

## BCS-BEC Crossover at Finite Temperature for Superfluid Trapped Fermi Atoms

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We consider the BCS-BEC (Bose-Einstein-condensate) crossover for a system of trapped Fermi atoms at finite temperature, both below and above the superfluid critical temperature, by including fluctuations beyond mean field. We determine the superfluid critical temperature and the pair-breaking temperature as functions of the attractive interaction between Fermi atoms, from the weak- to the strong-coupling limit (where bosonic molecules form as bound-fermion pairs). Density profiles in the trap are also obtained for all temperatures and couplings.

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Recent experimental advances with trapped Fermi atoms enable one to reach considerably lower temperatures than obtained previously, as well as to vary the effective attraction between Fermi atoms via Fano-Feshbach resonances [1]. It then becomes possible to reach conditions where Cooper pairs of Fermi atoms form in weak coupling below the superfluid critical temperature  $T_c$ , and composite bosons form and Bose-Einstein condense in strong coupling. It thus appears relevant to formulate a theory of the BCS-BEC crossover for trapped Fermi atoms for *all* temperatures in the broken-symmetry phase below  $T_c$ , connecting it with continuity to the results for the normal phase above  $T_c$ . This is the main task of the present Letter, where a unified theoretical framework is set up for all temperatures and couplings.

Limited theoretical results are so far available for the BCS-BEC crossover in a trap. A previous study of the density profiles over the whole crossover has dealt with the zero-temperature case within a mean-field approach [2]. Finite temperatures below  $T_c$  have been considered within mean field for a single coupling value in the weak-to-intermediate region [3]. Fluctuations over and above mean field have been included over the whole crossover for temperatures above  $T_c$  [4,5].

In the present Letter, we provide a systematic study of the whole BCS-BEC crossover in a trap by including fluctuations beyond mean field, for all temperatures below and above  $T_c$ , and up to the pair-breaking temperature  $T^*$ . Below the critical temperature, our theory recovers the BCS results in weak coupling and the Bogoliubov description for the composite bosons in strong coupling, and provides an interpolation scheme in the intermediate (crossover) region where no small parameter exists for controlling the approximations of many-body theory.

Study of the BCS-BEC crossover started with the pioneering work by Eagles for low-carrier doped superconductors [6]. A systematic approach to the problem was later given by Leggett [7], who showed that a *smooth* crossover from a BCS ground state of overlapping Cooper pairs to a condensate of composite bosons occurs as the strength of the fermionic attraction is increased.

This study was later extended to finite temperatures above  $T_c$  by Nozières and Schmitt-Rink with the use of diagrammatic methods [8]. Extension of this approach to trapped fermions has relied so far mostly on a local Thomas-Fermi (TF) approximation [2–4]. This local approximation is also adopted in the present Letter.

Our main results for the BCS-BEC crossover in a trap at finite temperature are the following:

(i) We find that the critical temperature  $T_c$  increases monotonically from weak to strong coupling, reaching eventually the value of the Bose-Einstein temperature for the composite bosons in the trap. Correspondingly, *no maximum* is found in the intermediate-coupling region for the trapped case. The presence of this maximum was instead found with the same diagrammatic theory formulated for the homogeneous case [8].

(ii) We find that in the intermediate-to-strong coupling region the density profiles show a characteristic *secondary peak* located away from the trap center, at temperatures below but close to  $T_c$ . The occurrence of this peak is due to the combined presence of condensed and noncondensed composite bosons. We find that this peak survives up to couplings near the crossover region, such that the residual interaction between the composite bosons is strong enough for the peak to be well pronounced. In this way, this peak could be experimentally accessible, providing one with a characteristic feature of the superfluid state.

(iii) We find that the “pairing-fluctuation region” between  $T_c$  and  $T^*$ , where precursor pairing effects occur, is considerably reduced in the trap with respect to the homogeneous case. Pseudogap phenomena are thus expected to be very much reduced for trapped Fermi atoms, with respect to what occurs for high-temperature superconductors [9].

