/z}{1+\cfrac{\Delta_2/z^2}{1+\cfrac{\Delta_3/z^2}{1+\cfrac{\Delta_4/z^2}{1+\ddots}}}} \,, \tag{C.20}$$

We will see in the next section that to study the convergence of the continued fraction representation of $\tilde{b}_1(z)$ it is convenient to write it in terms of a *finite part* and an *infinite part*. The finite part corresponds to the first $M-1$ steps of the continued fraction. The positive integer $M$ can be set arbitrarily as long as it is kept *finite*. The infinite part comprises from the $M$th-step to infinity, i.e.

$$\underset{\mathrm{j}=M}{\overset{\infty}{\mathrm{K}}} \left[(\Delta_\mathrm{j}/z^2)/1\right] \,, \tag{C.21}$$

and is sometimes referred to as the *tail* of the continued fraction.

Let's write out explicitly a few steps before and after an arbitrary $M$th-step in the continued fraction representation of $\tilde{b}_1(z)$

$$\tilde{b}_1(z) = \cfrac{1/z}{1+\cfrac{\Delta_2/z^2}{1+\cfrac{\Delta_3/z^2}{1+\cdots+\cfrac{\vdots}{1+\cfrac{\Delta_{M-1}/z^2}{1+\cfrac{\Delta_M/z^2}{1+\cfrac{\Delta_{M+1}/z^2}{1+\cfrac{\Delta_{M+2}/z^2}{1+\ddots}}}}}}}} = \cfrac{1/z}{1+\cfrac{\Delta_2/z^2}{1+\cfrac{\Delta_3/z^2}{1+\cdots+\cfrac{\vdots}{1+\cfrac{\Delta_{M-1}/z^2}{1+\underset{\mathrm{j}=M}{\overset{\infty}{\mathrm{K}}}\left[(\Delta_\mathrm{j}/z^2)/1\right]}}}}} \,, \tag{C.22}$$

and define the $M$th-*tail* as

$$\mathfrak{T}_M(z) \equiv \cfrac{\Delta_M/z^2}{1+\cfrac{\Delta_{M+1}/z^2}{1+\cfrac{\Delta_{M+2}/z^2}{1+\cfrac{\Delta_{M+3}/z^2}{1+\ddots}}}} = \underset{\mathrm{j}=M}{\overset{\infty}{\mathrm{K}}}\left[(\Delta_\mathrm{j}/z^2)/1\right] \ . \tag{C.23}$$

Thus, in terms of the infinite $M$th-*tail* part and the corresponding finite part, the continued fraction representation of $\tilde{b}_1(z)$ is written

$$\tilde{b}_1(z) = \cfrac{1/z}{1+\cfrac{\Delta_2/z^2}{1+\cfrac{\Delta_3/z^2}{1+\cdots+\cfrac{\vdots}{1+\cfrac{\Delta_{M-1}/z^2}{1+\mathfrak{T}_M(z)}}}}} \ . \tag{C.24}$$

Note that we are <u>*not*</u> truncating the continued fraction and that we <u>*do not*</u> need to be concerned at all with the size (or any estimate of it) of the tail. We only need to notice that the connection between the infinite $M$th-*tail* $\mathfrak{T}_M(z)$ and the full continued fraction representation of $\tilde{b}_1(z)$ is a *finite relation* and therefore their convergence or non–convergence behaviors are the same.

## C.8 Absolute convergence of the continued fraction representation of $\tilde{b}_1(z)$

The continued fraction representation of $\tilde{b}_1(z)$, given in Eq. (C.20) with all the partial denominators set to unity (PDSU)

$$\tilde{b}_1(z) = \cfrac{1/z}{1+\cfrac{\Delta_2/z^2}{1+\cfrac{\Delta_3/z^2}{1+\cfrac{\Delta_4/z^2}{1+\ddots}}}} \ , \tag{C.25}$$

belongs to the class of $\gamma$-fractions defined in §C.5. From Table 10.1 (that we reproduce below for convenience) and Eqs. (10.6) that give the odd and the even Deltas (also reproduced below for

Table C.1: Delta sequence $\sigma = (\Delta_1, \Delta_2, \ldots, \Delta_{d-1})$, in units of $k/m \equiv \Omega^2$. In the thermodynamic limit, $N \to \infty$, it is completely regular since then we do not have to worry about the special value (10.4) of the end-Delta breaking the sequence. $N$ is the length of the harmonic oscillators chain.

| | $\sigma =$ | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| $N$ | $(\Delta_1$ | $\Delta_2$ | $\Delta_3$ | $\Delta_4$ | $\Delta_5$ | $\Delta_6$ | $\Delta_7$ | $\Delta_8$ | $\Delta_9$ | $\Delta_{10}$ | $\Delta_{11})$ |
| 2 | $\big($ $\lambda(1+\kappa)$ | $\frac{1}{\kappa+1}$ | $\frac{\kappa}{\kappa+1}$ $\big)$ | | | | | | | | |
| 3 | $\big($ $\lambda(1+\kappa)$ | $\frac{1}{\kappa+1}$ | $\frac{2\kappa+1}{\kappa+1}$ | $\frac{\kappa+1}{2\kappa+1}$ | $\frac{\kappa}{2\kappa+1}$ $\big)$ | | | | | | |
| 4 | $\big($ $\lambda(1+\kappa)$ | $\frac{1}{\kappa+1}$ | $\frac{2\kappa+1}{\kappa+1}$ | $\frac{\kappa+1}{2\kappa+1}$ | $\frac{3\kappa+1}{2\kappa+1}$ | $\frac{2\kappa+1}{3\kappa+1}$ | $\frac{\kappa}{3\kappa+1}$ $\big)$ | | | | |
| 5 | $\big($ $\lambda(1+\kappa)$ | $\frac{1}{\kappa+1}$ | $\frac{2\kappa+1}{\kappa+1}$ | $\frac{\kappa+1}{2\kappa+1}$ | $\frac{3\kappa+1}{2\kappa+1}$ | $\frac{2\kappa+1}{3\kappa+1}$ | $\frac{4\kappa+1}{3\kappa+1}$ | $\frac{3\kappa+1}{4\kappa+1}$ | $\frac{\kappa}{4\kappa+1}$ $\big)$ | | |
| 6 | $\big($ $\lambda(1+\kappa)$ | $\frac{1}{\kappa+1}$ | $\frac{2\kappa+1}{\kappa+1}$ | $\frac{\kappa+1}{2\kappa+1}$ | $\frac{3\kappa+1}{2\kappa+1}$ | $\frac{2\kappa+1}{3\kappa+1}$ | $\frac{4\kappa+1}{3\kappa+1}$ | $\frac{3\kappa+1}{4\kappa+1}$ | $\frac{5\kappa+1}{4\kappa+1}$ | $\frac{4\kappa+1}{5\kappa+1}$ | $\frac{\kappa}{5\kappa+1}$ $\big)$ |

convenience)

Odd Deltas, with the thermodynamic limit taken,

$$\Delta_{2\rho-1} = \frac{\rho\kappa + 1}{(\rho-1)\kappa + 1}\,\Omega^2 \ , \qquad\qquad \rho = 2, 3, 4, \ldots \tag{C.26a}$$

Even Deltas, with the thermodynamic limit taken,

$$\Delta_{2\rho} = \frac{(\rho-1)\kappa + 1}{\rho\kappa + 1}\,\Omega^2 \ , \qquad\qquad \rho = 2, 3, 4, \ldots \tag{C.26b}$$

one sees that, *taking first the thermodynamic limit*, then the Deltas sequence satisfies

$$\lim_{\nu\to\infty} \Delta_\nu = \Omega^2 \ . \tag{C.27}$$

Thus, the elements (partial numerators) of the continued fraction representation of $\tilde{b}_1(z)$ with the (PDSU) approach a *finite* complex limit

$$\lim_{\nu\to\infty} \Delta_\nu / z^2 = \Omega^2 / z^2 \ , \tag{C.28}$$

and consequently (see §C.5) the continued fraction representation of $\tilde{b}_1(z)$, with the PDSU[5] belongs to the class of $\gamma$-fractions as claimed at the beginning of this section. Evidently, any infinite $M$th-tail $\mathfrak{T}_M(z)$ (*see* Eq. (C.23) p. 198) of the continued fraction representation $\tilde{b}_1(z)$ with PDSU, is also a $\gamma$-fraction.

We showed in the previous section, §C.7, that the convergence properties of the continued fraction representation of $\tilde{b}_1(z)$ (with the PDSU) and any of its infinite $M$th-tails $\mathfrak{T}_M(z)$ are the same. We have just shown that both are $\gamma$-fractions. Therefore we can now proceed (finally!) to use the theorems of §C.6.

