Series in Contemporary Applied Mathematics
CAM 12

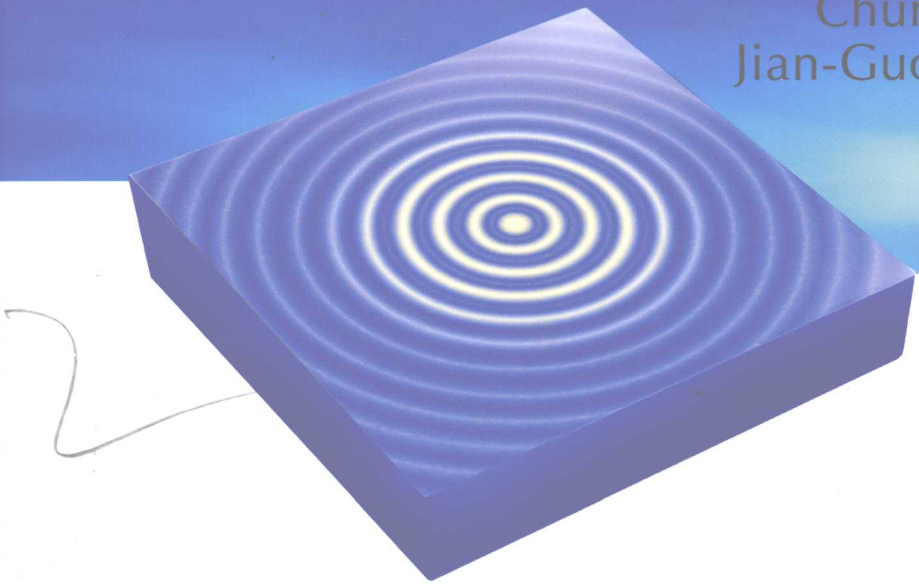
# Multi-Scale Phenomena in Complex Fluids

## Modeling, Analysis and Numerical Simulation

## 复杂流体中的多尺度问题

### 建模、分析与数值模拟

Thomas Y Hou
Chun Liu
Jian-Guo Liu
*editors*



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# Multi-Scale Phenomena in Complex Fluids

Modeling, Analysis and Numerical Simulation

# 复杂流体中的多尺度问题

建模、分析与数值模拟

# Preface

This volume is a collection of lecture notes generated from the first two series of mini-courses of "Shanghai Summer School on Analysis and Numerics in Modern Sciences" held during the summers of 2004 and 2006 at Fudan University, Shanghai, China. The summer school programs attracted more than 130 participants each year, including graduate students, postdoctors, and junior faculty members from more than 30 universities in China and USA.

The purpose of the summer school is to promote the interaction and collaboration of researchers with expertise in scientific modeling, mathematical analysis and numerical simulations. The focus of the year 2004's program was on the study of the multi-scale phenomena in complex fluids. The focus of the year 2006's program was on multi-scale analysis in nonlinear partial differential equations and their applications.

The summer school hosted several mini-courses each year. During the summer of 2004, the instructors are Weizhu Bao (National University of Singapore), Thomas Hou (California Institute of Technology, USA), Chun Liu (Penn State University, USA), Jianguo Liu (University of Maryland, USA), Tiehu Qin (Fudan University, PRC) and Qi Wang (Florida State University, USA). During the summer of 2006, the mini-courses were taught by Zhaojun Bai and Albert Fannjiang (University of California at Davis, USA), Thomas Hou, Wenbin Chen and Feng Qiu (Fudan University, PRC), Chun Liu, and Xiaoming Wang (Florida State University, USA). There are also short lectures given by many distinguished visitors from around the world.

There are five chapters in this volume, covering a wide range of topics in both analysis and numerical simulation methods, as well as their applications.

Chapter 1, by Zhaojun Bai, Wenbin Chen, Richard Scalettar and Ichitaro Yamazaki, is on the numerical methods for quantum Monte Carlo simulations of the Hubbard Models.

Chapter 2, by Albert Fannjiang, is on the wave propagation and imaging in random media.

Chapter 3, by Thomas Hou, is on multi-scale computations for flow and transport in porous media.

Chapter 4, by Chun Liu, is on the energetic variational approaches of elastic complex fluids.

