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Resonant hole configurations and hole pairing

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Abstract. Probabilistic diagonalization methods are used to analyse the structure of the ground state of the two-dimensional Hubbard model for a less than half-filled band. It is found that the ground state is dominated by resonant hole configurations and, for $2t/U < 1$, hole pairing is suppressed.

Hole pair condensation will occur only if an additional pairing interaction of strength $\varepsilon > 2t - 4\eta(t^2/U)$ is introduced, η being a parameter related to the probability of antiferromagnetic correlations between nearest neighbours. Provided that the additional pairing interaction is present, local antiferromagnetic correlations are seen to favour pair condensation, although no long-range antiferromagnetic order is to be expected.

The search for mechanisms of high-temperature superconductivity has highlighted the beauty and complexity of spin fluctuations and magnetic coupling mechanisms. The complexity is evident for example from the fact that one of the simplest such models, the two-dimensional one-band Hubbard model [1–3], remains basically unsolved despite the fact that it has played a central role in many discussions and has been written about in many papers.

The one-band Hubbard model, by itself, is probably not the right model to describe the high-T_c materials. However, its basic feature, which is the interplay of the role of itinerant and localized electrons, may already contain some of the basic ingredients needed to understand these materials. The aim here is to use probabilistic techniques to try to understand some of the dynamical mechanisms of this model. No claim is made concerning the construction of a realistic model for pairing or superconductivity in actual materials.

The Hamiltonian of the one-band Hubbard model is

$$H_b = -\sum_{\substack{\langle i,j\rangle \\ \sigma}} t c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \tag{1}$$

where $\langle i, j\rangle$ denotes ordered nearest-neighbour pairs and $n_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma}$. For a less than half-filled band it is convenient to split the hopping term

$$V = \sum_{\substack{\langle i,j\rangle \\ \sigma}} t c_{i\sigma}^{\dagger} c_{j\sigma} \tag{2a}$$

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into

$$V = tV_0 + tV_1 + tV_M \tag{2b}$$

where

$$V_0 = \sum_{\substack{\langle i,j\rangle \\ \sigma}} (1 - n_{i-\sigma}) c^\dagger_{i\sigma} c_{j\sigma} (1 - n_{j-\sigma}) \tag{2c}$$

$$V_1 = \sum_{\substack{\langle i,j\rangle \\ \sigma}} n_{i-\sigma} c^\dagger_{i\sigma} c_{j\sigma} n_{j-\sigma} \tag{2d}$$

$$V_M = \sum_{\substack{\langle i,j\rangle \\ \sigma}} [n_{i-\sigma} c^\dagger_{i\sigma} c_{j\sigma} (1 - n_{j-\sigma}) + (1 - n_{i-\sigma}) c^\dagger_{i\sigma} c_{j\sigma} n_{j-\sigma}]. \tag{2e}$$

V_0 transfers electrons from singly occupied sites to empty sites. It does not change the eigenvalue of $D = \Sigma_i n_{i\uparrow} n_{i\downarrow}$. V_1 transfers electrons from doubly occupied sites to sites which already have an electron. It does not change the eigenvalue of D as well, and it vanishes in the $D = 0$ subspace. V_M transfers electrons from singly occupied sites to sites which already have an electron and from doubly occupied sites to empty sites. It therefore changes D by one unit.

In the characterization of the dynamics of the ground state for a less than half-filled band, in the $D = 0$ subspace, the important contributions are the hole dynamics induced by the V_0-term and the second-order transitions mediated by virtual excited states of excitation energy U induced by the V_M-term.

The first step in our discussion is traditional. A canonical transformation

$$\exp(\mathrm{i}S)\, H_b \exp(-\mathrm{i}S) = H_{\mathrm{eff}} + \mathrm{O}(t^2)$$

with S determined by

$$V_M + \mathrm{i}[S, H_0] = 0 \qquad \left(H_0 = U \sum_i n_{i\uparrow} n_{i\downarrow} - tV_0\right)$$

is performed to eliminate the V_M-term (in order t) and to obtain an effective Hamiltonian in the $D = 0$ subspace:

$$H_{\mathrm{eff}} = -tV_0 - (t^2/U) V_M^2. \tag{3}$$

Let t be greater than zero. Concentrate first on the diagonalization problem for V_0 in the $D = 0$ sector [4]. Consider a less than half-filled band with N sites and n_h holes. The situations that we are mostly concerned with are situations where there is a macroscopic number of holes, i.e. n_h/N is of the order of at least a few per cent. States with n_h holes will be denoted by $|i, \beta\rangle$, i and β being the labels respectively for the hole configuration and the electron spin configuration. V_0 has matrix elements between $|i, \beta\rangle$ and $|j(i), \beta'\rangle$, $j(i)$ being the hole configurations that are connected to i by the motion of a hole to a nearest-neighbour site and $\beta' = \beta'(\beta, j(i))$ is the spin configuration obtained from β by the hole motion from i to $j(i)$.

