Pairing effects in the normal phase of a two-dimensional Fermi gas

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In a recent experiment,1,2 a pairing gap was detected in a two-dimensional (2D) Fermi gas with attractive interaction at temperatures where superfluidity does not occur. The question remains open whether this gap is a pseudogap phenomenon or is due to a molecular state. In this paper, we demonstrate that pseudogap phenomena occurring in 2D and 3D can be related through a variable spanning the BCS-BEC crossover in a universal way.

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Introduction. It is commonly believed that the normal phase of high-temperature (cuprate) superconductors is more intriguing than the superfluid phase below the critical temperature $T_c$, owing especially to the appearance of a pseudogap from the observation of a suppression of low-energy weight in the single-particle spectral function above $T_c$.2,4,5 Two alternative mechanisms have been proposed in this respect, namely, the presence of a competing order which affects directly the single-particle properties, and the occurrence of precursor pairing in the normal phase through strong pairing fluctuations which are amplified by the (quasi) 2D nature of these systems and affect the single-particle properties only indirectly through two-particle effects.2,3,4

Since it is hard to isolate these two mechanisms in a solid-state material, experiments have recently been performed with ultra-cold Fermi gases using momentum-resolved radio-frequency spectroscopy (in analogy to angle-resolved photoemission spectroscopy in solid state), originally in 3D10,11 and more recently in 2D1,2. This is because in ultra-cold gases one can tune the inter-particle attractive interaction in a controlled way, from weak coupling with largely overlapping Cooper pairs to strong coupling where composite bosons form, amplifying in this way the occurrence of pairing fluctuations and leaving aside other forms of long-range order not connected with pairing.

Above $T_c$ pairing correlations between opposite-spin fermions still extend over a finite distance. While 3D and 2D are not qualitatively different in this respect, the temperature window above $T_c$ in which precursor pairing occurs is expected to be wider in 2D than in 3D, making 2D systems best suited for the study of pseudogap phenomena in the normal phase. The problem is, however, that in 2D a two-body bound state occurs for any value of the inter-particle coupling, so that one may not a priori be confident that the measured pairing gap is truly a pseudogap due to collective (many-body) effects like the pairing gap below $T_c$, or is rather a molecular binding energy. We shall address this crucial issue by performing a theoretical study of the dispersion relation associated with the single-particle spectral function for various couplings and temperatures, determining in this way the fate of the underlying Fermi surface whose presence guarantees that the pairing gap is a truly many-body effect.

This study carries along another important issue, about the use of a more fundamental variable than the coupling to follow the evolution from the weak (BCS) to the strong (BEC) coupling limits. This issue was raised in Ref.12 to connect the physics of the BCS-BEC crossover with high-temperature superconductors. Also for ultra-cold gases, however, it would be preferable to deal with 3D and 2D systems on a comparable footing through the use of a unifying variable. It will turn out that in terms of this variable (identified as the ratio of the pair coherence length to the average inter-particle distance) the collapse of the Fermi surface occurs simultaneously in 3D and 2D, thus establishing a coherent framework for precursor-pairing phenomena in different dimensions.

The t-matrix approach in 2D. Our calculations rests on a non-self-consistent t-matrix approach, which was extensively used in 3D and is extended here to 2D. For an inter-particle interaction of the contact type, the pair propagator is given by

$$\Gamma_0(q, \Omega_{\nu}) = -\frac{1}{\frac{2\pi}{k_F^2} \eta + R_{pp}(q, \Omega_{\nu})} \tag{1}$$

where $q$ is a wave vector, $\Omega_{\nu} = 2\pi k_B T \nu$ ($\nu$ integer) a bosonic Matsubara frequency, and $\eta = -\ln(k_F a_{2D})$ the coupling parameter defined in terms of the Fermi wave vector $k_F$ and the 2D scattering length $a_{2D}$ (in turn identified from the two-body binding energy $\varepsilon_0 = (m a_{2D}^2)^{-1}$). In the above expression, $R_{pp}$ is the regularized particle-particle bubble

$$R_{pp}(q, \Omega_{\nu}) = \int \frac{dk}{(2\pi)^2} \left\{ [1 - f_F(\xi(k)) - f_F(\xi(k+q))] \frac{-m}{k^2} \Theta(|k| - k_F) \right\} \tag{2}$$
where $\xi(k) = \frac{k^2}{2m} - \mu$ ($\mu$ being the chemical potential and $h = 1$) and $f_F(e) = (\exp(e/k_BT) + 1)^{-1}$ is the Fermi function ($k_BT$ being the Boltzmann constant).