We write the (upper case) Deltas in units of $\Omega^2$ by introducing the following (lower case) deltas

$$\Delta_\nu \equiv \delta_\nu \Omega^2 \tag{C.29}$$

Then, from Eq. (C.27) the deltas sequence satisfies

$$\lim_{\nu\to\infty} \delta_\nu = 1 \ . \tag{C.30}$$

Let's start with the

## C.9 Application of the Borwein–Crandall first theorem to $\mathfrak{T}_M(z)$

The assumption (C.17a) $|c| < 1/4$ (see Eq. (C.16b) in §C.5), together with the definition of $\mathfrak{T}_M(z)$ (see Eq. (C.23)), and with the limit given by Eq. (C.28) demands

$$\left|\frac{\Omega^2}{z^2}\right| < \frac{1}{4} \ ,$$

or

$$4\Omega^2 < |z^2| \ . \tag{C.31}$$

The positive quantity $\varepsilon \equiv 1/4 - |c|$ defined in Eq. (C.17b) of §C.6 is

$$\varepsilon \equiv \frac{1}{4} - \left|\frac{\Omega^2}{z^2}\right| \ . \tag{C.32}$$

[5]The continued fraction representation of $\tilde{b}_1(z)$, without the partial denominators set to unity, also belongs to the class of $\gamma$-Fractions. See §C.5

The condition (C.17c) $|\gamma_n - c| < \varepsilon/2$ (see §C.5) has to be fulfilled *for all n* of the $\gamma$-fraction being considered ($\mathfrak{T}_M(z)$ in this case), to have absolute convergence. This requirement together with the definition of $\mathfrak{T}_M(z)$ (*see* Eq. (C.23)) demands, *for all*[6] $\mathrm{j} \neq 1$,

$$\left|\frac{\Delta_\mathrm{j}}{z^2} - \frac{\Omega^2}{z^2}\right| < \frac{1}{2}\left(\frac{1}{4} - \left|\frac{\Omega^2}{z^2}\right|\right) ,$$
$$|\Delta_\mathrm{j} - \Omega^2| < \frac{1}{2}\left(\frac{|z^2|}{4} - \Omega^2\right) = \frac{1}{2}\,\frac{|z^2| - 4\Omega^2}{4} ,$$

and with definition (C.29),

$$|\delta_\mathrm{j} - 1| < \frac{1}{2}\,\frac{|z^2| - 4\Omega^2}{4\Omega^2} . \tag{C.33}$$

The convergence (see Eq. (C.30)) of the $\delta_\nu$'s to 1 is *oscillatory* (see Table C.1) —the even $\delta_\nu$'s converge uniformly from below, the odd ones from above— but *uniform*: The following sequence decreases steadily

$$|\delta_{2\rho} - 1| = |\delta_{2\rho+1} - 1| = \frac{\kappa}{\rho\kappa + 1} , \qquad \rho = 1, 2, 3, 4, \ldots . \tag{C.34}$$

The limit (C.30) $\lim_{\nu\to\infty} \delta_\nu = 1$ ensures that one can always find at least one value of j, say $\mathrm{j}^*$, to satisfy the inequality (C.33), as long as its right hand side, no matter how small, remains *positive*. To satisfy the inequality (C.33), *for all* the values of j that enter into $\mathfrak{T}_M(z)$, it suffices to set $M \leftarrow \mathrm{j}^*$, since then, from Eq. (C.34),

$$|\delta_M - 1| \geqslant |\delta_{M+1} - 1| \geqslant |\delta_{M+2} - 1| \geqslant |\delta_{M+3} - 1| \geqslant \cdots > 0 . \tag{C.35}$$

In other words, one can always find a $M$th-tail $\mathfrak{T}_M(z)$, with $M$ *finite*,

$$\mathfrak{T}_M(z) \equiv \cfrac{\delta_M\Omega^2/z^2}{1 + \cfrac{\delta_{M+1}\Omega^2/z^2}{1 + \cfrac{\delta_{M+2}\Omega^2/z^2}{1 + \cfrac{\delta_{M+3}\Omega^2/z^2}{1 + \ddots}}}} = \underset{\mathrm{j}=M}{\overset{\infty}{\mathrm{K}}}\left[(\delta_\mathrm{j}\Omega^2/z^2)/1\right] , \tag{C.36}$$

such that *all* its partial numerators satisfy the inequality (C.33), implying the *absolute convergence* of $\mathfrak{T}_M(z)$ and of the continued fraction representation of $\tilde{b}_1(z)$.

[6] $\Delta_1$ is special (see Table C.1), it depends on $\lambda$. Anyway $\Delta_1$ does not appear in either the continued fraction representation of $\tilde{b}_1(z)$ or in any of its infinite $M$th-tails $\mathfrak{T}_M(z)$

This is a *sufficient* but *no necessary* condition, that can always be fulfilled, with $M$ *finite*, if $z$ is outside the circle $|z|^2 = 4\Omega^2$, i.e., the right hand side of inequality (C.33) is *positive*, no matter how small.

Thus, to satisfy the first theorem *it is sufficient* that

$$|z| > 2\Omega \; . \tag{C.37}$$

## C.10 Application of the Borwein–Crandall second theorem to $\mathfrak{T}_M(z)$

It is assumed in (C.18a) that $\theta = |\arg(c)| < \pi$. Here (see Eq. (C.16b), the definition of $\mathfrak{T}_M(z)$, Eq. (C.23), and the limit given by Eq. (C.28)),

$$c = \frac{\Omega^2}{z^2} \; , \tag{C.38}$$

is the limit of the sequence of partial numerators of $\mathfrak{T}_M(z)$. We are interested in singling out the *biggest* region of the complex plane compatible with the assumption (C.18a). Set

$$z = r\, \mathrm{e}^{\mathrm{i}\,\phi} \; . \tag{C.39}$$

Then, assumption (C.18a) gives

$$\theta = |2\phi| < \pi \, . \tag{C.40}$$

In detail

$$-\frac{\pi}{2} < \phi < \frac{\pi}{2} \; . \tag{C.41}$$

Since $\mathfrak{T}_M(z)$ is a function only of $z^2$, to the above interval we have to add $\pi/2 < \phi < 3\pi/2$. Therefore to satisfy the assumption (C.18a) $\theta = |\arg(c)| < \pi$

$$\arg(z) \in \{(-\pi/2, \pi/2) \cup (\pi/2, 3\pi/2)\} \, , \tag{C.42}$$

or, equivalently

$$\arg(z) \notin \{\text{open neighborhood of } \pm\, \pi/2\} \, . \tag{C.43}$$

The quantity $h$ that appears in the condition for absolute convergence required by the second theorem is

$$h = \frac{2}{9} \cos^2(\theta/2) = \cos^2 \frac{|2\phi|}{2} = \frac{2}{9} \cos^2 \phi \; , \tag{C.44}$$

with $\theta$ given by (C.40).

The condition (C.18b) $|\gamma_n - c| < h$ (see §C.5) has to be fulfilled *for all n* of the $\gamma$-fraction being considered ($\mathfrak{T}_M(z)$ in this case), to have absolute convergence. This condition together with the definition of $\mathfrak{T}_M(z)$ (*see* Eq. (C.23)) requires, *for all* (see [6] in page 201) $\mathfrak{j} \neq 1$,

$$\left|\frac{\Delta_{\mathfrak{j}}}{z^2} - \frac{\Omega^2}{z^2}\right| < h = \frac{2}{9}\cos^2\phi \ ,$$

$$|\Delta_{\mathfrak{j}} - \Omega^2| < \frac{2}{9}\,|z^2|\cos^2\phi \ ,$$

and with definition (C.29),

$$|\delta_{\mathfrak{j}} - 1| < \frac{2}{9}\,\frac{|z^2|}{\Omega^2}\cos^2\phi \ . \tag{C.45}$$

The limit (C.30) $\lim_{\nu\to\infty}\delta_\nu = 1$ ensures that one can always find at least one value of $\mathfrak{j}$, say $\mathfrak{j}^{**}$, to satisfy the inequality (C.45), as long as its (always positive) right hand side, no matter how small, remains *different from zero*. To satisfy the inequality (C.33), *for all* the values of $\mathfrak{j}$ that enter into $\mathfrak{T}_M(z)$, it suffices to set $M \leftarrow \mathfrak{j}^{**}$ , since then, from Eq. (C.34),

$$|\delta_M - 1| \geqslant |\delta_{M+1} - 1| \geqslant |\delta_{M+2} - 1| \geqslant |\delta_{M+3} - 1| \geqslant \cdots > 0 \ . \tag{C.46}$$

The right hand side of the inequality (C.45) will be different form zero if $|z^2| \neq 0$ and $\cos^2\phi \neq 0$. This last condition requires $\phi \neq \pm\pi/2$. Thus, to satisfy the second theorem *it is sufficient* that

$$|z| \neq 0 \quad \textit{and} \quad \arg(z) \in \{(-\pi/2, \pi/2) \cup (\pi/2, 3\pi/2)\} \, . \tag{C.47}$$

## C.11 The first theorem and the second theorem, together

The result (C.37) $|z| > 2\Omega$ from the first theorem, and the result (C.47) from the second theorem just above, each of them is, a *sufficient* but no necessary condition.

The *biggest* region of the complex plane in which *at least* one of them is fulfilled is

$$z \in \{\mathbb{C} - [-\,\mathrm{i}\,2\Omega, +\,\mathrm{i}\,2\Omega]\} \, , \tag{C.48a}$$

or

$$z \notin [-\,\mathrm{i}\,2\Omega, +\,\mathrm{i}\,2\Omega] \ . \tag{C.48b}$$

Again, (C.48) is a *sufficient* condition. □

# Appendix D

## Some useful operator identities and linear response theory relations

### D.1 Time dependent response function

The unperturbed quantum many body system (MBS) *time-independent* Hamiltonian is $H$, with eigenvalues $E_i$ and eigenstates $|i>\equiv|i(t=0)>$

$$H|i>=E_i|i>\ . \tag{D.1}$$

We set

$$|i(t)>\equiv \mathrm{e}^{-\,\mathrm{i}Ht/\hbar}\,|i>=\mathrm{e}^{-\,\mathrm{i}E_it/\hbar}\,|i>\,, \tag{D.2}$$

so that Schrödinger's equation reads

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\big(\,\mathrm{e}^{-\,\mathrm{i}E_it/\hbar}\,|i>\,\big)=\mathrm{e}^{-\,\mathrm{i}E_it/\hbar}\;\mathrm{i}\hbar\frac{-\,\mathrm{i}E_i}{\hbar}|i>=E_i\;\big(\,\mathrm{e}^{-\,\mathrm{i}E_it/\hbar}\,|i>\,\big)=H\,|i(t)>\,, \tag{D.3}$$

as expected. This interpretation: state vectors evolve in time and operators are constant, corresponds to the "Schhrödinger picture". In the "Heisenberg picture" the state vectors remain constant and the operators evolve according to Heisenberg's equation of motion

$$\frac{\mathrm{d}O(t)}{\mathrm{d}t}=\frac{\mathrm{i}}{\hbar}[H,O(t)]+\frac{\partial O}{\partial t}\,. \tag{D.4}$$

If $H$ is *time-independent*, the operators time evolution is[1]

$$O(t)=\mathrm{e}^{\mathrm{i}Ht/\hbar}\,O\,\mathrm{e}^{-\,\mathrm{i}Ht/\hbar} \tag{D.5}$$

with $O\equiv O(t=0)$. Since $H$ is <u>*time-independent*</u> the physical situation of the unperturbed MBS is <u>*stationary*</u> and therefore the choice of the $t=0$ instant in either Eq. (D.1) on the current page or Eq. (D.5) above is immaterial.

