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Interlayer pair hopping: Superconductivity from the resonating-valence-bond state

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Superconductivity in the high-T_c materials is interpreted as $\langle e_k e_{-k}\rangle$ condensation of hole bosons. Coherent interlayer tunneling of boson pairs results in order-parameter equations which are quite different from those of the Bardeen-Cooper-Schrieffer theory. A model is presented which suggests how this condensation is affected by charge-carrying boson interactions.

In the resonating-valence-bond[1] theory, the quasiparticle excitations of the simple two-dimensional (2D) Hubbard model at sufficiently low doping and temperature are believed to be one charge-carrying boson species (the "holon" e) and a spin-carrying fermion (the "spinon" S).[2] The holon must give rise to the observed superconductivity, though the question of the exact nature of this condensation must be clarified. One approach[3] has been to consider free bosons with weak dispersion along the c axis, which has been shown to lead to Bose condensation of a "$2+\epsilon$ dimensional Bose gas." We, however, do not make the assumption of a well-developed interlayer band, but consider the Josephson-like coupling between the layers. We will argue that the dominant process at sufficiently low temperatures is a coherent tunneling of quasiparticle holon pairs. This drives holon $\langle e^\dagger e^\dagger\rangle$ pairing and we have a $2e$ condensate.

The effective layer Hamiltonian we consider is

$$\mathcal{H}=\sum_{k,\sigma}(\Gamma_k-\mu^s)S^\dagger_{k,\sigma}S_{k,\sigma}+\sum_k(\varepsilon_k-\mu)e^\dagger_k e_k + \sum_{kpq}V^{\text{pseudo}}_q e^\dagger_{k+q}e_k e^\dagger_{p-q}e_p \ . \tag{1}$$

We will discuss V^{pseudo} later. $\Gamma\sim J$.

Let us first mention single electron tunneling.[4] This involves the transport of both spin and charge, and therefore the hopping of a spinon and a holon [Fig. 1(a)]. At temperatures small compared to the exchange energy J (estimated in these materials to be 1000 K), the spinon hopping is suppressed by the factor T/J, as the spinon must find an empty state in the adjacent layer. This picture accounts quite well for the interlayer resistivity data where $\rho\propto 1/T$ has been observed.[5]

The dominant process when $T\ll J$ is singlet pair tunneling. In 2D quasiparticle language we tunnel a holon pair and the spinon is involved only as a virtual excitation. The appropriate vertex $\Lambda(k,\omega)$ is [Fig. 1(b)]

$$\Lambda(k,\omega)=t^2_{ab}\chi^S(k,\omega) \ . \tag{2}$$

t_{ab} is the interlayer electron hopping matrix element where a,b label adjacent layers. The spinon response χ^S will be approximated by a k,ω independent constant $\chi^S\sim(2\pi J)^{-1}$ up to $k\sim 2k_F$ and $\omega\sim J^{-1}$. (The frequency dependence of χ^S is unimportant for $t\delta\ll J$ except insofar as we have found that the upper cutoff allows retardation to overcome repulsive interlayer effects in a manner identical to the Coulomb psuedopotential in Bardeen-Cooper-Schrieffer superconductors.) Another way to view this is to note that the intermediate state in question is a real electron-hole excitation in adjacent layers. The lifetime of these excitations is short (at most $\sim J^{-1}$) in the resonating-valence-bond state, and this determines the energy denominator.

Let us first discuss pairing for the unrealistic case of free bosons $V^{\text{pseudo}}=0$,[6]

$$H=\sum_k(\varepsilon_k-\mu)e^{a\dagger}_k e^a_k - \frac{\Lambda}{2}\sum_{k,q}(e^{a\dagger}_{-k}e^{a\dagger}_k e^b_q e^b_{-q}+\text{H.c.})+a\leftrightarrow b \ .$$

Note that a single boson hopping term here would constitute a strong pair-breaking effect. The equations of