Chapter 5, by Qi Wang, is on the kinetic theories of complex fluids.

We would like to express our gratitude to all the authors for their contributions to this volume, all the instructors for their contributions to the Shanghai Summer Schools in 2004 and 2006 and, in particular, thanks also go to all the participants in the Summer School programs. We want to thank Ms. Chunlian Zhou for her assistance, without which will be impossible for the success of the Summer School. The editors are grateful to Fudan University, the Mathematical Center of Ministry of Education of China, the National Natural Science Foundation of China (NSFC) and the Institut Sino-Francais de Mathematiques Appliquees (ISFMA) for their help and support. Finally, the editor wish to thank Tianfu Zhao (Senior Editor, Higher Education Press) for his patience and professional assistance.

Tomas Y. Hou, Chun Liu and Jianguo Liu

Editors

April 2008

# Contents

# Numerical Methods for Quantum Monte Carlo Simulations of the Hubbard Model*

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**Abstract**

One of the core problems in materials science is how the interactions between electrons in a solid give rise to properties like magnetism, superconductivity, and metal-insulator transitions. Our

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ability to solve this central question in quantum statistical mechanics numerically is presently limited to systems of a few hundred electrons. While simulations at this scale have taught us a considerable amount about certain classes of materials, they have very significant limitations, especially for recently discovered materials which have mesoscopic magnetic and charge order.

In this paper, we begin with an introduction to the Hubbard model and quantum Monte Carlo simulations. The Hubbard model is a simple and effective model that has successfully captured many of the qualitative features of materials, such as transition metal monoxides, and high temperature superconductors. Because of its voluminous contents, we are not be able to cover all topics in detail; instead we focus on explaining basic ideas, concepts and methodology of quantum Monte Carlo simulation and leave various part for further study. Parts of this paper are our recent work on numerical linear algebra methods for quantum Monte Carlo simulations.

# 1 Hubbard model and QMC simulations

The Hubbard model is a fundamental model to study one of the core problems in materials science: How do the interactions between electrons in a solid give rise to properties like magnetism, superconductivity, and metal-insulator transitions? In this lecture, we introduce the Hubbard model and outline quantum Monte Carlo (QMC) simulations to study many-electron systems. Subsequent lectures will describe computational kernels of the QMC simulations.

## 1.1 Hubbard model

The two-dimensional Hubbard model [8,9] we shall study is defined by the Hamiltonian:

$$\mathcal{H} = \mathcal{H}_K + \mathcal{H}_\mu + \mathcal{H}_V, \tag{1.1}$$

where $\mathcal{H}_K$, $\mathcal{H}_\mu$ and $\mathcal{H}_V$ stand for kinetic energy, chemical energy and potential energy, respectively, and are defined as

$$\begin{aligned}
\mathcal{H}_K &= -t \sum_{\langle i,j\rangle,\sigma} (c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma}), \\
\mathcal{H}_\mu &= -\mu \sum_i (n_{i\uparrow} + n_{i\downarrow}) \\
\mathcal{H}_V &= U \sum_i \left(n_{i\uparrow} - \frac{1}{2}\right)\left(n_{i\downarrow} - \frac{1}{2}\right)
\end{aligned}$$

and

- $i$ and $j$ label the spatial sites of the lattice. $\langle i,j\rangle$ represents a pair of nearest-neighbor sites in the lattice and indicates that the electrons only hopping to nearest neighboring sites,
- the operators $c_{i\sigma}^{\dagger}$ and $c_{i\sigma}$ are the fermion creation and annihilation operators for electrons located on the $i$th lattice site with $z$ component of spin-up ($\sigma=\uparrow$) or spin-down ($\sigma=\downarrow$), respectively,
- the operators $n_{i\sigma}=c_{i\sigma}^{\dagger}c_{i\sigma}$ are the number operators which count the number of electrons of spin $\sigma$ on site $i$,
- $t$ is the hopping parameter for the kinetic energy of the electrons, and is determined by the overlap of atomic wave functions on neighboring sites,
- $U$ is the repulsive Coulomb interaction between electrons on the same lattice site. The term $Un_{i\uparrow}n_{i\downarrow}$ represents an energy cost $U$ for the site $i$ has two electrons and describes a local repulsion between electrons,
- $\mu$ is the chemical potential parameter which controls the electron numbers (or density).

