Unconventional high-temperature superconductivity from repulsive interactions: theoretical constraints

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Unconventional symmetries of the order parameter allowed some researchers to maintain that a purely repulsive interaction between electrons provides superconductivity without phonons in a number of high-temperature superconductors. It is shown that the Cooper pairing in p and d states is not possible with the realistic Coulomb repulsion between fermions at relevant temperatures in any dimension.

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In the theoretical analysis, the pairing mechanism of carriers could be not only phononic as in the BCS theory or its strong-coupling bipolaronic extension [1], but also excitonic, plasmonic, magnetic, kinetic, or due to some purely repulsive interaction combined with the unconventional pairing symmetry of the order parameter. Actually, following the original proposal by P. W. Anderson, many authors [2] 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 the d-wave pairing channel \( (l=2) \). A motivation for this concept can be found in the earlier work by Kohn and Luttinger (KL) [3], who showed that the Cooper pairing of fermions with any weak repulsion was possible since the two-particle interaction induced by 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 [4] found that a system of the actual angular momentum of condensed Cooper pairs, Fay and Layzer [4] found that a system of

$$\lambda \Delta(p) = \frac{\Omega}{(2\pi \hbar)^d} \int \frac{dS_{p'}}{v_F(S)} K(p,p') \Delta(p')$$

with the most negative eigenvalue \( \lambda \). Here the integral is taken over the Fermi surface (or contour in 2D), \( \Omega \) is the normalisation volume in 3D \( (d=3) \) or area in 2D \( (d=2) \), \( v_F \) is the Fermi speed, and \( K(p,p') \) is the two-particle vertex. The sum of the first and second order diagrams, Fig. (1), for the two-particle vertex is evaluated from [2, 3]:

$$K(p,p') = v(p-p') + v(p-p') \sum_k [2v(p-p')$$

$$- v(k+p') - v(k-p)Q(p-p',k)$$

$$- \sum_k v(p-k)v(k+p')Q(p+p',k)$$

with \( Q(q,k) = (f_k - f_{k-q})/(E_k - E_{k-q}) \). \( f_k \) is the Fermi-Dirac distribution function, and \( E_k \) is the Bloch-band dispersion.

The second-order terms in Eq. (2) are prohibitively difficult to evaluate when the Fourier transform of the re-
pulsive 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 this case the first order does not contribute to \( \Lambda \) in any unconventional channel with \( I \geq 1 \), and the only (attractive) contribution comes from the last sum in Eq. (2) providing p-wave pairing in 3D for parabolic dispersion \(^4\) and d-wave pairing in 2D for the tight-binding dispersion \(^6\) \(^8\) \(^9\).

Different from those studies we consider here a more realistic Coulomb repulsion with \( v(q) = 4\pi e^2/\Omega(q^2 + \kappa^2) \) in 3D and \( v(q) = 2\pi e^2/\Omega(q + \kappa) \) in 2D, where \( \kappa \) is the inverse screening length. To elucidate the role of a finite potential radius we first take \( \kappa \) as an independent large parameter \( \kappa \gg k_F \), where \( \hbar k_F \) is the Fermi momentum. Such a short screening length could be due to another component of heavy carriers. In this limit, which mimics the Hubbard U model, one can neglect the \( q \) dependence of the potential in the second-order diagrams, while taking it into account in the first-order contribution. Then the first sum in Eq. (2) cancels. In the case of the 3D parabolic dispersion \( E_k = k^2/2m \) one can expand the order parameter in a series of the Legendre polynomials, \( P_l(\cos \Theta) \) on the spherical Fermi surface \(^3\) to obtain from Eq. (1) the l-channel eigenvalue as

\[
\lambda_l = \int_0^\pi d\Theta \sin(\Theta) P_l(\cos \Theta) \Gamma(\cos \Theta), \quad (3)
\]

