A solution of fermion sign problem for large fermion systems

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The exchange antisymmetry between identical fermions gives rise to infamous fermion sign problem, e.g. both path integral Monte Carlo and path integral molecular dynamics could only give accurate result for only a few noninteracting fermions at low temperatures. By considering fictitious particles with a real parameter interpolating continuously between bosons and fermions, we use path integral molecular dynamics to propose a general strategy to solve fermion sign problem in polynomial time. We verify that our method can efficiently give accurate energy values for large fermion systems through a series of numerical experiments.

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The partition function is the starting point of quantum statistical physics. Based on Feynman’s idea of path integral\cite{1,2}, we can transform the partition function of many-particle Fermi systems into classical interacting ring polymers\cite{4,5,6} and use Monte Carlo\cite{8,9} or molecular dynamics (MD)\cite{10,11} approaches to sample the probability distribution in the partition function to obtain physical quantities such as the average energy. However, due to the exchange antisymmetry of fermions, the distribution function in the partition function is not positive definite, rendering existing sampling methods ineffective. Despite the development of various approaches to alleviate the fermion sign problem\cite{9,10}, there are still insurmountable difficulties for large fermion systems at low temperatures\cite{12,17}. For a long time it is widely believed that fermion sign problem is a NP-hard problem\cite{14}.

In this work (see Fig. 1 and Fig. 2 for a brief summary of our method and idea), we notice that the partition function $Z(\xi)$ of a fictitious quantum system is an analytical function of a real variable $\xi$ with $\xi = -1$ for fermions, $\xi = 0$ for distinguishable particles, and $\xi = 1$ for bosons. By using a recursion formula\cite{10,11,18,19} for identical particles, we can accurately and efficiently calculate the average energy $E(\xi)$ for $\xi \geq 0$, without suffering from the fermion sign problem. Because both $Z(\xi)$ and $E(\xi)$ are analytical function of $\xi$, we find that the analytical continuation to fermions of $\xi = -1$ can give us accurate energy for fermions with the computational scaling of $O(N^3)$, which provides excellent strategy to solve the fermion sign problem.

We used numerical experiments to verify our idea with large fermion systems greatly exceeding the computational power of traditional methods in path integral formalism. For example, in our numerical experiments, we obtain the predicted results accurately even for a system consisting of 20 fermions without interactions. Traditional method cannot obtain the same result even with millions times more computational resources. Needless to say, the strategy for fermion sign problem we propose here will produce novel ways to solve significant problems in many disciplines such as physics, chemistry and astronomy.
\[ Z(\beta, \xi) = \text{Tr}(e^{-\beta \hat{H}}) \]

\[ N = 4 \]

\[ \text{Ratio of Computational Steps} \]

\[ N \]

FIG. 1. (a) Illustration of all the ring polymer configurations for 2 identical particles to calculate the partition function. \( \xi \) denotes the exchange effect between particles. (b) shows roughly the ratio of computational steps between the traditional method and our method to consider the fermion sign problem. The big difference is due to the computational scaling of \( O(e^{\beta N}) \) in the traditional method and \( O(PN^3) \) in our method. As shown in (c), in our method, we first calculate the energy \( E(\beta, \xi) \) for different positive \( \xi \) without suffering from fermion sign problem. Then, the fitting with parabolic function is used to get the energy of 4 interacting fermions with \( \beta = 1 \) and \( \lambda = 0.5 \). The red circle gives the energy of the traditional method. (d) shows perfect agreement between parabolic function and the traditional method in the whole region \( -1 \leq \xi \leq 1 \) for 4 interacting fermions. In our simulations, 12 beads and 3 independent trajectories each consisting of \( 5 \times 10^6 \) MD steps are used to assure convergence.

