Gapped spin liquid phase in the $J_1-J_2$ Heisenberg model by a Bosonic resonating-valence-bond ansatz

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We study the ground-state phase diagram of the spin-1/2 $J_1-J_2$ Heisenberg model on the square lattice with an accurate Bosonic resonating valence-bond (RVB) wave function. In contrast to the RVB ansatz based on Schwinger Fermions, the representation based on Schwinger Bosons, supplemented by a variational Monte Carlo technique enforcing the exact projection onto the physical subspace, is able to describe a fully gapped spin liquid in the strongly frustrated regime. In particular, a fully symmetric $Z_2$ spin liquid is stable between two antiferromagnetic phases; a continuous transition at $J_2 = 0.4J_1$, when the Marshall sign rule begins to be essentially violated, and a first-order transition around $J_2 = 0.6J_1$ are present. Most importantly, the triplet gap is found to have a non-monotonic behavior, reaching a maximum around $J_2 = 0.51J_1$, when the lowest spinon excitation moves from the $\Gamma$ to the $M$ point, i.e., $k = (\pi,0)$.

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I. INTRODUCTION

The search for quantum spin liquids in frustrated quantum antiferromagnets has a long history. In recent years, thanks to the advance of numerical techniques, several candidates for spin liquids have emerged in two-dimensional (2D) systems. These include the Hubbard model on the honeycomb lattice, the spin-1/2 Heisenberg model on Kagome lattice, and more recently the spin-1/2 $J_1-J_2$ Heisenberg model on the square lattice. In all these cases, a small but finite spin gap has been found and, according to generalizations of the Lieb-Schultz-Mattis theorem for higher dimensionalities, a topological degeneracy is expected. In spite of these results, descriptions based upon Fermionic resonating valence-bond (RVB) theory predict more often the existence of gapless spin-liquid states. For example, for the $J_1-J_2$ model on the square lattice, the Heisenberg model on the triangular or the Kagome lattices, and, more recently, also for the unfrustrated honeycomb lattice, the Fermionic RVB theory always predicts a gapless spin liquid phase with a Dirac-type spinon dispersion as the best variational state.

The $J_1-J_2$ model represents the simplest model to study the effect of frustration in a (low-dimensional) magnetic system; for this reason it has been investigated by many different approaches in the last 20 years. At the classical level, the system is magnetically ordered for $J_2 < 0.5J_1$ with the standard antiferromagnetic pattern at $q = (\pi, \pi)$. For $J_2 > 0.5J_1$, the ordering wave vector is moved to $q = (\pi,0)$ or $(0,\pi)$; these two ordered phases are separated by a first-order transition. Within the linear spin-wave approach, which goes beyond the classical theory, quantum fluctuations destroy the magnetic order in the intermediate region of $0.4J_1 \lesssim J_2 \lesssim 0.6J_1$, hence leading to a magnetically disordered state. However, the nature of this disordered phase is still elusive and several proposals have been raised. These include valence-bond solids with broken spatial symmetries or gapless spin-liquid states. The latter proposal is especially attractive, since it provides a simple and very accurate Fermionic RVB wave function for $0.4J_1 \lesssim J_2 \lesssim 0.55J_1$. This state has a Dirac-type spinon dispersion and $Z_2$ gauge structure and becomes stable for $J_2 \gtrsim 0.4J_1$.

More recently, density-matrix renormalization group (DMRG) calculations provided some evidence for a fully gapped spin liquid in the intermediate region of $0.4J_1 \lesssim J_2 \lesssim 0.62J_1$. Within this numerical approach, the spin gap increases linearly from $J_2 \simeq 0.4J_1$, reaches a maximum around $J_2 \approx 0.59J_1$, and then rapidly decreases. For $J_2 \gtrsim 0.62J_1$, a collinear magnetic order takes place. The spin-liquid phase determined by these DMRG calculations is thus inconsistent with the Fermionic RVB theory, due to presence of a finite spin gap.

