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Simple mean-field model for condensates in the BEC-BCS crossover regime

Cheng Chin
James Franck Institute and Department of Physics, University of Chicago, Chicago, Illinois 60637, USA
and Institut für Experimentalphysik, Universität Innsbruck, Technikerstrasse 25, 6020 Innsbruck, Austria

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We present a mean-field model to describe condensates in the BEC-BCS crossover regime based on pairs of fermionic atoms. 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 many-body 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 [1] address an intriguing topic, the crossover from a Bose-Einstein condensate (BEC) of composite bosons to a fermionic Bardeen-Cooper-Schrieffer superfluid (BEC-BCS crossover) [2]. By magnetically tuning the interaction strength near a Feshbach resonance [3], a molecular BEC can be smoothly converted into a degenerate Fermi gas and vice versa. Experimental [4–6] and theoretical research [7,8] into the quantum gases in the crossover regime are highly active and may provide 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 [9], theoretical models on fermionic 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, first, the lack of a small expansion parameter. The full range of atomic scattering length a should be taken into account. Second, 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 system 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 [5] and on the pairing gap [10] also indicate that near the Feshbach resonance, a large fraction of fermionic atoms are paired at low temperatures. From these observations, we propose a mean-field model based on a condensate of composite bosons to describe the atom pairs in the crossover regime. This mean-field approach is relatively simple and allows us to calculate the chemical potential, the equation of states and pair correlation in the crossover regime. Our results agree very well with other many-body calculations. In particular, we find the chemical potential in the unitarity limit is ~0.4357 times that in the BCS limit, in excellent agreement with the recent quantum Monte Carlo calculations of 0.42–0.44 [12,13].

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 $\psi_0(r)=\sqrt{4\pi}r\psi_0(\vec{r})$ with $r=|\vec{r}|$ the atomic separation. Given the atomic scattering length a, $\psi_0(r)$ satisfies Schrödinger's equation,

$$-\frac{\hbar^2}{m}\psi_0''(r)=-E_b\psi_0(r), \tag{1}$$

and 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 $\psi_0(r)=(2/a)^{1/2}e^{-r/a}$ 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 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

$$\left(-\frac{\hbar^2\nabla_R^2}{4m}-\frac{\hbar^2\partial_r^2}{m}+V+\hat{U}\right)\Psi(\vec{R})\psi(r)=\mu_m\Psi(\vec{R})\psi(r), \tag{2}$$

$$\psi(0)=-a\partial_r\psi(0). \tag{3}$$

Here μ_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 directly given by the scattering length of the bosons. For molecules, however, their interaction is determined by that of the constituent atoms. Recent four-body calculation shows that the molecular interaction is effectively repulsive and the molecular scattering length is $a_m=0.60a>0$ [14].

This linear dependence can be understood with a simple picture. Scattering with a repulsive interaction leads to a scattering length proportional to the size of the scatterer. For the molecules here, we expect $a_m \sim \langle r\rangle = a/2$. From this picture, we hypothesize that the interaction term depends on the atomic degrees of freedom as $\hat{g} = g(r)$

To proceed, we consider a uniform gas with density $|\Psi(\vec{R})|^2 = n = \text{const}$. Equation (2) reduces to

$$\left(-\frac{\hbar^2}{m}\partial_r^2 + g(r)n\right)\psi(r) = \mu_m \psi(r). \tag{4}$$

To determine $g(r)$, 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 $\psi_0(r)$ should yield the molecular mean field shift $4\pi\hbar^2 a_m n/2m$,

$$\int_0^\infty \psi_0^*(r) g(r) n \psi_0(r) dr = \frac{2\pi\hbar^2 a_m n}{m}. \tag{5}$$

This equation can be satisfied for all small scattering lengths when $g(r)$ is given by a linear function

$$g(r) = c\frac{\hbar^2}{m}r, \tag{6}$$

where $c = 4\pi a_m/a \approx 7.5$ is a dimensionless constant.