**Partition function of identical particles and fermion sign problem**—For the following Hamiltonian operator of \( N \) identical particles

\[ \hat{H} = \frac{1}{2m} \sum_{i=1}^{N} \hat{p}_i^2 + \hat{V}(r_1, \cdots, r_N), \]  

\[ (1) \]
the partition function \(Z(\beta, \xi) = Tr(e^{-\beta H})\) is given by

\[
Z(\beta, \xi) = \frac{1}{N!} \sum_{p \in S_N} \xi^{N_p} \int d\mathbf{r}_1 d\mathbf{r}_2 \cdots d\mathbf{r}_N \langle p(\{\mathbf{r}\}) | e^{-\beta H} | \{\mathbf{r}\} \rangle.
\]  

(2)

Here \(\beta = 1/k_B T\), with \(k_B\) being the Boltzmann constant and \(T\) being the system temperature. \(S_N\) represents the set of \(N!\) permutation operations denoted by \(p\). The factor \(\xi^{N_p}\) is due to the exchange effect of identical particles, with \(N_p\) a number defined to be the minimum number of times for which pairs of indices must be interchanged to recover the original order. \(\xi = +1\) for boson partition function, while \(\xi = -1\) for fermion partition function. In addition, \(\{\mathbf{r}\}\) denotes \(\{\mathbf{r}_1, \cdots, \mathbf{r}_N\}\). Using \(e^{-\beta H} = e^{-\Delta \beta H} \cdots e^{-\Delta \beta H}\) with \(\Delta \beta = \beta/P\) and the technique of path integral, the partition function \(Z(\beta, \xi)\) can be mapped as a classical system of interacting ring polymers. See Fig. 1(a) as an example for two identical particles.

In recent works by Hirshberg et al., a recursion formula is found to calculate the partition function for both bosons (\(\xi = 1\)) and fermions (\(\xi = -1\)). Based on the path integral ring polymer, the fermion partition function (\(Z_F\)) and boson partition function (\(Z_B\)) are expressed as an analytical function of the coordinates of interacting ring polymers

\[
Z_{F/B} \sim \int d\mathbf{R}_1 \cdots d\mathbf{R}_N e^{-\beta U^{(N)}_{F/B}}.
\]  

(3)

Here \(Z_{F/B}\) becomes a function of a set of ring polymer coordinates \((\mathbf{R}_1, \cdots, \mathbf{R}_N)\), with \(\mathbf{R}_i = (\mathbf{r}^i_1, \cdots, \mathbf{r}^i_P)\) corresponding to \(P\) ring polymer coordinates for the \(i\)th particle. The recursion formula is found to calculate \(U^{(N)}_F\) for fermions and \(U^{(N)}_B\) for bosons. For bosons, \(U^{(N)}_B\) is always real and \(e^{-\beta U^{(N)}_B}\) may be sampled for large boson systems. However, because of the factor \((-1)^{N_p}\) for fermions, \(U^{(N)}_F\) is a complex function, which can not be sampled with available methods.

Based on the traditional method to deal with the fermion sign problem, the fermion partition function may be written as

\[
Z_F \sim \int d\mathbf{R}_1 \cdots d\mathbf{R}_N e^{-\beta U^{(N)}_B} e^{\beta (U^{(N)}_B - U^{(N)}_F)}.
\]  

(4)

In this case, we may still use molecular dynamics to sample \(e^{-\beta U^{(N)}_B}\), while the energy is \(E(\beta) = \langle \epsilon s \rangle_B / \langle s \rangle_B\). Here \(s = e^{\beta (U^{(N)}_B - U^{(N)}_F)}\) and \(\epsilon\) is the estimator for energy. The average \(\langle \cdots \rangle_B\) is about the samples based on the partition function \(Z_B\) for bosons.

However, because of the factor \(s\), it is extremely hard to calculate the energy, both in path integral Monte Carlo and path integral molecular dynamics. General
consideration shows that the simulation becomes exponentially hard to converge with increasing numbers of fermions and decreasing temperatures\cite{12}. This is known as the infamous fermion sign problem\cite{12,17,25,28}, which is the biggest obstacle for almost all first-principle calculations for large fermion systems. It was declared by Troyer and Wiese\cite{14} that an algorithm that converges in polynomial time—is “almost certainly unattainable”. In this work, however, we will show that we have effective strategies to solve the fermion sign problem with polynomial time for a wide range of large fermion systems. Fig. 1(b) shows roughly the ratio of computational steps between the traditional method and our method to consider the fermion sign problem.