In this paper, we investigate the spin-liquid phase of the $J_1-J_2$ model with a Bosonic RVB wave function. This is motivated by the following reasons. First, while the Fermionic RVB state is found to be unable to open a spin gap for this system, a Bosonic spin-liquid state is by definition gapped, because otherwise the (Bosonic) spinon would condense and the system would develop magnetic order. Second, since the spin-liquid phase is found to exist in a quite small region between two magnetically ordered phases (for which a Bosonic description is quite accurate), it is natural to expect that the intermediate spin-liquid phase inherits some Bosonic characteristic.

The Bosonic RVB state has been adopted in many previous studies and is found to describe quite well both the magnetic ordered state and the disordered state for unfrustrated systems. For frustrated magnetic systems, the use of the Bosonic RVB wave function is very limited, since the loop gas algorithm for the Bosonic RVB
state encounters serious sign problems; moreover, the computation of the wave function amplitude in the orthogonal Ising basis involves permanents of matrices,\textsuperscript{25} implying a computational cost that grows exponentially with the size of the system. Only very recently, this approach has been implemented on small clusters for the Kagome lattice.\textsuperscript{15}

Here, the Bosonic RVB state is obtained after projecting the ground state of the mean-field Schwinger Boson Hamiltonian\textsuperscript{26} into the physical subspace with one spin per site. After this projection, the wave function turns out to be equivalent to the standard Liang-Doucet-Anderson RVB ansatz defined only in terms of a bosonic pairing function (that connects opposite sublattices). To enforce the physical symmetry of the model in the RVB state, we have made a full symmetry classification of the Schwinger Boson mean-field ansatz on the square lattice with the projective symmetry group (PSG) technique.\textsuperscript{28-30} Then, we have performed variational Monte Carlo simulations in order to optimize such a Bosonic RVB state, by using both the permanent Monte Carlo algorithm and the loop gas algorithm.

We find that the Bosonic RVB wave function gives a rather good variational description of the system. In addition, we find that the phase diagram predicted by the DMRG calculations can be well reproduced. Moreover, we find that the phase diagram predicted by the variational Monte Carlo simulations in order to optimize such a bosonic RVB state, by using both the permanent Monte Carlo algorithm and the loop gas algorithm.

Finally, by PSG symmetry considerations, it can be shown that the spin gap is always finite at the \( M \) point in the spin-liquid state around \( J_2 = 0.4J_1 \) through a continuous transition, when the Marshall sign rule in the ground state begins to be essentially violated. A level crossing of the spinon excitation is observed around \( J_2 = 0.51J_1 \), when the gap minimum of the spinon excitation branch is moved from the \( \Gamma \) to the \( M \) point, i.e., \( k = (\pi, 0) \) point and a kink appears in the spin gap as a function of \( J_2 \).

The paper is organized as follows: in Sec. III we describe the model and the method; in Sec. IV we present our numerical results; finally, in Sec. V we draw our conclusions.

II. THE MODEL AND METHODS

In this paper, we consider the following model:

\[
H = J_1 \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_i,
\]

where \( \langle i,j \rangle \) and \( \langle\langle i,j \rangle\rangle \) indicate nearest-neighbor and next-nearest-neighbor sites on the square lattice, respectively; \( \mathbf{S}_i \) denotes the spin operator at site \( i \).

In the Schwinger Boson representation,\textsuperscript{27} the spin operator is written as \( \mathbf{S} = \frac{1}{2} \sum_{\alpha,\beta} b_\alpha^\dagger \vec{\sigma}_\alpha b_\beta \), where \( b_\alpha \) is a Boson operator, \( \vec{\sigma} \) is the Pauli matrix. Bosons should satisfy the no double occupancy constraint \( \sum_\alpha b_\alpha^\dagger b_\alpha = 1 \), in order to be a faithful representation of the spin-1/2 operator. Within this representation, the Heisenberg superexchange coupling can be written as (apart from additive constants) \( \hat{S}_i \cdot \hat{S}_j = -\frac{1}{2} \hat{A}_{i,j} \hat{A}_{i,j} + \frac{1}{2} \hat{B}_{i,j} \hat{B}_{i,j} \), where \( \hat{A}_{i,j} = b_\uparrow b_\downarrow - b_\downarrow b_\uparrow \) and \( \hat{B}_{i,j} = b_\uparrow^\dagger b_\downarrow^\dagger + b_\downarrow b_\uparrow \).

