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Phase transition to the resonating valence bond state

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A Ginzburg-Landau expansion for the free energy functional of the resonating valence bond state is performed for the mean field approximation (MFA) and for a functional integral approach (FIA) which includes correlations. Phase diagrams obtained in both approximations are presented. The FIA differs form the MFA in three main aspects: *(i)* Above the mean field transition temperature an instability exists towards the formation of degenerate singlet pair states, indicating the onset of the RVB state. *(ii)* The extended *s*-wave phase is favoured over the extended *d*-wave phase. *(iii)* Phase fluctuations are included, destroying off-diagonal order in the absence of holes.

I. Introduction

Since the discovery of high T_c superconductors initiated by Bednorz and Müller [1] a great deal of experimental and theoretical work has been done to identify the mechanism of high T_c superconductivity. As one common feature the high T_c superconductors $La_{2-x}(Ba, Sr)_xCuO_y$, $YBa_2Cu_3O_{7-\delta}$ and the recently discovered Bi [2] or Tl compounds [3] possess Cu−O planes where the main physics is believed to happen. It is known as well that pure La_2CuO_4 is an antiferromagnetic insulator [4]. Doping by Ba or Sr destroys the antiferromagnetism and leads to superconductivity. Similarly $YBa_2Cu_3O_{6+\delta}$ shows antiferromagnetism [5] for $0 \leqq \delta \leqq 0.4$ and superconductivity for an oxygen content $\delta > 0.5$.

All experimental facts strongly suggest that physically active [6] $3d_{x_2-y_2}$ Cu and $2p_{x,y}$ O electrons of Cu−O planes are strongly correlated and form a system which is close to the metal-insulator Mott transition. A "minimum model" appropriate for such systems is therefore a Hubbard model on a square lattice with nearest neighbour hopping integral t and on-site Coulomb repulsion U – the starting point of much theoretical work. In the strong correlation limit $U/t \gg 1$ the Hubbard Hamiltonian is usually transformed into an effective Hamiltonian, describing an antiferromagnetic insulator in the half filled band case. It has been suggested [7] that a small concentration of holes removes the antiferromagnetic order, and a non-magnetic resonating valence bond state (RVB) is stabilized by quantum fluctuations arising from the holes. The preexisting singlet pairs on nearest neighbour sites in the RVB state can be considered an excellent stockpile of Cooper pairs and will lead to superconductivity as soon as the doping introduces sufficient phase coherence.

In fact, in the half filled band case the model has a local $U(1)$ gauge symmetry [8] which reflects the conservation of the number of electrons at each site. According to Elitzur's theorem [9] this local symmetry can not be spontaneously broken excluding any off diagonal order for zero doping. Doping by holes reduces the local gauge symmetry to a global one which can be spontaneously broken and which provides a chance for having superconductivity.

In this paper we present a Ginzburg-Landau (GL) free energy expansion for the RVB state. Using a path integral approach we compare the correlated theory with the mean field approximation in order to study the stability of various phases of different symmetry. The paper is organized as follows: The model to which we apply our method is given in Sect. II. In Sect. III the mean field approximation (MFA) originally suggested by Baskaran, Zou and Anderson

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(BZA) [10] is presented and its deficiences are discussed. The functional integral approach (FIA) and the resulting GL free energy expansion obtained in a static approximation as well as the phase diagram are analyzed in Sect. IV. Contrary to MFA results we find: *(i)* An instability exists towards the formation of a degenerate singlet pair state indicating the onset of the RVB state for small hole concentration δ and for temperatures above the mean field transition temperature. *(ii)* The proper treatment of the electronic correlations leads to an extended s-wave solution for finite doping concentration, contrary to the d-wave solution found in MFA. In both approximations, at low T and very small δ, a chiral phase is found to be stable in agreement with recent results of Fukuyama and Hasegawa [11].

II. Choice of model

Band structure calculations [6] and standard arguments of crystal chemistry [12] tell us that copper $3d_{x_2-y_2}$ and oxygen $2p_{x,y}$ orbitals form an antibonding band around the Fermi energy in the $La_{2-x}(Sr, Ba)_xCuO_y$ and 123 compounds. It can be argued [13] and there is experimental evidence [14] that holes introduced by doping will go into the oxygen sites but we will assume here that they are copper $3d$ holes [15]. Having in mind that band structure calculations give metallic behaviour for these systems we must add strong correlations between electrons to account for the possibility of a Mott metal-insulator phase transition. The minimum model appropriate is therefore the two dimensional Hubbard model on a square lattice.

$$H = -t \sum_{\langle ij\rangle\sigma} (c_{i\sigma}^+ c_{j\sigma} + \text{h.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow} \tag{1}$$

with the nearest neighbour hopping integral t and the on-site Coulomb repulsion U (Hubbard U). Both, the metal-insulator transition and the appearance of antiferromagnetism find a natural explanation in this simple one band model with a proper choice of parameters (say, $U \approx 5$ eV and $t \approx 0.5$ eV) which puts the model in the strong correlation limit.

