

MONTE CARLO SIMULATION
OF INTERACTING ELECTRON MODELS
BY A NEW DETERMINANT APPROACH

by

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(Under the direction of Robert W. Robinson and Heinz-Bernd Schüttler)

ABSTRACT

This work discusses the calculation of determinants and Monte Carlo simulation of Hubbard models by a new determinant approach which is derived from a Feynman diagram expansion for the single particle Green's function of the Hubbard model. We developed a determinant formalism for the extended Hubbard model and a Monte Carlo summation algorithm to evaluate the relevant diagram determinant sums.

INDEX WORDS: Monte Carlo Simulation, Hubbard Model, Feynman diagram,
Determinant

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DEDICATED TO MY DEAR WIFE CAO LIN

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CHAPTER 1

INTRODUCTION

Monte Carlo simulation of interacting electron models (in particular, the Hubbard models) has been an active topic of investigation in computational physics since the 1970s.

The Hubbard model, named after John Hubbard, is used to describe magnetism and superconductivity in strongly correlated electron systems. It was originally developed to explain the metal-insulator transition in strongly correlated electronic materials, and has subsequently been applied to the study of magnetism. Over the last 20 years, the two-dimensional (2D) Hubbard model has been used as a “minimal” model to describe high-temperature superconductors and has been applied extensively in that context.

Mathematically, it is very difficult to solve the Hubbard model. There are some reliable numerical solution methods, including quantum Monte Carlo, exact diagonalization and density matrix renormalization (see [2]), but these methods are limited to only small 2D clusters with typically fewer than 16 lattice sites. Recently, cluster mean-field embedding approaches have been developed which allow small cluster calculations to be effectively extrapolated to larger and even infinite lattice sizes (see [4],[5], [7] and [1]). The infinite limit, also referred to as the thermodynamic limit, is the appropriate limit of the model to describe macroscopic crystalline materials.

In this dissertation, we introduce a new determinant approach to these studies. Our approach is derived from a Feynman diagram expansion for the so-called single particle Green’s function of the Hubbard model. Green’s functions are mathematical objects of particular interest in the quantum theory of many-electron systems, since they model predictions

which can be directly compared to the data obtained in real materials by the various experimental probes. For example, the single-particle Green's function can be used to predict the results of photo-emission spectroscopy experiments. A similar determinant formalism was recently derived by functional integral techniques (see [10]) and used for Monte Carlo simulations of small 2D Hubbard model clusters. In the present work, we have developed a determinant formalism for the extended Hubbard model and developed an alternative Monte Carlo summation algorithm to evaluate the relevant determinant diagram sums. We have tested it on small 2×2 Hubbard clusters.

This dissertation is organized as follows. In Chapter 2, we review methods for the calculation of determinants of general matrices. We describe Feynman diagram expansions in chapter 3 and the extended Hubbard model on a 2D rectangular lattice in Chapter 4. In Chapter 5 we detail our new method for Monte Carlo simulation of the extended Hubbard model. Finally, we present the results of our tests in Chapter 6.

CHAPTER 2

CALCULATION OF DETERMINANTS

In this chapter, we will review preliminaries for determinants in §2.1, then introduce several algorithms for calculating determinants of general matrices in §2.2 and compare these algorithms in §2.3.

Throughout, n is a positive integer, \vec{x} is a column vector with components x_1, x_2, \dots, x_l , \vec{e}_k is the k th canonical vector

$$\overbrace{(0, \dots, 0, 1, 0, \dots, 0)}^{k-1}, \overbrace{(0, \dots, 0, 1, 0, \dots, 0)}^{n-k}^T,$$

0_n is the $n \times n$ zero matrix, I_n is the identity matrix of order n , $A = (a_{ij})$ is a real $n \times n$ matrix, A^T is the transpose of A , and $A(i_1 : i_2, j_1 : j_2)$ is the submatrix

$$(a_{ij} : i_1 \leq i \leq i_2, j_1 \leq j \leq j_2)$$

of A . We will write i_1 for $i_1 : i_1$ and $:$ for $1 : n$. For two subsets $I = \{i_1, \dots, i_s\}$ and $J = \{j_1, \dots, j_t\}$ of $\{1, \dots, n\}$, $A_{I,J}$ denotes the submatrix

$$(a_{ij} : i \in I, j \in J).$$

2.1 PRELIMINARIES

2.1.1 SIGNS OF PERMUTATIONS

Let S_n be the set of all *permutations* of the numbers $\{1, 2, \dots, n\}$. A permutation $\pi \in S_n$ can be produced by k_π exchanges of two elements (these exchanges are called *transpositions*), and π is called an *even permutation* (or *odd permutation*, respectively) if k_π is an even number

(or odd number, respectively). The *sign* of a permutation π is defined by

$$\operatorname{sgn}(\pi) = \begin{cases} 1 & \text{if } \pi \text{ is an even permutation;} \\ -1 & \text{otherwise.} \end{cases}$$

From algebra, we know that $\pi \in S_n$ can be uniquely written as a product of disjoint *cycles*. If k is the number of these cycles (including 1-cycles), then we have

$$\operatorname{sgn}(\pi) = (-1)^{n-k}. \quad (2.1)$$

2.1.2 DETERMINANTS

The determinant of a $n \times n$ matrix $A = (a_{ij})$, denoted by $\det A$, is defined by

$$\det A = \sum_{\pi \in S_n} \left(\prod_{i=1}^n a_{i\pi(i)} \right). \quad (2.2)$$

The determinant has the following properties.

(1) If matrix B results from A by exchanging two rows or columns, then

$$\det B = -\det A. \quad (2.3)$$

(2) If B results from A by multiplying one row or column with a constant c , then

$$\det B = c \det A. \quad (2.4)$$

(3) If B results from A by adding a multiple of one row to another row, or a multiple of one column to another column, then

$$\det B = \det A. \quad (2.5)$$

(4) For any $n \times n$ matrix B , we have

$$\det(AB) = \det A \cdot \det B. \quad (2.6)$$

2.1.3 THE LAPLACE EXPANSION THEOREM

The determinant of $A = (a_{ij})$ can be expanded along a row i :

$$\det A = \sum_{j=1}^n (-1)^{i+j} a_{ij} B_{i,j}, \quad (2.7)$$

where the $B_{i,j}$ is the determinant of the matrix that results from A by removing the i -th row and the j -th column.

More generally, let I be a k -subset of $\{1, 2, \dots, n\}$, $1 \leq k < n$, then we have the *Laplace expansion theorem*:

$$\det A = \sum_J (-1)^{s(I,J)} \cdot \det A_{I,J} \cdot \det A_{I^c,J^c}, \quad (2.8)$$

where J goes through all k -subsets of $\{1, 2, \dots, n\}$, $s(I, J)$ is the sum of numbers in I and J , and I^c is the complement of I . In particular, if for $a_{ij} = 0$ for all $i \in I$ and $j \notin I$, then

$$\det A = \det A_{I,I} \cdot \det A_{I^c,I^c}. \quad (2.9)$$

Formula (2.9) is useful for our simulation.

2.1.4 DETERMINANTS OF SOME SPECIAL MATRICES

Now, we consider the determinants of some special matrices.

(1) **Triangular matrix** If A is an *upper triangular matrix* (i.e., $a_{ij} = 0$ for $1 \leq j < i \leq n$) or *lower triangular matrix* (i.e., $a_{ij} = 0$ for $1 \leq i < j \leq n$), then

$$\det A = \prod_{i=1}^n a_{ii}. \quad (2.10)$$

(2) **Elementary matrices** Let $i, j \in \mathbb{N}$ with $i \neq j$. An *elementary transformation matrix* $L(i, j, \alpha) = (l_{kl})$ is the identity matrix with the correction

$$l_{ij} = \alpha,$$

and an *elementary permutation matrix* $E(i, j)$ is obtained by exchanging the i th row and the j th row of I_n . Using $L(i, j, \alpha)$ to premultiply a matrix M will add $\alpha M(j, :)$ to the i th

row of M , and using $E(i, j)$ to premultiply M will exchange the i th row and the j th row of M . It is clear that we have

$$\det(L(i, j, \alpha)) = 1, \quad \det(E(i, j)) = -1. \quad (2.11)$$

(3) **Orthogonal matrix** A is an *orthogonal matrix* if $AA^T = I_n$, where A^T is the transpose of A . It is clear that if A is orthogonal, then

$$\det A = \pm 1. \quad (2.12)$$

(4) **Vandermonde matrix** If

$$A = \begin{pmatrix} 1 & 1 & 1 & \cdots & 1 \\ x_1 & x_2 & x_3 & \cdots & x_n \\ x_1^2 & x_2^2 & x_3^2 & \cdots & x_n^2 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ x_1^{n-1} & x_2^{n-1} & x_3^{n-1} & \cdots & x_n^{n-1} \end{pmatrix}$$

where x_1, \dots, x_n are real numbers, then A is called a *Vandermonde matrix*, and

$$\det A = \prod_{i=2}^j \prod_{j=1}^{i-1} (x_i - x_j). \quad (2.13)$$

(5) **Cauchy matrix** If

$$A = \begin{pmatrix} \frac{1}{x_1+y_1} & \frac{1}{x_1+y_2} & \cdots & \frac{1}{x_1+y_n} \\ \frac{1}{x_2+y_1} & \frac{1}{x_2+y_2} & \cdots & \frac{1}{x_2+y_n} \\ \cdots & \cdots & \cdots & \cdots \\ \frac{1}{x_n+y_1} & \frac{1}{x_n+y_2} & \cdots & \frac{1}{x_n+y_n} \end{pmatrix}$$

where x_1, \dots, x_n and y_1, y_2, \dots, y_n are real numbers such that for each pair (i, j) , $x_i + y_j \neq 0$, then A is called a *Cauchy matrix*, and

$$\det A = \frac{\prod_{i=2}^j \prod_{j=1}^{i-1} (x_i - x_j)(y_i - y_j)}{\prod_{i=1}^n \prod_{j=1}^n (x_i + y_j)}. \quad (2.14)$$

2.2 DETERMINANTS OF ARBITRARY MATRICES

In general, we can calculate $\det A$ in the following way: First, write A in the form

$$A = LBR,$$

where B is an upper triangular matrix, and L and R are products of triangular or orthogonal matrices. Then we have

$$\det A = \det L \cdot \det B \cdot \det R. \quad (2.15)$$

The following algorithms are adapted from the algorithms that find the LU or QR factorizations. The running time for each of the algorithms is determined by the number of multiplications required by the algorithm.

2.2.1 GAUSSIAN ELIMINATION WITH PARTIAL PIVOTING (GEP)

A *Gaussian transformation* is a matrix of the form

$$M_k = I_m - \vec{\tau} \vec{e}_k^T = \prod_{j=k+1}^m L(j, k, -\tau_j),$$

where the first k components of $\vec{\tau}$ are zeros. It is clear that M_k is lower triangular and $\det M_k = 1$. The vector $\vec{\tau}$ is called the *Gauss vector* and its nonzero components are called *multipliers*.

Suppose $\vec{x} \in \mathbb{R}^m$ with $x_k \neq 0$. Let

$$\vec{\tau}^T = (0, \dots, 0, \tau_{k+1}, \dots, \tau_m), \quad \tau_i = \frac{x_i}{x_k}, \quad i = k+1, \dots, m.$$

Then we have

$$M_k \vec{x} = (x_1, \dots, x_k, 0, \dots, 0)^T. \quad (2.16)$$

Hence, we can upper-triangularize A by applying a series of Gaussian transformations to A . This method is called *Gaussian elimination*.

The following algorithm uses Gaussian elimination to upper-triangularize the $n \times n$ matrix A .

```

GEP( $A, n$ )
1   $sign \leftarrow 1$ ;
2  for  $i = 1$  to  $n - 1$  do
3    Determine  $t$  so that  $a_{it} = \max\{a_{ii}, \dots, a_{ni}\}$ ;
4    if  $t \neq i$  then
5      Exchange the  $t$ th row and the  $i$ th row of  $A$ ,  $sign \leftarrow -sign$ ;
6    for  $j = i + 1$  to  $n$  do
7       $a_{ji} \leftarrow \frac{a_{ji}}{a_{ii}}$ ;
8       $A(j, i + 1 : n) = A(j, i + 1 : n) - a_{ji}A(i, i + 1 : n)$ ;

```

The Lines 3–5 are doing *partial pivoting* that guarantees that no multiplier is greater than one in absolute value (large multipliers may cause large errors).

This algorithm requires at most $\frac{2}{3}n^3$ multiplications, and can be used to compute the *LU* factorization of a row permuted version of A ([3], pp.113-114).

2.2.2 GIVENS ROTATION (GR)

A *Givens rotation* is a matrix $G = G(i, k, \theta)$ that is the identity matrix with corrections

$$g_{ii} = g_{kk} = c, g_{ik} = s, g_{ki} = -s, c = \cos(\theta), s = \sin(\theta).$$

It is orthogonal with $\det G = 1$. Premultiplying a matrix A by G is equivalent to a counter-clockwise rotation of θ radians in the (i, k) coordinate plane that affects just two rows of A . By choosing the values of i, k and θ , we can zero selected elements in A , so we can upper triangularize A by a series of Givens rotations.

Given scalars a and b , the following function computes a unit vector $\vec{v} = (c, s)$ such that

$$\begin{pmatrix} c & s \\ -s & c \end{pmatrix}^T \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} r \\ 0 \end{pmatrix}. \quad (2.17)$$

$\vec{v} = \mathbf{givens}(a, b)$

1 **if** $b = 0$ **then**


```

2    $\vec{v} \leftarrow (1, 0);$ 
3   else
4      $t \leftarrow \frac{1}{\sqrt{a^2 + b^2}};$ 
5     if  $|a| < |b|$  then  $\vec{v} \leftarrow (-at, bt);$ 
6     else  $\vec{v} \leftarrow (at, -bt).$ 

```

Now, the following algorithm uses Givens rotations to upper-triangularize the $n \times n$ matrix A .

```

GR( $A, n$ )
1  for  $j = 1$  to  $n - 1$  do
2    for  $i = j + 1$  to  $n$  do
3      if  $a_{ij} \neq 0$  then
4         $\vec{v} \leftarrow \text{givens}(a_{jj}, a_{ij})$ 
5         $\vec{x} \leftarrow v_1 A(j, j : n) - v_2 A(i, j : n);$ 
6         $A(i, j : n) \leftarrow v_1 A(i, j : n) + v_2 A(j, j : n);$ 
7         $A(j, j : n) \leftarrow \vec{x}.$ 

```

This algorithm requires at most $2n^3$ multiplications, and can be used to compute the QR factorization of A ([3], pp.226-227).

