Rapid Communication

Quantum Monte Carlo study on the phase transition for a generalized two-dimensional staggered dimerized Heisenberg model*

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In order to gain a deeper understanding of the quantum criticality in the explicitly staggered dimerized Heisenberg models, we study a generalized staggered dimer model named the J_0–J_1–J_2 model, which corresponds to the staggered J–J' model on a square lattice and a honeycomb lattice when J_1/J_0 equals 1 and 0, respectively. Using the quantum Monte Carlo method, we investigate all the quantum critical points of these models with J_1/J_0 changing from 0 to 1 as a function of coupling ratio $\alpha = J_2/J_0$. We extract all the critical values of the coupling ratio α_c for these models, and we also obtain the critical exponents ν, β/ν, and η using different finite-size scaling ansätz,. All these exponents are not consistent with the three-dimensional Heisenberg universality class, indicating some unconventional quantum critical points in these models.

Keywords: staggered dimer model, VBS–Neel transition, finite-size scaling, universality class

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1. Introduction

Two-dimensional (2D) $S = 1/2$ antiferromagnetic Heisenberg-type models have received considerable attention in the past two decades since the discovery of high T_c superconductivity in the cuprate materials.[1] As the appropriate model for the undoped CuO_2 layers of the cuprate superconductors, the 2D antiferromagnetic Heisenberg model has become one of the fundamental starting-points for researching strongly correlated systems. It also provides a useful template for studying quantum phase transition.[2] By introducing frustration caused by lattice geometry or competitive couplings, these models may undergo a quantum phase transition from Neel state to spin liquid state.[3] For instance, doping the cuprate oxides would drive them into a resonating valence bond (RVB) liquid state.[4] For models with locally different nearest-neighbour couplings but without frustration, the competition among these couplings may lead to an explicit valence bond solid (VBS) ground state, while for models with homogeneous couplings which keep lattic symmetry, an implicit VBS ground state may also be formed by breaking the translational symmetry spontaneously.[5,6] Much effort have been devoted to study the VBS–Neel transition in these dimerized Heisenberg models. Usually the transition can be well described by the three-dimensional Heisenberg O(3) classical universality class by mapping to a nonlineal σ model.[5−8] However, it is argued that for some models which have an implicit VBS ground state, the Berry phase terms may be relevant and thus lead to the so-called deconfined quantum critical point (DQCP),[9,10] which challenges the standard Landau–Ginzburg–Wilson (LGW) paradigm.[11,12] Afterwards, many theoretical and numerical studies[13−20] tried to confirm the validity of the DQCP theory, some of which extend to different scenarios showing that this issue is still highly controversial.

Despite of the similarity of coupled spin ladder model and staggered J–J' model, which both have spatially anisotropic interactions, while the former provides a sophisticated example of a phase transition

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that fits well with the LGW paradigm,[21] the latter is argued to be a candidate that has a DQCP,[22,23] leading to critical exponents which differ from the Heisenberg universality class in three dimensions, even though it has an explicit VBS ground state. The quantum Monte Carlo study of the staggered J–J' model by Wenzel *et al.*[24] offers unexpected critical exponents and, indeed, indicates some nontrivial contributions to the quantum critical point that may be triggered by the staggered arrangement of couplings. However, it is argued that this unconventional phase transition is due to a cubic irrelevant term[25] which leads to the unexpected $\nu = 0.689(5)$ obtained in Wenzel's work. In addition, simulation results obtained by Jiang and Gerber[26] show that, for a staggered J–J' model on a honeycomb lattice, the unconventional $\nu = 0.689(5)$ can be obtained by a finite-size scaling ansatz using most of the available data points in conjunction with a sub-leading correction term, while the most accurate Monte Carlo value[28] of $\nu = 0.7112(5)$ for the O(3) universality class can be obtained by using the data points of large lattice sizes and considering only the leading term in finite-size scaling. However, there is no explicit answer to whether the staggered arrangement of couplings in 2D lattices will lead to an unconventional phase transition.

