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Double Exchange Model in Triangular Lattice Studied by Truncated Polynomial Expansion Method

Gui-Ping Zhang*

Department of Physics, Renmin University of China, Beijing 100872, China.

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Abstract. The low temperature properties of double exchange model in triangular lattice are investigated via truncated polynomial expansion method (TPEM), which reduces the computational complexity and enables parallel computation. We found that for the half-filling case a stable 120° spin configuration phase occurs owing to the frustration of triangular lattice and is further stabilized by antiferromagnetic (AF) superexchange interaction, while a transition between a stable ferromagnetic (FM) phase and a unique flux phase with small finite-size effect is induced by AF superexchange interaction for the quarter-filling case.

AMS subject classifications: 82B05, 26C99, 65F99, 15A30

Key words: Manganite, Monte Carlo simulation, polynomial moment expansion, triangular lattice, frustration, finite-size effect.

1 Introduction

Doped manganite has become one of the most important strongly correlated systems, since colossal magnetoresistance (CMR) effect was discovered in 1990s (see [1,2]). CMR is referred to the resistivity of material change orders of magnitude under external magnetic field and it may have a potential application in computer technology or even spintronics. There are rich phase diagrams and many ordered phase [3], rising from delicate interaction between electron, spin and orbit degree of freedoms. Further it is found that the phase separation [4] (PS) may be crucial to CMR effect.

Double-exchange model, as a starting point to study manganite, describes the Hund interaction between itinerant electron and localized spin of Mn atoms and is expressed by

$$H_{DE} = -t \sum_{\langle ij\rangle,\alpha} (C^{\dagger}_{i,\alpha} C_{j,\alpha} + h.c.) - J_H \sum_{i,\alpha,\beta} C^{\dagger}_{i,\alpha} \sigma_{\alpha\beta} C_{i,\beta} \cdot S_i, \tag{1.1}$$

*Corresponding author. *Email address:* zhanggp96@ruc.edu.cn (G.-P. Zhang)

where the nearest-neighbor hopping integral t is adopted as the energy unit, J_H is the Hund interaction strength, $C^{\dagger}_{i,\alpha}$ ($C_{i,\alpha}$) creates (annihilates) one electron at site i with spin α, $\langle ij\rangle$ stands for the nearest neighbors of lattice site, and $\sigma_{\alpha\beta}$ is the Pauli matrix. The localized spin S_i at site i is assumed as 1 here. In addition, antiferromagnetic (AF) superexchange is crucial to stabilize AF phase of some underdopped narrow-band manganite, and this interaction is expressed by $H_{AF}=J_{AF}\sum_{\langle ij\rangle}S_i\cdot S_j$. So the total hamiltonian is $H=H_{DE}+H_{AF}$. In this model, localized spins is treated as a classic field ϕ and electron degree of freedom can be integrated for any given localized spin configuration. The partition function is expressed by

$$Z=\mathrm{Tr_c}\,\mathrm{Tr_F}\left(e^{-\beta[H(\phi)-\mu n_e]}\right)=\mathrm{Tr_c}\,e^{-S_{\mathrm{eff}}(\phi)},$$

and the effective action is

$$S_{\mathrm{eff}}(\phi)=-\sum_{\nu}\ln\left(1+e^{-\beta(\epsilon_\nu-\mu)}\right)+\beta E(\phi).$$

Here ϵ_ν is the ν-th eigenvalue of one-electron sector's Hamiltonian matrix $H(\phi)$, $E(\phi)$ is the interaction energy between spins, β is the inverse temperature, μ is the chemical potential, and n_e is the electron number operator, respectively. The fluctuation of localized spins is suitable for Monte Carlo (MC) simulation, and the partition sum is replaced by stochastic samplings with the Boltzmann weight $e^{-S_{\mathrm{eff}}(\phi)}/Z$. With MC simulation, an intrinsic PS between high electron density and low electron density has been reproduced in doped manganites [5].

Despite the success of reproducing PS, the above method is suffered from finite-size effect, since the computational complexity of exact diagonalizing (DIAG) $H(\phi)$ scales as $\mathcal{O}(N^4)$, with N being the system size. In order to overcome the above restriction, Furukawa and Motome [6, 7] proposed Chebyshev polynomials expansion method(PEM) and the computational complexity became $\mathcal{O}(MN^3)$ at a finite cutoff M. In 2004 they further reduced the computational complexity to $\mathcal{O}(N)$ via truncated polynomial expansion method (TPEM) [8, 9]. The system size [10] is extended to 40×40, compared with 10×10 via DIAG [5]. Not only the computational complexity is greatly reduced, but also parallel computation is capable under PEM and TPEM, which would increase the computational speed very much. Finally, from the viewpoint of physical properties, one-body quantity such as energy and electron density, but also dynamical quantity or two-body quantity such as conductance are able to be investigated under PEM and TPEM, and there have been several examples of application to large scale system [10–13].

Up to date, most studies focus on the double-exchange model in one- and two-dimensional square lattice. In this paper, we present our results on this model in two dimensional triangular lattice. One famous layered triangular lattice is the superconductor $Na_{0.35}CoO_2\cdot1.35H_2O$ discovered in 2003 (see [14]). Though triangular lattice structure is not found in manganite yet, it is still meaningful to study the interplay between electron, spin and lattice for double exchange model in two dimensional triangular lattice.