A simple mean field equation for condensates in the BEC-BCS crossover regime

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We present a mean field approach based on pairs of fermionic atoms to describe condensates in the BEC-BCS crossover regime. By introducing an effective potential, the mean field equation allows us to calculate the chemical potential, the equation of states and the atomic correlation function. The results agree surprisingly well with recent quantum Monte Carlo calculations. We show that the smooth crossover from the bosonic mean field repulsion between molecules to the Fermi pressure among atoms is associated with the evolution of the atomic correlation function.

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Recent studies on ultracold Fermi gases and molecular condensates address an intriguing topic, the crossover from a Bose-Einstein condensate of composite bosons to a fermionic Bardeen-Cooper-Schrieffer superfluid (BEC-BCS crossover). By magnetically tuning the interaction strength near a Feshbach resonance, a molecular BEC can be smoothly converted into a degenerate Fermi gas in the crossover regime are highly active and may provide new insights into other strongly interacting Fermi systems.

In contrast to weakly interacting atomic BECs, for which a simple mean field description based on the Gross-Pitaevskii equation has been very successful, theoretical models on the condensates in the crossover regime are generally very sophisticated and require expertise borrowed from condensed matter theory. The difficulty in providing a simple model for the fermionic system comes from, firstly, the lack of a small expansion parameter. The full range of atomic scattering length should be taken into account to describe the crossover. Secondly, quantum many-body correlations are intrinsically more complicated for fermionic systems than for bosonic ones.

The BEC-BCS crossover, however, suggests an alternative approach to model the strongly interacting fermions based on composite bosons. This is possible since a Fermi gas in the crossover regime constitutes the same quantum phase as of a condensate of interacting pairs. Recent experiments on the wave function projection and on the pairing gap indeed indicate that near the Feshbach resonance, a large fraction of fermionic atoms are paired at low temperatures. From these observations, we propose a bosonic mean field equation, complementary to the fermion-based BCS approaches, to describe the atom pairs in the crossover regime. Our mean-field approach is relatively simple and well-behaved near the resonance. We obtain analytic expressions for the chemical potential and the equation of states, which agree very well with other calculations. In particular, we find the chemical potential in the unitarity limit is \( \sim 0.4357 \) times that in the BCS limit, in excellent agreement with the recent quantum Monte Carlo calculations of 0.42 \( \sim 0.44 \).

We consider an ultracold gas of two-component fermionic atoms. At low temperatures, only atoms in different internal states can pair via s-wave interaction. For simplicity, we assume the interaction range is zero. In the absence of many-body effects, the center-of-mass motion of an atom pair \( \Psi_0(\vec{R}) \) is decoupled from the internal relative atomic motion \( \psi_0(\vec{r}) = (4\pi r^2)^{-1/2}\psi_0(r) \) with \( r = |\vec{r}| \) the atomic separation. Given the atomic scattering length \( a \), \( \psi_0(r) \) satisfies Schrödinger’s equation,

\[
\frac{\hbar^2}{m} \psi_0''(r) = -E_b \psi_0(r)
\]

with the boundary condition \( \psi_0(0) = -a \psi_0'(0) \). Here \( m \) is the atomic mass, \( 2\pi\hbar \) is Planck’s constant, and \( E_b \) is the molecular binding energy.

For positive scattering lengths \( a > 0 \), the bound state is described by \( \psi_0 = (2/a)^{1/2}e^{-r/a} \) with \( E_b = \hbar^2/(ma^2) \). The size of the molecule is given by \( \langle r \rangle = a/2 \). For negative scattering lengths \( a < 0 \), the bound state does not exist and the ground state energy is \( -E_b = 0 \).

Now consider a condensate of pairs with a density distribution \( n(\vec{R}) \) in a slow-varying potential well \( V(\vec{R}) \). We introduce the many-body wave function to include the condensate of the bosonic pairs \( \Psi(\vec{R}) = n(\vec{R})^{1/2} \) as well as the internal atomic correlation \( \psi(r) \). The mean field equation for the composite bosons is then

\[
\left( -\frac{\hbar^2}{4m} \nabla^2 + \frac{\hbar^2 \alpha^2}{m} + V + \hat{U} \right)\Psi(\vec{R})\psi(r) = \mu_m \Psi(\vec{R})\psi(r) \tag{2}
\]

\[
\psi(0) = -a \partial_r \psi(0).
\]

Here \( \mu_m \) is the chemical potential, \( \hat{U} = \hat{g} |\Psi(\vec{R})|^2 \) is the mean field interaction and \( \hat{g} \) is the interaction term.

