A Monte Carlo Method for Fermion Systems Coupled with Classical Degrees of Freedom

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A new Monte Carlo method is proposed for fermion systems interacting with classical degrees of freedom. To obtain a weight for each Monte Carlo sample with a fixed configuration of classical variables, the moment expansion of the density of states by Chebyshev polynomials is applied instead of the direct diagonalization of the fermion Hamiltonian. This reduces a cpu time to scale as \( O(N_{\text{dim}}^2 \log N_{\text{dim}}) \) compared to \( O(N_{\text{dim}}^3) \) for the diagonalization in the conventional technique; \( N_{\text{dim}} \) is the dimension of the Hamiltonian. Another advantage of this method is that parallel computation with high efficiency is possible. These significantly save total cpu times of Monte Carlo calculations because the calculation of a Monte Carlo weight is the bottleneck part. The method is applied to the double-exchange model as an example. The benchmark results show that it is possible to make a systematic investigation using a system-size scaling even in three dimensions within a realistic cpu timescale.

KEYWORDS: Monte Carlo method, moment expansion, Chebyshev polynomials, parallel computation, double-exchange model

§1. Introduction

Lattice fermion models interacting with classical degrees of freedom have a wide range of application. In many realistic cases, localized spins or lattice distortions for instances are handled as classical degrees of freedom under the adiabatic approximation. In this work, we are interested in the cases where these interactions are primarily important and many-body interactions between fermions can be neglected. Although models are simplified in these cases, they are still very useful to discuss physical properties in some realistic systems. For instance, many experimental results in perovskite Mn oxides have been successfully explained by the double-exchange (DE) model with classical localized \( t_{2g} \) spins.

In such systems, the Hamiltonian is given by \( \mathcal{H}(\{x_i\}) \) and the partition function is written as

\[
Z = \text{Tr}_C \text{Tr}_F \exp \left( -\beta \left[ \mathcal{H}(\{x_i\}) - \mu N \right] \right),
\]

where \( \text{Tr}_C \) and \( \text{Tr}_F \) are traces over classical degrees of freedom denoted by classical variables \( \{x_i\} \) and fermion degrees of freedom, respectively. Here, \( \beta \) is the inverse temperature, \( \mu \) is the chemical potential and \( N \) is the particle-number operator.

A prescription to calculate the partition function in eq. (1) is Monte Carlo (MC) sampling on configurations of classical degrees of freedom. In this method, fermion degrees of freedom are traced out beforehand as follows. The Hamiltonian \( \mathcal{H}(\{x_i\}) \) defined for a fixed configuration of classical variables \( \{x_i\} \) can be represented by \( N_{\text{dim}} \times N_{\text{dim}} \) matrix where \( N_{\text{dim}} \) is proportional to the system size because there is no many-body interaction between fermions. Then the trace over fermion degrees of freedom is easily calculated by the diagonalization of the Hamiltonian matrix as

\[
\text{Tr}_F \exp \left( -\beta \left[ \mathcal{H}(\{x_i\}) - \mu N \right] \right) = \prod_{\nu=1}^{N_{\text{dim}}} \left[ 1 + \exp \left( -\beta (E_{\nu}(\{x_i\}) - \mu) \right) \right],
\]

with the effective action

\[
S_{\text{eff}}(\{x_i\}) = -\sum_{i=1}^{N_{\text{dim}}} \log \left[ 1 + \exp \left( -\beta (E_{\nu}(\{x_i\}) - \mu) \right) \right].
\]

Trace over classical variables in eq. (3) is effectively calculated by a MC sampling. The MC update is performed using the Boltzmann weight of the configuration \( \{x_i\} \) which is given by \( \exp [-S_{\text{eff}}(\{x_i\})] \). Configurations of classical variables \( \{x_i\} \) are updated by using the Metropolis algorithm. Because eq. (2) is positive definite, we do not have a negative sign problem in this fermionic MC calculation.