In order to further clarify this issue, we investigate a generalized Heisenberg-type dimer model with spatially staggered anisotropy, which is named the J_0–J_1–J_2 model (see Fig. 1). The Hamiltonian is given by

$$H = J_0 \sum_{\langle i,j\rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j + J_1 \sum_{\langle i,j\rangle'} \boldsymbol{S}_i \cdot \boldsymbol{S}_j + J_2 \sum_{\langle i,j\rangle''} \boldsymbol{S}_i \cdot \boldsymbol{S}_j, \quad (1)$$

where $\boldsymbol{S}_i$ is the onsite spin, and J_0, J_1, and J_2 are antiferromagnetic nearest-neighbour exchange couplings, as shown in Fig. 1(a). When $J_1/J_0 = 1$, this model becomes the staggered J–J' model on a square lattice (see Fig. 1(b)), with J_0 and J_2 corresponding to J and J', respectively. Obviously, for $J_1/J_0 = 0$, this model will be equivalent to the staggered J–J' model on a honeycomb lattice (see Fig. 1(c)). By means of quantum Monte Carlo simulation, we study all the transition points at the critical coupling ratio α_c, where $\alpha = J_2/J_0$, with J_1/J_0 changing from 0 to 1. We obtain the exact relation between α_c and J_1/J_0. By finite-size scaling of different observables, we extract the critical exponents, which are then used to compare with earlier results.

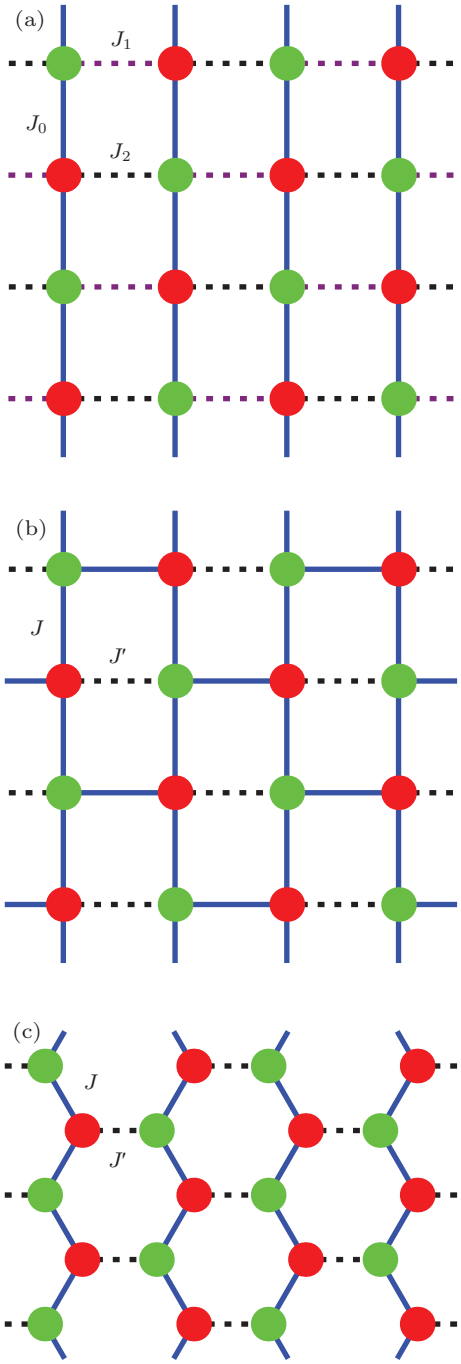


Fig. 1. (colour online) (a) Schematic of the J_0–J_1–J_2 model. (b) For $J_1/J_0 = 1$, this model becomes the staggered J–J' model on a square lattice. (c) For $J_1/J_0 = 0$, this model becomes the staggered J–J' model on a honeycomb lattice.

The rest of this paper is organized as follows. In the next section we briefly describe the observables used to detect the critical point, and then present the finite-size scaling ansatz for data analysis. The simula-

tion results are given in Section 3. In the last section, we shall discuss our results and give a summary.

2. Computational details

We perform the simulations using the loop algorithm based on the libraries of ALPS project[29] on each model for 16 different lattice sizes from $L = 10$ to $L = 80$. To detect the quantum critical point, we calculate the standard observables including staggered magnetization M_s, its second-order Binder cumulant Q_2, and the spin stiffness ρ_s, which are defined as follows:

$$M_s = \frac{1}{N}\sum_i^N (-1)^{x_i+y_i} S_i, \tag{2}$$

$$Q_2 = \frac{\langle (M_s^z)^4 \rangle}{\langle (M_s^z)^2 \rangle^2}, \tag{3}$$

$$\rho_s = \frac{3}{4\beta N}\langle W_x^2 + W_y^2 \rangle. \tag{4}$$

The W_x and W_y in Eq. (4) correspond to the winding number of worldlines along the x and y directions, and $\beta = 1/(k_B T)$ with k_B being the Boltzmann constant.