The system we consider is a gas of Fermi atoms confined in a trap by a harmonic spherical potential  $V(r)$  (where  $r$  measures the distance from the trap center). The Fermi atoms equally populate two spin (hyperfine) states and are mutually interacting via a point-contact ( $s$ -wave) attraction. This attraction is suitably regularized via the

scattering length  $a_F$  of the associated (fermionic) two-body problem. The coupling strength is then identified with the dimensionless parameter  $(k_F a_F)^{-1}$ , where the Fermi wave vector  $k_F$  is related to the Fermi energy  $E_F = (3N)^{1/3} \omega$  for noninteracting fermions in the trap [10] by  $E_F = k_F^2/(2m)$ . Here,  $N$  is the total number of Fermi atoms,  $\omega$  the trap frequency, and  $m$  the fermion mass (we set  $\hbar = 1$  throughout). In principle,  $(k_F a_F)^{-1} \approx -\infty$  corresponds to the (extreme) weak coupling and  $(k_F a_F)^{-1} \approx +\infty$  to the (extreme) strong-coupling limit. In practice, the crossover between these limits occurs in the limited interval  $-1 \lesssim (k_F a_F)^{-1} \lesssim +1$ .

The many-body diagrammatic structure for the homogeneous case is considerably simplified by the use of the above regularization [11]. In particular, in the broken-symmetry phase below  $T_c$  a diagrammatic theory for the BCS-BEC crossover can be set up [12] in the spirit of the  $t$ -matrix approximation [13]. This theory includes fluctuation corrections to the BCS results in weak coupling and describes the composite bosons in strong coupling by the Bogoliubov theory [14]. In the present Letter, we extend this approach to the trapped case, by adopting a *local* TF approximation to take into account the trapping potential. This local approximation is implemented by replacing the chemical potential  $\mu$ , whenever it occurs in the single-particle self-energy and Green's functions, by the local expression  $\mu(r) = \mu - V(r)$ . At the same time, the order parameter  $\Delta$  is replaced by a local function  $\Delta(r)$  to be determined consistently.

Quite generally, in the BCS-BEC crossover approach the chemical potential is strongly renormalized when passing from the weak- to the strong-coupling limit. In our case, the coupled equations for the chemical potential and the local order parameter  $\Delta(r)$  are

$$\Delta(r) = - \frac{4\pi a_F}{m} \int \frac{d\mathbf{k}}{(2\pi)^3} \left[ \frac{1}{\beta} \sum_s \mathcal{G}_{12}(\mathbf{k}, \omega_s; \mu(r), \Delta(r)) - \frac{m \Delta(r)}{|\mathbf{k}|^2} \right], \quad (1)$$

$$N = 8\pi \int dr r^2 \int \frac{d\mathbf{k}}{(2\pi)^3} \times \frac{1}{\beta} \sum_s e^{i\omega_s 0^+} G_{11}(\mathbf{k}, \omega_s; \mu(r), \Delta(r)), \quad (2)$$

where  $\mathbf{k}$  is a wave vector and  $\omega_s = (2s + 1)\pi/\beta$  ( $s$  integer) a fermionic Matsubara frequency ( $\beta$  being the inverse temperature). In the above expressions,  $\mathcal{G}_{12}(\mathbf{k}, \omega_s; \mu(r), \Delta(r))$  is obtained from the BCS anomalous single-particle Green's function  $\Delta/(E(\mathbf{k})^2 + \omega_s^2)$  [with  $E(\mathbf{k}) = \sqrt{\xi(\mathbf{k})^2 + \Delta^2}$  and  $\xi(\mathbf{k}) = \mathbf{k}^2/(2m) - \mu$ ], by replacing  $\mu$  with  $\mu(r)$  and  $\Delta$  with  $\Delta(r)$ ; the dressed normal single-particle Green's function  $G_{11}(\mathbf{k}, \omega_s; \mu(r), \Delta(r))$  is obtained by a similar replacement made on the function  $G_{11}(\mathbf{k}, \omega_s)$ , which contains fluctuation corrections beyond mean field.