In the mean-field treatment, we replace \( \hat{A}_{i,j} \) and \( \hat{B}_{i,j} \) with their mean-field expectation value \( A_{i,j} \) and \( B_{i,j} \), so to have:

\[
H_{MF} = -\frac{1}{2} \sum_{i,j} \left( \Delta_{i,j} \hat{A}_{i,j}^\dagger + h.c. \right) + \frac{1}{2} \sum_{i,j} \left( F_{i,j} \hat{B}_{i,j}^\dagger + h.c. \right) + \lambda \sum_i \left( \sum_\alpha b_\alpha^\dagger b_\alpha - 1 \right),
\]

where \( \Delta_{i,j} = J_{i,j} A_{i,j} \), \( F_{i,j} = J_{i,j} B_{i,j} \), and the chemical potential \( \lambda \) is introduced to fulfill, on average, the single-occupancy constraint. The mean-field ground state has the general form of

\[
\langle MF \rangle \propto \exp \left\{ \sum_{i,j} a(R_i, R_j)(b_i^\dagger b_{i,j} - b_{i,j}^\dagger b_i) \right\} |0\rangle.
\]

Then, a suitable RVB wave function in the physical Hilbert space with one Boson per site may be obtained by projecting the mean-field state, namely

\[
|RVB\rangle = P_G |MF\rangle,
\]

where \( P_G \) is a Gutzwiller projector that enforces the constraint of one Boson per site. The equivalence of the RVB state with the standard Liang-Doucet-Anderson state\textsuperscript{29} is clear after projection onto the physical subspace.

The form of the RVB amplitude \( a(R_i, R_j) \) is determined by the parameters \( \Delta_{i,j}, F_{i,j}, \lambda \). At the mean-field level, \( \Delta_{i,j} \) and \( F_{i,j} \) are non-zero only on those bonds with \( J_{i,j} \neq 0 \). However, from the variational point of view, we can take \( \{\Delta_{i,j}, F_{i,j}, \lambda\} \) as a set of free parameters to construct the RVB state. In such a case, we can also introduce \( \Delta_{i,j} \) and \( F_{i,j} \) on longer bonds, for which \( J_{i,j} = 0 \).

In order to describe a spin liquid state with the full symmetry of the model, the mean-field parameters \( \{\Delta_{i,j}, F_{i,j}, \lambda\} \) must satisfy certain symmetry conditions. Since there exists a U(1) gauge degree of freedom in the Schwinger Boson representation of the spin operator (i.e., \( b_{i,\alpha} \rightarrow b_{i,\alpha} e^{i\phi_i} \) leaves \( \hat{S}_i \) unchanged), the symmetry requirement on the mean-field Hamiltonian is actually the U(1) gauge projective extension of the physical symmetry of the model. Such symmetry conditions on the mean-field ansatz can be readily worked out by the so called PSG technique developed by Wen\textsuperscript{28} for the Fermionic representation. The Bosonic version of the PSG is the
U(1) subset of the Fermionic PSG. Here, we will just point out some basic structures that are relevant to our study.

In the Schwinger Boson formalism, the mean-field parameters $\Delta_{i,j}$ and $F_{i,j}$ describe antiferromagnetic and ferromagnetic local correlations, respectively (see Appendix A for the possible phases implied by this ansatz). Here, we assume a non-zero $\Delta_{i,j}$ between nearest-neighbor sites. Then, we find that a non-zero $\Delta_{i,j}$ between next-nearest-neighbor sites is compatible only with the so-called type B translational property of the mean-field Hamiltonian, which implies a unit cell with two sites. We find that such state is much higher in energy than any state in the so-called type A class, characterized by a manifestly translational invariant mean-field ansatz. Therefore, in the following we restrict our analysis only to translationally invariant states. Within the type A states, we find the following general rules for the mean-field ansatz for a symmetric spin liquid state. First, for sites belonging to different sub-lattices, only a real $\Delta_{i,j}$ is allowed. Second, for sites in the same sub-lattice, only a real $F_{i,j}$ is allowed. Considering the site $i$ as belonging to $A$ sub-lattice, the allowed mean-field parameters up to the fourth-neighbor are given by:

