Shrinking of a condensed fermionic cloud in a trap approaching the Bose-Einstein condensation limit

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We determine the zero-temperature density profile of a cloud of fermionic atoms in a trap subject to a mutual attractive interaction, as the strength of the interaction is progressively increased. We find a significant decrease of the size of the atomic cloud as it evolves from the weak-coupling regime of overlapping Cooper pairs to the strong-coupling (Bose-Einstein) regime of nonoverlapping bound-fermion pairs. Most significantly, we find a pronounced increase of the value of the density at the center of the trap (even by an order of magnitude) when evolving between the two regimes. Our results are based on a generalized Thomas-Fermi approximation for the superfluid state, which covers continuously all coupling regimes.

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The impressive experimental realization of Bose-Einstein condensation (BEC) of ultracold bosonic atoms in a trap over the past few years $\lceil 1 \rceil$ has prompted the expectation that also the properties of ultracold fermionic atoms in a trap could be revealed in a regime of quantum degeneracy $[2]$. In addition, the possibility that the study of Fermi gases may lead to a superfluid phase analogous to the BCS state has added excitement to the field. In particular, experimental proposals are under investigation for realizing Cooper pairs with ultracold dilute fermionic atoms in a trap, either via the enhanced interaction between fermionic atoms with a tunable scattering (Feshbach) resonance $\lceil 3 \rceil$ or via sympathetic cooling with a mixture of fermions and bosons $[4]$.

Given these rapid experimental advances, it seems timely to explore theoretically the even more intriguing question of the *crossover* between the weak-coupling (BCS) regime of overlapping Cooper pairs and the strong-coupling (Bose-Einstein) regime of nonoverlapping bound-fermion pairs for a gas of ultracold Fermi atoms in a trap, thus dealing simultaneously with two basic quantum phenomena that share the same spontaneous broken-symmetry (superfluid) behavior. In particular, novel and interesting physics may result in the intermediate-coupling regime where neither one of the two limits is fully realized.

Detection of density profiles of ultracold trapped atoms is routinely used to explore their degeneracy properties. This feature could also be explored to detect the continuous evolution from Cooper pairs to bound-fermion pairs as the strength of the attractive interaction between fermions is increased, with the expectation that the density profile shrinks upon approaching the strong-coupling regime owing to the diminished Fermi pressure. In this respect, partial results have already been obtained as a function of temperature in the broken-symmetry phase for a single coupling toward the weak-coupling side of the BCS-BEC crossover $[5]$, as well as a function of coupling in the normal phase above the critical temperature $[6]$.

In this paper, we calculate the density profile of a cloud of fermionic atoms in a trap subject to a mutual attractive interaction, as its strength is progressively increased from weak to strong coupling. To this end, we extend the coupled meanfield equations determining the gap function and the chemical potential for the BCS-BEC crossover problem of a homogeneous system to the case of a *spatially varying gap function* in the presence of a harmonic trap, and study in a systematic way the evolution of the density profile at zero temperature where the mean-field equations are expected to be reliable. Our approach generalizes the fermionic Thomas-Fermi (TF) approximation to the superfluid state at zero temperature for any coupling, and recovers the TF approximation for the composite bosons $[7]$ in the strong-coupling limit. We find a significant decrease of the size of the atomic cloud as the strong-coupling limit is approached; even more significantly, we find a pronounced increase of the value of the density at the center of the trap when evolving between the two regimes. This increase can thus be regarded as a signature of the achieved BCS-BEC crossover. Numerical calculations for the density profile, gap function, and chemical potential, as well as analytic results for the radius of the cloud and related quantities are presented.

A central issue of the BCS-BEC crossover problem $[8]$ is to obtain for all coupling regimes *a single theory* expressed in terms of fermionic variables, which recovers known results for weakly interacting fermions (on the weak-coupling side) and for weakly interacting bosons (on the strongcoupling side), thus providing an interpolation scheme over the intermediate-coupling regime. The treatment of the intermediate-coupling regime is necessarily an approximate one, because in this regime a small parameter to control the approximations is lacking. For these reasons, the interpolation via a single fermionic theory represents at present the only manageable approach to the BCS-BEC crossover. (Effects going beyond the BCS theory in weak coupling have been included for the homogeneous case in Ref. [9]. In the present treatment of the inhomogeneous case, we shall limit to consider the crossover from BCS theory to the BEC limit, thus leaving out these additional effects.)