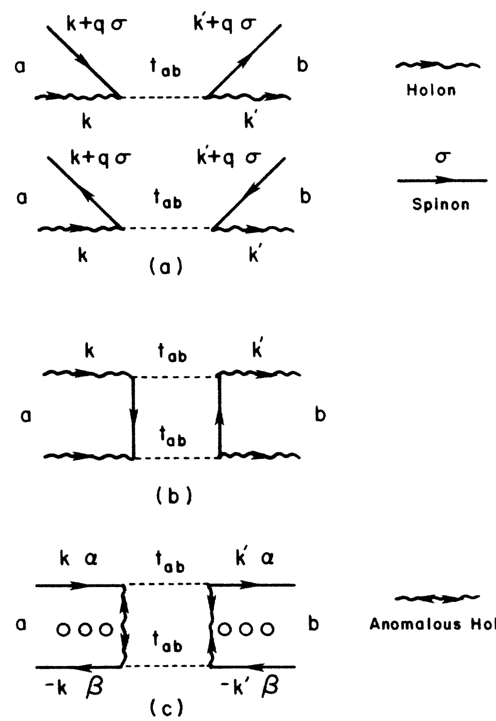

FIG. 1. (a) Processes contributing to interlayer conductance. The spinon required may come from either the a or b layer. (b) The vertex Λ describing the pair hopping process. (c) Spinon pair hopping involving anomalous holon propagator.

motion are

$$[H,e_k^a] = -(\varepsilon_k - \mu)e_k^a - \Lambda \sum_q e_q^b e_{-q}^b e_{-k}^{a\dagger} \ .$$

Suppose layer b forms part of a bulk $\langle e^b e^b \rangle$ superconductor, and proceed self-consistently,

$$\langle e_k^b e_{-k}^b \rangle = \langle e_k^a e_{-k}^a \rangle \ .$$

Let

$$\Delta = \Lambda \sum_k \langle e_k^b e_{-k}^b \rangle \ . \tag{3}$$

This acts as a source of pairs of finite strength in layer a. Linearizing in this way one obtains the spectrum

$$E_k = [(\varepsilon_k - \mu)^2 - \Delta^2]^{1/2} \ , \tag{4}$$

and

$$n_k + \tfrac{1}{2} = \coth[\beta E_k/2] \frac{(\varepsilon_k - \mu)}{2E_k} \ , \tag{5}$$

$$1 = \Lambda \sum_k \frac{\coth[\beta E_k/2]}{2E_k} \ , \tag{6}$$

For the free 2D Bose gas

$$\mu = k_B T \ln(1 - e^{-T_0/T}) \ ,$$

where $T_0 = 4\pi\delta t$ and δ is the doping. (It is valid to approximate $\varepsilon_k = tk^2$, i.e., to neglect the lattice.) T_c is easily found in the limit $\Lambda \ll t$:

$$T_c = \frac{4\pi\delta}{\ln(8\pi t/\Lambda)} \ . \tag{7}$$

Equations (5) and (6) give rise to a second-order transition. At $T \approx 0$,

$$\Delta = \Lambda\delta - \frac{(k_B T)^2}{4\pi t\delta} \ . \tag{8}$$

We also find that $\mu \to \Delta$ as $T \to 0$:

$$\mu = -\Delta + \frac{2(k_B T)^2}{\Lambda\delta} \exp\left(-\frac{8\pi t\delta}{k_B T}\right) \ . \tag{9}$$

The result (9) is very interesting. It states that the boson spectrum is strictly gapless only at $T=0$. This is in accord with the Hugenholtz-Pines theorem which states that the single-particle spectrum in the presence of $\langle e \rangle$ must be gapless, as implied by the integer particle-number fluctuations present in such a state. At $T=0$ we have macroscopic occupation of $k=0$ and it is likely that the theorem applies. At finite T, there is no such theorem for $\langle ee \rangle$ alone nonzero and a gap which is always exponentially small compared to the temperature appears in our solution.

At T_c one finds that

$$\begin{aligned} \Delta &= \frac{\Lambda\delta}{\sqrt{\ln(8\pi t/\Lambda)}} \left[\frac{6(T_c - T)}{T_c}\right]^{1/2} \ , \\ \mu &= -\frac{\Lambda\delta}{\ln(8\pi t/\Lambda)} \left[1 + \frac{3(T_c - T)}{T} \ln\left(\frac{8\pi t}{\Lambda}\right)\right] \ . \end{aligned} \tag{10}$$

The situation is summarized in Fig. 2.