Within the non-self-consistent t-matrix approach, the pair propagator enters the fermionic single-particle self-energy, in the form

$$\Sigma(k, \omega_n) = -\int \frac{dq}{(2\pi)^2} k_BT \sum_\nu \Gamma_0(q, \Omega_\nu) G_0(q-k, \Omega_\nu-\omega_n)$$

(3)

where $G_0(k, \omega_n) = [i\omega_n - \xi(k)]^{-1}$ is the bare single-particle Green’s function and $\omega_n = (2n+1)\pi k_BT$ ($n$ integer) a fermionic Matsubara frequency. The dressed Green’s function $G(k, \omega_n) = [G_0(k, \omega_n)^{-1} - \Sigma(k, \omega_n)]^{-1}$ is then obtained in terms of the self-energy [3]. With the analytic continuation $i\omega_n \to \omega + i\eta^+$ to the real frequency $\omega$, one finally ends up with the retarded Green’s function $G^R(k, \omega)$ from which the desired spectral function $A(k, \omega) = -\frac{1}{\pi} \text{Im} \{G^R(k, \omega)\}$ can be calculated [4]. Knowledge of $A(k, \omega)$, in turn, yields the density of states

$$N(\omega) = 2 \int \frac{dk}{(2\pi)^2} A(k, \omega)$$

(4)

where the factor of 2 accounts for the spin degeneracy, as well as the density equation

$$n = \int_{-\infty}^{+\infty} d\omega N(\omega) f_F(\omega)$$

(5)

which fixes the chemical potential in terms of $n$.

The above definition of the coupling parameter $\eta$ in 2D complies with the requirement of ranging from $-\infty$ in extreme weak coupling to $+\infty$ in extreme strong coupling, in analogy with the coupling parameter $(k_Fa)^{-1}$ in 3D. With this choice, the comparison between the 2D and 3D pseudo-gap physics appears to be quite natural. Other works, which did not address this comparison, made a different choice for the coupling parameter in 2D [15, 10].

The non-self-consistent t-matrix approach offers some advantages over the self-consistent one which has been used in the literature also in 2D: (i) Analytic continuation to the real frequency $\omega$ is exact within the non-self-consistent approach and does not have to rely on numerical procedures. (ii) In 2D the self-consistent t-matrix approach unphysically predicts that composite bosons remain interacting even when extremely dilute. The non-self-consistent t-matrix approach does not suffer from this drawback and can thus better describes the BEC limit of the crossover. (iii) From the computational side, the non-self-consistent t-matrix approach is far less demanding than the self-consistent one. It is then more manageable to apply when an averaging over the trap is required. The lack of self-consistency, on the other hand, yields an unphysical behavior of the chemical potential when the $T = 0$ limit is approached, as originally discussed in Ref. [17]. To the extent that we are not interested in addressing such low temperatures, the non-self-consistent t-matrix approach appears to be ideally suited to address the problem of the spectral function of a 2D Fermi gas with strong pairing interactions.

Previous theoretical work. Recent theoretical approaches that have addressed the experiment of Ref. [1] include the work of: (a) Ref. [10] which used a non-self-consistent t-matrix approach limited to a homogeneous system and where the energy distribution curves were not wave-vector resolved; (b) Ref. [18] which considered the trapped case as well, where quantitative comparison with the experimental data was rather limited; (c) Ref. [19] which used a high-temperature expansion valid for $T \gg T_F$ limited to a homogeneous system and where no quantitative comparison with the experimental data was attempted; (d) Ref. [20] where a related quantum cluster (virial) expansion was used also under homogeneous conditions; (e) Ref. [21] which used instead a self-consistent t-matrix approach limited to a homogeneous system and where no quantitative comparison with the experimental data was attempted.