Based on Eqs. (3), (4), and (6), the pair wave function can be solved as

$$\psi(r) = N\text{Ai}(c^{1/3}n^{1/3}r - c^{-2/3}\mu_m/E_0), \tag{7}$$

$$\psi(0) = -a\partial_r\psi(0), \tag{8}$$

where N is the normalization constant, $\text{Ai}(x)$ is Airy's Ai function, and $E_0 = \hbar^2 n^{2/3}/m$. Notice that Eq. (8) relates chemical potential μ_m to the scattering length a.

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 $\sim r^{-1/4}\exp\left(-\frac{2}{3}r^{3/2}\right)$. 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. [15]

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

$$\int_0^\infty \psi^*(r)\left(-\frac{\hbar^2\partial_r^2}{m}\right)\psi(r)dr = -E_b[1 + o(na^3)]. \tag{9}$$

The binding energy correction $o(na^3)$ is positive. This effect is absent in the calculations for pointlike bosons [16] since it comes from the internal degree of freedom. This result explains the augmentation of the molecular binding energy in the BEC regime, 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 identify an effective potential that can best describe the system in the BEC-BCS crossover regime.

In this regime, the four-body calculation of $a_m = 0.60a$ 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, $\hat{U} = \hat{g}|\Psi(R)|^2 = \hat{g}n$. Secondly, we exploit the asymptotic behavior of the gas in the weak coupling limit $na^3 \to 0^-$, where the system approaches an ideal degenerate Fermi gas with the chemical potential

$$\lim_{na^3 \to 0^-} \mu_m = 2E_\text{F} = \frac{(6\pi^2 n)^{2/3}\hbar^2}{m}, \tag{10}$$

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

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

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 [8]. To model the system, we adopt the mean-field term that was determined in the BCS limit, $g(r) = c'(\hbar^2/m)r$. The self-consistency of this assumption will be checked in later paragraphs. Given $c' = 6\pi^2\alpha^{-3/2}$ and the boundary condition $\partial_r\psi(0) = 0$, we can solve the chemical potential from Eqs. (7) and (8) as $\mu_m/2 = (\alpha'/\alpha)E_\text{F} \approx 0.4357E_\text{F}$, where $-\alpha' \approx -1.019$ is the first zero of the $\text{Ai}'(x)$ function.

This result agrees very well with the recent quantum Monte Carlo calculations that give $\mu_m/2 = 0.44(1)E_\text{F}$ [12] and $0.42(1)E_\text{F}$ [13], and the measurements [4,17], where the uncertainties are larger. In the vicinity of the unitarity limit, we have

$$\frac{\mu_m}{2E_\text{F}} = \frac{\alpha'}{\alpha} - \frac{\alpha^{-1/2}}{\alpha' k_\text{F} a} + O\left(\frac{1}{k_\text{F}^2 a^2}\right). \tag{11}$$

The success in the unitarity limit prompts us to extend the above model to the BEC-BCS crossover regime. Using $g(r) = c'(\hbar^2/m)r$, we rewrite Eqs. (7) and (8) as

$$\psi(r) = N\,\text{Ai}\left(\alpha^{-1/2}k_\text{F}r - \alpha\frac{\mu_m}{2E_\text{F}}\right), \tag{12}$$

$$\frac{k_\text{F}a}{\alpha^{1/2}} = -\frac{\text{Ai}(-\alpha\mu_m/2E_\text{F})}{\text{Ai}'(-\alpha\mu_m/2E_\text{F})}. \tag{13}$$

The chemical potential μ_m calculated from Eq. (13) is shown in Fig. 1. We see that μ_m approaches $2E_\text{F}$ 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 Ref. [13]. We can also evaluate the equation of

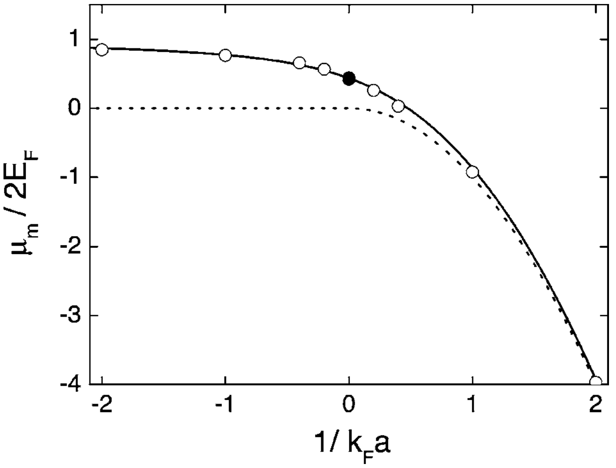

FIG. 1. Chemical potential μ_m in the crossover regime (solid line). For large $1/k_Fa$, the chemical potential μ_m approaches the energy of the molecular state $-E_b$ (dotted line). The solid dots and the open dots show the Monte Carlo calculations from Refs. [12,13], respectively.