**Partition function for a fictitious quantum system and analytical continuation**—

Because the operator $e^{-\beta H}$ is hermitian, it is clear that $Z(\beta, \xi)$ is a real function of $\beta$ and $\xi$ even for $\xi = -1$. For fermions, the transformation of $Z(\beta, \xi)$ as a multiple integral expression by path integral ring polymer is an important merit in the traditional method. However, after this transformation, for $\xi = -1$ (fermions), $U_F^{(N)}$ in the exponential function $e^{-\beta U_F^{(N)}}$ in the partition function becomes a complex function. This is a huge cost to solve fermions by path integral ring polymer. However, we should never forget that $Z(\beta, \xi)$ in essence is a problem of real number, and the emergence of complex exponential function and the resulting fermion sign problem is due to specific mathematical technique.

Fortunately, even for integral about complex exponential function, we still have mathematical method to solve the problem. A typical example is the calculation of $\int_{-\infty}^{\infty} e^{iax^2} dx$ for a real number $a$. If we use the usual numerical method to calculate this integral, we may have the illusion that this is a NP-hard problem. The method of analytical continuation makes this integral easy. If we try to consider directly the integral in $Z(\beta, \xi = -1)$, it would be a NP-hard problem too\cite{13}. However, this does not mean that the calculation of the energy of identical fermions must be a NP-hard problem.

To calculate the energy for identical fermions, we turn to consider the partition function $Z(\beta, \xi)$ given by Eq. (2). From the expression of $Z(\beta, \xi)$, it is clear that it is mathematically legitimate that we extend two discrete values $\xi = \{-1, 1\}$ for $Z(\beta, \xi)$ to the general case that $\xi$ becomes a continuous real variable (See Fig. 2). Generalizing the technique of the recursion formula discovered by Hirshberg et al.\cite{10,18}, from Eq. (2), we have

\begin{equation}
Z(\beta, \xi) \sim \int dR_1 \cdots dR_N e^{-\beta U_F^{(N)}}. \tag{5}
\end{equation}
FIG. 2. For the partition function $Z(\beta, \xi)$ with $\xi$ a real number ($\xi = -1$ for fermions, $\xi = 0$ for distinguishable particles and $\xi = 1$ for bosons), $U^{(N)}_\xi$ in the whole region $\xi \geq 0$ is a real function, which can be sampled accurately and efficiently. Hence, we can get many reliable values for the energy $E(\beta, \xi)$ in this region, and analytically continue to the energy of fermions (illustrated by blue solid line with arrow) if $E(\beta, \xi)$ has simple analytical property about $\xi$. In the traditional method, however, it is equivalent that the distribution of the partition function for a single point $\xi = 1$ is used to try to extend to the energy for fermions illustrated by red dashed line, which leads to an illusion of NP-hard problem.

The recursion formula of $U^{(N)}_\xi$ is given in SM (Supplementary Material). The energy of this fictitious quantum system for general real number $\xi$ is $E(\beta, \xi) = -\partial \ln Z(\beta, \xi) / \partial \beta$. It is obvious that both $Z(\beta, \xi)$ and $E(\beta, \xi)$ are analytical functions of $\beta$ and $\xi$.

From the recursion formula, $U^{(N)}_\xi$ is a real function for $\xi \geq 0$, while a complex function for $\xi < 0$ (See Fig. 2). Therefore, in the whole real number region $\xi \geq 0$, the partition function for this fictitious quantum system does not suffer from fermion sign problem. Because of
the analytical characteristic of $Z(\beta, \xi)$ and $E(\beta, \xi)$ about $\beta$ and $\xi$, it is expected that the analytical continuation will give us good chance to deal with fermions with $\xi = -1$. We consider in this paper the usual polynomial fitting so that $E(\beta, \xi) = a_0 + a_1 \xi + a_2 \xi^2 + \cdots a_n \xi^n + \cdots$. The accurate calculation of $E(\beta, \xi)$ for $\xi \geq 0$ means that we can obtain accurate evaluation of the coefficients $a_j$, in particular for analytical function $E(\beta, \xi)$ about $\xi$. In this case, it’s a matter of course that we have good chance to get accurate result of $E(\beta, \xi = -1)$ for fermions.