Comparison with the experimental data for the trapped system. Figure 1 compares the experimental data from Ref. [1] with our theoretical calculations. No fitting parameter is used in our theoretical calculations, which include an averaging over the trap. This rather good comparison gives us confidence about the validity of our theoretical approach, at least in the temperature range relevant to the experiment of Ref. [1]. After this favorable comparison for the trapped system, we turn to the properties of the homogeneous system which is of broader interest to other physical realizations as well, like those in condensed matter.

Properties of the underlying homogeneous system. We consider first the issue of the boundary between the pseudo-gap and molecular regimes. Figure 2 shows the frequency dependence of the single-particle density of states $N(\omega)$. Specifically, panel (a) shows $N(\omega)$ for the same couplings and temperature of Fig. 1 while panel (b) shows $N(\omega)$ for the coupling $\eta = -0.5$ and several temperatures about that of Fig. 1. In panel (a) the non-interacting function $N_0(\omega) = N_0(\Theta(\omega + \mu))$ (where $\Theta(x)$ is the Heaviside unit step function) is shown for comparison. From these curves one identifies the occurrence of a pseudo-gap whenever $N(\omega)$ has a local minimum about $\omega = 0$, and the closing of this pseudo-gap occurs as soon as $N(\omega)$ becomes a monotonically increasing function of $\omega$. In addition, Fig. 2(c) shows the temperature dependence of $N(\omega)$ for the weaker coupling $\eta = -2.0$, where a more symmetric shape of $N(\omega)$ results which resembles that obtained from tunneling experiments in cuprate superconductors [22]. Through this kind of analysis, we obtain the coupling dependence of the temperature $T^*$ at which the pseudo-gap closes according to the above
different values. The single-particle energy \( \eta \) where \( T = 0 \) in these panels, the temperature is fixed at the value 0.

The Fermi energy \( E_F \) the Fermi energy \( E_F = \omega_0 N^{1/2} \), where \( \omega_0 \) is the 2D average trap frequency and \( N \) the total particle number.

criterion. The result is shown in Fig.2(d).

What is not evident from the above analysis is whether what has been identified as a pseudo-gap is a truly many-body effect or rather a manifestation of two-body binding. To answer this question, we perform here for the 2D system an analysis similar to that done in Refs.\[24, 25\] for the 3D system. Accordingly, Fig.3(a) shows the dispersion relations obtained by following the evolution of the frequency position of the peak of the single-particle spectral function \( A(k, \omega) \) at negative frequencies when the magnitude \( k = |k| \) of the wave vector is increased from \( k = 0 \) to values larger than \( k_F \), for several values of coupling and temperature. For each coupling the temperature is chosen well below \( T^* \) (that is, \( T \approx 0.5 T^* \)), yet above the temperature range where the chemical potential is influenced by the effects originally discussed in Ref.\[17\] (see Ref.\[22\]). From these dispersions one can identify the values of \( k_L \) at which the curves “back-bend”, thereby signaling the presence of an underlying Fermi surface. The resulting coupling dependence of \( k_L \) is shown in Fig.3(b), where the error bars correspond to the statistical error of BCS-like fits to the curves of panel (a) \[22\]. We conclude from this analysis that in 2D the boundary between the pseudo-gap and molecular phases, where \( k_L \) vanishes and the underlying Fermi surface disappears, lies in the range \(-0.1 \leq \eta \leq 0.0 \). A similar analysis done in 3D \[22\] has shown that \( k_L \) vanishes at \( T_c \) for the coupling \((k_F a)^{-1} \approx 0.6 \) (\( k_F \) and \( a \) being the Fermi wave vector and scattering length in 3D).