[1]This can be immediately verified by taking the time derivative of Eq. (D.5) on this page.

In §12.1 we considered the particular situation in which the quantum MBS with Hamiltonian $H$ is perturbed by a weak applied field $h(t)$ that we *turn on* at a remote past $t = -T$, $T \to \infty$. The applied field $h(t)$ couples to the MBS observable variable $B$ giving rise to a time-dependent potential

$$\mathcal{V} \equiv \mathcal{V}(t) = -h(t)B\,. \tag{D.6}$$

For the perturbed system the Hamiltonian is

$$H' \equiv H + \mathcal{V}(t)\,, \tag{D.7}$$

the eigenstate $|i>$ is altered, and its time dependence is <u>*no longer stationary*</u> as was given by Eq. (D.2). For conciseness, we will write for it just

$$\begin{aligned} |i'(t)> &\equiv |i(t)> + \sum_j c_j(t)\,|j(t)>\,, \\ &= \mathrm{e}^{-\,\mathrm{i}E_i t/\hbar}\,|i> + \sum_j c_j\,\mathrm{e}^{-\,\mathrm{i}E_j t/\hbar}\,|j>\,. \end{aligned} \tag{D.8}$$

The coefficients $\{a_j(t)\}$ will be obtained by solving, up to first order in $\mathcal{V}$, Schrödinger's equation

$$\mathrm{i}\hbar\frac{\partial|i'>}{\partial t} = (H+\mathcal{V})|i'>\ . \tag{D.9}$$

Thus, we write the lhs and the rhs of Eq. (D.9) above, with $|i'>$ given by Eq. (D.8):

$$\mathrm{i}\hbar\frac{\partial|i'>}{\partial t} = E_i\,\mathrm{e}^{-\,\mathrm{i}E_i t/\hbar}\,|i> + \mathrm{i}\hbar\sum_j \dot{c}_j\,\mathrm{e}^{-\,\mathrm{i}E_j t/\hbar}\,|j> + \sum_j E_j c_j\,\mathrm{e}^{-\,\mathrm{i}E_j t/\hbar}\,|j>\,. \tag{D.10a}$$

$$\begin{aligned} (H+\mathcal{V})|i'> = E_i\,\mathrm{e}^{-\,\mathrm{i}E_i t/\hbar}\,|i> + \sum_j E_j c_j\,\mathrm{e}^{-\,\mathrm{i}E_j t/\hbar}\,|j> + \mathcal{V}\,\mathrm{e}^{-\,\mathrm{i}E_i t/\hbar}\,|i> \\ + \mathcal{V}\sum_j c_j\,\mathrm{e}^{-\,\mathrm{i}E_j t/\hbar}\,|j>\,. \end{aligned} \tag{D.10b}$$

The last term in Eq. (D.10b) above is of second order in $\mathcal{V}$ since the coefficients $c_j$ are already of first order in $\mathcal{V}$, thus we omit it. Then, comparing Eqs. (D.10a) and (D.10b) on the current page we obtain

$$\mathrm{i}\hbar\sum_j \dot{c}_j\,\mathrm{e}^{-\,\mathrm{i}E_j t/\hbar}\,|j> = \mathcal{V}\,\mathrm{e}^{-\,\mathrm{i}E_i t/\hbar}\,|i>\,. \tag{D.11}$$

Multiplying by $<n|$ on the right

$$\mathrm{i}\hbar\dot{c}_n\,\mathrm{e}^{-\,\mathrm{i}E_nt/\hbar} = \mathrm{e}^{-\,\mathrm{i}E_it/\hbar}\,<n|\mathcal{V}|i>\,, \tag{D.12}$$

that is

$$\dot{c}_n(t) = \frac{1}{\mathrm{i}\hbar}\,\mathrm{e}^{\mathrm{i}(E_n-E_i)t/\hbar}\,<n|\mathcal{V}(t)|i>\,, \tag{D.13}$$

and

$$c_n(t) = \frac{1}{\mathrm{i}\hbar}\int_{-\infty}^{t}\mathrm{e}^{\mathrm{i}(E_n-E_i)t'/\hbar}\,<n|\mathcal{V}(t')|i>\,\mathrm{d}t'\,. \tag{D.14}$$

We wish to obtain the time dependent ensemble-expectation-value $\langle A(t)\rangle_{H'(t)}$ of an operator $A$ in the perturbed system. This involves performing a trace with the corresponding density matrix as we will show below. Therefore, we need to know how the matrix element

$$<i(t)|A|i(t)>=<i|A|i> \tag{D.15}$$

in the unperturbed system, is altered by the time-dependent perturbation $\mathcal{V}(t)$. We will obtain this result accurate up to linear order in $\mathcal{V}$. Using the expression of $|i'(t)>$ given in Eq. (D.8) on the preceding page we can obtain the needed diagonal matrix elements of $A$ in the perturbed system as follows[2]:

$$\begin{aligned}
&<i'(t)|A|i'(t)> \\
&\quad= \big(\,\mathrm{e}^{\mathrm{i}E_it/\hbar}\,<i| + \sum_j c_j^*\,\mathrm{e}^{\mathrm{i}E_jt/\hbar}\,<j|\big)A\big(\,\mathrm{e}^{-\,\mathrm{i}E_it/\hbar}\,|i> + \sum_n c_n\,\mathrm{e}^{-\,\mathrm{i}E_nt/\hbar}\,|n>\,\big)\,, && \text{(D.16a)}\\
&\quad=<i|A|i> + \sum_j c_j\,\mathrm{e}^{\mathrm{i}(E_i-E_j)t/\hbar}\,<i|A|j> + \sum_j c_j^*\,\mathrm{e}^{\mathrm{i}(E_j-E_i)t/\hbar}\,<j|A|i> \\
&\qquad\qquad + \sum_{j,n} c_j^*c_n\,\mathrm{e}^{\mathrm{i}(E_j-E_n)t/\hbar}\,<j|A|n>\,, && \text{(D.16b)}
\end{aligned}$$

and using Eq. (D.5) on page 204:

$$=<i|A|i> + \sum_j c_j\,<i|A(t)|j> + \sum_j c_j^*\,<j|A(t)|i>\ . \tag{D.16c}$$

The $\{c_j\}$ coefficients are of first order in $\mathcal{V}$ thus, the second order term $\sum_{j,n} c_j^*c_n\ldots$ in Eq. (D.16b) above can be omitted. Now we substitute the solutions for the coefficients $c_j$ that we obtained in

[2]The dummy index in the second sum in Eq. (D.16a) on the current page was relabeled as $n$. Afterwards, it was relabeled again as $j$ in Eq. (D.16b).

Eq. (D.14)

$$
\begin{aligned}
&<i'(t)|A|i'(t)> \\
&\quad =<i|A|i> + \frac{1}{\mathrm{i}\hbar}\int_{-\infty}^{t}\sum_{j}\Big[\,\mathrm{e}^{\mathrm{i}(E_j-E_i)t'/\hbar}\,<j|\mathcal{V}(t')|i><i|A(t)|j> \\
&\qquad\qquad - \mathrm{e}^{\mathrm{i}(E_i-E_j)t'/\hbar}\,<i|\mathcal{V}(t')|j><j|A(t)|i>\,\Big]\,\mathrm{d}t'\,. \qquad \text{(D.17)}
\end{aligned}
$$

The time dependence in $\mathcal{V}(t)$ is from the applied field $h(t)$ [Eq. (D.6)] Substituting $\mathcal{V}(t') = -h(t')B$ allows us to use the symmetry of the terms in the square brackets above:

$$
\begin{aligned}
&=<i|A|i> + \frac{\mathrm{i}}{\hbar}\int_{-\infty}^{t}\sum_{j}\Big[\,\mathrm{e}^{\mathrm{i}(E_j-E_i)t'/\hbar}\,h(t')\,<j|B|i><i|A(t)|j> \\
&\qquad\qquad - \mathrm{e}^{\mathrm{i}(E_i-E_j)t'/\hbar}\,h(t')\,<i|B|j><j|A(t)|i>\,\Big]\,\mathrm{d}t'\,. \qquad \text{(D.18)}
\end{aligned}
$$

Aqain using Eq. (D.5):

$$
\begin{aligned}
&=<i|A|i> + \frac{\mathrm{i}}{\hbar}\int_{-\infty}^{t}\sum_{j}\Big[\,<j|B(t')|i><i|A(t)|j> \\
&\qquad\qquad - <i|B(t')|j><j|A(t)|i>\,\Big]h(t')\,\mathrm{d}t'\,, \qquad \text{(D.19)}
\end{aligned}
$$

and assuming the completeness of the set $\{|j>\}$, i.e. $\sum_j |j><j| = 1$, we obtain the following result for the diagonal matrix elements of $A$ in the perturbed system

$$
\begin{aligned}
&<i'(t)|A|i'(t)> \\
&\quad =<i|A|i> + \frac{\mathrm{i}}{\hbar}\int_{-\infty}^{t} <i|\big[A(t),B(t')\big]|i>\,h(t')\,\mathrm{d}t'\,. \qquad \text{(D.20)}
\end{aligned}
$$