states $\mu_m + E_b \propto n^\gamma$, where the exponent γ plays a crucial role in the collective excitation frequencies [9,18]. From Eq. (12) and (13), we obtain

$$\gamma = \frac{d\ln(\mu_m + E_b)}{d\ln n}, \tag{14}$$

$$= \frac{2}{3}\left(1+\frac{E_b}{\mu_m}\right)^{-1}\left(1+\frac{2\alpha^{-3/2}k_FaE_F^2/\mu_m^2}{k_F^2a^2+2E_F/\mu_m}\right). \tag{15}$$

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

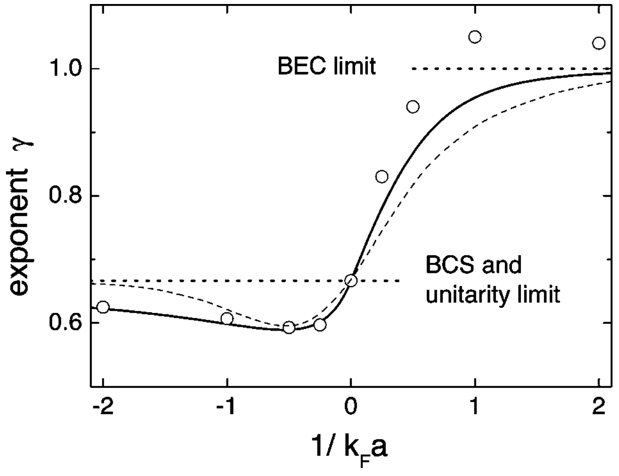

FIG. 2. Exponent γ for the equation of states from the mean-field calculation (solid line), the BCS calculation (dashed line) [19] and the fit to the quantum Monte Carlo calculation (open circles) [13,20]. The unitarity and BCS limit $\gamma=2/3$ and the BEC limit $\gamma=1$ are shown in dotted lines.

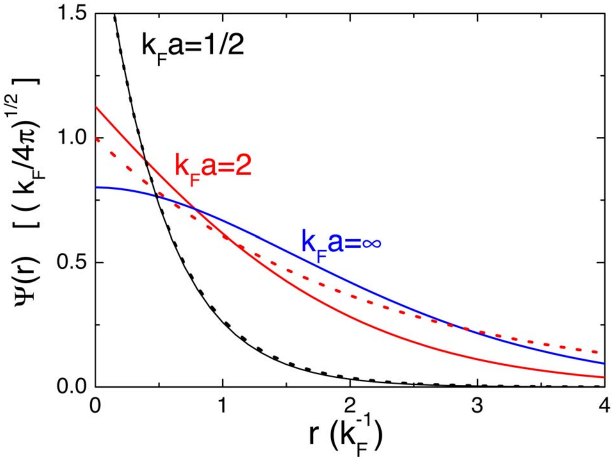

FIG. 3. (Color online) Pair wave functions in the crossover regime. Wave functions $\psi(r)$ at $k_Fa=1/2$, $k_Fa=2$, and $k_Fa=\pm\infty$, shown in solid lines, are calculated based on Eqs. (12) and (13). In the former two cases, the bare molecular wave functions $\psi_0(r)$ (dotted lines) are shown for comparison.

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 $\langle r\rangle \approx 2/k_F \approx 0.5n^{-1/3}$ suggests the size of the pairs is about half of the mean molecular spacing. Note that in our mean-field approach, $\psi(r)$ is the condensate wave function populated by all atom pairs, and should not be confused with the wave function of the Cooper pairs.

