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A Generic Solution of Fermion Sign Problem

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Abstract

The fermion sign problem, the biggest obstacle in quantum Monte Carlo calculations, is completely solved in this paper. Here, we find a strategy, in which the contribution from those negative-weighted paths is thoroughly cancelled or replaced by some positive-weighted paths. The crucial point lies on the Feynman path integral formula proposed in our group, which allows us to deeply analyze the Boltzmann weight of each path. Through mathematical proof, we demonstrate that physical quantities can be exactly calculated within a specific wavefunction space, in which all paths have positive Boltzmann weight. With this finding, a new Monte Carlo method is proposed, in which the fermion sign problem is absent. As an example, the current method is applied to the two-dimensional Hubbard model, and the results do manifest the correctness.

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Introduction

In quantum Monte Carlo (QMC) simulations, the notorious fermion sign problem (SP) has become a formidable obstacle for nonperturbative studies of various many-fermion systems, ranging from chemistry,[1] cold atoms,[2] condensed matter[3, 4] to particle and high-energy physics.[5, 6] Regarding to the SP, the computational physics seems to be in a helpless theoretical situation.[7, 8] For many years, albeit great efforts, the SP can only be relieved[9-46] or circumvented for some specific systems,[47-66] a generic solution is still missing. It is certain that, a complete solution of the SP will greatly promote the development of computational physics and many-fermion systems.

The SP has its roots in the antisymmetric character of many-fermion wave functions (WFs). The anti-symmetry makes most QMC calculations have to face a sum of numerically closed data but with the opposite sign or Boltzmann weight (BW), which results in the sign of data totally overwhelming QMC calculations. Far worse, the SP has the complicated dependence on systems,[67-70] the choice of basis,[57, 71-73] as well as algorithms.[74, 75] A recent study even shows that, the SP in determinant QMC could be quantitatively linked to quantum critical behavior.[7] Now, scientists have to accept the fact that, the SP is nondeterministic polynomial hard (NP-hard problem), and a generic solution is almost impossible within the known computational methods.[76]

Although the partition function of a many-fermion system is a sum of paths with both positive and negative BW, it must be a positive number. This implies that those negative-weighted paths must be completely cancelled out or replaced by some positive-weighted paths. If one can find out how those paths with negative BW are cancelled, the SP may be completely solved. Of course, this is not easy, because each path in the WF space is highly nonlocal and mutually entangled.

In this paper, based on the recently proposed formula of the path integral in field theory,[77] we are able to identify how these negative-weighted paths can be replaced. According to this finding, we suggest a new QMC framework, in which the SP is completely solved. We test our method on the two-dimensional Hubbard model, and the obtained results are in excellent with the previous ones.

Mathematical Proof and Discussion

To illustrate the current method, we choose Hubbard model[78] as an example. This model has been systematically and deeply studied, which provides various computational data for comparing.[79-82] However, it should be stressed that our method can be straightforwardly extended to any model or Hamiltonian.

General Formula: The current work is based on the path integral formula recently proposed in our group.[77] Here, we first present a brief introduction to this formula. The key step in this formula is to combine each off-diagonal term in Hamiltonian and its Hermitian conjugate into pairs. These paired operators are Hermitian, which will be used in the further mathematic deduction. For the Hubbard model, the paired operators look like $h_{ij\sigma} = -t_{ij}\left(c_{i\sigma}^{\dagger}c_{j\sigma} + c_{j\sigma}^{\dagger}c_{i\sigma}\right)$, in which t_{ij} is the hopping amplitude. In term of paired off-diagonal operators, the Hubbard Hamiltonian can be rewritten as:

$$H = \sum_{i,j,\sigma} h_{ij\sigma} + U\sum_{i} n_{i\uparrow}\, n_{i\downarrow}, \quad (1)$$

where all symbols have its standard meaning. For convenience, the spin index (σ) is omitted in the following context, it will be included later on to prevent confusion.

In the occupation number representation, let $|ijK\rangle$ denote a many-fermion WF, in which the occupancy of i-th and j-th sites is explicitly given and the occupancy of rest sites is simply labeled by K. For the i-th and j-th sites, the occupation can be classified into four cases, which are labeled as $|i\bar{j}K\rangle, |\bar{i}jK\rangle, |ijK\rangle,$ and $|\bar{i}\bar{j}K\rangle$. Here, $\bar{i}(\bar{j})$ indicates no electron occupying the i-th (j-th) site, while i (j) indicates one electron occupying the i-th (j-th) site.

According to the previous work,[77] the non-zero matrix element of a local Boltzmann operator, $e^{-\tau h}$ ($h = h_{ij}$ or $Un_{i\uparrow}n_{i\downarrow}$, and τ being a real number), is only presented in following cases:

$$\langle i\bar{j}K|e^{-\tau h_{ij}}|\bar{i}jK'\rangle = \langle \bar{i}jK|e^{-\tau h_{ij}}|i\bar{j}K'\rangle = \frac{1}{2}\delta_{K,K'}(e^{\theta_{ij}\tau t_{ij}} - e^{-\theta_{ij}\tau t_{ij}}) \quad (2.1)$$

$$\langle i\bar{j}K|e^{-\tau h_{ij}}|i\bar{j}K'\rangle = \langle \bar{i}jK|e^{-\tau h_{ij}}|\bar{i}jK'\rangle = \frac{1}{2}\delta_{K,K'}(e^{\theta_{ij}\tau t_{ij}} + e^{-\theta_{ij}\tau t_{ij}}) \quad (2.2)$$

