Evidence for an Unconventional Universality Class from a Two-Dimensional Dimerized Quantum Heisenberg Model

Sandro Wenzel,[1,*] Leszek Bogacz,[2] and Wolfhard Janke[1,+]

[1]*Institut für Theoretische Physik and Centre for Theoretical Sciences (NTZ), Universität Leipzig, Postfach 100 920, D-04009 Leipzig, Germany*

[2]*Department of Information Technology, Jagiellonian University, ul. Reymonta 4, 30-059 Krakow, Poland*

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The two-dimensional J-J' dimerized quantum Heisenberg model is studied on the square lattice by means of (stochastic series expansion) quantum Monte Carlo simulations as a function of the coupling ratio $\alpha = J'/J$. The critical point of the order-disorder quantum phase transition in the J-J' model is determined as $\alpha_c = 2.5196(2)$ by finite-size scaling for up to approximately 10 000 quantum spins. By comparing six dimerized models we show, contrary to the current belief, that the critical exponents of the J-J' model are not in agreement with the three-dimensional classical Heisenberg universality class. This lends support to the notion of nontrivial critical excitations at the quantum critical point.

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Dimerized quantum spin systems are important examples of low-dimensional antiferromagnets featuring a quantum phase transition (QPT) [1] which destroys a Néel ordered state by competition between different interactions. In contrast to other examples showing such criticality, in this class of models the actual transition is triggered by nonisotropic couplings where the dimers [2] are explicitly placed on the lattice. Because of the discovery of Bose-Einstein condensation of magnons in a magnetic field much effort has been spent to study their physics [3].

The characteristics of the QPT in two-dimensional (2D) dimerized models have been investigated in detail. By mapping to a nonlinear sigma model (NLSM) [4] it was argued that the transition is well described by the Heisenberg O(3) classical universality class in three dimensions. The role of Berry phase terms, which are present in the mapping to the NLSM, is argued to be irrelevant [5] and there are numerous numerical studies which support this claim. Examples include the CaVO lattice [6], bilayer models [7], and the 2D coupled ladder system [8].

Recently, the idea of deconfined quantum critical points has been put forward by Senthil *et al.* [9] who argue that there are, however, also important examples of QPTs where Berry phases and nontrivial excitations at the quantum critical point can change the critical behavior. These arguments are based on Heisenberg models with *isotropic* interactions exhibiting a transition between two ordered states such as an antiferromagnetic and a valence-bond solid phase, and numerical evidence for such a case was recently claimed by Sandvik [10]. This idea that challenges the standard Landau-Ginzburg-Wilson framework of phase transitions was also found to be relevant in other systems such as classical dimers [11] in three dimensions and has prompted further theoretical and numerical efforts [12–16], some of which extend to different scenarios or show that the field is still highly controversial.

In this context, it is in any case somewhat surprising that also a specific 2D dimerized spin model, which we refer to as the J-J' model, with *nonisotropic* interactions was suggested as a candidate for deconfinement at the quantum critical point by Yoshuika *et al.* [17] (see also Ref. [18]). In consequence this idea could lead to critical exponents characterizing the phase transition, which differ from those of the Heisenberg universality class in three dimensions. This conclusion was, however, questioned [19] because of the close relation of the J-J' model to the ladder model. In order to resolve this conflict and to give arguments in favor of one or the other alternative we report in this Letter on quantum Monte Carlo (QMC) simulations of various dimerized models, which signal the emergence of an unconventional phase transition for the J-J' model.