To obtain the time dependent ensemble-expectation-value $\langle A(t)\rangle_{H'(t)}$ in §12.1, Eq. (12.13b) on page 158 accurate to first order in $h(t)$, we have to take the trace of the diagonal matrix elements $A_{i'i'}$ obtained in Eq. (D.20) above with the density matrix of the <u>*unperturbed system*</u> since these matrix elements are already of first order in $h(t)$. Therefore

$$
\langle A(t)\rangle_{H'(t)} = \langle A\rangle_H + \frac{\mathrm{i}}{\hbar}\int_{-\infty}^{t}\langle\big[A(t),B(t')\big]\rangle_H\;h(t')\,\mathrm{d}t'\,, \qquad \text{(D.21a)}
$$

and using the *stationarity* of time correlation functions (TCF)s, [Eq. (D.95) on page 219]

$$
= \langle A\rangle + \int_{-\infty}^{t}\frac{\mathrm{i}}{\hbar}\langle\big[A(t-t'),B\big]\rangle h(t')\,\mathrm{d}t'\,. \qquad \text{(D.21b)}
$$

In Eq. (D.21) above —and everywhere else— the plain angular brackets denote [Eq. (12.11) on page 157] the ensemble average for the unperturbed MBS

$$
\langle\ldots\rangle \equiv \langle\ldots\rangle_H \equiv \frac{\mathrm{Tr}(\ldots\mathrm{e}^{-\beta H})}{\mathrm{Tr}(\mathrm{e}^{-\beta H})}\,. \qquad \text{(D.22)}
$$

## D.2 Static response

Let's suppose now that the applied field is constant

$$h(t) = h \tag{D.23}$$

in Equations (D.6)-(D.7) on page 205. Since the many body system (MBS) Hamiltonian [Eq. (D.1)] $H$ is time independent, the perturbed MBS Hamiltonian

$$H' = H + V\,, \quad \text{with } V \equiv -hB\,, \tag{D.24}$$

is also time independent. In this section we will calculate, accurate to first order in $V$, the *static response*

$$\langle A\rangle_{H'} - \langle A\rangle = \mathrm{Tr}(\rho' A) - \mathrm{Tr}(\rho A) \tag{D.25}$$

referred to in Eqs. (12.21)-(12.22) on page 159. We will *always* keep the plain angular brackets to denote the ensemble average on the unperturbed MBS

$$\langle \dots \rangle \equiv \langle \dots \rangle_H \equiv \frac{\mathrm{Tr}(\dots \mathrm{e}^{-\beta H})}{\mathrm{Tr}(\mathrm{e}^{-\beta H})}\,. \tag{D.26}$$

In Eq. (D.25) above $\rho$ is the density matrix for the unperturbed MBS and

$$\rho' = Z'^{-1}\,\mathrm{e}^{-\beta H'} = Z'^{-1}\,\mathrm{e}^{-\beta(H+V)}, \tag{D.27}$$

is the density matrix for the *perturbed* MBS, where $Z' = \mathrm{Tr}\,\mathrm{e}^{-\beta H'}$ is the partition function of the perturbed MBS.

To "split" the $\mathrm{e}^{-\beta(H+V)}$ exponential, following Marshall & Lowde [1968, p. 710], we write

$$\rho' = Z'^{-1}\,\mathrm{e}^{-\beta(H+V)} = Z'^{-1}\,\mathrm{e}^{-\beta H}(1+\alpha)\,, \tag{D.28}$$

with

$$\alpha \equiv \mathrm{e}^{\beta H}\,\mathrm{e}^{-\beta(H+V)} - 1\,. \tag{D.29}$$

Then

$$\begin{aligned}
\frac{\mathrm{d}\alpha}{\mathrm{d}\beta} &= \mathrm{e}^{\beta H}\,H\,\mathrm{e}^{-\beta(H+V)} - \mathrm{e}^{\beta H}(H+V)\,\mathrm{e}^{-\beta(H+V)}\,,\\
&= -\,\mathrm{e}^{\beta H}\,V\,\mathrm{e}^{-\beta(H+V)}\,,\\
&= -\,\mathrm{e}^{\beta H}\,V\,\mathrm{e}^{-\beta H} + \text{higher order terms in } V\,.
\end{aligned} \tag{D.30}$$

Integrating with respect to $\beta$

$$\alpha(\beta) - \alpha(\beta_0) = -\int_{\beta_0}^{\beta} \mathrm{e}^{\lambda H}\, V\, \mathrm{e}^{-\lambda H}\, \mathrm{d}\lambda\,. \tag{D.31}$$

But, since $\alpha(\beta = 0) = 0$, we can write

$$\alpha(\beta) = -\int_{0}^{\beta} \mathrm{e}^{\lambda H}\, V\, \mathrm{e}^{-\lambda H}\, \mathrm{d}\lambda\,. \tag{D.32}$$

Then, from Eq. (D.28) on the preceding page

$$\rho' = Z'^{-1}\, \mathrm{e}^{-\beta H} \Big(1 - \int_{0}^{\beta} \mathrm{e}^{\lambda H}\, V\, \mathrm{e}^{-\lambda H}\, \mathrm{d}\lambda\Big). \tag{D.33}$$

We still need to calculate $Z'^{-1}$ to first order in $V$. Equation (D.33) above is an *operator* equation and $Z'^{-1}$ is an *scalar* magnitude, so it suffices to pick any scalar invariant of Eq. (D.33). Taking the trace [Marshall & Lowde 1968, p. 710] we obtain the scalar equation

$$\begin{aligned} \mathrm{Tr}\rho' = 1 &= Z'^{-1}\Big[\mathrm{Tr}\,\mathrm{e}^{-\beta H} - \int_{0}^{\beta} \mathrm{Tr}(\mathrm{e}^{-\beta H}\, \mathrm{e}^{\lambda H}\, V\, \mathrm{e}^{-\lambda H})\, \mathrm{d}\lambda\Big]\,, \\ &= Z'^{-1}\Big[Z - \int_{0}^{\beta} \mathrm{Tr}(\mathrm{e}^{\lambda H}\, \mathrm{e}^{-\beta H}\, V\, \mathrm{e}^{-\lambda H})\, \mathrm{d}\lambda\Big]. \end{aligned} \tag{D.34}$$

where

$$Z = \mathrm{Tr}\,\mathrm{e}^{-\beta H} \tag{D.35}$$

is the partition function of the unperturbed MBS. Note that $\mathrm{e}^{-\beta H}$ and $\mathrm{e}^{-\lambda H}$ commute

$$\mathrm{e}^{-\beta H}\, \mathrm{e}^{\lambda H}\, V\, \mathrm{e}^{-\lambda H} = \mathrm{e}^{\lambda H}\, \mathrm{e}^{-\beta H}\, V\, \mathrm{e}^{-\lambda H}\,. \tag{D.36}$$

Also, the trace of a product of operators is invariant under cyclic permutations, for example

$$\begin{aligned} \mathrm{Tr}(ABCDEF) &= \mathrm{Tr}(FABCDE) = \mathrm{Tr}(EFABCD) \\ &= \mathrm{Tr}(BCDFEA) = \mathrm{Tr}(CDEFAB), \ldots \quad \text{etc.} \end{aligned} \tag{D.37}$$

Thus

$$\begin{aligned} \mathrm{Tr}(\mathrm{e}^{\lambda H}\, \mathrm{e}^{-\beta H}\, V\, \mathrm{e}^{-\lambda H}) &= \mathrm{Tr}(\mathrm{e}^{-\lambda H}\, \mathrm{e}^{\lambda H}\, \mathrm{e}^{-\beta H}\, V) \\ &= \mathrm{Tr}(\mathrm{e}^{-\beta H}\, V\, \mathrm{e}^{-\lambda H}\, \mathrm{e}^{\lambda H}) \\ &= \mathrm{Tr}(\mathrm{e}^{-\beta H}\, V)\,, \end{aligned} \tag{D.38}$$

then the integrand in the rhs of Eq. (D.34) on the preceding page becomes independent of $\lambda$

$$\begin{aligned}
\mathrm{Tr}\rho' = 1 &= Z'^{-1}\Big[Z - \int_0^\beta \mathrm{Tr}(\mathrm{e}^{-\beta H}\, V)\,\mathrm{d}\lambda\Big] \\
&= Z'^{-1}\Big[Z - \beta\,\mathrm{Tr}(\mathrm{e}^{-\beta H}\, V)\Big] \\
&= Z'^{-1}\Big[Z - Z\,\beta\,\mathrm{Tr}\big(\frac{1}{Z}\,\mathrm{e}^{-\beta H}\, V\big)\Big] \\
&= Z'^{-1} Z\,\big(1 - \beta\,\langle V\rangle\big)\,,
\end{aligned} \tag{D.39}$$

and then

$$Z'^{-1} = \frac{1}{Z\,\big(1 - \beta\,\langle V\rangle\big)} = Z^{-1}\big(1 - \beta\,\langle V\rangle\big)^{-1}\,. \tag{D.40}$$

Equation (D.40) above is correct [see Equations (D.27)-(D.33)] up to first order in $V$, therefore

$$Z'^{-1} = Z^{-1}\big(1 + \beta\,\langle V\rangle\big)\,, \tag{D.41}$$

is accurate to first order in $V$, where: $Z'^{-1}$ is the partition function for the *perturbed* many body system (MBS) [see Eq. (D.27) on page 208], and $Z$ is the partition function for the unperturbed MBS [see Eq. (D.35) on the previous page].