Let $|\psi\rangle$ be an eigenstate of V_0

$$V_0|\psi\rangle = \lambda|\psi\rangle = \lambda \sum_{i,\beta} c_{i\beta}|i, \beta\rangle = \sum_{i,\beta} \sum_{j(i)} \frac{c_{j(i)\beta'}}{c_{i\beta}} c_{i\beta}|i, \beta\rangle.$$

Then

$$\sum_{j(i)} \frac{c_{j(i)\beta'}}{c_{i\beta}} = \text{constant} = \lambda. \tag{4}$$

Because $t > 0$ for the energy of the ground state to be minimal, one requires $\mathrm{sgn}(c_{i\beta}) =$

$\mathrm{sgn}(c_{j(i)\beta'})$, i.e. configurations differing in the motion of a hole should have the same sign.

Successive applications of V_0 will connect states with all hole configurations and all electron spin distributions (preserving only the number of holes and the number of up and down spins). The eigenstates of V_0 are thus coherent superpositions of all hole configurations. The number of states to which a given $|i, \beta\rangle$ is connected by V_0 is called its 'connectivity number' $\nu(i)$ and varies from $4n_h$ for a state without hole clusters to about $4\sqrt{n_h}$ for a state with a global cluster.

The connectivity number $\nu(i)$ is the number of terms in the sum of equation (4). Because, for an eigenstate, the sum in (4) is a constant for all $|i, \beta\rangle$ and the connectivity varies with the formation of clusters, this provides a way to estimate the coefficients and hence the probability of cluster formation. An exact analytic calculation, i.e. an exact diagonalization of V_0 is not practical for a large number N of sites. However, the very fact that N is a large number may be turned to our profit to obtain 'exact' results in the probabilistic sense, i.e. to obtain ratios for the coefficients $c_{i\beta}$ which hold on the average. This is the basis of the method which we shall call 'probabilistic diagonalization'. Note that the quantum mechanical phases (signs) of the coefficients should be correctly taken into account. It is only for the amplitude of the coefficients and amplitude ratios that probabilistic estimates will be used.

In the expansion of the ground state $|\psi_0\rangle$ of V_0, consider the coefficients of the states with p hole pairs, which we denote by c_{2p}. When, starting from a given hole configuration, one hole is moved, the probability that a hole pair is formed by this motion is $3(n_h - 1)/(N - 1) \simeq 3n_h/N$. Noting that a hole pair contributes 6 to the connectivity as opposed to 8 for two isolated holes, one obtains from (4) the following, probabilistically rigorous equation:

$$4(n_h - 2p)[(1 - 3n_h/N) + (3n_h/N)(c_{2p+2}/c_{2p})] + 6p[(1 - 3n_h/N)(c_{2p-2}/c_{2p}) + 3n_h/N] = 4n_h[(1 - 3n_h/N) + (3n_h/N)(c_2/c_0)]. \quad (5)$$

Considering the addition of a hole pair to have a uniform effect on the ratio of the coefficients

$$c_{2p+2}/c_{2p} = c_{2p}/c_{2p-2} = c_2/c_0 = z \quad (6)$$

and defining $x = 3n_h/N$, one obtains

$$-4(1 - x) - 4xz + 3(1 - x)/z + 3x = 0. \quad (7)$$

The solution is $z = \frac{3}{4}$ (the other solution of (7) being negative for $x < 1$). This implies that

$$c_{2p} = (\tfrac{3}{4})^p c_0 \quad (8)$$

which means that the probability of finding a macroscopic number of hole pairs ($2p/n_h \sim O(1)$) vanishes in the thermodynamic limit ($N \to \infty$). Similar reasoning would lead to a similar conclusion for the probability of occurrence of other hole clusters in macroscopic numbers. The general conclusion is that the ground state $|\psi_0\rangle$ of V_0 is a coherent superposition dominated by sparse hole configurations with coefficients of similar magnitudes and the same sign. For each fixed number of up and down spins, one finds in $|\psi_0\rangle$ all possible spin configurations β with coefficients of similar magnitude, determined only by the cluster structure of the hole distribution. One therefore con-

cludes that the introduction of a macroscopic number of holes destroys any antiferromagnetic long-range order that might exist in the half-filled band.

The other eigenstates of V_0 are also coherent superpositions of all hole and spin configurations. The highest eigenvalue will correspond to coefficients of magnitude identical with those in $|\psi_0\rangle$ but such that configurations differing in the motion of a hole have opposite signs. We shall call this basis of V_0 eigenstates the 'resonant hole configuration' (RHC) basis.