The J-J' model is defined on a square lattice with $N = L^2$ spins by the Hamiltonian

$$\mathcal{H} = J\sum_{\langle i,j\rangle} \mathbf{S}_i\mathbf{S}_j + J'\sum_{\langle i,j\rangle'} \mathbf{S}_i\mathbf{S}_j. \tag{1}$$

Here, $\mathbf{S}_i = (1/2)(\sigma_x, \sigma_y, \sigma_z)$ denotes the usual spin-1/2 operator at lattice site i, and J and J' are the antiferromagnetic coupling constants defined on the bonds $\langle i, j\rangle$ and $\langle i, j\rangle'$, respectively. The ''staggered'' arrangements of the bonds on a square lattice with periodic boundary conditions can be seen in Fig. 1(a). The geometry of the ladder model results by a simple shift of every second dimer. We define $\alpha = J'/J$ as the parameter driving the phase transition.

Simulations are performed with the directed loop variant [20] of the stochastic series expansion (SSE) algorithm [21] for lattice sizes $L = 8$ up to $L = 72$ (in single cases $L = 96$) and inverse temperature up to $\beta = 256$. We checked that all quantities took on their ground-state values at the temperature simulated and we scaled $\beta \sim L$. Additional parallel tempering (PT) updates as well as

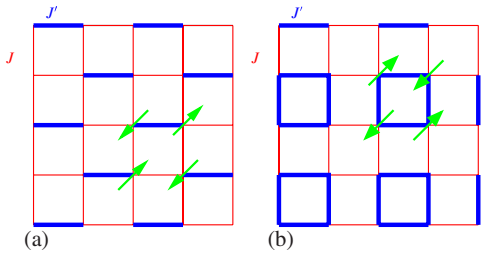

FIG. 1 (color online). (a) Visualization of the J-J' model on the 2D square lattice. The quantum spin ($S = 1/2$) degrees of freedom live on a square lattice with different nearest neighbor couplings J and J' (thin and thick). (b) Similar for the plaquette model, favoring quadrumer formation.

multihistogram reweighting were performed to further optimize sample statistics and data analysis.

To probe the nature of the quantum phase transition, we calculate several well-known observables starting from the staggered magnetization (the Néel order parameter) with

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

and its Binder parameters $Q_1 = \langle (m_s^z)^2\rangle/\langle |m_s^z|\rangle^2$ and $Q_2 = \langle (m_s^z)^4\rangle/\langle (m_s^z)^2\rangle^2$. These quantities are complemented by the second-moment correlation length obtained from structure factors S as

$$\xi_y = \frac{L_y}{2\pi}\sqrt{\frac{S(\pi,\pi)}{S(\pi,\pi+2\pi/L_y)} - 1}, \tag{3}$$

with the obvious relation for the imaginary time correlation length ξ_τ. Lastly, we determine the spin stiffness obtained from

$$\rho_s = \frac{3}{4\beta N}\langle w_x^2 + w_y^2\rangle, \tag{4}$$

where w_x^2 is the square of the difference of operator numbers S^+S^- and S^-S^+ in x direction. At a critical point the quantities Q_1, Q_2, ξ_y/L as well as $\rho_s L$ are expected to cross for different lattice sizes L (under the assumption that the imaginary time exponent $z = 1$, in case of the spin stiffness).

We first present QMC results for Q_2 and ξ_y/L in Fig. 2 where the crossing behavior becomes evident. A second-order phase transition is therefore very likely to happen. However, corrections to scaling terms are clearly present as the crossing points are not sharp but rather spread out for smaller lattice sizes. We exploit this fact by studying the scaling of the crossing points at lattice sizes L and $2L$ for the various quantities. In this way a bracketing of the critical coupling α_c is obtained in Fig. 2(c) and we can easily read off a preliminary estimate as $\alpha_c \in [2.5190, 2.5202]$. This value is made more precise by fitting to a function $\alpha_c(L, 2L) = \alpha_c + aL^{-1/\nu-\omega}$ yielding $\alpha_c = 2.5198(3)$. All observables agree in this picture, indicating a single phase transition and our estimate is in accordance to earlier quotes in the literature [22–25].