Nevertheless, for such seemingly natural idea, we must carry out numerical experiments to put it to the ultimate test. We have used many different fermion systems to justify our discoveries. The evaluation of the precision of $E(\beta, \xi = -1)$ can be shown through the degree of conformity of all the data for $\xi \geq 0$ in the fitting.

**Numerical experiments for noninteracting and interacting fermions**— Now we turn to consider numerical experiments to test our method. In our numerical simulations (more details are given in SI), the path integral ring polymers and molecular dynamics with separate Nosé-Hoover thermostat\[29–33\] are used to sample the partition function $Z(\beta, \xi)$ for $\xi \geq 0$, which is further used by polynomial fitting to calculate the energy for fermions. The number of beads $P$ used decreases as temperature increases to ensure numerical stability and assure convergence. In all of the following we checked convergence with respect to the number of beads and MD steps performed. For details of how to assure the convergence, one may refer to the supplementary material in Ref.\[18\]

We consider fermions in a two-dimensional harmonic trap $\frac{1}{2}m\omega^2(x^2 + y^2)$ with the units of $\hbar = 1, \omega = 1, m = 1$. The interparticle interactions are $V_{\text{int}} = \sum_{i<j}^N \lambda / |\mathbf{r}_i - \mathbf{r}_j|$. For $N = 4, \beta = 1$ and $\lambda = 0.5$ (not difficult both in traditional method and our method), the blue solid circle in Fig. 1(c) shows the numerical result of the energy for $0 \leq \xi \leq 1$. The solid line is the best fitting with the parabolic function. The red solid circle is the result of path integral Monte Carlo in Ref.\[19\]. In Fig. 1(d), we give the numerical results for the whole region $-1 \leq \xi \leq 1$ by using the traditional method to deal with the fermion sign problem. We give the parabolic function in the whole region, and perfect agreement is found. This verifies that $E(\beta, \xi)$ is a simple analytical function about $\xi$ in the whole region connecting bosons and fermions.

We consider further an example of noninteracting fermions with $N = 6$ and $\beta = 1$, which is very difficult but feasible in traditional method. It is worth pointing out that the
FIG. 3. Left figure for \( N=6 \): The blue circle and blue line give the results for \( \beta = 1 \) in our method. The red circle gives the result of traditional method\(^8\), while the green circle gives the result of grand canonical ensemble. Right figure for \( N=20 \): The blue circle and blue line give the results for \( \beta = 1 \) by polynomial fitting, while the red circle is the result of grand canonical ensemble. The inset shows that the parabolic function fails in the fitting. Hence, we should include the term \( \xi^4 \) for polynomial fitting.

Noninteracting fermions at low temperatures have the most severe fermion sign problem, which provide the best system to check the method to solve the fermion sign problem\(^9,10\). In Fig. 3(a), we give the numerical results for these parameters. The red circle shows the result of traditional method by path integral Monte Carlo\(^8\).

In Fig. 3(b), we consider noninteracting fermions of 20 particles in two-dimensional harmonic trap at \( \beta = 1 \), which is far beyond the capabilities of traditional method of path integral ring polymer. It is also much beyond the capabilities of the improved method to alleviate the fermion sign problem\(^9,10\) by introducing an extra fictitious interaction. We show our numerical result for \( 0 \leq \xi \leq 2 \) and the fitting to get the energy for fermions. The energy of fermions agrees perfectly with the result of grand canonical ensemble. Generally speaking, the actual interacting fermion systems have less severe fermion sign problem, compared with ideal fermions. Hence, the test of the principle of ideal fermions gives us strong support to
simulate efficiently and accurately large interacting fermion systems.