2.2.3 HOUSEHOLDER REFLECTIONS (HR)

Let $\vec{v} \in \mathbb{R}^m$. An $m \times m$ matrix P of the form

$$P = I_m - \beta \vec{v}^T \vec{v}, \quad \beta = \frac{2}{\vec{v}^T \vec{v}}$$

is called a *Householder reflection*. The vector \vec{v} is called a *Householder vector*. If a vector \vec{x} is multiplied by P , then it is reflected in the hyperplane $\text{span}\{\vec{v}\}^\perp$, and if we set

$$\vec{v} = \vec{x} - \|\vec{x}\| \vec{e}_1,$$

where $\|\vec{x}\| = \sqrt{x_1^2 + \cdots + x_m^2}$, then

$$P\vec{x} = \|\vec{x}\| \vec{e}_1. \tag{2.18}$$

It is readily checked that P is orthogonal, so $\det P = \pm 1$, and we have

$$\det P = -1 \iff \beta \|\vec{v}\| > 1. \quad (2.19)$$

Hence, we can compute $\det A$ by upper triangularizing A using a series of Householder reflections.

The following function computes the normalized Householder vector \vec{v} (i.e., $v_1 = 1$) and β for given $\vec{x} \in \mathbb{R}^m$.

```

[ $\vec{v}, \beta$ ] = house( $\vec{x}$ )
1   $m \leftarrow \mathbf{length}(\vec{x});$ 
2   $\sigma \leftarrow x(2 : m) \cdot x(2 : m);$ 
3   $\vec{v} \leftarrow x, v_1 \leftarrow 1;$ 
4  if  $\sigma = 0$  then
5     $\beta \leftarrow 0;$ 
6  else
7     $\mu \leftarrow \sqrt{x_1^2 + \sigma};$ 
8    if  $x_1 \leq 0$  then  $v_1 \leftarrow x_1 - \mu;$ 
9    else  $v_1 \leftarrow -\frac{\sigma}{x_1 + \mu};$ 
10    $\beta \leftarrow \frac{2v_1^2}{\sigma + v_1^2}; \vec{v} \leftarrow \frac{\vec{v}}{v_1};$ 

```

Now, the following algorithm uses Householder reflections to compute $\det A$.

```

HR( $A, n$ )
1   $k \leftarrow n, \mathit{sign} \leftarrow 1;$ 
2  for  $i = 1$  to  $n$  do
3    [ $\vec{v}, \beta$ ]  $\leftarrow \mathbf{house}(A(i : n, i));$ 
4     $W \leftarrow I_k - \beta \vec{v} \vec{v}^T;$ 
5     $A(i : n, i : n) \leftarrow WA(i : n, i : n);$ 
6    if  $\beta \vec{v} \cdot \vec{v} > 1$  then  $\mathit{sign} \leftarrow -\mathit{sign};$ 
7     $k \leftarrow k - 1;$ 
8   $\det A \leftarrow \mathit{sign} \cdot \prod_{i=1}^n a_{ii}.$ 

```

The algorithm HR requires at most $\frac{4}{3}n^3$ multiplications, and can be also used to compute the QR factorization of A ([3],pp.224-226).

2.2.4 FAST GIVENS TRANSFORMATION(FGT)

There are two types of *fast Givens transformations*. The “type 1” transformation is a matrix $F_1 = F_1(i, k, \alpha, \beta)$ that is the identity matrix with corrections

$$f_{ik} = f_{jk} = 1, f_{ii} = \beta, f_{kk} = \alpha,$$

and the ‘type 2’ transformation is a matrix $F_2 = F_2(i, k, \alpha, \beta)$ that is the identity matrix with corrections

$$f_{ik} = \alpha, f_{jk} = \beta, f_{ii} = f_{kk} = 1,$$

where α, β satisfy $-1 \leq \alpha\beta \leq 0$. It is clear that

$$\det F_1 < 0, \quad \text{and} \quad \det F_2 > 0.$$

From linear algebra (see [3], pp.219-221), applying a series of fast Givens transformations to the matrix A , we can get a diagonal matrix

$$D = \text{diag}(d_1, d_2, \dots, d_n)$$

with all $d_i > 0$, and an upper triangular matrix $T = M^T A = (T_{ij})$ where M is the product of the fast Givens transformations, such that

$$Q = MD^{-1/2}$$

is orthogonal, where

$$D^{-1/2} = \text{diag}\left(\frac{1}{\sqrt{d_1}}, \frac{1}{\sqrt{d_2}}, \dots, \frac{1}{\sqrt{d_n}}\right),$$

and if $R = D^{1/2}T$ where

$$D^{1/2} = \text{diag}(\sqrt{d_1}, \sqrt{d_2}, \dots, \sqrt{d_n}),$$

then $A = QR$ is the QR factorization of A . Note that

$$\det Q = \begin{cases} 1 & \text{if } t \text{ is even;} \\ -1 & \text{otherwise} \end{cases}$$

where t is the number of fast Givens transformations used, so we have

$$\det A = (-1)^t \frac{\prod_{i=1}^n T_{ii}}{\prod_{i=1}^n d_i}. \quad (2.20)$$

Given $\vec{x} \in \mathbb{R}^2$ and positive $\vec{d} \in \mathbb{R}^2$, the following function computes a 2×2 fast Givens transformation M and its *type*, such that $M^T \vec{d} M = \text{diag}(d_1, d_2)$.

```
[M, type] = fastgivens( $\vec{x}, \vec{d}$ )
1  if  $x_2 = 0$  then
2     $M \leftarrow I_2, \text{type} \leftarrow 1;$ 
3  else
4     $\alpha \leftarrow -\frac{x_1}{x_2}; \beta \leftarrow -\frac{\alpha d_2}{d_1}; \gamma \leftarrow -\alpha\beta;$ 
5    if  $\gamma > 1$  then
6       $\text{type} \leftarrow 1; \vec{d} \leftarrow (1 + \frac{1}{\gamma})\vec{d};$ 
7       $M \leftarrow I_2; t_{12} \leftarrow \frac{1}{\alpha}; t_{21} \leftarrow \frac{1}{\beta};$ 
8    else
9       $\text{type} \leftarrow -1; y \leftarrow d_1;$ 
10      $t_{11} \leftarrow \beta; t_{22} \leftarrow \alpha; t_{12} \leftarrow 1; t_{21} \leftarrow 1;$ 
11      $d_1 \leftarrow (1 + \gamma)d_2; d_2 \leftarrow (1 + \gamma)y.$ 
```

Now, the following algorithm computes $\det A$ by using fast Givens transformations (A is overwritten by T).

```
FGT( $A, n$ )
1   $\text{sign} \leftarrow 1; \vec{d} \leftarrow (1, \dots, 1);$ 
2  for  $j = 1$  to  $n - 1$  do
3    for  $i = n$  downto  $j + 1$  do
4      if  $a_{ij} \neq 0$  then
5         $[M, \text{type}] \leftarrow \text{fastgivens}(A(i - 1 : i, j), d(i - 1 : i));$ 
```

```

6         if type = -1 then sign = -sign;
7          $A(i - 1 : i, j : n) \leftarrow MA(i - 1 : i, j : n)$ ;
8   $\det A \leftarrow \textit{sign} \cdot \frac{\prod_{i=1}^n A(i,i)}{\sqrt{\prod_{i=1}^n d(i)}}$ 

```

The algorithm requires at most $\frac{4}{3}n^3$ multiplications.

Each of the four algorithms requires $O(n^3)$ multiplications. However, the running times of these algorithms differ systematically and significantly from each other. This is discussed in the next section.

2.3 COMPARISONS OF THE ALGORITHMS

To determine the most efficient and accurate of the algorithms in §1.2, we have performed several experiments. The programs were written in FORTRAN90 based on these algorithms, and were run on the machine origin.rcr.uga.edu. In the experiments, we used Vandermonde matrices and Cauchy matrices since the true values of determinants of these matrices can be easily computed by (2.13) and (2.14).

Throughout this section, T_1, T_2, T_3, T_4 and E_1, E_2, E_3, E_4 denote the CPU times and relative errors of GEP, GR, HR and FGT, respectively.

2.3.1 EXPERIMENT 1

In Experiment 1, we compute determinants of Vandermonde matrices with $\{x_1, \dots, x_n\}$ taken to be the first n numbers of the randomly generated sequence

$$\{2.87076397, 2.62174494, 0.46096613, 1.79393912, 1.73782442, 2.40223898$$

$$3.06015478, 0.96327602, 2.09695352, 1.16681509, 0.52530896, 0.38936178$$

$$3.89913013, 1.72542264, 0.00551535, 2.09386799, 0.27771812, 0.00571990\}$$

The results are in Table 2.1 and 2.2.

Table 2.1: CPU time in Experiment 1.

n	T_1 (ms)	T_2/T_1	T_3/T_1	T_4/T_1
10	0.018	2.22	9.33	11.5
12	0.026	2.31	8.96	12.2
14	0.038	2.26	8.21	12.0
16	0.053	2.25	7.60	11.8
18	0.072	2.22	7.10	11.8

Table 2.2: Relative errors in Experiment 1.

n	E_1	E_2/E_1	E_3/E_1	E_4/E_1
10	5.0×10^{-10}	1.15	1.37	0.83
12	1.1×10^{-9}	1.29	2.90	1.36
14	2.31×10^{-7}	3.87	0.72	5.22
16	1.16×10^{-5}	1.56	4.47	13.7
18	1.16×10^{-5}	3.98	6.98	13.5

2.3.2 EXPERIMENT 2

In Experiment 2, we compute determinants of Vandermonde matrices with $x_i = \frac{i}{5}$. The results are in Table 2.3 and 2.4.

2.3.3 EXPERIMENT 3

In Experiment 3, we compute determinants of Cauchy matrices with $\{x_1, \dots, x_n\}$ taken to be the first n numbers of the randomly generated sequence

$$\{ 0.07176910, 0.06554362, 0.01152415, 0.04484848, 0.04344561 \\ 0.06005598, 0.07650387, 0.02408190, 0.05242384, 0.02917038 \}$$

and $\{y_1, \dots, y_n\}$ be the first n numbers of the randomly generated sequence

$$\{ 0.09747825, 0.04313557, 0.00013788, 0.05234670, 0.00694295 \\ 0.00014300, 0.07939814, 0.08336780, 0.07268485, 0.06766319 \}$$

The results are in Table 2.5 and 2.6.

Table 2.3: CPU time in Experiment 2.

n	T_1 (ms)	T_2/T_1	T_3/T_1	T_4/T_1
10	0.018	2.17	9.22	11.7
12	0.026	2.35	8.73	12.3
14	0.037	2.35	8.19	12.5
16	0.053	2.31	7.58	12.2
18	0.071	2.25	7.14	11.8

Table 2.4: Relative errors in Experiment 2.

n	E_1	E_2/E_1	E_3/E_1	E_4/E_1
10	2.37×10^{-11}	2.96	11.5	14.3
12	6.94×10^{-10}	2.62	4.61	14.4
14	1.59×10^{-6}	0.08	0.08	2.50
16	1.42×10^{-4}	0.61	0.67	2.25
18	6.25×10^{-2}	0.01	0.11	0.02

2.3.4 EXPERIMENT 4

In this Experiment, we compute determinants of Cauchy matrices with $x_i = \frac{i}{10}$ and $y_i = \frac{i}{5}$, and the results are in Table 2.7 and 2.8.

2.3.5 CONCLUSION

The data in Tables 2.1 to 2.8 show that among the algorithms given in §2.2, GEP is the most efficient, and, in most cases, the most accurate. So in terms of efficiency and accuracy, GEP is a good algorithm for evaluating determinants. However, when GEP produced large errors, GR may be a good alternative method. HR and FGT have their advantages when finding QR factorizations, but they are not as good for evaluating determinants.

We used GEP to calculate determinants in our simulations.

Table 2.5: CPU time in Experiment 3.

n	T_1 (ms)	T_2/T_1	T_3/T_1	T_4/T_1
6	0.008	1.75	10.6	8.5
7	0.008	2.38	13.1	11.8
8	0.012	2.00	10.5	10.3
9	0.014	2.29	10.8	11.6
10	0.016	2.50	10.9	13.0

Table 2.6: Relative errors in Experiment 3.

n	E_1	E_2/E_1	E_3/E_1	E_4/E_1
6	2.40×10^{-8}	1.50	2.87	1.06
7	7.82×10^{-8}	2.68	11.9	3.76
8	8.37×10^{-7}	1.00	0.02	1.11
9	7.09×10^{-5}	2.84	1.27	1.56
10	1.55×10^{-3}	5.31	2.54	2.87

Table 2.7: CPU time in Experiment 4.

n	T_1 (ms)	T_2/T_1	T_3/T_1	T_4/T_1
6	0.007	2.00	11.7	9.7
7	0.009	2.11	11.4	10.6
8	0.011	2.27	12.2	11.5
9	0.014	2.21	10.7	11.6
10	0.018	2.22	9.78	11.6

Table 2.8: Relative errors in Experiment 4.

n	E_1	E_2/E_1	E_3/E_1	E_4/E_1
6	8.70×10^{-11}	0.08	6.54	12.5
7	9.50×10^{-9}	2.33	2.07	2.72
8	2.98×10^{-7}	2.37	0.56	3.69
9	8.53×10^{-7}	7.32	17.9	14.0
10	1.51×10^{-6}	1.99	3.86	2.52

CHAPTER 3

FEYNMAN DIAGRAM EXPANSIONS

A Feynman diagram is a tool invented by Richard Feynman for performing scattering calculations in quantum field theory. To simulate an electron system, we need to expand it to a series of Feynman diagrams. In this chapter, we describe the elements of Feynman diagrams for general 1–electron spaces in §3.1, then introduce the Feynman diagram series §3.2 and calculation of them in §3.3. Finally, we discuss the m –electron Green’s function in §3.4 and the integral padding functions in §3.5.

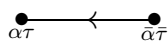
Throughout, \mathcal{E} denotes the (general) 1–*electron space*, $T \in (0, \infty)$ is the *temperature*, $\beta_T = \frac{1}{T}$ is the *inverse temperature*, and the interval $[0, \beta_T]$ is called the *imaginary–time interval*.

3.1 ELEMENTS OF FEYNMAN DIAGRAMS FOR 1–ELECTRON SPACES

There are two kinds of elements of Feynman diagrams for \mathcal{E} : fermions and bosons. The *order* of a Feynman diagram is the number of bosons in it. A vertex that incidents with a boson is called an *internal vertex* and denoted by \bullet . A diagram of order n has exactly $2n$ internal vertices that labeled by $1, 2, \dots, 2n$, and we will identify a vertex with its label.

3.1.1 FERMIONS

A *fermion* (or *g –line*) is a directed edge denoted by



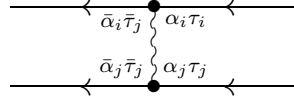
or

$$g(\alpha, \tau | \bar{\alpha}, \bar{\tau})$$

Where $\alpha, \bar{\alpha} \in \mathcal{E}$ and $\tau, \bar{\tau} \in [0, \beta_T]$.

