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HOLE PAIRING IN AN EXACT MODEL

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Abstract : A model is presented for a hole doped tight-binding half-filled band, in a plane square lattice, which incorporates strong intra-atomic repulsion, kinetic delocalization and hole-induced hopping.
The model has an exact hole-paired ground state. Some general conclusions are drawn concerning the requirements for hole pairing in more realistic models.

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Exact models are nice in the sense that, having rigorous control over their solutions, one can accurately check the validity of the hypothesis without being misled by the artifacts of the approximation that otherwise would be required to estimate a solution. In particular if, in a physical problem, one is looking for the kind of interactions that lead to some conjectured phenomenon, the availability of an exact model provides a way to pin down what is the nature and range of parameters, that bring about the required behavior.

In this paper this philosophy is applied to the study of hole pairing in a model for a half-filled tight-binding band, doped with holes, in a plane square lattice. However, before presenting the model, the terms in the model Hamiltonian will be motivated by a discussion of an effective Hamiltonian derived from the Hubbard model. In the Hubbard model one has

$$H_b = \sum_{i,\sigma} \epsilon_i \, c^{\dagger}_{i\sigma} \, c_{i\sigma} + \sum_{\substack{<i,j> \\ \sigma}} t_{ij} \, c^{\dagger}_{i\sigma} \, c_{j\sigma} + U \sum_i n_{i\uparrow} \, n_{i\downarrow} \tag{1}$$

where $<i,j>$ denotes nearest neighbor pairs and $n_{i\sigma} = c^{\dagger}_{i\sigma} \, c_{i\sigma}$. For a less than half-filled band it is convenient to split the hopping term

$$V = \sum_{\substack{<i,j> \\ \sigma}} t_{ij} \, c^{\dagger}_{i\sigma} \, c_{j\sigma} \tag{2.a}$$

into

$$V = V_0 + V_1 + V_M \tag{2.b}$$

where

$$V_0 = \sum_{\substack{<i,j> \\ \sigma}} t_{ij} \, (1 - n_{i-\sigma}) \, c^{\dagger}_{i\sigma} \, c_{j\sigma} \, (1 - n_{j-\sigma}) \tag{2.c}$$

$$V_1 = \sum_{\substack{<i,j> \\ \sigma}} t_{ij} \, n_{i-\sigma} \, c^{\dagger}_{i\sigma} \, c_{j\sigma} \, n_{j-\sigma} \tag{2.d}$$

$$V_M = \sum_{\substack{<i,j> \\ \sigma}} t_{ij} \left\{ n_{i-\sigma} \, c^{\dagger}_{i\sigma} \, c_{j\sigma} \, (1 - n_{j-\sigma}) + (1 - n_{i-\sigma}) \, c^{\dagger}_{i\sigma} \, c_{j\sigma} \, n_{j-\sigma} \right\} \tag{2.e}$$

V_0 transfers electrons from single occupied sites to empty sites. It does not change the eigenvalue of $D = \sum_i n_{i\uparrow} \, n_{i\downarrow}$.

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 single occupied sites to sites which already have an electron and

conversely. It therefore changes D by one unit.

In the characterization of the dynamics of the ground state (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 . The effective Hamiltonian in the D=0 subspace is usually obtained by performing a canonical transformation to eliminate the V_M term. However, when this is done, one is neglecting part of the effect, on virtual transitions, of the electrons placed near the holes, which also contribute to $\|\Delta D\|=1$ transitions through the second order process $(V_0 G_0 V_M + V_M G_0 V_0)$, G_0 being the free particle Green's function $G_0=(E-H_0+i\epsilon)^{-1}$. Therefore, to take into account as much of the relevant physics as possible, and before one applies a canonical transformation to eliminate the $\|\Delta D\|=1$ transitions, one should write an effective Hamiltonian containing explicitely (in lowest order) all the transitions of this type.

From the Born series for the transition T−matrix, keeping leading order terms and neglecting V_1 which does not contribute to the ground state dynamics one obtains

$$H_{eff1} = H_0 + V_0 + V_M + V_0 G_0 V_M + V_M G_0 V_0 \tag{3}$$

where we have defined

$$H_0 = \sum_{i,\sigma} \epsilon_i \, c^{\dagger}_{i\sigma} \, c_{i\sigma} + U \sum_i n_{i\uparrow} \, n_{i\downarrow} \tag{4}$$

The operator H_{eff1} leads (now in first order) to the same $\|\Delta D\|=0$ and $\|\Delta D\|=1$ matrix elements as H_b .