In this limit ($U/t \gg 1$) and close to the half filled band case elimination of energetically unfavourable double occupancy by a canonical transformation leads to an effective hamiltonian [16]:

$$H_{\text{eff}} = H_t + H_{\text{ex}}, \tag{2}$$

where the hopping hamiltonian

$$H_t = -t \sum_{\langle ij\rangle\sigma} (P_{0+1} c_{i\sigma}^+ c_{j\sigma} P_{0+1} + \text{h.c.}). \tag{3}$$

is to be understood as restricted to singly occupied and unoccupied sites and the exchange hamiltonian

$$H_{\text{ex}} = J \sum_{\langle ij\rangle} P_1 (\underline{S}_i \cdot \underline{S}_j - 1/4) P_1 \tag{4}$$

acts only on neighbouring pairs of singly occupied sites as indicated by the projection operator P_1. $J = 4t^2/U$ is the antiferromagnetic coupling constant between the electron spins $\underline{S}_i = c_{i\alpha}^+ \underline{\sigma}_{\alpha\beta} c_{i\beta}$ and $\langle ij\rangle$ indicates summation over nearest neighbour pairs (bonds) only and every bond is counted once.

It is immediately seen from (3) that for half filling the effective hopping is zero (Mott insulator) and the system is described by the $s = 1/2$ antiferromagnetic Heisenberg model. This model has an antiferromagnetic ground state in three dimensions and probably in two dimensions as well. But doping by a small number of holes introduces frustration into the system and destabilizes the AF order. This observation and earlier studies of a $2D$ Heisenberg model on a triangular lattice lead Anderson to suggest the resonating valence bond state (RVB) as an alternative ground state for the spin system [17]. This spin liquid state can be imagined approximately as a proper superposition of states where neighbouring spins are paired into separate singlets.

To emphasize the RVB type character, the exchange interaction may alternatively be written as:

$$H_A = -J \sum_{\langle ij\rangle} b_{ij}^+ b_{ij} \tag{5}$$

where

$$b_{ij}^+ = 1/\sqrt{2}(c_{i\uparrow}^+ c_{j\downarrow}^+ - c_{i\downarrow}^+ c_{j\uparrow}^+) \tag{6}$$

is a creation operator for a singlet pair on the bond $\langle ij\rangle$.

The hamiltonian (5) is invariant under the local gauge transformation $c_{i\sigma} \to \exp(\mathrm{i}\varphi_i) c_{i\sigma}$ [8]. This local $U(1)$ symmetry implies [9], that there is no spontaneous symmetry breaking and therefore $\langle b_{ij}\rangle = 0$.

Doping by holes converts the local gauge symmetry into a global one (see (3)), and allows $\langle b_{ij}\rangle$ to be nonzero. This symmetry which governs the physics in the weak doping regime must be included in the free energy expansion. This requires the order parameter $\Delta_{ij} = \langle b_{ij}\rangle$ to be a complex number.

III. Mean field approximation

Using the form (5) of H_A, Baskaran et al. [10] have suggested to apply a BCS type mean field approximation (MFA) with a simplified trial hamiltonian:

$$h = h_t + h_\Delta \tag{7}$$

where

$$h_\Delta = \sum_{\langle ij \rangle} (\Delta_{ij} b_{ij}^+ + \text{h.c.}) \tag{8}$$

and

$$h_t = -\delta t \sum_{\langle ij \rangle \sigma} (c_{i\sigma}^+ c_{j\sigma} + \text{h.c.}) - \mu N. \tag{9}$$

As we see in (9) the projection operators P_{0+1} are crudely replaced by the hole concentration δ. In (8), Δ_{ij} is the complex order parameter representing the pairing correlation.

Assuming the translational symmetry of the square lattice for the hamiltonian (7) we end up with only two independent order parameters Δ_x and Δ_y for the two nearest neighbour bond orientations. The quasiparticle spectrum corresponding to h, is given by:

$$E(\underline{k}) = [\varepsilon^2(\underline{k}) + |\Delta(\underline{k})|^2]^{1/2} \tag{10}$$

where

$$\varepsilon(\underline{k}) = -2\delta t (c_x + c_y) - \mu, \tag{11}$$

$$\Delta(\underline{k}) = \sqrt{2} (\Delta_x c_x + \Delta_y c_y), \tag{12}$$

with $c_x = \cos(a k_x)$, $c_y = \cos(a k_y)$. "a" is the lattice constant.