The present calculations are based on a local-density approximation, whereby the fermionic chemical potential entering the BCS gap and density equations are replaced by a *local chemical potential* that adapts to the spatial position in the harmonic trap. We thus set $\mu(\mathbf{r}) = \mu - V(\mathbf{r})$, where μ is the equilibrium chemical potential and $V(\mathbf{r}) = m\omega^2 r^2/2$ is the harmonic potential for the Fermi atoms at position **r** in the

trap (*m* being the fermionic mass and ω the characteristic trap frequency). Correspondingly, the gap function takes the local value $\Delta(\mathbf{r})$. With the replacement of μ by $\mu(\mathbf{r})$ and of Δ by $\Delta(\mathbf{r})$, the *s*-wave BCS gap equation at zero temperature becomes **r** dependent and reads in dimensionless form:

$$
-\frac{\pi}{k_F a_F} = \int_0^\infty d\tilde{E} \sqrt{\tilde{E}} \left(\frac{1}{\sqrt{[\tilde{E} - \tilde{\mu}(\tilde{r})]^2 + \tilde{\Delta}(\tilde{r})^2}} - \frac{1}{\tilde{E}} \right).
$$
\n(1)

We have here introduced the dimensionless variables \vec{r} $= |\mathbf{r}|/R_F$, $\tilde{\Delta}(\tilde{r}) = \Delta(|\mathbf{r}|)/E_F$, and $\tilde{\mu}(\tilde{r}) = \mu(|\mathbf{r}|)/E_F = \tilde{\mu} - \tilde{r}^2$ for a spherical trap, where $E_F = (3N)^{1/3}\omega$ ($\hbar = 1$ throughout) is the Fermi energy for noninteracting fermions in the trap [7], R_F is identified by the condition $m\omega^2 R_F^2/2 = E_F$, and $\tilde{\mu} = \mu/E_F$. We have further defined the Fermi wave vector k_F by $E_F = k_F^2/(2m)$.

The above equation has been obtained by considering a contact potential for the attractive fermionic interaction active between two equally populated fermionic species with different internal ("spin") states, and then regularizing the ensuing ultraviolet divergence of the gap equation in terms of the *scattering length* a_F of the associated fermionic twobody problem $[10,11]$. This regularization, in fact, considerably simplifies dealing with the BCS-BEC crossover and parametrizes the interaction in terms of the measurable scattering length a_F .

Dealing with the BCS-BEC crossover requires us to supplement the gap equation by the density equation *N* $= \int d\mathbf{r} n(\mathbf{r}) = \int d\tilde{\mathbf{r}} \tilde{n}(\tilde{\mathbf{r}})$, yielding

$$
\frac{\pi}{24} = \int_0^{\tilde{r}_c} d\tilde{r}\tilde{r}^2 \int_0^{\infty} d\tilde{E} \sqrt{\tilde{E}} \left(1 - \frac{\tilde{E} - \tilde{\mu}(\tilde{r})}{\sqrt{[\tilde{E} - \tilde{\mu}(\tilde{r})]^2 + \tilde{\Delta}(\tilde{r})^2}} \right). \tag{2}
$$

Here, \tilde{r}_c is the *radius of the atomic cloud* defined by the condition $\tilde{n}(\tilde{r}) = 0$ for $\tilde{r} \geq \tilde{r}_c$ (which, in turn, requires $\Delta(\tilde{r})$ $=0$ for $\tilde{r} \geq \tilde{r}_c$ as a necessary condition. It can be readily verified that \overline{r}_c is determined by the equation $\overline{\mu}(\overline{r}_c) = 0$ for $a_F < 0$, yielding $\tilde{r}_c = \sqrt{\tilde{\mu}}$, and by the equation $\tilde{\mu}_B(\tilde{r}_c) = 0$ for $a_F > 0$, yielding $\tilde{r}_c = \sqrt{\tilde{\mu} + (k_F a_F)^{-2}}$. In the above expression, we have introduced the local *bosonic* chemical potential $\mu_B(r) = \mu_B - V_B(r)$, where $\mu_B = 2\mu + \epsilon_0$ is the equilibrium bosonic chemical potential, $V_B(\mathbf{r}) = 2V(\mathbf{r}) = m_B\omega^2\mathbf{r}^2/2$ is the harmonic potential for the bosonic molecules of mass $m_B = 2m$, and $\epsilon_0 = (ma_F^2)^{-1}$ is the molecular binding energy. Contrary to Eq. (1) , Eq. (2) couples different positions in the trap, since obtaining a uniform chemical potential μ requires knowledge of $\Delta(\mathbf{r})$ and $\mu(\mathbf{r})$ over the whole trap region.