$$\langle ijK|e^{-\tau h_{ij}}|ijK'\rangle = \langle \bar{\imath}\bar{\jmath}K|e^{-\tau h_{ij}}|\bar{\imath}\bar{\jmath}K'\rangle = \delta_{K,K'} \qquad (2.3)$$

where θ_{ij} is the sign produced by particle exchange as h_{ij} acting on $|i\bar{\jmath}K\rangle$ or $|\bar{\imath}jK\rangle$. For the diagonal operator $e^{-\tau U n_{i\uparrow}n_{i\downarrow}}$, the only non-zero matrix element reads:

$$\langle i_\uparrow i_\downarrow K|e^{-\tau U n_{i\uparrow}n_{i\downarrow}}|i_\uparrow i_\downarrow K'\rangle = \delta_{K,K'}e^{-\tau U} \qquad (2.4)$$

The matrix element in Eq. 2.2-2.4 is the diagonal scattering, which value is independent on the sign of θ_{ij} and always positive. The matrix element in Eq. 2.1 can be positive or negative depending the sign of both θ_{ij} and t_{ij}. For $\theta_{ij} = 1\ (-1)$, Eq. 2.1 represents the off-diagonal scattering with the positive (negative) local sign. It is worth noting that, θ_{ij} is not the sign of the whole path. The sign of a path is determined by the number of occurrences of matrix element of Eq. 2.1 in the path (see Ref.[77] for details). In the following, we will call θ_{ij} as the *local sign*, and call the sign of a path as the *global sign*.

According to the standard path integral formula and Suzuki-Trotter decomposition,[83] the partition function of the Hubbard model is,

$$Z = Tre^{-\beta H} = Tr\prod_{ij} e^{-\tau h_{ij}} \prod_i e^{-\tau U n_{i\uparrow}n_{i\downarrow}} \cdots \prod_{ij} e^{-\tau h_{ij}} \prod_i e^{-\tau U n_{i\uparrow}n_{i\downarrow}} \qquad (3)$$

where the imaginary time or reciprocal temperature ($\beta = \frac{1}{k_B T}$) is divided into M time-slices with "time step" $\tau = \beta/M$. To calculate the partition function, a complete set of states are inserted between each local Boltzmann operator ($e^{-\tau h}$, $h = h_{ij}$ or $Un_{i\uparrow}n_{i\downarrow}$). If the matrix element for all $e^{-\tau h}$ in Eq.3 is non-zero, we call the corresponding WF sequence a **closed path** in WF spaces (or a **closed world line**). The partition function is denoted as $Z = \sum_\omega \rho(\omega)$, where $\rho(\omega)$ represents the BW of the closed path ω.

According to our strategy mentioned above, we try to divide the closed paths into two classes, ω_+ and ω_-. ω_+ contains these paths, in which not only the global sign is positive, but also all off-diagonal scatterings have the positive local sign, *i.e*, θ_{ij} equals to 1 in Eq. 2.1 (Hereafter **OP paths**). All rest paths belong to ω_- (Hereafter **ON paths**). An ON path either has a global negative sign or contains at least one negative off-diagonal scattering. Evidently, OP paths always have the global positive sign or positive weight, while ON paths may have the global positive or negative sign. Now the partition function can be written as,

$$Z=\sum_{\omega}\rho(\omega)=\sum_{\omega_+}\rho(\omega_+)+\sum_{\omega_-}\rho(\omega_-)=Z_++Z_-.$$

Obviously, if $\frac{Z_-}{Z_+}$ is a constant, the negative-weighted paths can be well cancelled or replaced, and the physical quantities can be exactly calculated within OP paths, accordingly the SP will be solved automatically. Our following proof is based on this idea.

Our proof starts from analyzing the contribution of $e^{-\tau h_{12}}$ in 1st time slice (1ST) to energies. For that, we further write $Z_+=Z_+^{(0)}+Z_+^{(1)}+Z_+^{(2)}$ and $Z_-=Z_-^{(0)}+Z_-^{(1)}+Z_-^{(2)}$. Here $Z_\pm^{(0)}$ only contains these paths, at which the matrix element of $e^{-\tau h_{12}}$ in 1ST takes Eq. 2.3. $Z_+^{(1)}$ and $Z_-^{(1)}$ only contain these paths, at which the matrix element of $e^{-\tau h_{12}}$ in 1ST appears as Eq. 2.2. $Z_+^{(2)}$ and $Z_-^{(2)}$ only contain these paths, at which the matrix element of $e^{-\tau h_{12}}$ in 1ST appears as Eq. 2.1. It is worth noting that, θ_{12} in 1ST could be +1 or -1 in $Z_+^{(1)}$, $Z_-^{(1)}$ and $Z_-^{(2)}$, but it can only take +1 in $Z_+^{(2)}$. Evidently, $Z_+^{(0,1,2)}$ is always non-negative, while $Z_-^{(0,1,2)}$ can be positive or negative.

It needs to point out that, $Z_\pm^{(0)}$, $Z_\pm^{(1)}$ and $Z_\pm^{(2)}$ are classified regarding to $e^{-\tau h_{12}}$ in 1TS, however this classification will change for other $e^{-\tau h_{ij}}$ at other time slices. For example, a path in $Z_\pm^{(0)}$ defined according to $e^{-\tau h_{12}}$ in 1TS may become one in $Z_\pm^{(1)}$ or $Z_\pm^{(2)}$ regarding to $e^{-\tau h_{ij}}$ at other time slices. However according to our definition of $Z_\pm$, paths in $Z_+^{(\alpha)}$ can only transfer into $Z_+^{(\alpha')}$, but not into $Z_-^{(\alpha'')}$; Similarly, paths in $Z_-^{(\alpha)}$ can only transfer into $Z_-^{(\alpha')}$, but not into $Z_+^{(\alpha'')}$. This point will be used in the following proof.