The spectrum (10) is formally of BCS type. Due to the spatially extended structure of the order parameter, its Fourier transform $\Delta(\underline{k})$ does not necessarily create a gap in the excitation spectrum. Explicitly we have three possible phases which will be discussed later:

a) Extended s-wave phase: $\Delta_x = \Delta_y = \Delta$, $\Delta(\underline{k}) = \Delta(c_x + c_y)$. In this case the energy gap vanishes only for $\mu = 0$, which corresponds to a half filled band. We then have a line of zeros in the first Brillouin zone of the two dimensional square lattice.

b) d-wave phase: $\Delta_x = -\Delta_y = \Delta$, $\Delta(\underline{k}) = \Delta(c_x - c_y)$. The d-wave phase has no gap in the energy spectrum, for zero doping as well as for any finite doping.

c) Chiral phase, $\Delta_y = \Delta_x \exp(\mathrm{i}\varphi)$, $\Delta_x = \Delta$ for $\pi/2 \leqq \varphi \leqq \pi$. In the chiral phase the gap vanishes only for $\mu = 0$ (half filled band) on 4 separate points of the first Brillouin zone.

The absence of an energy gap results in a power law behaviour of the heat capacity at low temperature, so the symmetry of the phase that minimizes the free energy manifests itself in the thermodynamics of the system.

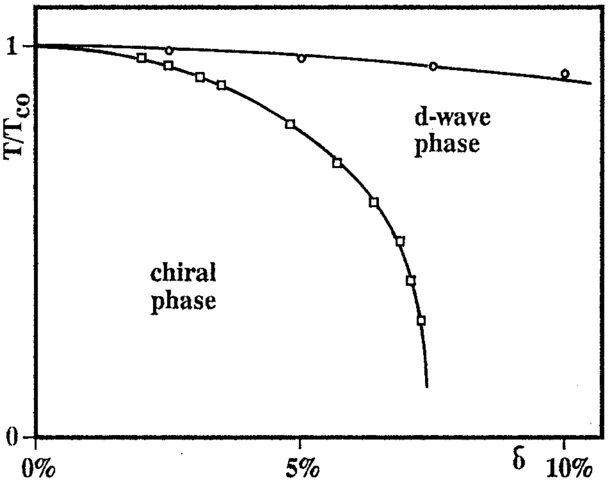

Fig. 1. MFA phase diagram for $U/t = 10$. The chiral phase is found to be stable for small doping δ and temperature T, whereas the extended d-wave phase is stable everywhere else

The free energy of (5) in the mean field approximation (7) is given by:

$$\begin{aligned} \Delta F = \sum_{\underline{k}} \Bigg\{ & \frac{|\Delta(\underline{k})|^2}{E(\underline{k})} \tanh\left(\frac{\beta E(\underline{k})}{2}\right) \\ & - \frac{2}{\beta} \ln\left[\frac{\cosh(\beta E(\underline{k})/2)}{\cosh(\beta \varepsilon(\underline{k})/2)}\right]\Bigg\} \\ & - 2\frac{J}{N} \sum_{\underline{k}, \underline{k}'} (c_x c_x' + c_y c_y') \frac{\Delta^*(\underline{k})}{2E(\underline{k})} \\ & \cdot \tanh\left(\frac{\beta E(\underline{k})}{2}\right) \frac{\Delta(\underline{k}')}{2E(\underline{k}')} \tanh\left(\frac{\beta E(\underline{k}')}{2}\right). \end{aligned} \tag{13}$$

The equation for the chemical potential μ is derived by fixing the number of electrons, $N = \partial \Delta F / \partial \mu$, leading to

$$\delta = \frac{1}{N} \sum_{\underline{k}} \frac{\varepsilon(\underline{k})}{E(\underline{k})} \tanh\left(\frac{\beta E(\underline{k})}{2}\right). \tag{14}$$

The order parameter $\Delta(\underline{k})$ has to satisfy the selfconsistency equations

$$\Delta_x = \frac{J}{N} \sum_{\underline{k}} c_x \frac{\Delta(\underline{k})}{E(\underline{k})} \tanh\left(\frac{\beta E(\underline{k})}{2}\right), \tag{15a}$$

$$\Delta_y = \frac{J}{N} \sum_{\underline{k}} c_y \frac{\Delta(\underline{k})}{E(\underline{k})} \tanh\left(\frac{\beta E(\underline{k})}{2}\right). \tag{15b}$$

From (14) we can see that $\mu = 0$ for $\delta = 0$ and the chemical potential vanishes proportional to δ for small doping concentration, $\mu \sim \delta t^2/U$. In the limit $t/U \to 0$, where $\mu/\delta t \to 0$, and for fixed $\delta U/t$ we have computed the complete phase diagram by minimizing the free energy (13), subject to the constraints of the selfconsistency equations (14) and (15) (see Fig. 1).