The weak- and strong-coupling limits of Eqs. (1) and (2) are essentially determined by the behavior of the chemical potential μ , which almost coincides with the Fermi energy E_F in the weak-coupling limit and with (minus half) the binding energy ϵ_0 in the strong-coupling limit. These values represent, in fact, the energy required to extract one fermion

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from the system in the two limits, namely, from the Fermi sea and from a bound molecule, respectively.

In analogy to the homogeneous case [12], *analytic* results can be obtained from the coupled equations (1) and (2) both in the weak- and strong-coupling limits, defined, in the order, by the conditions $\tilde{\mu}(\tilde{r}) > 0$ and $\tilde{\Delta}(\tilde{r}) \leq \tilde{\mu}(\tilde{r})$, and $\tilde{\mu}(\tilde{r}) < 0$ and $\tilde{\Delta}(\tilde{r}) \ll |\tilde{\mu}(\tilde{r})|$ (for $0 \le \tilde{r} \le \tilde{r}_c$). In weak coupling, one obtains $\widetilde{\Delta}(\widetilde{r}) = [8\widetilde{\mu}(\widetilde{r})/e^2] \exp\{-\pi/(2k_F|a_F|\sqrt{\widetilde{\mu}(\widetilde{r})})\}$ with the typical essential singularity behavior as $k_F|a_F| \rightarrow 0$, and the associated density profile $\tilde{n}(\tilde{r}) = (8N/\pi^2)(1-\tilde{r}^2)^{3/2}$ which is the standard result within the TF approximation for noninteracting fermions. For the radius of the atomic cloud one gets correspondingly $r_c = R_F$. In strong coupling, one obtains instead $\tilde{\Delta}(\tilde{r})^2 = 2(\epsilon_0 / E_F) \tilde{\mu}_B(\tilde{r})$ with the associated bosonic density $n_B(r) = n(r)/2 = (m_B/4\pi a_B)\mu_B(r)$ in terms of the original variables, where $a_B = 2a_F$ identifies the bosonic scattering length. The TF result for bosons $[7]$ is thus properly recovered by our calculation in the strong-coupling limit, with a residual bosonic interaction $U_0 = 4 \pi a_B / m_B$. [A more sophisticated theory for the homogeneous case $[11]$ has shown that the correct value for the bosonic scattering length a_B is smaller by about a factor of 3 than the value $2a_F$. Owing to the very slow dependence of the size of the Thomas-Fermi density profile on a_B in strong coupling (see below), this difference makes practically no change in this quantity.] Using eventually the expression of μ_B for bosons in a trap [7], one gets the value $\tilde{r}_c = \sqrt{\tilde{\mu}_B/2}$ $=0.69(k_Fa_F)^{1/5}$, showing a nontrivial dependence of \tilde{r}_c on the coupling parameter in the strong-coupling limit.

Recovering from Eqs. (1) and (2) the TF results for both noninteracting fermions (in the weak-coupling limit) and for weakly interacting bosons (in the strong-coupling limit) should not be surprising, since these equations can also be obtained by generalizing the TF procedure for fermions to the superfluid state. To this end, one introduces an energy functional $E[n(\mathbf{r}), \Delta(\mathbf{r})]$ that depends on the local variables $n(\mathbf{r})$ and $\Delta(\mathbf{r})$, such that minimizing $E[n(\mathbf{r}),\Delta(\mathbf{r})]$ with respect to variations of $\Delta(\mathbf{r})$ and $n(\mathbf{r})$ [subject to the constraint $N = \int d\mathbf{r} n(\mathbf{r})$] leads to Eqs. (1) and (2), respectively. Within the present approach, this functional is given by the expression

