Hubbard Model

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1 The Hubbard model

The **Hubbard model** is a famous lattice model of strongly correlated electrons. In the following we denote the coordinates of the grid points by $\boldsymbol{i}, \boldsymbol{j}$, etc. as usual. The Hamiltonian without the chemical potential is

$$H = \underbrace{-t \sum_{\langle \boldsymbol{i},\boldsymbol{j}\rangle,\sigma} c^\dagger_{\boldsymbol{i}\sigma} c_{\boldsymbol{j}\sigma} + \text{h.c.}}_{H_0} + \underbrace{U \sum_{\boldsymbol{i}} n_{\boldsymbol{i}\uparrow} n_{\boldsymbol{i}\downarrow}}_{H_\text{I}}. \tag{1}$$

Or, redefining the chemical potential for Monte Carlo simulations later, we also have

$$H = -t \sum_{\langle \boldsymbol{i},\boldsymbol{j}\rangle,\sigma} c^\dagger_{\boldsymbol{i}\sigma} c_{\boldsymbol{j}\sigma} + \text{h.c.} + U \sum_{\boldsymbol{i}} \left(n_{\boldsymbol{i}\uparrow} - \frac{1}{2}\right)\left(n_{\boldsymbol{i}\downarrow} - \frac{1}{2}\right). \tag{2}$$

2 Hubbard model for quantum Monte Carlo simulation

2.1 Trotter decomposition and auxiliary field introduction

Now we perform a Trotter decomposition to the Hubbard model, and rewrite the partition function into a discrete path integral. Let the imaginary time interval be $\Delta\tau$, and there are m imaginary time points in total, $\tau = m\Delta\tau$. For the Hubbard model, there is a special decomposition of

$$\mathrm{e}^{-\Delta\tau H_\text{I}} = \gamma \sum_{s_1,s_2,\ldots,s_N=\pm 1} \mathrm{e}^{\alpha \sum_{\boldsymbol{i}} s_{\boldsymbol{i}}(n_{\boldsymbol{i}\uparrow} - n_{\boldsymbol{i}\downarrow})}, \quad \gamma = \frac{1}{2^N}\mathrm{e}^{\Delta\tau U N/4}, \quad \cosh(\alpha) = \mathrm{e}^{\Delta\tau U/2}, \tag{3}$$

It can be seen that γ is a quantity unrelated to the auxiliary field $\{s_{\boldsymbol{i}}\}$ (as usual we note its timeline as $\mathbf{s}$ below), and considering that the constant factor of the partition function is irrelevant, omitting this factor, the partition function is

$$\begin{aligned} Z &= \operatorname{tr} \prod_{n=1}^{m} \sum_{\mathbf{s}_n} \mathrm{e}^{\alpha \sum_{\boldsymbol{i}} s_{\boldsymbol{i}}(n_{\boldsymbol{i}\uparrow} - n_{\boldsymbol{i}\downarrow})} \mathrm{e}^{\Delta\tau t \sum_{\langle \boldsymbol{i},\boldsymbol{j}\rangle,\sigma} c^\dagger_{\boldsymbol{i}\sigma} c_{\boldsymbol{j}\sigma} + \text{h.c.}} \\ &= \sum_{\mathbf{s}} \prod_{n=1}^{m} \mathrm{e}^{\alpha c^\dagger_\uparrow \operatorname{diag} \mathbf{s}_n c_\uparrow} \mathrm{e}^{-\alpha c^\dagger_\downarrow \operatorname{diag} \mathbf{s}_n c_\downarrow} \mathrm{e}^{-\Delta\tau c^\dagger_\uparrow \mathbf{T} c_\uparrow} \mathrm{e}^{-\Delta\tau c^\dagger_\downarrow \mathbf{T} c_\downarrow}, \end{aligned}$$

where we specify $\mathbf{T}$ as the coefficient matrix of the kinetic energy part H_0 in the single-particle manifold, i.e.

$$T_{\boldsymbol{ij}} = \begin{cases} -t, & \langle \boldsymbol{i}, \boldsymbol{j}\rangle, \\ 0, & \text{otherwise.} \end{cases} \tag{4}$$

Applying the formula

$$\operatorname{tr}(\mathrm{e}^{-\sum_{i,j} c^\dagger_i A_{ij} c_j} \mathrm{e}^{-\sum_{i,j} c^\dagger_i B_{ij} c_j} \cdots) = \det\bigl(1 + \mathrm{e}^{-\mathbf{A}} \mathrm{e}^{-\mathbf{B}} \cdots\bigr), \tag{5}$$

We integrate out the fermion degrees of freedom to obtain

$$Z = \sum_{\mathbf{s}} \det\left(1 + \prod_{n=1}^{m} \exp(\alpha \operatorname{diag} \mathbf{s}_n \oplus (-\mathbf{s}_n)) \exp\left(-\Delta\tau \begin{pmatrix} \mathbf{T} & \\ & \mathbf{T} \end{pmatrix}\right)\right).$$

Since the quantum number of electrons includes both position and spin, the operators involved in the partition function have to be represented by $2N \times 2N$ (in $2N$ dimensions, the first N

dimension corresponds to the spin-up state and the second N dimension corresponds to the spin-down state) matrices. However, the spin rotational invariance implies that the above matrices are block diagonal. In the end, we have

$$Z = \det\left(1 + \prod_{\sigma=\uparrow,\downarrow} \prod_{n=1}^{m} \mathbf{B}_{\mathbf{s}}^{\sigma}(\tau)\right), \tag{6}$$

where

$$\mathbf{B}_{\mathbf{s}}^{\uparrow}(\tau) = \mathrm{e}^{\alpha \operatorname{diag} \mathbf{s}_n} \mathrm{e}^{-\Delta\tau \mathbf{T}}, \quad \mathbf{B}_{\mathbf{s}}^{\downarrow}(\tau) = \mathrm{e}^{-\alpha \operatorname{diag} \mathbf{s}_n} \mathrm{e}^{-\Delta\tau \mathbf{T}}. \tag{7}$$

All $\mathbf{B}_\sigma$ are $N \times N$ matrices, not $2N \times 2N$ ones.