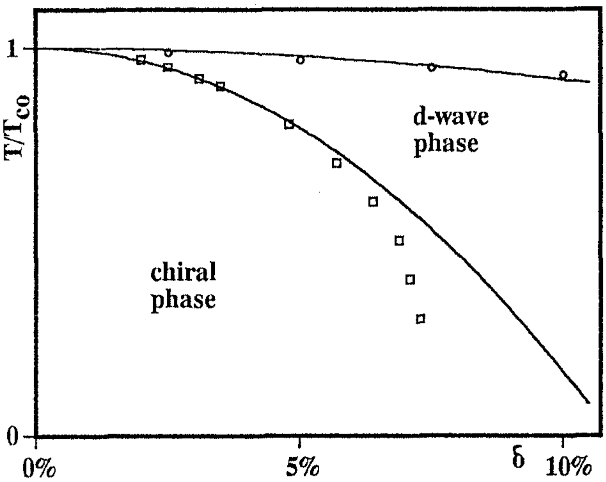

Fig. 2. Phase diagram for $U/t=10$, following from the Landau expansion of the MFA free energy. For comparison, the open circles and squares indicate the data for the phase boundaries of Fig. 1

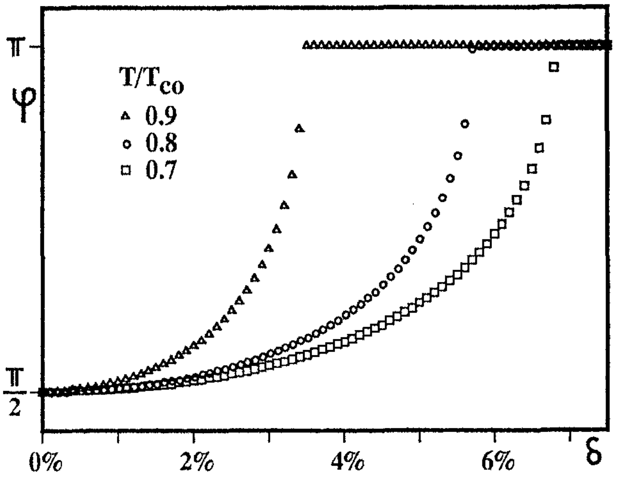

Fig. 3. The phase difference φ of the order parameters Δ_x and Δ_y in MFA for $U/t=10$ vs. doping δ for fixed temperature T. Starting from $\varphi=\pi/2$ for $\delta=0$, the phase difference continuously changes to $\varphi=\pi$ at the boundary to the d-wave phase

This phase diagram can be easily understood by inspection of the Landau expansion of ΔF (13) up to fourth order in Δ and to second order in δ,

$$\begin{aligned}\frac{\Delta F\cdot T_{c0}}{N}\approx\; & a_2(|\Delta_x|^2+|\Delta_y|^2)+a_4(|\Delta_x^2|+|\Delta_y^2|)^2\\ & +\tfrac{2}{3}a_4(\Delta_x\Delta_y^*+\Delta_x^*\Delta_y)^2\\ & -\frac{2}{3}a_4|\Delta_x|^2|\Delta_y|^2+\frac{p}{2}(\Delta_x^*\Delta_y+\Delta_x\Delta_y^*),\end{aligned}\tag{16}$$

where the short notation

$$T_{c0}=J/4,\quad a_2=\frac{T-T_{c0}}{8T_{c0}},\quad a_4=\frac{1}{64T_{c0}^2},$$
$$p=\frac{1}{12}\left(\frac{\delta t}{T_{c0}}\right)^2$$

has been used. For the order parameter (Δ_x, Δ_y) we use the parametrization $\Delta_x=\Delta\cos\psi\exp(\mathrm{i}\varphi_x)$, $\Delta_y=\Delta\sin\psi\exp(\mathrm{i}\varphi_y)$ with $\Delta\geqq 0$ and phases $0\leqq\psi\leqq\pi/2$, $0\leqq\varphi_x, \varphi_y<2\pi$. Denoting the relative phase by $\varphi=\varphi_x-\varphi_y$ the Landau expansion (16) can be rewritten as:

$$\begin{aligned}\frac{\Delta F\cdot T_{c0}}{N}\approx & \left(a_2+\frac{5p}{4}\right)\Delta^2+a_4\Delta^4\\ & +\frac{a_4}{6}\Delta^4\sin 2\psi(4\cos^2\varphi-1)\\ & +p\Delta^2\sin 2\psi\cos\varphi.\end{aligned}\tag{17}$$

The free energy expansion (17) is valid only for temperatures close to T_{c0} and for $\delta\ll 1$.