In order to avoid mathematical ambiguous in the following derivation, $e^{-\tau h_{12}}$ in 1TS is formally replaced by $e^{-\tilde{\tau} h_{12}}$, and taking $\tilde{\tau}=\tau$ at the final step. Evidently,

$$Z_+^{(0)} = \sum_K \Big[\langle \overline{12}K|e^{-\beta H'}|\overline{12}K\rangle\langle \overline{12}K|e^{-\tilde{\tau}h_{ij}}|\overline{12}K\rangle_+$$

$$+ \langle 12K|e^{-\beta H'}|12K\rangle\langle 12K|e^{-\tilde{\tau}h_{ij}}|12K\rangle_+\Big]$$

$$= \sum_K \Big[\langle \overline{12}K|e^{-\beta H'}|\overline{12}K\rangle_+ + \langle 12K|e^{-\beta H'}|12K\rangle_+\Big] \quad (4.1)$$

$$Z_-^{(0)} = \sum_K \Big[\langle \overline{12}K|e^{-\beta H'}|\overline{12}K\rangle\langle \overline{12}K|e^{-\tilde{\tau}h_{ij}}|\overline{12}K\rangle_-$$

$$+ \langle 12K|e^{-\beta H'}|12K\rangle\langle 12K|e^{-\tilde{\tau}h_{ij}}|12K\rangle_-\Big]$$

$$= \sum_K \Big[\langle \overline{12}K|e^{-\beta H'}|\overline{12}K\rangle_- + \langle 12K|e^{-\beta H'}|12K\rangle_-\Big] \quad (4.2)$$

$$Z_+^{(1)} = \sum_K \Big[\langle 1\overline{2}K|e^{-\beta H'}|1\overline{2}K\rangle\langle 1\overline{2}K|e^{-\tilde{\tau}h_{12}}|1\overline{2}K\rangle_+$$

$$+ \langle \overline{1}2K|e^{-\beta H'}|\overline{1}2K\rangle\langle \overline{1}2K|e^{-\tilde{\tau}h_{12}}|\overline{1}2K\rangle_+\Big]$$

$$= \sum_K \Big[\langle 1\overline{2}K|e^{-\beta H'}|1\overline{2}K\rangle_+ + \langle \overline{1}2K|e^{-\beta H'}|\overline{1}2K\rangle_+\Big]\frac{(e^{\tilde{\tau}\theta_{12}t_{12}}+e^{-\tilde{\tau}\theta_{12}t_{12}})}{2} \quad (4.3)$$

$$Z_-^{(1)} = \sum_K \Big[\langle 1\overline{2}K|e^{-\beta H'}|1\overline{2}K\rangle\langle 1\overline{2}K|e^{-\tilde{\tau}h_{12}}|1\overline{2}K\rangle_-$$

$$+ \langle \overline{1}2K|e^{-\beta H'}|\overline{1}2K\rangle\langle \overline{1}2K|e^{-\tilde{\tau}h_{12}}|\overline{1}2K\rangle_-\Big]$$

$$= \sum_K \Big[\langle 1\overline{2}K|e^{-\beta H'}|1\overline{2}K\rangle_- + \langle \overline{1}2K|e^{-\beta H'}|\overline{1}2K\rangle_-\Big]\frac{(e^{\tilde{\tau}\theta_{12}t_{12}}+e^{-\tilde{\tau}\theta_{12}t_{12}})}{2} \quad (4.4)$$

$$Z_+^{(2)} = \sum_K \Big[\langle \overline{1}2K|e^{-\beta H'}|1\overline{2}K\rangle\langle 1\overline{2}K|e^{-\tilde{\tau}h_{12}}|\overline{1}2K\rangle_+$$

$$+ \langle 1\overline{2}K|e^{-\beta H'}|\overline{1}2K\rangle\langle \overline{1}2K|e^{-\tilde{\tau}h_{12}}|1\overline{2}K\rangle_+\Big]$$

$$= \sum_K \Big[\langle \overline{1}2K|e^{-\beta H'}|1\overline{2}K\rangle_+ + \langle 1\overline{2}K|e^{-\beta H'}|\overline{1}2K\rangle_+\Big]\frac{(e^{\tilde{\tau}t_{12}} - e^{-\tilde{\tau}t_{12}})}{2} \quad (4.5)$$

$$Z_-^{(2)} = \sum_K \Big[\langle \overline{1}2K|e^{-\beta H'}|1\overline{2}K\rangle\langle 1\overline{2}K|e^{-\tilde{\tau}h_{12}}|\overline{1}2K\rangle_-$$

$$+ \langle 1\overline{2}K|e^{-\beta H'}|\overline{1}2K\rangle\langle \overline{1}2K|e^{-\tilde{\tau}h_{12}}|1\overline{2}K\rangle_-\Big]$$

$$= \sum_K \left[\langle \bar{1}2K|e^{-\beta H'}|1\bar{2}K\rangle_- + \langle 1\bar{2}K|e^{-\beta H'}|\bar{1}2K\rangle_-\right] \frac{(e^{\tilde{\tau}\theta_{12}t_{12}} - e^{-\tilde{\tau}\theta_{12}t_{12}})}{2} \quad (4.6)$$

with $H' = H - \frac{\tilde{\tau}}{\beta} h_{12}$. The subscription $+$ and $-$ in above equations refer **OP** and **ON** paths, respectively. In the process of above deduction (Eq. 4.1-4.6), Eq. 2.1-2.3 are used.