Actual numerical calculation along the above conventional procedures is time-consuming and serious to handle large-sized systems. The bottleneck is the numerical diagonalization of the Hamiltonian \( \mathcal{H}(\{x_i\}) \). It costs a cpu time scaling as \( O(N_{\text{dim}}^3) \). If there are classical degrees of freedom proportional to \( N_{\text{dim}} \), as actually seen in many systems, one MC sweep to update all the values of \( \{x_i\} \) totally scales as \( O(N_{\text{dim}}^4) \). Let us consider the DE models for instance. We are especially interested in three-dimensional cases as realistic models for Mn oxides.
According to our estimation described later, a cpu time for 1,000 MC sweeps in $6 \times 6 \times 6$-sites system costs about 10 days and that in $8 \times 8 \times 8$ costs about 10 months on a standard workstation. This makes it extremely difficult to make a systematic size-scaling analysis, especially in three dimensions. So far, MC studies have been performed mainly in one and two dimensions without the system-size scaling in many cases.

In this work, we propose an alternative technique of MC calculations which is of great advantage to reduce the cpu time. In our method, the numerical diagonalization of the Hamiltonian is replaced by a moment expansion of the density of states by using orthogonal polynomials. This moment expansion costs a cpu time scaling as only $O(N_{\text{dim}}^3 \log N_{\text{dim}})$ compared to $O(N_{\text{dim}}^3)$ in the diagonalization. Moreover, the procedure can be done by parallel computations whereas the parallelization is difficult for the diagonalization in the conventional method. Efficiency of the parallelization is very high especially for large-sized systems. These significantly save a total cpu time for MC calculations by accelerating the bottleneck part to obtain the MC weights.

The paper is organized as follows: In §2 the new algorithm is introduced. It is applied to DE models in §3 to demonstrate its advantages. The benchmark results for a cpu time are also shown in §3. Sec. 3 is devoted to summary.

§2. Algorithm

In the conventional MC technique for the class of models considered here, as mentioned in §1, the Hamiltonian is numerically diagonalized for each configuration of $\{x_i\}$ to give all the eigenvalues. The effective action $S_{\text{eff}}$ is exactly calculated through eq. (3) by using these eigenvalues. However, the exact eigenvalues contain more than enough information for the purpose of performing practical MC calculations: It is sufficient to know the density of states within required accuracy.

In our algorithm, instead of the eigenvalues of the Hamiltonian, the density of states is estimated by using a moment expansion with orthogonal polynomials. This technique has been originally formulated to handle huge-sized matrix numerically. The Chebyshev polynomials are convenient in the moment expansion, which are defined recursively by

$$T_{m+1}(x) = 2xT_m(x) - T_{m-1}(x), \quad (5)$$

with $T_0 = 1$ and $T_1 = x$ for $-1 \leq x \leq 1$.

First, we define a renormalized Hamiltonian $X(\{x_i\})$ whose eigenvalues are $-1 \leq \varepsilon_\nu \leq 1$ by $H = aX + b$ with

$$a = (E_{\text{max}} - E_{\text{min}})/2, \quad b = (E_{\text{max}} + E_{\text{min}})/2, \quad (6)$$

where $E_{\text{max}}$ ($E_{\text{min}}$) is a highest (lowest) eigenvalue of the Hamiltonian $H$. Then, the $m$-th Chebyshev moment of the density of states $D(\varepsilon) \equiv \sum_{\nu} \delta(\varepsilon - \varepsilon_\nu)$ is defined by

$$\mu_m = \int_{-1}^{1} T_m(\varepsilon) D(\varepsilon) d\varepsilon. \quad (7)$$

Once the moments $\mu_m$ are calculated, the density of states is inversely obtained by

$$D(\varepsilon) = \frac{1}{\pi \sqrt{1 - \varepsilon^2}} \left[ \mu_0 + 2 \sum_{m \geq 1} \mu_m T_m(\varepsilon) \right]. \quad (8)$$

The expectation value of an operator $A$ is calculated by

$$\langle A \rangle = \int_{-1}^{1} A(\varepsilon) D(\varepsilon) d\varepsilon = \mu_0 \nu_0 + 2 \sum_{m \geq 1} \mu_m \nu_m, \quad (9)$$

where the moments of $A$ is given by

$$\nu_m = \int_{-1}^{1} \frac{d\varepsilon}{\pi \sqrt{1 - \varepsilon^2}} A(\varepsilon) T_m(\varepsilon). \quad (10)$$