Note that we consider the case of a half-filled band. Hence the Hamiltonian is explicitly written in particle-hole symmetric form.

The expected value of a physical observable $\mathcal{O}$ of interest, such as density-density correlation, spin-spin correlation or magnetic susceptibility, is given by

$$\langle\mathcal{O}\rangle=\mathrm{Tr}(\mathcal{O}\mathcal{P}), \tag{1.2}$$

where $\mathcal{P}$ is a distribution operator defined as

$$\mathcal{P}=\frac{1}{\mathcal{Z}}e^{-\beta\mathcal{H}}, \tag{1.3}$$

and $\mathcal{Z}$ is the partition function defined as

$$\mathcal{Z}=\mathrm{Tr}(e^{-\beta\mathcal{H}}), \tag{1.4}$$

and $\beta$ is proportional to the inverse of the product of the Boltzmann's constant $k_B$ and the temperature $T$:

$$\beta=\frac{1}{k_BT}.$$

$\beta$ is referred to as an *inverse temperature*.

"Tr" is a trace over the Hilbert space describing all the possible occupation states of the lattice:

$$\mathrm{Tr}(e^{-\beta\mathcal{H}})=\sum_i\langle\psi_i|e^{-\beta\mathcal{H}}|\psi_i\rangle,$$

where $\{|\psi_i\rangle\}$ is an orthonormal basis of the Hilbert space. Note that the trace does not depend on the choice of the basis. A convenient choice of the basis is the so-called "occupation number basis (local basis)" as described below.

In a classical problem where $\mathcal{H} = E$ is the energy, a real variable, then $\exp(-\beta E)/Z$ is the probability, where $Z = \int e^{-\beta E}$. In quantum mechanics, as we shall see, we will need to recast the operator $\exp(-\beta\mathcal{H})$ into a real number. The "path integral representation" of the problem to do this was introduced by Feynman and Hibbs [3].

*Remark* 1.1. According to Pauli exclusion principle of electrons, there are four possible states at every site:

$|\cdot\rangle$ no particle,
$|\uparrow\rangle$ one spin up particle,
$|\downarrow\rangle$ one spin down particle,
$|\uparrow\downarrow\rangle$ two particles with different spin directions.

Therefore the dimension of the Hilbert space is $4^N$, where $N$ is the number of sites.

The actions of the spin creation operators $c_\sigma^\dagger$ on the four states are

| | $\|\cdot\rangle$ | $\|\uparrow\rangle$ | $\|\downarrow\rangle$ | $\|\uparrow\downarrow\rangle$ |
|---|---|---|---|---|
| $c_\uparrow^\dagger$ | $\|\uparrow\rangle$ | 0 | $\|\uparrow\downarrow\rangle$ | 0 |
| $c_\downarrow^\dagger$ | $\|\downarrow\rangle$ | $\|\uparrow\downarrow\rangle$ | 0 | 0 |

The actions of the spin annihilation operators $c_\sigma$ are

| | $\|\cdot\rangle$ | $\|\uparrow\rangle$ | $\|\downarrow\rangle$ | $\|\uparrow\downarrow\rangle$ |
|---|---|---|---|---|
| $c_\uparrow$ | 0 | $\|\cdot\rangle$ | 0 | $\|\downarrow\rangle$ |
| $c_\downarrow$ | 0 | 0 | $\|\cdot\rangle$ | $\|\uparrow\rangle$ |

*Remark* 1.2. The states $|\cdot\rangle$ and $|\uparrow\rangle$ are the eigen-states of the number operator $n_\uparrow = c_\uparrow^\dagger c_\uparrow$:

$$n_\uparrow|\cdot\rangle = 0|\cdot\rangle = 0, \quad n_\uparrow|\uparrow\rangle = |\uparrow\rangle.$$

When the operator $n_\uparrow$ takes the actions on the states $|\downarrow\rangle$ and $|\uparrow\downarrow\rangle$, we have

$$n_\uparrow|\downarrow\rangle = 0, \quad n_\uparrow|\uparrow\downarrow\rangle = |\uparrow\downarrow\rangle.$$