Considering $y_{\pm} = R\left(e^{\tilde{\tau}\theta t} \pm e^{-\tilde{\tau}\theta t}\right)$, where θ could be +1 or -1, and R is independent on $\tilde{\tau}$. It is easily to prove,

$$-\frac{1}{y_{\pm}}\frac{\partial y_{\pm}}{\partial \tilde{\tau}} = -\theta t \frac{e^{\tilde{\tau}\theta t} \mp e^{-\tilde{\tau}\theta t}}{e^{\tilde{\tau}\theta t} \pm e^{-\tilde{\tau}\theta t}} = -t\frac{(e^{\tilde{\tau}t} \mp e^{-\tilde{\tau}t})}{(e^{\tilde{\tau}t} \pm e^{-\tilde{\tau}t})} \quad (5)$$

Using this equation, the contribution of $e^{-\tilde{\tau}h_{12}}$ in 1TS to energies reads,

$$\varepsilon_{12} = -\frac{1}{M}\frac{1}{Z}\frac{\partial Z}{\partial \tilde{\tau}}$$

$$= -\frac{t_{12}}{M} \frac{(Z_+^{(1)} + Z_-^{(1)}) \frac{e^{\tilde{\tau}t_{12}} - e^{-\tilde{\tau}t_{12}}}{e^{\tilde{\tau}t_{12}} + e^{-\tilde{\tau}t_{12}}} + (Z_+^{(2)} + Z_-^{(2)}) \frac{e^{\tilde{\tau}t_{12}} + e^{-\tilde{\tau}t_{12}}}{e^{\tilde{\tau}t_{12}} - e^{-\tilde{\tau}t_{12}}}}{Z_+^{(0)} + Z_+^{(1)} + Z_+^{(2)} + Z_-^{(0)} + Z_-^{(1)} + Z_-^{(2)}} \quad (6)$$

Proof of $\frac{Z_-^{(1)}}{Z_+^{(1)}} = \frac{Z_-^{(2)}}{Z_+^{(2)}}$: Consider a quantity $\bar{A}$, which is defined as, $\bar{A} = \frac{\partial Z_+^{(1)}}{\partial \tilde{\tau}}$. Now we formally write $Z_+^{(1)}$ as $Tr_+^{(1)} e^{-\beta H'} e^{-\tilde{\tau}h_{12}}$, where $Tr_+^{(1)}$ refers the trace evaluated over paths in OP paths. If we take the derivation first then evaluating the trace, $\bar{A}$ can be calculated as,

$$\bar{A} = \frac{\partial Z_+^{(1)}}{\partial \tilde{\tau}} = \sum_K \left[\langle 1\bar{2}K|e^{-\beta H'}|1\bar{2}K\rangle_+ + \langle \bar{1}2K|e^{-\beta H'}|\bar{1}2K\rangle_+\right] \frac{\partial(e^{\tilde{\tau}\theta_{12}t_{12}} + e^{-\tilde{\tau}\theta_{12}t_{12}})}{2\partial\tilde{\tau}}$$

$$= \theta_{12}t_{12} \sum_K \left[\langle 1\bar{2}K|e^{-\beta H'}|1\bar{2}K\rangle_+ + \langle \bar{1}2K|e^{-\beta H'}|\bar{1}2K\rangle_+\right] \frac{(e^{\tilde{\tau}\theta_{12}t_{12}} - e^{-\tilde{\tau}\theta_{12}t_{12}})}{2}$$

$$= \theta_{12}t_{12} \sum_K \left[\langle 1\bar{2}K|e^{-\beta H'}|1\bar{2}K\rangle_+ \right.$$

$$\left. + \langle \bar{1}2K|e^{-\beta H'}|\bar{1}2K\rangle_+\right] \frac{(e^{\tilde{\tau}\theta_{12}t_{12}} + e^{-\tilde{\tau}\theta_{12}t_{12}})}{2} \frac{(e^{\tilde{\tau}\theta_{12}t_{12}} - e^{-\tilde{\tau}\theta_{12}t_{12}})}{(e^{\tilde{\tau}\theta_{12}t_{12}} + e^{-\tilde{\tau}\theta_{12}t_{12}})}$$

$$= t_{12} Z_+^{(1)} \frac{(e^{\tilde{\tau}t_{12}} - e^{-\tilde{\tau}t_{12}})}{(e^{\tilde{\tau}t_{12}} + e^{-\tilde{\tau}t_{12}})} \quad (7a)$$