3.1.2 BOSONS

A *boson* (or *interaction*, or *V-line*) stands for an *instantaneous interaction*. and is denoted by



or

$$V(\bar{\alpha}_j, \bar{\alpha}_i | \alpha_i, \alpha_j) \delta(\tau_j - \tau_i) \delta(\bar{\tau}_j - \bar{\tau}_i) \delta(\tau_j - \bar{\tau}_i),$$

where i, j are two vertices, $\alpha_i, \alpha_j, \bar{\alpha}_i, \bar{\alpha}_j \in \mathcal{E}$, $\tau_i, \tau_j, \bar{\tau}_i, \bar{\tau}_j \in [0, \beta_T]$, and δ is the *Dirac δ -function* defined by

$$\delta(x) = \begin{cases} 0 & \text{if } x \neq 0; \\ \infty & \text{if } x = 0. \end{cases}$$

3.2 THE FEYNMAN DIAGRAM SERIES

In this section, we will describe the Feynman diagrams and the Feynman diagram series for m -electron systems.

3.2.1 THE FEYNMAN DIAGRAMS

Each internal vertex in a diagram has exactly 1 incident boson, 1 incoming fermion and 1 outgoing fermion. We will assume that the k -th boson connects vertices $2k - 1$ and $2k$.

In the case $m = 0$, all vertices are internal vertices, the fermions of a diagram F of order n determine a permutation $\pi_F \in S_{2n}$ on its vertices, and the closed fermion loops form a cycle decomposition of π_F . Then

$$\text{sgn}(\pi_F) = (-1)^k \tag{3.1}$$

by (2.1), where k is the number of closed fermion loops in F .

More generally, let $m \geq 0$; for each electron in the m -electron system, an *exterior vertex* (denoted by a pair of \otimes s) with an outgoing fermion and an incoming fermion is included in

the diagram. The fermions in a diagram F of order n determine a permutation $\pi_F \in S_{2n+m}$ on the vertices, and the closed fermion loops form a cycle decomposition of π_F . Then by (2.1), we have

$$\text{sgn}(\pi_F) = (-1)^{k+m} \quad (3.2)$$

where k is the number of closed fermion loops in F

The *Feynman diagram series* for m -electron systems

$$R_m(\beta_1, \dots, \beta_m | \bar{\beta}_1, \dots, \bar{\beta}_m, \theta_1, \dots, \theta_m | \bar{\theta}_1, \dots, \bar{\theta}_m)$$

is the sum of all Feynman diagrams for m -electron systems, where $\beta_i, \bar{\beta}_i \in \mathcal{E}$ and $\theta_i, \bar{\theta}_i \in [0, \beta_T]$. As examples, we give more details for $m = 0$ and $m = 1$.

3.2.2 THE SERIES R_0

Let R_0^n be the series of Feynman diagrams of order n for 0-electron system, $\alpha_i, \bar{\alpha}_i \in \mathcal{E}$ and $\tau_i, \bar{\tau}_i \in [0, \beta_T]$. Then we have

$$R_0 = \sum_{n=1}^{\infty} R_0^n,$$

where $R_0^0 = 1$, and

$$R_0^1 = \begin{array}{c} \alpha_1 \tau_1 \\ \bullet \quad \bullet \\ \bar{\alpha}_1 \bar{\tau}_1 \end{array} \begin{array}{c} \leftarrow \\ \leftarrow \\ \leftarrow \end{array} \begin{array}{c} \bar{\alpha}_2 \bar{\tau}_2 \\ \bullet \quad \bullet \\ \alpha_2 \tau_2 \end{array} \quad + \quad \begin{array}{c} \bar{\alpha}_1 \bar{\tau}_1 \\ \bullet \quad \bullet \\ \alpha_1 \tau_1 \end{array} \begin{array}{c} \leftarrow \\ \leftarrow \\ \leftarrow \end{array} \begin{array}{c} \alpha_2 \tau_2 \\ \bullet \quad \bullet \\ \bar{\alpha}_2 \bar{\tau}_2 \end{array}$$

3.2.3 THE SERIES $R_1(\beta | \bar{\beta}, \theta | \bar{\theta})$

Let R_1^n be the series of Feynman diagrams of order n for 1-electron systems, $\alpha_i, \bar{\alpha}_i \in \mathcal{E}$ and $\tau_i, \bar{\tau}_i \in [0, \beta_T]$. Then we have

$$R_1(\beta | \bar{\beta}, \theta | \bar{\theta}) = \sum_{n=1}^{\infty} R_1^n,$$

where

$$R_1^0 = \otimes_{\beta, \theta} \leftarrow \otimes_{\bar{\beta}, \bar{\theta}}$$

and

$$\begin{aligned}
R_1^1 = & \quad \begin{array}{c} \text{Diagram 1: } \bigotimes_{\beta,\theta} \leftarrow \bar{\alpha}_2, \bar{\tau}_2 \xrightarrow{\alpha_2 \tau_2} \bar{\alpha}_1, \bar{\tau}_1 \xrightarrow{\alpha_1 \tau_1} \bigotimes_{\bar{\beta}, \bar{\theta}} \\ \text{Diagram 2: } \begin{array}{c} \text{Loop } \bar{\alpha}_2, \bar{\tau}_2, \alpha_2 \tau_2 \\ | \\ \bigotimes_{\beta,\theta} \leftarrow \bar{\alpha}_1, \bar{\tau}_1 \xrightarrow{\alpha_1 \tau_1} \bigotimes_{\bar{\beta}, \bar{\theta}} \end{array} \\ \\ \text{Diagram 3: } \begin{array}{c} \alpha_1 \tau_1 \\ \curvearrowright \\ \bar{\alpha}_1, \bar{\tau}_1 \\ \curvearrowleft \\ \alpha_2 \tau_2 \\ \curvearrowright \\ \bar{\alpha}_2, \bar{\tau}_2 \\ \curvearrowleft \\ \alpha_1 \tau_1 \end{array} \\ \text{Diagram 4: } \begin{array}{c} \bar{\alpha}_1, \bar{\tau}_1 \\ \curvearrowright \\ \alpha_1 \tau_1 \\ \curvearrowleft \\ \bar{\alpha}_2, \bar{\tau}_2 \\ \curvearrowright \\ \alpha_2 \tau_2 \\ \curvearrowleft \\ \bar{\alpha}_1, \bar{\tau}_1 \end{array} \\ \\ \text{Diagram 5: } \bigotimes_{\beta,\theta} \leftarrow \bar{\beta}, \bar{\theta} \bigotimes \\ \text{Diagram 6: } \bigotimes_{\beta,\theta} \leftarrow \bar{\beta}, \bar{\theta} \bigotimes \end{array}
\end{aligned}$$

3.3 CALCULATION OF FEYNMAN DIAGRAM SERIES

In this section, we will discuss the calculation of Feynman diagram series for m -electron systems.

3.3.1 COMPACT NOTATION

In the remainder of this dissertation, we will use the following compact notation.

Given $\hat{\alpha} = (\alpha_1, \dots, \alpha_{2n}, \bar{\alpha}_1, \dots, \bar{\alpha}_{2n}) \in \mathcal{E}^{4n}$ and $\hat{\beta} = (\beta_1, \dots, \beta_m, \bar{\beta}_1, \dots, \bar{\beta}_m) \in \mathcal{E}^{2m}$, let

$$V(n, \hat{\alpha}) := \begin{cases} \prod_{k=1}^n V(\bar{\alpha}_k, \bar{\alpha}_{k+n} | \alpha_{k+n}, \alpha_k) & \text{if } n > 0; \\ 1 & \text{if } n = 0. \end{cases}$$

and

$$\hat{\gamma} := \hat{\alpha} \oplus \hat{\beta} := (\alpha_1, \dots, \alpha_{2n}, \beta_1, \dots, \beta_m, \bar{\alpha}_1, \dots, \bar{\alpha}_{2n}, \bar{\beta}_1, \dots, \bar{\beta}_m) \in \mathcal{E}^{2(2n+m)}$$

Given $\hat{\tau} = (\tau_1, \dots, \tau_n, \bar{\tau}_1, \dots, \bar{\tau}_n) \in [0, \beta_T]^{4n}$ with

$$\tau_{k+n} = \tau_k, \bar{\tau}_j = \tau_j, \quad 1 \leq k \leq n, 1 \leq j \leq 2n,$$

and given $\hat{\theta} = (\theta_1, \dots, \theta_m, \bar{\theta}_1, \dots, \bar{\theta}_m) \in [0, \beta_T]^{2m}$, let

$$\hat{\varphi} := \hat{\tau} \oplus \hat{\theta} := (\tau_1, \dots, \tau_{2n}, \theta_1, \dots, \theta_m, \bar{\tau}_1, \dots, \bar{\tau}_{2n}, \bar{\theta}_1, \dots, \bar{\theta}_m) \in [0, \beta_T]^{2(2n+m)}$$

Let $\hat{\alpha}, \hat{\tau}, \hat{\gamma}$ and $\hat{\varphi}$ as above. For $i, j \in \{1, \dots, 2n\}$, let

$$g_{\hat{\alpha}\hat{\tau}}(i, j) = g(\alpha_i, \tau_j | \bar{\alpha}_i, \bar{\tau}_j),$$

and for $i, j \in \{1, \dots, 2n+m\}$, let

$$g_{\hat{\gamma}\hat{\varphi}}(i, j) = g(\gamma_i, \varphi_j | \bar{\gamma}_i, \bar{\varphi}_j).$$

Then we define matrices

$$\hat{g}_{\hat{\alpha}\hat{\tau}} := (g_{\hat{\alpha}\hat{\tau}}(i, j))_{1 \leq i, j \leq 2n}$$

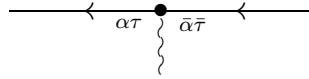
and

$$\hat{g}_{\hat{\gamma}\hat{\varphi}} := (g_{\hat{\gamma}\hat{\varphi}}(i, j))_{1 \leq i, j \leq 2n+m}.$$

3.3.2 FEYNMAN RULES FOR \mathcal{E}

To calculate diagrams for \mathcal{E} , we have the following rules that are called *Feynman rules*.

- (1) Each fermion gives a factor g .
- (2) Each boson gives a factor V .
- (3) At each internal vertex



sum over $\alpha, \bar{\alpha}$:

$$\sum_{\alpha \in \mathcal{E}} \sum_{\bar{\alpha} \in \mathcal{E}} \dots$$

and integrate over $\tau, \bar{\tau}$:

$$\int_0^{\beta_T} d\tau \int_0^{\beta_T} d\bar{\tau} \dots$$

- (4) For each diagram F for m -electron system, multiply by the prefactor

$$\frac{(-1)^n}{2^n n!} (-1)^{m+N_L} = \frac{(-1)^n}{2^n n!} \text{sgn}(\pi_F),$$

where N_L is the number of closed fermion loops in F , n is the order of F and $\pi_F \in S_{2n+m}$ is the permutation determined by F .

3.3.3 CALCULATION OF FEYNMAN DIAGRAM SERIES

For each $n \geq 0$, let

$$\alpha_1, \dots, \alpha_{2n}, \bar{\alpha}_1, \dots, \bar{\alpha}_{2n} \in \mathcal{E},$$

and

$$\tau_1, \dots, \tau_{2n}, \bar{\tau}_1, \dots, \bar{\tau}_{2n} \in [0, \beta_T]$$

with

$$\bar{\tau}_j = \tau_j, \tau_{k+n} = \tau_k, 1 \leq j \leq 2n, 1 \leq k \leq n.$$

Then, applying Feynman rules to the series R_0 , we have

$$\begin{aligned} R_0 &= \sum_{n=0}^{\infty} \frac{(-1)^n}{2^n n!} \sum_{\alpha_1 \dots \alpha_{2n}} \sum_{\bar{\alpha}_1 \dots \bar{\alpha}_{2n}} \prod_{k=1}^n V(\bar{\alpha}_k, \bar{\alpha}_{k+n} | \alpha_{k+n}, \alpha_k) \\ &\times \int_0^{\beta_T} d\tau_1 \cdots \int_0^{\beta_T} d\tau_n \sum_{\pi \in S_{2n}} \text{sgn}(\pi) \prod_{j=1}^{2n} g(\alpha_{\pi(j)}, \tau_{\pi(j)} | \bar{\alpha}_j, \bar{\tau}_j) \end{aligned}$$

Rewriting in the compact notation, we have

$$R_0 = \sum_{n=0}^{\infty} \sum_{\hat{\alpha} \in \mathcal{E}^{4n}} \int_0^{\beta_T} d\tau_1 \cdots \int_0^{\beta_T} d\tau_n \frac{(-1)^n}{2^n n!} V(n, \hat{\alpha}) \det(\hat{g}_{\hat{\alpha}\hat{\tau}}). \quad (3.3)$$

Note that $\det(\hat{g}_{\hat{\alpha}\hat{\tau}}) = 1$ for $n = 0$.

Similarly, given $\hat{\beta} = (\beta, \bar{\beta}) \in \mathcal{E}^2$ and $\hat{\theta} = (\theta, \bar{\theta}) \in [0, \beta_T]^2$, then we have

$$R_1(\hat{\beta}, \hat{\theta}) = \sum_{n=0}^{\infty} \sum_{\hat{\alpha} \in \mathcal{E}^{4n}} \int_0^{\beta_T} d\tau_1 \cdots \int_0^{\beta_T} d\tau_n \frac{(-1)^n}{2^n n!} V(n, \hat{\alpha}) \det(\hat{g}_{\hat{\alpha} \oplus \hat{\beta}, \hat{\tau} \oplus \hat{\theta}}). \quad (3.4)$$

More generally, given

$$\hat{\beta} = (\beta_1, \dots, \beta_m, \bar{\beta}_1, \dots, \bar{\beta}_m) \in \mathcal{E}^m, \quad \hat{\theta} = (\theta_1, \dots, \theta_m, \bar{\theta}_1, \dots, \bar{\theta}_m) \in [0, \beta_T]^m$$

we have

$$R_m(\hat{\beta}, \hat{\theta}) = \sum_{n=0}^{\infty} \sum_{\hat{\alpha} \in \mathcal{E}^{4n}} \int_0^{\beta_T} d\tau_1 \cdots \int_0^{\beta_T} d\tau_n \frac{(-1)^n}{2^n n!} V(n, \hat{\alpha}) \det(\hat{g}_{\hat{\alpha} \oplus \hat{\beta}, \hat{\tau} \oplus \hat{\theta}}). \quad (3.5)$$

3.4 THE m -ELECTRON GREEN'S FUNCTION

The m -electron Green's Function G_m on $\mathcal{E}^{2m} \times [0, \beta_T]^{2m}$ is defined by

$$G_m(\hat{\beta}, \hat{\theta}) = \frac{1}{R_0} R_m(\hat{\beta}, \hat{\theta}).$$

This function is what we want to calculate by Monte Carlo simulation.

Note that the fermion g can be viewed as a function on $\mathcal{E}^2 \times [0, \beta_T]^2$, and is called *1-electron Green's function*. We will give some important properties of g below, and these properties also hold for the function G_m .