In particular, the effective action in eq. (3) is obtained by

$$S_{\text{eff}} = \mu_0 \nu_0 + 2 \sum_{m \geq 1} \mu_m s_m, \quad (11)$$

where

$$s_m = -\int_{-1}^{1} \frac{N_{\text{dim}} d\varepsilon}{\pi \sqrt{1 - \varepsilon^2}} \log \left[ 1 + e^{-\beta (\varepsilon + b - \mu)} \right] T_m(\varepsilon) \quad (12)$$

with the coefficients $a$ and $b$ in eq. (3). Eqs. (8) and (9) are straightforwardly confirmed by using the orthonormality of Chebyshev polynomials.

From the definition (3), the moments of the density of states are calculated by

$$\mu_m = \frac{1}{N_{\text{dim}}} \text{Tr} \{T_m(X)\} = \frac{1}{N_{\text{dim}}} \sum_{\nu=1}^{N_{\text{dim}}} \langle \nu \rangle T_m(X) \langle \nu \rangle, \quad (13)$$

where $|\nu\rangle$ are convenient complete basis of the Hamiltonian $\langle \nu_1 | \nu_2 \rangle = \delta_{\nu_1 \nu_2}$. If we obtain the vectors $|\nu;m\rangle \equiv T_m(X) |\nu\rangle$, the calculation of a moment is a vector product;

$$\mu_m = \frac{1}{N_{\text{dim}}} \sum_{\nu=1}^{N_{\text{dim}}} \langle \nu ; m \rangle \langle \nu ; 0 | \nu ; m \rangle, \quad (14)$$

which costs a cpu time scaling as $O(N_{\text{dim}})$. The vectors $|\nu;m\rangle$ are calculated recursively by using the relation (5) as

$$|\nu;m+1\rangle = 2X |\nu;m\rangle - |\nu;m-1\rangle. \quad (15)$$

For a sparse Hamiltonian, the matrix-vector product in eq. (12) costs a cpu time scaling as only $O(N_{\text{dim}})$. Furthermore, we use recursive relations of Chebyshev polynomials;

$$T_{2m} = 2T_m^2 - 1, \quad T_{2m+1} = 2T_m T_{m+1} - T_1, \quad (16)$$

which enable us to obtain moments up to $M$-th order from those only up to $M/2$-th order. A total cpu time to compute the moments $\mu_m$ up to the order of $m = M$ scales as $O(N_{\text{dim}}^2 M)$.

The present method becomes ‘exact’, that is, equivalent to the direct diagonalization of the Hamiltonian in the conventional technique when we take the summations in eqs. (6) and (9) up to infinite order. In actual calculations, we approximate the summations in eqs. (6) and (9) by finite summations up to $m = M$. The approximation by the truncation at a finite value of $M$
is controllable since we can always estimate the errors through comparison with ‘exact’ results obtained by the conventional technique within the range of system sizes we are interested in. In particular, the truncation error of the effective action, $\Delta S_{\text{eff}}$, which is a crucial quantity in MC updates, becomes exponentially small as a function of $M$, as shown in §2 for DE models as an example. This comes from the fact that the moments $s_m$ in eq. (12) become exponentially small to the value of $m$. This justifies our approximation even for small values of $M$.

We discuss here $N_{\text{dim}}$ dependence of the truncation number $M$ which keeps $\Delta S_{\text{eff}}$ (the truncation error of $S_{\text{eff}}$) small enough to perform MC calculations practically. This is crucial for a cpu time. From the definition (13), $\Delta S_{\text{eff}}$ consists of the sum of errors for each eigenvalue $E_j$. Hence, if these exponentially-small errors are statistically independent of each other, $\Delta S_{\text{eff}}$ is proportional to $\sqrt{N_{\text{dim}}}$. In the case of correlated errors, $\Delta S_{\text{eff}}$ can be proportional to $N_{\text{dim}}$. For either case, therefore, to estimate $S_{\text{eff}}$ within required accuracy, the necessary truncation number $M$ should be proportional to $\log N_{\text{dim}}$ because $\Delta S_{\text{eff}} \sim \exp(-M)$. This indicates that a total cpu time to obtain moments for actual MC calculations scales as $O(N_{\text{dim}}^2 \log N_{\text{dim}})$. These properties of the truncation errors will be examined for DE models as an example in the next section.