Alternatively, we can take the derivation first then evaluating the trace, $\bar{A}$ becomes

$$\bar{A} = \frac{\partial Z_+^{(1)}}{\partial \tilde{\tau}} = \sum_K \Big[\langle 1\bar{2}K|e^{-\beta H'}h_{12}|1\bar{2}K\rangle_+ + \langle \bar{1}2K|e^{-\beta H'}h_{12}|\bar{1}2K\rangle_+\Big]\frac{(e^{\tilde{\tau}\theta_{12}t_{12}}+e^{-\tilde{\tau}\theta_{12}t_{12}})}{2}$$

$$= \theta_{12}t_{12}\sum_K \Big[\langle 1\bar{2}K|e^{-\beta H'}|\bar{1}2K\rangle_+ + \langle \bar{1}2K|e^{-\beta H'}|1\bar{2}K\rangle_+\Big]\frac{(e^{\tilde{\tau}\theta_{12}t_{12}}+e^{-\tilde{\tau}\theta_{12}t_{12}})}{2}$$

$$= \theta_{12}t_{12}\sum_K \Big[\langle 1\bar{2}K|e^{-\beta H'}|\bar{1}2K\rangle_+ + \langle \bar{1}2K|e^{-\beta H'}|1\bar{2}K\rangle_+\Big]\frac{(e^{\tilde{\tau}\theta_{12}t_{12}}-e^{-\tilde{\tau}\theta_{12}t_{12}})}{2}\frac{(e^{\tilde{\tau}\theta_{12}t_{12}}+e^{-\tilde{\tau}\theta_{12}t_{12}})}{(e^{\tilde{\tau}\theta_{12}t_{12}}-e^{-\tilde{\tau}\theta_{12}t_{12}})}$$

$$= t_{12}Z_+^{(2)}\frac{(e^{\tilde{\tau}t_{12}}+e^{-\tilde{\tau}t_{12}})}{(e^{\tilde{\tau}t_{12}}-e^{-\tilde{\tau}t_{12}})} \qquad (7b)$$

In deriving Eq. 7b, if $\theta_{12} = -1$ occurs at IST in a path ($\omega \in Z_+^{(1)}$), the above deduction will result in a new path belonging to $Z_-^{(2)}$. To avoid this situation, we can search the value of θ_{12} along this path ($\omega \in Z_+^{(1)}$) until $\theta_{12} = 1$ at a certain time slice. Then we can perform the above deduction at the new time slice, Eq.7b is still hold. In principle, the number of time slices M can be taken as any large number, this condition ($\theta_{12} = 1$ at a certain time slice) can always be met. Because $\bar{A}$ calculated by above two methods should be identical, combining Eq. 7a and 7b, we arrive,

$$\frac{Z_+^{(1)}}{Z_+^{(2)}} = \frac{(e^{\tilde{\tau}t_{12}}+e^{-\tilde{\tau}t_{12}})^2}{(e^{\tilde{\tau}t_{12}}-e^{-\tilde{\tau}t_{12}})^2} \qquad (8)$$

Using the similar procedure above, we can obtain,

$$\frac{Z_-^{(1)}}{Z_-^{(2)}} = \frac{(e^{\tilde{\tau}t_{12}}+e^{-\tilde{\tau}t_{12}})^2}{(e^{\tilde{\tau}t_{12}}-e^{-\tilde{\tau}t_{12}})^2} \qquad (9)$$

Combining Eq. 8 and 9, we have $\frac{Z_+^{(2)}}{Z_+^{(1)}} = \frac{Z_-^{(2)}}{Z_-^{(1)}}$. By reforming this equation, we obtain,

$$\frac{Z_-^{(1)}}{Z_+^{(1)}} = \frac{Z_-^{(2)}}{Z_+^{(2)}} = \gamma \qquad (10)$$

where γ is defined.

Proof of $\frac{Z_-^{(0)}}{Z_+^{(0)}} = \frac{Z_-^{(1)}}{Z_+^{(1)}} = \frac{Z_-^{(2)}}{Z_+^{(2)}}$: In the subset path space of $Z^{(1+2)} = Z_+^{(1)} + Z_+^{(2)} + Z_-^{(1)} + Z_-^{(2)}$, the expectation value of h_{12} at 1TS can be calculated according to the thermodynamic estimator of energies,

$$\langle h_{12} \rangle_{Z^{(1+2)}} = -\frac{1}{M}\frac{1}{Z^{(1+2)}}\frac{\partial Z^{(1+2)}}{\partial \tilde{\tau}}$$

$$= -\frac{t_{12}}{M}\frac{(Z_+^{(1)} + Z_-^{(1)})\frac{e^{\tilde{\tau}t_{12}} - e^{-\tilde{\tau}t_{12}}}{e^{\tilde{\tau}t_{12}} + e^{-\tilde{\tau}t_{12}}} + (Z_+^{(2)} + Z_-^{(2)})\frac{e^{\tilde{\tau}t_{12}} + e^{-\tilde{\tau}t_{12}}}{e^{\tilde{\tau}t_{12}} - e^{-\tilde{\tau}t_{12}}}}{Z_+^{(1)} + Z_+^{(2)} + Z_-^{(1)} + Z_-^{(2)}}$$

$$= -\frac{t_{12}}{M}\frac{Z_+^{(1)}(1+\gamma)\frac{e^{\tilde{\tau}t_{12}} - e^{-\tilde{\tau}t_{12}}}{e^{\tilde{\tau}t_{12}} + e^{-\tilde{\tau}t_{12}}} + Z_+^{(2)}(1+\gamma)\frac{e^{\tilde{\tau}t_{12}} + e^{-\tilde{\tau}t_{12}}}{e^{\tilde{\tau}t_{12}} - e^{-\tilde{\tau}t_{12}}}}{Z_+^{(1)}(1+\gamma) + Z_+^{(2)}(1+\gamma)}$$

$$= -\frac{t_{12}}{M}\frac{Z_+^{(1)}\frac{e^{\tilde{\tau}t_{12}} - e^{-\tilde{\tau}t_{12}}}{e^{\tilde{\tau}t_{12}} + e^{-\tilde{\tau}t_{12}}} + Z_+^{(2)}\frac{e^{\tilde{\tau}t_{12}} + e^{-\tilde{\tau}t_{12}}}{e^{\tilde{\tau}t_{12}} - e^{-\tilde{\tau}t_{12}}}}{Z_+^{(1)} + Z_+^{(2)}} \qquad (11a)$$