Although ideal fermions have already provided the best and harshest example to test our method, as the final example, we consider interacting fermions in two-dimensional harmonic trap. In Fig. 4(a), we show our result for $N = 8$, $\beta = 1$ and $\lambda = 0.5$, which agrees with the traditional method (red circle) by Dornheim, while our method is much more efficient and has much smaller statistical fluctuations. In Fig. 4(b), we show the numerical simulation of $N = 20$, $\beta = 1$ and $\lambda = 0.5$. The successful application of our method to large fermion systems is not so surprising, because the partition function $Z$ and total energy $E$ are also regular functions of $N$. This means that the success of our method for several examples of different $N$ will ensure the validity for all $N$ in principle, with computational scaling of $O(PN^3)$.

It is not the purpose of the present work to prove or argue that our polynomial-time algorithm can be used to study any large fermion system. The present method relies on the assumption that $E(\beta, \xi)$ has simple analytical property for $\xi \geq -1$. In SM, we provide other examples to suggest strongly that the simple analytical property is a very common
situation. The simple analytical property of $E(\beta, \xi)$ has physical reason that the exchange effect of fermions has equivalently repulsive statistical interaction, while the exchange effect of bosons leads to equivalently attractive statistical interaction. This suggests strongly that $E(\beta, \xi)$ has monotonic or simple behavior, for the vast majority of quantum systems we have interests. Of course, for some specific quantum systems, we may find better function than polynomial function for data fitting. It depends on the quantum system studied, and the comparison with experiments may also improve the choice of the fitting function.

In all the results based on our method, the statistical error is negligible. Hence, we do not give error bar for the energy in our method. This provides strict criteria to test whether our method is applicable for specific and eccentric quantum systems in future work. In practical application, one may first check our method with ideal fermions to avoid potential problem, and then use it to interacting fermions (see details in SM).

**Conclusion**—Compared with the traditional method, at first sight, our method and result for solving the fermion sign problem is an unbelievable miracle. However, the miracle is due to the fact that in our method, more informations (the reliable importance sampling for many different values of $\xi \geq 0$ for $Z(\beta, \xi)$) are given to the analytical property of $Z(\beta, \xi)$ to extend the result to $\xi = -1$ (See Fig. [2]). As a comparison, we see that in the traditional method, we only consider the distribution of the partition function $Z(\beta, \xi)$ for a single point $\xi = 1$ and try to analytically extend to the result to $\xi = -1$. This traditional method for extrapolation is obviously hard and dangerous. Based on this comparison, the superiority of our method is self-evident. It is expected that the present work will stimulate new surges of scientific research in many fields such as physics, chemistry and astronomy.

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Appendix A: Methods

(I) Recursion formula for $Z(\beta, \xi)$

We consider $N$ fictitious identical particles, so that the normalized position eigenstates are

$$|N_\xi\rangle = \frac{1}{\sqrt{N!}} \sum_{p \in S_N} \xi^{N_p} |p\{r\}\rangle. \quad (A.1)$$

$S_N$ represents the set of $N!$ permutation operations denoted by $p$. The factor $\xi^{N_p}$ is due to the exchange effect of the fictitious particles, with $N_p$ a number defined to be the minimum number of times for which pairs of indices must be interchanged to recover the original order.

We have the unit operator

$$\hat{1}_\xi = \frac{1}{N!} \int d\mathbf{r}_1 d\mathbf{r}_2 \cdots d\mathbf{r}_N |N_\xi\rangle \langle N_\xi|. \quad (A.1)$$

We also have another unit operator

$$\hat{1} = \int d\mathbf{r}_1 d\mathbf{r}_2 \cdots d\mathbf{r}_N |\{r\}\rangle \langle \{r\}|. \quad (A.1)$$

By dividing $\beta$ into $P$ segments, with $\Delta \beta = \beta/P$, and using the identity

$$e^{-\beta \hat{H}} \hat{1}_\xi = e^{-\Delta \beta \hat{H}} \hat{1} e^{-\Delta \beta \hat{H}} \hat{1}_\xi \cdots \hat{1} e^{-\Delta \beta \hat{H}} \hat{1}_\xi,$$  