The original formulation of this moment-expansion technique has been proposed by sampling a few random basis for the sum in eq. (13). This reduces a cpu time to scale as $O(N_{\text{dim}} M I)$, where $I$ is the number of the random basis. However, this sampling method works well only for huge-sized matrix for which $(N_{\text{dim}} I)^{-1/2}$ is small enough. In our MC calculations, since the matrix sizes for the systems we are interested in are not so large ($N_{\text{dim}} \simeq 10^3$), errors are not small and accumulate through MC updates to lead wrong samplings. From this, we take a sum over complete basis in eq. (13).

Another important point to reduce a cpu time is that the calculations of the moments in eq. (13) are computed very efficiently as far as the bandwidth $N_{\text{dim}}$ is proportional to $N_{\text{dim}}^2 M/N_{\text{PE}}$ whereas a time to communicate the calculated moments to add up is proportional to $MN_{\text{PE}}$. Here, $N_{\text{PE}}$ is the number of processors used in parallel calculations. This indicates that the parallel computation is performed very efficiently as far as $(N_{\text{dim}}/N_{\text{PE}})^2$ is large. High efficiency of this parallelization is demonstrated in the last part of the next section. Since it is difficult to make an efficient parallelization of the matrix diagonalization when all the eigenvalues are required, the present algorithm has another advantage in accelerating the calculation by parallelization. A cpu time to compute $S_{\text{eff}}$ is much shortened by both the reduction from $O(N_{\text{dim}})$ to $O(N_{\text{dim}}^2 \log N_{\text{dim}})$ and the parallel calculation. As mentioned in §2, since the calculation of $S_{\text{eff}}$ is the bottleneck in MC calculations, a total cost is much reduced; when there are $O(N_{\text{dim}})$ classical variables to be updated, a cpu time for one MC sweep on all these variables scales as $O(N_{\text{dim}}^3 \log N_{\text{dim}}/N_{\text{PE}})$ in our algorithm whereas that in the conventional method scales as $O(N_{\text{dim}}^3)$.

§3. Application

In this section, we show efficiency of the new algorithm introduced in §2 by an application to DE models with classical localized spins. The Hamiltonian is given by:

$$\mathcal{H} = -t \sum_{\langle ij \rangle, \sigma} \left( c_{i\sigma}^\dagger c_{j\sigma} + h.c. \right) - J \sum_i \mathbf{\sigma}_i \cdot \mathbf{S}_i, \quad (17)$$

where $c_{i\sigma}^\dagger (c_{i\sigma})$ creates (annihilates) a $\sigma$-spin electron at site $i$; $\mathbf{\sigma}_i$ is the spin operator whereas $\mathbf{S}_i$ denotes the localized spin at site $i$. We consider the nearest-neighbor hopping $t$ and the ferromagnetic Hund’s-rule coupling $J > 0$. Here the localized spin $\mathbf{S}_i$ is approximated as a classical rotator. The configuration of the classical rotator is described by two angles in each site: $\mathbf{S}_i = (\cos \theta_i \cos \phi_i, \sin \theta_i \cos \phi_i, \sin \phi_i)$. Then, the classical variables $\{x_i\}$ in eq. (17) are $2N$ variables, $\{\theta_i, \phi_i\}$ ($i = 1, 2, \ldots, N$), in this model (17). $N$ is the number of sites. The Hamiltonian for a fixed configuration $\{\theta_i, \phi_i\}$ can be written as $2N \times 2N$ matrix. Hereafter we take the bandwidth $W = zt = 1$ as an energy unit, where $z = 2D$ is the coordination number in a $D$-dimensional hypercubic lattice. Throughout the paper we take $J = 4$ which is an appropriate value to investigate the model in comparison with Mn oxides experiments. This model (17) has been intensively studied to understand physical properties of perovskite Mn oxides.