In deriving Eq. 11a, Eq. 10 is used. According to $Z^{(1+2)} = (1+\gamma)(Z_+^{(1)} + Z_+^{(2)})$, $\langle h_{12} \rangle_{Z^{(1+2)}}$ can also be calculated as,

$$\langle h_{12} \rangle_{Z^{(1+2)}} = -\frac{1}{M}\frac{1}{Z^{(1+2)}}\frac{\partial Z^{(1+2)}}{\partial \tilde{\tau}}$$

$$= -\frac{t_{12}}{M}\frac{Z_+^{(1)}\frac{e^{\tilde{\tau}t_{12}} - e^{-\tilde{\tau}t_{12}}}{e^{\tilde{\tau}t_{12}} + e^{-\tilde{\tau}t_{12}}} + Z_+^{(2)}\frac{e^{\tilde{\tau}t_{12}} + e^{-\tilde{\tau}t_{12}}}{e^{\tilde{\tau}t_{12}} - e^{-\tilde{\tau}t_{12}}}}{\left(Z_+^{(1)} + Z_+^{(2)}\right)} - \frac{t_{12}}{M}\frac{\partial \gamma}{(1+\gamma)\partial \tilde{\tau}} \quad (11b)$$

$\langle h_{12} \rangle_{Z^{(1+2)}}$ obtained in Eq. 10a and 10b must be identical, which implies $\frac{\partial \gamma}{\partial \tilde{\tau}} = 0$, namely γ is independent on temperature!

Recall $h_{12} = -t_{12}\left(c_1^\dagger c_2 + c_1^\dagger c_2\right)$, within the subset path space of $Z^{(1+2)}$, the expectation value of $c_1^\dagger c_2 + c_1^\dagger c_2$ at 1TS can be calculated as,

$$\langle c_i^\dagger c_j + c_j^\dagger c_i \rangle_{Z^{(1+2)}} = \frac{1}{Z^{(1+2)}}\frac{\partial Z^{(1+2)}}{\partial(\tilde{\tau}t_{12})}$$

$$= \frac{(Z_+^{(1)} + Z_-^{(1)})\frac{e^{\tilde{\tau}t_{12}} - e^{-\tilde{\tau}t_{12}}}{e^{\tilde{\tau}t_{12}} + e^{-\tilde{\tau}t_{12}}} + (Z_+^{(2)} + Z_-^{(2)})\frac{e^{\tilde{\tau}t_{12}} + e^{-\tilde{\tau}t_{12}}}{e^{\tilde{\tau}t_{12}} - e^{-\tilde{\tau}t_{12}}}}{Z_+^{(1)} + Z_+^{(2)} + Z_-^{(1)} + Z_-^{(2)}}$$

$$= \frac{Z_+^{(1)}(1+\gamma)\frac{e^{\tilde{\tau}t_{12}} - e^{-\tilde{\tau}t_{12}}}{e^{\tilde{\tau}t_{12}} + e^{-\tilde{\tau}t_{12}}} + Z_+^{(2)}(1+\gamma)\frac{e^{\tilde{\tau}t_{12}} + e^{-\tilde{\tau}t_{12}}}{e^{\tilde{\tau}t_{12}} - e^{-\tilde{\tau}t_{12}}}}{Z_+^{(1)}(1+\gamma) + Z_+^{(2)}(1+\gamma)}$$

$$= \frac{Z_+^{(1)} \frac{e^{\tilde{\tau} t_{12}} - e^{-\tilde{\tau} t_{12}}}{e^{\tilde{\tau} t_{12}} + e^{-\tilde{\tau} t_{12}}} + Z_+^{(2)} \frac{e^{\tilde{\tau} t_{12}} + e^{-\tilde{\tau} t_{12}}}{e^{\tilde{\tau} t_{12}} - e^{-\tilde{\tau} t_{12}}}}{Z_+^{(1)} + Z_+^{(2)}} \qquad (12a)$$

Similarly, according to $Z^{(1+2)} = (1+\gamma)(Z_+^{(1)} + Z_+^{(2)})$, we also have,

$$\langle c_i^\dagger c_j + c_j^\dagger c_i \rangle_{Z^{(1+2)}} = \frac{1}{Z^{(1+2)}} \frac{\partial Z^{(1+2)}}{\partial(\tilde{\tau} t_{12})}$$

$$= \frac{Z_+^{(1)} \frac{e^{\tilde{\tau} t_{12}} - e^{-\tilde{\tau} t_{12}}}{e^{\tilde{\tau} t_{12}} + e^{-\tilde{\tau} t_{12}}} + Z_+^{(2)} \frac{e^{\tilde{\tau} t_{12}} + e^{-\tilde{\tau} t_{12}}}{e^{\tilde{\tau} t_{12}} - e^{-\tilde{\tau} t_{12}}}}{\left(Z_+^{(1)} + Z_+^{(2)}\right)} + \frac{\partial \gamma}{(1+\gamma)\partial(\tilde{\tau} t_{12})} \quad (12b)$$