In conventional approaches, \( \hat{g} \) is given by the scattering length of the bosons. For pairs of fermions, scattering length \( a_m \) is determined by that of the constituent atoms as \( a_m = 0.60a \), resulting from an effective repulsive potential between molecules. This dependence can be understood in a simple picture. Low-energy collision with a repulsive interactions acquires a scattering length which is proportional to the size of the scatterer. For pairs of atoms, we have \( a_m \sim (r) = a/2 \).

From the above considerations, we hypothesize that the interaction term \( \hat{g} \) is effectively proportional to the...
interatomic separation $r$ as
\[
g = g(r) = \frac{\hbar^2}{m} r,
\]
where $c$ is a dimensionless constant.

To proceed with minimum algebra, we consider a uniform gas with a density $|\Psi(R)|^2 = n$. Eq. (2) becomes
\[
(-\frac{\hbar^2}{m} \frac{\partial^2}{\partial r^2} + \hat{g}) \psi(r) = \mu_m \psi(r).
\]

To determine $c$, we consider the BEC limit ($na_m^3 \ll 1$), where the mean field term can be treated perturbatively. That is, the expectation value of $\hat{U}$ based on the bare molecular wave function $\psi_0(r) = (2/a)^{1/2} e^{-r/a}$ should yield the molecular mean field shift $4\pi \hbar^2 a_m n/2m$,
\[
\int_0^\infty \psi^*_0(r) \hat{g} n \psi_0(r) dr = \frac{2\pi \hbar^2 a_m n}{m}.
\]

Using $a_m = 0.6a$, we find Eq. (6) can indeed hold for arbitrary scattering lengths $a_m$ based on the linear mean field potential in Eq. (4). We determine $c = 4\pi a_m / a \approx 7.5$.

From Eq. (3), (4), and (5), the exact solution of the pair wave function is given by
\[
\psi(r) = N \text{Ai}(c^{1/3} n^{1/3} r - c^{-2/3} \mu_m / E_0) \quad (7)
\]
\[
\psi(0) = -a \partial_r \psi(0), \quad (8)
\]
where $N$ is the normalization constant, $\text{Ai}(x)$ is Airy'sAi function, and $E_0 = \hbar^2 n^{2/3} / m$. Notice that the chemical potential $\mu_m$ in Eq. (7) is determined from Eq. (8).

In the weak interaction limit $0 < na_m^3 \ll 1$, the wave function $\psi(r)$ obtained from Eq. (7) is identical to the unperturbed one $\psi_0(r)$ for $r \ll n^{-1/3}$. For $r \gg n^{-1/3}$, $\psi(r)$ is exponentially smaller than $\psi_0(r)$ and approaches $\sim r^{-1/4} \exp(-r^{3/2})$. This suppression for large atomic separation is expected since the interaction energy increases when the pairs start overlapping. As a consequence, the pair wave function $\psi(r)$ is compressed to a smaller size than that of a bare molecule. Similar effect is also discussed in Ref. [17].

The distortion of the pair wave function can be characterized by an effective shift in the binding energy $E_b$. In the weak interaction limit, the shift can be defined as
\[
\int_0^\infty \psi^* \psi(-\frac{\hbar^2 \partial^2}{m}) \psi dr = -E_b(1 + o(na^3)).
\]

The binding energy correction $o(na^3)$ is positive. This effect is absent in the calculations for point-like bosons [10] since it originates comes from the internal degree of freedom. This increase in binding energy is expected since the pair is compressed. This result also provides a simple picture to understand the augmentation of the molecular binding energy reported in Ref. [10].

We extend the mean field model to the crossover and the BCS regime, where the atom pairs strongly overlap. Although it becomes less clear if the mean field approach can fully capture the Fermionic nature of the gas, our aim here is to determine an effective potential which can best describe the system in the BEC-BCS crossover regime.

