First-Order Phase Transition in Easy-Plane Quantum Antiferromagnets

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Quantum phase transitions in Mott insulators do not fit easily into the Landau-Ginzburg-Wilson paradigm. A recently proposed alternative to it is the so-called deconfined quantum criticality scenario, providing a new paradigm for quantum phase transitions. In this context it has recently been proposed that a second-order phase transition would occur in a two-dimensional spin $1/2$ quantum antiferromagnet in the deep easy-plane limit. A check of this conjecture is important for understanding the phase structure of Mott insulators. To this end we have performed large-scale Monte Carlo simulations on an effective gauge theory for this system, including a Berry-phase term that projects out the $S = 1/2$ sector. The result is a first-order phase transition, thus contradicting the conjecture.

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The Landau-Ginzburg-Wilson (LGW) theory for phase transitions has been an immensely successful paradigm of physics for the last 50 years. It is one of the cornerstones of statistical and condensed matter physics, providing deep insight into phase transitions [1]. The standard example is the well-known paramagnetic-ferromagnetic phase transition. Recently, examples of phase transitions that do not fit into the LGW paradigm have been discussed [2–4]. A prominent example is the *continuous* quantum phase transitions from a Néel state with conventional antiferromagnetic order into a paramagnetic valence-bond solid (VBS) state [5]. In the Néel state, an $SU(2)$ symmetry is broken, while in the VBS phase translation invariance of the lattice is broken. The LGW paradigm does not describe this phase transition correctly, since it predicts a first-order phase transition in this case. In view of the failure of the LGW paradigm in this and other cases, a new scenario has recently been proposed [2,3], introducing the concept of deconfined quantum criticality (DQC). This concept applies to systems where the order parameter can be viewed as being composed by elementary building blocks. For instance, in the case of the Néel-VBS transition the spinons are the building blocks of the spin field. Similarly to quarks in hadrons, the spinons are confined in both the Néel and VBS phases. The DQC scenario asserts that the spinons are deconfined only at the critical point. This claim is based on a subtle destructive quantum interference mechanism between instantons and the Berry phase [2].

An attempt to provide proof of evidence for these ideas has recently been put forth [2]. It involves a deformation of the two-dimensional Heisenberg model into an easy-plane quantum antiferromagnet. The effective theory of a spin $1/2$ quantum antiferromagnet is a $O(3)$ nonlinear σ model with a staggered Berry-phase factor [4]. Such a nonlinear σ model describes the fluctuations of the orientation $\mathbf{n}_j$ of the order parameter. The easy-plane deformation adds a term proportional to n_{zj}^2 to the action, which explicitly breaks the $O(3)$ symmetry down to $U(1)$. This lower symmetry simplifies considerably the analysis, especially when the CP^1 representation $\mathbf{n}_j = z_{ja}^* \boldsymbol{\sigma}_{ab} z_{jb}$ is used, with $|z_{j1}|^2 + |z_{j2}|^2 = 1$ due to the local constraint $\mathbf{n}_j^2 = 1$. The CP^1 representation naturally introduces a local Abelian gauge symmetry, since $\mathbf{n}_j$ is invariant under the local gauge transformation $z_{ja} \to e^{i\theta_{aj}} z_{ja}$. A deep easy-plane deformation forces $n_{zj}^2 \approx 0$, thus inducing the additional local constraint $|z_{j1}|^2 \approx |z_{j2}|^2$. This allows us to write $z_{ja} = e^{i\theta_{ja}}/\sqrt{2}$. The requirement of local $U(1)$ gauge invariance and the deep easy-plane limit naturally leads to an effective lattice gauge theory for a quantum antiferromagnet proposed in Ref. [6], which for $S = 1/2$ has the lattice Lagrangian

$$\mathcal{L}_j = -\beta \sum_{a=1}^{2} \cos(\Delta_\mu \theta_{ja} - A_{j\mu}) - \kappa \cos(\epsilon_{\mu\nu\lambda} \Delta_\nu A_{j\lambda}) + i\eta_j A_{j\tau}, \tag{1}$$

where $\mathbf{A}_j$ is a compact gauge field which here is doing more than just being an auxiliary field, like in the case of the CP^1 model. It determines also the Berry phase for the above model. The index τ corresponds to imaginary time and the staggering factor is given by $\eta_j = (-1)^j$. Note that the present gauge field is a function of the spacetime coordinates, in contrast to the usual Berry gauge potential appearing in spin models [4], which is a functional of the spin field.

