Effective Ruderman-Kittel-Kasuya-Yosida-like interaction in diluted double-exchange model: self-learning Monte Carlo approach

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We study the site-diluted double exchange (DE) model and its effective Ruderman-Kittel-Kasuya-Yosida-like interactions, where localized spins are randomly distributed, with the use of the Self-learning Monte Carlo (SLMC) method. The SLMC method is an accelerating technique for Markov chain Monte Carlo simulation using trainable effective models. We apply the SLMC method to the site-diluted DE model to explore the utility of the SLMC method for random systems. We check the acceptance ratios and investigate the properties of the effective models in the strong coupling regime. The effective two-body spin-spin interaction in the site-diluted DE model can describe the original DE model with a high acceptance ratio, which depends on temperatures and spin concentration. These results support a possibility that the SLMC method could obtain independent configurations in systems with a critical slowing down near a critical temperature or in random systems where a freezing problem occurs in lower temperatures.

I. INTRODUCTION

Interactions between itinerant electrons and localized spins have attracted much attention in magnetic materials such as Manganese.\textsuperscript{[10]} The double-exchange (DE) model, a fundamental model of the itinerant magnetism, has also attracted much attention from theoretical and experimental points of view, since its itinerant nature yields various rich phases.\textsuperscript{[6–11]}

The electron-spin interaction in weak coupling regime in the DE model is approximated by the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction between localized spins, whose coupling constant oscillates and decays with the distance between localized spins.\textsuperscript{[12–14]} In the diluted magnetic alloys (e.g., AuFe and CuMn)\textsuperscript{[15]} the spin glass (SG) order, where spins freeze in the spatially random manner, is explained by existence of the RKKY interaction between randomly localized spins. The SG state shows novel transport phenomena due to the random spin structure.\textsuperscript{[16–17]} The nature of SG, however, is still under debate even if it is treated as a simplified classical spin model, so-called Edwards-Anderson model, whose exchange coupling constants are given by a certain probability distribution.\textsuperscript{[18–20]}

Even treating localized spins as classical ones, the studies beyond the weak coupling regime are not trivial since itinerant electrons play a more important role in the DE model due to its quantum nature. For example, the existence of the SG order in the site-diluted DE model has not been theoretically confirmed yet. A standard method to simulate classical spins is the Markov chain Monte Carlo (MCMC) method. In the DE model, however, computational complexity is huge due to a fermion determinant for itinerant electrons. For example, this naive calculation takes $\mathcal{O}(N^4)$ per sweep with the system size $N$ since a full diagonalization is needed to estimate the fermion determinant for each Monte Carlo step. Many alternative algorithms to simulate electrons coupled to given spin configurations for each Monte Carlo step. Many alternative algorithms to simulate electrons coupled to classical fields have been developed.\textsuperscript{[21–27]}

In MCMC methods for physics, obtaining independent configurations sometimes becomes hard near a critical temperature or at low temperatures. A critical slowing down of the autocorrelation time near the critical temperature is a famous effect when the update algorithm for generating configurations is local. Cluster global update algorithms such as the Wolff algorithm\textsuperscript{[28]} and the Swendsen-Wang algorithm\textsuperscript{[29]} are usually adopted for reducing the autocorrelation time if one can consider a model where these algorithms are available. The freezing problem is caused by the multi-valley structure of the energy landscape manifested at low temperatures, and the states are trapped in the local minima. The freezing problem appears in random systems such as the SG systems and makes difficult its MCMC simulations. In principle, one can reach the true minima in finite-temperature systems after many Monte Carlo (MC) steps.

