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Ferromagnetic transition in the double-exchange model on the pyrochlore lattice

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Abstract. The double-exchange model, which has been extensively studied in the context of colossal magneto-resistance in perovskite manganese oxides, is known to exhibit a ferromagnetic metallic state at low temperatures because of the interplay between localized moments and itinerant electrons through the Hund’s-rule coupling. Here we investigate numerically the ferromagnetic transition in the double-exchange model defined on the frustrated pyrochlore lattice as a simple model for ferromagnetic pyrochlore oxides. We demonstrate that the finite-size corrections are largely reduced by implementing averages over the twisted boundary conditions in the Monte Carlo simulation, which enables to estimate the ferromagnetic transition temperature in relatively small size clusters. The estimate is compared with that for the non-frustrated cubic lattice system.

1. Introduction
The double-exchange (DE) model is a minimal model which explicitly incorporates the interplay between itinerant electrons and localized magnetic moments. The Hamiltonian is given by

$$H = -\sum_{\langle ij \rangle\sigma} t (c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}) - J_H \sum_i \mathbf{s}_i : \mathbf{S}_i - \mu \sum_i n_i,$$

where $c_{i\sigma}$ ($c_{i\sigma}^\dagger$) is an annihilation (creation) operator of an electron with spin $\sigma$ at site $i$, $t$ is the transfer integral for nearest-neighbor sites $\langle ij \rangle$, $\mathbf{s}_i$ and $\mathbf{S}_i$ are spin operators of itinerant electron and localized spin, respectively, which are coupled by the Hund’s-rule coupling $J_H$, $n_i = \sum_{\sigma} c_{i\sigma}^\dagger c_{i\sigma}$ is the density operator, and $\mu$ is the chemical potential. The localized spins $\mathbf{S}_i$ are treated as classical vectors. The model was originally introduced by Zener [1], and has been studied for understanding the physics of perovskite manganese oxides [2, 3]. In particular, the rediscovery of colossal magneto-resistance phenomena have stimulated extensive studies for the DE systems, including some extensions of the model such as the super-exchange interaction between localized moments, orbital degeneracy of itinerant electrons, and electron-phonon couplings [4, 5].

The model (1) is known to exhibit a ferromagnetic metallic state at low temperature ($T$) to gain the kinetic energy of electrons by aligning localized moments in parallel. This is called the DE mechanism [1]. There have been many efforts to estimate the ferromagnetic transition temperature $T_c$ [6]. For the model on the three-dimensional cubic lattice, $T_c$ was determined...
precisely by a large-scale Monte Carlo simulation: For example, $T_c/t = 0.136(2)$ at the electron density $n = 0.5$ in the limit of $J_H/t \to \infty$ [7].

In this contribution, we present our numerical results for the ferromagnetic transition when the model is defined on the geometrically frustrated lattice structure. Among many frustrated lattice structures, we consider the pyrochlore lattice, which is a three-dimensional network of corner-sharing tetrahedra as shown in Fig. 1(a). One of the experimental motivations is found in a family of Mo pyrochlore oxides $R_2\text{Mo}_2\text{O}_7$: When the ionic size of rare earth element $R$ is relatively large such as $R = \text{Nd}$ and $\text{Sm}$, the compounds become ferromagnetic metal at low $T$ [8, 9], and it was pointed out by the first principle calculations that the DE mechanism plays a key role for this behavior [10]. As a first step toward the understanding of thermodynamic properties of the pyrochlore systems, below we will investigate the ferromagnetic transition by Monte Carlo calculations for the simplest case, i.e., the model (1) in the limit of $J_H/t \to \infty$.

![Pyrochlore lattice structure.](image1)

**Figure 1.** (a) Pyrochlore lattice structure. The box indicates the cubic unit cell. (b) Density of states per site for the non-interacting model on the pyrochlore lattice.

### 2. Monte Carlo Simulation with Averaging over Twisted Boundary Conditions

We employ a Monte Carlo method to take account of large fluctuations in the frustrated system. The method is a standard one in which configurations of classical localized spins are sampled by Monte Carlo procedure; the Monte Carlo weight is calculated by the exact diagonalization of the fermion Hamiltonian matrix for a given spin configuration. The bottleneck of the calculations is the exact diagonalization, which usually limits the accessible system sizes to several hundreds sites. An improved method based on the polynomial expansion of the density of states was developed by the authors [11, 12], but for frustrated systems, in general, the method becomes less efficient because of singular form of the density of states: Indeed, in the present pyrochlore case, the density of states exhibits a $\delta$-functional peak due to two flat bands ($\omega/t = 2$) as well as two van-Hove singularities ($\omega/t = 0$ and $-4$) in the non-interacting model as shown in Fig. 1(b). Therefore we here employ the standard method.