$\langle c_i^\dagger c_j + c_j^\dagger c_i \rangle_{Z^{(1+2)}}$ obtained in Eq. 12a and 12b must be identical too, thus γ is also independent on the hopping amplitude. Finally, we reach the essential conclusion that γ **is independent on both** $\tilde{\tau}$ **and** t_{ij} **for any** $e^{-\tau h_{ij}}$ **at any time slice**. In other words, γ **is independent on both temperature and interaction.**

Define σ as, $\sigma = \frac{Z_-}{Z_+} = \frac{Z_-^{(0)} + Z_-^{(1)} + Z_-^{(2)}}{Z_+^{(0)} + Z_+^{(1)} + Z_+^{(2)}}$, we have,

$$\sigma = \gamma + \frac{(\vartheta - \gamma) Z_+^{(0)}}{Z_+^{(0)} + Z_+^{(1)} + Z_+^{(2)}}. \quad (13)$$

with $\vartheta = \frac{Z_-^{(0)}}{Z_+^{(0)}}$. It is self-evident that, no matter how the classification changes, both Z_- and Z_+, as well as the ratio of Z_- to Z_+, must have a definite value for a given system and temperature. For any $e^{-\tau h_{ij}}$ at any time slice, and whatever h_{ij} changing with i and j, Eq. 13 must hold. However, $Z_+^{(0)}$ is changeable with $e^{-\tau h_{ij}}$ and time slice. To guarantee σ unchanged, the only possibility is $\vartheta = \gamma$, namely,

$$\frac{Z_-^{(0)}}{Z_+^{(0)}} = \frac{Z_-^{(1)}}{Z_+^{(1)}} = \frac{Z_-^{(2)}}{Z_+^{(2)}} = \gamma \qquad (14)$$

Using this proportional relationship, Eq. 6 can be written as,

$$\varepsilon_{12} = -\frac{t_{12}}{M} \frac{Z_+^{(1)} \frac{e^{-\tilde{\tau} t_{12}} - e^{\tilde{\tau} t_{12}}}{e^{-\tilde{\tau} t_{12}} + e^{\tilde{\tau} t_{12}}} + Z_+^{(2)} \frac{e^{-\tilde{\tau} t_{12}} + e^{\tilde{\tau} t_{12}}}{e^{-\tilde{\tau} t_{12}} - e^{\tilde{\tau} t_{12}}}}{Z_+^{(0)} + Z_+^{(1)} + Z_+^{(2)}} = -\frac{t_{12}}{M} \frac{\partial Z_+}{Z_+ \partial \tilde{\tau}} \qquad (15)$$

Since h_{12} in 1TS is nothing special, Eq. 15 can be used to calculate expectation value of h_{ij} at any time slice in OP path space. Although the above analysis is focus on energies, other physics quantities can be analyzed in the similar way, and calculated only in OP paths. If $\hat{O}$ is a physics quantity, $\langle\hat{O}\rangle$ reads

$$\langle\hat{O}\rangle = \langle\hat{O}\rangle_{OP} = \left(\frac{Tr\hat{O}e^{-\beta H}}{Tre^{-\beta H}}\right)_{OP} \qquad (16)$$

Since all OP paths always have the global positive sign, thus SP completely disappears!

General Remarks: The following issues need to be stressed. **First of all**, the key step in the current proof lies on the combination of each off-diagonal term in Hamiltonian and its Hermitian conjugate. Without this combination, the strict mathematical proof is definitely impossible. **Second**, in above analysis, an implicit feature of $\frac{\partial Z_{+}^{(\alpha)}}{Z_{+}^{(\alpha)}\partial\tilde{\tau}} = \frac{\partial Z_{-}^{(\alpha)}}{Z_{-}^{(\alpha)}\partial\tilde{\tau}}$, namely OP and ON paths contributing the identical instantaneous energy, is crucial, especially in the mathematical derivation of Eq. 7-10. With this feature, we know that the cancellation only modifies the weight of paths, but does not change the instantaneous energy. This is the reason why we work on the local Boltzmann operator ($e^{-\tau h_{ij}}$) rather than the global Boltzmann operator ($e^{-\beta H}$).[84] **Third**, although the above proof is for one-body operators, it is straightforward to extend to two-body and even more complex operators, and the conclusion will not change. **Forth**, the abandoned paths that belong Z_{-} (or ON paths) can have either positive- or negative-weight. Clearly, we do not simply abandon negative-weighted paths. **Fifth**, the above discussion does not involve Hubbard-Stratonovich transformation, however the current method can be straightforwardly adopted to the effective Hamiltonian introduced by the Hubbard-Stratonovich transformation. And the current idea for solving the SP is independent on the specified QMC algorithm, the only requirement is to combine each off-diagonal term in Hamiltonian and its Hermitian conjugate into pairs, and constrains the sampling of QMC within the OP paths. **Finally**, the WF space contains a huge number of individual paths, a path can be defined as an individual path or a group of a few individual paths. In different QMCs, the meaning of a path may be quite different. In fact, a path defined in current work is different from that used in other QMCs. Thus, the most essential point is that, our strategy for SP and our path integral formula are inseparable, which should be considered as a whole.

Apply to Hubbard Model

The QMC simulation is based on the world-line algorithm recently proposed in our group.[77] In this method, to obtain a closed path (a non-zero weight path), we design an algorithm similar to the world-line algorithm[85] and the multiple time threading one.[3] In order to implement the current idea, or specifically, in order to calculate Eq.16, we need to make appropriate modifications to the QMC algorithm. In fact, this modification is very simple. We only need to make calculations in OP paths.