Based on the renormalization group (RG) prediction, in the vicinity of the quantum critical point, there is a scaling of the form

$$\mathcal{O}_L(t) = L^{\lambda/\nu}[1 + c(tL^{1/\nu})L^{-\omega}]g_{\mathcal{O}}(tL^{1/\nu}), \tag{5}$$

where t is the reduced coupling defined by $t = (\alpha - \alpha_c)/\alpha_c$, L is the lattice size, ν is the critical exponent of the correlation length, and λ is the critical exponent associated with the quantity $\mathcal{O}$. For the quantities Q_2 and $\rho_s L$, λ is equal to 0, while for the quantities $|m_s^z|$ and $L^2 m_s^z$, the λ/ν should be replaced by $-\beta/\nu$ and $d - z - \eta$, respectively. We set $d = 2$ so that we are dealing with a two-dimensional lattice, and we assume that the imaginary time exponent $z = 1$. $c(tL^{1/\nu})L^{-\omega}$ is the sub-leading correction term, ω is the confluent correction exponent, and $g_{\mathcal{O}}(tL^{1/\nu})$ is the universal scaling function. In practice, near the critical point, $c(x)$ with $x = tL^{1/\nu}$ can be approximated by a constant c, leading to the commonly employed form

$$\mathcal{O}_L(t) = L^{\lambda/\nu}(1 + cL^{-\omega})g_{\mathcal{O}}(x). \tag{6}$$

Near the critical point, the analytical universal function $g_{\mathcal{O}}(x)$ can be Taylor expanded. We do this up to the fourth order and thus obtain the final scaling form

$$\mathcal{O}_L(t) = L^{\lambda/\nu}(1 + cL^{-\omega})(g_0 + g_1 x + g_2 x^2 + g_3 x^3 + g_4 x^4 + \cdots), \tag{7}$$

which is used for data fitting and collapsing.

3. Main results

The results for Q_2 and $\rho_s L$ with $J_1/J_0 = 0.6$ are presented in Fig. 2, where the crossing behavior becomes more and more evident as the system size becomes larger. However, due to the restriction of computational resources and the confluent correction term, the critical coupling could only be estimated roughly by the crossing position of different large system sizes. To obtain a more precise critical point, it is better to fit the crossing points $\alpha_c(L, 2L)$ into the form[32]

$$\alpha_c(L, 2L) = \alpha_c + bL^{-1/\nu-\omega}, \tag{8}$$

which is shown in Fig. 2. Using this approach, we obtain the critical coupling $\alpha_c = 2.1904(4)$. The critical points α_c for all the situations with J_1/J_0 changing from 0 to 1 are shown in Table. 1. It can be seen that we obtain consistent results of the critical points with previous studies for both a square lattice[24] and a honeycomb lattice.[26]