Recently, an efficient MCMC algorithm combined with a machine-learning technique, the self-learning Monte Carlo (SLMC) method, was proposed.\textsuperscript{[30]} The SLMC method constructs effective models to generate the Boltzmann weight by means of machine learning from gathered original Markov chains. Once an effective model is prepared, we can perform MCMC simulations of the original models using the effective models trained. It was shown that SLMC reduces the number of the MC steps of the original model even near the critical slowing down.\textsuperscript{[30–31]} The SLMC method accelerates a simulation of a model where cluster algorithms are unavailable by using an effective model where cluster algorithms are available such as the Ising model.\textsuperscript{[30]} As shown in Fig. 1, with the use of the SLMC, we can bypass heavy numerical computations coming from an estimation of the original model. This
of the RKKY interaction, which was used also for the random systems. If one uses a very complicated effective model similar to the RKKY interaction even in strong coupling regime. To prove it, We employed the SLMC model as the learning data by performing MCMC simulation of the original model. We optimize the effective model by using the generated learning data so that it generates $W_{\text{eff}}(S)$ closer to original $W(S)$. We adopt a site-diluted two-body classical spin interaction up to 6th neighbor, as in the previous study for the regular DE model. The effective Hamiltonian is expressed as

$$ H_{\text{eff}} = E_0 - \sum_{\langle i,j \rangle} J_{\text{eff}} n p_i p_j S_i \cdot S_j, $$

where, $\{E_0, J_{\text{eff}} n\}$ are trainable parameters which we optimize. The difference from the previous study is that we only consider the interactions between randomly arranged spins. In the appendix, we explain details for optimizing the effective model.

"Earn" is the actual simulation of the original model using the effective model optimized. The acceptance ratio from current state $S$ to a new state generated by the MCMC of the effective model $S'$ is given by

$$ p(S \rightarrow S') = \min \left\{ 1, \frac{W(S')}{W(S)} \frac{W_{\text{eff}}(S)}{W_{\text{eff}}(S')} \right\}, $$

which is known as the Metropolis-Hastings test. We note that a proposed state $S'$ is cumulatively updated and the length of the effective Markov chain is not limited. We can update states as long as we need to reduce autocorrelations since the acceptance ratio is converged as a functional of the length of the effective Markov chain.

In the effective MCMC, we use the heatbath and the overrelaxation procedure, which is known as an effective update algorithm in classical spin systems. After 200 effective MC steps, where one step includes one heatbath seeps and four overrelaxations, the Metropolis-Hastings

property is also useful for solving the freezing problem.

It is not trivial whether the SLMC method is efficient for random systems. If one uses a very complicated effective model with deep neural networks, the original model might be reproduced by the effective model. However, in terms of the computational complexity of actual MCMC simulations, a simple effective model is needed to bypass heavy numerical computations. In the week coupling regime, there is a simple effective model known as the RKKY interaction, which was used also for the randomly distributed spin systems.

In this paper, we show that there is a simple effective model similar to the RKKY interaction even in strong coupling regime. To prove it, We employed the SLMC method with the cumulative update for fermions coupled to the classical field. We first checked success or failure through the acceptance ratio. Next, we investigated the properties of the effective models trained. The main issues are the dependencies of temperature and distance between localized spins of the effective models trained. The temperature dependence was not investigated in the site-diluted DE model and also in the regular DE model previously.

The letter is organized as follows. First, we introduce the site-diluted DE model. Next, we explain how to perform the SLMC simulation and show obtained results for the site-diluted DE model. Finally, we summarize and give some discussions.

II. MODEL AND METHOD

In this paper, we focus on the site-diluted DE model on three-dimensional cubic lattice to examine the efficiency of the SLMC method. The site-diluted DE model (i.e., site-diluted ferromagnetic Kondo model) is defined as follows:

$$ \hat{H} = -t \sum_{\sigma, \langle i, j \rangle} (\hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} + \text{h.c.}) - \frac{J}{2} \sum_i p_i S_i \cdot \hat{\sigma}_i - \mu \sum_{\sigma, i} \hat{c}^\dagger_{i\sigma} \hat{c}_{i\sigma}, $$

where $S_i$ and $\hat{\sigma}_i$ are the classical Heisenberg spins and the Pauli matrices respectively. $t > 0$ and $J > 0$ are the hopping and coupling constant. $p_i$ is a binary random number (0 or 1) which represents whether the site $i$ is occupied ($p_i = 1$) or not ($p_i = 0$) with a localized spin. When $p_i$ is always 1 for a arbitrary $i$, the model corresponds to the regular DE model. It is known the regular DE model holds the ferromagnetic order for enough large $J/t$. For simplicity, we utilize a semiclassical approximation where localized spins are classical ones and energy of the electrons changes instantaneously with change of the localized spins i.e., the localized spins are "time-independent".