A unifying variable for 2D and 3D. One can take advantage of the similarities between pseudo-gap phenomena in 3D and 2D to identify a variable alternative to the coupling, through which it is possible to unify the evolution from BCS to BEC in 3D and 2D. Following Ref.\[17\], we identify this variable with the ratio between the pair coherence length \( \xi \) and the average inter-particle distance \( d_n \) given by \([3/(4\pi n)]^{1/3}\) in 3D and \([1/(\pi n)]^{1/2}\) in 2D, where \( \xi \) is obtained at \( T = 0 \) within mean field in the two cases.\[12, 26\] Figure 4 shows the ratio \( \xi/d_n \) vs the respective couplings, in panel (a) for 3D and panel (b) for 2D. From these curves, a relationship between the couplings \((k_F a)^{-1}\) in 3D and \( \eta \) in 2D can be established, as shown in Fig.4(c). In addition, one verifies that the critical values of the couplings at which \( k_L \) vanishes in 3D and 2D correspond to the same value \( \xi/d_n \approx 0.4 \). From panel (c) one also verifies that to the unitary limit
\[(k_F a)^{-1} = 0\] in 3D corresponds the value \(\eta \approx -0.6\) in 2D with \(\xi/d_n \approx 0.6\). In terms of the universal variable \(\xi/d_n\), we can again consider the issue of the temperature \(T^*\) up to which pseudo-gap phenomena survive. The dependence of \(T^*\) on \(\xi/d_n\) is shown in Fig. 4(d) both for the 3D and 2D cases, which evidences the strong enhancement of pseudo-gap effects in 2D. For instance, to the “unitary” value \(\xi/d_n \approx 0.6\) there correspond \((T^*/T_F)_{3D} = 0.3\) and \((T^*/T_F)_{2D} = 0.7\), with a 2.3 amplification factor.

**Conclusions.** The above analysis allows us to interpret the panels of Fig. 4 where a comparison is made with the experimental data of Ref. [1]. By extracting the local couplings and temperatures in terms of the local density in the trap (see Ref. [22]), we are led to conclude that the data of panel (a) are below \(T^*\) and at the boundary between the pseudo-gap and molecular phases, those of panel (b) are just below \(T^*\) and well within the pseudo-gap phase, and those of panel (c) are above \(T^*\) although at couplings consistent with the pseudo-gap phase at lower temperatures. The analysis presented here, using both the pseudo-gap and the Luttinger wave vector, has allowed us to make these distinctions and to answer the question raised at the beginning.

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See Supplemental Material for more details on the comparison with the experimental data, the behavior of the chemical potential vs. temperature for the homogeneous system, and report the theoretical values of the local couplings and normalized temperatures relevant for the discussion of the experimental data.

Comparison with the experimental data

In the absence of final-state effects (as appropriate to $^{40}$K atoms), the radio-frequency spectral intensity is given by:

$$\text{RF}(\tilde{\omega}) = \frac{2}{N} \int d\mathbf{k} \int d\mathbf{r} \langle \mathbf{k}, \xi(\mathbf{k}; \mathbf{r}) \rangle f(\xi(\mathbf{k}; \mathbf{r}) - \tilde{\omega}).$$

(6)

Here, $\tilde{\omega} = \omega_{\text{rf}} - \omega_0$ is the detuning frequency, i.e., the difference between the radio-frequency $\omega_{\text{rf}}$ and the atomic transition frequency $\omega_0$ for the free atoms, $\mathbf{r}$ the position in the trap, and $\xi(\mathbf{k}; \mathbf{r}) = k^2/(2m) - \mathbf{r}$, with $\mu(\mathbf{r}) = \mathbf{r} - V(\mathbf{r})$, where $V(\mathbf{r}) = \tfrac{1}{2}m\omega_0^2 r^2$ trapping $N$ atoms. The prefactor in Eq. (6) is chosen to make the total area of the radio-frequency spectral intensity equal unity, namely, $\int_{-\infty}^{+\infty} d\tilde{\omega} \text{RF}(\tilde{\omega}) = 1$. The spectral function $A(\mathbf{k}, \xi(\mathbf{k}; \mathbf{r}) - \tilde{\omega})$ is calculated at position $\mathbf{r}$ in the trap, within a local-density approximation.