In this free-boson approximation, the heat-capacity jump ΔC at T_c is of order $k_B \Lambda\delta/t$. It is small compared to the boson background ($C \approx k_B^2 T_c/t$) and the spinon background ($C \approx k_B^2 T_c/J$). A jump $\Delta C/C$ of order 1 is required for qualitative agreement with experiment.[7]

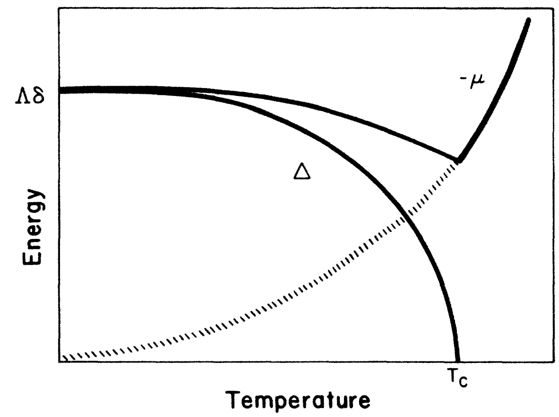

FIG. 2. The temperature dependence of chemical potential and pairing amplitude for free bosons. The dotted line is the chemical potential below T_c for unpaired bosons.

While they are suggestive, the above results may not be directly applicable to the holon. Essentially they describe the stabilization of incipient layer ODLRO. The true holon occupation is smeared in k space so as to satisfy $n_k \le n_0$,[8] where n_0 is in general, not macroscopic. One may view this as a good approximation for strongly interacting bosons, especially in two dimensions, but given that the holon states are constructed by Gutzwiller projecting the appropriate Fermi sea it is required that no state should obtain a larger occupation.

We impose this constraint via a k-space pseudopotential in Hartree-Fock. We require a flat spectrum up to $k_0 = (4\pi\delta/n_0)^{1/2}$ and $\varepsilon_k \sim tk^2$ thereafter, at $T=0$. The required pseudopotential V_k is

$$\begin{aligned} V_k &= A - \frac{t}{\delta}|\mathbf{k}|^2, \ k < 2k_0 \ , \\ &= 0, \ k > 2k_0 \ , \end{aligned} \tag{11}$$

yielding

$$\begin{aligned} \varepsilon_k &= \varepsilon_k^0 + NV_0 + \sum_p V_{k-p} n_p \ , \\ &= \varepsilon_0, \ k < k_0 \ , \\ &\sim tk^2, \ k \gg k_0 \ . \end{aligned} \tag{12}$$

At finite T one finds

$$\varepsilon_k = \varepsilon_0(T) + \alpha T \exp - \left(\frac{4\pi t\delta}{n_0 T}\right) k^2 \ , \tag{13}$$

for $k < k_0$, arising from the change in occupation. Below the degeneracy temperature ε_k is quite flat. The chemical potential is fixed such that

$$\frac{\varepsilon_k - \mu}{T} \to \ln(n_0^{-1} + 1), \ k < k_0, \ T \to 0 \ . \tag{14}$$

This is consistent with the above very weak dispersion, i.e.,

$\varepsilon_k/T \rightarrow \varepsilon_0/T$ as $T \rightarrow 0$. The system crosses over to free bosons at a temperature $T_{\rm cross} \sim t\delta/\ln n_0$.

We now allow interlayer pair hopping to form a paired state from this Hartree-Fock holon gas. Now (12), in addition to (5) and (6), form a couplet set of integral equations.[6] However, for weak coupling the dispersion acquired at finite T or Δ is a small correction. One finds that all wave vectors up to k_0 contribute to the pairing. Now

$$T_c = \frac{(1/2n_0+1)}{\ln(n_0^{-1}+1)} \Lambda\delta \ . \qquad (15)$$

T_c is an increasing function of the maximum allowed occupation. [In fact T_c reaches $T_{\rm cross}$ at $T_c \simeq t\delta/\ln(t/\Lambda)$. One obtains the earlier expression when $n_0 > t/\Lambda$.]