with

\[
\Gamma(\cos \Theta) = \frac{s}{2(1 - \cos \Theta)} + \frac{(\kappa/k_F)^2}{s^2k_F^4} \frac{1 - \cos \Theta}{\kappa^4} \frac{\ln \sqrt{2 + \sqrt{1 + \cos \Theta}}}{\sqrt{2 - \sqrt{1 + \cos \Theta}}}, \quad (4)
\]

where we define the small expansion parameter as \( s = e^2/(\pi \hbar v_F) \approx r_s/6 \) \( (r_s \) is the dimensionless Wigner-Seitz radius, and \( v_F = \hbar k_F/m \) is the Fermi speed). Integrating in Eq. (3) over the scattering angle yields \( \lambda_1/s = (k_F/\kappa)^4[4/3 - 2s(2 \ln 2 - 1)/5] \) and \( \lambda_2/s = (k_F/\kappa)^4[16(k_F/\kappa)^2/15 - 4s(8 - 11 \ln 2)/105] \) for p and d-channels, respectively, at strong screening, \( \kappa/k_F \gg 1 \). For the p-wave symmetry a negative \( \lambda \) appears only if \( s > 10/[3(2 \ln 2 - 1)] \approx 9 \) no matter how small the screening length is. This surprising result is due to a nonvanishing repulsive contribution to the p-wave channel of the lowest-order \( q \)-correction to the Hubbard repulsion \( (\propto q^2/\kappa^2) \), which is proportional to the same power in the screening length \( (\kappa^{-4}) \) as the attraction. Different from the p-channel this lowest-order \( q \)-correction does not contribute to the repulsion in the d-channel, so that \( \lambda_2 \) becomes negative at some critical screening, \( (\kappa/k_F)^2 > 420/[15s(8 - 11 \ln 2)] \approx 75/s \). However, it is unrealistic to find the screening length one order of magnitude smaller than the lattice constant in real solids, so that neither p- nor d-wave pairing can be realised in the 3D Coulomb gas in the weak- and intermediate-coupling regimes, where \( s \lesssim 1 \), if the screening length, \( \kappa^{-1} \), is chosen to be small.

Actually the screening length in the single-component dense Coulomb gas, where the perturbation expansion in powers of \( s \) makes sense, is large, \( (\kappa/k_F)^2 = 4s \lesssim 1 \), so that it is unreasonable to treat the Coulomb repulsion as weak and at the same time as short-ranged, contrary to the suggestion of Ref.\(^3\). Following Refs.\(^6\) \(^8\) \(^9\) we now include all bubble diagrams in the screened potential replacing the screening momentum \( \kappa \) by the static Lindhard function,

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

It is sufficient to use the Fourier component of the potential with the long-wave screening, \( s(0) = 4s \) and the backward scattering \( p' = -p \) with \( p = q_-/2 \) where \( q_- = p - p' \) in diagrams of Fig. (1c,d), and the forward scattering with \( q_+ = p + p' \approx 2p \) in the diagram Fig. (1a) \(^9\). Then the all diagrams are readily simplified with the following result for \( \Gamma(\cos \Theta) \equiv \Gamma_a + \Gamma_b + \Gamma_c + \Gamma_d + \Gamma_e \) in the eigenvalue equation \(^3\)

\[
\Gamma_a + \Gamma_b = \frac{s}{q_-^2 + s(q_-)}.
\]

\[
\Gamma_c + \Gamma_d = \frac{4s^2}{q_-^2 + s(q_-)} \int_0^1 dk \frac{k^2 - q_-^2 + 4q_+}{k^2 + q_-^2 + 4q_+ + 4q_-} \left[ \frac{q_-/2 + k}{q_-/2 - k} \ln \frac{k^2 - q_-^2/4 + 4q_+}{k^2 + q_-^2/4 + 4q_+ + 4q_-} \right].
\]

\[
\Gamma_e = \frac{s}{4q_+} \left[ \frac{1 - q_+^2/4}{1 - q_+^2/4 + 4q_+} \ln \frac{1 + q_+/2}{1 - q_+/2} \right.
\]

\[
\left. - \frac{1 - q_+^2/4}{1 - q_+^2/4 + 4q_+} \ln \frac{1 + q_+/2}{(1 - q_+^2/4 + 4q_+)} \right].
\]

Finally, we want to comment on the choice of \( F \) in the 3D Coulomb gas. Inset shows the first order (a) and the second-order (b,c,d,e) contributions to the two-particle vertex.

