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Polynomial expansion Monte Carlo study of frustrated itinerant electron systems: Application to a spin-ice type Kondo lattice model on a pyrochlore lattice

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ABSTRACT

We present the benchmark of the polynomial expansion Monte Carlo method to a Kondo lattice model with classical localized spins on a geometrically frustrated lattice. The method enables us to reduce the calculation amount by using the Chebyshev polynomial expansion of the density of states compared to a conventional Monte Carlo technique based on the exact diagonalization of the fermion Hamiltonian matrix. Further reduction is brought about by a real-space truncation of the vector–matrix operations. We apply the method to the model with spin-ice type Ising spins on a three-dimensional pyrochlore lattice and carefully examine the convergence in terms of the order of polynomials and the truncation distance. We find that, in a wide range of electron density at a relatively weak Kondo coupling compared to the noninteracting bandwidth, the results by the polynomial expansion method show good convergence to those by the conventional method within reasonable numbers of polynomials. This enables us to study the systems up to $4 \times 8^3 = 2048$ sites, while the previous study by the conventional method was limited to $4 \times 4^3 = 256$ sites. On the other hand, the real-space truncation is not helpful in reducing the calculation amount for the system sizes that we reached, as the sufficient convergence is obtained when most of the sites are involved within the truncation distance. The necessary truncation distance, however, appears not to show significant system size dependence, suggesting that the truncation method becomes efficient for larger system sizes.

1. Introduction

Interplay between localized spins and itinerant electrons has been one of the major topics in the field of strongly correlated electrons. In the spin-charge coupled systems, the fluctuations of localized spins considerably affect the charge degree of freedom of itinerant electrons, leading to fascinating transport phenomena, such as non Fermi liquid behavior in the quantum critical region in rare-earth compounds [1] and the colossal magneto-resistance (CMR) in perovskite manganese oxides [2]. On the other hand, for the localized spin degree of freedom, the kinetic motion of itinerant electrons results in effective interactions between localized spins, such as the Ruderman–Kittel–Kasuya–Yosida (RKKY) interaction [3] and double-exchange (DE) interaction [4]. These effective interactions give rise to peculiar magnetic orderings in the spin–charge coupled systems. Hence, in these systems, the charge and spin degrees of freedom affect each other in an entangled way, and it is not allowed to treat only one degree of freedom by fixing the other; the equilibrium state is obtained by optimizing the total free energy of the system.

The study on the spin–charge coupling has recently been extended to frustrated magnetic conductors in which itinerant electrons are coupled to localized spins on geometrically frustrated lattices. Experimentally, metallic pyrochlore oxides have attracted considerable attention [5], in which itinerant d electrons interact with localized f electrons. Theoretically, however, geometrical frustration brings further difficulty into the problem of spin–charge coupled systems. First, in the presence of frustration, the coupling between itinerant electrons and localized quantum spins leads to the negative sign problem, which hampers precise calculations at low temperatures. Meanwhile, when the localized spins are approximated as classical vectors and the electrons do not have any direct interaction between them (the situation that we focus on in the present work), the negative sign problem can be avoided. Even in this simplified situation, however, systematic calculations are still challenging; in order to examine the effect of large fluctuations, it is desired to make numerical simulations, but the calculation amount is usually large and increases rapidly as the system size increases.

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For the spin–charge coupled systems with classical localized spins, unbiased Monte Carlo (MC) calculations have been developed and used in the field of CMR manganites in which the geometrical frustration does not play a major role [6]. Originally, the MC method was implemented by using the exact diagonalization (ED) for the electronic degree of freedom to calculate the MC weight for sampling the configuration of the classical spins [7]. We call this algorithm EDMC. Later, several alternative methods were proposed for reducing the calculation amount [8–13]. One of the sophisticated methods is the polynomial expansion MC (PEMC) method proposed by one of the authors and his collaborators [8,9]. In this method, the polynomial expansion of the density of states (DOS) is used to calculate the MC weight, which reduces the calculation amount than ED; the method was further improved by introducing the truncation in the vector–matrix operations [10,11]. Hence, PEMC allows analyses on much larger system sizes compared to EDMC [14–19].

Because of the growing interests in frustrated magnetic conductors, it is desired to apply such MC simulations to the models with geometrical frustration. The application of PEMC, however, is anticipated to be less efficient for frustrated systems as, in general, DOS has a singular form under frustration. For example, a δ-function peak can appear associated with a flat band in the case of a kagome (corner-sharing triangles) and a pyrochlore (corner-sharing tetrahedra) lattice. A large number of polynomial bases are required to reproduce such a δ function in DOS with high accuracy, implying slow convergence in the PEMC framework and larger computational amount. Another difficulty is that the spin–charge coupling in frustrated magnetic conductors is often very weak compared to the large Hund's-rule coupling in CMR materials, and hence, the RKKY mechanism is dominant to make the effective spin interactions long-ranged and oscillating. This makes the truncation scheme less efficient since subtle energy differences originating from further-neighbor interactions play a decisive role.