As we can see from Fig. 2, the phase diagram following from (17) agrees almost quantitatively with the phase diagram resulting from the full MFA free energy given by (13) (Fig. 1). This justifies to expect the Landau expansion of the free energy to be qualitatively correct in the whole range of parameters.

The first two terms in (17) are invariant with respect to spatial rotations of bonds. The third term favours the chiral phase while the last term favours the d-wave symmetry for a finite doping concentration. It is the competition between these two terms which determines the structure of the phase diagram.

For finite doping ($\delta>0$) and with decreasing temperature a first transition to a d-wave phase ($\psi=\pi/4$, $\varphi=\pi$) appears driven by the last term in (17) with a transition temperature

$$T_d=T_{c0}(1-p).\tag{18}$$

This phase has also been discussed by Cyrot [18] and others [19]. With further decreasing temperature the third term proportional to Δ^4 grows in weight and below the temperature

$$T_{ch}=T_{c0}(1-10p)\tag{19}$$

the chiral phase with $\psi=\pi/4$, $\pi/2\leqq\varphi\leqq\pi$ is stable and persists down to zero temperature. This chiral phase disappears for a doping fraction δ corresponding to $p>p_c\approx 0.1$, corresponding to $\delta\approx t/U$, and the phase difference φ continuously changes from $\varphi=\pi$ to $\varphi=\pi/2$ with decreasing δ. The phase difference φ of the chiral phase is plotted in Fig. 3 as a function of the doping δ for different temperatures. In fact, the s-wave phase ($\psi=\pi/4$, $\varphi=0$) which was suggested in [10] never wins in MFA.

Besides the expansion (13) which is based on the trial hamiltonian (7) we have performed a GL expansion of the free energy without any symmetry restrictions on the order parameter Δ_{ij}. Using the mean field version h_t (9) of the kinetic energy a conventional Hubbard-Stratonovich transformation can be employed (see Chapt. IV). The resulting cumulant expansion of the free energy functional then reads:

$$\begin{aligned}\Delta F\cdot T_{c0}=&\left(a_2+\frac{7p}{4}\right)\sum_{\langle ij\rangle}|\Delta_{ij}|^2+\frac{a_4}{3}\sum_{\langle ij\rangle}|\Delta_{ij}|^4\\&+\frac{2a_4}{3}\Big[\sum_{\substack{\langle ijk\rangle\\ \text{--}\,\llcorner}}|\Delta_{ij}|^2|\Delta_{jk}|^2\\&+\sum_{\substack{\langle ijkl\rangle\\ \square}}(\Delta^*_{ij}\Delta_{jk}\Delta^*_{kl}\Delta_{li}+\text{h.c.})\Big]\\&+\frac{p}{4}\Big[\sum_{\substack{\langle ijk\rangle\\ \llcorner}}(\Delta_{ij}\Delta^*_{jk}+\text{h.c.})\\&-\sum_{\substack{\langle ijkl\rangle\\ \shortparallel\;\;=}}(\Delta_{ij}\Delta^*_{kl}+\text{h.c.})\Big].\end{aligned}\tag{20}$$

The indicated figures show the spatial bond orientations to be summed over in the corresponding sum. In addition to quadratic and quartic single bond terms ($|\Delta_{ij}|^2$ and $|\Delta_{ij}|^4$) the r.h.s. of (20) also contains quartic double bond terms ($|\Delta_{ij}|^2|\Delta_{jk}|^2$) and plaquette terms ($\Delta\Delta^*\Delta\Delta^*$) which are all invariant under local gauge transformations. The last two quadratic $\pi/2$ bond rotating ($\Delta_{ij}\Delta^*_{jk}$) and bond shifting ($\Delta_{ij}\Delta^*_{kl}$) terms are due to doping and break the local gauge invariance. An expansion of this type was suggested by Anderson and coworkers [15] for vanishing doping fraction δ and without double bond contributions.