\[
F_{i,i+\delta_1} = 0, \quad \Delta_{i,i+\delta_1} = \Delta, \quad (5)
\]

\[
F_{i,i+\delta_2} = F, \quad \Delta_{i,i+\delta_2} = 0, \quad (6)
\]

\[
F_{i,i+\delta_3} = F_{2x}, \quad \Delta_{i,i+\delta_3} = 0, \quad (7)
\]

\[
F_{i,i+\delta_4} = 0, \quad \Delta_{i,i+\delta_4} = \Delta_{2xy}, \quad (8)
\]

where $\delta_\mu$ (with $\mu = 1, \ldots, 4$) denotes the vectors connecting the site $i$ to its neighbors, up to the fourth distance. Here, $\{\lambda, F, \Delta, F_{2x}, \Delta_{2xy}\}$ are a set of real parameters. An illustration of the ansatz used in this study is shown in Fig. 1. For the sites $i$ belonging to $B$ sub-lattice, the sign of $\Delta$ and $\Delta_{2xy}$ should be reversed (since $\Delta_{i,j}$ is odd by interchanging $i$ and $j$).

At the mean-field level, both $F_{2x}$ and $\Delta_{2xy}$ are zero, and the Hamiltonian is given by

\[
H_{MF} = \sum_{k \in MBZ} \psi_k^\dagger \begin{pmatrix}
\epsilon_k & 0 & 0 & \Delta_k \\
0 & \epsilon_k & -\Delta_k & 0 \\
0 & -\Delta_k & \epsilon_k & 0 \\
\Delta_k & 0 & 0 & \epsilon_k
\end{pmatrix} \psi_k, \quad (9)
\]

in which $MBZ$ indicates the reduced (magnetic) Brillouin zone, $\psi_k^\dagger = (b_{4k+1}^\dagger, b_{4k+2}^\dagger, b_{4k+3}^\dagger, b_{4k+4}^\dagger)$, $\epsilon_k = \lambda + 2F g(k)$, and $\Delta_k = 2\Delta g(k)$. Here $g(k) = \cos(k_x) \cos(k_y)$, $\gamma(k) = (\cos(k_x) + \cos(k_y))/2$. The mean-field spectrum is given by $E_k = \sqrt{\epsilon_k^2 - \Delta_k^2}$ and the minimal spinon gap is given by

\[
E_{min} = \begin{cases}
\sqrt{(\lambda + 2F)^2 - (2\Delta)^2}, & 2\lambda F < \Delta^2, \\
\lambda - 2F, & 2\lambda F > \Delta^2.
\end{cases}
\]

For the first case, the gap minimum is located at the $\Gamma$ point, while for the second case the gap minimum is at the $M$ point.

Finally, the RVB amplitudes derived from the mean-field ground state are given by

\[
a(R_i - R_j) = \frac{1}{N} \sum_{k \in MBZ} \frac{\Delta_k}{\epsilon_k + E_k} e^{i k (R_i - R_j)}, \quad (10)
\]

where $N$ is the number of sites, $i \in A$ and $j \in B$. The RVB amplitudes between sites in the same sub-lattice are...
identically zero. We would like to mention that, within
the standard formulation based upon Monte Carlo sam-
ing only positive pairing functions $a(R_i - R_j)$ have
been considered so far. In our formulation this restric-
tion applies only for standard antiferromagnetic phases,
while negative amplitudes are found in the much more
interesting spin-liquid phase.

III. RESULTS

The mean-field Hamiltonian has been studied by
Mila and collaborators, showing that no spin-liquid
phases are stabilized and a direct transition between two
ordered phases is present, with a phase diagram that is
very similar to the classical limit.

