Phononic pairing glue in cuprates and related high-temperature superconductors

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Along with some other researches we have realised that the true origin of high-temperature superconductivity should be found in the strong Coulomb repulsion combined with a significant electron-phonon interaction. Both interactions are strong (on the order of 1 eV) compared with the low Fermi energy of doped carriers which makes the conventional BCS-Eliashberg theory inapplicable in cuprates and related doped insulators. Based on our recent analytical and numerical results I argue that the high-temperature superconductivity from repulsion is impossible for any strength of the Coulomb interaction. Major steps of our alternative polaronic theory are outlined starting from the generic Hamiltonian with the unscreened (bare) Coulomb and electron-phonon interactions accounting for critical temperatures of high-temperature superconductors without any adjustable parameters.

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I. HIGH-TEMPERATURE SUPERCONDUCTIVITY FROM REPULSION: IMPOSSIBILITY

With a few exceptions [1] many researchers share the view that the electron-phonon interaction (EPI) is insufficient for high temperature superconductivity at least in the framework of the conventional Bardeen-Cooper-Schrieffer (BCS) theory or its intermediate-coupling Eliashberg extension [2]. Phenomenologically, the pairing mechanism of carriers could be not only phononic as in the BCS theory or its strong-coupling bipolaronic extension [3], but also excitonic, plasmonic, magnetic, kinetic, or due to some purely repulsive interactions combined with the unconventional pairing symmetry of the order parameter.

Quite naturally, a number of authors assumed that the electron-electron interaction in high-temperature superconductors was strong but repulsive providing high $T_c$ without phonons via superexchange and/or spin-fluctuations in unconventional (e.g. d-wave) pairing channel. A motivation for this concept can be found in the earlier work by Kohn and Luttinger (KL) [4], who showed that the Cooper pairing of fermions with any weak repulsion was possible since the two-particle interaction induced by the many-body effects is attractive for pairs with large orbital momenta, $l \gg 1$. While the KL work did not provide the specification of the actual angular momentum of condensed Cooper pairs, Fay and Layzer [5] found that a system of hard-sphere fermions condenses at low densities into p-orbital state ($l = 1$). The critical transition temperature $T_c$ of repulsive fermions was estimated well below 0.1 K with very little enhancement due to flatness of the Fermi surface [6]. In two dimensions (2D) the KL effect is absent for the parabolic band dispersion, but the d-wave low-$T_c$ pairing was found with the repulsive Hubbard $U$ (i.e. hard-sphere) potential when tight-binding corrections to the electron energy spectrum are taken into account [7].

More recent studies claimed that even a weak repulsive Hubbard $U$ combined with lattice induced band-structure effects results in higher values of $T_c$ in the spin singlet d-wave channel near half-filling "encouragingly similar to what is found in the cuprate high-temperature superconductors" [8, 9].

Different from these studies we have analysed the KL problem with the realistic Coulomb repulsion rather than with the hard-core Hubbard $U$ [10]. The second-order diagrams, responsible for the unconventional pairing in the KL theory Fig. 1, are prohibitively difficult to evaluate when the Fourier transform of the repulsive potential, $v(q)$, depends on $q$, so that most previous and recent studies [8, 9] confined to the hard-sphere Hubbard $U$ repulsion with $v(q)=\text{constant}$. In that case the first order does not contribute to the pairing vertex in any unconventional channel with $l \gg 1$, and the only (attractive) contribution comes from the second-order exchange diagram providing p-wave pairing in 3D for parabolic dispersion [2] and d-wave pairing in 2D for the tight-binding dispersion $\pi e^2/\hbar k_F$ [9].

Actually the screening length in the dense Coulomb gas, where the perturbation expansion in powers of $s = e^2/\pi \hbar v_F$ makes sense, is large compared with the characteristic electron wavelength $\sim 1/k_F$, so that it is unreasonable to treat the weak Coulomb repulsion as short-ranged as in Ref. [9] ($v_F$ and $k_F$ are the Fermi speed and the wave-vector, respectively). We have included all bubble diagrams in the screened Coulomb potential, $v(q) = 4\pi e^2/[q^2 + s(q)]$ with the static Lindhard func-
due to vHs proximity. Numerically solving the enhancement of the unconventional Tc level, the tight-binding energy dispersion, any realistic Fermi energy density of states, screening length κ the need for additional mechanisms such as spin fluctuations.

