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Instability of the long-range resonating-valence-bond state in the mean-field approach

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We show the instability of the mixed $s+id$ flux phase by showing that a continuous path connects it to a lower-energy dimerized phase without crossing any energy barriers. We discuss the consequences of this result for possible expansions around mean-field theory.

After Anderson[1] suggested a possible connection between the resonating-valence-bond (RVB) phase of the quantum Heisenberg antiferromagnet and high-temperature superconductivity there has been substantial effort in trying to elucidate the existence and the physical properties of magnetic phases which are disordered because of quantum fluctuations.

At this point there are only two ways of modeling these phases; one uses variational wave functions[2] and the other decouples bond variables by introducing auxiliary gauge fields. The leading approximation in the second approach is a mean-field theory first proposed by Baskaran, Zou, and Anderson (BZA).[3] This approach is very appealing because of its simplicity and because it naturally leads to a spectrum of fermionic excitations which is known to be the correct spectrum of excitations in one dimension.[4]

This approach can describe different phases of the resonating-valence-bond theory depending on the different expectation values of the bond variables. In their original paper,[3] BZA considered an order parameter with equal amplitude and phases in all bonds. It describes a phase with a pseudo-Fermi-surface and a Fermi-liquid type of excitation spectrum which is responsible for a constant low-temperature susceptibility and a linear specific heat. Later Kotliar[5] and independently Affleck and Marston[6] found a lower-energy solution within mean-field theory by taking the relative phase of certain bond variables to be $\pi/2$. The equivalence of the approaches of Refs. 5 and 6 was established in an elegant paper by Affleck, Zou, Hsu, and Anderson.[7] This mixed $s+id$ or flux phase has an excitation spectrum of particle and hole pairs with a quasiparticle dispersion vanishing at four points in the Brillouin zone. As a result this phase has a specific heat which is quadratic in temperature and a susceptibility which vanishes linearly at low temperatures. This choice of phases has a deep physical meaning. Indeed it is needed in the fermion representation of the variational wave functions to obtain the correct Marshall sign of the wave function in the spin representation.[8] Affleck and Marston[6] also found a Peierls spin phase with perfect dimerization, having the lowest energy. This phase is highly degenerate and a combination of different dimerization patterns could describe a short-range RVB phase[9] with a gap to spin excitations and exponentially vanishing susceptibility and specific heat.

Even though the gauge-theory formulation of RVB (Refs. 7 and 10) is in principle exact, all the calculations, so far, have been done at the level of mean-field theory which is exact in the limit of large number of fermions.[6] It has been shown that the uniform BZA solution is unstable to phase fluctuations[5,6] but it is widely believed that the flux phase is locally stable.[6]

We studied the effect of Gaussian fluctuations of arbitrary frequency and wave vector around the flux $s+id$ solution, to see how the free fermion spectrum of excitations is modified by the interaction with the gauge fields. We found that while this phase is stable against phase fluctuations with an arbitrary wave vector and frequency it is *unstable* against amplitude fluctuation with wave vector $(0,\pi),(\pi,0)$. These fluctuations produce *umklapp* scattering between the different species of low-energy fermions and dimerizes the lattice, opening up a gap in the fermionic spectrum.

In this communication we will prove the instability of the flux phase by studying the free-energy functional allowing for the most unstable modes of wave vector $(0,\pi),(\pi,0)$. This we do by doubling the periodicity of the flux phase.

We recall[6] the derivation of the free-energy functional. Starting from the exchange Hamiltonian

$$H=\frac{J}{N}\sum_{(i,j)}\sum_{\sigma,\sigma'}c_{i\sigma}^{\dagger}c_{i\sigma'}c_{j\sigma'}^{\dagger}c_{j\sigma}\,, \tag{1}$$

with (i,j) denoting nearest-neighbor pairs of sites, and σ and σ' flavor indices running from 1 to N. In the spin-$\frac{1}{2}$ problem $N=2$ and σ and σ' are the up and down spin indices, respectively. We write the partition function of model (1) introducing a Hubbard-Stratonovich field for the valence-bond operator

$$\Delta_{ij}=\frac{J}{N}\sum_{\sigma}c_{i\sigma}^{\dagger}c_{j\sigma}\,. \tag{2}$$

Now the partition function is given as a functional integral over all time-dependent histories of the bonds Δ_{ij} and a static field λ_i which enforces the constraint of $N/2$ flavors per site:

$$e^{-\beta F}=Z=\int dc_{i\sigma}^{\dagger}dc_{i\sigma}d\Delta_{ij}\exp\left[-\int_0^{\beta}d\tau\sum_{i,\sigma}c_{i\sigma}^{\dagger}\frac{d}{d\tau}c_{i\sigma}+N\sum_{(i,j)}\frac{|\Delta_{ij}|^2}{J}+\sum_{(i,j)}(\Delta_{ij}c_{\sigma i}^{\dagger}c_{\sigma j}+\text{H.c.})+\sum_{i,\sigma}\lambda_i(c_{\sigma i}^{\dagger}c_{\sigma i}-\tfrac{1}{2})\right]. \tag{3}$$