The quantity  $G_{11}(\mathbf{k}, \omega_s)$  results from the solution of the  $2 \times 2$  Dyson's equation in Nambu notation, with self-energy

$$\begin{aligned} \Sigma_{11}(\mathbf{k}, \omega_s) &= - \Sigma_{22}(\mathbf{k}, -\omega_s) \\ &= - \int \frac{d\mathbf{k}'}{(2\pi)^3} \frac{1}{\beta} \sum_{\nu} \Gamma_{11}(\mathbf{q}, \Omega_{\nu}) \\ &\quad \times \mathcal{G}_{11}(\mathbf{q} - \mathbf{k}, \Omega_{\nu} - \omega_s), \end{aligned} \quad (3)$$

$$\Sigma_{12}(\mathbf{k}, \omega_s) = \Sigma_{21}(\mathbf{k}, \omega_s) = - \Delta, \quad (4)$$

where  $\Omega_{\nu} = 2\pi\nu/\beta$  ( $\nu$  integer) is a bosonic Matsubara frequency. Here,  $\mathcal{G}_{11}(k) = -(\xi(\mathbf{k}) + i\omega_s)/(E(\mathbf{k})^2 + \omega_s^2)$  is the BCS normal single-particle Green's function and  $\Gamma_{11}(q) = \chi_{11}(-q)/[\chi_{11}(q)\chi_{11}(-q) - \chi_{12}(q)^2]$  is the normal pair propagator, with

$$-\chi_{11}(q) = \int \frac{d\mathbf{k}}{(2\pi)^3} \left[ \frac{1}{\beta} \sum_s \mathcal{G}_{11}(k+q) \mathcal{G}_{11}(-k) - \frac{1}{2E(\mathbf{k})} \right], \quad (5)$$

$$\chi_{12}(q) = \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{1}{\beta} \sum_s \mathcal{G}_{12}(k+q) \mathcal{G}_{21}(-k), \quad (6)$$

and the four-vector notation  $k = (\mathbf{k}, \omega_s)$  and  $q = (\mathbf{q}, \Omega_{\nu})$ .

Neglecting the diagonal elements (3) of the self-energy results in the BCS (mean-field) approximation. When extrapolated toward strong coupling, this approximation accounts for the formation of bound-fermion pairs upon lowering the temperature below  $T^*$ . Inclusion of the diagonal elements (3) of the self-energy is required to describe condensation of these pairs at the lower temperature  $T_c$ . In strong coupling, the normal pair propagator  $\Gamma_{11}$  (together with its anomalous counterpart) reduce to the propagators for composite bosons within the Bogoliubov approximation [16]. Above  $T_c$ , the diagonal elements (3) correspond to the  $t$ -matrix approximation in the normal phase.

Figure 1 compares the temperature vs coupling phase diagram for the trapped ( $t$ ) and homogeneous ( $h$ ) case, where  $T_c$  and  $T^*$  are identified. The temperatures  $T_c$  and  $T^*$  are obtained by solving the coupled equations (1) and (2) when  $\Delta(r) = 0$ , with and without inclusion of the diagonal self-energy (3), in the order.

Note that  $T_c^t$  increases *monotonically* from weak to strong coupling, approaching the value  $T_{BE} = 0.94\omega(N/2)^{1/3}$  of the Bose-Einstein temperature for the composite bosons in the trap [10] (with the same trap frequency for fermions and composite bosons). No maximum for  $T_c$  is thus found in the intermediate-coupling region for the trapped case, contrary to the homogeneous case where a maximum occurs at  $(k_F a_F)^{-1} \cong 0.35$ . This behavior is consistent with the fact that, for a dilute Bose gas, interaction effects lead to a positive (negative) shift of the critical temperature in the homogeneous (trapped) case [17]. Together with the vanishing of  $T_c$  in weak

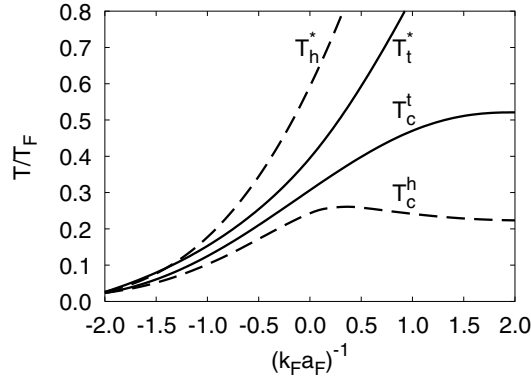


FIG. 1. Temperature vs coupling phase diagram for the trapped (solid lines) and homogeneous (dashed lines) case, with the critical temperature  $T_c$  and the pair-breaking temperature  $T^*$  shown for the two cases. Each temperature is normalized to the respective Fermi temperature  $T_F$ . With this normalization, the phase diagram also holds for anisotropic traps.

coupling, this implies that (at least) one maximum must be present for the homogeneous case, while the presence of a maximum is not required for the trapped case. It is encouraging that our approximate theory leads to curves for the critical temperature in line with these general expectations.