To enable systematic analysis within the limited system sizes, we apply a technique of averaging over the twisted boundary conditions [13, 14]. In this technique, a twisted boundary condition is imposed with replacing the transfer integral $t$ by $t \exp(i\phi \cdot \delta_{ij})$, where $\phi$ denotes a magnetic flux and $\delta_{ij}$ represents the vector connecting the nearest-neighbor sites $(ij)$. The average is taken by the integral over $\phi$, which is approximately calculated by the sum over $N_{\phi}$ grid points. It has been shown that the procedure reduces finite size effects originating from the discreteness of the wave numbers.

It is shown for the model (1) that in the limit of $N_{\phi} \to \infty$, the averaging procedure for a state of a finite size cluster with a given set of spin configurations provides results for the infinite size system which consists of a periodic array of the finite size cluster. For example, for the perfectly ordered ferromagnetic state, the averaging procedure with $N_{\phi} \to \infty$ for any
finite size cluster gives the exact result in the thermodynamic limit. In order to take this advantage, we apply the averaging procedure to each Monte Carlo snapshot for calculating the Monte Carlo weight. This corresponds to ensemble average over the independent systems with different boundary conditions. In the following calculations, we take the average over the grid points with \( \phi = ((2m_x - 1)\Delta \phi, (2m_y - 1)\Delta \phi, (2m_z - 1)\Delta \phi) \), where \( \Delta \phi_{\nu} = \pi / 2L_{\nu}l_{\nu} \) and \( m_{\nu} = 1, 2, \cdots, l_{\nu} (\nu = x, y, z) \). Here, \( N_{\phi} = l_x \times l_y \times l_z \) and \( N_s = L_x \times L_y \times L_z \times 16 \).

We demonstrate here the efficiency of the averaging technique by calculating the electron density \( n \) as a function of \( T \). We show the Monte Carlo results at \( \mu = 0 \) in Figs. 2 and 3 as an example. In Fig. 2, we present \( N_{\phi} \) dependence for two different system sizes. In both cases, the results converge onto a single curve as increasing \( N_{\phi} \). Furthermore, the necessary \( N_{\phi} \) for the convergence becomes smaller as the system size \( N_s \) increases. Figure 3 shows \( N_s \) dependence with and without taking averages. In the case without taking averages, the results are largely scattered for different system sizes as shown in Fig. 3(a). In contrast, as in Fig. 3(b), when we take averages over a sufficient number of \( N_{\phi} \) chosen for each system size, all the results converge onto a single curve and the finite size effects are sufficiently small, even for the rectangular-shaped clusters. We have checked the efficiency in wide parameter regions of \( \mu \) and \( T \) and confirmed that the averaging procedure is efficient enough to suppress the finite size effects coming from the discreteness of the wave numbers. We adopt \( N_{\phi} \) used in Fig. 3(b) for each \( N_s \) in the following calculations.

![Figure 2](image1.png)

**Figure 2.** \( T \) dependence of the electron density \( n \) at \( \mu = 0 \) for different numbers of grid points \( N_{\phi} \). (a) The system size \( N_s = 1 \times 1 \times 1 \times 16 \) and (b) \( N_s = 2 \times 2 \times 2 \times 16 \). The lines are guides for the eyes.

![Figure 3](image2.png)

**Figure 3.** \( T \) dependence of \( n \) at \( \mu = 0 \) for different system sizes \( N_s \) (a) without taking average \( (N_{\phi} = 1 \times 1 \times 1) \) and (b) with taking average \( N_{\phi} \) (the numbers are shown in the legend). The lines are guides for the eyes.
3. Results and Discussion

Applying the method above, we investigate the magnetic behavior of the model (1) in the limit of $J_H/t \to \infty$ at the electron density $n = 0.5$. The results are presented in Fig. 4. At $T/t \simeq 0.14$, the square of total magnetization per site $m = \sum_i S_i/N_s$ grows rapidly [Fig. 4(a)] and the uniform magnetic susceptibility $\chi = (\langle |m|^2 \rangle - \langle |m| \rangle^2)N_s/T$ exhibits a peak [Fig. 4(b)], signaling a ferromagnetic transition. We estimate $T_c$ from the crossing point of the Binder parameter $g = 1 - (\langle |m|^2 \rangle^2 / 3 \langle |m|^2 \rangle^2)$ for different system sizes: The estimate is $T_c/t = 0.135(15)$.

Figure 4. $T$ dependences of (a) square of total magnetization per site, (b) uniform magnetic susceptibility, and (c) Binder parameter for the total magnetization per site. The electron density is fixed at $n = 0.5$ by controlling $\mu$.

The value of $T_c$ is quite similar to that for the cubic lattice model, $T_c/t = 0.136(2)$ [7]. This is reasonable because the DE ferromagnetism is governed by the kinetic energy of electrons, and does not strongly depend on the details of the lattice structure.

Our results demonstrate that systematic and quantitative study of the phase diagram is feasible within relatively small size clusters by implementing the averaging procedure over twisted boundary conditions in the Monte Carlo calculations. This gives a starting point for further study of frustrated DE-based models and for understanding the physics of pyrochlore-based ferromagnets such as Mo pyrochlore oxides. Studies of phase competitions in the model including the super-exchange coupling between localized moments are in progress.

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