The flux-phase mean-field solution takes Δ_{ij} to be static and doubles the unit cell; the lattice sites are divided into even and odd sites depending on the parity of the sum of the coordinates. The bonds emanating from an even site have all the same amplitude but are assigned different phases as shown in Fig. 1. To allow for fluctuations with wave vectors $(\pi,0)$ we consider a unit cell containing four sites and therefore eight bonds (see Fig. 2). We assign to the bonds emanating from the first even site of the new unit cell four independent amplitudes while keeping their relative phases as in the flux phase (the variable Q_i in Fig. 2 is taken to be real). Bonds attached to the second even site are obtained from those in the first even site by a π rotation. This is not the most general solution compatible with the new periodicity but is general enough to illustrate our point. For $Q_1=Q_3=Q_2=Q_4$, our phase is just the flux phase. The free energy per flavor and per site for the configuration of the bonds described in Fig. 2 is simply given by

$$F=\frac{(\delta_1^2+\delta_3^2+\delta_2^2+\delta_4^2)}{J}-\frac{1}{(2\pi)^2}\int_{-\pi}^{\pi}\int_{\pi}^{-\pi}(\delta_1^2\cos^2k_x+\delta_3^2\sin^2k_x+\delta_2^2\cos^2k_y+\delta_4^2\sin^2k_y)^{1/2}, \tag{4}$$

with

$$\delta_1=\frac{Q_1+Q_3}{2},\quad \delta_3=\frac{Q_1-Q_3}{2},$$
$$\delta_2=\frac{Q_2+Q_4}{2},\quad \delta_4=\frac{Q_2-Q_4}{2}.$$

For $\delta_3=\delta_4=0$ we recover the spectrum of the flux phase. In the limit $\delta_1=\delta_3=\delta_2=\delta_4$ we have a dispersionless spectrum characteristic of localized dimers. Minimizing the free energy we find that the free energy of this phase is given by $-J/8$ (in fact the same as the dimer phase). This is lower than the free energy of the flux phase (which is given by $-0.115J$). Formula (4) interpolates continuously between the two suggesting that the flux phase is unstable. This is confirmed directly by calculating the second derivatives of the free-energy function (4) at the flux-phase saddle point. Indeed, the flux phase corresponds to $\delta_3=\delta_4=0$ and $\delta_1=\delta_2=\delta$ where δ is the solution of

$$\frac{2}{J}=\frac{1}{(2\pi)^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\frac{\cos^2k_x}{\delta(\cos^2k_x+\cos^2k_y)^{1/2}}dk_x\,dk_y. \tag{5}$$

At this point, the second derivative with respect to δ_3 is given by

$$\frac{2}{J}-\frac{1}{(2\pi)^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\frac{\sin^2k_x}{\delta(\cos^2k_x+\cos^2k_y)^{1/2}}, \tag{6}$$

which by using (5) can be rewritten as

$$\frac{1}{(2\pi)^2}\frac{1}{\delta}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\frac{\cos2k_x}{(\cos^2k_x+\cos^2k_y)^{1/2}}$$
$$=-\frac{1}{(2\pi)^2}\frac{1}{4\delta}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\frac{\sin^22k_x}{(\cos^2k_x+\cos^2k_y)^{3/2}}<0, \tag{7}$$

where the last result comes from an integration by parts. This shows that the energy of the flux phase can be lowered by an infinitesimal variation of δ_3 or δ_4 and therefore proves its instability. In fact, it is easy to convince oneself by a similar argument that inside our family of phases parametrized by δ_1, δ_2, δ_3, and δ_4 local minima can exist only at $\delta_1=\delta_3$, $\delta_2=\delta_4$, i.e., for phases with localized fermions.

It is surprising that the minimum of the functional[4] describes a phase where the bonds form disconnected squares, and which has the same energy as the dimer state considered by Affleck and Marston.[6] We also proved that this is indeed the absolute minimum of the *full* free energy. Creating bond patterns more complicated than

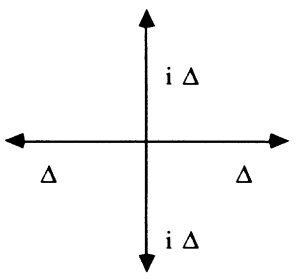

FIG. 1. Expectation value of the bond variables in the flux phase.

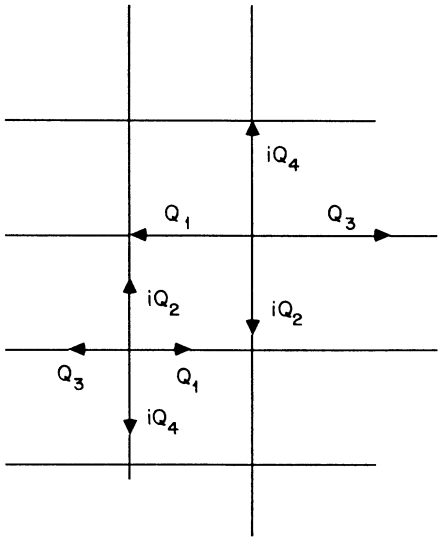

FIG. 2. Expectation value of the bond variables in the doubled unit cell, in the phase treated in this paper.

squares or pure dimers only raises the free energy.

In this communication we found an instability in a mean-field theory of RVB based on a factorization in the particle-hole channel. This is the correct factorization in the limit of a large number of fermion flavors. It is clear, however, that the same instability will be present in the SU(2) formulation[7] of the mean-field theory, which might be more suitable to treat the $N=2$ case.

Recently, several papers[11] have addressed the role of the gauge fields and the low-energy fermions exploiting connections with the theory of anomalies in quantum field theory. Our calculation shows that these subtleties might not complicate the study of fluctuations around mean-field theory. The most dangerous fluctuations eliminate the low-energy fermions by opening up a dimerization gap.

For the reasons given at the beginning of this paper the flux phase is theoretically appealing. It seems that we have lost a good starting point to investigate the resonating-valence-bond state at zero doping and it would be interesting to find terms in the Hamiltonian that could stabilize the flux phase. An obvious possibility is that a finite concentration of holes will eliminate the instability discussed in this paper. A theoretical description of this scenario will certainly require new techniques.

There seems to be a rather close parallel between mean-field calculations and numerical evaluation of the energy of Gutzwiller-projected wave functions.[12,13] It would be interesting to confirm the instability found here using variational Monte Carlo techniques.

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