![Fig. 1: Angular momentum of the order parameter as the function of the dimensionless repulsion \( s = e^2/\pi \hbar v_F \) in the 3D Coulomb gas. Inset shows the first order (a) and the second-order (b,c,d,e) contributions to the two-particle vertex.](image-url)
where $q_x^2 = 2(1 \pm \cos \Theta)$.

Eqs. (10) allows us to find the symmetry (i.e. the angular momentum $l$) of the order parameter with the most negative value of $\lambda$, shown in Fig. (1) as the function of the interaction strength. As in the case of independent screening we do not observe the p and d-wave pairing in the whole region of the Kohn-Luttinger perturbation expansion and beyond (up to $s = 3$) in agreement with Refs. [14, 15]. There is a pairing in higher momentum states, $l \geq 3$, but the corresponding eigenvalues are numerically so small ($\lambda_3 \approx 0.0011$ for $s = 3$), that the corresponding $T_c \approx (E_F/k_B) \exp(-1/\lambda)$ is virtually zero for any realistic Fermi energy $E_F$.

Finally, let us analyse the unconventional pairing in a two-dimensional electron gas on the square lattice with a tight-binding energy dispersion,

$$E_p = -2t(\cos(p_x a/\hbar) + \cos(p_y a/\hbar)) - \mu$$ \hspace{1cm} (7)

($a$ is the lattice constant). 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 [8]. The repulsion between electrons is modeled by a strongly screened Coulomb potential with the Fourier component $2\pi e^2/\Omega(q + \kappa) \approx 2\pi e^2(1 - q/\kappa)/\Omega \kappa$, where the inverse screening length is taken as an independent large parameter, $\kappa a \gg 1$.

Similar to the 3D case, the short screening length allows one to neglect $q$ dependence of the potential in the second-order diagrams slightly overestimating their contribution, while taking $q$ into account in the first-order contribution. Then the diagrams b,c,d in Fig. (1) cancel each other. The remaining second-order contribution (e), proportional to the static susceptibility of the noninteracting electrons, can be reduced to a one-fold integration, so that the two-particle vertex contribution to the unconventional pairing is expressed as $K(p, p') = (2\pi e^2/\Omega \kappa^2) \Gamma(\alpha p/\hbar, \alpha p'/\hbar)$ with

$$\Gamma(k, k') = -|k - k'| - \frac{U}{4\pi} \int_{k_m}^{k_m} dx \ln \frac{(a_1 - b)(a_2 + b)}{(a_1 + b)(a_2 - b)},$$ \hspace{1cm} (8)

$a_{1, 2} = \sin(x + q_y/2) \sin(q_y/2) \tan(\pi z/2 + q_x/4) + \sin(q_x/2), b = [\sin(q_x/2)^2 - \sin(x + q_y/2)^2 \sin(q_y/2)]^{1/2}, z = \cos^{-1}(\cos(x) - \mu), \mu = \mu/2t, q = k + k'$, and $k_m = \cos^{-1}(1 - \mu)$. Here one assumes that $|\sin(q_x/2)| > |\sin(q_y/2)|$ and if otherwise, one should replace $q_x \equiv q_y$. No matter what the screening length is, the relative contribution of the second-order diagram (e) depends on a single dimensionless interaction parameter $U \equiv e^2/\alpha t \approx r_s$, which is supposed to be small in the framework of the KL approach.