In this regime, the four-body calculation of $a_m = 0.6a$ is no longer valid, and we determine the mean field interaction $\hat{U}$ from the properties of the Fermi gas. First of all, in the dilute gas limit, we still expect the interaction to be proportional to the square of the bosonic field, $\hat{U} = \hat{g} |\Psi(R)|^2$. Secondly, we exploit the asymptotic behavior of the gas in the weak coupling limit $na^3 \rightarrow 0^-$, where the system approaches an ideal degenerate Fermi gas with the chemical potential
\[
\lim_{na^3 \rightarrow 0^-} \mu_m = 2E_F = \frac{(6\pi^2 n)^{2/3} \hbar^2}{m}.
\]

where $E_F = \hbar^2 k_F^2 / 2m$ is the Fermi energy and $k_F = (6\pi^2 n)^{1/3}$ is the Fermi wave number.

Based on Eq. (5), we find that the above density dependence $\mu_m \propto n^{2/3}$ can be satisfied only when the interaction term $\hat{g}$ is again a linear function of $r$. Taking the limit of $a = 0^-$ and assuming $g(r) = c'(\hbar^2 / m) r$, we can solve the chemical potential from Eq. (7) and Eq. (8) as $\mu_m = \alpha'^{2/3}E_0$ where $-\alpha' \approx -2.338$ is the first zero of the Ai(x) function. Equating $\mu_m$ to $2E_F$ yields $c' = 6\pi^2 \alpha'^{-3/2} \approx 16.56$. This value is about twice as large as $c$.

We first test the equation in the unitarity limit $a = \pm \infty$. Fermi gases in this limit have been extensively studied, for which a universal and fermionic behavior is expected [3]. Due to the divergence of the scattering length, we expect the only energy scale in the system is the Fermi energy $E_F$. From the boundary condition $\partial_r \psi(0) = 0$ and $g = c'(\hbar^2 / m) r$, we determine the chemical potential as $\mu_m = \alpha' c'^{2/3} E_0$, where $-\alpha' \approx -1.019$ is the first zero of the Ai'(x) function. Given $c' = 6\pi^2 \alpha'^{-3/2}$, we get $\mu_m / 2 = (\alpha' / \alpha) E_F \approx 0.4357 E_F$. This result agrees excellently with recent quantum Monte Carlo calculations which gives $\mu_m / 2 = 0.44(1) E_F$ [12] and $0.42(1) E_F$ [13], and the measurements [14, 17], where the uncertainties are larger. We, however, cannot exclude this agreement is coincidental. Near the unitarity limit, we have
\[
\frac{\mu_m}{2E_F} = \frac{\alpha'}{\alpha} - \frac{\alpha^{-1/2}}{\alpha' k_F a} + O\left(\frac{1}{k_F^2 a^2}\right).
\]

Next, we investigate the BEC-BCS crossover regime. Rewriting Eq. (7) and (8) using $c' = 6\pi^2 \alpha'^{-3/2}$, we get
lower amplitude for $r > k$ with a higher probability amplitude for unitarity limits. In the range of $1 < k$ effect we discussed. In the unitarity limit $k$ associate at this point. The mean atomic separation of the atomic pairing is fermionic since bare molecules dissociate at this point. The mean atomic separation of a dramatic variation is directly linked to the crossover nature.

\[ \psi(r) = N \text{Ai}(\alpha^{-1/2}k_Fr - \alpha \frac{\mu_m}{2E_F}) \]  
\[ \frac{k_Fa}{\alpha^{1/2}} = -\frac{\text{Ai}(\alpha \mu_m/2E_F)}{\text{Ai}'(-\alpha \mu_m/2E_F)}. \]

The chemical potential $\mu_m$ calculated from Eq.(13) is shown in Fig. 1. We see that $\mu_m$ approaches $2E_F$ in the BCS limit and $-E_b$ in the BEC limit, as expected. In the crossover regime, the values agree well with the Monte Carlo calculation from [12]. We can also evaluate the equation of states $\mu_m + E_b \propto n^\gamma$, where the exponent $\gamma$ plays a crucial role in the collective excitation frequencies. From Eq.(12) and Eq.(13), we obtain

\[ \gamma = \frac{d \ln(\mu_m + E_b)}{d \ln n} \]
\[ = \frac{2}{3} \left(1 + \frac{E_b}{\mu_m}\right)^{-1} \left(1 + \frac{2\alpha^{-3/2}k_FaE_F^2/\mu_m^2}{k_F^2a^2 + 2E_F/\mu_m}\right). \]

The exponent $\gamma$ (see Fig. 2) shows the expected behavior: $\gamma = 1$ in the BEC limit and $\gamma = 2/3$ in the BCS and unitarity limits. In the range of $1 < k_Fa < \infty$, $\gamma$ shows a dramatic variation. In the following, we show that this dramatic variation is directly linked to the crossover nature of the quantum gas and is a result of the distortion of the pair wave function $\psi(r)$.