Introducing $Z'^{-1}$ given in expression (D.41) above into Eq. (D.33) on the previous page

$$\begin{aligned}
\rho' &= Z^{-1}\big(1 + \beta\,\langle V\rangle\big)\,\mathrm{e}^{-\beta H}\,\Big(1 - \int_0^\beta \mathrm{e}^{\lambda H}\, V\,\mathrm{e}^{-\lambda H}\,\mathrm{d}\lambda\Big)\,, \\
&= \rho\,\big(1 + \beta\,\langle V\rangle\big)\Big(1 - \int_0^\beta \mathrm{e}^{\lambda H}\, V\,\mathrm{e}^{-\lambda H}\,\mathrm{d}\lambda\Big)\,,
\end{aligned} \tag{D.42}$$

where $\rho'$ is the density matrix of the *perturbed* MBS introduced in Eq. (D.27), and

$$\rho = Z^{-1}\,\mathrm{e}^{-\beta H} \tag{D.43}$$

is the density matrix of the unperturbed MBS.

Expanding Eq. (D.42) above

$$\rho' = \rho\,\Big[1 + \beta\,\langle V\rangle - \int_0^\beta \mathrm{e}^{\lambda H}\, V\,\mathrm{e}^{-\lambda H}\,\mathrm{d}\lambda - \beta\,\langle V\rangle \int_0^\beta \mathrm{e}^{\lambda H}\, V\,\mathrm{e}^{-\lambda H}\,\mathrm{d}\lambda\Big]\,, \tag{D.44}$$

and writing $\beta\,\langle V\rangle = \int_0^\beta \mathrm{e}^{\lambda H}\langle V\rangle\,\mathrm{e}^{-\lambda H}\,\mathrm{d}\lambda$, and discarding the —second order in $V$— last term, we obtain

$$\rho' = \rho\,\Big[1 + \int_0^\beta \mathrm{e}^{\lambda H}(\langle V\rangle - V)\,\mathrm{e}^{-\lambda H}\,\mathrm{d}\lambda\Big]\,. \tag{D.45}$$

In terms of the MBS dynamic variable $B$ that couples to the —constant— applied field $h$, the *perturbed* Hamiltonian is $H' = H + V$ with $V = -hB$ [see Eqs. (D.23)–(D.24) on page 208] and the *perturbed* density matrix $\rho'$ reads

$$\rho' = \rho \left[ 1 + h \int_0^\beta \mathrm{e}^{\lambda H} (B - \langle B \rangle) \, \mathrm{e}^{-\lambda H} \, \mathrm{d}\lambda \right] . \tag{D.46}$$

Then, the ensemble average of an operator $A$ on the *perturbed* MBS is

$$\begin{aligned} \langle A \rangle_{H'} &= \mathrm{Tr}(\rho' A) \\ &= \mathrm{Tr}(\rho A) + h \, \mathrm{Tr} \Big[ \int_0^\beta \rho \, \mathrm{e}^{\lambda H} (B - \langle B \rangle) \, \mathrm{e}^{-\lambda H} \, A \, \mathrm{d}\lambda \Big] , \\ &= \langle A \rangle + h \int_0^\beta \mathrm{Tr} [ \rho \, \mathrm{e}^{\lambda H} (B - \langle B \rangle) \, \mathrm{e}^{-\lambda H} \, A ] \, \mathrm{d}\lambda \, . \end{aligned} \tag{D.47}$$

The static response function [Eq. (D.25) on page 208] is, therefore,

$$\begin{aligned} \langle A \rangle_{H'} - \langle A \rangle &= h \Big[ \int_0^\beta \mathrm{Tr} [ \rho \, \mathrm{e}^{\lambda H} (B - \langle B \rangle) \, \mathrm{e}^{-\lambda H} \, A ] \, \mathrm{d}\lambda \Big] , \\ &= h \Big[ \int_0^\beta \mathrm{Tr} [ \rho \, \mathrm{e}^{\lambda H} \, B \, \mathrm{e}^{-\lambda H} \, A ] \, \mathrm{d}\lambda - \beta \, \langle B \rangle \, \mathrm{Tr}(\rho A) \Big] , \\ &= h \Big[ \int_0^\beta \langle \, \mathrm{e}^{\lambda H} \, B \, \mathrm{e}^{-\lambda H} \, A \rangle \, \mathrm{d}\lambda - \beta \, \langle B \rangle \, \langle A \rangle \Big] . \end{aligned} \tag{D.48}$$

Comparing this result with the definition of the *Kubo scalar product* [Eq. (2.1) on page 5]

$$(X, Y) = \int_0^\beta \langle \mathrm{e}^{\lambda H} X^\dagger \mathrm{e}^{-\lambda H} Y \rangle \mathrm{d}\lambda - \beta \langle X^\dagger \rangle \langle Y \rangle \tag{D.49}$$

we finally obtain

$$\langle A \rangle_{H'} - \langle A \rangle = h \, (B^\dagger, A) \tag{D.50}$$

for the *static response*.

## D.3 Time reversal symmetry (TRS) of the autocorrelation function: $R_A(-t) = R_A(t)$

The autocorrelation function $R_A(t)$ was defined in §12.1, p. 160, Eq. (12.27) as

$$R_A(t) \equiv R_{AA}(t) \, , \tag{D.51}$$

where

$$R_{AB}(t) \equiv (B^\dagger, A(t))\,, \tag{D.52}$$

is the *Kubo relaxation function* [Eq. (12.24) on page 159], and $(X, Y)$ is the *Kubo scalar product* (KSP) whose definition is reproduced in Eq. (D.82) on page 217.

Let's check first the time reversal symmetry (TRS) of $R_{AB}(t)$:

$$\begin{aligned} R_{AB}(-t) &= (B^\dagger, A(-t)) \\ &= (A(-t)^\dagger, B) && \text{since } (X,Y) = (Y^\dagger, X^\dagger) \text{ [Eq. (D.89)]}, \\ &= (A^\dagger(-t), B) && \text{using Eq. (D.106)}, \\ &= (A^\dagger, B(t)) = R_{BA}(t) && \text{since } (X(-t), Y) = (X, Y(t)) \text{ [Eq. (D.93)]}. \end{aligned} \tag{D.53}$$

Therefore, if $B = A$ then

$$R_{AA}(-t) = (A^\dagger, A(t)) = R_{AA}(t)\,. \quad \square \tag{D.54}$$

## D.4 The autocorrelation function and the time dependent susceptibility

We show in this section that

$$\frac{\mathrm{d}R_A(t)}{\mathrm{d}t} = -\chi_A(t)\,. \tag{D.55}$$

Here, $\chi_A(t) \equiv C_{AA}(t) = (\mathrm{i}/\hbar)\langle\,[A(t), A]\,\rangle$ is the time dependent susceptibility defined in Eq. (12.16) on page 158, and $R_A(t)$ is the autocorrelation function [Eq. (D.51) on the previous page]

$$R_A(t) = R_{AA}(t)\,, \tag{D.56}$$

where

$$R_{AB}(t) = (B^\dagger, A(t))\,, \tag{D.57}$$

$$= \int_0^\beta \langle\, \mathrm{e}^{\lambda H}\, B\, \mathrm{e}^{-\lambda H}\, A(t)\,\rangle\, \mathrm{d}\lambda - \beta\langle B\rangle\langle A(t)\rangle\,, \quad \text{[See Eq. (D.82)]} \tag{D.58}$$

$$= \int_0^\beta \langle\, \mathrm{e}^{\lambda H}\, B\, \mathrm{e}^{-\lambda H}\, A(t)\,\rangle\, \mathrm{d}\lambda - \beta\langle B\rangle\langle A\rangle\,, \tag{D.59}$$

is the *Kubo relaxation function* [Eq. (D.52)] written in terms of the Kubo scalar product (KSP) (X,Y) [Eq. (D.82) on page 217]. Also note that $\langle A(t)\rangle = \langle A\rangle$, see Eq. (D.90) p. 218.

We first calculate the time derivative of the Kubo relaxation function given in Eq. (D.59) on the previous page, and afterwards we set $B = A$

$$\frac{\mathrm{d}R_{AB}(t)}{\mathrm{d}t} = \frac{\mathrm{i}}{\hbar}\int_0^\beta \langle\, \mathrm{e}^{\lambda H}\, B\, \mathrm{e}^{-\lambda H}[H, A(t)]\,\rangle\, \mathrm{d}\lambda\,. \tag{D.60}$$

Before going on we need the following identity, valid for any operator $O$

$$\mathrm{e}^{\beta H}\, O\, \mathrm{e}^{-\beta H} - O = \int_0^\beta \mathrm{e}^{\lambda H}[H, O]\, \mathrm{e}^{-\lambda H}\, \mathrm{d}\lambda\,. \tag{D.61}$$

Also, making the change $H \leftarrow -H$

$$\mathrm{e}^{-\beta H}\, O\, \mathrm{e}^{\beta H} - O = -\int_0^\beta \mathrm{e}^{-\lambda H}[H, O]\, \mathrm{e}^{\lambda H}\, \mathrm{d}\lambda\,, \tag{D.62}$$

or, equivalently

$$O - \mathrm{e}^{-\beta H}\, O\, \mathrm{e}^{\beta H} = \int_0^\beta \mathrm{e}^{-\lambda H}[H, O]\, \mathrm{e}^{\lambda H}\, \mathrm{d}\lambda\,. \tag{D.63}$$

Let's check this result.