The states $|\cdot\rangle$ and $|\downarrow\rangle$ are the eigen-states of the number operator $n_\downarrow = c_\downarrow^\dagger c_\downarrow$:

$$n_\downarrow|\cdot\rangle = 0|\cdot\rangle = 0, \quad n_\downarrow|\downarrow\rangle = |\downarrow\rangle.$$

When the operator $n_\downarrow$ on the state $|\uparrow\rangle$ and $|\uparrow\downarrow\rangle$, we have

$$n_\downarrow|\uparrow\rangle = 0, \quad n_\downarrow|\uparrow\downarrow\rangle = |\uparrow\downarrow\rangle.$$

The operator $U(n_\uparrow - \frac{1}{2})(n_\downarrow - \frac{1}{2})$ describes the potential energy of two electrons with different spin directions at the same site:

$$U(n_\uparrow - \tfrac{1}{2})(n_\downarrow - \tfrac{1}{2}) \ : |\cdot\rangle = +\tfrac{U}{4}|\cdot\rangle, \quad |\uparrow\rangle = -\tfrac{U}{4}|\uparrow\rangle,$$
$$|\downarrow\rangle = -\tfrac{U}{4}|\downarrow\rangle, |\uparrow\downarrow\rangle = +\tfrac{U}{4}|\uparrow\downarrow\rangle.$$

These eigenenergies immediately illustrate a key aspect of the physics of the Hubbard model: The single occupied states $|\uparrow\rangle$ and $|\downarrow\rangle$ are lower in energy by $U$ (and hence more likely to occur). These states are the ones which have nonzero magnetic moment $m^2 = (n_\uparrow - n_\downarrow)^2$. One therefore says that the Hubbard interaction $U$ favors the presence of magnetic moments. As we shall see, a further question (when $t$ is nonzero) is whether these moments will order in special patterns from site to site.

*Remark* 1.3. The creation operators $c^\dagger_{i\sigma}$ and the annihilation operators $c_{i\sigma}$ anticommute:

$$\{c_{j\sigma}, c^\dagger_{\ell\sigma'}\} = \delta_{j\ell}\delta_{\sigma\sigma'},$$
$$\{c^\dagger_{j\sigma}, c^\dagger_{\ell\sigma'}\} = 0,$$
$$\{c_{j\sigma}, c_{\ell\sigma'}\} = 0,$$

where the anticommutator of two operators $a$ and $b$ is defined by $ab+ba$, i.e., $\{a, b\} = ab + ba$, and $\delta_{j\ell} = 1$ if $j = \ell$, and otherwise, $\delta_{j\ell} = 0$.

If we choose $\ell = j$ and $\sigma = \sigma'$ in the second anticommutation relation, we conclude that $(c^\dagger_{j\sigma})^2 = 0$. That is, one cannot create two electrons on the same site with the same spin (Pauli exclusion principle). Thus the anticommutation relations imply the Pauli principle. If the site or spin indices are different, the anticommutation relations tell us that exchanging the order of the creation (or destruction) of two electrons introduces a minus sign. In this way the anticommutation relations also guarantee that the wave function of the particles being described is *antisymmetric*, another attribute of electrons (fermions). Bosonic particles (which have *symmetric* wave functions) are described by creation and destruction operators which commute.

*Remark* 1.4. When the spin direction $\sigma$ and the site $i$ are omitted, a quantization to describe the states is

$$|0\rangle : \text{no particle},$$
$$|1\rangle : \text{one particle}.$$

The actions of the creation and destruction operators on the states are

$$\begin{aligned} c &: |0\rangle \to 0, \quad |1\rangle \to |0\rangle, \\ c^\dagger &: |0\rangle \to |1\rangle, |1\rangle \to 0. \end{aligned} \tag{1.5}$$

Subsequently, the eigen-states of the number operator $n = c^\dagger c$ are

$$n \ : \ |0\rangle = 0, \quad |1\rangle = |1\rangle.$$

In addition, the operator $c_i^\dagger c_{i+1}$ describes the kinetic energy of the electrons on nearest neighbor sites:

$$\begin{aligned} c_i^\dagger c_{i+1} : |00\rangle \to 0, |01\rangle \to |10\rangle, \\ |10\rangle \to 0, |11\rangle \to c_i^\dagger |10\rangle \to 0. \end{aligned}$$

Therefore, if there is one particle on the $(i+1)$th site, and no particle on the $i$th site, the operator $c_i^\dagger c_{i+1}$ annihilates the particle on the $(i+1)$th site and creates one particle on the $i$th site. We say that the electron hops from site $i+1$ to site $i$ after the action of the operator $c_i^\dagger c_{i+1}$.