Some experimental results have been explained; such as the ferromagnetic metal in carrier-doped region, the transition to paramagnetic state by increasing temperature and the negative magnetoresistance near the transition. As far as we use the conventional MC technique described in [1], it is difficult to study realistic three-dimensional cases based on the size-scaling analysis, because of a diverging cpu-time as increasing the system sizes. So far, numerical studies have been performed mainly in one and two dimensions. In the following, we show that the new algorithm formulated in §2 reduces a cpu time significantly and makes it possible to investigate much larger-sized systems than the conventional technique.

First, we discuss the truncation error in the moment expansion. Figure 1 shows the truncation errors of the effective action when we truncate the summation in eq. (13) at $m = M$. The errors are estimated as deviations from the results by the direct diagonalization of the Hamiltonian in the conventional method. The errors become exponentially small to the value of $M$ as shown in the figures. The exponential decay depends on the temperature. Approximately, we find a relation: $\Delta S_{\text{eff}} \sim \exp(-M/\beta)$.

Although the necessary value of the truncation number $M$ for practical MC is proportional to $\log N_{\text{dim}}$ as mentioned in [2], actual values of $M$ may depend on models and parameters. It should be determined in MC results for each case. We examine here the condition for $M$ by changing temperatures in the DE model (17). Fig-
Figure 2 shows $M$ dependence of physical quantities. We calculate here the electron density and the spin structure factor at the wave number $k = 0$ (ferromagnetic component) by the 1,000 MC samplings with $S_{\text{eff}}$ whose moment expansion is truncated at $m = M$. In all the figures, the values by the conventional technique with direct diagonalization of the Hamiltonian are shown at $1/M = 0$ because our results should agree with them in the limit of $M \to \infty$. For small values of $M$, the truncation errors are so large that the estimated values deviate from those by the conventional method. However, for $M > \sim 40$, the expectation values converge on those by the conventional method within statistical error bars in the temperature range of $10 \lesssim \beta \lesssim 50$ which we are interested in. (The ferromagnetic transition temperature is estimated around $\beta = 20$ by the $D = \infty$ technique\(^7\).) The behavior is similar between data for different sizes. This is consistent with the weak $N_{\text{dim}}$-dependence of $M (M \sim \log N_{\text{dim}})$ as mentioned in §2. Therefore, in order to obtain these quantities of the present model eq. (17) within this accuracy, the value of $M$ can be taken at around 40 throughout the parameter range of our interests.

Finally, we show the benchmark results for a cpu time of our algorithm. Figure 3 shows the benchmark result on a workstation with Alpha-processor 21164 533MHz. A cpu time for MC sweeps on whole lattice sites in our technique is proportional to $N^3$, whereas the conventional technique costs a time proportional to $N^4$. When we take the value of $M$ as 40 based on the above observation in Fig. 2, our algorithm becomes faster than the conventional one for $N \gtrsim 80 - 90$ even in a single CPU.

![Figure 1](image1.png)

**Fig. 1.** The error of the effective action for a configuration of classical variables when the moment expansion is truncated at $m = M$; (a) $N = 16$ and (b) $N = 64$ in one dimension. We take $J = 4$ and $\mu = -4$. The circles, squares and triangles correspond to the data for $\beta = 10, 50$ and 100, respectively.

![Figure 2](image2.png)

**Fig. 2.** The truncation $M$ dependence of MC estimations for physical quantities: (a) and (b) show the electron density, and (c) and (d) show the spin structure factor at the wave number $k = 0$. (a) and (c) are the results for $N = 16$, and (b) and (d) are for $N = 64$ in one dimension. The results are for $J = 4$ and $\mu = -3.5$ by 1,000 MC sweeps on whole lattice sites. The circles, squares and triangles are for $\beta = 10, 20$ and 50, respectively. The filled symbols at $1/M = 0$ are the values obtained by the conventional MC technique using the diagonalization of the Hamiltonian.

As mentioned in \(^7\) moreover, our algorithm has an advantage to be performed on a parallel computer. Figure 4 shows efficiency of the parallelization. The parallel calculations have been performed using SR-2201 at the computer center of University of Tokyo. We find that
in Fig. 4 (a), a cpu time is reduced almost inversely proportional to the number of processors for large-sized systems. Figure 4 (b) shows the efficiency of the parallelization defined by

\[ R = \frac{1}{N_{PE}} \frac{t(N_{PE})^{-1}}{t(N_{PE} = 1)^{-1}}. \] (18)

Here \( t(N_{PE}) \) is a cpu time on \( N_{PE} \) processors. Note that \( R \) takes a value between 0 and 1, and that \( R = 1 \) when the parallelization is perfect. The parallelization is more effective for larger-sized systems for the reason mentioned in §2; for instance, \( R \) remains around 0.9 for \( 6 \times 6 \times 6 \) systems even when we use 64 processors.

