PATH INTEGRAL STUDY OF THE PHASE TRANSITION TO THE RESONATING VALENCE BOND STATE

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Phase fluctuations in the RVB approach to the strong coupling Hubbard model are studied in mean field approximation, reflecting the change from local to global gauge symmetry induced by hole doping.

The discovery of the ceramic high temperature superconductors [1] has produced a new strong motivation for a better understanding of various aspects of the physics of strongly correlated Fermi systems. Among these aspects are the Mott–Hubbard insulating state and superexchange antiferromagnetism. One line of thought tries to let high-temperature superconductivity originate from the antiferromagnetic exchange interaction via the resonating valence bond (RVB) concept [2]. In order to put such ideas on a more profound basis it is necessary to properly include the strong electronic on site correlations and to improve the understanding of quantum fluctuations. The present paper suggests a proper mean field treatment that takes both aspects into account.

The RVB concept makes use of the idea that in the presence of strong quantum fluctuations antiferromagnets can be described in terms of singlet pair states. A first attempt to formalize this idea was put forward by Baskaran et al. [3] who proposed a mean field theory for a singlet pair phase. The order parameter used in this mean field theory is suited to describe superconducting states as well. The mean field approximation is, however, not sufficient for an appropriate description of possible superconducting phases for at least two reasons: (1) it ignores certain essential correlation effects and (2) it also ignores the features due to local gauge invariance. Various attempts to go beyond the mean field approximation and avoid these deficiencies have been made [4–6].

In ref. [4] a functional integral formulation was introduced which is able to retain the important phase fluctuations due to the local gauge properties and which permits to include all correlation effects, although only in a high temperature expansion. A static approximation – which is a standard and almost unavoidable approximation in evaluating functional integrals – was used in this work. The static approximation certainly has its problems at low temperatures, where it was shown to give e.g. the wrong answer for the ground state energy for a single bond [7]. Nevertheless, more reliable information can be obtained about the symmetry properties of the or-

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dered phases. In fact, the path integral formulation of ref. [4] shows a phase transition to an extended s-wave state which smoothly turns into a state with a chiral symmetry at lower temperatures. This chiral state has in the meantime become known as the flux phase [8,9], which is most recently also discussed in the context of fractional statistics [10] and time reversal symmetry (T) and parity (P) violating ground states [11–13].

We start from the t–J model as the strong coupling limit $U/t \gg 1$ of a two-dimensional Hubbard model on a square lattice:

$$H = -t \sum_{\langle ij\rangle,\sigma} (P_{1+0} c_{i\sigma}^{+} c_{j\sigma} P_{0+1} + \text{h.c.}) - J \sum_{\langle ij\rangle} b_{ij}^{+} b_{ij} . \tag{1}$$

$J = 4t^2/U$ is the exchange energy and

$$b_{ij}^{+} = \frac{1}{\sqrt{2}} (c_{i\uparrow}^{+} c_{j\downarrow}^{+} - c_{i\downarrow}^{+} c_{j\uparrow}^{+}) \tag{2}$$

is a singlet creation operator for the bond $\langle ij\rangle$. The projection operators P_{0+1} in the kinetic energy avoid double occupancy of sites. In the half filled band case (1) reduces to an insulating antiferromagnetic Heisenberg model which is invariant under the local gauge transformation $c_{i\sigma} \to \exp(i\varphi_i) c_{i\sigma}$ [5]. This local U(1) symmetry cannot be spontaneously broken according to Elitzur's theorem [14], and therefore $\langle b_{ij}\rangle = 0$ in the half-filled band case. Doping with holes converts the local gauge symmetry into a global one, which can be spontaneously broken and allows the order parameter $\langle b_{ij}\rangle$ to be nonzero. A proper mean field theory has to take into account these symmetry requirements and should avoid to break the local symmetry "by hand".