$$
E[n(\mathbf{r}), \Delta(\mathbf{r})] = \int d\mathbf{r} \left\{ n(\mathbf{r}) V(\mathbf{r}) - \frac{m}{4 \pi a_F} \Delta(\mathbf{r})^2 + \int \frac{d\mathbf{k}}{(2 \pi)^3} \times \left[\epsilon_{\mathbf{k}} - \frac{\epsilon_{\mathbf{k}}(\epsilon_{\mathbf{k}} - \lambda) + \Delta(\mathbf{r})^2}{\sqrt{(\epsilon_{\mathbf{k}} - \lambda)^2 + \Delta(\mathbf{r})^2}} + \frac{\Delta(\mathbf{r})^2}{2 \epsilon_{\mathbf{k}}} \right] \right\}, \quad (3)
$$

where $\epsilon_{\mathbf{k}} = k^2/(2m)$ and λ is here an implicit function of $n(\mathbf{r})$ and $\Delta(\mathbf{r})$ via the equation

$$
n(\mathbf{r}) = \int \frac{d\mathbf{k}}{(2\pi)^3} \left[1 - \frac{\epsilon_{\mathbf{k}} - \lambda}{\sqrt{(\epsilon_{\mathbf{k}} - \lambda)^2 + \Delta(\mathbf{r})^2}} \right].
$$
 (4)

In particular, in the strong-coupling limit [whereby $n(r)$ $\propto \Delta(r)^2$] functional (3) reduces to

FIG. 1. Density profile (divided by N) vs the radial coordinate for several values of the coupling parameter $(k_F a_F)^{-1}$.

$$
E[n(\mathbf{r})] = \int d\mathbf{r} \left[\frac{U_0}{8} n(\mathbf{r})^2 + \left(V(\mathbf{r}) - \frac{\epsilon_0}{2} \right) n(\mathbf{r}) \right], \quad (5)
$$

from which the bosonic TF expression for $n_B(\bf{r})$ can be obtained by minimizing with respect to $n(r)$ and taking the constraint into account. The absence of the kinetic-energy term in the bosonic TF approximation results in the present approach by the neglecting of the center-of-mass motion of the pairs in expression (3) for the energy.] This result implements at the level of the TF approximation the density functional theory for superconductors described in Ref. [13].

Rescaled equations (1) and (2) depend *only* on the dimensionless coupling parameter $(k_F a_F)^{-1}$ and not on the total number of particles, *N*. This is due to the fact that, as expected, the kinetic energy is not properly taken into account in the present local-density treatment that reduces to the TF approximation for fermions in weak coupling and for bosons in strong coupling. What is missing in our equations is the presence of the length scale of the harmonic trap, which for a bosonic molecule equals $a_{osc}^B = (m_B \omega)^{-1/2}$ and to which there would be associated the *N*-dependent dimensionless ratio $R_F/a_{osc}^B = 2.402N^{1/6}$. The physical lower bound r_c $=a_{\text{osc}}^B$, however, can never be reached in practice, since it would correspond to the condition $(k_F a_F)^{-1} = 12.5N^{5/6}$, yielding the totally unrealistic value $a_F \sim 10^{-3}a_0$ (a_0 being the Bohr radius) in the case of a fermionic atom such as 40 K for $N \sim 10^6$ and a typical trap value $\omega \sim 10^3$ s⁻¹.

Similarly, it can be shown that the local-density approximation for the trapped Fermi gas holds, provided $k_F R_F \ge 1$ (such that the energy quantization in the trap is irrelevant with respect to E_F) and $\Delta(\mathbf{r}=0)/\omega \ge 1$ (such that the pairs are well contained within the trap) [14]. When $N \sim 10^6$, $k_F R_F \sim 10^2$ while $\Delta(\mathbf{r}=0)/\omega \sim 10$ already for the weakcoupling value $(k_F a_F)^{-1} = -2$.

Figure 1 shows the density profile $\tilde{n}(\tilde{r})$ along the radial coordinate (in units of R_F) for several values of the coupling parameter $(k_Fa_F)^{-1}$. The TF profiles for noninteracting fermions as well as for interacting pointlike bosons [with $(k_Fa_F)^{-1}$ =5] are also shown for comparison. Note from the figure that the noninteracting fermion density profile is recovered in weak coupling and the interacting pointlike boson

FIG. 2. Radius of the atomic cloud (full line) and its strongcoupling approximation (dashed line) vs the coupling parameter $(k_Fa_F)^{-1}$. Inset: corresponding values of the dimensionless density at the center of the trap.

density profile is recovered in strong coupling, respectively. Note also the shrinking of the size of the atomic cloud as it evolves from the weak-coupling to the strong-coupling regime, the critical radius \tilde{r}_c being reduced by about a factor of 2 across the crossover region. Correspondingly, the density at the center of the trap increases significantly (by about a factor of 6 for the coupling values shown in the figure).