(1) *Anti-periodicity*: for an integer l , we have

$$g(\alpha, \tau | \bar{\alpha}, \bar{\tau} + l\beta_T) = (-1)^l g(\alpha, \tau | \bar{\alpha}, \bar{\tau})$$

and

$$g(\alpha, \tau + l\beta_T | \bar{\alpha}, \bar{\tau}) = (-1)^l g(\alpha, \tau | \bar{\alpha}, \bar{\tau}).$$

(2) *Time translation invariance*: for a real number δ , we have

$$g(\alpha, \tau + \delta | \bar{\alpha}, \bar{\tau} + \delta) = g(\alpha, \tau | \bar{\alpha}, \bar{\tau}).$$

In particular, setting $\delta = -\bar{\tau}$, we have

$$g(\alpha, \tau - \bar{\tau} | \bar{\alpha}, 0) = g(\alpha, \tau | \bar{\alpha}, \bar{\tau}).$$

Hence we can write

$$g(\alpha, \tau | \bar{\alpha}, \bar{\tau}) \equiv g(\alpha | \bar{\alpha}, \tau - \bar{\tau}).$$

(3) *Jump discontinuity*: Let $\tau_g = \tau - \bar{\tau}$. Then the function $g(\alpha | \bar{\alpha}, \tau_g)$ is continuous (actually, holomorphic) for $\tau_g \in (0, \beta_T)$, but it has jump discontinuities (assume orthonormal 1-electron basis states “ $|\alpha$ ”) at $\tau_g = l\beta_T$, where l is an integer. In particular, at $\tau_g = 0$, we have

$$\lim_{\tau_g \rightarrow 0^+} g(\alpha | \bar{\alpha}, \tau_g) - \lim_{\tau_g \rightarrow 0^-} g(\alpha | \bar{\alpha}, \tau_g) = \delta_{\alpha, \bar{\alpha}}.$$

Here δ is the *Kronecker* δ , defined by

$$\delta_{ij} = \begin{cases} 1 & \text{if } i = j, \\ 0 & \text{otherwise.} \end{cases}$$

3.5 INTEGRAL PADDING FUNCTIONS

Given a positive integer N , let $n \in \{0, \dots, N\}$, $p = N - n$ and $\tilde{\psi} = (\psi, \dots, \psi_p) \in [0, \beta_T]^p$.

Then, the *integral padding function* (for short, *padding function*) is defined by

$$Q_p(\tilde{\psi}) = \begin{cases} \prod_{l=1}^p g_l(\psi_l) & \text{if } p > 0, \\ 1 & \text{if } p = 0. \end{cases} \quad (3.6)$$

Here for each $l \in \{1, \dots, p\}$, g_l is a non-negative real function such that

$$\int_0^{\beta_T} g_l(\psi_l) d\psi_l = 1. \quad (3.7)$$

It is readily seen that

$$\int_0^{\beta_T} d\psi_1 \cdots \int_0^{\beta_T} d\psi_p Q_p(\tilde{\psi}) = 1. \quad (3.8)$$

Let $\hat{\alpha}, \hat{\tau}, \hat{\beta}$ and $\hat{\theta}$ be as in (3.4). Recall that $\hat{\tau} = (\tau_1, \dots, \tau_n, \bar{\tau}_1, \dots, \bar{\tau}_n) \in [0, \beta_T]^{4n}$ with

$$\tau_{k+n} = \tau_k, \bar{\tau}_j = \tau_j, \quad 1 \leq k \leq n, 1 \leq j \leq 2n.$$

Now, let

$$\tilde{\tau} := (\tau_1, \dots, \tau_n) \in [0, \beta_T]^n$$

and

$$\tilde{\tau} \oplus \tilde{\psi} := (\tau_1, \dots, \tau_n, \psi_1, \dots, \psi_{N-n}) \in [0, \beta_T]^N.$$

Then we define

$$F_m(\hat{\beta}, \hat{\theta}, n, \hat{\alpha}, \hat{\tau}, \tilde{\psi}) := \frac{(-1)^n}{2^n n!} V(n, \hat{\alpha}) \det \left(\hat{g}_{\hat{\beta} \oplus \hat{\beta}, \hat{\tau} \oplus \hat{\theta}} \right) Q_{N-n}(\tilde{\psi}).$$

In particular, if $m = 0$, we write

$$F_0(n, \hat{\alpha}, \hat{\tau}, \tilde{\psi}) = \frac{(-1)^n}{2^n n!} V(n, \hat{\alpha}) \det \left(\hat{g}_{\hat{\beta}, \hat{\tau}} \right) Q_{N-n}(\tilde{\psi}).$$

Then the m -electron Green's function can be rewritten as

$$G_m(\hat{\beta}, \hat{\theta}) = \lim_{N \rightarrow \infty} \frac{\sum_{n=0}^N \sum_{\hat{\alpha} \in \mathcal{E}^{4n}} \int_{[0, \beta_T]^N} d^N(\tilde{\tau} \oplus \tilde{\psi}) F_m(\hat{\beta}, \hat{\theta}, n, \hat{\alpha}, \hat{\tau}, \tilde{\psi})}{\sum_{n=0}^N \sum_{\hat{\alpha} \in \mathcal{E}^{4n}} \int_{[0, \beta_T]^N} d^N(\tilde{\tau} \oplus \tilde{\psi}) F_0(n, \hat{\alpha}, \hat{\tau}, \tilde{\psi})}. \quad (3.8)$$

CHAPTER 4

EXTENDED HUBBARD MODEL (EHM)

The *Hubbard model*, is the simplest model of interacting particles in a lattice. If interactions between particles on different sites of the lattice are included, the model is often referred as the *extended Hubbard model*.

In this chapter, we introduce an extended Hubbard model (for short, EHM) on a 2-dimensional rectangular lattice that can be used to describe strongly interacting electrons in 3-dimensional transition metal compounds, such as high temperature superconductors. We will describe the 2-dimensional real space lattice \mathcal{L} and 1-electron space on it in §4.1 and discuss the interaction potential function V for EHM on \mathcal{L} in §4.2. Then, we define the \vec{k} -space and reciprocal lattice of \mathcal{L} in §4.3. Finally, we will discuss the 1-electron Green's function g and m -electron Green's function for EHM in real space representations in §4.4 and §4.5, respectively.

4.1 THE LATTICE \mathcal{L} AND 1-ELECTRON SPACE

Given two positive integers L_x and L_y , a 2-dimensional rectangle *lattice* \mathcal{L} of *size*

$$|\mathcal{L}| = L_x \cdot L_y$$

is defined by

$$\mathcal{L} := \{\vec{r} = (r_x, r_y) \mid r_x \in \{0, \dots, L_x - 1\}, r_y \in \{0, \dots, L_y - 1\}\}.$$

The following *periodic boundary condition* (PBC) holds for any $\vec{r}_1, \vec{r}_2 \in \mathcal{L}$:

$$\vec{r}_1 \oplus \vec{r}_2 = ((r_{1x} + r_{2x}) \bmod(L_x), (r_{1y} + r_{2y}) \bmod(L_y)). \quad (4.1)$$

Now, let the *spin space* \mathcal{S} be defined by

$$\mathcal{S} := \left\{ \frac{1}{2}, -\frac{1}{2} \right\}.$$

Then the 1–electron space \mathcal{E} is defined by

$$\mathcal{E} := \mathcal{L} \times \mathcal{S} = \{ \alpha = (\vec{r}, s) \mid \vec{r} \in \mathcal{L}, s \in \mathcal{S} \}.$$

4.2 INTERACTION POTENTIAL FUNCTION V

In this section, we will discuss the *interaction potential function* V and its properties.

4.2.1 DEFINITION

Suppose that $\alpha_l = (\vec{r}_l, s_l) \in \mathcal{E}$, $l = 1, \dots, 4$. Then the interaction potential function is given by

$$V(\alpha_1, \alpha_2 | \alpha_3, \alpha_4) \equiv \begin{array}{c} \alpha_2 \longleftarrow \bullet \longleftarrow \alpha_3 \\ \text{~~~~~} \updownarrow \text{~~~~~} \\ \alpha_1 \longleftarrow \bullet \longleftarrow \alpha_4 \end{array} = V_c(\Delta\vec{r}) \delta_{\vec{r}_1 \vec{r}_4} \delta_{\vec{r}_2 \vec{r}_3} \delta_{s_1 s_4} \delta_{s_2 s_3},$$

where $V_c(\Delta\vec{r})$ is called the *Coulomb potential function*, and δ is the Kronecker δ . We may write $V(\vec{r}_1, s_1, \vec{r}_2, s_2 | \vec{r}_3, s_3, \vec{r}_4, s_4)$ for $V(\alpha_1, \alpha_2 | \alpha_3, \alpha_4)$.

Note that comparing this to the definition of boson in § 3.1.2, τ –labels and the Dirac δ for τ 's are removed, and spins and the Kronecker δ for spins are added.

4.2.2 THE SIMPLEST EHM FOR V_c

Let $\vec{R}_x := (L_x, 0)$ and $\vec{R}_y := (0, L_y)$ (called *lattice size vectors*) and

$$\mathcal{L}_\infty := \{ \vec{r} = (r_x, r_y) \mid r_x \in \mathbb{Z}, r_y \in \mathbb{Z} \}.$$

Then the *norm* of $\Delta\vec{r} = \vec{r}_1 - \vec{r}_2 \in \mathcal{L}_\infty$ is defined by

$$|\Delta\vec{r}|_{\mathcal{L}} := \min_{(n_x, n_y) \in \mathbb{Z}^2} |\Delta\vec{r} - n_x \vec{R}_x - n_y \vec{R}_y|.$$

Here the norm

$$|\vec{a}| = \sqrt{a_x^2 + a_y^2}, \quad \vec{a} = (a_x, a_y) \in \mathbb{Z}^2$$

is the Euclidean distance.

Now, let V_0 be the *Hubbard on-site repulsion energy*, V_1 the *first neighbor repulsion energy* and R_c the *Coulomb cut-off radius*. Then the Coulomb potential function V_c is defined by

$$V_c(\Delta\vec{r}) = \begin{cases} V_0 & \text{if } |\Delta\vec{r}|_{\mathcal{L}} = 0; \\ V_1 \frac{\theta_c(R_c - |\Delta\vec{r}|_{\mathcal{L}})}{|\Delta\vec{r}|_{\mathcal{L}}} & \text{otherwise.} \end{cases} \quad (4.2)$$

Here

$$\theta_c(x) = \begin{cases} 1 & \text{if } x \geq 0, \\ 0 & \text{otherwise} \end{cases}$$

is the *step function*.

4.2.3 LTI AND PBC FOR FUNCTION V

Let $\vec{r}_1, \dots, \vec{r}_4 \in \mathcal{L}$ and $s_1, \dots, s_4 \in \mathcal{S}$. The function V has the following *lattice translation invariance* property (LTI): for $\vec{r}_0 \in \mathcal{L}_\infty$, we have

$$\begin{aligned} V(\vec{r}_1, s_1, \vec{r}_2, s_2 | \vec{r}_3, s_3, \vec{r}_4, s_4) &= V(\vec{r}_1 - \vec{r}_0, s_1, \vec{r}_2 - \vec{r}_0, s_2 | \vec{r}_3 - \vec{r}_0, s_3, \vec{r}_4 - \vec{r}_0, s_4) \\ &= V_c(\vec{r}_1 - \vec{r}_2) \delta_{\vec{r}_1 \vec{r}_4} \delta_{s_1 s_4} \delta_{\vec{r}_2 \vec{r}_3} \delta_{s_2 s_3} \end{aligned} \quad (4.3)$$

The PBC also holds for V : let $l_x, l_y \in \mathbb{Z}$ and let $\vec{R} := l_x \vec{R}_x + l_y \vec{R}_y$, then

$$\begin{aligned} V(\vec{r}_1, s_1, \vec{r}_2, s_2 | \vec{r}_3, s_3, \vec{r}_4, s_4) &= (\vec{r}_1 + \vec{R}, s_1, \vec{r}_2, s_2 | \vec{r}_3, s_3, \vec{r}_4, s_4) \\ &= V(\vec{r}_1, s_1, \vec{r}_2 + \vec{R}, s_2 | \vec{r}_3, s_3, \vec{r}_4, s_4) \\ &= V(\vec{r}_1, s_1, \vec{r}_2, s_2 | \vec{r}_3 + \vec{R}, s_3, \vec{r}_4, s_4) \\ &= V(\vec{r}_1 + \vec{R}, s_1, \vec{r}_2, s_2 | \vec{r}_3, s_3, \vec{r}_4, s_4) \end{aligned} \quad (4.4)$$

since $V_c(\Delta\vec{r} + R) = V_c(\Delta\vec{r})$.

4.3 THE \vec{k} -SPACE AND RECIPROCAL LATTICE OF \mathcal{L}

In this section, we will define the \vec{k} -space and *reciprocal lattice* of \mathcal{L}

4.3.1 THE \vec{k} -SPACE OF \mathcal{L}

The \vec{k} -space $\mathcal{K}_{\mathcal{L}_\infty}$ of \mathcal{L} is defined by

$$\mathcal{K}_{\mathcal{L}_\infty} := \left\{ \vec{k} = \left(\frac{2\pi m_x}{L_x}, \frac{2\pi m_y}{L_y} \right) \mid (m_x, m_y) \in \mathbb{Z}^2 \right\}$$

and the \vec{k} -zone $\mathcal{K}_{\mathcal{L}}$ of \mathcal{L} is defined by

$$\mathcal{K}_{\mathcal{L}} := \left\{ \vec{k} = \left(\frac{2\pi m_x}{L_x}, \frac{2\pi m_y}{L_y} \right) \mid (m_x, m_y) \in \mathcal{L} \right\}.$$

Let $\mathcal{R}_{\mathcal{L}}$ be the *PB vector space* defined by

$$\mathcal{R}_{\mathcal{L}} := \{ \vec{R} = (l_x L_x, l_y L_y) \equiv l_x \vec{R}_x + l_y \vec{R}_y \mid (l_x, l_y) \in \mathbb{Z}^2 \};$$

then we have

$$\begin{aligned} \vec{k} \in \mathcal{K}_{\mathcal{L}_\infty} &\iff \vec{k} \bullet \vec{R} \in \{2\pi j \mid j \in \mathbb{Z}\}, \quad \forall \vec{R} \in \mathcal{R}_{\mathcal{L}} \\ &\iff e^{i\vec{k} \bullet \vec{R}} = 1, \quad \forall \vec{R} \in \mathcal{R}_{\mathcal{L}}. \end{aligned} \tag{4.5}$$

Here “ \bullet ” is the dot (or inner) product of vectors.