Using Eq. (8) we can solve the eigenvalue problem, Eq. (1), numerically as in Ref. [8] by discretization of the Fermi surface and diagonalization of the kernel in the following integral equation,

$$\lambda \Delta(k) = \frac{U}{4\pi(\kappa a)^2} \int_{-k_m}^{k_m} dq \frac{\Gamma(k, k') \Delta(k') + \Gamma(k, -k') \Delta(-k')}{\sin(k_y') \sin(k_y) |\sin(k_y')/\sin(k_y)|^{1/2}}.$$ \hspace{1cm} (9)

Here vectors $k$ and $k'$ are taken on the Fermi surface, so that $k_{y'}$ in the integral is defined via $k_y'$ using $\cos(\pi k_{y'}) + \cos(\pi k_{y'}) = -\mu$.

With 800 discretization points we reproduce fairly well the results of Ref. [8] for the 2D Hubbard model, if we...
drop the first term in $\Gamma(k,k')$, Eq.\(^3\) arising from the expansion of the bare Coulomb potential in powers of $1/\kappa$, Fig.\(\mathbf{2}\). As shown in the inset of Fig.\(\mathbf{2}\) the ground state is $B_{1g}$ spin singlet with the d-wave symmetry $x^2-y^2$ close to the half-filling for any weak Hubbard repulsion.

In fact, there is no reason to neglect the first-order $q$-correction in the two-particle vertex Eq.\(\mathbf{6}\), since this correction is larger than the spin-fluctuation contribution at any screening, if the repulsion is weak. Using the correct vertex Eq.\(\mathbf{6}\) qualitatively changes the ground state, Fig.\(\mathbf{3}\). Contrary to Ref.\(\mathbf{4}\),\(\mathbf{5}\),\(\mathbf{6}\),\(\mathbf{7}\) neither p- nor d-wave pairing are possible in the ground state at any filling until the effective interaction becomes so strong that the perturbation theory does not apply, $U \gtrsim 1$, Fig.\(\mathbf{3}\), similar to the 3D case discussed above. As in the continuum 3D Coulomb gas, Fig.\(\mathbf{1}\), there is a pairing in higher momentum states (e.g. $A_{2g}$ with the symmetry $(x^2-y^2)xy$), but as shown in Fig.\(\mathbf{4}\) the corresponding eigenvalues are numerically very small, and the corresponding $T_c$ is about zero.

In cuprate superconductors and many other metallic compounds the Coulomb interaction is rather strong $r_s \gg 1$, 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, $U > 1$ sometimes with conflicting conclusions. In particular, recent studies by Aimi and Imada\(\mathbf{11}\) 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 was confirmed in the variational Monte Carlo (vMC) studies by Baeriswyl \etal\(\mathbf{12}\);\(\mathbf{13}\), who found, however, some condensation energy away from the optimum doping and also adding next-nearest neighbor hoppings. Importantly, a similar vMC method\(\mathbf{12}\) found that even a relatively weak finite-range electron-phonon interaction with the BCS coupling constant $\lambda \approx 0.1$ induces a d-wave superconducting state in strongly correlated metals with the condensation energy several times larger than can be obtained with the Hubbard repulsion alone. Moreover, the unconventional superconductivity has been shown to exist due to a finite-range electron-phonon interaction\(\mathbf{12}\),\(\mathbf{13}\) without the need for additional mechanisms such as spin fluctuations.

In conclusion, we have shown that the p- and d-wave Cooper pairing from the weak Coulomb repulsion is not possible between fermions at any screening length and in any dimension. Pairing in higher momentum states ($l \geq 3$) has virtually zero $T_c$ for any realistic Fermi energy. The unconventional pairing from the strong Coulomb repulsion is not possible either since the corresponding condensation energy, if any, is several times lower than the condensation energy caused by the electron-phonon interaction.

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