The radio-frequency spectral intensity can be analyzed into its individual $\mathbf{k}$-components by exchanging the order of the two integrals in Eq. (6). One may then define

$$\text{RF}(\mathbf{k}, \tilde{\omega}) = \frac{2}{N} \int d\mathbf{r} A(\mathbf{k}, \xi(\mathbf{k}; \mathbf{r}) - \tilde{\omega}) f(\xi(\mathbf{k}; \mathbf{r}) - \tilde{\omega}),$$

(7)

such that $\text{RF}(\tilde{\omega}) = \int d\mathbf{k} \text{RF}(\mathbf{k}, \tilde{\omega})$. By expressing wave vectors in units of $k_F$, energies in units of $E_F$, and radial positions in units of the Thomas-Fermi radius $R_F$, one gets:

$$\text{RF}(\mathbf{k}, \tilde{\omega}) = 8 \int d\mathbf{r} A(\mathbf{k}, \xi(\mathbf{k}; \mathbf{r}) - \tilde{\omega}) f(\xi(\mathbf{k}; \mathbf{r}) - \tilde{\omega}).$$

(8)

Finally, to obtain an expression that can be directly compared with the experimental Energy Distribution Curve (EDC), it is sufficient to express the frequency $\tilde{\omega}$ in terms of the single-particle energy $E_s \equiv k^2/(2m) - \omega_0$. This yields eventually:

$$\text{EDC}(\mathbf{k}, E_s) = 8 \int d\mathbf{r} A(\mathbf{k}, E_s - \mu(\mathbf{r})) f(E_s - \mu(\mathbf{r})).$$

(9)

In particular, since the experimental data reported in Fig. 1 of the main text were taken at $\mathbf{k} = 0$, the corresponding theoretical curves were calculated with Eq. (9) evaluated at $\mathbf{k} = 0$. For given coupling strength and temperature, the value of the chemical potential $\mu$ required
to calculate $EDC(k = 0, E_r)$ was calculated by inverting numerically the number equation $N = \int d\mathbf{r} n(\mathbf{r})$, where $n(\mathbf{r})$ is the particle number density obtained from the local spectral weight function at position $\mathbf{r}$. The reported experimental resolution of 1.5 kHz (see online supplementary material of ref. [S1]) was finally included in the comparison with the experimental data, by convolving the results of Eq. (9) with a normalized Gaussian with variance $\sigma = 1.5$ kHz (converted in units of $E_F$). For completeness, Fig. 1 of the main text reports the theoretical curves obtained both without (green thin lines) and with (blue thick lines) this convolution.

The value of $E_F$ for the experimental data at temperature $T/T_F = 0.65$ reported in Fig. 1 of the main text was determined to be 11 kHz. One should note that the value $k_F = 8.1 \mu m^{-1}$ reported in ref. [S1] would yield a Fermi energy $E_F = 8.4$ kHz. This value refers, however, to a lower temperature ($T/T_F = 0.27$), with less atoms in the sample (due to evaporative cooling). The dependence of the number of particles on temperature in the experimental setup of ref. [S1] was analyzed in ref. [S2] by the same group. A linear interpolation of the Fermi wave vector data reported there for $T/T_F = 0.27$ and $T/T_F = 1.09$ (see the caption of their Fig. 3) enables us to conclude that the value of the Fermi energy at $T/T_F = 0.27$ has to be multiplied by a factor 1.3, in order to obtain the value of $E_F$ at $T/T_F = 0.65$. This leads eventually to the value $E_F = 11$ kHz quoted above, which fixes the horizontal scale of the experimental spectra. The vertical scale of the experimental spectra was instead set by making the height of the right experimental peak to coincide with the theoretical prediction.

Note further that it was not possible to compare also with the experimental data at $T/T_F = 0.27$ (reported in the top panels of Fig. 2a of ref. [S1]). The present non-self-consistent t-matrix approach yields, for the couplings $\eta = (-0.8, -0.5, 0)$ considered in ref. [S1], the values $T_c/T_F = (0.37, 0.45, 0.58)$, respectively, for the the superfluid critical temperature $T_c$ of the trapped system (cf. ref. [S3]). The temperature $T/T_F = 0.27$ is then lower than $T_c$, which does not allow us to compare with the experimental data for this temperature (at least with the present theory, which is formulated in the normal phase). In this context, a reference value for $T_c$ is provided by the BEC limit $T_c/T_F = \sqrt{3}/\pi \approx 0.55$ for an ideal Bose gas of molecules trapped in a harmonic two-dimensional potential. The superfluid critical temperature of the trapped two-dimensional Fermi gas should converge to this value when $\eta \to +\infty$. A comparison with this value suggests that the values of $T_c$ quoted above for $\eta = -0.8, -0.5, 0$, while a priori not expected to be quantitatively correct, are probably not unrealistic.