4.3.2 THE RECIPROCAL LATTICE OF \mathcal{L}

The reciprocal lattice $\mathcal{Q}_{\mathcal{L}}$ of \mathcal{L} is defined by

$$\mathcal{Q}_{\mathcal{L}} := \{ \vec{K} = (2\pi m_x, 2\pi m_y) \mid (m_x, m_y) \in \mathbb{Z}^2 \}.$$

It is readily seen that

$$\begin{aligned} \vec{K} \in \mathcal{Q}_{\mathcal{L}} &\iff \vec{r} \bullet \vec{K} \in \{2\pi j \mid j \in \mathbb{Z}\}, \quad \forall \vec{r} \in \mathcal{L}_\infty \\ &\iff e^{i\vec{r} \bullet \vec{K}} = 1, \quad \forall \vec{r} \in \mathcal{L}_\infty \end{aligned} \tag{4.6}$$

4.4 THE 1-ELECTRON GREEN'S FUNCTION g

Through this section, i denotes an imaginary unit (that is, $i^2 = -1$).

4.4.1 ENERGY BAND

Let t_l ($l = 1, 2, 3$) be the l -th neighbor hopping (or hybridization) energy and μ be the chemical potential. Then the energy band $\mathcal{E}_{\vec{k}}$ of $\vec{k} = (k_x, k_y) \in \mathcal{K}_{\mathcal{L}_\infty}$ is defined by

$$\mathcal{E}_{\vec{k}} := -2t_1(\cos k_x + \cos k_y) - 4t_2 \cos k_x \cos k_y - 2t_3(\cos(2k_x) + \cos(2k_y)) - \mu.$$

The following LTI property for $\mathcal{E}_{\vec{k}}$ holds:

$$\mathcal{E}_{\vec{k}+\vec{K}} = \mathcal{E}_{\vec{k}}, \quad \forall \vec{k} \in \mathcal{K}_{\mathcal{L}_\infty}, \quad \forall \vec{K} \in \mathcal{Q}_{\mathcal{L}} \quad (4.7)$$

4.4.2 THE FOURIER SUM OVER MATSUBARA FREQUENCIES

Let \mathcal{F}_- be the set of Matsubara frequencies defined by

$$\mathcal{F}_- := \{i\nu \mid \nu = (2m+1)\pi T, m \in \mathbb{Z}\}$$

and let

$$\tilde{g}_0(\vec{k}, i\nu) := \frac{1}{i\nu - \mathcal{E}_{\vec{k}}}, \quad i\nu \in \mathcal{F}_-, \quad \vec{k} \in \mathcal{K}_{\mathcal{L}_\infty}.$$

Then, the Fourier sum over Matsubara frequencies

$$\tilde{g}_0(\vec{k}, \Delta\tau) := T \sum_{i\nu \in \mathcal{F}_-} \tilde{g}_0(\vec{k}, i\nu) e^{-i\nu\Delta\tau} \quad (4.8)$$

can be evaluated analytically by complex contour integration. This yields

$$\tilde{g}_0(\vec{k}, \Delta\tau) = e^{\mathcal{E}_{\vec{k}}\Delta\tau} [f(\mathcal{E}_{\vec{k}}) - \theta_c(\Delta\tau)] \quad (4.9)$$

and

$$\tilde{g}_0(\vec{k}, \Delta\tau + l\beta_T) = (-1)^l \tilde{g}_0(\vec{k}, \Delta\tau) \quad (4.10)$$

for

$$-\beta_T < \Delta\tau < \beta_T, \quad l \in \mathbb{Z}.$$

Where

$$\theta_c(x) = \begin{cases} 1 & \text{if } x \geq 0; \\ 0 & \text{if } x < 0. \end{cases}$$

and f is the *Fermi function* defined by

$$f(\mathcal{E}) := \frac{1}{e^{\beta\tau\mathcal{E}} + 1}.$$

By (4.7) and (4.9), the LTI property for \tilde{g}_0 holds:

$$\tilde{g}_0(\vec{k} + \vec{K}, \Delta\tau) = \tilde{g}_0(\vec{k}, \Delta\tau) \quad (4.11)$$

4.4.3 THE FUNCTION g

For $\alpha_1 = (\vec{r}_1, s_1) \in \mathcal{E}$, $\alpha_2 = (\vec{r}_2, s_2) \in \mathcal{E}$ and $\tau_1, \tau_2 \in [0, \beta_T]$, the 1–electron Green’s function g is defined by

$$g(\alpha_1, \tau_1 | \alpha_2, \tau_2) \equiv g(\vec{r}_1, s_1 | \vec{r}_2, s_2, r_1 - r_2) := \delta_{s_1 s_2} \frac{T}{|L|} \sum_{\vec{k} \in \mathcal{K}_{\mathcal{L}}} \sum_{i\nu \in \mathcal{F}_-} \tilde{g}_0(\vec{k}, i\nu) e^{i\vec{k} \bullet \Delta\vec{r} - i\nu \Delta\tau}$$

Let

$$g_0(\Delta\vec{r}, \Delta\tau) := \frac{1}{|L|} \sum_{\vec{k} \in \mathcal{K}_{\mathcal{L}}} \tilde{g}_0(\vec{k}, \Delta\tau) e^{i\vec{k} \bullet \Delta\vec{r}}; \quad (4.12)$$

then we have

$$g(\vec{r}_1, s_1 | \vec{r}_2, s_2, r_1 - r_2) = \delta_{s_1 s_2} g_0(\Delta\vec{r}, \Delta\tau). \quad (4.13)$$

Note that in the sum on the right side of (4.11), the conjugate of each summand is also a summand, so the sum is a real number.

Both LTI and PBC hold for the function g . That is, for $\vec{r}_1, \vec{r}_2 \in \mathcal{L}$, $\vec{r}_0 \in \mathcal{L}_\infty$ and $\vec{R} \in \mathcal{R}_{\mathcal{L}}$, we have

$$g(\vec{r}_1, s_1 | \vec{r}_2, s_2, \Delta\tau) = g(\vec{r}_1 - \vec{r}_0, s_1 | \vec{r}_2 - \vec{r}_0, s_2, \Delta\tau) \quad (4.14)$$

and

$$g(\vec{r}_1, s_1 | \vec{r}_2, s_2, \Delta\tau) = g(\vec{r}_1 + \vec{R}, s_1 | \vec{r}_2, s_2, \Delta\tau) = g(\vec{r}_1, s_1 | \vec{r}_2 + \vec{R}, s_2, \Delta\tau) \quad (4.15)$$

4.5 THE m –ELECTRON GREEN’S FUNCTION G_m FOR EHM

We now turn to the m –electron Green’s function G_m ($m \geq 0$) for EHM in the real space representation.

4.5.1 NOTATION

Let n, N be integers with $0 \leq n \leq N$.

Let the external vertices be denoted by

$$\hat{\beta} := (\hat{r}^{(\beta)}, \hat{s}^{(\beta)}),$$

where

$$\hat{r}^{(\beta)} := (\vec{r}_1^{(\beta)}, \dots, \vec{r}_m^{(\beta)} | \vec{r}_1^{(\beta)}, \dots, \vec{r}_m^{(\beta)}) \in \mathcal{L}^{2m}$$

and

$$\hat{s}^{(\beta)} := (s_1^{(\beta)}, \dots, s_m^{(\beta)} | \bar{s}_1^{(\beta)}, \dots, \bar{s}_m^{(\beta)}) \in \mathcal{S}^{2m}.$$

Given $\tilde{r} = (\vec{r}_1, \dots, \vec{r}_{2n}) \in \mathcal{L}^{2n}$, let

$$\hat{r} := (\vec{r}_1, \dots, \vec{r}_{2n} | \vec{r}_1, \dots, \vec{r}_{2n}) \in \mathcal{L}^{4n}$$

and

$$\hat{r}^{(g)} := \hat{r} \oplus \hat{r}^{(\beta)} = (\vec{r}_1, \dots, \vec{r}_{2n}, \vec{r}_1^{(\beta)}, \dots, \vec{r}_m^{(\beta)} | \vec{r}_1, \dots, \vec{r}_{2n}, \vec{r}_1^{(\beta)}, \dots, \vec{r}_m^{(\beta)}) \in \mathcal{L}^{2(2n+m)}$$

where $\vec{r}_j = \vec{r}_j$ for $j = 1, \dots, 2n$.

Given $\tilde{s} = (s_1, \dots, s_{2n}) \in \mathcal{S}^{2n}$, let

$$\hat{s} := (s_1, \dots, s_{2n} | \bar{s}_1, \dots, \bar{s}_{2n}) \in \mathcal{S}^{4n}$$

and

$$\hat{s}^{(g)} := \hat{s} \oplus \hat{s}^{(\beta)} = (s_1, \dots, s_{2n}, s_1^{(\beta)}, \dots, s_m^{(\beta)} | \bar{s}_1, \dots, \bar{s}_{2n}, \bar{s}_1^{(\beta)}, \dots, \bar{s}_m^{(\beta)}) \in \mathcal{S}^{2(2n+m)}$$

with $\bar{s}_j = s_j$ for $j = 1, \dots, 2n$.

Given $\tilde{\tau} := (\tau_1, \dots, \tau_n) \in [0, \beta_T]^n$ and

$$\hat{\theta} := (\theta_1, \dots, \theta_m | \bar{\theta}_1, \dots, \bar{\theta}_m) \in [0, \beta_T]^{2m},$$

let

$$\hat{\tau} := (\tau_1, \dots, \tau_{2n} | \bar{\tau}_1, \dots, \bar{\tau}_{2n}) = \tilde{\tau} \oplus \tilde{\tau} \oplus \tilde{\tau} \oplus \tilde{\tau} \in [0, \beta_T]^{4n}$$

and

$$\tau^{(g)} := \hat{\tau} \oplus \hat{\theta} = (\tau_1, \dots, \tau_{2n}, \theta_1, \dots, \theta_m | \bar{\tau}_1, \dots, \bar{\tau}_{2n}, \bar{\theta}_1, \dots, \bar{\theta}_m) \in [0, \beta_T]^{2(2n+m)}.$$

with $\tau_{k+n} = \tau_k$, $1 \leq k \leq n$ and $\bar{\tau}_j = \tau_j$, $1 \leq j \leq 2n$.

Let

$$\hat{\alpha} = (\alpha_1, \dots, \alpha_{2n}, \bar{\alpha}_1, \dots, \bar{\alpha}_{2n}) \in \mathcal{E}^{4n}$$

with

$$\alpha_j = (\vec{r}_j, s_j), \quad \bar{\alpha}_j = (\vec{r}_j, \bar{s}_j), \quad 1 \leq j \leq 2n.$$

4.5.2 THE FUNCTION G_m

Given $\tilde{\psi} := (\psi_1, \dots, \psi_{N-n}) \in [0, \beta_T]^{N-n}$, let

$$\begin{aligned} F_m(\hat{r}^{(\beta)}, s^{(\beta)}, \hat{\theta}, n, \tilde{r}, \tilde{s}, \tilde{\tau}, \tilde{\psi}) &\equiv F_m(\hat{\beta}, \hat{\theta}, n, \hat{\alpha}, \hat{\tau}, \tilde{\psi}) \\ &= \frac{(-1)^n}{2^n n!} (\prod_{k=1}^n V_c(\vec{r}_{k+n} - \vec{r}_k)) \det \hat{g}_{\vec{r}^{(g)}, s^{(g)}, \hat{\tau}^{(g)}} Q_{N-n}(\tilde{\psi}) \end{aligned} \quad (4.16)$$

where the Coulomb potential function V_c is given in (4.2), the padding function Q_{N-n} is given in (3.6), and

$$\hat{g}_{\vec{r}^{(g)}, s^{(g)}, \hat{\tau}^{(g)}} := \left[g(\vec{r}_i^{(g)}, s_i^{(g)} | \vec{r}_j^{(g)}, s_j^{(g)}, \tau_i^{(g)} - \tau_j^{(g)}) \right]_{1 \leq i, j \leq 2n+m} \quad (4.17)$$

is a $(2n+m) \times (2n+m)$ matrix. Then the m -electron diagram series is given by

$$R_m(\hat{r}^{(\beta)}, s^{(\beta)}, \hat{\theta}) = \lim_{N \rightarrow \infty} \sum_{n=0}^N \sum_{\tilde{r} \in \mathcal{L}^{2n}} \sum_{\tilde{s} \in \mathcal{S}^{2n}} \int_{[0, \beta_T]^n} d^m \tilde{\tau} \int_{[0, \beta_T]^{N-n}} d^{N-n} \tilde{\psi} F_m(\hat{\beta}, \hat{\theta}, n, \hat{\alpha}, \hat{\tau}, \tilde{\psi}). \quad (4.18)$$

Now, the m -electron Green's function is defined by

$$G_m(\hat{r}^{(\beta)}, s^{(\beta)}, \hat{\theta}) := \frac{R_m(\hat{r}^{(\beta)}, s^{(\beta)}, \hat{\theta})}{R_0}. \quad (4.19)$$

CHAPTER 5

MONTE CARLO EVALUATION OF EHM

In this chapter, we will discuss the Monte Carlo evaluation of the extended Hubbard model defined in Chapter 4. We first discuss the Monte Carlo simulation of EHM in §4.1. Then, we discuss the Metropolis Markov Chain Monte Carlo method in §5.2 and MC move types in §5.3.

5.1 MONTE CARLO SIMULATION OF EHM

Let $n, N \in \mathbb{N}$ with $0 \leq n \leq N$, $\tilde{\alpha} = (\alpha_1, \dots, \alpha_n) \in \mathcal{E}^{2n}$ and $\hat{\alpha} = \tilde{\alpha} \oplus \tilde{\alpha} \in \mathcal{E}^{4n}$. Let $\tilde{\tau}, \hat{\tau}, \tilde{\psi}, \hat{\beta}$ and $\hat{\theta}$ be as in §4.5. Then we define the *domain* to be the set of all tuples $(n, \tilde{\alpha}, \tilde{\tau}, \tilde{\psi})$:

$$\mathcal{D} := \{X \mid X = (n, \tilde{\alpha}, \tilde{\tau}, \tilde{\psi})\}.$$

For short, we will write \int_X for

$$\sum_{n=0}^N \sum_{\tilde{\alpha} \in \mathcal{E}^{2n}} \int_{[0, \beta_T]^N} d^N(\tilde{\tau} \oplus \tilde{\psi}).$$

5.1.1 SCORE, WEIGHT AND PROBABILITY FUNCTIONS FOR EHM

The *weight* function W on \mathcal{D} for EHM is defined by

$$W(X) := |F_0(X)| \tag{5.1}$$

and the *score* function S_m is defined by

$$S_m(\hat{\beta}, \hat{\theta}, X) := \frac{F_m(\hat{\beta}, \hat{\theta}, X)}{W(X)}. \tag{5.2}$$

Let

$$P(X) := \frac{1}{\int_X W(X)} W(X). \quad (5.3)$$

Then we have

$$\int_X P(X) = 1$$

and

$$P(X) \geq 0, \quad \forall X \in \mathcal{D}.$$

Hence, P is a probability distribution on \mathcal{D} .

