Antiferromagnetic long-range order in the uniform resonating valence bond state on the square lattice

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Abstract – With an extensive variational Monte Carlo simulation, we show that the uniform resonating valence bond (U-R VB) state on the square lattice is antiferromagnetic long-range ordered. The ordered moment is estimated to be \( m \approx 0.186 \). Such a behavior is quite unexpected from the slave boson mean-field treatment or the Gutzwiller approximation of the uniform RVB state.

The resonating valence bond (RVB) state plays an important role in our understanding of exotic physics in quantum antiferromagnet and the high-\( T_c \) superconductors [1]. The RVB state is a quantum many-body spin singlet constructed from the coherent superposition of different pairing patterns of the spins on the lattice.

In practice, the most studied RVB states are those generated from the Gutzwiller projection of a fermionic or bosonic mean-field state with condensed singlet pairs. It is well known that the RVB states generated from these two routes differ in their property qualitatively. For example, a bosonic RVB state can be either short ranged in its spin correlation when the spinon excitation spectrum has a full gap, or, long-range ordered when the bosonic spinon condenses. On the other hand, a fermionic RVB state can have more choices for its spin correlation. Beside being short ranged with an exponentially decaying spin correlation, the spin can also choose to stay in various kinds of critical states. For example, a fermionic RVB state can have a large spinon Fermi surface or various kinds of node structure in its spinon dispersion. The spin correlation in such critical state generally follows a power law behavior. However, a condensation of triplet pairs will inevitably break the spin rotational symmetry.

The relation between the bosonic and fermionic RVB state has been studied by many authors [2,3]. It was found that when the RVB amplitude is extremely short ranged, or extending only between nearest-neighbor sites, and the lattice is planar, a fermionic RVB state can be transformed into a bosonic RVB state with suitable redefinition of the RVB amplitudes. For fermionic RVB states with longer-range RVB amplitudes, their relation with the bosonic RVB states is still elusive. More generally, it was found that on the bipartite lattice, both the bosonic and the fermionic RVB state satisfy the well-known Marshall sign rule for unfrustrated antiferromagnets, if they are both derived from a bipartite mean-field Hamiltonian.

An analytical treatment of the RVB state is difficult. The most commonly adopted method to study the fermionic RVB state is the slave boson mean-field theory. Beyond the mean-field theory, there is also the more elaborate effective gauge field theory treatment [4–6]. However, it is well known that the mean-field theory may fail qualitatively as the no-double-occupancy constraint is relaxed to a global one in such treatment. The gauge fluctuation corrections, which can in principle improve the result of the mean-field theory, are accounted for only at the Gaussian level in most cases and may miss the singular gauge fluctuation effect at the lattice scale. As a variational state, the fermionic RVB state is also studied by the Gutzwiller approximation [7], which tries to estimate the effect of the local constraint by correcting the mean-field expectation value with some correction factor. However,
the Gutzwiller approximation cannot produce any qualitatively different prediction from the mean-field theory as to the spin correlation in the RVB state [8].

The variational Monte Carlo (VMC) method is a direct way to study the properties of the fermionic RVB state. It is found that in certain cases the VMC result can be quite different from the mean-field prediction. For example, on a bipartite lattice, a well-defined sign structure (the Marshall sign rule) may emerge out of a general mean-field state through the Gutzwiller projection, even if the mean-field state breaks the time-reversal symmetry and has a complex valued wave function. Such a sign structure will restore the time-reversal symmetry in the projected state and remove from the system the possible topological degeneracy [9].

In this paper, we present another example in which the mean-field prediction is qualitatively changed by the Gutzwiller projection. We show that the well-known uniform RVB state on the square lattice with a large Fermi surface for the spinon actually describes a state with magnetic long-range order.

The uniform RVB state first appears as a variational state for the high-\(T_c\) superconductors in Anderson’s original paper on the RVB theory of the cuprates [10]. The state has a large nested Fermi surface for the fermionic spinon. Although it is later found that the \(d\)-wave RVB state is energetically more favorable than the uniform RVB state [11], the uniform RVB state is nevertheless still an interesting state of its own right.

At the mean-field level, the uniform RVB state is described by a filled Fermi sea with a nested Fermi surface. The spin correlation function decays algebraically with distance as \(1/k^2\). The spin structure factor at the antiferromagnetic wave vector is given by \(S_q=(\pi,\pi) = \frac{3}{2N}\), in which \(N\) is number of lattice sites [12]. Thus, at the mean-field level, the uniform RVB state describes a state with no magnetic long-range order. However, as the system presents a nested Fermi surface, the mean-field state is unstable with respect to an infinite small perturbation toward antiferromagnetic ordering. Thus, it is highly possible that the Gutzwiller projection may induce finite antiferromagnetic order in the uniform RVB state, in a way that the spin rotational symmetry remains intact.