The partition function of the model $Z$ is given by

$$ Z = \sum_{S} W(S), $$

where $W(S) \equiv \prod_n (1 + e^{\beta E_n(S)})$ is the Boltzmann weight with a spin configuration $S$. Here, $\{E_n(S)\}$ is the eigen spectrum.

We show a summary of the procedure of the SLMC simulation in Fig. 1. The SLMC method is based on two procedures: "learn" and "earn". "Learn" is the training procedure of the effective models. We generate $W(S)$ of the original models as the learning data by performing MCMC simulation of the original model. We optimize the effective model by using the generated learning data so that it generates $W_{\text{eff}}(S)$ closer to original $W(S)$. We adopt a site-diluted two-body classical spin interaction up to 6th neighbor, as in the previous study for the regular DE model. The effective Hamiltonian is expressed as

$$ H_{\text{eff}} = E_0 - \sum_{\langle i,j \rangle} J_{\text{eff}} n p_i p_j S_i \cdot S_j, $$

where, $\{E_0, J_{\text{eff}} n\}$ are trainable parameters which we optimize. The difference from the previous study is that we only consider the interactions between randomly arranged spins. In the appendix, we explain details for optimizing the effective model.

"Earn" is the actual simulation of the original model using the effective model optimized. The acceptance ratio from current state $S$ to a new state generated by the MCMC of the effective model $S'$ is given by

$$ p(S \rightarrow S') = \min \left\{ 1, \frac{W(S')}{W(S)} \frac{W_{\text{eff}}(S)}{W_{\text{eff}}(S')} \right\}, $$

which is known as the Metropolis-Hastings test. We note that a proposed state $S'$ is cumulatively updated and the length of the effective Markov chain is not limited. We can update states as long as we need to reduce autocorrelations since the acceptance ratio is converged as a functional of the length of the effective Markov chain.

In the effective MCMC, we use the heatbath and the overrelaxation procedure, which is known as an effective update algorithm in classical spin systems. After 200 effective MC steps, where one step includes one heatbath seeps and four overrelaxations, the Metropolis-Hastings

FIG. 1. A brief schematic summary of the SLMC procedure. The computational costs of the SLMC method are cheaper than one of the naive Monte Carlo calculation.
test determined by Eq. (11) is done with the proposed spin configuration. We use an annealing-like training process to obtain effective models with different temperatures. We first gather training data set and train the effective model \( H_{\text{eff}} \) at a higher temperature (at \( T = 0.4 \) in this paper). To obtain the effective models in lower temperatures, we use the SLMC with the effective model constructed in the higher temperature and update the model using current data.

We set \( t \) as unity and \( J/t = 16 \) and \( \mu = 8 \), which possesses the ferromagnetic order in the regular case and keep near the quarter filling. We used the 3d cubic lattice \( N = 4^3 \) and we averaged over 5 different realizations with the fixed spin concentration and investigated with decreasing spin concentrations.

III. RESULTS

A. Acceptance ratios

We investigate the averaged acceptance ratio of the SLMC. The acceptance ratio shows how many proposed spin configurations are accepted during simulations. If the learning procedure is failed, the effective model cannot fit the original Boltzmann weight \( W(S) \) with a given spin configuration \( S \). Such as bad proposal is almost rejected and the acceptance ratio becomes very low, which means a failure of a simulation. The averaged acceptance ratio is estimated as \( p \sim e^{-\sqrt{\text{MSE}_{H}}} \) with the use of mean-squared error (MSE) between the original and effective energy given as:

\[
\text{MSE} = \frac{1}{N_S} \sum_S \left( \log W(S) - \log W_{\text{eff}}(S) \right)^2,
\]

where \( N_S \) is the number of spin configurations. A high acceptance ratio is important for reducing an autocorrelation time\(^6\). We define the autocorrelation time \( \tau_A \) for the observable \( A \) in the original MC simulation. If the number of effective MC steps is larger than \( \tau_A \), the proposed spin configuration is uncorrelated. Since the proposed configuration is accepted with the probability \( p \), an uncorrelated configuration is obtained after \( 1/p \) times Metropolis-Hastings tests. Therefore, the acceptance ratio represents the quality of the effective model and criteria whether the simulations work well or not.