5.1.2 MONTE CARLO EVALUATION OF G_m

For any function $A = A(X)$ on \mathcal{D} , the *average of A for the probability distribution P* is defined by

$$\langle A(\bullet) \rangle_P := \int_X A(X) P(X). \quad (5.4)$$

Then the function G_m can be rewritten as

$$G_m(\hat{\beta}, \hat{\theta}) = \lim_{N \rightarrow \infty} \frac{\langle S_m(\hat{\beta}, \hat{\theta}, \bullet) \rangle_P}{\langle S_0(\bullet) \rangle_P} \quad (5.5)$$

To evaluate $\langle A(\bullet) \rangle_P$, we generate a random sample of K points

$$X^{(1)}, \dots, X^{(K)}, \quad X^{(j)} \in \mathcal{D}$$

that is distributed according to $P(X)$. Let

$$\langle A(\bullet) \rangle^{(K)} := \frac{1}{K} \sum_{j=1}^K A(X^{(j)}). \quad (5.6)$$

Then, by the central limit theorem, we have

$$\lim_{K \rightarrow \infty} \langle A(\bullet) \rangle^{(K)} = \langle A(\bullet) \rangle_P. \quad (5.7)$$

5.1.3 EVALUATION OF $\det \hat{g}$

To evaluate the scores, we need to calculate the determinant of the $(2n + m) \times (2n + m)$ matrix

$$\hat{g} = \hat{g}_{\vec{r}^{(g)}, s^{(g)}, \hat{\tau}^{(g)}} = (g_{ij})_{1 \leq i, j \leq 2n+m},$$

where $\vec{r}^{(g)}, s^{(g)}, \hat{\tau}^{(g)}$ are as in §4.5, and

$$g_{ij} = g(\vec{r}_i, s_i | \vec{r}_j, s_j, \tau_i - \tau_j).$$

Let $I = \{i \mid s_i = 0.5, 1 \leq i \leq 2n + m\}$ and $J = \{j \mid s_j = -0.5, 1 \leq j \leq 2n + m\}$. Then $\{I, J\}$ is a partition of $\{1, \dots, 2n + m\}$ such that $g_{ij} = 0$ for all $i \in I$ and $j \in J$ by (4.13). Hence,

$$\det \hat{g} = \det \hat{g}_{II} \cdot \det \hat{g}_{JJ} \tag{5.8}$$

by (2.9). In particular, if $V_1 = 0$ and $m = 0$, $\det \hat{g} \neq 0$ implies that

$$\vec{r}_j = \vec{r}_{j+n}, s_j \neq s_{j+n}, 1 \leq j \leq n \tag{5.9}$$

by (4.2) and (4.13). It follows that $|I| = |J|$ and $\det \hat{g}_{II} = \det \hat{g}_{JJ}$, so we have

$$\det \hat{g} = (\det \hat{g}_{II})^2. \tag{5.10}$$

5.2 METROPOLIS MCMC METHOD

The Metropolis method is one of the most important MCMC (Markov Chain Monte Carlo) methods. It is used to generate a Markov chain by reject sampling.

Let $\{1, \dots, M\}$ be the set of available *move types*. We assign to each move type u a number $p_M(u) \geq 0$, such that

$$\sum_{u=1}^m p_M(u) = 1.$$

Then $p_M = \{p_M(1), \dots, p_M(M)\}$ defines a probability distribution on $\{1, \dots, M\}$.

Let $P(X) > 0$ ($\forall X \in \mathcal{D}$) be a probability distribution on \mathcal{D} ; we want to generate a Markov chain

$$X^{(1)}, \dots, X^{(K)}, K \in \mathbb{N}, X^{(j)} \in \mathcal{D}, 1 \leq j \leq K, \tag{5.11}$$

from $P(X)$.

5.2.1 METROPOLIS METHOD

Given $X \in \mathcal{D}$ with $W(X) > 0$, we generate X^\oplus from X (*i.e.*, do an *MC move*) as follows.

(1) Randomly select a move type $u \in \{1, \dots, M\}$ according to the probability distribution p_M .

(2) Randomly generate $X' \in \mathcal{D}$ with *proposed probability* $T_u^{(P)}(X \rightarrow X')$ according to the rule for move type u . X' is called the *proposal*.

(3) Accept X' as X^\oplus (*i.e.*, set $X^\oplus = X'$) with *acceptance probability* $T_u^{(A)}(X \rightarrow X')$ defined by

$$T_u^{(A)}(X \rightarrow X') := \min \left\{ 1, \frac{T_u^{(P)}(X' \rightarrow X)P(X')}{T_u^{(P)}(X \rightarrow X')P(X)} \right\}. \quad (5.12)$$

That is, generate a random variable $p \sim U[0, 1]$, where $U[0, 1]$ is the uniform distribution on $[0, 1]$. If $p \leq T_u^{(A)}(X \rightarrow X')$, then accept the proposal and set $X^\oplus = X'$. Otherwise, reject the proposal and set $X^\oplus = X$.

5.2.2 GENERATING THE CHAIN

Let $L, S \in \mathbb{N}$ with $L > 0, S > 0$. To generate the chain (5.11), we start with a randomly generated $Y^{(1-L)} \in \mathcal{D}$ with $W(Y^{(1-L)}) > 0$, then do MC moves $L + KS - 1$ times and obtain a chain of length $L + KS$:

$$Y^{(1-L)}, \dots, Y^{(0)}, Y^{(1)}, \dots, Y^{(KS)}.$$

Now, for $j = 1, \dots, K$ we set $X^{(j)} = Y^{(jS)}$ for the chain (5.11).

5.2.3 CONVERGENCE

Since the set $\{1, \dots, M\}$ of available move types is obviously *ergodic* (that is, they enable any configuration to be reached from any other with positive probability), and the *transition probabilities*

$$T_u(X \rightarrow X') := T_u^{(P)}(X \rightarrow X') \cdot T_u^{(A)}(X \rightarrow X')$$

obviously satisfy the *detailed balance relation* (DBR)

$$T_u(X \rightarrow X')P(X) = T_u(X' \rightarrow X)P(X'),$$

the points $X^{(j)}$ in the chain (5.11) will have probabilities distributed according to $P(X)$ as $L \rightarrow \infty$. Hence, these points can be used as MC samples for calculating $\langle A(\bullet) \rangle^{(K)}$.

5.3 MC MOVE TYPES FOR EHM

There are 7 available (MC) move types for EHM, and move type 6 contains two subtypes of equal probabilities. We will give the rules and acceptance probabilities for each move type.

Let

$$X = (n, (\vec{r}_1, s_1), \dots, (\vec{r}_{2n}, s_{2n}), \tau_1, \dots, \tau_n, \psi_1, \dots, \psi_{N-n}) \in \mathcal{D},$$

with

$$|\vec{r}_k - \vec{r}_{k+n}|_{\mathcal{L}} \leq R_c, \quad \forall k \in \{1, \dots, n\},$$

so that $V_c(\vec{r}_k - \vec{r}_{k+n}) \neq 0$ and $P(X) \neq 0$.

For each $\vec{r} \in \mathcal{L}$, we define the *interaction sphere* by

$$C_{\mathcal{L}}(\vec{r}) := \{\vec{r}' \in \mathcal{L} \mid |\vec{r}' - \vec{r}|_{\mathcal{L}} \leq R_c\}.$$

Hereafter, we assume that the value of R_c is chosen so that $C_{\mathcal{L}}(\vec{r})$ contains 1 or 5 elements.

For each move type u , we define

$$R_u^{(P)}(X \rightarrow X') := \frac{T_u^{(P)}(X' \rightarrow X)}{T_u^{(P)}(X \rightarrow X')}.$$

5.3.1 MOVE TYPE 1: MOVE A PAIR OF V-LINES.

Randomly select $k_0 \in \{1, \dots, n\}$ and $\vec{r}_0 \in \mathcal{L}$. Then propose $X \rightarrow X'$ with

$$\vec{r}_{k_0} \rightarrow \vec{r}'_{k_0} = \vec{r}_{k_0} \oplus \vec{r}_0$$

and

$$\vec{r}_{k_0+n} \rightarrow \vec{r}'_{k_0+n} = \vec{r}_{k_0+n} \oplus \vec{r}_0.$$

It is clear that

$$T_1^{(P)}(X' \rightarrow X) = T_1^{(P)}(X \rightarrow X').$$

Hence we have $R_1^{(P)}(X \rightarrow X') = 1$ and

$$T_1^{(A)}(X \rightarrow X') = \min \left(1, \frac{W(X')}{W(X)} \right). \quad (5.13)$$

5.3.2 MOVE TYPE 2: FLIP THE SPIN AT A VERTEX.

Randomly select $j_0 \in \{1, \dots, 2n\}$, and propose $X \rightarrow X'$ with

$$s_{j_0} \rightarrow s'_{j_0} = -s_{j_0}.$$

Similarly to move type 1, we have

$$T_2^{(A)}(X \rightarrow X') = \min \left(1, \frac{W(X')}{W(X)} \right). \quad (5.14)$$

Note that in the case of $V_1 = 0$, we must have $W(X') = 0$ by (5.9), and hence $X \rightarrow X'$ is always rejected.

5.3.3 MOVE TYPE 3: MOVE THE \vec{r} AT A VERTEX.

Randomly select $j_0 \in \{1, \dots, 2n\}$, and let

$$k_0 = \begin{cases} j_0 - n & \text{if } j_0 > n; \\ j_0 + n & \text{otherwise.} \end{cases}$$

Then, randomly select

$$\vec{r}_0 \in C_{\mathcal{Z}}(\vec{r}_{j_0})$$

with $\vec{r}_0 \neq \vec{r}_{k_0}$ and propose $X \rightarrow X'$ with

$$\vec{r}_{j_0} \rightarrow \vec{r}'_{j_0} = \vec{r}_0.$$

Similarly to move type 2, we have

$$T_3^{(A)}(X \rightarrow X') = \min \left(1, \frac{W(X')}{W(X)} \right), \quad (5.15)$$

and in the case of $V_1 = 0$, X' is always rejected.

5.3.4 MOVE TYPE 4: MOVE τ AT A V-LINE.

Randomly select $k_0 \in \{1, \dots, n\}$, and randomly generate a homogeneously distributed number $\delta \in [-\Delta_\tau, \Delta_\tau]$ with $0 \leq \Delta_\tau \leq \beta_T$. Let $\tau_0 = \tau_{k_0} + \delta$. Then, propose $X \rightarrow X'$ with

$$\tau_{k_0} \rightarrow \tau'_{k_0} = \begin{cases} \tau_0 & \text{if } \tau_0 \in [0, \beta_T]; \\ 2\beta_T - \tau_0 & \text{if } \tau_0 \in (\beta_T, 2\beta_T]; \\ -\tau_0 & \text{otherwise.} \end{cases}$$

Similarly to move type 1, we have

$$T_4^{(A)}(X \rightarrow X') = \min\left(1, \frac{W(X')}{W(X)}\right). \quad (5.16)$$

5.3.5 MOVE TYPE 5: UPDATE τ -PADDING VARIABLE ψ .

Randomly select $l_0 \in \{1, \dots, N - n\}$, and randomly generate $\psi_0 \in [0, \beta_T]$ according to $g_{l_0}(\psi)$ (see (3.7)). Then propose $X \rightarrow X'$ with

$$\psi_{l_0} \rightarrow \psi'_{l_0} = \psi_0.$$

It is readily seen that

$$T_5^{(P)}(X' \rightarrow X) = \frac{1}{N - n} g_{l_0}(\psi'_{l_0}).$$

Hence

$$R_5^{(P)}(X' \rightarrow X) = \frac{g_{l_0}(\psi_{l_0})}{g_{l_0}(\psi'_{l_0})}$$

and

$$T_5^{(A)}(X \rightarrow X') = 1. \quad (5.17)$$

That is, this move type has 100% acceptance probability.

5.3.6 MOVE TYPE 6: RAISE OR LOWER DIAGRAM ORDER.

Move type 6 has two subtype: move type 6^+ and 6^- . Once move type 6 is selected, we randomly choose 6^+ or 6^- with equal probabilities.

MOVE TYPE 6^+ : RAISE DIAGRAM ORDER

If $n = N$, we reject this move type and proceed to the next move.

Now, assume $n < N$. We randomly select $k_0 \in \{1, \dots, n+1\}$, $l_0 \in \{1 \dots N - n\}$, $\vec{r}_0 \in \mathcal{L}$, $\vec{r}_{-1} \in C_{\mathcal{L}}(\vec{r}_0)$ and $s_0, s_{-1} \in \mathcal{S}$. Then, we construct X' from X by inserting a new V-line $(k_0, k_0 + n)$ with τ -value

$$\tau'_{k_0} = \psi_{l_0},$$

and new vertex \mathcal{E} -coordinates

$$(\vec{r}'_{k_0}, s'_{k_0}) = (\vec{r}_0, s_0), (\vec{r}'_{k_0+n'}, s'_{k_0+n'}) = (\vec{r}_{-1}, s_{-1})$$

and deleting the old ψ_{l_0} from the list of $\tilde{\psi}$ -variables. That is, we propose $X \rightarrow X'$ with

$$n \rightarrow n' = n + 1$$

and

$$\dots \rightarrow (\tau'_k, \vec{r}'_k, s'_k, \vec{r}'_{k+n'}, s'_{k+n'}) = \begin{cases} (\tau_k, \vec{r}_k, s_k, \vec{r}_{k+n}, s_{k+n}) & \text{if } 1 \leq k < k_0; \\ (\psi_{l_0}, \vec{r}_0, s_0, \vec{r}_{-1}, s_{-1}) & \text{if } k = k_0; \\ (\tau_{k-1}, \vec{r}_{k-1}, s_{k-1}, \vec{r}_{k+n-1}, s_{k+n-1}) & \text{if } k_0 < k \leq n' \end{cases}$$

and

$$\dots \rightarrow \psi'_l = \begin{cases} \psi_l & \text{if } 1 \leq l < l_0; \\ \psi_{l+1} & \text{if } l_0 < l \leq N - n'. \end{cases}$$

MOVE TYPE 6^- : LOWER DIAGRAM ORDER

If $n = 0$, we reject this move type and proceed to the next move.