To analyse the unconventional pairing in a two-dimensional (2D) electron gas on the square lattice with two-particle vertex. (Reproduced from Ref. [10], ©American Physical Society, 2011.)

\[
s(q) = 4s k_F^2 \left[ \frac{1}{2} + \frac{k_F^2 - q^2/4}{2qk_F} \ln \frac{k_F + q/2}{k_F - q/2} \right],
\]

and carefully calculated all second-order diagrams in the 3D Cooper channel. Then solving the linearised BCS equation allowed us to find the symmetry (i.e. the angular momentum l) of the order parameter, shown in Fig. 1 as the function of the interaction strength s. Remarkably we did not observe p and d-wave pairing in the whole region of the Kohn-Luttinger perturbation expansion and beyond (up to s = 3). There is a pairing in higher momentum states, l ≥ 3, but the corresponding eigenvalues are numerically so small (λ3 ≈ 0.0011 at s = 3), that the corresponding Tc ≈ EF exp(−1/λ) is virtually zero for any realistic Fermi energy EF.

To analyse the unconventional pairing in a two-dimensional (2D) electron gas on the square lattice with the tight-binding energy dispersion,

\[
E_p = -2t[\cos(p_x a/h) + \cos(p_y a/h)] - \mu
\]

(\(a\) is the lattice constant) we used the model 2D Coulomb potential \(v(q) = 2\pi e^2/(q + \kappa)\) with a constant inverse screening length \(\kappa\). For the half-filled band the Fermi level, \(\mu\) is found at the van-Hove singularity (vHs) of the density of states, \(\mu = 0\), so that one might expect a strong enhancement of the unconventional \(T_c\) near half-filling due to vHs proximity. Numerically solving the linearised BCS equation by discretization of the Fermi surface we reproduced fairly well the results of Ref. [8] for the 2D Hubbard model, where the ground state is \(B_{1g}\) spin singlet with the d-wave symmetry \(x^2 − y^2\) close to the half-filling. However, using the screened Coulomb repulsion instead of the Hubbard one qualitatively changed the ground state, so that contrary to Ref. [7] neither p- nor d-wave pairing is possible at any filling while the repulsion is weak [10]. This surprising result is due to a nonvanishing first-order repulsive contribution to unconventional channels from the finite range interaction.

In cuprate and related superconductors the Coulomb repulsion is believed rather strong \(s ≫ 1\), so that the perturbative KL approach might have no direct relevance to these materials. Different numerical techniques have been applied to elucidate the ground state of the repulsive Hubbard model in the intermediate to strong-coupling regime, sometimes with conflicting conclusions. In particular, recent studies by Aimi and Imada [11] using a sign-problem-free Gaussian-basis Monte Carlo (GBMC) algorithm showed that the simplest Hubbard model with the nearest-neighbor hopping has no superconducting condensation energy at optimum doping. This striking result has been confirmed in the variational Monte Carlo (VMC) studies by Baeriswyl et al. [12], who found, however, some condensation energy away from optimum doping and also adding next-nearest neighbor hopping.

Using similar VMC simulations of the Hubbard model but including a realistic finite-range electron-phonon interaction, we found that even a relatively weak EPI with the BCS coupling constant \(\lambda ≈ 0.1\) induces the d-wave superconducting state in the model with the condensation energy several times larger than can be obtained with the Hubbard repulsion alone [13], Fig. 2. Moreover, the unconventional superconductivity has been shown to exist due to a finite-range EPI [12, 13] without the need for additional mechanisms such as spin fluctuations.

Based on these findings one concludes that the p- and d-wave Cooper pairing from the weak Coulomb repulsion is not possible between fermions in any dimension. Pairing in higher momentum states (\(l ≥ 3\)) has the corresponding \(T_c\) virtually zero for any realistic Fermi energy. The unconventional pairing from the strong Coulomb repulsion is highly unrealistic either since the corresponding condensation energy, if any, is many times lower than the condensation energy caused by the realistic electron-phonon interaction.