### 1.1.1 Hubbard model with no hopping

Let us consider a special case of the Hubbard model, namely, there is only one site and no hopping, $t = 0$. Then the Hamiltonian $\mathcal{H}$ is

$$\mathcal{H} = U\left(n_\uparrow - \frac{1}{2}\right)\left(n_\downarrow - \frac{1}{2}\right) - \mu(n_\uparrow + n_\downarrow).$$

It can be verified that the orthonormal eigen-states $\psi_i$ of the operator $n_\sigma$ are the eigen-states of the Hamiltonian $\mathcal{H}$:

$$\begin{aligned} \mathcal{H} : |\cdot\rangle = \tfrac{U}{4}|\cdot\rangle, \qquad & |\uparrow\rangle = \left(\tfrac{U}{4} - (\mu + \tfrac{U}{2})\right)|\uparrow\rangle, \\ |\downarrow\rangle = \left(\tfrac{U}{4} - (\mu + \tfrac{U}{2})\right)|\downarrow\rangle, \ & |\uparrow\downarrow\rangle = \left(\tfrac{U}{4} - 2\mu\right)|\uparrow\downarrow\rangle. \end{aligned}$$

The Hamiltonian $\mathcal{H}$ is diagonalized under the basis $\{\psi_i\}$:

$$\mathcal{H} \longrightarrow \left(\langle\psi_i|\mathcal{H}|\psi_j\rangle\right) = \begin{bmatrix} \frac{U}{4} & & \\ & \frac{U}{4} - (\mu + \frac{U}{2}) & \\ & & \frac{U}{4} - (\mu + \frac{U}{2}) \\ & & & \frac{U}{4} - 2\mu \end{bmatrix}.$$

Consequently, the operator $e^{-\beta\mathcal{H}}$ is diagonalized:

$$e^{-\beta\mathcal{H}} \longrightarrow e^{-\frac{U\beta}{4}} \mathrm{diag}\left(1, e^{\beta(U/2+\mu)}, e^{\beta(U/2+\mu)}, e^{2\mu\beta}\right).$$

The partition function $\mathcal{Z}$ becomes

$$\mathcal{Z} = \mathrm{Tr}(e^{-\beta\mathcal{H}}) = \sum_i \langle\psi_i|e^{-\beta\mathcal{H}}|\psi_i\rangle \longrightarrow Z = e^{-\frac{U\beta}{4}}\left(1 + 2e^{\left(\frac{U}{2}+\mu\right)\beta} + e^{2\mu\beta}\right).$$

The operators $\mathcal{H}e^{-\beta\mathcal{H}}$, $n_\uparrow e^{-\beta\mathcal{H}}$, $n_\downarrow e^{-\beta\mathcal{H}}$ and $n_\uparrow n_\downarrow e^{-\beta\mathcal{H}}$ required for calculating physical observables $\mathcal{O}$ of interest become

$$\begin{aligned}
\mathcal{H}e^{-\beta\mathcal{H}} &\longrightarrow e^{-\frac{U\beta}{4}}\operatorname{diag}\left(\frac{U}{4}, \left(-\mu-\frac{U}{4}\right)e^{\beta(U/2+\mu)},\right.\\
&\qquad \left.\left(-\mu-\frac{U}{4}\right)e^{\beta(U/2+\mu)}, \left(\frac{U}{4}-2\mu\right)e^{2\mu\beta}\right),\\
n_\uparrow e^{-\beta\mathcal{H}} &\longrightarrow e^{-\frac{U\beta}{4}}\operatorname{diag}\left(0, e^{\beta(U/2+\mu)}, 0, e^{2\mu\beta}\right),\\
n_\downarrow e^{-\beta\mathcal{H}} &\longrightarrow e^{-\frac{U\beta}{4}}\operatorname{diag}\left(0, 0, e^{\beta(U/2+\mu)}, e^{2\mu\beta}\right),\\
n_\uparrow n_\downarrow e^{-\beta\mathcal{H}} &\longrightarrow e^{-\frac{U\beta}{4}}\operatorname{diag}\left(0, 0, 0, e^{2\mu\beta}\right).
\end{aligned}$$