The physics properties of the two-dimensional Hubbard model with the size of 4×4 are calculated at finite temperature. In all calculations, $t_{ij} = t$ is taken as the unit of energy and set $t = 1.0$ and $U = 4$. We focus on the system with 14 electrons, $i.e., N = 14$, corresponding to the electron density $\rho = 0.875$. And the number of spin-up and spin-down electrons is equal. The system with $\rho = 0.875$ has the heaviest SP in the standard Hubbard model.[67] For most simulations, the total number of QMC steps at each temperature or M is more than 10^7, where the first third of the steps are used to equilibrate the system and the remaining two thirds of the steps are used to calculate the physical properties. According to thermodynamics, the energy is calculated according to $E = -\frac{1}{Z} \cdot \frac{\partial Z}{\partial \beta}$, and the double occupancy are calculated as $O_d = \sum_i < n_{i\uparrow} n_{i\downarrow} >$.

The convergence tests of τ for the system at the temperature of 0.5 are shown in Fig. 1. It can be seen that, with the increase of M, namely τ being decreased, the energy is quickly convergent. From $M = 40$, *i.e.*, $\tau = 0.05$, the change in QMC results is much slowly, indicating the convergence. In the rest QMC simulations, τ is fixed at the value of 0.05.

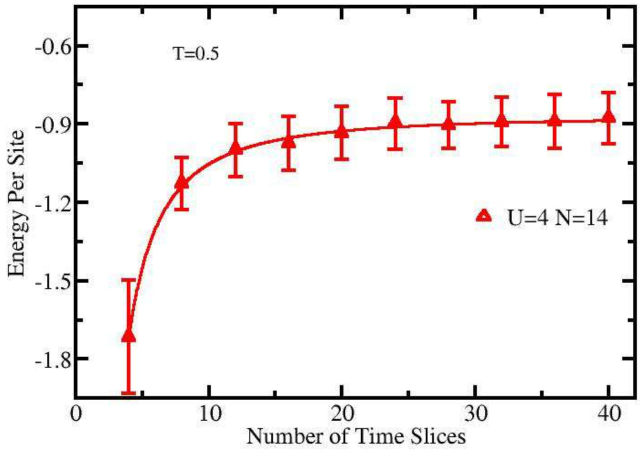

Figure 1: The energy with the number of time slices (*M*) at the temperature of 0.5 for $N = 14$ and $U = 4.0$ system. The QMC calculation becomes convergent for $M \geq 40$.

Since the current QMC is limited in OP paths, the SP is automatically absent. In the following, we will compare the current results to that presented in literatures. We find that, the energy and double occupancy calculated by current QMC simulations are in excellent agreement with that from various techniques[79] in the entire range of temperatures. Fig. 2 depicts the energy (upper panel) and double occupancy (lower panel) via temperature for $N = 14$ and $U = 4.0$. From this figure, one can see that, both the energy and double occupancy vs temperature show the same trend as that shown in Ref.[79].

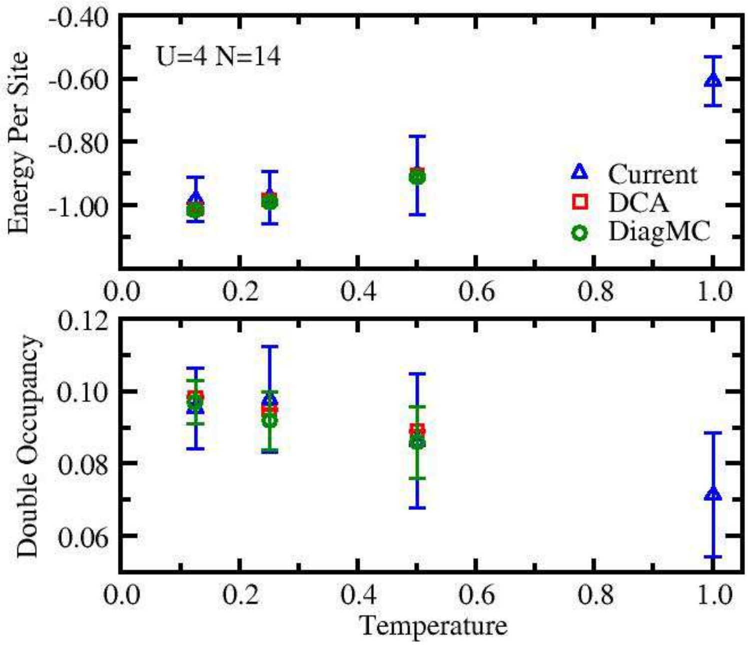

Figure 2: Temperature dependence on the energy (upper panel) and double occupancy (lower panel) for $N = 14$ and $U = 4.0$. The triangles represent the current results, while the circle and square represent the results from various techniques.[79]

V. Summary

In summary, we have found a rigorous solution for the fermion sign problem. The basic idea behind this solution is to look for a way to completely cancel or replace those paths with negative weights. By analyzing the contribution of a local Boltzmann operator to the partition function, we have proved that, the physical quantities can be exactly calculated in partial positive-weighted paths, thus the fermion sign problem is completely and rigorously solved. As an example, we have calculated the thermodynamic quantities of two-dimensional Hubbard model at finite temperature. Our results are in excellent agreement with previous values, which confirms the reliability of the current method.

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