# Superconducting condensation energy and an antiferromagnetic exchange-based pairing mechanism

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For the traditional low-$T_c$ superconductors, the superconducting condensation energy is proportional to the change in energy of the ionic lattice between the normal and superconducting state, providing a clear link between pairing and the electron-ion interaction. Here, for the $t$-$J$ model, we discuss an analogous relationship between the superconducting condensation energy and the change in the exchange energy between the normal and superconducting states. We point out the possibility of measuring this using neutron scattering and note that such a measurement, while certainly difficult, could provide important evidence for an exchange interaction-based pairing mechanism. [S0163-1829(98)07638-3]

During the past several years, a variety of experiments ranging from NMR (Refs. 1,2) and penetration depth[3] studies to angle-resolved photoemission spectroscopy[4,5] and Josephson phase interference measurements[6,7] have provided clear evidence for $d_{x^2-y^2}$ pairing in the high-$T_c$ cuprates. This type of pairing was in fact predicted from a variety of theoretical studies on Hubbard and $t$-$J$ models in which a short-range Coulomb potential leads to a near-neighbor exchange interaction and short-range antiferromagnetic correlations.[8] Thus, in spite of the differences in the interpretations of some of these calculations, one might have concluded that the basic mechanism which is responsible for pairing in the cuprates arises from the antiferromagnetic exchange interaction and the short-range exchange correlations. However, there is far from a consensus on this, and a variety of different basic models and pairing mechanisms have been proposed.[9]

In the traditional low-temperature superconductors one could see an image of the phonon density of states $F(\omega)$ in the frequency dependence of the gap $\Delta(\omega)$.[10] One also had a clear isotope effect in some of the simpler materials and Chester[11] showed that in this case the superconducting condensation energy could be related to the change in the ion kinetic energy. Thus, while the kinetic energy of the electrons is increased in the superconducting state relative to the normal state, the decrease in the ion lattice energy is sufficient to give the condensation energy. This provided a further link between the electron lattice interaction and the pairing mechanism in the traditional superconductors.

Now, in the high-$T_c$ cuprates, we believe that one can see the image of the $k$ dependence of the interaction in $\Delta(k)$ and that this supports the Hubbard and $t$-$J$ pictures.[12,13] However, as noted, this remains an open question and it would be useful to look for the analogue of the decrease in lattice energy and the condensation energy. From density matrix renormalization group studies of the $t$-$J$ model,[13] we know that while the kinetic energy of a pair of holes is increased relative to having two separate holes, the exchange energy is reduced. Thus, if the short-range antiferromagnetic spin-lattice correlations play a similar role to the ion lattice in the traditional low-temperature superconductors, the condensation energy would be proportional to the change in the exchange energy between the normal and superconducting states.

Here we examine this and look for its possible experimental consequences. Unfortunately, just as in the case of the traditional electron-phonon systems where the fractional change in the lattice energy between the normal and superconducting ground states is small, of order $T_c^2/\mu_F\omega_D$, and hence hard to detect, here we find that the fractional change in the exchange energy, of order $T_c^2/\mu_F J$, will also be difficult to observe. Nevertheless, on a formal level it is interesting to contrast the relationship between the superconducting condensation energy and the change in the exchange energy with a recent proposal by Leggett[14] in which he argues that the condensation energy arises from a change in the long-wavelength Coulomb energy associated with the midinfrared dielectric response.

Our basic idea originated from the results of numerical density matrix renormalization-group calculations[13] for the $t$-$J$ model. The $t$-$J$ Hamiltonian in the subspace in which there are no doubly occupied sites is given by

$$H=-t\sum_{\langle ij\rangle s}(c_{is}^{\dagger}c_{js}+\text{H.c.})+J\sum_{\langle ij\rangle}\left(\mathbf{S}_i\cdot\mathbf{S}_j-\frac{n_in_j}{4}\right). \quad (1)$$

Here $ij$ are near-neighbor sites, $s$ is a spin index, $\vec{S}_i=(c_{is}^{\dagger}\vec{\sigma}_{ss'}c_{is'})/2$, and $c_{i,s}^{\dagger}$ are electron spin and creation operators, and $n_i=c_{i\uparrow}^{\dagger}c_{i\uparrow}+c_{i\downarrow}^{\dagger}c_{i\downarrow}$. The near-neighbor hopping and exchange interactions are $t$ and $J$. We have calculated the ground-state energy of Eq. (1) for zero ($E_0$), one ($E_1$), and two ($E_2$) holes. For $J/t=0.35$ we find, for an $8\times8$ system, that the binding energy of a pair of holes is

 

$$\Delta_B = 2E_1 - (E_2 + E_0) = 0.23J. \tag{2}$$

We also find that the dominant contribution to this binding comes from the change in the exchange energy

$$2\left\langle J\sum_{\langle ij\rangle} \vec{S}_i\cdot\vec{S}_j\right\rangle_1 - \left(\left\langle J\sum_{\langle ij\rangle} \vec{S}_i\cdot\vec{S}_j\right\rangle_2 + \left\langle J\sum_{\langle ij\rangle} \vec{S}_i\cdot\vec{S}_j\right\rangle_0\right). \tag{3}$$

Here 0, 1, and 2 refer to the number of holes in the ground state.