After imposing translational symmetry, the expansion (20) turns into (17). Thus we realize that the plaquette term is the source of the chiral phase, whereas the quadratic $\pi/2$ bond rotating term is responsible for the *d*-wave phase.

Using (20) we have tested the stability of the "twitch phase" proposed by Anderson et al. [20]. This phase has a doubled unit cell and it is described by a $++--$ sequence of order parameter signs obtained by moving along the boundary of a plaquette. It is gauge equivalent to the *d*-wave solution which has signature $+-+-$. This implies that these two phases have the same free energy for $\delta=0$. But we know that the chiral phase wins in that case. For $\delta>0$ the quadratic bond-rotating and bond-shifting terms in (14) disfavour the twitch phase strongly in comparison to the *d*-wave phase. Therefore within the MFA the twitch phase has no chance anywhere in the phase diagram of the model investigated here. This picture has also been confirmed by Monte Carlo calculations on finite systems based on the expansion (20).

The mean field theory discussed above has three major deficiencies:

(i) MFA gives a finite transition temperature T_{c0} for $\delta=0$, where the local gauge invariance suppresses any long range order due to Elitzur's theorem [9]. This is because phase fluctuations of the order parameter are neglected in MFA.

(ii) The exclusion of double occupancy of sites is ignored. Traces are performed over the complete Hilbert space.

(iii) The projection operator P_{0+1} in the kinetic energy (3) is simply replaced by the hole concentration δ as a *c*-number.

These deficiencies influence the results in an uncontrolled way. They will now be avoided in a functional integral ansatz, which explicitly takes electronic correlations into account.

IV. Functional integral approach

There are various ways to linearize the exchange hamiltonian (5) with a Hubbard-Stratonovich transformation. Since we want to introduce complex order parameters as in (8) in order to incorporate the local gauge symmetry, we use a two field scheme starting from the identity:

$$\begin{aligned}b^+_{ij}\,b_{ij}=&1/2\,[b^+_{ij},b_{ij}]+1/4(b_{ij}+b^+_{ij})^2\\&-1/4(b_{ij}-b^+_{ij})^2,\end{aligned}\tag{21}$$

where the commutator is given by

$$[b^+_{ij},b_{ij}]=1/2((n_i-1)+(n_j-1)).\tag{22}$$

The partition function $Z=\operatorname{Tr}P_{0+1}\exp(-\beta H)$ can thus be written as:

$$\begin{aligned}Z=&\operatorname{Tr}P_{0+1}\exp(-\beta[H_t+H_0])\\&\cdot T\exp\left(\int_0^\beta d\tau\,\frac{J}{4}\sum_{\langle ij\rangle}[(b_{ij}(\tau)+b^+_{ij}(\tau))^2\right.\\&\left.-(b_{ij}(\tau)-b^+_{ij}(\tau))^2]\right)\end{aligned}\tag{23}$$

where

$$H_0=(\mu_h-J)\sum_i(n_i-1)=:\tilde{\mu}_h\sum_i(n_i-1)\tag{24}$$

results from the commutator (22). μ_n is the chemical potential for holes. In (23) T is the time ordering operator, and the imaginary time dependence of the operators is given by:

$$A(\tau)=\mathrm{e}^{\tau(H_0+H_t)}A\,\mathrm{e}^{-\tau(H_0+H_t)}. \tag{25}$$

$\mathrm{Tr}\,P_{0+1}$ means that the trace is taken only over states with empty or singly occupied sites.

Applying the Hubbard-Stratonovich identity [21] to (23) we arrive at

$$\begin{aligned}Z=&\int\prod_{\langle ij\rangle}\left(D^2\Delta_{ij}(\tau)\frac{\beta}{\pi J}\right)\mathrm{Tr}\,P_{0+1}\,\mathrm{e}^{-\beta[H_0+H_t]}\\ &\cdot\;T\exp\left(-\sum_{\langle ij\rangle}\int_0^\beta \mathrm{d}\tau\,[1/J|\Delta_{ij}|^2+\Delta_{ij}(\tau)\,b_{ij}^+(\tau)\right.\\ &\left.+\Delta_{ij}^*(\tau)\,b_{ij}(\tau)]\vphantom{\int_0^\beta}\right)\end{aligned} \tag{26}$$

where the operators $b_{ij}(\tau)$ and $b_{ij}^+(\tau)$ depend on time τ according to (25). The partition function can then be expressed as:

$$Z=\int\prod_{\langle ij\rangle}\left(D^2\Delta_{ij}(\tau)\frac{\beta}{\pi J}\right)\mathrm{e}^{-\beta\Delta F[\Delta]} \tag{27}$$

