First order phase transitions in the square lattice “easy-plane” J-Q model

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We study the quantum phase transition between the superfluid and valence bond solid in “easy-plane” J-Q models on the square lattice. The Hamiltonian we study is a linear combination of two model Hamiltonians: (1) an SU(2) symmetric model, which is the well known J-Q model that does not show any direct signs of a discontinuous transition even on lattices as large as $512 \times 512$ and is presumed continuous, and (2) an easy plane version of the J-Q model, which shows clear evidence for a first order transition even on $L \approx 16$. A parameter $0 \leq \lambda \leq 1$ ($\lambda = 1$ being the symmetric J-Q model) allows us to smoothly interpolate between these two limiting models. We use stochastic series expansion (SSE) quantum Monte Carlo (QMC) to investigate the nature of this transition for $\lambda = 0.5$ and 0.75. While we find that the first order transition weakens as $\lambda$ is increased from 0 to 1, we find no evidence that the transition becomes continuous before the SU(2) symmetric point, $\lambda = 1$. We thus conclude that the square lattice superfluid-VBS transition in the two-component easy-plane model is generically first order.

I. INTRODUCTION

The quantum transition from Néel or superfluid to a valence bond solid (VBS) has been proposed to be described by the deconfined criticality scenario. In this scenario it is generically possible to have a direct continuous Néel-VBS transition. A number of field theoretic formulations that describe this putative critical point at long distances have been put forward and interesting connections between different representations have been conjectured via duality arguments. Establishing these fascinating connections non-perturbatively by lattice simulations is an exciting field of current research. In the original study two kinds of symmetries were highlighted for their possibility as platforms for deconfined criticality, an SU(2) symmetric system and a $U(1) \times Z_2$ symmetric system. Physically, the SU(2) field theory could be a description for a rotationally symmetric $S = 1/2$ antiferromagnet and its transition to a valence bond solid. The $U(1) \times Z_2$ system can be thought of as a model for the same Néel-VBS transition in magnet with easy-plane anisotropy or alternatively as a model for a superfluid to Mott transition.

In the years since the original proposal, it has been demonstrated that the Néel-VBS transition and many of its variants can be studied in sign-free quantum spin Hamiltonian models on large lattices. Through extensive numerical simulations in the SU(2) symmetric models many aspects of the proposal have been borne out and no direct evidence for a first order transition has been observed. Numerical studies of classical statistical mechanics models of tightly packed loops and dimer models in three dimensions that have been argued to realize the same universal physics as the SU(2) Néel-VBS transition are also consistent with the deconfined criticality scenario. Despite this large body of evidence for the deconfined criticality scenario, numerical studies have observed scaling violations whose origin is currently unclear.

In contrast in the easy-plane case where SU(2) is broken to $U(1) \times Z_2$ a number of numerical studies have concluded that the transition is first order. Recently however it has been claimed that a continuous transition has been found in a square lattice model with somewhat weaker easy-plane anisotropy, suggesting that perhaps a large easy-plane anisotropy could result in a first order transition, and the first order and second order regime are separated by a multicritical point. Motivated by this study, we address the issue of how the easy-plane transition is connected to the symmetric one, by studying a model that interpolates between these two limiting cases on the square lattice. For the symmetric model we use the popular J-Q model which shows no direct evidence for first order behavior even on lattices as