The situation at $T=0$ is also radically changed. μ must differ from Δ to ensure $n_k \leq n_0$ which leads to a charge gap Δ_g in the superconducting state. From (5),

$$\varepsilon_0 - \mu = (2n_0+1)E_0 \ \text{or} \ E_0 = \frac{1}{2\sqrt{n_0(n_0+1)}}\Delta \ , \qquad (16)$$

where Δ is defined by (3). Solving (6) for $E_0 \equiv \Delta_g$,

$$\Delta_g = \frac{\Lambda\delta}{2n_0} \ . \qquad (17)$$

So for $n_0 = 1$ for example,

$$\frac{\Delta_g}{T_c} = 0.23 \ . \qquad (18)$$

We display these results in Fig. 3. Three-dimensional Coulomb interactions are expected to raise the collective modes out of the gap.

How would things differ for hypothetical fermion holons? The gap parameter and T_c are uncharacteristic of fermions, despite the Fermi-like occupation. The systems differ strongly mainly from the point of view of their coherence properties. The situation is similar to ^{4}He vs ^{3}He. For fermion holes we would obtain, for example, $T_c \sim t\exp(-t/\Lambda)$.

Our model predicts that T_c is proportional to doping. Data from Shafer, Penney, and Olsen and Batlogg[9] display this behavior. From these and the estimate[4] $(t_{ab}/t)^2 < 0.1$ from the anisotropic conductivity we must set $n_0 \sim 1$, as expected. If the Josephson pair mechanism dominates as suggested here, one would expect that T_c is an increasing function of the $1/T$ part of the c-axis conductance divided by carrier concentration, which appears to be direct measure of Λ.[4] By the same token, T_c should increase as the in-plane resistivity divided by carrier concentration, as in-plane scattering by spinons and χ^S both are proportional to the spinon density of states at the pseudo-Fermi surface.

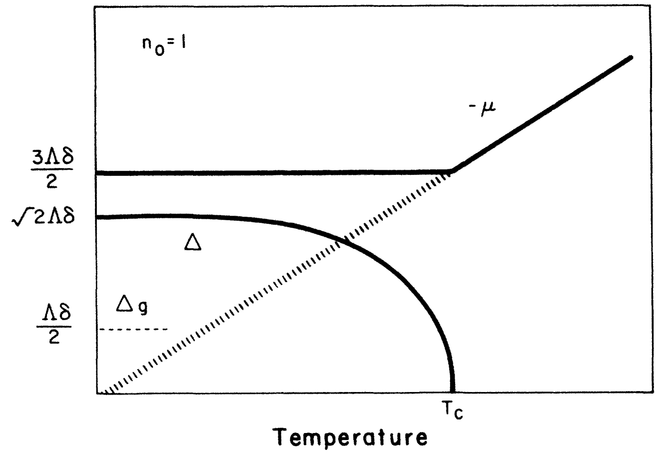

FIG. 3. The temperature dependence of chemical potential, pair amplitude, and gap Δ_g for $n_0 = 1$.

Returning to the heat capacity, we find that the heat capacity jump is of order $\Delta C_H \sim k_B\delta$. The background heat capacity of the holons is now $C_H \sim k_B\delta(\Lambda/t)^{2/3}$, much reduced from that of the free-boson case. The precise numerical factors and powers are artefacts of Hartree-Fock, but the jump is now comparable in magnitude to the spinon background in the regime $\delta \sim 0.1-0.2$. Below T_c, C_H is activated, roughly $\delta(\Delta_g/T)^2 \exp - (\Delta_g/T)$.

What of the spin degrees of freedom in (1)? Because of the separation of charge and spin, we have the possibility of distinct boson and fermion gaps in the superconducting state. When hole pairs tunnel, the singlet pair bonds left behind modify the length distribution of valence bonds which might lead to a gap in the spinon spectrum. However, consider Fig. 1(c). Here, for example, a spinon pair in layer a absorb charge $2e$ from the condensate and dump charge $2e$ in the b layer. A holon gap will act to strongly suppress this process. Conversely, a spinon gap would appear to suppress holon pair hopping. Work is in progress on these questions.

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