The traces of these operators are

$$\begin{aligned}
\operatorname{Tr}(\mathcal{H}e^{-\beta\mathcal{H}}) &= e^{-\frac{U\beta}{4}}\left(\frac{U}{4}+2\left(-\mu-\frac{U}{4}\right)e^{\beta(U/2+\mu)}\right.\\
&\qquad \left.+\left(\frac{U}{4}-2\mu\right)e^{2\mu\beta}\right),\\
\operatorname{Tr}((n_\uparrow+n_\downarrow)e^{-\beta\mathcal{H}}) &= e^{-\frac{U\beta}{4}}\left(2e^{\beta(U/2+\mu)}+2e^{2\mu\beta}\right),\\
\operatorname{Tr}(n_\uparrow n_\downarrow e^{-\beta\mathcal{H}}) &= e^{-\frac{U\beta}{4}}e^{2\mu\beta}.
\end{aligned}$$

By definition (1.2), the following physical observables $\mathcal{O}$ can be computed exactly:

1. The one-site density $\rho = \langle n_\uparrow\rangle + \langle n_\downarrow\rangle$ to measure the average occupation of each site:

$$\begin{aligned}
\rho = \langle n_\uparrow\rangle + \langle n_\downarrow\rangle &= \frac{\operatorname{Tr}\left((n_\uparrow+n_\downarrow)e^{-\beta\mathcal{H}}\right)}{\operatorname{Tr}(\mathcal{Z})}\\
&= \frac{2e^{\left(\frac{U}{2}+\mu\right)\beta}+2e^{2\mu\beta}}{1+2e^{\left(\frac{U}{2}+\mu\right)\beta}+e^{2\mu\beta}}.
\end{aligned}$$

   When there is no chemical potential, i.e., $\mu = 0$, $\rho = 1$ for any $U$ and $\beta$, it is referred to as "half-filling" because the density is one-half the maximal possible value.

2. The one-site energy $E = \langle\mathcal{H}\rangle$:

$$\begin{aligned}
E = \langle\mathcal{H}\rangle &= \frac{\operatorname{Tr}(\mathcal{H}e^{-\beta\mathcal{H}})}{\operatorname{Tr}(\mathcal{Z})}\\
&= \frac{U}{4} - \frac{(2\mu+U)e^{\left(\frac{U}{2}+\mu\right)\beta}+2\mu e^{2\mu\beta}}{1+2e^{\left(\frac{U}{2}+\mu\right)\beta}+e^{2\mu\beta}}.
\end{aligned}$$

When there is no chemical potential, i.e., $\mu = 0$,

$$E = \frac{U}{4} - \frac{U}{2(1 + e^{-\frac{U\beta}{2}})}.$$

Figure 1.1 shows the plot of $E$ versus $U$ and $\beta$.

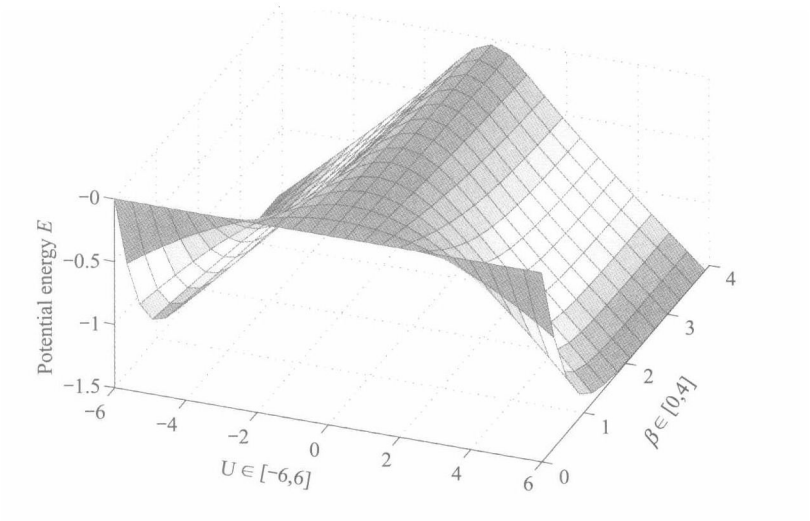


Figure 1.1. Potential energy $E$ for $t = 0, \mu = 0$.