One now performs on H_{eff1} a canonical transformation $e^{iS} H_{eff1} e^{-iS}$ with S determined by

$$V_M + V_0 G_0 V_M + V_M G_0 V_0 + i\,[S\,,\, H_0+V_0] = 0 \tag{5}$$

to obtain the following effective Hamiltonian, P_0−projected in the D=0 subspace.

$$P_0 \, H_{eff} \, P_0 = P_0 \left(H_0 + V_0 - \frac{1}{U} \left(V_M + V_0 G_0 V_M + V_M G_0 V_0 \right)^2 \right) P_0 \tag{6}$$

One notices from (6) that besides the usual nearest neighbor kinetic delocalization terms induced by V_M^2 , one also obtains kinetic delocalizations involving next-to-nearest neighbors, in the imediate vicinity of the hole positions. These terms are of higher order in t_{ij} , but of the same order in 1/U . One now uses (6) as an inspiration to define a model Hamiltonian. Some simplifications are introduced to make the model solvable and the V_0 term has been neglected, because the main purpose is to discuss the forces leading to hole pairing and not to describe hole mobility. This term will, of

course, have to be reintroduced in a more realistic model for it is hole mobility (paired or otherwise) that leads to electric conductivity.

The model Hamiltonian is as follows :

$$H = H_0 + H_1 + H_2 + H_3 + H_4 \tag{7}$$

where

$$H_0 = \sum_{i,\sigma} \epsilon_i \, c^{\dagger}_{i\sigma} \, c_{i\sigma} \tag{7a}$$

$$H_1 = U \sum_{i,\sigma} c^{\dagger}_{i\sigma} \, c_{i\sigma} \, c^{\dagger}_{i-\sigma} \, c_{i-\sigma} \tag{7b}$$

$$H_2 = - b \sum_{\substack{<i,j> \\ \sigma}} c^{\dagger}_{i\sigma} \, c_{j\sigma} \, c^{\dagger}_{j\sigma} \, c_{i\sigma} \tag{7c}$$

$$H_3 = k \sum_{\substack{<i,j> \\ \sigma}} \{ c_{i\sigma} \, c^{\dagger}_{i\sigma} \, c_{i-\sigma} \, c^{\dagger}_{i-\sigma} \} \{ c_{j\sigma} \, c^{\dagger}_{j\sigma} \, c_{j-\sigma} \, c^{\dagger}_{j-\sigma} \} \tag{7d}$$

$$H_4 = - J \sum_{i,\sigma} \{ c_{i\sigma} \, c^{\dagger}_{i\sigma} \, c_{i-\sigma} \, c^{\dagger}_{i-\sigma} \} \sum_{\substack{v_i \neq v'_i \\ \sigma'}} c^{\dagger}_{v_i\sigma'} \, c_{v'_i\sigma'} \, c^{\dagger}_{v'_i\sigma'} \, c_{v_i\sigma'} \tag{7e}$$

$c^{\dagger}_{i\sigma}$ and $c_{i\sigma}$ are electron creation and annihilation operators in the Wannier-function representation , $<i,j>$ denotes nearest neighbor pairs and v_i (or v'_i) is a nearest neighbor to the site i.

H_0 is the diagonal contribution of the Wannier orbital energies and H_1 represents the intra-atomic Coulomb repulsion favoring, for large U, the single electron per site configuration.

H_2 contains a delocalization decrease in the electron energy due to a charge fluctuation to a neighboring site. A simplification has been introduced in that only charge fluctuations leading back exactly to the same electron spin configuration are taken into account. This is imposed on the model to simplify the structure of the exact vacuum state, but it is reasonable to assume that it captures the essence of the nearest-neighbor delocalization contributions to the energy.

In H_3 the operator products inside curly brackets are hole number operators, equal to one if the site is vacant and zero otherwise. H_3 represents therefore a positive contribution to the energy due to hole repulsion at neighboring sites.