The diagonalization of the full effective Hamiltonian $-tV_0 - (t^2/U)V_M^2$ may now be carried out in this basis or, using equation (4), we may estimate directly the change in the coefficient ratios introduced by the V_M^2 interaction. From (2*e*) one sees that V_M^2 has non-vanishing diagonal matrix elements for states with electrons of opposite spin in nearest-neighbour sites, as well as matrix elements between states that differ in the spin interchange of two neighbouring anticorrelated electrons. The magnitude of these matrix elements is proportional to the number of electron pairs in nearest-neighbour sites with opposite spins (anticorrelated spins).

For a configuration of N sites, $n_h - 2p$ isolated holes and p hole pairs, the maximum possible number of anticorrelated spins is

$$n_{a,p} = 2N - 4(n_h - 2p) - 7p.$$

Hence, when a new hole pair is created, $n_{a,p} \to n_{a,p} + 1$. Let us denote by η the fraction of the n_a allowed links that is actually anticorrelated. Using now equation (4), as before, to estimate the ratios of the coefficients of states differing by one hole pair, one obtains

$$\begin{aligned} -t\left[4(n_h - 2p)\left((1-x) + x\frac{c_{2p+2}}{c_{2p}}\right) + 6p\left((1-x)\frac{c_{2p-2}}{c_{2p}} + x\right)\right] \\ - \frac{t^2}{U} 2\left(\sum_{\beta''} \frac{c_{2p,\beta''}}{c_{2p,\beta}} + \eta(n_{a,0} + p)\right) \\ = -t4n_h\left((1-x) + x\frac{c_2}{c_0}\right) - \frac{t^2}{U}2\left(\sum_{\beta''}\frac{c_{0,\beta''}}{c_{0,\beta}} + \eta n_{a,0}\right). \end{aligned} \tag{9}$$

The sum $\Sigma_{\beta''}$ is over the spin configurations that differ from β in the exchange of spins in two neighbouring anticorrelated electrons. It is reasonable to assume that $c_{2p,\beta''}/c_{2p,\beta} \simeq 1$, leading to

$$\sum_{\beta''} \frac{c_{2p,\beta''}}{c_{2p,\beta}} \simeq \eta(n_{a,0} + p).$$

Defining the ratio z as in (6), one finally obtains

$$-4(1-x) - 4xz + 3(1-x)/z + 3x + 2(t/U)\eta = 0 \tag{10}$$

with the solution

$$z = (1/8x)\{-4 + 7x + \delta + \sqrt{(x-4)^2 + \delta^2 - 8\delta + 14x\delta}\} \tag{11}$$

where

$$\delta = 2(t/U)\eta.$$

z in equation (11) varies with δ from $\frac{3}{4}$ at $\delta = 0$ to 1 at $\delta = 1$, the variation in this range

being largely independent of x. For $\delta > 1$, one has $z > 1$. This implies that for $\delta < 1$ we have the same situation as in the diagonalization of V_0, i.e.

$$c_{2p} = z^p c_0$$

and the probability of having a macroscopic number of hole pairs vanishes in the thermodynamic limit. Conversely, if $\delta > 1$, then $z > 1$ and the ratio c_{2p}/c_0 diverges for a macroscopic number of pairs, leading to hole pair condensation.

Our treatment and in particular the construction of the effective Hamiltonian (3) is based on the assumption that $t \ll U$ (which seems to hold for the physical parameters in oxide materials [5]). Therefore $\delta < 1$ and the interactions of the Hubbard model are insufficient for pair formation and hole superconductivity.

We now modify slightly the two-dimensional Hubbard model and introduce an explicit ('chemical') pairing interaction

$$H_{\text{eff}} = -tV_0 - (t^2/U)V_M^2 - \varepsilon V_p$$

where V_p is a hole-pairing interaction with unit matrix elements for each hole pair. Applying the same reasoning as before, one would simply modify equation (9) by adding a term $-\varepsilon p$ to the left-hand side. The solution for z is the same as in equation (11) with

$$\delta \to \delta' = \varepsilon/2t + 2(t/U)\eta.$$

Hole pair condensation therefore requires that

$$\varepsilon/t > 2 - 4(t/U)\eta.$$

The interaction $(t^2/U)\, V_M^2$ lifts the degeneracies in the RHC basis, the lowest energies being obtained for the largest number ηn_a of anticorrelated pairs. This favours approximately equal numbers of up and down spins. Furthermore pair condensation is favoured by a large η. This favours, for condensed states, the occurrence of local spin anticorrelations, although there is no reason to expect any long-range antiferromagnetic order.

We conclude from this study that, although the interactions of the Hubbard model are not sufficient to explain hole pair formation, together with an additional pairing interaction they provide an effective mechanism for hole pair condensation. The fact that some other factor besides the Hubbard interaction might be needed has already been suggested by some workers [6]. This might for example be associated with hole polarization (contraction) of the oxygen p orbitals. Anharmonic interactions might also be enhanced by the effect of the apex electrons.

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