Define $O(\lambda) \equiv \mathrm{e}^{\lambda H}\, O\, \mathrm{e}^{-\lambda H}$. Then

$$\begin{aligned}
\frac{\mathrm{d}O(\lambda)}{\mathrm{d}\lambda} &= HO(\lambda) - O(\lambda)H \\
&= H\, \mathrm{e}^{\lambda H}\, O\, \mathrm{e}^{-\lambda H} - \mathrm{e}^{\lambda H}\, O\, \mathrm{e}^{-\lambda H}\, H \\
&= \mathrm{e}^{\lambda H}\, HO\, \mathrm{e}^{-\lambda H} - \mathrm{e}^{\lambda H}\, OH\, \mathrm{e}^{-\lambda H} = \mathrm{e}^{\lambda H}[H, O]\, \mathrm{e}^{-\lambda H}\,.
\end{aligned} \tag{D.64}$$

Thus, $\mathrm{d}O(\lambda) = \mathrm{e}^{\lambda H}[H, O]\, \mathrm{e}^{-\lambda H}\, \mathrm{d}\lambda$, and therefore

$$\int_0^\beta \mathrm{d}O(\lambda) = O(\beta) - O(0) = \mathrm{e}^{\beta H}\, O\, \mathrm{e}^{-\beta H} - O = \int_0^\beta \mathrm{e}^{\lambda H}[H, O]\, \mathrm{e}^{-\lambda H}\, \mathrm{d}\lambda\,. \quad \square \tag{D.65}$$

Returning to the time derivative of the Kubo relaxation function on Eq. (D.60), we write

$$\begin{aligned}
\frac{\mathrm{d}R_{AB}(t)}{\mathrm{d}t} &= Z^{-1}\,\frac{\mathrm{i}}{\hbar}\int_0^\beta \mathrm{Tr}\big\{\ \mathrm{e}^{\lambda H}\,B\,\mathrm{e}^{-\lambda H}[H,A(t)]\,\mathrm{e}^{-\beta H}\ \big\}\,\mathrm{d}\lambda\,,\\
&= Z^{-1}\,\frac{\mathrm{i}}{\hbar}\int_0^\beta \mathrm{Tr}\big\{\ B\,\mathrm{e}^{-\lambda H}[H,A(t)]\,\mathrm{e}^{\lambda H}\,\mathrm{e}^{-\beta H}\ \big\}\,\mathrm{d}\lambda\,,\\
&= Z^{-1}\,\frac{\mathrm{i}}{\hbar}\,\mathrm{Tr}\bigg\{B\,\bigg[\int_0^\beta \mathrm{e}^{-\lambda H}[H,A(t)]\,\mathrm{e}^{\lambda H}\,\mathrm{d}\lambda\bigg]\,\mathrm{e}^{-\beta H}\ \bigg\}\,,\\
&= Z^{-1}\,\frac{\mathrm{i}}{\hbar}\,\mathrm{Tr}\Big\{B\big[A(t)-\mathrm{e}^{-\beta H}A(t)\,\mathrm{e}^{\beta H}\big]\,\mathrm{e}^{-\beta H}\ \Big\}\,,\quad \text{[using Eq. (D.63)]}\\
&= Z^{-1}\,\frac{\mathrm{i}}{\hbar}\,\Big[\mathrm{Tr}\big\{BA(t)\,\mathrm{e}^{-\beta H}\ \big\}-\mathrm{Tr}\big\{B\,\mathrm{e}^{-\beta H}\,A(t)\big\}\Big]\,,\\
&= Z^{-1}\,\frac{\mathrm{i}}{\hbar}\,\Big[\mathrm{Tr}\big\{BA(t)\,\mathrm{e}^{-\beta H}\ \big\}-\mathrm{Tr}\big\{A(t)B\,\mathrm{e}^{-\beta H}\ \big\}\Big]\,,\\
&= \frac{\mathrm{i}}{\hbar}\langle\,[B,A(t)]\,\rangle = -\frac{\mathrm{i}}{\hbar}\langle\,[A(t),B]\,\rangle\,.
\end{aligned}\tag{D.66}$$

We had already encountered the function $(\mathrm{i}/\hbar)\langle\,[A(t),B]\,\rangle$ in the calculation of the many body system time dependent response in Eq. (D.21b), p. 207 of this appendix. It is the *response function* $C_{AB}(t)$ defined in Eq. (12.15) on page 158.

Thus, we have shown that

$$\frac{\mathrm{d}R_{AB}(t)}{\mathrm{d}t} = -\frac{\mathrm{i}}{\hbar}\langle\,[A(t),B]\,\rangle \equiv -C_{AB}(t)\,. \tag{D.67}$$

Setting $B \leftarrow A$ we obtain the corresponding result [Eq. (D.55) on page 212] for the autocorrelation function, i.e.

$$\frac{\mathrm{d}R_{A}(t)}{\mathrm{d}t} = -\chi_{A}(t)\,. \tag{D.68}$$

## D.5 The time average of the time dependent susceptibility or response function in the ergodic hypotheses statement

In this section we show that

$$\lim_{T\to\infty}\frac{1}{T-b}\int_b^T \mathrm{d}t\int_b^t \mathrm{d}t'\,\chi_A(t-t') = \tilde{\chi}_A(0) + \lim_{T\to\infty}\Big[R_A(T)-\frac{1}{T-b}\tilde{R}_A(0)\Big]\,. \tag{D.69}$$

Here, $\tilde{\chi}_A(z)$ and $\tilde{R}_A(z)$ are the Laplace transforms of the *time-dependent response function* $\chi_A(t-t')$ [Eq. (12.16), p. 158], and the *autocorrelation function* $R_A(t)$ [Eq. (12.27), p. 160], respectively.

We designate with the letter $b$ the "beginning" time such that the applied field (AF) $h(t)$

$$h(t < b) \equiv 0\,. \tag{D.70}$$

It corresponds to the lower limit of both time integrals in Eq. (D.69). From that instant one generally assumes that $h(t)$ is gradually turned on. In our case we have taken $h(t) = h$, i.e., the AF is constant [See Eq. (D.23)] and the only time dependence stems from the switching on of the AF at $t = b$.

The time average in the left hand side of Eq. (D.69) with the " beginning" time set to $-\infty$, that is, $b = -T$ with $T \to \infty$, appears in (the lhs too of) the ergodic hypotheses (EH) given in Eq. (12.28), §12.1 in p. 160.

The assumption that the applied field (AF) is constant, i.e., $h(t) = h$, also results in an expression for the EH written totally in terms of intrinsic properties of the many body system (MBS): the AF does not appear inside the time integrals and cancels out in both sides of EH given in Eq. (12.28). Usually one chooses either $b = 0$ or $b \to \infty$. We will consider both cases, although any other value may be chosen.

To obtain the time average in Eq. (D.69) we will follow closely M. Howard Lee in [Lee 2007*b*, §§3–4]. We shall time average the time dependent susceptibility over a long time. The stationarity property $\chi(t, t') = \chi(t - t')$ makes it convenient [Lee 2007*b*, §3] to write for the inner integral

$$\int_b^t \chi(t - t')\,\mathrm{d}t' = \int_{t-b}^0 \chi(t')(-\,\mathrm{d}t') = \int_0^{t-b} \chi(t')\,\mathrm{d}t' \equiv \varphi(t - b)\,. \tag{D.71}$$

The change $t' \leftarrow t - t'$ helps to reduce the double integral into a single one. The new function $\varphi(t)$ satisfies $\varphi(t = 0) = 0$, and $\mathrm{d}\varphi(t)/\,\mathrm{d}t = \chi(t)$.

Using the definition of $\phi(t)$ [Eq. (D.71)] we write the time integrals of the time average in Eq. (D.69) as

$$\int_b^T \mathrm{d}t \int_b^t \mathrm{d}t'\, \chi_A(t - t') = \int_b^T \varphi(t - b)\,\mathrm{d}t\,. \tag{D.72}$$

The variable change $t \leftarrow t - b$ gives

$$\int_b^T \varphi(t - b)\,\mathrm{d}t = \int_0^{T-b} \varphi(t)\,\mathrm{d}t\,. \tag{D.73}$$

One partial integration using $\varphi(t=0)=0$, and $\mathrm{d}\varphi(t)/\,\mathrm{d}t=\chi(t)$ gives

$$\int_0^{T-b}\varphi(t)\,\mathrm{d}t=(T-b)\varphi(T-b)-\int_0^{T-b}t\,\chi(t)\,\mathrm{d}t\,. \tag{D.74}$$

We do another partial integration using $\mathrm{d}R_A(t)/\,\mathrm{d}t=-\chi_A(t)$ [Eq. (D.68)], and summarizing these results we finally obtain for the double time integral

$$\begin{aligned}\int_b^T\mathrm{d}t\int_b^t\mathrm{d}t'\,\chi_A(t-t')&=\int_b^T\varphi(t-b)\,\mathrm{d}t\,,\qquad\text{using the definition of }\varphi(t),\text{ [Eq. (D.71)]}\\&=\int_0^{T-b}\varphi(t)\,\mathrm{d}t\,,\qquad\text{making the variable change } t\leftarrow t-b\\&=(T-b)\varphi(T-b)+(T-b)R_A(T-b)-\int_0^{T-b}R_A(t)\,\mathrm{d}t\,.\end{aligned} \tag{D.75}$$

The time average then becomes

$$\lim_{T\to\infty}\frac{1}{T-b}\int_b^T\mathrm{d}t\int_b^t\mathrm{d}t'\,\chi_A(t-t')=\lim_{T\to\infty}\left[\varphi(T-b)+R_A(T-b)-\frac{1}{T-b}\int_0^{T-b}R_A(t)\,\mathrm{d}t\right]. \tag{D.76}$$

We use the Laplace transform definition to make this result look simpler [Lee 2007*b*, §3] and thus we obtain the result [Eq. (D.69)] we were seeking

$$\lim_{T\to\infty}\frac{1}{T-b}\int_b^T\mathrm{d}t\int_b^t\mathrm{d}t'\,\chi_A(t-t')=\tilde{\chi}_A(0)+\lim_{T\to\infty}\left[R_A(T)-\frac{1}{T-b}\tilde{R}_A(0)\right].\quad\square \tag{D.77}$$

Here we used Eq. (D.71) to write

$$\lim_{T\to\infty}\varphi(T-b)=\lim_{T\to\infty}\varphi(T)=\lim_{T\to\infty}\int_0^T\chi(t')\,\mathrm{d}t'\equiv\tilde{\chi}_A(z=0)\,. \tag{D.78}$$

And similarly

$$\lim_{T\to\infty}\int_0^{T-b}R_A(t)\,\mathrm{d}t=\lim_{T\to\infty}\int_0^T R_A(t)\,\mathrm{d}t\equiv\tilde{R}_A(z=0)\,. \tag{D.79}$$

As an example, setting $b=0$ in Eq. (D.69) or Eq. (D.77) we obtain

$$\lim_{T\to\infty}\frac{1}{T}\int_0^T\mathrm{d}t\int_0^t\mathrm{d}t'\,\chi_A(t-t')=\tilde{\chi}_A(0)+R_A(T)-\frac{1}{T}\tilde{R}_A(0)\,,\quad\text{with } T\to\infty\,. \tag{D.80}$$

This is Eq. (9) of [Lee 2007*b*, §3].