The averaged acceptance ratios are shown in Fig. 2. In systems with different classical spin concentrations. In the regular model where classical spins are located on all lattice points (\( N_{\text{spin}} = 64 \)), there is a ferromagnetic transition at \( T_c \sim 0.1 \).\(^7\) We find that there is no drastic change of the acceptance ratio around a critical temperature. This is naturally explained by that the effective interactions do not change between different phases. The temperature dependence of the acceptance ratio is explained by the temperature dependence of the MSE as follows. The temperature dependence of the effective action \( \log W_{\text{eff}}(S) \) is described by \( \log W_{\text{eff}}(S, \beta) = -\beta H_{\text{eff}}(S, \beta) \). Therefore, the averaged acceptance ratio is estimated as

\[
p \sim \exp \left( -\sqrt{\text{MSE}_{H}} \sqrt{T} \right),
\]

where \( \text{MSE}_{H} = \frac{1}{N_S} \sum_S \left| \log W(S) - H_{\text{eff}}(S, \beta) \right|^2 \). Since the temperature dependence of the acceptance ratio shown in Fig. 2 is well explained by the function \( e^{-a\sqrt{1/T}} \), the mean-squared error of the original and effective Hamiltonian does not depend on the temperature much. We note that the effective Hamiltonian itself depends on the temperature as shown in the latter part of this paper.

The above analysis can be applied to cases of different spin concentrations. The acceptance rates are kept 40% below to \( T = 0.1 \). This means the SLMC method works well with the site-diluted DE model. We find that if a system has less localized spins the acceptance ratio becomes high. This suggests that there is an effective two-body classical spin-spin interaction in the strong coupling regime where \( J/t = 16 \) in this paper.

B. Spin concentration and temperature dependence of the effective models

We investigate the spin concentration and temperature dependence of the effective model with the use of the SLMC. In the weak coupling regime, it is well known that the RKKY interaction does not depend on temperature since the RKKY interaction is derived from the second-order perturbation method. It is also known that the RKKY interaction does not depend on the spin configuration since this is a two-body interaction between spins. In the regular DE model reported in the previous

![Fig. 2. The acceptance ratios versus the temperature with different spin concentrations for localized spins. The acceptance ratios keep at least 40% until \( T = 0.1 \) for all spin concentrations.](image)
TABLE I. Effective long-range interactions $T = 0.4$

| $N_{\text{spin}}$ | $E_0$     | $J_1$     | $J_2$     | $J_3$     | $J_4$     | $J_5$     | $J_6$     |
|------------------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
| 64               | -55.253(1)| 0.0691(1) | -0.00739(9)| 0.00234(5)| -0.00158(6)| 0.00047(4)| -0.00033(3)|
| 56               | -48.02(1) | 0.0732(2) | -0.00747(9)| 0.00222(2)| -0.00202(9)| 0.00047(9)| -0.00034(5)|
| 48               | -40.85(2) | 0.0781(2) | -0.0072(2) | 0.0017(2) | -0.00231(1)| 0.00051(9)| -0.00027(8)|
| 40               | -33.77(3) | 0.0837(7) | -0.0069(2) | 0.00120(6)| -0.00152(2)| 0.00024(5)| -0.00003(10)|
| 32               | -26.86(3) | 0.091(1)  | -0.0068(2) | 0.0011(1) | -0.0017(2) | 0.00028(6)| -0.00006(10)|
| 24               | -20.02(2) | 0.095(1)  | -0.0064(4) | 0.0006(2) | -0.0021(2) | 0.00092(12)|
| 16               | -13.36(2) | 0.101(1)  | -0.0070(5) | 0.00006(42)| -0.0017(2) | 0.00009(11)|