Compactness of the gauge field gives rise to instanton configurations [7] which are known to spoil the phase transition in a corresponding model with only one phase field and no Berry phase [8]. In the absence of Berry phase and with two phase fields present, on the other hand, a phase transition in the 3Dxy universality class occurs [9,10] regardless of whether the gauge field is compact or not. Since only one gauge field is present and there are two phase fields available, the Higgs mechanism is able to suppress only one out of two massless modes. The remaining massless mode is charge neutral and drives the 3Dxy transition [10].

Recently, it has been argued that the Berry phase, which is crucial to describe the phase inside the paramagnetic phase [2,3], suppresses the instantons at the critical point. Here we will investigate this point by monitoring the phase transitions in the model (1) in the presence and absence of a Berry phase. In the former case a phase transition is expected in the charged sector, contrasting with the transition driven only by the neutral sector in absence of the Berry phase. The result will be shown to be a first-order phase transition.

The DQC scenario implies that the critical point is governed by an easy-plane system Lagrangian featuring a noncompact gauge field, i.e.,

$$\mathcal{L}_i = -\beta \sum_{a=1}^{2} \cos(\Delta_\mu \theta_{ia} - A_{i\mu}) + \frac{\kappa}{2}(\mathbf{\Delta} \times \mathbf{A}_i)^2. \quad (2)$$

This model with unequal bare phase stiffnesses has been studied in great detail [10]. It features two distinct second-order phase transitions, one belonging to the 3Dxy universality class and another one corresponding to the so-called inverted 3Dxy transition [11]. In the limit where the bare phase stiffnesses are equal, clear signals of non-3Dxy behavior are seen [10,12,13]. In Ref. [12], strong indications of a first-order phase transition in a loop-gas representation of the noncompact model Eq. (2), were found. We will consider both Eqs. (1) and (2) in detailed Monte Carlo (MC) simulations.

For performing MC simulations on the model with a Berry-phase term, it is convenient to introduce a dual representation of the model Eq. (1). In such a representation the action is real, with a Lagrangian given by [4]

$$\mathcal{L}_i = \frac{1}{2\beta} \sum_{a=1}^{2} (\mathbf{\Delta} \times \mathbf{h}_i^{(a)})^2 + \frac{1}{2\kappa}(\mathbf{h}_i^{(1)} + \mathbf{h}_i^{(2)} + \mathbf{f}_i + \mathbf{\Delta} s_i)^2. \quad (3)$$

Here, $\mathbf{h}^{(a)}$ are integer-valued dual gauge fields, and $\varepsilon_{\mu\lambda\nu}\Delta^\nu f_i^\lambda = \delta_{\mu\tau}\eta_i$. Note that we would obtain Eq. (3) both for Eqs. (1) and (2), with $f_i = 0$ for Eq. (2). For Eq. (1) with compact $A_{i\mu}$, s_i is integer valued. For Eq. (2) with a noncompact $A_{i\mu}$, s_i is real valued. Therefore, in the former case s_i can be gauged away since the $\mathbf{h}^{(a)}$-fields are integer valued. We have chosen a gauge where $s_i = 0$. The MC computations were performed using Eqs. (2) and (3). For both Eqs. (2) and (3), we have used $\kappa = \beta$. We have used the standard Metropolis algorithm with periodic boundary conditions on a cubic lattice of size $L \times L \times L$. For Eq. (3) we have used $L = 4, 8, 12, 16, 20, 24, 32, 36, 48, 60, 64, 72, 80, 96, 120$, while for Eq. (2) we have used $L = 48, 64, 80, 96, 112, 120$. A large number of sweeps is required in order to get adequate statistics in the histograms (see below) for the largest system sizes. First, we have computed the second moment of the action $M_2 \equiv \langle (S - \langle S \rangle)^2 \rangle$ for the model with and without a Berry-phase term, where $S = \sum_i \mathcal{L}_i$. Second, we have focused on a number of quantities that provide information on the character of the phase transition associated with the specific heat anomaly. The first of these quantities is the third moment of the action, $M_3 \equiv \langle (S - \langle S \rangle)^3 \rangle$. At a second-order phase transition this quantity should scale as follows. The peak-to-peak height scales as $L^{(1+\alpha)/\nu}$, whereas the width between the peaks scales as $L^{-1/\nu}$ [14]. At a first-order phase transition, these quantities scale as L^6 and L^{-3}, respectively [15]. We also study the probability distribution $P(S, L)$ of the action S for various system sizes. At a first-order phase transition, $P(S, L)$ will exhibit a double-peak structure associated with the two coexisting phases.