In a previous paper [4] we have developed a path integral formulation and used the Hubbard Stratonovich identity to decouple the exchange interaction. The grand canonical statistical sum can then be written as a functional integral,

$$\text{Tr}\, P_{0+1} e^{-\beta H} = \int \prod_{\langle ij\rangle} \mathscr{D}^2 \left(\frac{\beta}{\pi J} \Delta_{ij}(\tau) \right) e^{-\beta F[\Delta(\tau)]} , \tag{3}$$

where the effective free energy F is a functional of fluctuating bond order parameters $\Delta_{ij}(\tau)$. In a static approximation and up to leading orders in Δ and in the hole fugacity $z = \exp(\beta\tilde{\mu})$, where $\tilde{\mu} = \mu_{\text{hole}} - J$, the free energy F is given by [4]

$$\begin{aligned} F T_{c0} = {} & b_2 \sum_{\langle ij\rangle} |\Delta_{ij}|^2 - b_4 (1 - 3z) \sum_{\langle ij\rangle} |\Delta_{ij}|^4 \\ & + b_4 \sum_{\langle ijk\rangle} |\Delta_{ij}|^2 |\Delta_{jk}|^2 \\ & + b_4 \sum_{\square} (\Delta_{ij} \Delta_{jk}^{*} \Delta_{kl} \Delta_{li}^{*} + \text{c.c.}) \\ & - \frac{qz}{2} \sum_{\Gamma} (\Delta_{ij} \Delta_{jk}^{*} + \text{c.c.}) \end{aligned} \tag{4}$$

The indicated figures show the spatial bond orientation to be summed over in the corresponding sum. The coefficients in (4) are given by

$$q = \frac{3}{16} \left(\frac{t}{T_{c0}} \right)^2 , \quad b_2 = \frac{T - T_{c0}}{4 T_{c0}} , \quad b_4 = \frac{1}{96 T_{c0}^2}$$

and $T_{c0} = J/4$. The local constraints of no double occupancy, as enforced by the projection operators, are handled by using a localized basis (states $|\uparrow\rangle$, $|\downarrow\rangle$, $|0\rangle$ per site) in performing traces.

In the following we consider only effects up to first order in the hole doping concentration δ, which are missing in the mean field version of Baskaran et al. [3]. In this small doping limit the hole fugacity is directly proportional to δ. We identify

$$\langle b_{ij} \rangle \equiv \langle \Delta_{ij} \rangle = \frac{\int \prod_{\langle ij\rangle} \mathscr{D}^2 \Delta_{ij} e^{-\beta F} \Delta_{ij}}{\int \prod_{\langle ij\rangle} \mathscr{D}^2 \Delta_{ij} e^{-\beta E}} \tag{5}$$

and emphasize the role of the phase fluctuations for the order parameter. Assuming that the amplitudes of Δ_{ij} depend only weakly on position, $\Delta_{ij} \simeq \Delta_0 \exp(i\varphi_{ij})$ [5], we obtain from (4) a simplified version of the free energy

$$F = F[\Delta_0] + \Delta F_1[\varphi] + \Delta F_2[\varphi] , \tag{6}$$

where

$$\Delta F_1[\varphi] = \frac{2 b_4 \Delta_0^4}{T_{c0}} \sum_{\square} \cos(\varphi_{ij} - \varphi_{jk} + \varphi_{kl} - \varphi_{li}) , \tag{7a}$$

$$\Delta F_2[\varphi] = \frac{qz \Delta_0^2}{T_{c0}} \sum_{\Gamma} \cos(\varphi_{ij} - \varphi_{jk}) . \tag{7b}$$

We may use the $F[\Delta_0]$ part of the free energy to determine $\Delta_0(T)$ [5] leading to

$$\Delta_0(T)=\frac{6T_{c0}}{1+\frac{3}{2}z}\frac{T-T_{c0}}{T_{c0}}, \tag{8}$$

which next enters $\Delta F_1[\varphi]$ and $\Delta F_2[\varphi]$ as an input parameter. The average

$$\langle \Delta_{ij}\rangle+\Delta_0\langle \exp(i\varphi_{ij})\rangle=\Delta_0\langle\cos\varphi_{ij}\rangle$$

is then performed with $\Delta F_1[\varphi]+\Delta F_2[\varphi]$ only.

ΔF_1 contains only the plaquette term which is invariant under local gauge transformations. $\Delta F_2[\varphi]$, however, is only globally gauge invariant and vanishes at half filling where $z=0$.