![Phase Diagram of $H_{\lambda}^{JQ}$ described by Eq. 1 as a function of $\lambda$ and $g \equiv Q/J$. Using the model $H_{\lambda}^{JQ}$ we can access the phase boundary between the Néel and VBS phases. The transition at $\lambda = 0$ was demonstrated to be first order previously. We find that this transition is first order for $\lambda = 0.5$ and $\lambda = 0.75$. The signals of first order that we detect vanish at the symmetric point $\lambda = 1$ even on the largest lattices simulated here.](image-url)
large as \( L = 512 \). For the easy plane case we use an easy-plane J-Q that was shown to have a first order transition already visible on \( L \approx 16 \). The interpolating model introduced in detail below is slightly different from the one studied in Ref. 32,33 where the easy-plane anisotropy was introduced only in the J-term; both models are believed to have the same universal features however. In this work we present studies on larger lattices and a more thorough analysis. Contrary to the previous study, we find no evidence for new continuous easy-plane criticality. Instead we find a first order transition for \( 0 \leq \lambda < 1 \) that weakens as \( \lambda \) is increased and we approach the symmetric point \( (\lambda = 1) \) at which all our direct signals of a first order transition vanish and the transition is presumed continuous. This is the primary result of our paper and is summarized in Fig. 1. Although no numerical study can rule out that the transition becomes continuous for a very small but finite window close to \( \lambda = 1 \) (with finite easy-plane anisotropy), we find this rather unlikely given our results below. We thus conclude that the easy-plane Néel-VBS transition is generically first order on the square lattice.

II. THE MODEL

The Hamiltonian studied here is an \( S = 1/2 \) system on an \( L \times L \) square lattice,

\[
H^{JQ}_\lambda = \lambda H^{JQ}_s + (1 - \lambda) H^{\text{ep}}_\lambda,
\]

and is a linear combination of two parts, \( H^{JQ}_s \) is the SU(2) symmetric part and \( H^{\text{ep}}_\lambda \) is the easy plane part that explicitly breaks the SU(2) symmetry. \( \lambda \) is an anisotropy parameter that allows us to smoothly interpolate between the easy plane limit (\( \lambda = 0 \)) and the SU(2) symmetric limit (\( \lambda = 1 \)). We define the singlet projection operator on a bond between two sites \( i \) and \( j \) as,

\[
P_{ij} = \frac{1}{4} - \hat{S}_i \cdot \hat{S}_j.
\]

Then \( H^{JQ}_s \), which is the well known J-Q model,\(^7\) can be written as,

\[
H^{JQ}_s = -J \sum_{\langle ij \rangle} P_{ij} - Q \sum_{\langle ijk \rangle} P_{ij} P_{kl}
\]

\( H^{JQ}_s \) has full SU(2) inherited from \( P_{ij} \). Similarly if we define

\[
\tilde{P}_{ij} = S_i^x S_j^x + S_i^y S_j^y
\]

the easy plane Hamiltonian, \( H^{\text{ep}}_{nxJQ} \) can be written as,\(^27\)

\[
H^{\text{ep}}_{\lambda} = J \sum_{\langle ij \rangle} \tilde{P}_{ij} - Q \sum_{\langle ijk \rangle} \tilde{P}_{ij} \tilde{P}_{kl}
\]

\( \tilde{P}_{ij} \) has a symmetry of \( U(1) \times Z_2 \), which corresponds to \( U(1) \) rotations about the \( \hat{z} \)-axis and the \( Z_2 \) operation of a \( \pi \) rotation about the \( \hat{x} \)-axis.

We study the quantum phase transition from the magnetic phase to the valence-bond solid (VBS) phase as \( g \equiv Q/J \) is varied for a fixed \( \lambda \). While in the easy plane limit, i.e. \( \lambda = 0 \), this transition has been found to be first order,\(^27\) it has been argued to be to continuous in the SU(2) symmetric limit, \( \lambda = 1 \).\(^7,8,10,13\) In this work we interpolate between the two limiting models with the aim of elucidating the evolution of the nature of the quantum transition and in particular to investigate whether the transition is continuous for any \( \lambda < 1 \).

III. NUMERICAL SIMULATIONS

The numerical results presented below have been obtained using the stochastic series expansion (SSE) quantum Monte Carlo method.\(^34\) We use the directed loop algorithm\(^35\) to carry out global loop updates on our Monte Carlo configurations (see Appendix A 1). 