The specific heat M_2 is shown in Fig. 1. Panel (a) shows the anomaly for the model Eq. (3) with no Berry-phase term, i.e., $\mathbf{\Delta} \times \mathbf{f} = (0, 0, \eta) = 0$. The anomaly has the characteristic asymmetric shape of the 3Dxy model. In this case, there are no Berry phases to suppress the instantons of the compact gauge-field $\mathbf{A}$ at the critical point. Hence, the charged sector does not feature critical fluctuations that can interfere with those of the neutral sector. When the Berry-phase field $\mathbf{f}$ is included, the specific heat is notably more symmetric and the anomaly develops into a δ-function peak, consistent with a first-order phase transition. This is shown in panel (b).

To investigate more precisely the character of the phase transition when a Berry-phase term is present, we have performed finite-size scaling (FSS) of the third moment of the action, M_3 [14]. The results are shown in Fig. 2, panel (a). It is seen that for small and intermediate system sizes, the height increases with L in a manner which might appear consistent with that of a second-order phase transition. However, the quality of the scaling is not satisfactory, since a clear curvature in the scaling plots is seen (red

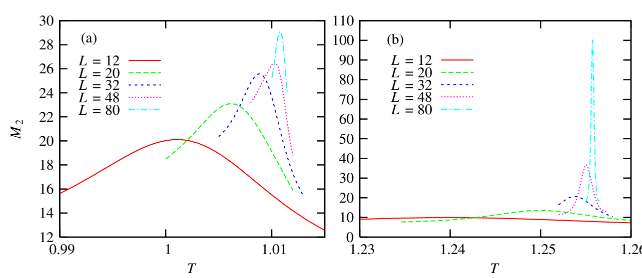

FIG. 1 (color online). Specific heat M_2 of Eq. (3) for various system sizes. Panel (a): Without Berry-phase term. The peak develops into a singularity of the 3Dxy type. Panel (b): With Berry-phase term. The peak develops into a δ-function singularity with a peak scaling as L^3, consistent with a first-order transition. Note the symmetry and asymmetry of the peaks in the right and left panels, respectively. This is to be expected, since the peaks in the right panel originate with the superposition of a 3Dxy peak and an inverted 3Dxy peak.

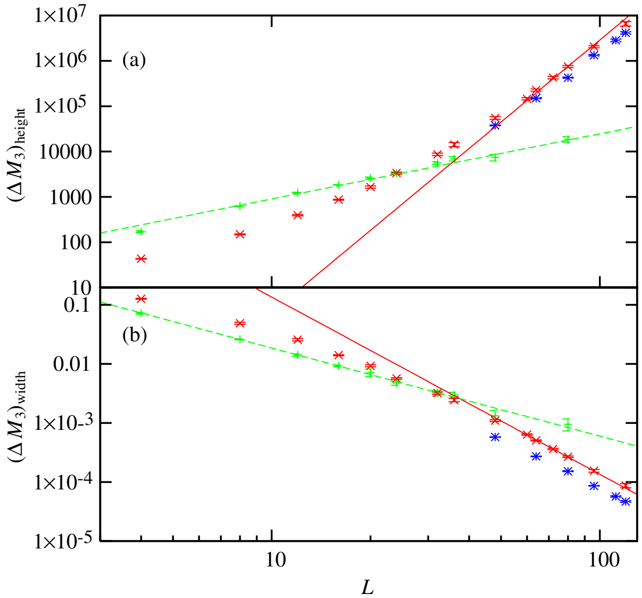

FIG. 2 (color online). Scaling of the height [panel (a)] and width [panel (b)] of M_3 of the action in Eqs. (2) and (3). The lines in panel (a) represent $L^{1.43}$ and L^6. The former is the 3Dxy result. The lines in panel (b) represent $L^{-1.49}$ and L^{-3}. The former is the 3Dxy result. For large system sizes, the height and width scale in manner consistent with a first-order phase transition. Also shown are results for Eq. (3) with no Berry-phase term $\mathbf{f} = 0$ (green symbols). These results follow the 3Dxy scaling lines. The red symbols are the results for Eq. (3) while the blue symbols are results for Eq. (2).