Note further that the “pairing-fluctuation region” of the phase diagram, delimited in each case by the curves  $T^*$  and  $T_c$ , is considerably reduced in the trap with respect to the homogeneous case. In the strong-coupling limit, the reduction of the pairing-fluctuation region stems from the difference in the density of states  $D(\epsilon)$  at energy  $\epsilon$  for noninteracting particles, when passing from the homogeneous [ $D_h(\epsilon) \propto \epsilon^{1/2}$ ] to the trapped [ $D_t(\epsilon) \propto \epsilon^2$ ] case. This difference is, in fact, known to account for the larger value of  $(T_{BE}/T_F)_t$  with respect to  $(T_{BE}/T_F)_h$  [10]. By a similar token, it can be shown that the same difference in the density of states accounts for the smaller value of  $(T^*/T_F)_t$  with respect to  $(T^*/T_F)_h$ .

Figure 2 shows the density profiles  $n(r)/N$  [such that  $4\pi \int dr r^2 n(r)/N = 1$ ] vs  $r/R_F$  for three characteristic couplings, from  $T = 0$  to  $T^*$  [where  $R_F = \sqrt{2E_F/(m\omega^2)}$  is the TF radius for noninteracting fermions in the trap]. On the weak-coupling side of the crossover [ $(k_F a_F)^{-1} = -1.0$ ],  $n(r)$  depends mildly on temperature. In weak coupling, no information can thus be extracted from  $n(r)$  about when the superfluid phase is entered. For intermediate couplings [ $(k_F a_F)^{-1} = 0.0$ ],  $n(r)$  starts to depend sensibly on temperature. Eventually in strong coupling [ $(k_F a_F)^{-1} = 1.0$ ],  $n(r)$  shows a marked temperature dependence. In this case, the broad density profile at  $T^*$  corresponds to a system of noninteracting fermions at the same temperature. Upon lowering the temperature, the density profile shrinks considerably and  $n(r=0)$  increases correspondingly, as expected for a system of weakly interacting (composite) bosons [18].

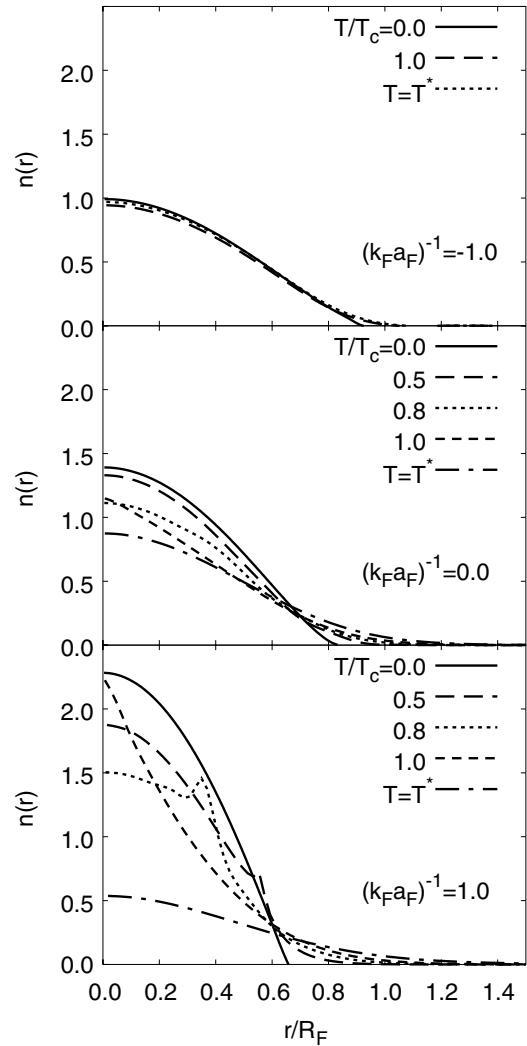


FIG. 2. Density profile  $n(r)/N$  vs  $r/R_F$  for three coupling values and several temperatures from  $T = 0$  to  $T^*$ .