In order to go beyond this approximation, we now
move to the projected RVB state of Eq. (4), to assess
the possibility that quantum fluctuations may induce a
finite spin gap and, therefore, a stable spin liquid. We
thus determine the parameters in the Bosonic RVB state
by optimizing the energy of the original $J_1 - J_2$ model,
rather than solving the self-consistent equations. Then,
the spinon gap can be estimated by inserting back the
optimized parameters into the mean-field dispersion re-
elation $E_k$. Note that the RVB wave function does not
depend on the overall energy scale of the system. As a
result, the spinon gap can be determined only up to a
normalization constant. Here we will use the chemical
potential $\lambda$ as the unit of energy. To have an estimate
of the absolute scale of the spinon gap, we determine the
pairing potential $\Delta$ from the

$$\Delta = J_1 \langle \hat{A}_{i,i+x} \rangle = \frac{J_1}{N} \sum_{k \in MBZ} \Delta_k \gamma(k)$$

by inserting on the right-hand side the optimized values
of $\Delta / \lambda$ and $F / \lambda$, which are $(\Delta / \lambda)^{\text{opt}}$ and $(F / \lambda)^{\text{opt}}$. Then $\lambda$ can be determined by requiring that $\Delta / \lambda = (\Delta / \lambda)^{\text{opt}}$.

The computation of the Bosonic RVB wave function is
very expensive in the Ising basis, since it requires the
calculation of permanents, for which no polynomial algo-
rithm exists. However, on small clusters it is affordable.
In this work, we have used a $6 \times 6$ cluster to perform the optimization of the parameters in the
RVB wave function. It is important to note the key
difference between the mean-field theory and the pro-
jected RVB wave function. In the mean-field theory, the
chemical potential $\lambda$ is determined by the self-consistent
equation for the total Boson number. When the spinon
gap approaches zero, the number of Boson will diverge.
Then, on any finite lattice, the spinon gap can never be
zero and a finite-size gap must exist (see Appendix C for
the details on the spinon gap in the mean-field approach).
On the contrary, after projection, the constraint of one
Boson per site is satisfied exactly and such a divergence
will not appear. Therefore, the RVB wave function is
well behaved even when the spinon gap is zero. This fact
implies that a vanishing spinon gap can be realized ex-
actly after optimization of the corresponding projected
RVB wave function on a relatively small cluster.

From our numerical optimization, we find that a spin
gap can not be opened if we keep $\Delta / \lambda$ and $F / \lambda$ only.
Moreover, by a direct optimization of the pairing ampli-
tudes $a(R_i - R_j)$, a good accuracy can be achieved only
by including a third-neighbor parameter $F_{2x}$, while the
fourth-neighbor parameter $\Delta_{xy}$ is found to be
always negligibly small. Therefore, in the following, we
optimize the wave function with $\Delta / \lambda$, $F / \lambda$ and $F_{2x}$ as variational parameters. In particular, we find that the
inclusion of $F_{2x}$ is crucial for the opening of the spin
gap. The optimized value of the parameters in the RVB
wave function are shown in Fig. 2.

The spinon gap at the $\Gamma$ and the $M$ points is shown
in Fig. 3(a). Around $J_2 = 0.5J_1$, a level crossing in the
spinon excitation occurs and the gap minimum changes
from $\Gamma$ to $M$. By further increasing $J_2$, the spinon
gap at $M$ decreases and eventually approaches zero around
$J_2 = 0.6J_1$. At this point the system becomes unstable
with respect to magnetic ordering at $q = (\pi, 0)$. It
should be noted that, although the spinon gap at the $M$
point approaches zero continuously for $J_2 = 0.6J_1$, our
state cannot be continuously connected to the collinear
ordered state, and a first-order transition must exist be-
tween the fully symmetric spin liquid and the collinear
ordered magnetic phase. This is clearly seen in the static
spin structure factor:

$$S(q) = \frac{1}{2} \sum_{k} \left( \frac{\epsilon_k \epsilon_{q-k} - \Delta_k \Delta_{q-k}}{E_k E_{q-k}} - 1 \right).$$

Since $\Delta_k(\pi, 0) = 0$ by symmetry (see Appendix D),
the singularity in the coherence factor for $E_{k=(\pi,0)} \rightarrow 0$ is
removed and the spin structure factor at $q = (\pi, 0)$ is
always finite. Thus, the state cannot be connected to
the collinear ordered phase, in which $S(\pi, 0)$ diverges.
Therefore, we conclude that a first-order transition must
exist between the spin liquid and the collinear ordered
phase.