From Eq. (12), we calculate $\psi(r)$ for $k_Fa = 1/2$, 2, and $\pm \infty$, shown in Fig. 3. For $k_Fa = 1/2$, we see very small deviation of $\psi(r)$ from the bare molecular wave function $\psi_0(r)$. For $k_Fa = 2$, $\psi(r)$ is clearly different from $\psi_0(r)$ with a higher probability amplitude for $r < k_F^{-1}$ and a lower amplitude for $r > k_F^{-1}$. This is the compression effect we discussed. In the unitarity limit $k_Fa = \pm \infty$, the atomic pairing is fermionic since bare molecules dissociate at this point. The mean atomic separation of

\[ \langle r \rangle \approx 2/k_F \approx 0.5 n^{-1/3} \] suggests the size of the pairs is about half of the mean molecular spacing.

The distortion of the wave functions leads to significant consequences for the quantum gas. Given the mean field energy as $\langle \hat{U} \rangle \propto n\langle r \rangle$, the evolution of the pair size from $\langle r \rangle \propto a$ in the BEC regime to $\langle r \rangle \propto n^{-1/3}$ in the unitarity limit underlies the crossover nature of the interactions from the bosonic mean field repulsion $\langle \hat{U} \rangle \propto na$ to the Fermi pressure $\langle \hat{U} \rangle \propto n^{2/3}$. This explains the variation of the exponent $\gamma$ in Fig. (2). From these observations, we can qualitatively define the BCS regime to be $k_Fa < 0$, crossover regime $1/2 < k_Fa < \infty$, and BEC regime $0 < k_Fa < 1/2$. The use of $c' \approx 16.56$ in the mean field term is appropriate in the BCS and crossover regimes and $c \approx 7.5$ in the BEC regime.

The pair wave functions can be directly probed experimentally by radio-frequency (rf) excitations as demon-
excite the bound pairs into another spin state in which the atomic separation is small compared to the intermolecular distance. In the crossover regime, $K_{pk}$ approaches a small fraction of $E_F$. The persistence of the resonance structure at unitarity and in the BCS regime indicates the correlation of the atoms in momentum space. This dependence is recently reported in [10, 11]. A quantitative comparison with the measurements, however, must include the effects of the trapping potential and the finite temperature $T$, which is outside the scope of this paper.

In conclusion, we provide a simple mean field model to describe the BEC-BCS crossover. From this equation, many properties of the strongly interacting gas can be analytically calculated with high accuracy. Our model can also be easily generalized to include the external potential and to study crossover effects in systems with lower or higher dimension.

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$F_f(K) = \frac{m}{\pi \hbar^2 k} \int_0^{\infty} \sin(kr + \delta)\psi_0(r)dr^2,$ (16)

where $K = h^2 k^2/m$, $k$, and $\delta$ are the energy, relative wave number and the scattering phase shift of the outgoing atoms, respectively.

To calculate Franck-Condon factors in the crossover regime, we replace $\psi_0(r)$ by $\psi(r)$ and assume the atoms in the outgoing channel do not interact $\delta = 0$. In Fig. 4 we show that the Franck-Condon factors display a resonance structure in the crossover regime. The location of the peak Franck-Condon factor $K_{pk}$ provides a sensitive measure of the atomic correlation length. In the BEC regime, $K_{pk}$ approaches $\frac{1}{2}E_b \gg E_F$ [22] and suggests that the atomic separation is small compared to the intermolecular distance. In the crossover regime, $K_{pk}$ approaches a small fraction of $E_F$. The persistence of the resonance structure at unitarity and in the BCS regime indicates the correlation of the atoms in momentum space. This dependence is recently reported in [10, 11]. A quantitative comparison with the measurements, however, must include the effects of the trapping potential and the finite temperature $T$, which is outside the scope of this paper.

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