Fig. 1 shows a phase diagram obtained from numerical
for a phase transition between the XY order (superfluid) and VBS phases. We define the following quantities to detect magnetic order,

\[ S_{m_1^2}(\vec{k}) = \sum_{\vec{r}} e^{i \vec{k}.\vec{r}} \langle S_0^x S_0^x + S_0^y S_0^y \rangle \]

\[ S_{\phi_2}(\vec{k}) = \sum_{\vec{r}} e^{i \vec{k}.\vec{r}} (P_x(\vec{0}) P_x(\vec{r})) \]  

Here \( P_x(\vec{r}) \) is a plaquette operator which equals the sum of all the operators in the Hamiltonian acting on the plaquette at \( \vec{r} \) as described in Appendix A.

The spin stiffness \( \rho_s \) is defined as,

\[ \rho_s = \frac{\partial^2 E(\phi)}{\partial \phi^2} \bigg|_{\phi=0} \] (7)

Here \( E(\phi) \) is the energy of the system with a twist of \( \phi \) in the boundary condition in either the \( x \) or the \( y \) direction. In the QMC, this quantity is related to the winding number of loops in the direction that the twist has been added,

\[ \rho_s = \frac{\langle W^2 \rangle}{\beta} \] (8)

where \( \beta \) is the inverse temperature. \( \rho_s \) goes to a finite value in the magnetically ordered phase but goes to 0 otherwise. The quantity \( L \rho_s \) is expected to show a crossing at the coupling at which magnetic order is destroyed.

In order to detect the ordered phase we make use of ratios defined as,

\[ R_{op} = 1 - \frac{|S_{\phi}(k_o)|}{|S_{\phi}(k_o')|} \] (9)

Here \( o_p = m_{1,2}^2, \phi_2, k_o \) and \( k_o' \) are the ordering momentum and momentum closest to the ordering momentum respectively. In the ordered phase \( R_{op} \) goes to 1 and in the disordered phase it goes to 0 on increasing system size, therefore they are expected to cross for different system sizes at the critical point.

**A. Measurements**

When \( \lambda < 1 \), the presence of a small amount of anisotropy makes the spins preferentially align in the XY plane. Therefore as we vary \( g \) in our simulations, we look

**FIG. 3:** The values of \( \langle m_1^2 \rangle \) and \( \langle \phi_2^2 \rangle \) where \( R_{m_1^2} \) and \( R_{\phi_2} \) for the same value of \( L \) cross each other extrapolated as a function of system size. This extrapolation has been carried out for two different fit forms, (a) Power law: \( C_0 + \frac{C_1}{L} \) (left) (b) Polynomial: \( C_0 + \frac{C_1}{L} + \frac{C_2}{L^2} \) (right). The biggest system size used for the fits is \( L = 128 \). We find that the numerical values to which \( \langle m_1^2 \rangle \) and \( \langle \phi_2^2 \rangle \) extrapolate depend on the fit form itself and are inconsistent with the stochastic errors (shown in the legend). The best fitted functions are shown with dashed lines for reference. In both fit forms the extrapolated order parameters go unambiguously to finite values for \( \lambda = 0.5 \) and \( \lambda = 0.75 \). For \( \lambda = 1 \) on the other hand they are consistent with a zero extrapolated value. The \( \langle m_1^2 \rangle \) data shows this effect much more clearly than in the \( \langle \phi_2^2 \rangle \), where it is nonetheless also evident.
B. Numerical Results

In this work, we focus on two values of the anisotropy parameter, $\lambda = 0.5$ and $\lambda = 0.75$. We have included a comparison with the symmetric case $\lambda = 1$ when appropriate.

1. Crossing Analysis

Fig. 2 (a) and (b) show ratios $\mathcal{R}_{m_2^\perp}$ and $\mathcal{R}_{\phi_2^2}$ (defined above) crossing for different $L$ for $\lambda = 0.5$. This indicates a transition from the magnetic to VBS phase. Fig. 2(c) shows crossing of these ratios for the same $L$. As shown in 2(d), the crossing analysis from 2(c) yields the transition point to be at $g_c^* = 12.111(3)$, which is close to the value at which the couplings at the crossing points, $g_c(L)$, converge. This extrapolation has been done only using small system sizes, $L \leq 64$. We notice that smaller system sizes can be seen to smoothly converge to $g_c^* \approx 12.1$, bigger system sizes start deviating from this trend. This is because of the double peaked structure that starts to develop in the order parameter estimators, making it difficult to reliably extrapolate $g_c(L)$ using bigger lattices.