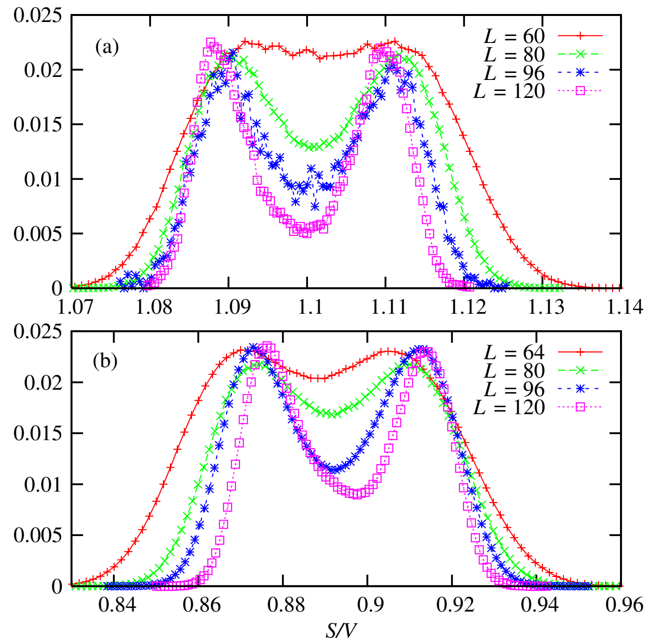

FIG. 3 (color online). Histograms for the probability distribution $P(S, L)$ as a function of S/L^3 for various system sizes L. (a): results for Eq. (1) in the representation Eq. (3). (b): results Eq. (2). A double-peak structure develops with the latent heat per unit volume approaching a finite constant as L is increased. This is a hallmark of a first-order transition. For the largest systems, up to 120×10^6 sweeps over the lattice were performed. A total of approximately 500 000 CPU hours were used to obtain these results.

data points). As system sizes increase we see a gradual increase in the apparent value of $(1 + \alpha)/\nu$, until for large system sizes, we clearly have $M_3 \sim L^6$, consistent with a first-order phase transition [15].

Panel (b) of Fig. 2 shows the scaling of the width of M_3. Again, the line with the smallest negative slope is the line one would obtain for the 3Dxy model, while the line with the most negative slope is $\sim L^{-3}$, characteristic of a first-order phase transition. Again we obtain apparent scaling, with a crossover regime at intermediate length scales into a regime where the width scales as it would in a first-order phase transition [15]. The results of Fig. 2 provide further support to the notion that the phase transition in the model with a compact gauge-field and a Berry-phase term is a first-order phase transition.

To investigate this further, we have computed the probability distribution $P(S, L)$ for various system sizes. The results are shown in Fig. 3. Panel (a) shows results for Eq. (1) in the representation Eq. (3). Panel (b) shows results for Eq. (2). The Ferrenberg-Swendsen algorithm has been used to reweight the histograms [16]. For $L \leq 48$, we essentially have not been able to resolve a double-peak structure at all, showing that the phase transitions in the models Eqs. (1) and (2) are weakly first order. We have located the transition temperature from the peak structures in the specific heat and M_3, and performed long simulations at this temperature for each L. For the largest systems, $L = 96$, 120, up to 120×10^6 sweeps over the lattice were done. A clear double-peak structure in $P(S, L)$ is seen to develop for system sizes $L > 60$. The fact that such large system sizes are required to bring out the double-peak structure, implies that this phase transition is weakly first order.

We also perform FSS of the height of the peak between the two degenerate minima in the free energy $-\ln[P(S, L)]$. This height should scale as L^2 in a first-order phase transition, since it represents the energy of an area which separates two coexisting phases [17]. The results are shown in panel (a) of Fig. 4. For large enough systems, the height clearly approaches the dotted line $\sim L^2$, as in a first-order transition. This is corroborated by extracting the latent heat per unit volume in the transition, shown in the lower panel of Fig. 4. It approaches a nonzero constant as L is increased, as it should in a first-order phase transition.