Given the results for the spinon spectrum of Fig. 3(a),
it is possible to make some prediction on the behavior of
the triplet gap as a function of $J_2$. Indeed, to construct
a triplet excitation at $q = (\pi, \pi)$, we can use two spinons
both from the $\Gamma$ point and the $M$ point. On the con-
trary, for a triplet excitation with momentum $q = (\pi, 0)$,
we should use one spinon from the $\Gamma$ point and another
spinon from the $M$ point. Therefore, the lowest triplet
excitation is always realized at $q = (\pi, \pi)$ and the energy
of triplet excitation at $q = (\pi, 0)$ is always finite, see
Fig. 3(b). This is consistent with the result of the static
spin structure factor mentioned above and points to the
fact that our spin-liquid state cannot be continuously
connected to the collinear ordered phase. We note that
the peculiar behavior of the triplet excitations found in
this work represents an astonishing consequence of frac-
tionalized spinon excitations in the spin-liquid phase.
We would like to mention that our results for the spin gap are quite similar to the DMRG ones.\textsuperscript{4} Indeed, within both approaches, the spin gap is found to open around $J_2 = 0.4J_1$ and close around $J_2 = 0.62J_1$. In addition, a sharp maximum is present, though its position in the Bosonic RVB approach is found to correspond to a lower value of $J_2$ with respect to the DMRG study. Moreover, taking the value of $\lambda$ estimated from Eq.\textsuperscript{11}, which is $\lambda \approx 1.02J_1$ at $J_2 = 0.5J_1$, we have that the maximal spin gap is quite consistent with the DMRG prediction.

In this work, the sharp maximum in the spin gap is interpreted as the result of a level crossing in the minimum of the spinon spectrum (from the $\Gamma$ to the $M$ point). In such a picture the lowest triplet excitation within the symmetric spin liquid phase is always at $q = (\pi, \pi)$. However, other possibilities for this structure may exist, among which a spin nematic liquid phase, which breaks the reflection symmetry $x \rightarrow y$ but with all other physical symmetries intact, is especially interesting.\textsuperscript{35} Since the DMRG calculations have been done on rectangular clusters, the nematic liquid phase can be connected to the symmetric state continuously on finite lattices.

To further check the accuracy of the Bosonic RVB wave function, we computed the relative error in the ground-state energy, namely $\Delta E = |E_0 - E_{\text{var}}|/|E_0|$, where $E_0$ is the exact ground-state energy and $E_{\text{var}}$ is the variational energy of the RVB state. In Fig.\textsuperscript{4} we report the accuracy of the Bosonic RVB wave function on the $6 \times 6$ cluster, in comparison with the best Fermionic RVB wave function.\textsuperscript{2} For small $J_2$, the Bosonic RVB wave function is much more accurate than the Fermionic RVB wave function, which cannot describe magnetically ordered states. In this region, our results for the Bosonic wave function agree with previous calculations reported in Ref.\textsuperscript{36} obtained with a different algorithm\textsuperscript{21} or a different parametrization.\textsuperscript{22} For $J_2 \gtrsim 0.45J_1$, the Fermionic wave function becomes more accurate. However, the error in both wave functions are similar and both increase with the same trend by increasing $J_2$ up to $J_2 = 0.6J_1$.