Fig. 4 shows crossings of the quantity $L\rho_s$ for both $\lambda = 0.5$ and $\lambda = 0.75$, which also indicates transition out of the magnetic phase. To investigate the nature of the transition, we study the extrapolation of observables with system size at the critical point. For a continuous transition, all the observables described above ($\rho_s$, $\langle m^2 \rangle$, $\langle \phi^2 \rangle$), should go to zero at the critical point as $L \to \infty$. Fig. 3 shows values of $\langle m_2^\perp \rangle$ and $\langle \phi_2^2 \rangle$ at the crossing points of $\mathcal{R}_{m_2^\perp}$ and $\mathcal{R}_{\phi_2^2}$ at $L$ extrapolated to the infinite system size limit using two different fitting forms (as described in the caption). The extrapolated values of $\langle m_2^\perp \rangle$ and $\langle \phi_2^2 \rangle$ are finite for both $\lambda = 0.5$ and $\lambda = 0.75$. These values for $\lambda = 0.75$ are smaller than that of $\lambda = 0.5$, indicating that the first order nature weakens on increasing $\lambda$. The stiffness extracted from crossings of $L\rho_s$ for $L$ and $L/2$ in Fig 4(a),(b) is plotted as a function of $1/L$ in 4(c). $\rho_s$ clearly extrapolates to a finite value for $1/L \to 0$ for both $\lambda = 0.5$ and $\lambda = 0.75$. Our analysis thus points to a first order transition for $\lambda = 0.5$ and $\lambda = 0.75$. For $\lambda = 1$, on the other hand it is apparent from our data that is hard to argue for a finite order parameter for $\langle m_2^\perp \rangle$ and $\langle \phi_2^2 \rangle$ from the data we have. A more through analysis of the $\lambda = 1$ is available in Ref. 15. We note that these extrapolations become hard to do on very large system sizes because of ergodicity issues that we discuss below and that we argue arise fundamentally at first order transitions.
we found the phase diagram shown in Fig. 1. Our main conclusion is that whenever the easy-plane anisotropy is present the transition is first order. All signs of discontinuity vanish only at the symmetric point $\lambda = 1$

We acknowledge helpful discussions with A. Sandvik. Partial financial support was received through NSF DMR-1611161. Computing resources were obtained through NSF’s XSEDE award TG-DMR-140061 and the DLX computer at the University of Kentucky.

Appendix A: Details of Numerical Simulations and Checks

1. Lattice Hamiltonian

The Hamiltonian defined by Eq. 1 is sign free and therefore we use the SSE QMC algorithm with directed loop updates to simulate it. The easy plane limit of this model ($\lambda = 0$) has no diagonal terms. Hence, to make the model easier to simulate in this limit, we add a constant to the Hamiltonian to generate diagonal matrix elements. The easy plane part of the model defined in Eq. 5 then becomes:

$$H_{ns}^{JQ} = J \sum_{\langle ij \rangle} (\tilde{P}_{ij} + \mathbb{1}_{ij}) - Q \sum_{\langleijkl\rangle} \tilde{P}_{ij} \tilde{P}_{kl}$$

(A1)

To make the loop update more convenient we treat all bonds as plaquettes by multiplying an identity to the adjacent bond, for e.g. the $P_{ij}$ operator in Eq. 2 gets replaced in the following way:

$$P_{ij} = \frac{1}{N_{plaq}^{b}} \sum_{kl} P_{ij} \mathbb{1}_{kl}$$

(A2)