with a free energy functional

$$\begin{aligned}\Delta F[\Delta]=&\frac{1}{J}\sum_{\langle ij\rangle}|\Delta_{ij}|^2\\ &-\frac{1}{\beta}\ln\left\langle T\exp\left(-\int_0^\beta \mathrm{d}\tau\,h_\Delta(\tau)\right)P_{0+1}\right\rangle_{H_0+H_t},\end{aligned} \tag{28}$$

where

$$h_\Delta=\sum_{\langle ij\rangle}(\Delta_{ij}(\tau)\,b_{ij}^+(\tau)+\Delta_{ij}^*(\tau)\,b_{ij}(\tau)) \tag{29}$$

and the expectation value is evaluated with H_0+H_t only.

If we neglect the electronic correlations arising from the exclusion of double occupancy, we may perform the traces over the complete Hilbert space and simply disregard the projection operators P_{0+1}. Using the mean field version of the kinetic energy h_t, a subsequent cumulant expansion then leads to the static approximation to the free energy (20), which was discussed in the last chapter. However, this version suffers the same deficiencies as the BZA mean field approach.

In order to avoid these deficiencies the projection operators P_{0+1} have to be explicitly taken into account. In a leading order cumulant expansion of the free energy functional (28) this was achieved using a localized basis for the Hilbert space. In a static approximation the free energy can then be expanded up to the fourth order in Δ and to second order in the hole fugacity $z=\exp(\beta\tilde{\mu}_h)$. ΔF then turns out to have the following form:

$$\begin{aligned}\Delta F\cdot T_{c0}=&(b_2-3qz^2)\sum_{\langle ij\rangle}|\Delta_{ij}|^2\\ &-b_4(1-3z+\tfrac{5}{4}z^2)\sum_{\langle ij\rangle}|\Delta_{ij}|^4\\ &+b_4\{(1+\tfrac{7}{4}z^2)\sum_{\substack{\langle ijk\rangle\\ \text{-\,-}\llcorner}}|\Delta_{ij}|^2|\Delta_{jk}|^2\\ &+(1+z^2)\sum_{\substack{\langle ijkl\rangle\\ \square}}[\Delta_{ij}\Delta_{jk}^*\Delta_{kl}\Delta_{li}^*+\text{h.c.}]\}\\ &-\frac{q}{4}\{(6z-10z^2)\sum_{\llcorner}(\Delta_{ij}\Delta_{jk}^*+\text{h.c.})\\ &+(6z-11z^2)\sum_{-\,-}(\Delta_{ij}\Delta_{jk}^*+\text{h.c.})\\ &+4z^2\sum_{|\,|\;=}(\Delta_{ij}\Delta_{pq}^*+\text{h.c.})\}\end{aligned} \tag{30}$$

where the coefficients

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

have been introduced.

Comparison with (20) shows that the exclusion of double occupancy and the proper treatment of the projection operators in the kinetic energy, employed in the derivation of (30), make two profound differences:

(i) The quartic single bond term has become negative for small z. This implies that ΔF possesses absolute minima for nonzero isolated order parameters at a temperature $T_1>T_{c0}$. Such degenerate singlet pair states may be considered an incipient RVB state. For small but finite doping these isolated singlets gain additional energy by parallel ordering due to the last term in (30). This illustrates the formation of phase coherence in the RVB state.

(ii) The local gauge symmetry breaking terms now favour an extended *s*-wave symmetry for finite δ (contrary to the *d*-wave solution in MFA). This is due to terms linear in δ, which were absent in MFA.

In order to study the local minima at $T>T_{c0}$ higher order terms are required to remove the instability due to the negative quartic term. It turns out that the single bond (sb) terms of ΔF can be calculated to all orders. They are given by:

$$\begin{aligned}\Delta F_{\text{sb}}=\sum_{\langle ij\rangle}\Bigg[&\frac{|\Delta_{ij}|^2}{4T_{c0}}-T\ln(3+\cosh(\sqrt{2}\beta|\Delta_{ij}|)\\ &+4z\cosh(\beta|\Delta_{ij}|/\sqrt{2}))\\ &+\frac{z^2}{2}(1+\cosh(\sqrt{2}\beta|\Delta_{ij}|))\Bigg].\end{aligned} \tag{31}$$

