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Angaben zur Veröffentlichung / Publication details:

Müller-Hartmann, E., M. Drzazga, Arno P. Kampf, and H. A. Wischmann. 1988. "Phase transition to the resonating valence bond state." *Physica C: Superconductivity* 153-155: 1261–62. https://doi.org/10.1016/0921-4534(88)90271-7.

PHASE TRANSITION TO THE RESONATING VALENCE BOND STATE

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A path integral formulation for the resonating valence bond concept (RVB) is suggested. Within a Landau expansion three main differences arise compared to a conventional mean field treatment: (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) S-wave symmetry is favoured for the low temperature phase. (iii) Phase fluctuations can be included, destroying off-diagonal order in the absence of holes.

I. INTRODUCTION

There is strong evidence both theoretically and experimentally, that the new High-T_c compounds are examples of strongly correlated fermi systems. The CuO planes may be described by a two dimensional single band Hubbard model on a square lattice in the strong correlation limit U/t>>1. In the spirit of Anderson's resonating valence bond idea (1) the effective Hamiltonian is written as

$$H= -t \sum_{<ij>\sigma} [P_i c^+_{i\sigma} c_{j\sigma} P_i + h.c.] - J \sum_{<ij>} b^+_{ij} b_{ij}$$

with the singlet creation operator

$$b^+_{ij} = (1/\sqrt{2})(c^+_{i\uparrow} c^+_{j\downarrow} - c^+_{i\downarrow} c^+_{j\uparrow})$$

and the exchange energy $J=4t^2/U$. The projection operators P_i in the kinetic energy avoid double occupancy of sites, which is strongly disfavoured due to the large onsite Coulomb repulsion. For an exactly half filled band the effective Hamiltonian reduces to an antiferromagnetic Heisenberg model.

II.MEAN FIELD APPROXIMATION (MFA)

Reminiscent of BCS theory H is replaced in a mean field treatment by the trial Hamiltonian

$$h = \delta t \sum_{<ij>\sigma} (c^+_{i\sigma} c_{j\sigma} + h.c.) - \mu_c N + \sum_{<ij>} (\Delta_{ij} b^+_{ij} + h.c.)$$

as originally suggested by Baskaran et al. (2). δ is the concentration of holes. Without any symmetry restrictions for the complex order parameters Δ_{ij} a Landau expansion for the change of the free energy functional due to finite Δ_{ij} can be derived from h :

$$\Delta F\ T_{co} = (a_2 + \frac{7p}{4}) \sum_{<ij>} |\Delta_{ij}|^2 + \frac{2a_4}{3} \{ \sum_{<ij>} |\Delta_{ij}|^4 /2 + \sum_{<ijk>} |\Delta_{ij}|^2 |\Delta_{jk}|^2 + \sum_{\square} (\Delta_{ij} \Delta^*_{jk} \Delta_{kl} \Delta^*_{li} + h.c.) \} + \frac{p}{4} \{ \sum'_{<ijk>} (\Delta_{ij} \Delta^*_{jk} + h.c.) - \sum_{\square} (\Delta_{ij} \Delta^*_{kl} + h.c.) \}$$

Here the parameters are defined as $T_{co}=J/4$, $a_2=(T-T_{co})/T_{co}$, $a_4=(1/8T_{co})^2$ and $p=(\delta t/T_{co})^2/12$. In addition to quadratic and quartic single bond terms it contains quartic double bond terms which are all invariant under local gauge transformations

$$\Delta_{ij} \rightarrow \exp(i\varphi_i) \Delta_{ij} \exp(i\varphi_j)$$

For $\delta=0$ we therefore have a local U(1) gauge theory (3).The last two quadratic $\pi/2$ bond-rotating and bond shifting terms are due to doping with holes and break the local gauge symmetry. (Note that the sum with a prime couples only nearest neighbour bonds perpendicular to each other.)

Assuming that the translational symmetry of the square lattice is preserved the (mean field) free energy can be calculated to all orders of Δ. The resulting phase diagram is shown in Fig.1.