In H_4 the sum on v_i,v'_i runs over the neighbors of the site i. Because of the first factor, H_4 is a delocalization term that operates only between the neighbors of a hole. It corresponds to hole-induced

hopping between next-to-nearest neighbors.

Define $n_{i\sigma} = c^{\dagger}_{i\sigma} c_{i\sigma}$. It is now easy to rewrite H as follows :

$$H = \sum_{i,\sigma} (\epsilon_i - 4b)\, n_{i\sigma} + U \sum_{i,\sigma} n_{i\sigma}\, n_{i-\sigma} + b \sum_{\substack{<i,j>\\ \sigma}} n_{i\sigma}\, n_{j\sigma} +$$

$$+ \sum_{i,\sigma} (1 - n_{i\sigma})(1 - n_{i-\sigma}) \left\{ J \left(\sum_{v_i} n_{v_i} - \frac{4J+k}{2J} \right)^2 - (2J+k) \sum_{v_i} n_{v_i\uparrow}\, n_{v_i\downarrow} - \right.$$

$$\left. - \frac{(4J+k)^2}{4J} + 4k - 2J \sum_{v_i \neq v_i'} n_{v_i\uparrow}\, n_{v_i'\downarrow} \right\} \qquad (8)$$

where $n_{v_i} = n_{v_i\uparrow} + n_{v_i\downarrow}$.

Let us assume $U >> b$, $b > 2J$ and consider states with a fixed number of electrons and holes. To minimize the energy, the second and third terms in Eq.(8) require respectively single occupancy per site and antiferromagnetic order. Then the terms $-(2J+k) \sum_{v_i} n_{v_i\uparrow}\, n_{v_i\downarrow}$ and $-2J \sum_{v_i \neq v_i'} n_{v_i\uparrow}\, n_{v_i'\downarrow}$ vanish when applied to one-electron-per-site antiferromagnetic configurations.

The minimum of the energy is now obtained by minimizing $\left(\sum_{v_i} n_{v_i} - \frac{4J+k}{2J} \right)^2$

i. e. choosing, in the neighborhood of each hole site i, an electron configuration such that $\sum_{v_i} n_{v_i}$ is as close as possible to $(4J+k)/2J$. In particular for $3J > k > J$

one obtains $\sum_{v_i} n_{v_i} = 3$, i. e. all holes are paired.

The exact ground state of the system, in this case, may be written

$$\psi_o = \sum_{h_i} \left\{ \prod_{k \notin h_i} c^{\dagger}_{k,\sigma_k} + \prod_{k \notin h_i} c^{\dagger}_{k,-\sigma_k} \right\} |O> \qquad (9)$$

where the sum is over all possible distributions of hole pairs throughout the lattice and the two terms in Eq.(9) correspond to the two distinct antiferromagnetic configurations for the remaining electrons.

The interpretation of the pairing mechanism is clear. Once the next-to-nearest neighbor transition probabilities are enhanced by the modification introduced by the hole, the delocalization of the electrons to next-to-nearest neighbors becomes energetically favorable. However, if the nearest neighbor hopping interaction is still sufficiently strong to maintain local antiferromagnetic order, the delocalization to next-to-nearest neighbors becomes frustrated. Then, the only possible solution, to

lower the energy, is to attract another hole.

The gap associated to the energy of a hole pair is $6J-2k$.

We have assumed $b>2J$. If this condition is not satisfied the term

$-2J \sum_{i,\sigma} (1 - n_{i\sigma})(1 - n_{i-\sigma}) \sum_{v_i \neq v_i'} n_{v_i\uparrow} n_{v_i'\downarrow}$ implies that it is energetically

favorable to have different spin orientations in the neighborhood of a hole. The electrons around the hole site may then delocalize not only through the presence of another hole, but also through vacant spin states in their next-to-nearest neighbors. I. e., if b is not larger than 2J, the hole leads to a partial destruction of local antiferromagnetic order.

The main conclusions that may be extracted concerning the behavior of more realistic models, for physical systems of a similar nature, are the following:

1- With Coulomb repulsion between neighboring holes, the only way for pairing to become favorable, is through a hole-induced modification (enhancement) of the electron transition probabilities. If the Wannier wave functions of the electrons in the half-filled shell are well localized near atomic sites, this mechanism naturally requires the enhancement of hopping between next-to-nearest-neighbors.