Further insight into the nature of the first-order phase transition can be obtained by means of the renormalization group (RG). In the field theory Lagrangian the interaction of an easy-plane system reads $\mathcal{L}_{\rm int} = u_0(|z_1|^2 + |z_2|^2)^2/2 + v_0|z_1|^2|z_2|^2 = u_0(|z_1|^4 + |z_2|^4)/2 + w_0|z_1|^2|z_2|^2$, where $w_0 = u_0 + v_0$. Consider a generalized situation where

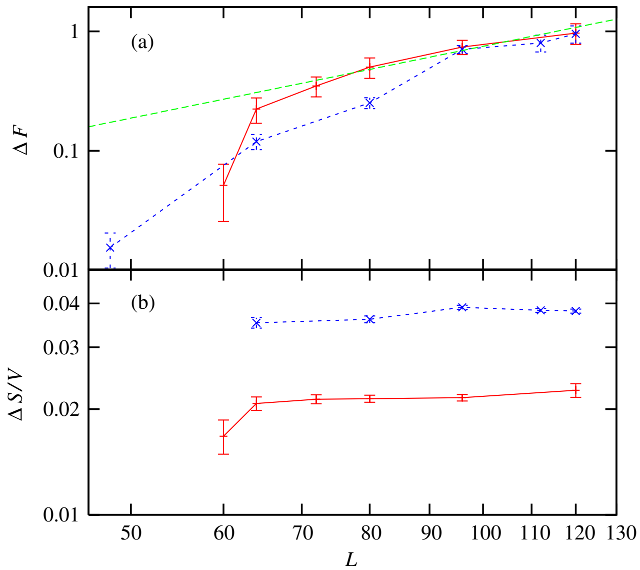

FIG. 4 (color online). Panel (a) shows the scaling of the height ΔF of the peak between the two minima in $-\ln P(S, L)$ both for Eqs. (3) (red curve) and (2) (blue curve). Dotted line is the line $\sim L^2$. The height scales as $\Delta F \sim L^{d-1}$. This is a hallmark of a first-order transition. Panel (b) shows latent heat per unit volume $\Delta S/V$ as a function of L. The upper (blue) curve is from Eq. (2), the lower (red) curve is from Eq. (3). $\Delta S/V$ approaches a nonzero value as L is increased.

the complex fields have each $N/2$ components. The renormalized dimensionless couplings in $d = 4 - \varepsilon$ dimensions are $g = u\mu^{-\varepsilon}$, $h = w\mu^{-\varepsilon}$, and f, where f is the dimensionless gauge coupling and μ is an arbitrary mass scale. The β functions at one-loop order are [18] $\beta_g = -\varepsilon g - 6gf + (N + 8)g^2/2 + 2Nh^2 + 6f^2$, $\beta_h = -\varepsilon h - 6hf + 3(N + 2)gh + 6f^2$, and $\beta_f = -\varepsilon f + Nf^2/3$. Nontrivial fixed points with $f = 3\varepsilon/N$ and $h < 0$ are found for $N \geq 300$, while in the deep easy-plane limit $h = 0$ no fixed points with $f = 3\varepsilon/N$ are found for all values of N. In a Ginzburg-Landau (GL) theory of superconductors, the existence of a critical value of N above which nontrivial fixed points are found actually reflects the strong-coupling behavior at much lower values of N. It turns out that the phase transition for one complex order parameter is second order in the type II regime [11], while a first-order transition occurs in the type I regime [19–21]. Inspired by the GL case, we interpret the complete absence of a critical value of N for $h = 0$ as a clear signature of a first-order phase transition in the deep easy-plane regime. This is a further confirmation of our MC results; see also Ref. [12], where a first-order transition in a closely related model has also been found.

In summary, our large-scale MC simulations of the deep easy-plane quantum antiferromagnet confirm the instanton-Berry-phase suppression mechanism proposed in Ref. [2]. Therefore, the spinons are indeed deconfined at the phase transition. However, the phase transition in this case is first order, which contradicts the DQC picture for this model, where a second-order phase transition has been predicted.

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