As pointed out in Ref.\textsuperscript{6}, the sign structure of the ground state is crucial for the origin of the spin liquid phase. For $J_2 = 0$, the ground-state wave function satis-
fies the Marshall sign rule. However, the Marshall sign rule is essentially violated only for $J_2 \gtrsim 0.4J_1$ and, in the Fermionic RVB approach, a $Z_2$ spin liquid phase emerges just at the same point. A similar scenario also appear in the Bosonic representation. In this case, when the RVB amplitudes from sub-lattice A to sub-lattice B are positive, then the wave function satisfies the Marshall sign rule, otherwise (if some amplitudes are negative) the Marshall sign rule is violated. In Fig. 5, we plot all the independent RVB amplitudes $a(R_i, R_j)$ on a 6 x 6 lattice of the optimized wave function (with the amplitude between the nearest-neighbor sites equal to one). For $J_2 < 0.4J_1$, all amplitudes are positive and thus the wave function has the Marshall sign. For $J_2 > 0.4J_1$, the amplitude on bond (1, 2) becomes negative and the Marshall sign rule is violated. It is just at this point that the spin gap opens. Thus, the origin of the spin gap and the existence of the spin liquid phase can be understood as a result of violation of the Marshall sign rule. Such an understanding is consistent with several previous studies in which the topological degeneracy, which is a hallmark of gapped spin liquid, is argued to be absent in system satisfying the Marshall sign rule.

Finally, we report in Fig. 5 the average Marshall signs in the Bosonic and Fermionic RVB wave functions:

$$\langle S \rangle = \sum_x |\langle x|RVB\rangle|^2 \text{sign} \left\{ \langle x|RVB\rangle(-1)^{N_1(x)} \right\},$$

where $|RVB\rangle$ denotes the RVB variational state (either Bosonic or Fermionic) and the sum is over the orthogonal Ising basis $|x\rangle$; for comparison, we also report the results for the exact ground state, where $|RVB\rangle$ is replaced by $|\Psi_0\rangle$. The Fermionic RVB wave function is better in the sense of sign structure and this is consistent with the fact that the Fermionic wave function has a lower energy for large $J_2$. However, it is clearly seen that both the Bosonic and the Fermionic RVB wave function underestimate seriously the frustration of the sign in the spin-liquid regime.

### IV. CONCLUSIONS

In conclusion, we find the Bosonic RVB wave function generates a ground-state phase diagram of the $J_1 - J_2$ model on the square lattice that is qualitatively consistent with DMRG results. A gapped spin-liquid phase is found for $0.4J_1 < J_2 < 0.6J_1$. The spin-liquid phase is connected to the staggered magnetic ordered state through a continuous transition but cannot be connected continuously to the collinear magnetic ordered state and a first-order transition between the two must exist. The spin gap is found to have a maximum around $J_2 = 0.5J_1$ as a result of the level crossing between the spinon at $\Gamma$ and $M$ points. This fact implies that the lowest triplet excitation is found to be always at $q = (\pi, \pi)$ in the spin-liquid phase. We also found that the spin gap opens at the same point where the system violates the Marshall sign rule. This fact provides strong support for previous arguments for the absence of topological order in systems satisfying the Marshall sign rule. Despite that these outcomes are in good agreement with recent DMRG calculations of Ref. 4, the gapless Dirac-type Fermionic RVB ansatz remains slightly more accurate at the variational level in the highly-frustrated regime.

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### Appendix A: The various phases described by the wave function studied in this work

The various phases described by the wave function studied in this work are shown in Fig. 6. Here, we report the various properties as a function of two parameters, namely $F/\lambda$ and $\Delta/\lambda$. The case with non-zero $F_{2x}/\lambda$ is qualitatively similar. The condensation lines denote the magnetically ordered states with staggered or collinear patterns. The three regions, A, B and C, denote spin-liquid phases. In regions A and B, the spinon gap minimum is realized at the $\Gamma$ point, while in the region C the gap minimum is moved to the $M$ point. In region B, the Marshall sign rule is violated while it is satisfied in region A. The region with slanted lines is physically non-accessible.
FIG. 7: (Color on-line) The spinon gap predicted by mean-field theory both at Γ and M points. For the Γ point, we show the scaling of the mean-field gap with the linear size of the system. The mean-field gap at the M point in the thermodynamic limit is also reported (dashed line).