Chemical potential vs. temperature for the homogeneous system

Figure 5 presents the chemical potential vs. temperature as obtained within the present non-self-consistent t-matrix approach. One sees that, for all couplings considered in Fig. 5, the chemical potential presents a non-monotonic behavior. This behavior was already discussed some time ago by Schmitt-Rink, Varma, and Ruckenstein [S4] (within a Nozieres-Schmitt-Rink approach, which corresponds to a simplified variant of the present formalism where the Dyson’s equation for the one-body Green’s function is expanded to first order in the self-energy). It originates from the infrared divergence of the single-particle self-energy when the Thouless’ criterion curve, defined by the equation $\Gamma_0^{-1}(q = 0, N_r = 0) = 0$, is approached. More specifically, the equation $\Gamma_0^{-1}(0, 0) = 0$ defines, for each value of the coupling parameter $\eta$, a curve $\mu_\eta(T)$ (dotted lines in Fig. 5) that cannot be crossed by the curve $\mu(T)$ because along it the self-energy would be infinite. The solution of the particle number equation makes then the chemical potential to osculate the curve $\mu_\eta(T)$ when the temperature is lowered, and eventually to approach the limiting value $-\epsilon_0/2$ when $T \to 0$. This behavior, albeit correct in the strong-coupling regime, is unphysical for weak and intermediate couplings. Empirically, one can identify the temperature where $\mu(T)$ reaches its maximum, as the temperature below which the proximity to this unphysical divergence begins to matter. The temperature $T^*$ is well above this region. When determining $k_L$, on the other hand, it is desirable to work at the lowest temperature as possible in order to reduce the importance of thermal broadening relative to interaction effects. The temperature used for calculating $k_L$ was then chosen to correspond to about the maximum of $\mu(T)$ (being approximately 0.5 $T^*$ for the couplings considered in Fig. 3 of the main text).
Local couplings and normalized temperatures

Once the density profile $n(r)$ in the trap has been calculated for given values of the coupling parameter $\eta$ and temperature $T$, one may determine the local coupling parameter $\eta(r) \equiv -\ln[k_F(r) a]$ and normalized temperature $T/T_F(r)$, where $k_F(r) = \sqrt{2\pi n(r)}$ and $T_F(r) = k_F(r)^2/(2m)$. Table I reports two examples of these local values for the three different cases considered in Fig. 1 of the main text, corresponding to the trap coupling parameter $\eta = 0, -0.5, -0.8$ for panels a,b,c, respectively, and $T = 0.65T_F$. Specifically, we report in Table I the local values both at $r = |r| = 0$ and at $r = r_{\text{max}}$, defined as the value of $r$ where $rn(r)$ attains its maximum, such that the corresponding radial shell has the largest particle number.

The region $r \lesssim r_{\text{max}}$ is expected to contribute most to the measured EDC spectral intensity. The local values of coupling and normalized temperature at $r = 0$ and $r = r_{\text{max}}$ can be compared with the curve for $T^*$ and with the boundary between the pseudo-gap and molecular phases presented in Fig. 2d and 3b of the main text, so as to establish the coupling and temperature regimes of the homogeneous gas explored by the experimental data of Fig. 1 of the main text.

This is done in Fig. 6 from which one concludes that the data of Fig. 1a of the main text are below $T^*$ and at the boundary between the pseudo-gap and molecular phases, those of Fig. 1b are just below $T^*$ and well within the pseudo-gap phase, while those Fig. 1c are above $T^*$ although at couplings consistent with the pseudo-gap phase at lower temperatures.

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