As another example, setting $b=-T$ with $T\to\infty$ in Eq. (D.69) or Eq. (D.77) we find

$$\lim_{T\to\infty}\frac{1}{2T}\int_{-T}^T\mathrm{d}t\int_{-T}^t\mathrm{d}t'\,\chi_A(t-t')=\tilde{\chi}_A(0)+R_A(T)-\frac{1}{2T}\tilde{R}_A(0)\,,\quad\text{with } T\to\infty\,. \tag{D.81}$$

This is Eq. (A.6) of [Lee 2007*b*, App. A]. It also corresponds to Eq. (12.31), p. 161 that was used to write the ergodic hypotheses (EH) given in Eq. (12.32). $\square$

## D.6 Three identities related to the Kubo scalar product (KSP)

The Kubo scalar product (KSP) was defined in Eq. (2.1) on page 5 as

$$(X,Y) = \int_0^\beta \langle \mathrm{e}^{\lambda H}\, X^\dagger\, \mathrm{e}^{-\lambda H}\, Y\rangle \,\mathrm{d}\lambda - \beta\langle X^\dagger\rangle\langle Y\rangle\,, \tag{D.82}$$

where

$$\langle \dots \rangle \equiv Z^{-1}\mathrm{Tr}(\mathrm{e}^{-\beta H}\dots) = Z^{-1}\mathrm{Tr}(\dots \mathrm{e}^{-\beta H})\,. \tag{D.83}$$

### D.6.1 Complex conjugation of the KSP: $(X,Y) = (Y,X)^*$

Let's look first at the trace in the integrand:

$$\begin{aligned}\mathrm{Tr}(\mathrm{e}^{\lambda H}\, X^\dagger\, \mathrm{e}^{-\lambda H} Y\, \mathrm{e}^{-\beta H}) &= \mathrm{Tr}(\mathrm{e}^{\lambda H}\, X^\dagger\, \mathrm{e}^{-\lambda H}\, Y\, \mathrm{e}^{-\beta H})^{\mathrm{t}} = [\mathrm{Tr}(\mathrm{e}^{\lambda H}\, X^\dagger\, \mathrm{e}^{-\lambda H}\, Y\, \mathrm{e}^{-\beta H})^{\mathrm{t}*}]^*\,,\\ &= [\mathrm{Tr}(\mathrm{e}^{\lambda H}\, X^\dagger\, \mathrm{e}^{-\lambda H}\, Y\, \mathrm{e}^{-\beta H})^\dagger]^* = [\mathrm{Tr}(\mathrm{e}^{-\beta H^\dagger}\, Y^\dagger\, \mathrm{e}^{-\lambda H^\dagger}\, X\, \mathrm{e}^{\lambda H^\dagger})]^*\,,\end{aligned}$$

we assume $H$ is hermitian

$$= [\mathrm{Tr}(\mathrm{e}^{-\beta H}\, Y^\dagger\, \mathrm{e}^{-\lambda H}\, X\, \mathrm{e}^{\lambda H})]^* = [\mathrm{Tr}(\mathrm{e}^{\lambda H}\, Y^\dagger\, \mathrm{e}^{-\lambda H}\, X\, \mathrm{e}^{-\beta H})]^*\,. \quad \square \tag{D.84}$$

Now the second term in the KSP

$$-\beta\langle X^\dagger\rangle\langle Y\rangle = -\beta\langle (X^\dagger)^{\mathrm{t}}\rangle\langle Y^{\mathrm{t}}\rangle = -\beta\langle X^*\rangle\langle (Y^\dagger)^*\rangle = (-\beta\langle Y^\dagger\rangle\langle X\rangle)^*\,. \quad \square \tag{D.85}$$

Thus

$$(X,Y) = (Y,X)^*\,. \tag{D.86}$$

### D.6.2 KSP of complex conjugated and transposed (dagged) operators: $(X,Y) = (Y^\dagger, X^\dagger)$

The first term of $(X,Y)$ maybe rewritten as follows

$$\begin{aligned}Z^{-1}\int_0^\beta \mathrm{Tr}(\mathrm{e}^{\lambda H}\, X^\dagger\, \mathrm{e}^{-\lambda H}\, Y\, \mathrm{e}^{-\beta H})\,\mathrm{d}\lambda &= Z^{-1}\int_0^\beta \mathrm{Tr}(Y\, \mathrm{e}^{(\lambda-\beta)H}\, X^\dagger\, \mathrm{e}^{-\lambda H})\,\mathrm{d}\lambda\\ &= Z^{-1}\int_0^\beta \mathrm{Tr}(\mathrm{e}^{(\beta-\lambda)}\, Y\, \mathrm{e}^{(\lambda-\beta)H}\, X^\dagger\, \mathrm{e}^{-\beta H})\,\mathrm{d}\lambda\\ &= Z^{-1}\int_\beta^0 \mathrm{Tr}(\mathrm{e}^{\xi H}\, Y\, \mathrm{e}^{-\xi H}\, X^\dagger\, \mathrm{e}^{-\beta H})(-\,\mathrm{d}\xi)\\ &= Z^{-1}\int_0^\beta \mathrm{Tr}(\mathrm{e}^{\xi H}\, Y\, \mathrm{e}^{-\xi H}\, X^\dagger\, \mathrm{e}^{-\beta H})\,\mathrm{d}\xi\,. \quad \square\end{aligned} \tag{D.87}$$

For the second term of $(X, Y)$ we write

$$-\beta\langle(Y^\dagger)^\dagger\rangle\langle X^\dagger\rangle = -\beta\langle X^\dagger\rangle\langle Y\rangle\,. \quad \square \tag{D.88}$$

Therefore

$$(X, Y) = (Y^\dagger, X^\dagger)\,. \tag{D.89}$$

### D.6.3 KSP TIME SHIFT: $(X, Y(t)) = (X(-t), Y)$

The ensemble average in the unperturbed many body system (MBS) of any operator is

$$\begin{aligned}\langle A(t)\rangle &= Z^{-1}\mathrm{Tr}(\mathrm{e}^{-\beta H}\,\mathrm{e}^{\mathrm{i}Ht/\hbar}\,A\,\mathrm{e}^{-\,\mathrm{i}Ht/\hbar})\\ &= Z^{-1}\mathrm{Tr}(\mathrm{e}^{-\,\mathrm{i}Ht/\hbar}\,\mathrm{e}^{-\beta H}\,\mathrm{e}^{\mathrm{i}Ht/\hbar}\,A)\end{aligned}$$

$\mathrm{e}^{-\,\mathrm{i}Ht/\hbar}$ and $\mathrm{e}^{-\beta H}$ commute, hence

$$= Z^{-1}\mathrm{Tr}(\mathrm{e}^{-\beta H}\,A) = \langle A\rangle\,. \tag{D.90}$$

Thus, for the second term of $(X, Y(t))$ we have

$$-\beta\langle X\rangle\langle Y(t)\rangle = -\beta\langle X\rangle\langle Y\rangle = -\beta\langle X(-t)\rangle\langle Y\rangle\,. \quad \square \tag{D.91}$$

Now, consider the trace inside the integral in the first term of $(X, Y(t))$

$$\begin{aligned}\mathrm{Tr}(\mathrm{e}^{\lambda H}\,X^\dagger\,\mathrm{e}^{-\lambda H}Y(t)\,\mathrm{e}^{-\beta H}) &= \mathrm{Tr}(\mathrm{e}^{\lambda H}\,X^\dagger\,\mathrm{e}^{-\lambda H}\,\mathrm{e}^{\mathrm{i}Ht/\hbar}\,Y\,\mathrm{e}^{-\,\mathrm{i}Ht/\hbar}\,\mathrm{e}^{-\beta H})\\ &= \mathrm{Tr}(\mathrm{e}^{\lambda H}\,\mathrm{e}^{-\,\mathrm{i}Ht/\hbar}\,X^\dagger\,\mathrm{e}^{\mathrm{i}Ht/\hbar}\,\mathrm{e}^{-\lambda H}\,Y\,\mathrm{e}^{-\beta H})\\ &= \mathrm{Tr}(\mathrm{e}^{\lambda H}[\mathrm{e}^{-\,\mathrm{i}H^\dagger t/\hbar}\,X\,\mathrm{e}^{\mathrm{i}H^\dagger t/\hbar}]^\dagger\,\mathrm{e}^{-\lambda H}\,Y\,\mathrm{e}^{-\beta H})\end{aligned}$$

since $H^\dagger = H^\dagger$, then

$$\begin{aligned}&= \mathrm{Tr}(\mathrm{e}^{\lambda H}[\mathrm{e}^{-\,\mathrm{i}Ht/\hbar}\,X\,\mathrm{e}^{\mathrm{i}Ht/\hbar}]^\dagger\,\mathrm{e}^{-\lambda H}\,Y\,\mathrm{e}^{-\beta H})\\ &= \mathrm{Tr}(\mathrm{e}^{\lambda H}[X(-t)]^\dagger\,\mathrm{e}^{-\lambda H}\,Y\,\mathrm{e}^{-\beta H})\,. \quad \square\end{aligned} \tag{D.92}$$