we can obtain the discrete form for the partition function by inserting the definition for the identity operators from the above equations. After that is done, the partition function is a function of a set of ring polymer coordinates $(\mathbf{R}_1, \cdots, \mathbf{R}_N)$, with $\mathbf{R}_i = (\mathbf{r}_{1i}, \cdots, \mathbf{r}_{Pi})$ corresponding to $P$ ring polymer coordinates for the $i$th particle. Explicitly, after considering all the permutation terms in Eq. (2) in the text, we have $U^{(N)}_\xi$ in Eq. (5) in the text given by

$$U^{(N)}_\xi = -\frac{1}{\beta} \ln W^{(N)}_\xi + \frac{1}{P} \sum_{j=1}^P V(\mathbf{r}_{1j}, \cdots, \mathbf{r}_{Nj}), \quad (A.1)$$

and $W^{(N)}_\xi$ is

$$W^{(N)}_\xi = \frac{1}{N} \sum_{k=1}^N \xi^{k-1} e^{-\beta E^{(k)}_N} W^{(N-k)}_\xi. \quad (A.1)$$
In addition,
\[ E^{(k)}_N = \frac{1}{2} m \omega_r^2 \sum_{l=N-k+1}^N \sum_{j=1}^P (r_i^{j+1} - r_i^j)^2. \] (A.1)

Here \( r_i^{P+1} = r_i^{1+k} \), except for \( l = N \) for which \( r_N^{P+1} = r_N^{1-k} \). In addition, \( \omega_r = \sqrt{P/\beta \hbar} \).

(II) Energy estimator and molecular dynamics

In order to perform molecular dynamics, we need the potential function and its gradient. From the fact that \( W^{(N)}_\xi = e^{-\beta V^{(N)}_\xi} \), we can evaluate the potential \( V^{(N)}_\xi \) recursively as
\[ V^{(N)}_\xi = -\frac{1}{\beta} \log -\frac{1}{\alpha} \sum_{k=1}^N \xi^{k-1} e^{-\beta (E^{(k)}_\alpha + V^{(\alpha-k)}_\xi)}. \] (A.1)

Taking gradient, we see that the forces are given by
\[ -\nabla_{r_i} V^{(N)}_\xi = -\frac{\sum_{k=1}^N \xi^{k-1} [\nabla_{r_i} E^{(k)}_\alpha + \nabla_{r_i} V^{(\alpha-k)}_\xi] e^{-\beta (E^{(k)}_\alpha + V^{(\alpha-k)}_\xi)}}{\sum_{k=1}^N \xi^{k-1} e^{-\beta (E^{(k)}_\alpha + V^{(\alpha-k)}_\xi)}}. \] (A.1)

From the relation between \( E(\beta, \xi) \) and \( Z(\beta, \xi) \), we have
\[ E(\beta, \xi) = \frac{P d N}{2 \beta} + \left< U \right> + \left< V^{(N)}_\xi + \beta \frac{\partial V^{(N)}_\xi}{\partial \beta} \right>, \] (A.1)

with \( d \) the spatial dimensions. \( V^{(N)}_\xi + \beta \frac{\partial V^{(N)}_\xi}{\partial \beta} \) may be evaluated as
\[ V^{(N)}_\xi + \beta \frac{\partial V^{(N)}_\xi}{\partial \beta} = \frac{\sum_{k=1}^N \xi^{k-1} [V^{(N-k)}_\xi + \beta \frac{\partial V^{(N-k)}_\xi}{\partial \beta} - E^{(k)}_N] e^{-\beta (E^{(k)}_N + V^{(\alpha-k)}_\xi)}}{\sum_{k=1}^N \xi^{k-1} e^{-\beta (E^{(k)}_N + V^{(\alpha-k)}_\xi)}}. \] (A.1)

with \( V^{(0)}_\xi + \beta \frac{\partial V^{(0)}_\xi}{\partial \beta} = 0 \).