![Graph](image1)

**Fig. 3.** The benchmark results for both our algorithm and the conventional one on a workstation with Alpha-processor 21164 (533MHz). The results are for 100 MC sweeps on whole lattice sites. The filled diamonds are for the conventional technique. The dotted line is a fit by \( N^4 \). The circles and squares are for our algorithm with \( M = 4 \) and 40, respectively. The data are fitted by \( N^3 \) as the gray lines.

Table I summarizes estimated cpu times for various system sizes of DE models. Our algorithm is powerful enough to study three-dimensional systems with several different sizes within a realistic timescale. Physical properties in three-dimensional DE models including the ferromagnetic transition temperature will be reported elsewhere.

| system size | conventional algorithm | present algorithm |
|-------------|------------------------|-------------------|
| \( 6 \times 6 \times 6 \) | \( \sim 10 \) days | \( \sim 10 \) hours |
| \( 8 \times 8 \times 8 \) | \( \sim 10 \) months | \( \sim 6 \) days |
| \( 10 \times 10 \times 10 \) | \( \sim 12 \) years | \( \sim 6 \) weeks |

Fig. 4. The benchmark results for our algorithm on the parallel computer, SR2201 at the computer center of University of Tokyo. The results are for 10 MC sweeps on whole lattice sites with \( M = 40 \). The circles, squares, triangles and crosses are for \( N = 16, 32, 64 \) and 128 in one dimension, respectively. The diamonds show the results for \( N = 6 \times 6 \times 6 \) in three dimensions. (a) is the-number-of-nodes-dependence of a cpu time. (b) shows the efficiency of the parallelization. See text for details. The lines are guides to eye.

§4. Summary

We have proposed the new algorithm of Monte Carlo calculation for fermion systems interacting with classical degrees of freedom under the adiabatic approximation. The moment expansion of the density of states by orthogonal polynomials is used, instead of the direct diagonalization of the Hamiltonian, to obtain a Monte Carlo weight for a fixed configuration of classical variables. Errors of the effective action by the truncation of the expansion become exponentially small with increasing the order of the expansion. This allows us to truncate the expansion at a small order in practical Monte Carlo calculations. These reduce a cpu time to scale as \( O(N_{dim}^2 \log N_{dim}) \) from \( O(N_{dim}^3) \) in the diagonalization, where \( N_{dim} \) is the dimension of the Hamiltonian matrix. This moment-expansion method is controllable since we can always estimate the truncation errors through comparison with results by the diagonalization. As another advantage, since the moment expansion is independent for each basis of the Hamiltonian, our new algorithm...
can be performed on parallel computers. Efficiency of the parallelization is very high especially for larger-sized systems since data to be communicated between nodes become smaller compared to calculations in each node. The reduction of the order of $N_{\text{dim}}$ and the parallelization significantly accelerate the procedure to obtain a Monte Carlo weight. This leads to much reduction of a total cpu time for Monte Carlo since the calculation of the weight is the bottleneck part.

In order to show the efficiency of our algorithm, we have applied it to the double-exchange model with classical localized spins. We have examined effects of the truncation of the moment expansion in actual Monte Carlo calculations. The condition for the truncation is clarified in the parameter region of interest. The benchmark results on both a single and multi cpu systems have been shown. Our algorithm is a powerful tool to investigate large-sized systems which are difficult to handle by the conventional technique within a realistic cpu timescale; for the double-exchange model, it may make possible to study three-dimensional systems systematically through system-size scaling analysis.

There are many other applications of our algorithm; such as double-exchange models including Jahn-Teller distortion, surface effects in double-exchange systems and some models for organic compounds. Our algorithm gives us a possible way to investigate these problems by using a numerical analysis for larger-sized systems.

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