Note, in addition, the presence of a secondary peak away from the trap center, that shows up at temperatures below but close to  $T_c$  (this peak is most evident at about  $0.7T_c$ ). The presence of this peak stems from the ability of our theory to recover the Bogoliubov approximation for the composite bosons. The presence of this peak was, in fact, predicted for a weakly interacting trapped Bose gas [19]. Our results show that this peak appears not only in the strong-coupling limit (which corresponds to weakly interacting bosons), but also in the crossover region. In this region, the residual interaction between the composite bosons is sufficiently strong for the peak to be well pronounced over the background, contrary to what occurs for weakly interacting bosons. In this way, the presence of the secondary peak in  $n(r)$  below  $T_c$  could be subject to experimental testing, providing one with a characteristic signature of the superfluid state.

It is interesting to separate the total density  $n(r)$  for a given coupling into three components, namely,  $n_F(r)$  for unbound fermions,  $n_0(r)$  for condensed pairs, and  $n'(r)$

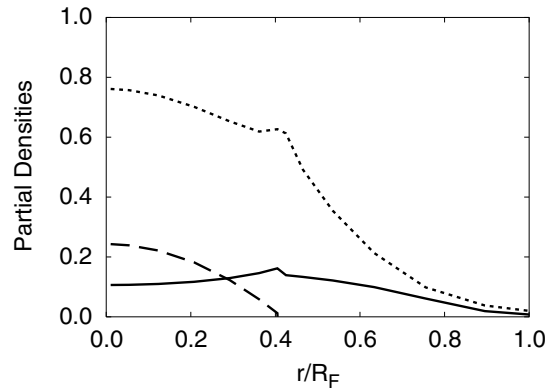


FIG. 3. Partial density profiles vs  $r/R_F$  for  $(k_F a_F)^{-1} = 0.0$  and  $T = 0.8T_c$ :  $n_F(r)/N$  (solid line),  $n_0(r)/N$  (dashed line), and  $n'(r)/N$  (dotted line).

for noncondensed pairs. These components are obtained from expressions similar to (2), with  $G_{11}$  therein replaced, respectively, by the Green's function  $\mathcal{G}_0$  for non-interacting fermions and by the differences  $\mathcal{G}_{11} - \mathcal{G}_0$  and  $G_{11} - \mathcal{G}_{11}$ . This procedure is meant to project out from the many-body state its fermionic and bosonic characters, not only in the strong-coupling regime (where  $n_0$  and  $n'$  have independent physical reality while  $n_F$  vanishes), but also in the intermediate-coupling region of interest.

The three components are plotted in Fig. 3 for the coupling value  $(k_F a_F)^{-1} = 0.0$  and the temperature  $0.8T_c$ . A layered structure results for these densities, from an inner core of Bose superfluid to an outer layer of normal Fermi liquid, in agreement with recent arguments for a dilute atomic-molecular Fermi cloud [20]. Note that, for this intermediate coupling, the component  $n'(r)$  obtained by including fluctuations dominates over the condensate component  $n_0(r)$  that results from mean field. This implies that, already in the intermediate-coupling region, it is not possible to rely only on a mean-field calculation [3] to obtain density profiles for trapped fermions at finite temperature.

In conclusion, with a single theory that includes fluctuations beyond mean field, both below and above the critical temperature, we have studied the BCS-BEC crossover for a system of trapped Fermi atoms at finite temperature. Novel features, peculiar to the trapped case, have been contrasted with the results for the homogeneous case.

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[13] The many-body  $t$  matrix depends on the energy and the wave vectors of the incoming particles, as well as on temperature  $T$  and chemical potential  $\mu$ . In this way, its value does not coincide with the two-body expression  $4\pi a_F/m$  and thus does not diverge when the two-body resonance is crossed. The  $t$ -matrix self-energy is thus "unitarity" limited in the many-body sense.

[14] The Bogoliubov description of the composite bosons is here associated with the value  $a_B = 2a_F$  for the bosonic scattering length  $a_B$ , which amounts to the Born approximation for the scattering between composite bosons [11]. A complete treatment of the composite-boson scattering problem leads to a reduction of  $a_B$  by about a factor of 3 [11,15]. Owing to the very slow dependence of the density profiles on  $a_B$  in strong coupling, we expect this difference in  $a_B$  to make no significant change in the density profiles.

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