Here $\mathbb{1}_{kl}$ is an identity operator, the sum in this equation is over all four site plaquettes $ijkl$ such that $kl$ is adjacent and parallel to $ij$. $N_{plaq}^{b}$ is number of such plaquettes for each bond, which is 2 in the square lattice case. After making these substitutions the full Hamiltonian described by Eq. 1 becomes:

$$H = \lambda \left\{ \frac{J}{2} \sum_{ijkl} (P_{ij} \mathbb{1}_{kl} + \mathbb{1}_{ij} \cdot P_{kl}) + Q \tilde{P}_{ij} \cdot \tilde{P}_{kl} \right\} +$$

$$(1 - \lambda) \left\{ \frac{J}{2} \sum_{ijkl} (\tilde{P}_{ij} \mathbb{1}_{kl} + \mathbb{1}_{ij} \cdot \tilde{P}_{kl} + \mathbb{1}_{ij} \cdot \mathbb{1}_{kl}) + Q \tilde{P}_{ij} \cdot \tilde{P}_{kl} \right\}$$

(A3)

2. Plaquette Operator

The plaquette operator, $P_{x}(\vec{r})$ in Eq. 6 is the sum of all operators in the Hamiltonian acting on the plaquette at $\vec{r}$. Let $\vec{r}_{ijkl}$ be the position vector of the lower left site of the plaquette $ijkl$.
Fig. 7: Observables $\rho_s, m_±^2$ and $\phi^2_±$ plotted vs $\beta$ can be seen to saturate on increasing $\beta$. This data has been taken at $g = 12$ for $\lambda = 0.5$ and $g = 16$ for $\lambda = 0.75$. These observables can be seen to saturate before $\beta = L$.

TABLE I: Comparison of ground state energy per unit site and spin stiffness values from QMC (for $\beta = 4L$) with ED for $4 \times 4$ square lattice

| $\lambda$ | $\frac{Q}{L}$ | $e^{\text{qmc}}$ | $e^{\text{exact}}$ | $\rho_s^{\text{qmc}}$ | $\rho_s^{\text{exact}}$ |
|----------|---------------|----------------|----------------|----------------|----------------|
| 0.5      | 0.5           | -0.99366(6)    | -0.99371       | 0.2737(1)      | 0.2738         |
| 0.5      | 1.0           | -0.96744(6)    | -0.96746       | 0.2375(1)      | 0.2374         |
| 0.75     | 10.0          | -0.80616(6)    | -0.80608       | 0.12102(7)     | 0.12090        |
| 0.75     | 18.0          | -0.76614(6)    | -0.76613       | 0.11319(7)     | 0.11324        |

\[ P_x(\vec{r}_{ijkl}) = \frac{J}{2} \{ \lambda(\hat{P}_{ij}.\hat{1}_{kl} + \hat{1}_{ij}.\hat{P}_{kl}) + (1 - \lambda)(\hat{P}_{ij}.\hat{1}_{kl} + \hat{1}_{ij}.\hat{P}_{kl}) + \hat{Q}\{\lambda \hat{P}_{ij}.\hat{P}_{kl} + (1 - \lambda) \hat{P}_{ij}.\hat{P}_{kl}\} \quad (A4) \]

3. QMC vs ED

Tables I and II show comparison of the groundstate energy per unit site ($e$), spin stiffness ($\rho_s$) and square of the order parameters, $\langle m_±^2 \rangle$ and $\langle \phi^2_± \rangle$, got from QMC and from exact diagonalization for $\lambda = 0.5$ and $\lambda = 0.75$ on $4 \times 4$ lattices. $\rho_s$, $m_±^2$ and $\phi^2_±$ are as defined in Sec. III A.

4. Convergence to $T = 0$

Fig. 7 shows the behaviour of the observables we have measured for $L \times L$ square lattices as a function of inverse temperature $\beta$. The measurements have been done close to the critical points ($g = 12$ for $\lambda = 0.5$ and $g = 16$ for $\lambda = 0.75$). These quantities can be seen to saturate to the $T = 0$ value on increasing the value of $\beta$. The $\beta$ at which this saturation occurs depends on the system size $L$. As we increase the system size these values saturate to the value at $\beta = L$ faster, therefore we pick $\beta = L$ for our simulations.

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