Pair formation temperature in jelliumlike two-dimensional electron gases

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A standard many-body method, based on the spherical-harmonics representation of the Bethe-Salpeter ladder solution for the two-particle scattering amplitude in two-dimensional jellium electron gases, is applied to determine a pair formation temperature T_p from the pole of the pairing vertex. In this method, pairing may occur due to attractive spherical harmonics in the input interparticle interaction. The comparative study was performed with parametrized models for this interaction obtained by considering the real-space aspects of screening holes around moving electrons. The theoretical, maximal pair formation temperatures are in the ~100 K range and appear at small values of the density of the jellium system.

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There are clear experimental indications[1] that cuprate superconductors can exhibit significant pairing correlation for a range of temperatures that extends above the highest measured superconducting T_c. The anomalous normal state of these materials is exemplified by their pseudogap in the excitation spectra, the proper characterization of which is a strong motivation behind various more recent experimental works[2–5] also. The problem of pair formation is an important issue to a successful theory in our understanding of high-temperature superconductivity in cuprates. A very recent observation[6] on the onset of a pseudogap in a nearly optimally doped pnictide superconductor ($T_c \simeq 50$ K) gives an additional strong motivation to the present attempt on pairing since the experimental onset temperature (about 180 K) is in the range of 100–250 K, estimated experimentally[1–5] for high-temperature cuprate superconductors. These data suggest us a search for clarification of *common* origin.

On the theoretical side of the pairing problem in jelliumlike systems, we should mention the earlier systematic studies[7,8] of the group of Jankó. Their method is based on the so-called pair-correlation approximation[9] of Kadanoff and Martin for superconductivity, with a *built-in* attractive interaction (to a conventional *s*-type channel) in momentum space. In brief, the key element of this approximation is the many-body scattering t matrix. This is expressed self-consistently in their framework in terms of the built-in attractive interaction in *momentum space* and the pair susceptibility. Then, a resonant (above T_c) pair scattering is characterized[7] by the condition that the real part of the inverse t matrix is zero.

Following the lead of a more recent work[10] by Galitski, where a built-in l wave ($l>1$) pairing was applied to analyze experimental[3] predictions, we shall use the T_p notation for this thermodynamical quantity in the present work on pair (p) formation in a two-dimensional (2D) fermionic system. Galitski discussed, within the framework of a disordered BCS theory, the fluctuational aspects of the local[3] pairing temperature above T_c and deduced a dome-shaped form for T_p as a function of doping.

In the present study on the onset temperature (T_p) for pairing in 2D electron gases we *combine* a well-known conventional many-body approximation[11–13] for the pairing vertex ($\bar{\Gamma}$) in momentum space and the modeling of the input effective interparticle interaction using real-space constraints. Such a transparent combination is motivated, apart from its intrinsic theoretical interest, by the experimentally established local pairing picture[3] and intricate duality[14] between real and momentum spaces. The obtained estimations for the onset temperature for pairing are in the above-mentioned experimental range. Thus, the underlying treatment could provide an important contribution to our general understanding of a phenomenon which appears in the normal state of *different* unconventional superconducting materials.

According to the many-body theory[11–13] in momentum space, in the temperature-dependent formalism of the two-particle Green's function for a normal Fermi system, the Cooper (opposite momenta) channel is characterized by zero total momentum at the Fermi surface. This implies a vanishing excitation energy (ω) for quasiparticle-quasiparticle scattering. In this formalism the signal for pair formation appears (at T_p) as a pole of the total pairing vertex function. In order to solve the Cooper problem one has to expand the irreducible interaction (Γ) in the eigenfunctions of the angular momentum[11] at the Fermi surface with zero total momentum.

Under *this* procedure, the integral equation for the pairing ($\bar{\Gamma}$) vertex decouples[11–13] to a set of algebraic equations for its partial (l) component $\bar{\Gamma}_l$. In each equation, a partial component of $\bar{\Gamma}_l$ is coupled to a component of Γ_l as given (Hartree atomic units are used) below:

$$\bar{\Gamma}_l = \frac{\Gamma_l}{(1+\nu\Gamma_l)}. \tag{1}$$

In this equation $\nu=(1/2\pi)\ln(E_F/k_BT)$ at vanishing excitation energy at the Fermi surface[13] of the 2D system. The decoupling in the Cooper channel has a profound consequence, as was emphasized[11] by Lifshitz and Pitaevski. The liquid state

is unstable against pairing if there is an attraction even for a single Γ_l, at which the denominator of the above equation becomes *zero*. If several $\Gamma_l<0$, the pair formation occurs[11] at that temperature (denoted here by T_p) which corresponds to the largest $|\Gamma_l|$ value, i.e., the strongest attraction.