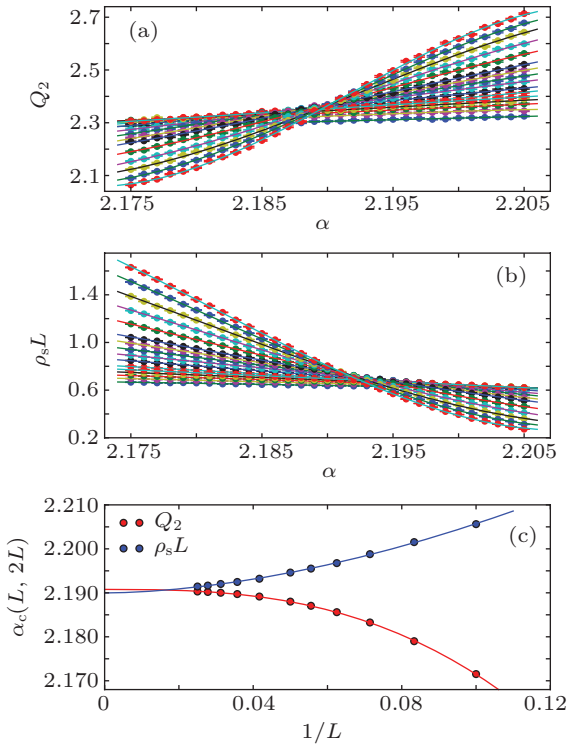


Fig. 2. (colour online) (a) The Binder cumulant Q_2 and (b) the multiplication of spin stiffness with lattice size $\rho_s L$ (middle) for various lattice sizes for $J_1/J_0 = 0.6$. The lines are the fitting results by expanding polynomial form up to the 8th order. (c) Critical coupling α_c derived from the scaling analysis of the crossing points between $Q_2(L)$ and $Q_2(2L)$ or between $\rho_s(L)$ and $\rho_s(2L)$. The lines are the fitting results according to Eq. (8).

Table 1. Fitting results for the critical couplings α_c and the critical exponents ν, β/ν, and $1-\eta$. The α_c^a is obtained from Eq. (8) using data of the crossing points, α_c^b and ν are extracted by fitting $\rho_s L$. The $L_{\min}$ is the smallest system size which is included by the data used for fitting $\rho_s L$. The β/ν and $1-\eta$ are obtained by finite-size scaling $|m_s^z|$ and $L^2 m_s^2$, respectively.

J_1/J_0	α_c^a	$L_{\min}$	α_c^b	ν	β/ν	$1-\eta$
0.0	1.7355(2)	28	1.7358(3)	0.680(7)	0.543(4)	0.914(3)
0.1	1.8067(3)	36	1.8065(4)	0.697(5)	0.541(3)	0.917(4)
0.2	1.8802(2)	28	1.8804(3)	0.687(5)	0.544(3)	0.912(4)
0.3	1.9553(3)	28	1.9553(3)	0.691(4)	0.541(3)	0.918(3)
0.4	2.0326(3)	28	2.0326(2)	0.687(4)	0.546(3)	0.908(3)
0.5	2.1110(3)	24	2.1106(4)	0.688(7)	0.546(4)	0.910(4)
0.6	2.1904(4)	24	2.1904(2)	0.685(4)	0.543(4)	0.915(3)
0.7	2.2715(2)	28	2.2714(2)	0.687(4)	0.547(3)	0.907(3)
0.8	2.3531(4)	28	2.3525(5)	0.693(8)	0.542(6)	0.916(5)
0.9	2.4358(2)	32	2.4358(2)	0.701(7)	0.541(5)	0.918(4)
1.0	2.5198(4)	40	2.5196(3)	0.689(6)	0.546(3)	0.909(3)

Another way of obtaining critical couplings as well as values of critical exponents is to fit the corresponding quantities according to Eq. (7). The Binder cumulant Q_2 we obtain is not smooth enough to make a reliable fitting. Therefore, we extract the value of α_c and ν by fitting $\rho_s L$. The fitting results of $\rho_s L$ for different values of J_1/J_0 are shown in Table. 1. A larger ν will be derived if we only fit data points of relatively large systems.[26] However, the results should be stable when the system sizes are large enough, so $L_{\min}$ determines the smallest size for the fitting result to be stable. When fitting $\rho_s L$ with large system sizes only, we could not detect a noticeable difference in the fitting results if we included a shift correction term[30,31] by replacing $x = tL^{1/\nu}$ with $x' = tL^{1/\nu} + dL^{-\phi/\nu}$. The critical couplings obtained in this way are in good agreement with the results extracted from $\alpha_c(L, 2L)$. We also obtain the same unconventional value of $\nu = 0.689$ for a square lattice.[24] Remarkably, all the values of ν for this generalized model are not consistent with the standard O(3) value $\nu = 0.7112(5)$. To check the quality of fitting results, we carry out the data collapsing for $\rho_s L$ near the critical point, as shown in Fig. 3, which displays a very good collapse quality. Recently, it was proposed that by considering the spatially staggered anisotropy, the quantity $\rho_s(\boldsymbol{x})L$ in a particular direction has much smaller confluent correction than the averaged $\rho_s L$, and will exhibit a good scaling behavior so that a consistent value of ν with the known O(3) result could be obtained.[27]