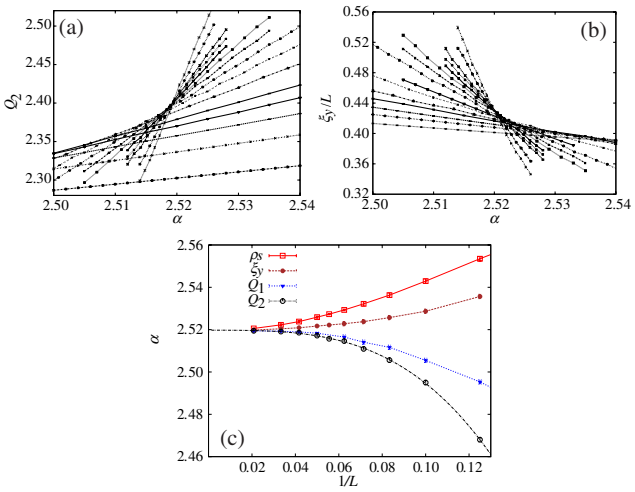

FIG. 2 (color online). (a) The Binder parameter Q_2 and (b) the correlation length ξ_y/L for various lattice sizes from $L = 8$ to $L = 72$. (c) Scaling of the crossing points can be used to extract the critical coupling α_c. All quantities seem to converge to the same estimate.

Finite-size scaling.—Having gained a fairly good estimate of the critical coupling α_c we now turn to determining the critical exponent ν. This is done by using the scaling ansatz for a second-order phase transition $\mathcal{O}_L(t) = L^{\lambda/\nu} g_{\mathcal{O}}(tL^{1/\nu})$, where λ is the scaling exponent associated with the quantity $\mathcal{O}$, $t = \alpha/\alpha_c - 1$ the reduced critical coupling and $g_{\mathcal{O}}$ a scaling function. For the quantities Q_2 and ξ_y/L, it is clear that $\lambda = 0$, which is indeed *verified* from the data in Fig. 2. In this work we follow Ref. [7] and take evident corrections to scaling explicitly into account by performing the data analysis according to a more general scaling ansatz

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

where ω is the usual confluent correction exponent and ϕ a shift correction contribution. This way we can directly compare with a very detailed study recently performed on two bilayer models favoring dimer formation which gave strong support for O(3) universality [7].

We perform our data analysis using this scaling ansatz in two ways. First, a Taylor expansion of $g_{\mathcal{O}}(x)$ up to fourth order in x is used in conjunction with multidimensional fitting. Second, we check this procedure by using a collapsing tool [26] which makes direct use of multihistogram reweighting. Both methods give consistent results for the critical coupling ratio as $\alpha_c = 2.5196(2)$ and the critical exponent $\nu = 0.689(5)$ which is more than 4σ smaller than the standard O(3) value [27] of $\nu = 0.7112(5)$. We arrive at this result conclusively for all observables of this study. The error bar reflects checking for different window sizes, as well as trying different correction terms. In fact, we find that in most cases the ω correction is sufficient; i.e., the inclusion of ϕ terms does not change the estimate for ν. Figure 3 contains a data collapse for all lattice sizes for

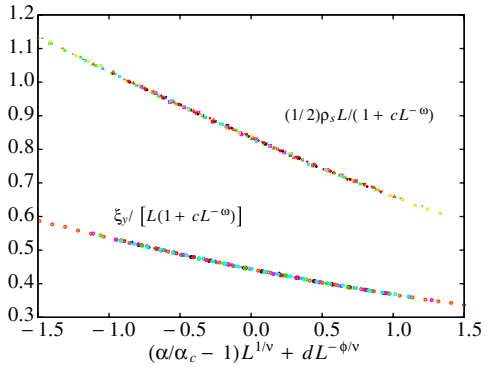

FIG. 3 (color online). Best collapse for the spin stiffness (upper data set) and the correlation length (lower data set) obtained from fitting data to the scaling ansatz (5).

quantities ξ_y and $\rho_s L$. The exponent z can best be estimated from the correlation length ξ_τ in imaginary time. As the result $\nu_\tau = 0.687(5)$ is almost equal to the previous value we can conclude $z = 1.01(1)$.