The uniform RVB state is given by the Gutzwiller projection of the ground state of the following mean-field ansatz:

\[
H_{U-RVB} = - \sum_{\langle i,j \rangle,\sigma} \left( \epsilon_{i\sigma} c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.} \right),
\]

where \(\epsilon_k = -2(\cos k_x + \cos k_y)\). The uniform RVB state can then be written as

\[
|U-RVB\rangle = P_G \prod_{k<k_F} c_{k\uparrow}^\dagger c_{-k\downarrow} \langle 0 |,
\]

where \(k_F\) denotes the Fermi momentum of the spinon and is determined by \(\epsilon_{k_F} = 0\). \(P_G\) denotes the Gutzwiller projection into the subspace of no double occupancy. The state can also be written in the form of condensed pairs,

\[
|U-RVB\rangle = P_G \left( \sum_{i,j} a(i-j) c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger \right)^{\frac{1}{2}} |0\rangle,
\]

in which \(a(i-j) = \sum_{k<k_F} e^{i k (R_i-R_j)}\). Due to the bipartite nature of the square lattice, it can be shown that the uniform RVB state satisfies the Marshall sign rule for an unfrustrated antiferromagnet [2,13]. More specifically, the wave function of the uniform RVB state in a Ising basis is real up to a global phase factor and its sign is given by \((-1)^{N_d}\), where \(N_d\) denotes the number of down spins in the \(A\) sublattice.

To detect possible magnetic long-range order in the uniform RVB state, we focus on the spin structure factor at the antiferromagnetic ordering wave vector

\[
S_{q=(\pi,\pi)} = \frac{1}{N^2} \sum_{i,j} e^{i q (R_i-R_j)} \langle S_i \cdot S_j \rangle.
\]

At the mean-field level, the spin structure factor can be found to be given by \(S_{q=(\pi,\pi)} = \frac{3}{2N}\). On the other hand, when the no-double-occupancy constraint is enforced by the Gutzwiller projection, the result is quite different.

In fig. 1, we show the VMC result for the spin structure factor of the uniform RVB state at \(q = (\pi,\pi)\) on a square lattice as a function of the inverse linear scale of the lattice, \(1/L\). Presented in this figure are the results for \(L = 6,8,10,12,14,16,18,20,22,24,26,30,36,40,44\) and \(50\). The periodic-antiperiodic boundary condition is adopted in the calculation to satisfy the closed-shell condition. The error bars are smaller than the size of the symbols. The black dot on the \(y\)-axis denotes the fitted value of \(S_0\).

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The statistical error estimated from the data is smaller than the size of the symbols in the figure. The spin structure factor of the uniform RVB state clearly extrapolates to a finite value in the thermodynamic limit.

To see the trend of the spin structure factor more clearly, we fit the data with the formula $S_q = S_0 + A/L + B/L^2$, which is the expected scaling form for a system with finite magnetic stiffness. The best fit to the data is found to be $S_0 = 0.03452$. Thus, the ordered moment in the uniform RVB state is given by $m = \sqrt{S_0} = 0.186$, which is not at all small if compared to the value predicted by the spin wave theory for the Heisenberg model on the square lattice ($m = \sqrt{S_0} = 0.3$).

As a comparison, we also present the spin structure factor of another well-known fermionic RVB state on the square lattice, namely, the $\pi$ flux phase in fig. 2. The $\pi$-flux phase is generated by the following mean-field ansatz:

$$H_{\pi,\text{flux}} = -\sum_{\langle i,j \rangle,\sigma} (e^{i\phi_{i,j}} c_{i,\sigma}^\dagger c_{j,\sigma} + \text{h.c.})$$

in which the phase factor $\phi_{i,j}$ is introduced to guarantee that each plaquette of the square lattice is threaded by a $U(1)$ flux of value $\pi$. In the $\pi$-flux phase, the spinon has a Dirac-type linear dispersion and the mean-field spin correlation also decays with distance as $1/R^2$. After the Gutzwiller projection, the spin correlation of the system is greatly enhanced. But as is clear from fig. 2, the $\pi$-flux phase does not support the antiferromagnetic long-range order. In fact, a finite-size scaling analysis shows that the spin structure factor decays as $1/L^2$ with the linear scale of the lattice and extrapolates to zero in the thermodynamic limit (fig. 3).

From these data, it is clear that the uniform RVB state indeed describes a state with antiferromagnetic long-range order. This is quite unexpected from the mean-field theory and it represents the first example of fermionic RVB state with magnetic order. Such an order does not originate from the condensation of spinons as in the bosonic RVB state and respects the spin rotational symmetry. In the uniform RVB state, the magnetic long-range order can be understood as a result of the induced magnetic ordering in a system with nested Fermi surface.

Following the above reasoning, it is quite interesting to ask the following question: does the uniform RVB state have antiferromagnetic long-range order in other spatial dimensions? In one dimension, the projected Fermi sea state is critical and the spin correlation function decays with distance as $1/L$, indicating no magnetic long-range order. This can be understood as the result of the strong quantum fluctuation in a one-dimensional system. As the fluctuation becomes weaker in higher spatial dimensions, it is quite possible that the uniform RVB state in three dimension (on a cubic lattice) also has antiferromagnetic long-range order. A study of this issue, which is numerically quite demanding for a large lattice, will be presented in another paper.

Additional remark: We have come to know that a recent preprint [14] independently confirmed part of the results of this manuscript.
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