Now, assume $n > 0$. We randomly select $k_0 \in \{1, \dots, n\}$ and $l_0 \in \{1 \dots N - n + 1\}$. Then, we construct X' from X by deleting the old V-line $(k_0, k_0 + n)$ and insert τ_{k_0} as new ψ_{l_0} into the list of $\tilde{\psi}$ -variables. That is, we propose $X \rightarrow X'$ with

$$n \rightarrow n' = n - 1$$

and

$$\dots \rightarrow (\tau'_k, \vec{r}'_k, s'_k, \vec{r}'_{k+n'}, s'_{k+n'}) = \begin{cases} (\tau_k, \vec{r}_k, s_k, \vec{r}_{k+n}, s_{k+n}) & \text{if } 1 \leq k < k_0; \\ (\tau_{k+1}, \vec{r}_{k+1}, s_{k+1}, \vec{r}_{k+n+1}, s_{k+n+1}) & \text{if } k_0 \leq k \leq n' \end{cases}$$

and

$$\dots \rightarrow \psi'_l = \begin{cases} \psi_l & \text{if } 1 \leq l < l_0; \\ \tau_{k_0} & \text{if } l = l_0; \\ \psi_{l+1} & \text{if } l_0 < l \leq N - n'. \end{cases}$$

ACCEPTANCE PROBABILITY OF MOVE TYPE 6

Let $|\mathcal{L}| = L_x \times L_y$ be the size of the lattice \mathcal{L} , $|C_{\mathcal{L}}|$ the size of the interaction sphere, and

$$|C_{\mathcal{L}}| = \begin{cases} 2 & \text{if } V_1 = 0 \text{ or } |C_{\mathcal{L}}| = 1; \\ 4 & \text{otherwise.} \end{cases}$$

Now, let $u = 6^+$ and $X \rightarrow X'$ with $n' = n + 1$. Then we have

$$T_u^{(P)}(X \rightarrow X') = \frac{1}{2n'(N-n)|\mathcal{L}| \cdot |C_{\mathcal{L}}| \cdot |C_{\mathcal{L}}|}$$

and

$$T_u^{(P)}(X' \rightarrow X) = \frac{1}{2n'(N-n)}.$$

It follows that

$$R_u^{(P)}(X \rightarrow X') = |\mathcal{L}| \cdot |C_{\mathcal{L}}| \cdot |C_{\mathcal{L}}|$$

and

$$R_u^{(P)}(X' \rightarrow X) = \frac{1}{|\mathcal{L}| \cdot |C_{\mathcal{L}}| \cdot |C_{\mathcal{L}}|}.$$

Hence, we have

$$T_u^{(A)}(X \rightarrow X') = \min \left(1, |\mathcal{L}| \cdot |C_{\mathcal{L}}| \cdot |C_{\mathcal{L}}| \cdot \frac{W(X')}{W(X)} \right). \quad (5.18)$$

Analogously, for $u = 6^-$, we have

$$T_u^{(A)}(X \rightarrow X') = \min \left(1, \frac{1}{|\mathcal{L}| \cdot |C_{\mathcal{L}}| \cdot |C_{\mathcal{L}}|} \cdot \frac{W(X')}{W(X)} \right). \quad (5.19)$$

5.3.7 MOVE TYPE 7: EXCHANGE A PAIR OF SPINS.

If $n = 0$, we reject this move type and proceed to the next move.

Now, assume that $n > 0$. Then we randomly select $j_0 \in \{1, \dots, 2n\}$, and propose $X \rightarrow X'$ with

$$s_{j_0} \rightarrow s'_{j_0} = s_{j_0+n}.$$

and

$$s_{j_0+n} \rightarrow s'_{j_0+n} = s_{j_0}.$$

Similarly to move type 1, we have

$$T_7^{(A)}(X \rightarrow X') = \min \left(1, \frac{W(X')}{W(X)} \right). \quad (5.20)$$

Note that in the case of $n > 0$ and $V_1 = 0$, we must have $W(X) = W(X')$ by (5.9), and hence $X \rightarrow X'$ is always accepted.

CHAPTER 6

RESULTS

We performed Monte Carlo simulations of EHM for 1-electron systems over 12 parameter sets using the evaluation method detailed in Chapter 5. We will describe briefly the experiments in §6.1, and present and discuss the results in §6.2. Finally, we draw conclusions about our method in §6.3.

6.1 THE EXPERIMENTS

In this section, we will briefly describe our experiments and give the parameter sets used in the experiments.

6.1.1 THE PROGRAM

Our program is written in C and MPI, and run at the computer `rlcluster.rcc.uga.edu`.

For each parameter set, the program uses R processors. Each of the processors randomly generates an $X \in \mathcal{D}$ with a common initial seed $seed_0$ for the random number generator, and then randomly generates a Markov chain of length K starting with X and initial seed $seed_j = Seed_0 + 1000j$, where j is the ordinal of the processor. Then, we collect the scores of the R chains and compute the final scores (S_0 , S_1 and G_1) and their standard deviations in the major processor.

We use the algorithm GEP (see §2.2.1) and the formula (5.8) or (5.10) to calculate determinants. Note that the running time of *GEP* is $O(n^3)$, so the use of (5.8) or (5.10) gives rise to a speed-up factor of up to 8.

Let the function $g_l(\psi)$ in (3.6) be defined by

$$g_l(\psi) := T, \quad \forall \psi \in [0, \beta_T].$$

It is the simplest function that satisfies (3.7). Then, the padding function is just

$$Q_{N-n}(\tilde{\psi}) = T^{N-n}.$$

6.1.2 CONTINUOUS TIME SCHEME

Let the external vertex be (\hat{r}, \hat{s}) , where

$$\hat{r} = (\vec{r} | \vec{r}) \in \mathcal{L}^2, \quad \hat{s} = (s | \bar{s}) \in \mathcal{S}$$

with $s = \bar{s}$, and let $\hat{\theta} = (\tau, \bar{\tau}) \in [0, \beta_T]$. By (4.13) and (4.16), we need to compute score S_1 and G_1 for selected pairs of the form

$$(\Delta \vec{r} = \vec{r}' - \vec{r}, \Delta \tau = \tau - \bar{\tau}).$$

We use the *continuous time scheme* to select these pairs as follows. Let L_τ be a large integer.

Given integers

$$0 = a_1 < b_1 < a_2 < b_2 < a_3 < b_3 = L_\tau,$$

and c_1, c_2, c_3 , such that $(c_k - 1) | (b_k - a_k)$ for $k = 1, 2, 3$, let

$$J = \{ \pm(a_k + j_k d_k) \mid k = 1, 2, 3; d_k = \frac{b_k - a_k}{c_k - 1}, j_k = 0, \dots, c_k - 1 \}.$$

Then, the scores will be computed at each point in the set

$$\{ (\vec{r}, \Delta \tau = \frac{j}{L_\tau} \beta_T) \mid \vec{r} \in \mathcal{L}, j \in J \}.$$

In our experiments, we set $L_\tau = 4096$, and the values of a_k, b_k, c_k are given in Table 6.1.

Table 6.1: Parameters a_k, b_k, c_k

k	a_k	b_k	c_k
1	0	112	8
2	256	3840	15
3	3984	4096	8

6.1.3 THE PARAMETER SETS

Our experiments used 12 parameter sets. The values of most parameters are the same, except N , V_0 , μ and T .

The parameter sets and the values of the three variable parameters N , V_0 and T are given in Table 6.2. Note that we always have $\mu = 0.5V_0$, and the values of N were chosen so that the orders of diagrams in the Markov chains never exceed them.

Table 6.2: Parameter Sets

Set	N	V_0	T
1a	32	1.0	1.0
1b	32	1.0	0.5
1c	32	1.0	0.25
1d	48	1.0	0.125
2a	32	2.0	1.0
2b	32	2.0	0.5
2c	64	2.0	0.25
2d	80	2.0	0.125
1a	48	4.0	1.0
1b	56	4.0	0.5
1c	84	4.0	0.25
1d	128	4.0	0.125

The values of the common parameters are given in Table 6.3. Note that we set

$$p_M(2) = p_M(3) = 0$$

because that in the case $V_1=0$, an MC move of type 2 or 3 is always rejected.

Table 6.3: Common Parameters

R	32	L	2×10^7	$p_M(3)$	0.0
L_x	2	K	10^8	$p_M(4)$	0.15
L_y	2	S	4	$p_M(5)$	0.15
V_1	0	$ C_{\mathcal{L}} $	1	$p_M(6)$	0.3
t_1	1.0	$seed_0$	1011	$p_M(7)$	0.2
t_2	0.0	$p_M(1)$	0.2		
t_3	0.0	$p_M(2)$	0.0		

6.2 RESULTS

In this section, we present and discuss the results of our experiments.

6.2.1 ACCEPT RATIOS OF MC MOVES

By Table 6.3, MC move types 2 and 3 are not used in our experiments and the accept ratio for move type 5 is 1. The accept ratios for other move types are given in Table 6.4. Note that the accept ratio of move type 7 tends to 1 as V_0 and β_T increase, meaning that the number of diagrams of order 0 tends to 0 as V_0 and β_T increase.

6.2.2 RUNNING TIME

The running time T_r of the program is the system time for the major processor. It is obvious that $T_r \propto K$, and the experiments show that $T_r \propto \beta_T^{1+c_T}$ and $T_r \propto V_0^{1+c_V}$ approximately, (see Figure 6.1), where c_T and c_V are some constants. Hence, we have

$$T_r \propto KV_0^{1+c_V} \beta_T^{1+c_T}.$$

6.2.3 ORDER FREQUENCIES

The order frequencies are important in our simulations.

Table 6.4: Accept ratios

u	V_0	$\beta_T = 1$	$\beta_T = 2$	$\beta_T = 4$	$\beta_T = 8$
1	1	0.510	0.646	0.691	0.688
	2	0.595	0.635	0.627	0.611
	4	0.554	0.553	0.536	0.512
4	1	0.564	0.719	0.791	0.818
	2	0.728	0.765	0.760	0.751
	4	0.795	0.744	0.703	0.653
6	1	0.581	0.695	0.715	0.698
	2	0.657	0.669	0.652	0.631
	4	0.593	0.586	0.571	0.554
7	1.0	0.598	0.804	0.925	0.977
	2.0	0.809	0.933	0.981	0.998
	3.0	0.938	0.988	0.999	1.000

Given a Markov chain C of length K on \mathcal{D} , let n^+ be the number of even-order points in C and n^- be the number of odd-order points in C (n^+ and n^- will be used hereafter). Assume $V_1 = 0$; then for each $X \in C$, we have

$$F_0(X) \begin{cases} > 0 & \text{if } n \text{ is even;} \\ < 0 & \text{if } n \text{ is odd} \end{cases}$$

by (5.10) and (4.16). It follows that for the chain C

$$S_0 = \frac{n^+ - n^-}{K} \tag{6.1}$$

by (5.2) and (5.7).

Our experiments show that the maximal order n_{max} and the most frequent order n_h of points in the R Markov chains generated increase as β_T or V_0 increases (see Figure 6.2 and 6.3, respectively).

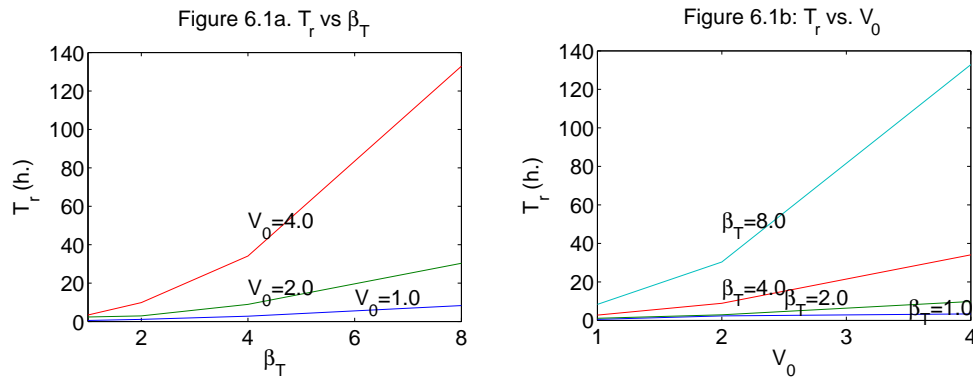


Figure 6.1: Running time

6.2.4 CONVERGENCE FOR PARAMETER SET 3b

Let $var(S_0)$ and $var(S_1)$ be the square of the standard deviations of S_0 and S_1 , respectively. The results for parameter set 3b (see Figure 6.4) show that as $K \rightarrow \infty$, S_0 becomes stable, and that $\frac{1}{var(S_1)}$ (at $\Delta\tau \in \{0.0078, 1.0, 1.9922\}$) and $\frac{1}{var(S_0)}$ increase quickly. This indicates that the simulation converged well. Note that the figure also shows that $\frac{1}{var(S_1)}$ increased significantly faster at $\Delta\tau = 1.0$ than at $\Delta\tau = 0.0078$ or $\Delta\tau = 1.9922$, indicating that S_1 converged faster in the middle than near the two ends of the interval $[0, \beta_T]$.

6.2.5 S_0 OR S_1 VS. β_T

Figure 6.5 shows the relation between $\lg(|S_1|)$ and β_T at $((0,0),0)$, and the relation between $\lg(|S_0|)$ and β_T . From the figure, we have

$$|S_0| = e^{c_0\beta_T}$$

and

$$|S_1| = e^{c_1\beta_T},$$

where c_0 and c_1 are nearly constant.

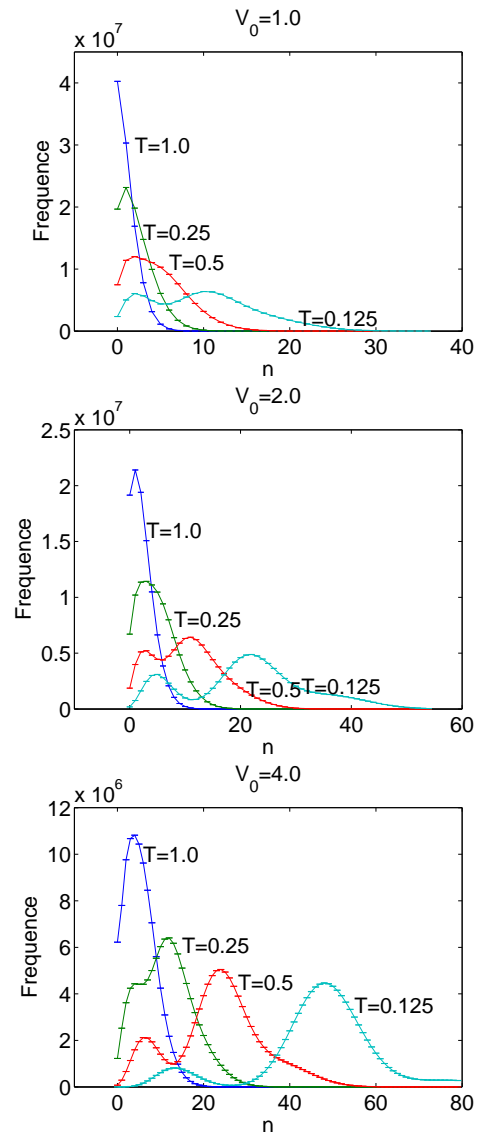
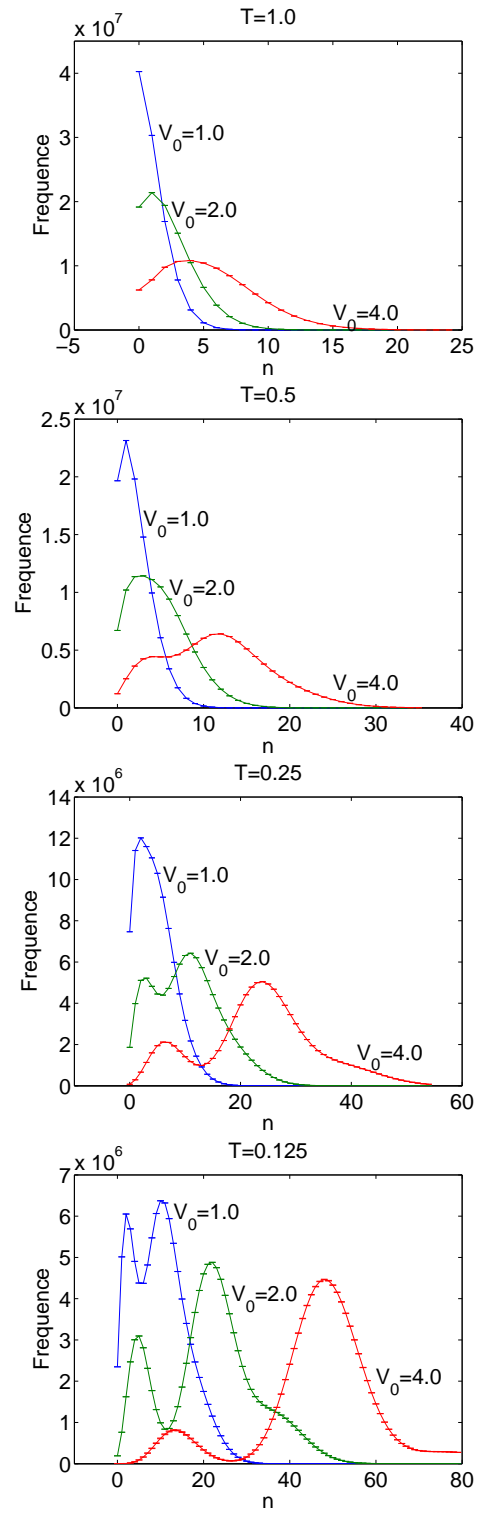


Figure 6.2: Order frequencies vs. β_T

Figure 6.3: Order frequencies vs. V_0

6.2.6 THE GREEN'S FUNCTION G_1

The 1–electron Green's functions for the 12 parameter sets are plotted in Figure 6.6 and Figure 6.7. In the figures, the anti-periodicity and jump discontinuity are easy seen. Note that the relative errors were large for parameter sets 2d, 3c and 3d, and we only plotted the three parameter sets for $\Delta\vec{r} = (0, 0)$.