Cross-checks and critical scaling.—Since the discrepancy between ν and the standard O(3) value is rather small we have performed multiple checks of the algorithm and our numerical procedure in different categories. First, we repeat the study for a different aspect ratio $2L_y \times L_y$ ($L_x = 2L_y$) (and larger β), where the correlation lengths in the x and in the y direction are approximately equal, giving a consistent result of $\nu = 0.688(5)$. Second, we carefully ran simulations on various dimerized models known to be described by exponents in the three-dimensional Heisenberg universality class. These include the CaVO, the bilayer, and the ladder model discussed before. In all cases we arrive easily at Heisenberg universality. This is also true for the plaquette model of Fig. 1(b), being a model not previously investigated to high precision. There, we obtain a critical point of $\alpha_c = 1.8228(4)$ and a critical exponent of $\nu = 0.709(8)$ using exactly the same procedure (even at smaller lattice sizes of up to $L = 48$) [28]. Those checks on known and hitherto less studied models indicate that the critical exponent ν is indeed smaller for the J-J' model.

To further investigate the "mismatch" of the universality class we proceed with determining other critical exponents by studying the scaling at the quantum critical point α_c. In this case the staggered magnetization scales as $\langle |m_s^z| \rangle \sim L^{-\beta/\nu}$ and we can obtain the exponent η (as well as z) from $\langle m_s^2 \rangle$ and the staggered susceptibility from

$$\langle L^2 m_s^2 \rangle \sim L^{d-z-\eta}, \qquad \chi_s \sim L^{\gamma/\nu}. \tag{6}$$

Using this approach, we obtain in Fig. 4(a) the estimates $\beta/\nu = 0.515(4)$ for the bilayer, the ladder and the plaquette model at the known critical points (see Table I), and $\beta/\nu = 0.545(4)$ for the J-J' model, which should be compared to the O(3) value of $\beta/\nu = 0.518(1)$ [27]. The error bars on the data reflect uncertainties in α_c and the straight line fits are all excellent and results are independent of different fitting windows. Our results are quoted for the five largest lattice sizes. To make the discrepancy in β/ν more apparent we have rescaled the original data to start at a common point in the plot. Second, we compute ν again from the slope $s_Q = dQ_2/d\alpha$ and $s_\xi = (1/L)d\xi_y/d\alpha$ at the critical point which should scale with lattice size as $L^{1/\nu}$. Figure 4(b) shows this for s_ξ in comparison for the J-J', the ladder, and the plaquette model. Fits for the ladder and the plaquette model yield a common $\nu = 0.709(6)$ while $\nu = 0.689(5)$ is obtained for the J-J' model, in accordance with the previous analysis. Similarly, the remaining exponents η and z are determined to be $d - z - \eta = 0.908(5)$ (J-J') as well as $d - z - \eta = 0.971(2)$ (other models) with the