Introducing the $\Gamma_l=(1/2k_F)\gamma_l$ notation, this T_p is determined (for a $\gamma_l<0$) from

$$k_B T_p = \frac{1}{r_s^2}\exp\left(-\frac{4\sqrt{2}\pi}{r_s|\gamma_l|}\right), \tag{2}$$

since $E_F=1/r_s^2$ and $k_F=\sqrt{2}/r_s$ in 2D. With a *fixed* $|\gamma_l|$ there is (for $\gamma_l<0$) an optimal (o) density parameter $[r_s^{(o)}=2\sqrt{2}\pi/|\gamma_l|]$ *at which* the pair formation temperature T_p has its maximum (m) value (in a.u.) of

$$k_B T_p^{(m)} = \frac{(|\gamma_l|)^2}{8\pi^2}\exp(-2). \tag{3}$$

Thus, we get $T_p^{(m)}=540(|\gamma_l|)^2$ in thermodynamical units, K. The l-dependent partial component is

$$\gamma_l = \left(\frac{k_F}{\pi}\right)\int_0^\pi d\phi\,\cos(l\phi)V_{\rm eff}[q=2k_F\sin(\phi/2)], \tag{4}$$

where $V_{\rm eff}(q)$ is an effective (input) interaction in 2D which *models* the quasiparticle-quasiparticle irreducible vertex (Γ) in the Cooper channel. Notice that according to Mermin's theorem, for the $(\omega/q)\to 0$ limit this vertex is zero[11,15] on the Fermi surface at $q\to 0$.

The practical attempt in the present work rests, partly, on our previous[16,17] experience of modeling interparticle interactions in 2D jellium systems. In brief, we modeled the normalized holes surrounding moving electrons using *real-space* arguments such as the physically limited magnitude of charge depletion at a repulsive-particle position. Here, the following three models for an instantaneous hole are investigated. The Gaussian (G) distribution

$$\Delta n_G(r) = (\beta^2/2\pi)\exp(-\beta^2 r^2/2), \tag{5}$$

with $\Delta n_G(q)=\exp(-q^2/2\beta^2)$ Fourier transform. The more extended hydrogenic (H) distribution

$$\Delta n_H(r) = (\beta^2/2\pi)\exp(-\beta r), \tag{6}$$

for which we get $\Delta n_H(q)=\beta^3/(\beta^2+q^2)^{3/2}$. Finally, a very extended powerlike (P) distribution is introduced,

$$\Delta n_P(r) = \frac{(\beta^2/2\pi)}{[1+(\beta r)^2]^{3/2}}, \tag{7}$$

which also has a finite value at $r=0$. In this case one has $\Delta n_P(q)=\exp(-q/\beta)$. In our comparative study we fix $\beta=k_F=\sqrt{2}/r_s$; i.e., we apply the complete depletion at $r=0$. This is supported by recent Monte Carlo data[18] on the pair-correlation function at contact.

Next, by using a symmetry argument[17,19] for real-space screening of *two* (equivalent) charges in their many-body environment, and the rules of convolution, we write for the quasiparticle-quasiparticle effective interaction in wave vector (q) space

$$V_{\rm eff}^{(i)}(q) = [1-\Delta n_i(q)]V(q)[1-\Delta n_i(q)], \tag{8}$$

where $V(q)=2\pi/q$ in 2D for Coulomb potential. For *all* interaction $V_{\rm eff}^{(i)}(q=0)=0$, i.e., the properly weighted sum of scattering phase shifts[17,20] is zero. Thus, our effective interactions are well constrained considering the important[11,15] limit value of a renormalized scattering vertex at $q\to 0$ on the Fermi surface.