TABLE II. Effective long-range interactions $T = 0.1$

| $N_{\text{spin}}$ | $E_0$     | $J_1$     | $J_2$     | $J_3$     | $J_4$     | $J_5$     | $J_6$     |
|------------------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
| 64               | -52.30(1) | 0.0744(7) | -0.0087(2) | 0.0041(1) | -0.0004(4)| 0.0007(2) | -0.0004(2)|
| 56               | -45.33(1) | 0.0794(7) | -0.0099(4) | 0.0043(5) | -0.0015(2)| 0.0007(2) | -0.0004(2)|
| 48               | -38.38(2) | 0.0841(9) | -0.0087(5) | 0.0035(5) | -0.0023(5)| 0.0001(2) | -0.0005(2)|
| 40               | -31.58(6) | 0.090(2)  | -0.0099(9) | 0.0041(1) | -0.0017(8)| 0.0006(1) | -0.0006(5)|
| 32               | -24.97(5) | 0.101(3)  | -0.010(1)  | 0.0034(7) | -0.0015(5)| 0.0009(2) | -0.0012(2)|
| 24               | -18.46(2) | 0.111(2)  | -0.0103(8) | 0.0028(2) | -0.0025(7)| 0.0012(2) | -0.0007(2)|
| 16               | -12.25(3) | 0.116(3)  | -0.013(2)  | 0.002(1)  | -0.0015(9)| 0.0001(4) | 0.0003(4)|

FIG. 3. The coupling constants $J_n^{\text{eff}}$ of the trained effective models versus distances between localized spins at $T = 0.1$ and $T = 0.4$.

It was found that the effective coupling constants oscillate and decay as a function of the distance between localized spins, which is similar to the RKKY interactions. In Fig. 3, we show the coupling constants $J_n^{\text{eff}}$ of the trained effective models against distances between spins at $T = 0.1$ and $T = 0.4$ in different spin concentration systems. In the Table II ($T = 0.4$) and the Table I ($T = 0.1$), we summarize the obtained values of $J_n^{\text{eff}}$. Here, $n = 1$ means the nearest neighbor coupling and $n = 2$ the next-nearest neighbor coupling, and so on.

As shown in Fig. 3, we find the RKKY features, oscillating and decaying behavior as a functional of the distance between spins, for all spin concentrations at both a higher temperature $T = 0.4$ and a lower temperature $T = 0.1$. However, the amplitude of the couplings depends on the spin concentrations and the temperatures. The spin concentration dependence suggests that this effective "RKKY" interaction in the strong coupling regime can not be derived from second-order perturbation theory. The high acceptance ratio is shown in Fig. 2 indicates that this effective two-body interaction well describes the original model and there are some renormalizations from many-body effects.

We show the temperature dependence of the effective coupling constants $J_n^{\text{eff}}$ in the trained effective models for each distance $n$ with different spin concentrations, as shown in Fig. 3. The characteristics are different for the nearest neighbor $n = 1$ and other cases. For the nearest neighbor $n = 1$, temperature dependencies are relatively smaller with small error bars. On the other hand, for other cases, temperature dependencies are nonmonotonic and relatively larger. The number of further interactions is fewer than nearer ones, therefore, they are relatively irrelevant and can easily fluctuate. Since the temperature dependence of the effective coupling constants is not so strong, the "annealing" procedure that we use to obtain the effective model in lower temperature works well in the site-diluted DE model.

As seen in the acceptance ratios calculated, the temperature dependence of the effective model is small. On the other hand, we observed temperature-dependent be-
FIG. 4. The coupling constants $J_{\text{eff}}^n$ of the trained effective models versus temperature. The error bars are defined as standard error over different localized spin realizations.

Behavior in the effective coupling constant trained. The effective model $H_{\text{eff}}$ is optimized minimizing MSE$_{\text{H}}$ and satisfying $H_{\text{eff}}(S, \beta) \approx \log W(S, \beta)$. This means an effective model should mimicks not energy but local “free energy” at finite temperature. The “entropy”, therefore, may cause temperature-dependent behavior of effective models.