The three parameter sets for which $V_0\beta_T \geq 16$ had large relative errors because for each of the 3 sets, n^+ and n^- are very close. Thus in the R chains for each of these sets, the number of chains with positive score S_0 and the number of chains with negative score S_0 were close. This leads to a small sum due to cancellations, while the variance accumulates resulting in large relative errors. To verify this, we plotted S_1^+ and S_1^- for parameter set 3d in Figure 6.8, where

$$S_1^+ = \frac{\sum(S_1(X))}{K},$$

the sum goes through all points of even order, and S_1^- is defined analogously. As expected, the error bars in Figure 6.8 were small, and $S_1^+ \approx S_1^-$.

6.3 CONCLUSION

From the results, we conclude that our new method works well over a large region of the parameter space. Our program can be used for any rectangular lattice, and can be used for m –electron systems with $m > 1$ with only slight modifications. However, it appears impractical when $V_0\beta_T \geq 16$.

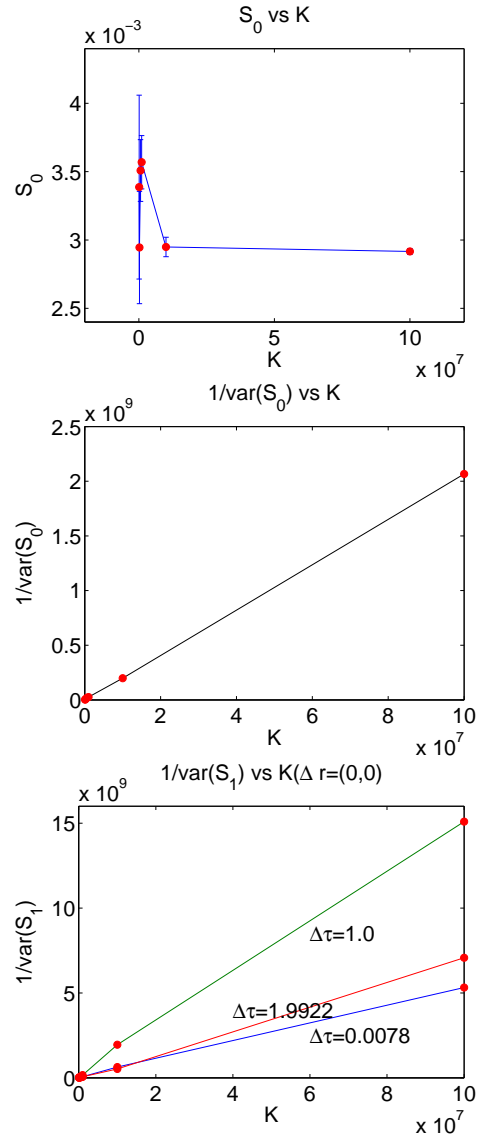
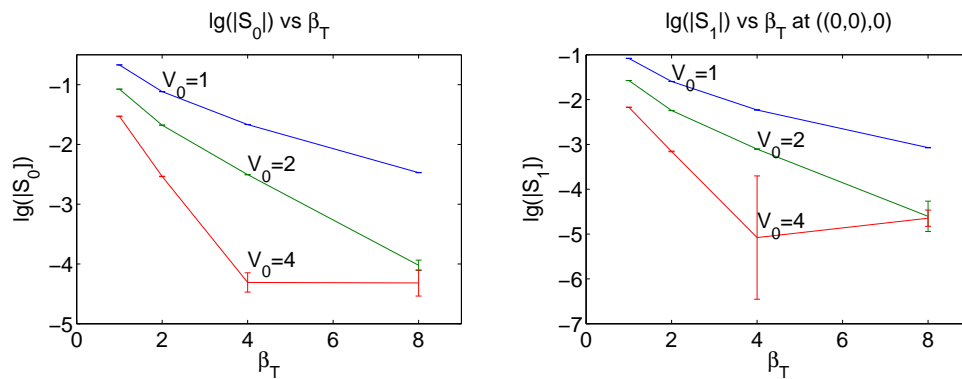


Figure 6.4: Convergence of parameter set 3b

Figure 6.5: $\lg(|S_1|)$ or $\lg(|S_0|)$ vs. β_T

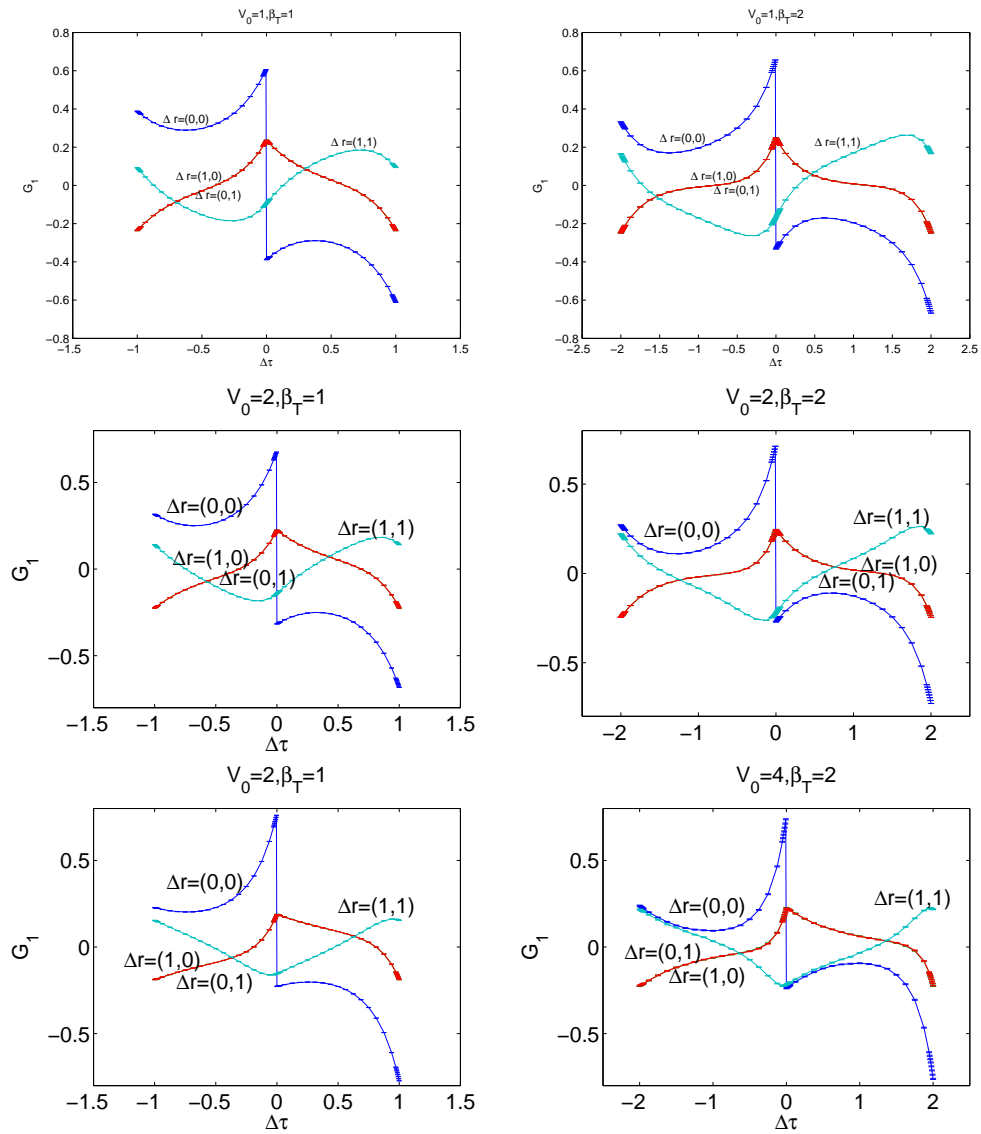


Figure 6.6: The Green's function G_1 ($\beta_T = 1, 2$)

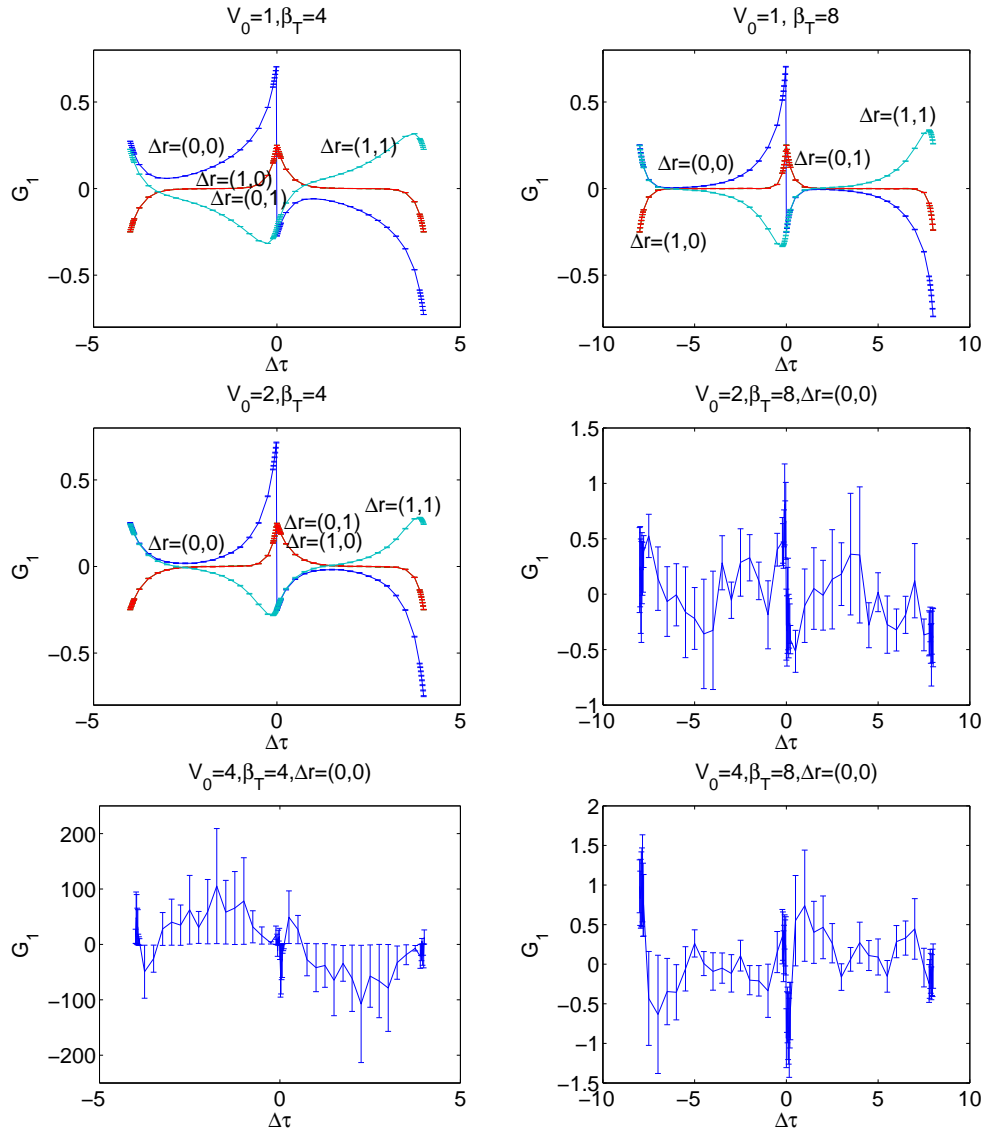


Figure 6.7: The Green's function G_1 ($\beta_T = 4, 8$)

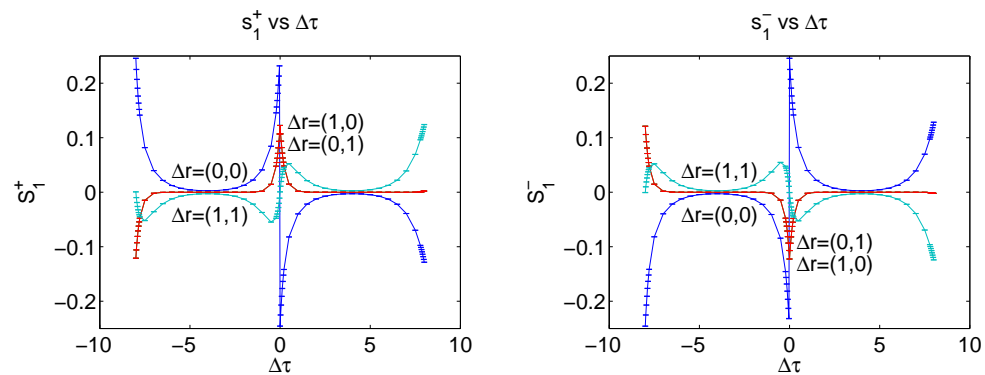


Figure 6.8: S_1^+ and S_1^- for $V_0 = 4, T = 8$

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