Appendix B: The mean-field finite size gap

In the mean-field theory, the spinon is always gapped when the system is defined on a finite lattice. We report in Fig. 7 the spinon gap obtained by solving the mean-field self-consistent equations. Here, we would like to emphasize that the origin of a spinon gap obtained on finite lattices with the projected Bosonic RVB wave function is totally different from that obtained within the mean-field approximation. Indeed, after projection, the number of spinons is fixed (each site is occupied by one and only one spinon) and the RVB wave function is always well defined.

In fact, we find that the spinon gap is exactly zero for \( J_2 < 0.4 J_1 \) from our optimization on the \( 6 \times 6 \) lattice, see Fig. 8. Instead, the finite size gap in the mean-field theory is much larger and smoother than that obtained with the projected Bosonic RVB wave function. In addition, we note that the mean-field theory always predicts a very large gap at the M point in the thermodynamic limit.

Appendix C: The proof of \( \Delta_{k=(\pi,0)} = 0 \)

For the ansatz of type A, which is manifestly translational invariant in the so-called uniform gauge, the gauge transformations of the PSG for symmetric Bosonic spin liquid state is found to be (we have adopted the convention of Ref. 28)

\[
G_{px} = \eta_x P_x e^{i\phi_x}, \\
G_{py} = \eta_y P_y e^{i\phi_y}, \\
G_{pxy} = e^{i\phi_{xy}},
\]

in which \( \eta_x P_x, \eta_y P_y = \pm 1, \phi_x, \phi_{xy} = 0, \pi/2 \).

If we require \( \Delta_{i,j} \) to be non-zero between nearest-neighbor sites, the PSG should satisfy

\[
\eta_x P_x = -\eta_y P_y, \\
\eta_x P_x = -e^{2i\phi_x}.
\]

In the uniform gauge, \( \Delta_{i,j} \) is only a function of \( R_j - R_i \), so we can write \( \Delta_{i,j} = \Delta_{(d_x,d_y)} \), in which the distance \( (d_x, d_y) = (j_x - i_x, j_y - i_y) \). By applying \( P_x \) and \( P_y \) successively, we have

\[
\Delta(-d_x,-d_y) = \left( \eta_x P_x \eta_y P_y \right) d_x + d_y \Delta_{(d_x,d_y)} = (-1)^{d_x + d_y} \Delta_{(d_x,d_y)}.
\]

However, from the fact that \( \Delta_{i,j} = -\Delta_{j,i} \), we have

\[
\Delta(-d_x,-d_y) = -\Delta_{(d_x,d_y)}.
\]

We thus conclude that \( \Delta_{i,j} \) is non-zero only between sites in the opposite sub-lattices.

To show further that \( \Delta_{k=(\pi,0)} = 0 \), we need to go to the sub-lattice uniform gauge. For \( \phi_{xy} = 0 \), the gauge transformation from the uniform gauge to the sub-lattice uniform gauge is given by

\[
W_i = (-1)^{\left\lfloor \frac{i_x + i_y}{2} \right\rfloor},
\]

while for \( \phi_{xy} = \pi/2 \), it is given by

\[
W_i = (-1)^{\left\lfloor \frac{i_x - i_y}{2} \right\rfloor},
\]

in which \( \lfloor r \rfloor \) means the largest integer that is not greater than \( r \). In the sub-lattice uniform gauge, the pairing term \( \Delta_{(d_x,d_y)} \) has s-wave symmetry from any site in the A or B sub-lattice (but has opposite signs for \( \Delta_{i,j} \) starting from the A and B sub-lattices). Thus the total contribution to the Fourier transform of \( \Delta_{(d_x,d_y)} \) from distance \( (d_x, d_y) \) and all the other symmetry-related distances is proportional to

\[
\Delta_{(d_x,d_y)} \left( \cos(k_x d_x) \cos(k_y d_y) + \cos(k_x d_y) \cos(k_y d_x) \right).
\]

Since \( \Delta_{(d_x,d_y)} \) is non-zero only when \( d_x + d_y \) is an odd integer, it is easy to see that \( \Delta_{k=(\pi,0)} = 0 \).

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