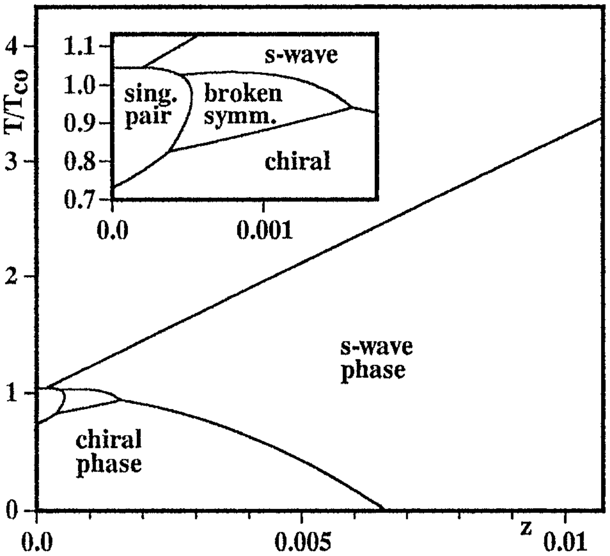

Fig. 4. FIA phase diagram for $U/t=10$. A chiral phase is found to be stable for small doping δ and low temperatures T. In contrast to the MFA phase diagram, the s-wave phase is stable at higher temperatures or larger doping. In addition, the singlet pair state is favoured for very small doping close to the MFA transition temperature. A phase of broken symmetry ($|\Delta_x| \neq |\Delta_y|$) is stable in an intermediate parameter range

The leading order terms of this expression are already contained in the expansion (30).

From (31) we immediately obtain the sixth order single bond term:

$$\frac{b_4}{2}\left(\frac{7}{15}-z+\frac{67}{60}z^2\right)\sum_{\langle ij\rangle}|\Delta_{ij}|^6 \qquad (32)$$

which should be added to (30) to stabilize the system.

We have calculated a "lowest free energy phase diagram" as shown in Fig. 4 by determining the minimum of the free energy as a function of temperature T and doping δ. We find that for very small z there is a small region where the singlet pair state is stable. In this singlet state the bonds are oriented in parallel along one of the axes of the square lattice. At a lower temperature a transition to the chiral phase takes place. This chiral phase region is the only common feature with the MFA phase diagram [see Fig. 2]. In both expansions it results from the plaquette term. For larger doping the extended s-wave phase is stable and the transition temperature T_{cs} initially increases with increasing z. Finally, there is another small region of the phase diagram where the symmetry between x- and y-bonds is broken, i.e. $|\Delta_x|$ and $|\Delta_y|$ have different values.

The path integral representation also allows a straightforward inclusion of phase fluctuations. As suggested by Baskaran and Anderson [8] the locally gauge invariant terms of the free energy functional (30) can be used to determine the absolute value of the order parameter $|\Delta_{ij}|=\Delta_0$ for all bonds. The plaquette term can then be expressed by fluctuating phases only. It is locally gauge invariant as well which implies $\langle\Delta_{ij}\rangle=0$ due to Elitzur's theorem [9]. Thus, T_c is suppressed to zero for $\delta=0$, when the phase fluctuations are properly included. A finite doping concentration $\delta>0$ reduces the local gauge invariance to a global one and allows $\langle\Delta_{ij}\rangle$ to be nonzero. The transition temperature will therefore grow to finite values with increasing z. (A detailed analysis of the phase fluctuations is currently in progress [23].)

V. Conclusion

We have calculated the Ginzburg-Landau expansion for the free energy in a mean field approximation and a functional integral approach for the RVB state, starting from the planar Hubbard model in its strong correlation limit close to the half filled band. In both approaches we have obtained the phase diagrams. In FIA, contrary to MFA, we have found an instability towards the formation of degenerate singlet pair states, indicating the onset of the RVB state for small hole concentration δ and for temperatures above the mean field transition temperature. For finite doping δ we found the extended s-wave phase to be more stable than the d-wave solution. For low temperatures and very small doping δ the chiral phase minimizes the free energy in both treatments.

We are aware that numerical evidence [22] provides arguments against the appearance of superconductivity in the "minimum model" on which our presentation is based, e.g. the inclusion of nearest neighbour Coulomb interactions in an extended Hubbard model is probably important for obtaining superconductivity. Nevertheless, we regard the development of appropriate analytic methods necessary, which would permit an elementary understanding of the various aspects of the problems. The work presented here is meant as a contribution towards this goal. Among the aspects which are relevant, some consequenes of correlations which were not found either in the MFA or in other work [19, 22] appeared in our treatment. In particular, the stabilization of the s-wave phase should be mentioned here again. Local gauge invariance and its being broken is also very important. It can be taken care of in the framework of our approach and will be discussed further elsewhere [23]. One important aspect which has not been treated systematically by any analytical approach we are aware of is the hole-hole correlation. As long as this aspect is not included in the description, the theory has to be considered preliminary.

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