In the absence of doping we can apply Elitzur's theorem [14] and show that

$$\langle\cos\varphi_{ij}\rangle\equiv\frac{1}{Z}\lim_{J\to 0}\lim_{N\to\infty}\int\prod_{k,l}d\varphi_{kl}\exp(-\beta\Delta F_1[\varphi])$$

$$\times\exp\left(J\sum_{kl}\cos\varphi_{kl}\right)\cos\varphi_{ij}=0, \tag{9}$$

using the gauge transformation

$$B_{lk}=\varphi_{lk}-\tfrac{1}{2}(\delta_{l,i}+\delta_{k,i}+\delta_{l,j}+\delta_{k,j})\varphi_{ij}$$
$$+\delta_{(l,k),(i,j)}\varphi_{ij}, \tag{10}$$

and following Elitzur's proof as outlined in ref. [14]. Consequently the RVB state is not coherent in the half-filled band case [5]. The result given by (9) is very strong. It implies that the plaquette term cannot be decoupled in any way in the calculation, because this always introduces artificially non-zero averages.

On the other hand $\Delta F_2[\varphi]$ possesses only global gauge symmetry which can be spontaneously broken. A proper mean field approximation for phase fluctuations can therefore be formulated by decoupling $\Delta F_2[\varphi]$ according to

$$\Delta F[\varphi]=\Delta F_1[\varphi]-\sum_i\left[K_x(a,b)\cos(\varphi_{i,i+x})\right.$$
$$\left.+K_y(a,b)\cos(\varphi_{i,i+y})\right], \tag{11}$$

where we have introduced

$$a=\langle\cos(\varphi_{i,i+x})\rangle,\quad b=\langle\cos(\varphi_{i,i+y})\rangle$$

and

$$K_x(a,b)=\frac{2qz\Delta_0^2}{T_{c0}}(a+2b)=K_y(b,a). \tag{12}$$

The expectation values a and b have to be determined self-consistently with the free energy $\Delta F[\varphi]$, following the prescription given in (5). In the vicinity of the phase boundary this leads to the equations

$$a=\frac{K_x}{2T}-\frac{1}{2}\left(\frac{K_x}{2T}\right)^3\left(1-\frac{K_y^2}{K_x^2}\frac{J_1(\gamma)}{J_0(\gamma)}\right), \tag{13a}$$

$$b=\frac{K_y}{2T}-\frac{1}{2}\left(\frac{K_y}{2T}\right)^3\left(1-\frac{K_x^2}{K_y^2}\frac{J_1(\gamma)}{J_0(\gamma)}\right), \tag{13b}$$

where

$$J_n(x)=\frac{1}{2\pi}\int_{-\pi}^{\pi}\cos(n\varphi)e^{x\cos\varphi}\,d\varphi$$

is a Bessel function of the first kind and $\gamma=-2b_4(\Delta_0^4/T)T_{c0}$.

The set of equations (13) has only one physical solution $a=b$ below a critical temperature

$$T_c=3qz\Delta_0^2/T_{c0}. \tag{14}$$

a and b have a mean field type temperature dependence close below T_c as given by

$$a=b=\left(\frac{T_c-T}{T_c[\frac{1}{2}-J_1(\gamma)/J_0(\gamma)]}\right)^{1/2}. \tag{15}$$

T_c increases linearly with the hole concentration $\delta\sim z$ for small doping. The plaquette term reflects itself only in the presence of the J_1/J_0 term and tends to lower the value of a and b. Since the order parameters attain the same value on the x- and y-bonds, $a=b$, the solution of the self-consistency equations has the extended s-wave symmetry. Similar results with T_c increasing linearly with doping were also obtained by Fukuyama et al. [15] and by Nakamura and Matsui [6] using Monte Carlo techniques. They observe, however, a transition to a d-wave phase.

In summary, we have presented here a RVB mean field theory for phase fluctuations that seems to reflect properly the fundamental change of gauge symmetry arising from hole doping. Away from half-filling the mean field theory shows a finite temperature transition to a coherent state with extended s-wave symmetry. From our earlier path integral analysis [4] we know that the chiral state (flux phase) minimizes the free energy at low temperatures for small doping and the extended s-wave phase will continuously change into the chiral phase with decreasing tem-

perature or decreasing doping. A similar result was recently obtained by Fradkin and Kivelson [16]. We therefore expect the chiral phase to be stable at low temperatures in contrast to a conclusion recently obtained by Dombre and Kotliar [17] in a large-n expansion. Nevertheless, we are aware that the effects of low dimensionality on T_c are not included in our mean field treatment [18].

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