Therefore,

$$(X, Y(t)) = (X(-t), Y)\ . \tag{D.93}$$

## D.7 Some properties of time correlation functions (TCF)s

The *Kubo scalar product* (KSP) [Eq. (2.1) on page 5], the *response function* [Eq. (12.15)] and the *time dependent susceptibility* [Eq. (12.16) on page 158] are all defined in terms of *time correlation functions*. Their scope and definition is most clearly and concisely stated by Balucani, Lee & Tognetti in their review of "Dynamical correlations" [2003, §1.1.2, p. 414]:

> Consider a physical system characterized by $N$ "particles" and a time-independent Hermitian Hamiltonian $H$. The system is assumed to be in thermal equilibrium at the temperature $T = (k_B\beta)^{-1}$ as a result of being in contact with a suitably large heatbath. Except for this, the system can be considered to be isolated from any external perturbation. Given two dynamical variables (operators) of the system, denoted by $A$ and $B$, the *time correlation function* (TCF) of $A$ and $B$ is defined by the following statistical average in a canonical ensemble:
>
> $$\langle B(0)A(t)\rangle \equiv (1/Z_N)\mathrm{Tr}[B(0)A(t)\,\mathrm{e}^{-\beta H}] = \mathrm{Tr}[B(0)A(t)\rho]\,. \tag{D.94a}$$
>
> $$= (1/Z_N)\mathrm{Tr}[\mathrm{e}^{-\beta H}\,B(0)A(t)] = \mathrm{Tr}[\rho B(0)A(t)]\,. \tag{D.94b}$$
>
> Here, $Z_N \equiv \mathrm{Tr}\,\mathrm{e}^{-\beta H}$ is the partition function and $\rho \equiv \mathrm{e}^{-\beta H}/[\mathrm{Tr}\,\mathrm{e}^{-\beta H}]$ In Eqs. (D.94) $A(t) = \mathrm{e}^{\mathrm{i}Ht/\hbar}\,A\,\mathrm{e}^{-\mathrm{i}Ht/\hbar}$ with $A(0) = A$ satisfies the Heisenberg equation of motion $\mathrm{d}A(t)/\,\mathrm{d}t = (1/\mathrm{i}\hbar)[A(t), H]$. In the classical limit $\hbar \to 0$, the trace is replaced by phase-space integrals and the commutator $(1/\mathrm{i}\hbar)[\ldots, H]$ by the classical Poisson bracket $\{\ldots, H\}$.

We need the following properties of the time correlation functions

### D.7.1 TCFs Stationarity: $\langle B(0)A(t)\rangle = \langle B(\tau)A(t+\tau)\rangle$

The unperturbed system Hamiltonian $H$ is *time independent*, therefore the time-dependence of the TCF must be stationary, in other words, the time origin in the statistical average must be irrelevant:

$$\langle B(0)A(t)\rangle = \langle B(\tau)A(t+\tau)\rangle \tag{D.95}$$

for arbitrary $\tau$. Let's write the trace in the rhs of Eq. (D.95)

$$\begin{aligned}\mathrm{Tr}[B(\tau)A(t+\tau)\,\mathrm{e}^{-\beta H}] &= \mathrm{Tr}[\mathrm{e}^{\mathrm{i}H\tau/\hbar}\,B\,\mathrm{e}^{-\,\mathrm{i}H\tau/\hbar}\,\mathrm{e}^{\mathrm{i}H(t+\tau)/\hbar}\,A\,\mathrm{e}^{-\,\mathrm{i}H(t+\tau)/\hbar}\,\mathrm{e}^{-\beta H}]\,,\\ &= \mathrm{Tr}[B\,\mathrm{e}^{-\,\mathrm{i}H\tau/\hbar}\,\mathrm{e}^{\mathrm{i}H(\tau+t)/\hbar}\,A\,\mathrm{e}^{-\,\mathrm{i}H(t+\tau)/\hbar}\,\mathrm{e}^{\mathrm{i}H\tau/\hbar}\,\mathrm{e}^{-\beta H}]\,,\\ &= \mathrm{Tr}[B\,\mathrm{e}^{\mathrm{i}Ht/\hbar}\,A\,\mathrm{e}^{-\,\mathrm{i}Ht/\hbar}\,\mathrm{e}^{-\beta H}]\,. \quad \square\end{aligned} \tag{D.96}$$

### D.7.2 TCF of complex conjugated and transposed (dagged) operators: $\langle B(0)A(t)\rangle = \langle A^\dagger(t)B^\dagger(0)\rangle^*$

We show below that

$$\langle B(0)A(t)\rangle = \langle A^\dagger(t)B^\dagger(0)\rangle^*. \tag{D.97}$$

Let's write out the trace in the lhs of Eq. (D.97)

$$\begin{aligned}\mathrm{Tr}(BA(t)\,\mathrm{e}^{-\beta H}) &= \mathrm{Tr}(BA(t)\,\mathrm{e}^{-\beta H})^{\mathrm{t}} = [\mathrm{Tr}(BA(t)\,\mathrm{e}^{-\beta H})^{\mathrm{t}*}]^* = [\mathrm{Tr}(BA(t)\,\mathrm{e}^{-\beta H})^\dagger]^*,\\ &= [\mathrm{Tr}(\mathrm{e}^{-\beta H^\dagger}A(t)^\dagger B^\dagger)]^*,\end{aligned}$$

but $H^\dagger = H$ and time independent $\Rightarrow$ $A(t)^\dagger = A^\dagger(t)$ [Eq. (D.106) on the next page]

$$= [\mathrm{Tr}(\mathrm{e}^{-\beta H}\,A^\dagger(t)B^\dagger)]^* = [\mathrm{Tr}(A^\dagger(t)B^\dagger\,\mathrm{e}^{-\beta H})]^*. \quad \square \tag{D.98}$$

### D.7.3 TCF shifted by $\mathrm{i}\hbar\beta$: $\langle B(0)A(t)\rangle = \langle A(t-\mathrm{i}\hbar\beta)B(0)\rangle$

In this subsection we show that

$$\langle B(0)A(t)\rangle = \langle A(t-\mathrm{i}\hbar\beta)B(0)\rangle\,. \tag{D.99}$$

Note first that

$$-\,\mathrm{i}\,\frac{Ht}{\hbar} - \beta H = -\,\mathrm{i}\,\frac{H}{\hbar}(t-\mathrm{i}\hbar\beta)\,. \tag{D.100}$$

The trace in the lhs of Eq. (D.99) is

$$\begin{aligned}\mathrm{Tr}(BA(t)\,\mathrm{e}^{-\beta H}) &= \mathrm{Tr}(B\,\mathrm{e}^{\mathrm{i}\frac{Ht}{\hbar}}\,A\,\mathrm{e}^{-\,\mathrm{i}\frac{Ht}{\hbar}}\,\mathrm{e}^{-\beta H}) = \mathrm{Tr}[\mathrm{e}^{-\beta H}\,\mathrm{e}^{\beta H}\,\mathrm{e}^{\mathrm{i}\frac{Ht}{\hbar}}\,A\,\mathrm{e}^{-\,\mathrm{i}\frac{Ht}{\hbar}(t-\mathrm{i}\hbar\beta)}\,B]\\ &= \mathrm{Tr}[\mathrm{e}^{-\beta H}\,\mathrm{e}^{\mathrm{i}\frac{Ht}{\hbar}(t-\mathrm{i}\hbar\beta)}\,A\,\mathrm{e}^{-\,\mathrm{i}\frac{Ht}{\hbar}(t-\mathrm{i}\hbar\beta)}\,B]\\ &= \mathrm{Tr}[\mathrm{e}^{\mathrm{i}\frac{Ht}{\hbar}(t-\mathrm{i}\hbar\beta)}\,A\,\mathrm{e}^{-\,\mathrm{i}\frac{Ht}{\hbar}(t-\mathrm{i}\hbar\beta)}\,B\,\mathrm{e}^{-\beta H}]. \quad \square\end{aligned} \tag{D.101}$$

## D.8 Time evolution of a complex conjugated and transposed (dagged) operator $A^\dagger$

If the Hamiltonian $H$ is time independent

$$O(t) = \mathrm{e}^{\mathrm{i}Ht/\hbar}\, O\, \mathrm{e}^{-\mathrm{i}Ht/\hbar}\,, \tag{D.102}$$

for *any* operator $O$. Thus, for an operator $A$ we have

$$A(t) = \mathrm{e}^{\mathrm{i}Ht/\hbar}\, A\, \mathrm{e}^{-\mathrm{i}Ht/\hbar}\,. \tag{D.103}$$

For the complex conjugated and transposed $A$, Eq. (D.102) on this page also applies

$$A^\dagger(t) = \mathrm{e}^{\mathrm{i}Ht/\hbar}\, A^\dagger\, \mathrm{e}^{-\mathrm{i}Ht/\hbar}\,. \tag{D.104}$$

Let's now check $[A(t)]^\dagger$. We obtain

$$\begin{aligned} [A(t)]^\dagger &= [\mathrm{e}^{\mathrm{i}Ht/\hbar}\, A\, \mathrm{e}^{-\mathrm{i}Ht/\hbar}]^\dagger \\ &= (\mathrm{e}^{-\mathrm{i}Ht/\hbar})^\dagger A^\dagger (\mathrm{e}^{\mathrm{i}Ht/\hbar})^\dagger \\ &= \mathrm{e}^{+\mathrm{i}H^\dagger t/\hbar}\, A^\dagger\, \mathrm{e}^{-\mathrm{i}H^\dagger t/\hbar}\,. \end{aligned} \tag{D.105}$$

Thus, if $H$ is time independent and hermitian, i.e., $H^\dagger = H$ , then

$$[A(t)]^\dagger = A^\dagger(t)\,. \tag{D.106}$$