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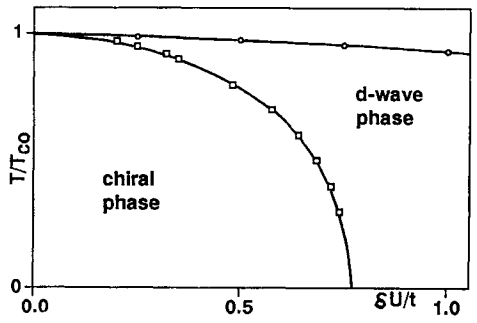

FIGURE 1
Mean field phase diagram

The above Landau expansion is sufficient for understanding the phase diagram almost quantitatively : For a finite hole concentration $\delta>0$ there is a transition to a d-wave state ($\Delta_x=-\Delta_y$) at $T_d=T_{co}(1-p)$. At the lower temperature $T_{ch}=T_{co}(1-10p)$ the d-wave phase smoothly turns into a "chiral phase", characterized by a phase difference of the order parameters on X and Y bonds, $\Delta_x=\Delta_y\exp(i\varphi)$, $\pi/2\le\varphi\le\pi$. The d-wave phase corresponds to $\varphi=\pi$. In the absence of doping the chiral phase with $\varphi=\pm\pi/2$ is stable.

II. FUNCTIONAL INTEGRAL APPROACH

The MFA treatment has three major deficiencies. (i) Local gauge invariance which suppresses T_c to zero for $\delta=0$, excluding any off-diagonal order in the absence of holes, is broken by the MFA. Phase fluctuations which are neglected in MFA have to be included. (ii) The mean field approximation ignores the exclusion of double occupancy. (iii) The hopping is not treated properly by replacing the projection operators by the hole concentration δ.

All three deficiences can be avoided in a functional integral approach. Using The Hubbard-Stratonovich identity the partition function Z is written as

$$Z \sim \int \prod_{<ij>\,n\beta} D^2\Delta_{ij}(\tau)\,\mathrm{Tr}P_{0i}\exp(-\beta[H_0+H_t])$$
$$\mathrm{T}\exp\Big(-\sum_{<ij>}\int_0 d\tau\{|\Delta_{ij}|^2/J+\Delta_{ij}b_{ij}^{+}(\tau)+\mathrm{h.c.}\}\Big)$$

where H_t is the hopping part of H and the concentration of holes is controlled by the chemical potential of holes μ_h in $H_0 = -(\mu_h+J)\Sigma_i(1-n_i)$. The operator P_{0i} projects on the subspace with no doubly occupied sites.

In a static approximation we perform a cumulant expansion of the free energy functional. Traces are performed using a localized basis, explicitly taking the projection operators into account. To leading orders in Δ and in the hole fugacity $z=\exp(\beta\mu_h)$ (and simultaneously in t) we obtain (see (4)):

$$\Delta F T_{co} = (b_2-qz^2)\sum_{<ij>}|\Delta_{ij}|^2 - b_4(1-3z)\sum_{<ij>}|\Delta_{ij}|^4$$
$$+ b_4\,(1-15z^2/2)\sum_{<ijk>}|\Delta_{ij}|^2|\Delta_{jk}|^2 +$$
$$+ b_4\,(1-4z^2)\sum_{\square}(\Delta_{ij}\Delta_{jk}^{*}\Delta_{kl}\Delta_{li}^{*}+\mathrm{h.c.})$$
$$- \frac{q}{2}\Big[\, z\sum_{<ijk>}(\Delta_{ij}\Delta_{jk}^{*}+\mathrm{h.c.}) +$$
$$+ z^2/3\sum_{||}(\Delta_{ij}\Delta_{kl}^{*}+\mathrm{h.c.})\Big]$$

where the coefficients $q=3(t/T_{co})^2/16$, $b_2=(T-T_{co}[1+z^2/4])/4T_{co}$ and $b_4=1/96T_{co}^2$ have been used. For small hole concentration z is proportional to δ.

Two profound differences arise compared to the MFA result: (i) Due to the exclusion of double occupancy the quartic single bond term has become negative. This indicates an instability towards the formation of isolated order parameters at a temperature $T_1>T_{co}$. These (degenerate) singlet pair states may be considered an incipient RVB state. (ii) The terms breaking the local gauge symmetry now favour s-wave symmetry, resulting from the proper treatment of the hopping and the exclusion of double occupancy.

The path integral representation allows for straightforward inclusion of phase fluctuations. For zero doping the local gauge symmetry thus leads to $\langle\Delta\rangle=0$ and T_c is suppressed. For small doping phase fluctuations appear to be the most relevant degrees of freedom.

We are aware that we have performed a simple high temperature expansion of the free energy. It seems reasonable, however, to assume that our conclusions remain valid at low temperature, as they obviously do for the MFA expansion.

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