II. ALTERNATIVE THEORY

Based on the above analytical and numerical results and numerous experimental facts supporting strong electron-lattice coupling [13] we trust that EPI should be the key in solving the high-\(T_c\) problem. However, a quantitative analysis of the doping-dependent EPI has remained elusive in cuprates and related compounds. Recent observations of the quantum magnetic oscillations in
some underdoped \cite{16} and overdoped \cite{17} cuprate superconductors has opened up the possibility for a quantitative assessment of EPI in these and related doped ionic lattices \cite{18}. The oscillations revealed cylindrical Fermi surfaces, enhanced effective masses of carriers (ranging from $2m_e$ to $6m_e$) and the astonishingly low Fermi energy, which appears to be well below 40 meV in underdoped \cite{16} and less than or about 400 meV in heavily overdoped cuprates \cite{17}. Such low Fermi energies make the Migdal-Eliashberg adiabatic approach to EPI inapplicable in these compounds. Since carriers in cuprates are in the non-adiabatic (underdoped) or near-adiabatic (overdoped) regimes with their Fermi energy about the optical phonon energy, our multi polaron theory of superconductivity \cite{3} should be more appropriate here.

The theory of dense polaronic systems in the intermediate coupling regime has remained rather cumbersome, in particular, when EPI competes with strong electron correlations. Corresponding microscopic models with the on-site Hubbard repulsion and the short-range Holstein EPI have been studied using analytical and powerful numerical techniques \cite{15}. In most analytical and numerical studies both interactions have been introduced as input parameters not directly related to the material. Quantitative calculations of the interaction matrix elements can be performed from pseudopotentials using the density functional theory (DFT) \cite{19}. On the other hand, one can express the bare Coulomb repulsion and EPI through material parameters rather than computing them from first principles in many physically important cases \cite{20}. In particular, for a polar coupling to longitudinal optical phonons (the Fröhlich EPI), which is the major EPI in polar crystals, both the momentum dependence of the matrix element, $M(q)$, and its magnitude are well known, $|M(q)| = \gamma(q)\hbar\omega_0\sqrt{2N}$. Here $\gamma(q) = \sqrt{4\pi e^2/\kappa\hbar\omega_0q^2}$ is a dimensionless coupling, $\Omega$ is a unit cell volume, $N$ is the number of unit cells in a crystal, $\omega_0$ is the optical phonon frequency, and $\kappa = \epsilon_\infty\epsilon_0/(\epsilon_0 - \epsilon_\infty)$ ($\epsilon_\infty$ and $\epsilon_0$ are high-frequency and static dielectric constants in a parent polar insulator).

Recently I have noticed that, in highly polarizable ionic lattices as cuprates with $\epsilon_0 \gg 1$ the bare long-range Coulomb and Fröhlich interactions almost negate each other allowing for the analytical multi-polaron theory in the strong-coupling regime \cite{21}. The dielectric response function of strongly correlated electrons is *apriori* unknown. Hence one has to start here with a generic Hamiltonian including unscreened Coulomb and Fröhlich interactions operating on the same scale since any ad-hoc assumption on their range and relative magnitude might fail,

$$H = - \sum_{ij} (T_{ij} \delta_{ss'} + \mu \delta_{ij}) c_{i}^\dagger c_{j} + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{\epsilon_\infty |\mathbf{m} - \mathbf{n}|} \hat{n}_i \hat{n}_j + \sum_{\mathbf{q}, \omega_n} \hbar\omega_0 \hat{n}_i [u(\mathbf{m}, \mathbf{q})d_{\mathbf{q}} + H.c.] + H_{ph}.$$  

Here $T_{ij} \equiv T(\mathbf{m} - \mathbf{n})$ is the bare hopping integral, $\mu$ is the chemical potential, $i = \mathbf{m}, s$ and $j = \mathbf{n}, s'$ include both site $(\mathbf{m}, \mathbf{n})$ and spin $(s, s')$ states, $u(\mathbf{m}, \mathbf{q}) = (2N)^{-1/2}\gamma(q) \exp(\mathbf{q} \cdot \mathbf{m})$, $c_{i}^\dagger$, $d_{\mathbf{q}}$ are electron and phonon operators, respectively, $\hat{n}_i = c_{i}^\dagger c_{i}$ is a site occupation operator, and $H_{ph} = \sum_{\mathbf{q}} \hbar\omega_0 (d_{\mathbf{q}}^\dagger d_{\mathbf{q}} + 1/2)$ is the polar vibration energy.