3. The double occupancy $\langle n_\uparrow n_\downarrow \rangle$ is

$$\langle n_\uparrow n_\downarrow \rangle = \frac{\mathrm{Tr}(n_\uparrow n_\downarrow e^{-\beta\mathcal{H}})}{\mathrm{Tr}(\mathcal{Z})} = \frac{e^{2\mu\beta}}{1 + 2e^{(\frac{U}{2}+\mu)\beta} + e^{2\mu\beta}}.$$

When there is no chemical potential, i.e., $\mu = 0$,

$$\langle n_\uparrow n_\downarrow \rangle = \frac{1}{2(1 + e^{\frac{U}{2}\beta})}.$$

Note that as $U$ or $\beta$ increases, the double occupancy goes to zero.

### 1.1.2 Hubbard model without interaction

When there is no interaction, $U = 0$, the spin-up and spin-down spaces are independent. $\mathcal{H}$ breaks into the spin-up ($\uparrow$) and spin-down ($\downarrow$) terms. We can consider each spin space separately. Therefore, by omitting the spin, the Hamiltonian $\mathcal{H}$ becomes

$$\mathcal{H} = -t \sum_{\langle i,j \rangle} (c_i^\dagger c_j + c_j^\dagger c_i) - \mu \sum_i n_i.$$

It can be recast as a bilinear form:

$$\mathcal{H} = \boldsymbol{c}^\dagger(-tK - \mu I)\,\boldsymbol{c},$$

where

$$\boldsymbol{c} = \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \end{bmatrix} \quad \text{and} \quad \boldsymbol{c}^\dagger = [c_1^\dagger,\ c_2^\dagger,\ \cdots,\ c_N^\dagger],$$

and $I$ is the identity matrix, $K = (k_{ij})$ is a matrix to describe the hopping lattice geometry $\langle i, j\rangle$:

$$k_{ij} = \begin{cases} 1, \text{ if } i \text{ and } j \text{ are nearest neighbors,} \\ 0, \text{ otherwise.} \end{cases}$$

For instance, for a one-dimensional (1D) lattice of $N_x$ sites, $K$ is an $N_x \times N_x$ matrix given by

$$K = K_x = \begin{bmatrix} 0 & 1 & & & 1 \\ 1 & 0 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & 0 & 1 \\ 1 & & & 1 & 0 \end{bmatrix}.$$

The $(1, N_x)$ and $(N_x, 1)$ elements of $K$ incorporate the so-called "periodic boundary conditions (PBCs)" in which sites 1 and $N_x$ are connected by $t$. The use of PBC reduces finite size effects. For example, the energy on a finite lattice of length $N$ with open boundary conditions (OBCs) differs from the value in the thermodynamic limit ($N \to \infty$) by a correction of order $1/N$ while with PBCs, the correction is order $1/N^2$.[①] The use of PBCs also makes the system translationally invariant. The density of electrons per site, and other similar quantities, will not depend on the site in question. With OBCs quantities will vary with the distance from the edges of the lattice.

For a two-dimensional (2D) rectangle lattice of $N_x \times N_y$ sites, $K$ is an $N_xN_y \times N_xN_y$ matrix given by

$$K = K_{xy} = I_y \otimes K_x + K_y \otimes I_x,$$

where $I_x$ and $I_y$ are identity matrices with dimensions $N_x$ and $N_y$, respectively; $\otimes$ is the matrix Kronecker product.

[①] A simple analogy is this: Consider numerical integration of $f(x)$ on an interval $a \leqslant x \leqslant b$. The only difference between the rectangle and trapezoidal rules is in their treatment of the boundary point contributions $f(a)$ and $f(b)$, yet the integration error changes from linear in the mesh size to quadratic.