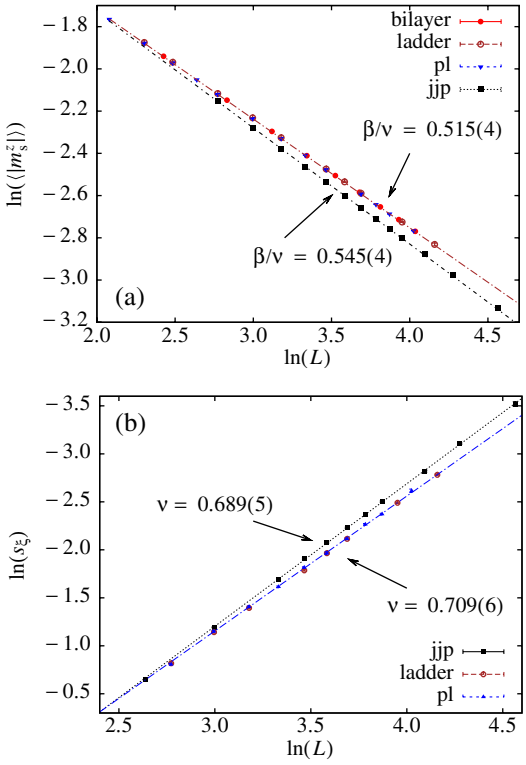

FIG. 4 (color online). Scaling of (a) the staggered magnetization and the (b) the slope s_ξ of ξ_y/L at the critical point. We compare the scaling of the J-J' model (jjp) against the plaquette (pl), the bilayer and the ladder models at the best known critical couplings. Both quantities indicate different critical exponents for the J-J' model.

TABLE I. Different Heisenberg models used for finite-size scaling comparison at the critical point.

Model	Type	α_c	Reference
Bilayer	Symm., dimer	2.5220(1)	[7]
Kondo	Symm., dimer	1.3888(1)	[7]
CaVO	Symm., plaquette	0.939(2)	[6]
Plaquette	Symm., plaquette	1.8228(4)	[28]
Ladder	Unsymm., dimer	1.909(1)	[8,28]
J-J'	Unsymm., dimer	2.5196(2)	this work, [28]

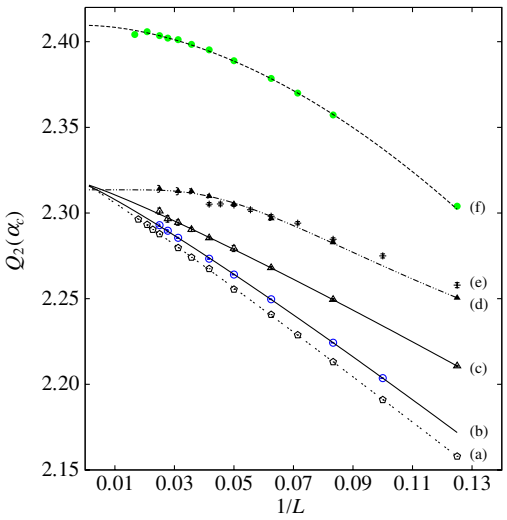

FIG. 5 (color online). The critical Binder parameter in dependence on the lattice size L for the (a) plaquette model, (b) ladder model, (c) bilayer, (d) Kondo lattice, (e) classical O(3) model, and (f) J-J' model. Data for the CaVO lattice are not shown as they overlap with curve (c).

obvious contrast. It is easily checked, that the scaling law $2\beta = (d + z - 2 + \eta)\nu$ is satisfied within error bars for all cases. The exponent η for the J-J' model is thus given by $\eta = 0.09(1)$, which is considerably larger than the standard O(3) value.

Our findings are finally reinforced by comparing the Binder parameter at the best known critical points for the models of Table I. It is evident from Fig. 5 that all cases apart from the J-J' model are in accordance with O(3) behavior. To make this comparison even stronger we also include in Fig. 5 the value from Wolff cluster simulations of the ordinary three-dimensional classical Heisenberg model [29].

Conclusion.—In this Letter we give comprehensive numerical evidence for an unconventional universality class of the J-J' model based on data collapsing analysis, scaling at criticality and by a comparison of the Binder parameter for six different dimerized models. This shows that there are nontrivial contributions to the quantum critical point changing the critical exponents. Those contributions are triggered by the special staggered arrangement of couplings. Our result challenges the current understanding of quantum phase transitions in dimerized quantum spin systems and it will be interesting to see which exact theoretical mechanism accounts for the observed discrepancy.

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*wenzel@itp.uni-leipzig.de
+janke@itp.uni-leipzig.de

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[29] Q_2 is then also computed for the z component of the magnetization and as an average over slices in z direction. Note that $\langle (m^z)^4 \rangle / \langle (m^z)^2 \rangle^2$ is equal to $(9/5)\langle m^4 \rangle / \langle m^2 \rangle^2$.