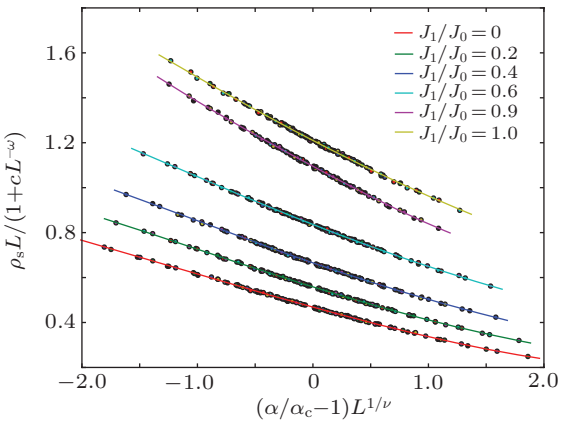


Fig. 3. (colour online) Data collapsing for $\rho_s L$. The lines represent the fitting results of the universal functions.

To obtain values of other exponents like β and η, we need to perform finite-size scaling of corresponding quantities at the quantum critical point. The critical couplings we use in this step are α_c^a resulting from $\alpha_c(L, 2L)$. The scaling graphs are shown in Fig. 4 and the resulting values of β/ν and $1-\eta$ are shown in Table 1; all results of these two exponents are quoted for lattice sizes $L > 24$. For a staggered square lattice with $J_1/J_0 = 1$, the exponents we obtain are in good accordance with previous analysis.[24] The values of β/ν and $1-\eta$ for all the situations with J_1/J_0 changing from 0 to 1 lie in the range of $(0.54, 0.55)$ and $(0.905, 0.92)$, respectively. Nevertheless, the standard O(3) values of these two exponents[28,31] should be 0.518(1) and 0.971(5). We may check the consistency of these two exponents by testing the (hyper)scaling relation $2\beta/\nu = (d + z - 2 + \eta)$, which holds true for

nearly all cases. However, as derived from almost the same quantity, β and η are likely to be strongly correlated.

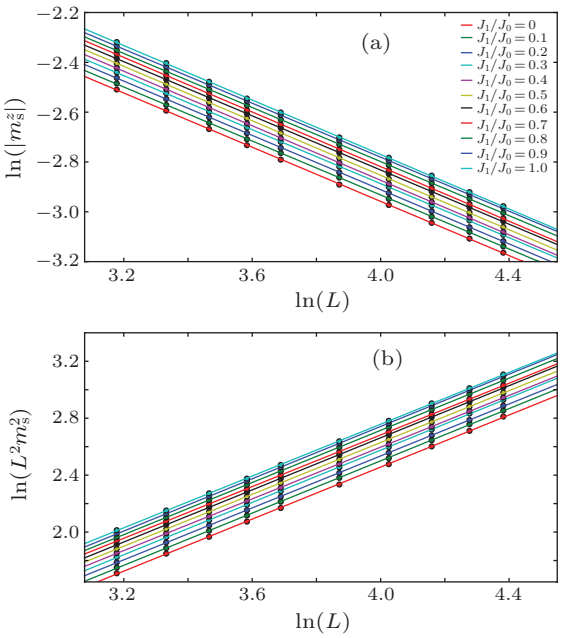


Fig. 4. (colour online) Finite-size scaling of (a) $|m_s^z|$ and (b) $L^2m_s^2$. The extracted values of β/ν and $1-\eta$ are shown in Table 1. A vertical shift is applied on each line to separate the original overlapping lines.

4. Discussion and conclusion

In this paper, we present results of the quantum Monte Carlo study of a generalized two-dimensional staggered dimer model. Using different finite-size scaling ansätz, we obtain the exact quantum critical point of VBS–Neel transition for all the situations that have been simulated, establishing a first benchmark for these models. The unconventional critical exponents are also extracted, indicating there may be a nontrivial contribution to the critical point which is triggered by the spatially staggered arrangement of couplings.

While for exponent ν, the inconsistency with standard O(3) values could be considered as the result of the large confluent correction for $\rho_s L$, and there still is a lack of a convincing explanation of the robust and large deviation from standard O(3) values for β/ν and $d-z-\eta$. The question whether the cubic irrelevant term suggested in Ref. [25] is the reason for the enhanced correction to the scaling for this transition and thus all the unexpected values of critical exponents still needs further numerical studies. It would be of great interest to recheck all these critical theories by simulating other staggered dimer models with larger system sizes or in higher dimensions, and carrying out finite-size scaling analysis in a more sophisticated manner.

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