There is another possible explanation for the existence of temperature dependence. In terms of the quantum field theory, one has to integrate out the electron degrees of freedom to obtain effective classical interactions. Two classical spins interact with each other through electron Green’s functions in the effective Lagrangian. At zero temperature, such a Green’s function has been obtained as a result of the exact summation of the Born series. At finite temperature, the electron Green’s function depends on temperatures. The SLMC imitates this effective model in the Hamiltonian formalism with the use of the temperature-dependent coupling constant.

We show that the SLMC works well in random systems and there is a simple effective model. There are two ways to study the SG transition in the site-diluted DE model. One is the MC simulation with effective two-body interactions obtained by the SLMC. We find that, even in the strong coupling regime, there is an effective two-body interaction to describe the original DE model. Therefore, without doing the Metropolis-Hastings test, one might have good accuracy in the classical MC simulation with this effective interaction. The other is the SLMC with the use of the two-body classical spin interactions. To grasp the tail of the SG transition, one has to calculate systems in various sizes with fixed spin concentration, which takes much time. By accelerating the MCMC simulations with the use of the SLMC, one can study whether the SG transition occurs in the DE model or not, which is still an open question. We note that a transition temperature of the SG transition would be much lower than one of the ferromagnetic transition due to spin frustrations. For the challenge to the problems of the SG transition in the itinerant electron systems, larger system sizes and much lower-temperature simulations are needed. The temperature exchange method is usually used for the classical localized SG models and will make our simulation better, but combinations of the temperature exchange method and the SLMC method are future work.

IV. SUMMARY

We performed the self-learning Monte Carlo methods to the semiclassical site-diluted double-exchange model. With decreasing localized spin concentrations, we observed modest acceptance rates and the effective models kept RKKY behavior, which oscillates and decays with distance. As well as the regular DE model, the SLMC method works well with the diluted DE model. We found that effective RKKY-like interaction depends on the spin
concentrations and temperature, while the RKKY interaction derived in the weak coupling regime does not depend on both. We showed that the SLMC works well in random systems and there is a simple effective model in a strong coupling regime.

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**Appendix: details of optimization procedure of effective models**

In this appendix, we will explain details how to optimize the effective models. We assume the effective model as $H_{\text{eff}}(S, \beta) = \sum_{(i,j)\in n} J_{n}^{\text{eff}}(\beta) S_i \cdot S_j(S)$ and consider up to $N_{\text{eff}}$th neighbor interactions at inverse temperature $\beta$.

We prepare $M$ states $S_1, \ldots, S_M$ as training data and $C_n(S) \equiv \sum_{(i,j)\in n} S_i \cdot S_j(S)$. A matrix $C$ and a vector $J$ are defined as follows:

$$C \equiv \begin{pmatrix} 1 & C_1(S_1) & \cdots & C_{N_{\text{eff}}}(S_1) \\ \vdots & \vdots & \ddots & \vdots \\ 1 & C_1(S_M) & \cdots & C_{N_{\text{eff}}}(S_M) \end{pmatrix},$$

$$J \equiv \begin{pmatrix} E_0 \\ J_1^{\text{eff}} \\ \vdots \\ J_{N_{\text{eff}}}^{\text{eff}} \end{pmatrix}.$$

We also define a vector $\mathcal{H} \equiv \{ \mathcal{H}(S_1), \ldots, \mathcal{H}(S_M) \}$ is aligned energies calculated via states as training data. For the actual simulation you should restore $C$ used the following procedure.

$J$ which give a minimum of $\| \mathcal{H} - C J \|^2$ is a solution of the normal equation $\mathcal{C} C J = \mathcal{C} \mathcal{H}$ and it becomes $J = (\mathcal{C} C)^{-1} \mathcal{C} \mathcal{H}$. The number of learning parameters to train is a few (only $N_{\text{eff}}$ parameters), a direct calculation of the $N_{\text{eff}} + 1$ dimensional inverse matrix $(\mathcal{C} C)^{-1}$ is not expensive. Of course, if the number of learning parameters is large, you should use an iterative method.
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