Due to these anticipated problems, MC studies of frustrated spin–charge coupled systems have been very limited so far. For instance, the DE model on a pyrochlore lattice was studied, but the accessible system sizes were small since the studies were made by using EDMC [20–22]. Models in two dimensions were also studied on a triangular lattice [23–25] and kagome lattice [26], using EDMC. While PEMC was recently applied to a triangular lattice model, the studies focused on the case with a large Hund's-rule coupling comparable to the bandwidth [27,28]. In addition, DOS of the triangular lattice model in the noninteracting limit does not have a flat band, in contrast to the kagome and pyrochlore models. Hence, it does not involve the difficulties due to the δ-function structure in DOS.

Recently, the authors applied PEMC to a model for metallic pyrochlore oxides, i.e., a spin-ice type Kondo lattice model on a pyrochlore lattice [29]. They calculated the magnetic and electronic properties of the three-dimensional model in a relatively weak-coupling regime up to 4×8^3 sites systematically, and clarified the phase diagram including a variety of different phases. In the course of the study, the applicability of PEMC was examined carefully, and a part of the benchmark was reported in Ref. [30]. The details, however, have not been discussed yet.

In this paper, we present the detailed benchmark on the application of PEMC to the spin-ice type Kondo lattice model on a pyrochlore lattice. We focus on the low electron density region in the relatively weak-coupling regime, which is considered to be relevant for the metallic pyrochlore oxides. We perform the benchmark on the convergence of PEMC in terms of the order of polynomials and the truncation of vector–matrix operations by calculating both the order parameters and local correlations. The results indicate that, although DOS has a singular form including a δ-function peak in the noninteracting limit, PEMC turns out to be applicable in a wide range of electron density except for the very low density region. The required order of polynomials is within the range comparable to the typical numbers in the previous studies for unfrustrated models. On the other hand, the weak spin–charge coupling makes the truncation less helpful to reduce the calculation amount for currently accessible systems sizes. However, our benchmark suggests that it will become efficient in the simulations on larger size systems than those used in the present study.

The organization of this paper is as follows. In Section 2, we introduce the model and method. The model Hamiltonian and parameters are described in Section 2.1. A brief introduction on the PEMC method is given in Sections 2.2 and 2.3. In Section 3, we present the results of the benchmark. In Section 3.1, we show the temperature dependence of the sublattice magnetization calculated by EDMC and PEMC. Detailed comparison of PEMC to EDMC for 4×4^3 site systems is shown in Sections 3.2 and 3.3. The results for larger system sizes are presented in Section 3.4. Discussions on the results are elaborated in Section 4. Finally, Section 5 is devoted to the summary.

2. Model and method

In this section, we introduce the model and method used in our benchmark study in the following sections. We use the PEMC method developed in the previous studies [8,10,11] with a minor modification in the truncation method. The procedure of PEMC is briefly reviewed to make the paper self-contained.

2.1. Model and parameters

We consider a Kondo lattice model with Ising spins on a pyrochlore lattice [29,31], whose Hamiltonian is given by

$$H = -t \sum_{\langle i,j\rangle,\sigma} (c^\dagger_{i\sigma} c_{j\sigma} + \text{H.c.}) - J \sum_{i,\sigma,\sigma'} c^\dagger_{i\sigma} \boldsymbol{\sigma}_{\sigma\sigma'} c_{i\sigma'} \cdot \mathbf{S}_i. \tag{1}$$

The first term represents hopping of itinerant electrons, where $c_{i\sigma}$ ($c^\dagger_{i\sigma}$) is the annihilation (creation) operator of an itinerant electron with spin $\sigma = \uparrow, \downarrow$ at ith site, and t is the transfer integral. The sum $\langle i, j\rangle$ is taken over nearest-neighbor sites on the pyrochlore lattice which consists of a three-dimensional network of corner-sharing tetrahedra (see Figs. 2(d)–(f)). The second term is the onsite interaction between itinerant electron spins ($\boldsymbol{\sigma}$ is the Pauli matrix) and localized Ising spins $\mathbf{S}_i$ ($|\mathbf{S}_i| = 1$), and J is the coupling constant (the sign of J does not matter, since the localized spins are classical). The anisotropy axis of Ising spin is given along the local [111] direction, i.e., along the line connecting the centers of two tetrahedra which the spin belongs to (see Figs. 2(d)–(f)).

Considering the situations in many pyrochlore oxides, we focus on the relatively low electron density region of $0 < n < 0.35$ at a weak spin–charge coupling $J = 2t$ compared to the noninteracting bandwidth $8t$. Here, the electron density is defined by

$$n = \frac{1}{2N} \sum_{i\sigma} \langle c^\dagger_{i\sigma} c_{i\sigma} \rangle, \tag{2}$$

where N is the number of sites. Hereafter, we set the unit of energy $t = 1$, the lattice constant of the cubic unit cell $a = 1$, and the Boltzmann constant $k_B = 1$.

2.2. Polynomial expansion Monte Carlo method

In the model in Eq. (1), itinerant electrons have no direct interaction between them, but are coupled only to the classical Ising spins. The model belongs to the category of models in which noninteracting fermions couple with classical fields. In general, the partition function for such models is obtained by taking two traces: one is over the classical fields and the other over the fermion