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Superlight bipolarons and criterion of BCS-BEC crossover in cuprates

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Most of the proposed models of high-temperature superconductivity (HTSC) are based on the short-range electron-electron correlations or/and on a short-range electron-phonon interaction. However, in the cuprates the screening is poor due to a low carrier density, layered crystal structure, and high ionicity of the lattice. We develop further the bipolaron model of HTSC, which explicitly takes into account the long-range origin of all interactions. The long-range electron-phonon (Froehlich) interaction binds carriers into real space pairs (small bipolarons) with surprisingly low mass but sufficient binding energy, while the long-range Coulomb repulsion keeps them from forming larger clusters. The model has explained many key features of cuprates. It is shown here that real-space pairing takes place in many cuprates at variance with some (incorrect) criteria of the BCS-BEC crossover.

I. INTRODUCTION: BIPOLARON MODEL OF CUPRATES

The electron-phonon interaction as an origin of high $T_c$ continues to gather support through isotope effect measurements, infrared, tunnelling, neutron and photoemission spectroscopies. To account for high values of $T_c$ in the cuprates, it is necessary to have a strong electron-phonon interaction, when a many-electron-phonon system collapses into the small (bi)polaron regime. At first sight these carriers have a mass too large to be mobile, however it has been shown that the inclusion of the on-site Coulomb repulsion leads to the favoured binding of intersite oxygen holes. The intersite bipolarons can then tunnel with an effective mass of only 10 electron masses.

Mott and the author proposed a simple model of the cuprates based on bipolarons, Fig.1. In this model all the holes (polarons) are bound into small intersite singlet and triplet bipolarons at any temperature. Above $T_c$ this Bose gas is non-degenerate and below $T_c$ phase coherence (ODLRO) of the preformed bosons sets in, followed by superfluidity of the charged carriers. The model accounts for the crossover regime at $T^*$ and normal state pseudogaps in cuprates. Here I show that real-space pairing takes place in many cuprates.

II. PAIRING IS ‘INDIVIDUAL’ IN MANY CUPRATES

The possibility of real-space pairing, as opposed to BCS-like pairing, has been the subject of much discussion. Experimental and theoretical evidence for an exceptionally strong electron-phonon interaction in high temperature superconductors is now so overwhelming, that even advocates of nonphononic mechanisms accept this fact. Nevertheless the same authors dismiss any real-space pairing claiming that pairing is collective in cuprates. They believe in a large Fermi surface with the number of holes $(1 + x)$ rather than $x$, where $x$ is the doping level like in $La_{2-x}Sr_{x}CuO_4$. As an alternative to a three-dimensional BEC of bipolarons these authors suggest a collective pairing (i.e. the Cooper pairs in the momentum space) at some temperature $T^* > T_c$, but without phase ordering. In this concept $T_c$ is determined by the superfluid density, which is proportional to doping $x$, rather then to the total density of carriers $(1 + x)$. On the experimental side a large Fermi surface is clearly incompatible with a great number of thermodynamic, magnetic, and kinetic measurements, which show that only holes doped into a parent insulator are carriers in the normal state. On the theoretical ground this preformed Cooper-pair (or phase-fluctuation) scenario contradicts a theorem, which proves that the number of supercarriers (at $T = 0$) and normal-state carriers is the same in any clean superfluid.

Here I show that objections against real-space pairing...
also contradict a parameter-free estimate of the Fermi energy. In cuprates the band structure is quasi-two-dimensional (2D) with a few degenerate hole pockets. Applying the parabolic approximation for the band dispersion we obtain the renormalized Fermi energy as 

\[ \epsilon_F = \frac{\hbar^2 \pi n_i d}{(m^*_i)} , \]

where \( d \) is the interplane distance, and \( n_i, m^*_i \) are the density of holes and their effective mass in each of the hole subbands \( i \) renormalized by the electron-phonon (and by any other) interaction. One can express the renormalized band-structure parameters through the in-plane magnetic-field penetration depth at \( T \approx 0 \), measured experimentally:

\[ \lambda^2_H = \frac{4\pi e^2}{\sum_i n_i / (m^*_i c^2)} \]

In the framework of the BCS theory this expression is applied to any clean superfluid, where \( m^*_i \) and \( n_i \) are the normal state mass and density of carriers, respectively. As a result, we obtain a parameter-free expression for the “true” Fermi energy as

\[ \epsilon_F = \frac{\hbar^2 dc^2}{4ge^2\lambda_H^2} \] (1)

where \( g \) is the degeneracy of the spectrum which might depend on doping in cuprates. Because Eq. (1) does not contain any other band-structure parameters, the estimate of \( \epsilon_F \) using this equation does not depend very much on the parabolic approximation for the band dispersion.

Parameter-free estimates of the Fermi energy using Eq. (1) show that the renormalised Fermi energy in many cuprates is certainly well below 100 meV and the pairing is individual. Indeed such pairing will occur when the size of a pair, \( \rho \) is smaller than the interpair separation, \( r \). The size of a pair is estimated as

\[ \rho = \hbar / (\sqrt{m^* \Delta}) \]

Separation of pairs is directly related to the Fermi energy in 2D

\[ r = \hbar \sqrt{\pi / (\epsilon_F m^*)} \]

We see that the true condition for real-space pairing is

\[ \epsilon_F \lesssim \pi \Delta \] (2)

The bipolaron binding energy is thought to be twice the pseudogap. Experimentally measured pseudogap of many cuprates is as large as \( \Delta/2 \gtrsim 50 \text{meV} \), so that Eq. (2) is well satisfied in underdoped and even in a few optimally and overdoped cuprates. One should notice that the coherence length in the charged Bose gas has nothing to do with the size of the boson as erroneously assumed by some authors. It depends on the interparticle distance and the mean-free path, and might be as large as in the BCS superconductor. Hence, it is incorrect to apply the ratio of the coherence length to the inter-carrier distance as a criterion of the BCS-Bose liquid crossover. The correct criterion is given by Eq. (2).

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