The pair binding energy can be used in a simple estimate of $T_c$: if we relate the superconducting gap to the binding energy via $2\Delta = \Delta_B$, and assume that $2\Delta/kT_c \approx 6$, we find $T_c \approx 0.04J/k$. Taking $J = 1500$ K, this gives $T_c \approx 60$ K, a quite reasonable value. Now, it is clear that superconductivity in the cuprates is a much more complicated phenomena than this simple picture of pair binding. For example, even in the $t$-$J$ model, we find that with a finite concentration of holes, domain walls form, rather than pairs.[15] However, the formation of domain walls in the $t$-$J$ model is also driven largely by the exchange energy. Therefore, it is reasonable to assume that whatever the precise mechanism of superconductivity in the cuprates, energetically it is driven by the exchange interaction.

Based upon this and in analogy with the electron phonon case, we suggest that if the basic interaction which is responsible for pairing in the high-$T_c$ cuprates is the antiferromagnetic exchange, the condensation energy will be proportional to the change in the exchange energy between the normal and superconducting phases

$$\frac{\alpha H_c^2(T)\Omega_0}{8\pi} = J(\langle \vec{S}_i\cdot\vec{S}_{i+x} + \vec{S}_i\cdot\vec{S}_{i+y}\rangle_N - \langle \vec{S}_i\cdot\vec{S}_{i+x} + \vec{S}_i\cdot\vec{S}_{i+y}\rangle_S). \tag{4}$$

Here $H_c(T)$ is the thermodynamic critical field at temperature $T$, $\Omega_0$ is the unit-cell volume per $CuO_2$, and $\alpha$ is a factor of order 1. Note that both expectation values in Eq. (4) are also taken at temperature $T$ with the subscript $N$ referring to a nominal normal state and $S$ to the superconducting state. Thus one needs to be able to extrapolate the normal-state data to temperatures $T < T_c$.

For the $t$-$J$ model we have[16]

$$\langle \vec{S}_i\cdot\vec{S}_j\rangle = 3\int \frac{d^2q}{(2\pi)^2}\int_0^\infty \frac{d\omega}{\pi}\mathrm{Im}\,\chi(q,\omega)\cos[\vec{q}\cdot(\vec{i}-\vec{j})], \tag{5}$$

where $\chi(q,\omega)$ is the magnetic susceptibility at temperature $T$. For $\vec{i}$ equal to $\vec{j}$ we have the sum rule

$$(1-x)S(S+1) = 3\int \frac{d^2q}{(2\pi)^2}\int_0^\infty \frac{d\omega}{\pi}\mathrm{Im}\,\chi(q,\omega) \tag{6}$$

with $S = 1/2$, and $x$ the hole doping. Using Eqs. (5) and (6), we can write Eq. (4) in the form

$$\frac{\alpha H_c^2(T)\Omega_0}{8\pi} = 3J\int \frac{d^2q}{(2\pi)^2}\int_0^\infty \frac{d\omega}{\pi}[\mathrm{Im}\,\chi_S(q,\omega) - \mathrm{Im}\,\chi_N(q,\omega)](2 - \cos q_x - \cos q_y). \tag{7}$$

In Eq. (7), we have added a constant 2 using the sum rule Eq. (6). The form factor $2 - \cos q_x - \cos q_y$ favors large momentum transfers $q_x \sim q_y \sim \pi$ and the energy scale is set by $\omega \lesssim J$.

For the optimally or possibly the overdoped materials, it may be that $\mathrm{Im}\,\chi_N(q,\omega)$ has reached its ''low-temperature normal form'' at temperatures above $T_c$. In this case, one could extract it from neutron-scattering data for $T > T_c$. Then, using low-temperature $T \ll T_c$ data for $\mathrm{Im}\,\chi_S(q,\omega)$ in Eq. (7), one would obtain the condensation energy. Because $H_c^2(0)\Omega_0/8\pi J \sim 10^{-3}$, it will require extremely careful neutron-scattering measurements to check Eq. (7). Furthermore, one will have to be satisfied that the normal-state measurements taken at temperatures above $T_c$ can be extrapolated to a temperature which is low compared to $T_c$. Clearly, this will be difficult. However, on a formal level, it is interesting to contrast the content of Eq. (7) with the recent proposal by Leggett.[14] He takes the point of view that the pairing mechanism is associated with the long-wavelength Coulomb energy and relates the condensation energy to a change in the dielectric function between the normal and superconducting state. He then argues that the important contributions are associated with momentum transfers which are small compared to $\pi$ and energy transfers in the midinfrared region, 0.1–1.5 eV.

Now, it is certainly true that if one goes all the way back, the Coulomb energy is responsible for the exchange interaction we have focused on. However, having integrated out the short-range part of the Coulomb interaction to arrive at an exchange interaction $J \sim 4t^2/U$, we conclude from Eq. (7) that the important part of the pairing interaction is associated with large momentum transfers $q \sim (\pi/a, \pi/a)$ and energies less than or of order $J \sim 0.1$ eV. Thus, contrary to Ref. 14, where one seeks to find a relationship between the condensation energy and the change in the *dielectric* response between the normal and superconducting state in the small momentum and higher energy 0.1–1.5 eV regime, we suggest that the condensation energy is related to changes in the *magnetic* spin response at large momentum transfer and energies $\omega \lesssim J$.

Thus, it would be very interesting if it were possible to confirm or contradict the relationship of the change in $\langle \vec{S}_i\cdot\vec{S}_{i+\hat{x}}\rangle$ between the normal and superconducting states and the superconducting condensation energy given by Eqs. (4) and (7).

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[16] For the Hubbard model the left-hand side of Eq. (6) is replaced by $\langle \vec{S}^2 \rangle$, which could change slightly in the superconducting state, so that one would not want to make the subtraction in Eq. (7) and the 2 in Eq. (7) should be dropped.