For the details on the real-space $V_{\rm eff}(R)$ forms we refer the interested reader to earlier[16,17] works, in the Gaussian and hydrogenic cases; R is the interparticle relative distance. In the powerlike case one gets via standard inverse Fourier-Hankel transformation

$$V_{\rm eff}^{(P)}(R) = \frac{1}{R} - \frac{2\beta}{\sqrt{1+(\beta R)^2}} + \frac{\beta}{\sqrt{4+(\beta R)^2}}. \tag{9}$$

This becomes attractive only at high R values.

A convenient representation of the key quantity (γ_l) to the above Eq. (2) is as follows:

$$\gamma_l^{(i)} = \int_0^\pi d\phi\frac{\cos(l\phi)}{\sin(\phi/2)}\left[1-\Delta n_i\left(q=2k_F\sin\frac{\phi}{2}\right)\right]^2. \tag{10}$$

This expression is used in our practical estimations based on three models with (common) complete depletion. Due to this physical constraint on normalized holes, the calculated $\gamma_l^{(i)}$ become *pure numbers*.

For completeness, we would like to emphasize at this point of evaluation that with a simple Thomas-Fermi (TF)-type model $[\Delta n_{\rm TF}(q)=2/(2+q)]$ we get

$$\gamma_l^{\rm (TF)} = 2k_F^2\frac{\cos(l\pi)}{1-(2l)^2} + O(k_F^3), \tag{11}$$

via Eqs. (4) and (8) in the *low* density limit. This becomes negative only for even l, with a maximum in $|\gamma_l^{\rm (TF)}|$ for $l=2$. This particular conclusion fits to the statement of Galitski and Das Sarma, who discussed[21] a *retarded* interaction to pairing in the d channel. We refer, at this point of discussing an effective interaction, to the particularly clear work[22] of Anderson on the *possible ways* of eliminating the elementary repulsive force between electrons. The high l *scaling*, i.e., $\log(T_p)\sim[-(2l)^2]$ obtained from Eq. (2), is in harmony with the 2D result[12] of Chubukov. The difference in comparison with the pioneering[23] three-dimensional (3D) case treated by Kohn and Luttinger is notable since in 3D one gets a $\log(T_p)\sim[-(2l)^4]$ dependence for high l.

It is clear from Eq. (2) with Eq. (11) that a TF modeling results in an exponentially decreasing (T_p/E_F) as a function of r_s at low densities. This r_s dependence of the exponent is *opposite* to the one obtained in our study where the relevant γ_l is a number. In our modeling of an *interparticle* interaction between system particles, the effective range is determined by the extension $[\propto(1/k_F)\sim r_s]$ of a normalized comoving hole. We stress that such a scaling in screening is the *only* one, according to detailed scattering[24,25] calculations, which can yield a perfect agreement with an exact limiting behavior in r_s of the pair-correlation function at contact.

We performed the numerical calculations, using Eq. (10), with the inputs based on Eqs. (5)–(7) and the prefixed β

$=k_F=\sqrt{2}/r_s$. For the Gaussian model[17] we obtained $\gamma_1^{(G)}=-0.6053$, $r_s^{(o)}\cong 14$, and $T_p^{(m)}\cong 200$ K. With the hydrogenic model for the normalized hole, we deduced $\gamma_1^{(H)}=-0.4225$, $r_s^{(o)}\cong 20$, and $T_p^{(m)}\cong 100$ K. The very extended, and therefore less physical, powerlike model results in $\gamma_2^{(P)}=-0.2317$, $r_s^{(o)}\cong 36$, and $T_p^{(m)}\cong 30$ K. The above values for $T_p^{(m)}$ with well-localized (Gaussian and hydrogenic) holes, which is the physically expected[16,17] character due to strong dynamical correlation, are in the experimental range. The powerlike model, due to its extension in real space, results in values which are out of this range.

In conclusion, motivated by experimental indications on the values of pair formation temperatures in the normal state of *different* unconventional superconductor materials, a model calculation is performed within the framework of the Bethe-Salpeter ladder method in order to point out a possible common origin to a proper phenomenology. We implemented the many-body approximation by physically constrained inputs.

The applied constraints are based on simple but *fundamental* aspects of modeling in real and momentum spaces simultaneously. The theoretical pair formation temperatures are in the experimentally established range. Our results show that it is the *extension* of comoving holes around electrons in their many-body environment which influences the quantitative prediction for pairing.

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