This Hamiltonian can be reduced to the polaronic "t-J$_p$" Hamiltonian using two successive canonical transformations \cite{21},

$$\mathcal{H} = - \sum_{ij} (t_{ij} \delta_{ss'} + \tilde{\mu} \delta_{ij}) c_{i}^\dagger c_{j} + 2 \sum_{\mathbf{m} \neq \mathbf{n}} J_p(\mathbf{m} - \mathbf{n}) \left( \frac{\hat{S}_m \cdot \hat{S}_n}{2} + \frac{1}{4} \hat{n}_m \hat{n}_n \right),$$

where $\hat{S}_m = (1/2) \sum_{s,s'} e_{ms}^\dagger \hat{s}_{ss'} e_{ms'}$ is the spin 1/2 operator ($\hat{\sigma}$ are the Pauli matrices), $\hat{n}_m = \sum_s \hat{n}_i$, and $\tilde{\mu}$ is the renormalized chemical potential.

There is a striking difference between this polaronic t-J$_p$ Hamiltonian Eq.\cite{4} and the familiar t-J model derived from the repulsive Hubbard U Hamiltonian in the limit $U \gg t$ omitting the so-called three-site hoppings and EPI \cite{22}. The latter model acts in a projected Hilbert space constrained to no double occupancy. Within this standard t-J model the bare transfer amplitude of electrons $(t)$ sets the energy scale for incoherent transport, while the Heisenberg interaction $(J \propto t^2/U)$ allows for spin flips leading to coherent hole motion with an effective bandwidth determined by $J \ll t$. On the contrary in our polaronic t-J$_p$ Hamiltonian, Eq.\cite{4} there is no constraint on the double on-site occupancy since the Coulomb repulsion is negated by the Fröhlich EPI. The polaronic
hopping integral $t$ leads to the coherent (bi)polaron band and the antiferromagnetic exchange of purely phononic origin $J_p \gg t$ bounds polarons into small superlight intersite bipolarons. Last but not least the difference is in the "+" sign in the last term of Eq.(3) proportional to $\hat{n}_m\hat{\sigma}_m$, which protects the ground superconducting state from the bipolaron clustering, in contrast with the "-" sign in the similar term of the standard t-J model, where the phase separation is expected at sufficiently large $J$.

The reduction of Eq.(3) to Eq.(4) is based on the so-called "inverse coupling constant (1/$\lambda$)" perturbation technique developed by us for the multi-polaron systems [3], where the residual polaron-phonon interaction creates multi-phonon vertexes in the diagrammatic technique. Different from any model proposed so far, all quantities in the polaronic $t$-$J_p$ Hamiltonian (4) are defined through the material parameters, in particular $t_{ij} = T(m - n)\exp[-g^2(m - n)]$ with

$$g^2(m) = \frac{2\pi e^2}{\kappa \hbar \omega_0 N \Omega} \sum_q \frac{1 - \cos(q \cdot m)}{q^2},$$

(5)

and

$$J_p(m) = \frac{T^2(m)}{2g^2(m)\hbar \omega_0},$$

(6)

Here the high-frequency, $\epsilon_\infty$ and the static, $\epsilon_0$ dielectric constants as well as the optical phonon frequency, $\omega_0$ and the bare hopping integrals in a rigid lattice, $T(m)$ are measured and/or found using the first-principle Density Functional Theory [19] in a parent polar insulator.

Solving the polaronic $t$-$J_p$ model with the appropriate material parameters, $\kappa, \omega_0$ and $T(m)$ exhibits a phase transition to a superconducting state with the critical temperature in excess of 100K at optimum doping [21]. The model provides an understanding of the spin and charge pseudogaps [22] and the unified parameter-free explanation of the observed oxygen-isotope effects on the critical temperature, the magnetic-field penetration depth, and on the normal-state pseudogap in underdoped cuprate superconductors [24].

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