We should take care to ensure numerical stability when evaluating the above formulas. For the potential, except for the case of \( \xi = 0 \), a numerically stable way to calculate potential is the following
\[ V^{(N)}_\xi = \log -\frac{1}{\alpha} \sum_{k=1}^N e^{(k-1) \log \xi - \beta (E^{(k)}_\alpha + V^{(\alpha-k)}_\xi)} + \log \alpha, \] (A.1)

where \( \tilde{E} \) is chosen as
\[ \tilde{E} = -\max_k [(k-1) \log \xi - \beta (E^{(k)}_\alpha + V^{(\alpha-k)}_\xi)]. \] (A.1)

(III) Polynomial fitting and applicability of our approach

Because in our method, the energy for \( \xi \geq 0 \) can be calculated accurately (it is routine to realize the precision far below 1%), the only potential problem to get the accurate value
for fermions is whether the fitting is reasonable. The good fitting depends on the good
analytical property of $E(\beta, \xi)$ between $-1 \leq \xi \leq \xi_{up}$. Here $\xi_{up}$ is a positive value in our
numerical calculations between $0 \leq \xi \leq \xi_{up}$. In this work, we use Mathematica for fitting,
while the energy between $0 \leq \xi \leq \xi_{up}$ is calculated by path integral molecular dynamics with
C++ codes. If $E(\beta, \xi)$ has singular behavior or highly irregular oscillating behavior about
$\xi$, it is hard to assure the extrapolation for fermions. However, even for these situations,
some unique methods such as Schlessinger point method may be helpful. Fortunately, the
exchange effect of fermions has equivalently repulsive statistical interaction, while the ex-
change effect of bosons leads to equivalently attractive statistical interaction. This suggests
strongly that $E(\beta, \xi)$ has simple monotonic behavior, for most quantum systems we have
interests. Of course, for any practical research, we should first check the numerical stability
and accuracy for $\xi \geq 0$ and judge the validity of the fitting also from physical considerations.
Before considering large fermion systems, one may first calculate a few fermions for the re-

gion $-1 \leq \xi \leq \xi_{up}$ to confirm the simple and monotonic behavior of $E(\beta, \xi)$, like Fig. 1(d)
in this paper. After this confirmation, it would be safe to get the energy for large fermion
systems using the data fitting for $\xi \geq 0$.

**Appendix B: Analytical property of $E(\beta, \xi)$ for other examples**

As discussed in the text, the applicability of our method relies on the good analytical
property of $E(\beta, \xi)$. In this supplementary material, we calculate $N = 4, \beta = 1$ for different
types of interparticle interaction by traditional method to deal with the fermion sign prob-
lem, to show good analytical property of $E(\beta, \xi)$ for the whole region of $-1 \leq \xi \leq 1$. Of
course, for any practical research, we suggest strongly that one confirms first the analytical
property of $E(\beta, \xi)$ for $\xi \geq -1$ for a few fermions by path integral molecular dynamics and
traditional method to deal with the fermion sign problem before the calculations for large
fermion systems with our method. See the general strategy to numerically simulate large
fermion systems in Fig. S.1.

In all the following simulations, we use parabolic function for fitting, and the good ana-
lytical property of $E(\beta, \xi)$ about $\xi$ is shown very clearly.

1. Fig. S.2: Coulomb repulsive interaction $V_{int} = \sum_{i<j}^N \frac{\lambda}{|\mathbf{r}_i - \mathbf{r}_j|}$ with $\lambda = 1$.

2. Fig. S.3: Dipole interaction $V_{int} = \sum_{i<j}^N \frac{\lambda}{|\mathbf{r}_i - \mathbf{r}_j|^3}$ with $\lambda = 1$. 


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The calculation of $E(\beta, \xi)$ for $\xi \geq -1$ with a few particles (4 particles recommended) by path integral molecular dynamics to check the analytical property.

The calculation of $E(\beta, \xi)$ for $\xi \geq 0$ with many particles by path integral molecular dynamics.

Fitting the data to get the energy for large fermion system.

FIG. S.1. The general strategy to safely simulate large fermion systems without suffering from fermion sign problem.

(3) Fig. S.4: Gaussian interaction $V_{int} = \sum_{i<j}^N \frac{g}{\pi s^2} e^{-\frac{(R_i-R_j)^2}{s^2}}$ with $g = 3.0$ and $s = 0.5$. 

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FIG. S.2. Coulomb repulsive interaction.

FIG. S.3. Dipole interaction.
FIG. S.4. Gaussian interaction.