Figure 2 shows the radius \tilde{r}_c of the atomic cloud (full line) vs the coupling parameter, as determined by entering the numerical values of the chemical potential (obtained from the solution of Eqs. (1) and (2)) into the analytic expressions of \tilde{r}_c reported previously. Three distinct regions of the coupling parameter are identified from this plot: (i) A weak-coupling region for $(k_F a_F)^{-1} \le -1$ where \tilde{r}_c is almost coupling independent and equal to 1 ; (ii) an intermediatecoupling region for $-1 \le (k_F a_F)^{-1} \le 1$ where \tilde{r}_c rapidly de-

FIG. 3. Chemical potential in units of E_F when $\mu > 0$ and of $\epsilon_0/2$ when $\mu<0$ (full line) and its strong-coupling approximation (dashed line) vs the coupling parameter $(k_F a_F)^{-1}$. Inset: gap parameter at the center of the trap (full line) and its strong-coupling approximation (dashed line) vs the coupling parameter [the value for three-dimensional homogeneous case (dash-dotted line) is also shown for comparison].

creases for increasing coupling, being reduced by about 35% when $(k_Fa_F)^{-1}=1$; (iii) a strong-coupling region for 1 $\leq (k_F a_F)^{-1}$ where \tilde{r}_c coincides with the analytic expression of the bosonic TF theory (dashed line). For completeness, we also show in the inset the value of the density $\overline{n}(\overline{r}=0)$ at the center of the trap vs the coupling parameter (full line). Following a flat behavior in the weak-coupling regime, a quite rapid increase of $\tilde{n}(\tilde{r}=0)$ occurs in the intermediatecoupling regime, approaching eventually the power-law dependence $\tilde{n}(\tilde{r}=0) \propto (k_F a_F)^{-3/5}$ obtained analytically in the strong-coupling regime (dashed line).

The chemical potential is finally shown in Fig. 3 (full line) vs the coupling parameter. The behavior of the chemical potential obtained from the expression $\mu = (\mu_B - \epsilon_0)/2$ in strong coupling (with the value of μ_B for bosons in a trap $[7]$) is also shown for comparison (dashed line). In the inset, the gap parameter $\tilde{\Delta}(\tilde{r}=0)$ at the center of the trap (full line) is shown vs the coupling parameter and compared with its strong-coupling approximation (dashed line) the value for the three-dimensional homogeneous case $\lceil 12 \rceil$ (dashed-dotted line) is also shown. Note the marked difference between the trapped and homogeneous cases, with the value for the trapped case increasing much faster than for the homoge-

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neous case as the coupling increases. Specifically, in strong coupling the analytical arguments discussed above yield $\Delta(\vec{r}) = (2\sqrt{2}/k_F a_F) \sqrt{0.476(k_F a_F)^{2/5} - \tilde{r}^2}$, producing the value $\tilde{\Delta}(0) = 1.951(k_F a_F)^{-4/5}$ at the center of the trap; for the homogeneous case, on the other hand, Δ/E_F $=1.303(k_{F}a_{F})^{-1/2}.$

As the data of Figs. 1–3 for the various physical quantities $n(r)$, $\Delta(r)$, r_c , and μ show, the BCS-BEC crossover takes place in practice over the rather narrow range -1 $\leq (k_F a_F)^{-1} \leq 1$ of the coupling parameter. This remark suggests that it would be especially interesting to explore experimentally this intermediate-coupling region, where deviations from the purely fermionic and bosonic behaviors occur.

In conclusion, we have shown that the density profile for superfluid fermionic atoms in a trap exhibits an interesting shrinking of the size of the atomic cloud as the strength of the attraction increases. This behavior should permit one to decide whether the superfluid behavior is either of the BCS type with strongly overlapping Cooper pairs or of the BEC type with nonoverlapping bound-fermion pairs.

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