2- Enhancement of the delocalization transitions, for the electrons around a hole, makes the existence of another hole in the neighborhood energetically favorable only if the electron transitions are frustrated. This means that the electrons around the first hole have the same spin orientation. I. e. the mechanism operates only if there is local antiferromagnetic order.

3- Provided the amplitude for nearest neighbor hopping is sufficient to maintain local antiferromagnetic order in the presence of holes, the transition temperature is determined by the parameters that characterize hole Coulomb repulsion and hole-induced hopping between next-to-nearest-neighbors.

4- A general inspiration for some of the features of the model was a particular reduction of the Hubbard Hamiltonian. The question of the applicability of the model to concrete physical situations may however be discussed independently from the Hubbard Hamiltonian. The essential ingredient in producing hole-pairing in the model was seen to be the enhancement of hopping between hole neighbors. Also the model is a single-band one. Hence, its applicability hinges mainly on the likelihood of the occurence of these conditions.

Spectroscopic methods have shown[1] that, in the Cu-O planes of high temperature superconductors the doped holes reside on the O sites. As shown by Zhang and Rice[2], they hybridize with the preexisting ($3d_{x^2-y^2}$) at the Copper sites leading, in first approximation, to a symetric state involving a $3d_{x^2-y^2}$ hole state in Copper and the ($2p_x$,$2p_y$) oxygen hole states. The hybridization leads to an effective single-band Hamiltonian. Furthermore the hybridized symmetric states, localized around Cu sites, are not orthogonal to each other because the neighboring squares share a common O site. The overlap will surely change (maybe enhance) the hopping probabilities between the Copper sites surrounding the doped hole.

The usual nearest-neighbor hopping interactions in magnetic insulators are due to superexchange[3] mediated by the ligand ion. What is being suggested here is an effect of hole enhanced hopping arising from an extended superexchange based on the hybridization of oxygen and copper hole states.

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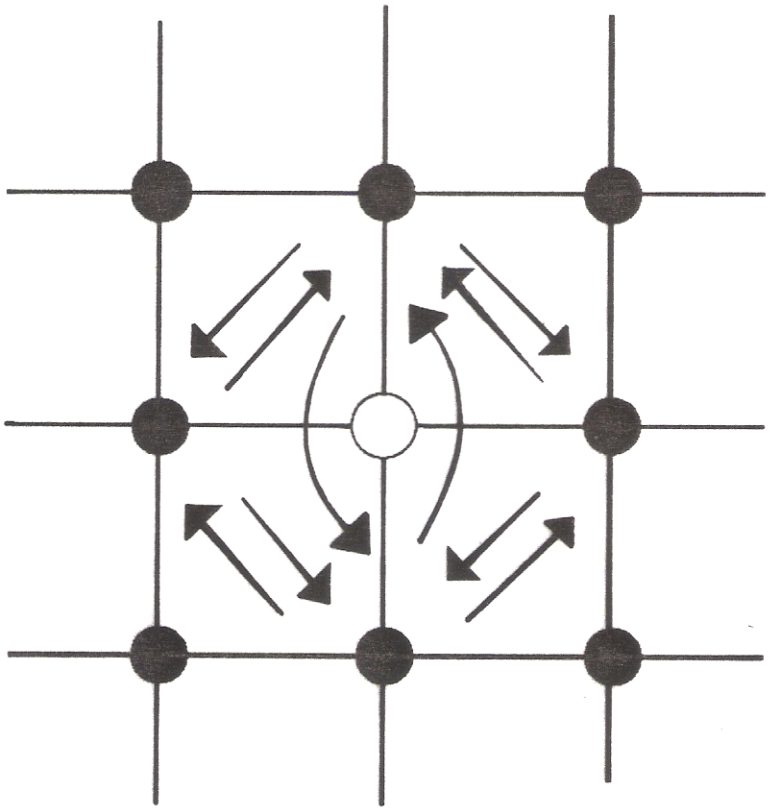

Hole enhanced hopping between next-to-nearest-neighbors