The distortion of the wave functions is in association with the BEC-BCS crossover phenomena. Given the mean-field energy as $\langle\hat{U}\rangle \propto n\langle r\rangle$, the evolution of the pair size from

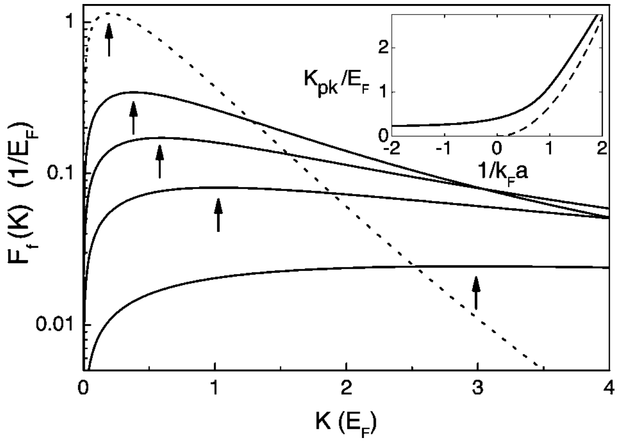

FIG. 4. Bound-free Franck-Condon factors $F_f(K)$ of the pairs for (from bottom to top) $k_Fa=1/2$, $k_Fa=1$, $k_Fa=2$, $k_Fa=\pm\infty$ (unitarity limit), and $k_Fa=0^-$ (BCS limit, dotted line). The arrows mark the peak positions K_{pk}. In the inset, K_{pk} is plotted as a function of $1/k_Fa$ (solid line) together with the K_{pk} for bare molecules (dashed line).

$\langle r\rangle \propto a$ 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 γ in Fig. 2.

The behavior of γ in Fig. 2 also shows that within the crossover regime $-1<(k_{\mathrm{F}}a)^{-1}<1$, the system is closer to a Fermi gas with $\gamma=2/3$ than to a Bose condensate with $\gamma=1$. Near the unitarity limit, γ exactly equals to that in an ideal Fermi gas. This result is consistent with many-body calculations and self-consistently supports the use of $g(r)=6\pi^2\alpha^{-3/2}(\hbar^2/m)r$ in the crossover regime.

The pair wave functions can be directly probed experimentally by radio-frequency (rf) excitations as demonstrated in Refs. [10,22]. In these experiments, rf photons excite the bound pairs into another spin state in which no bound state exists. The excited pairs then dissociate into free atoms. Theoretical calculation based on bare molecules shows that the excitation rate constant, or the bound-free Franck-Condon factor $F_f(K)$, reflects the pair wave function in the momentum space [21],

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

where $K=\hbar^2k^2/m$, k, and δ 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 $\frac{4}{3}E_b \gg E_{\mathrm{F}}$ [21] 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 [23]. These effects are outside the scope of this paper.

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[1] S. Jochim *et al.*, Science **302**, 2101 (2003); M. Greiner, C. A. Regal, and D. S. Jin, Nature (London) **426**, 537 (2003); M. W. Zwierlein *et al.*, Phys. Rev. Lett. **91**, 250401 (2003).

[2] D. M. Eagles, Phys. Rev. **186**, 456 (1969); A. J. Leggett, in *Modern Trends in the Theory of Condensed Matter* (Springer-Verlag, Berlin, 1980); P. Nozières and S. Schmitt-Rink, J. Low Temp. Phys. **59**, 195 (1985); Q. Chen, J. Stajic, S. Tan, and K. Levin, Phys. Rep. **412**, 1 (2005).

[3] E. Tiesinga, B. J. Verhaar, and H. T. C. Stoof, Phys. Rev. A **47**, 4114 (1993).

[4] M. Bartenstein *et al.*, Phys. Rev. Lett. **92**, 120401 (2004).

[5] C. A. Regal, M. Greiner, and D. S. Jin, Phys. Rev. Lett. **92**, 040403 (2004); M. W. Zwierlein *et al.*, *ibid.* **92**, 120403 (2004)

[6] J. Kinast *et al.*, Phys. Rev. Lett. **92**, 150402 (2004); M. Bartenstein *et al.*, *ibid.* **92**, 203201 (2004).

[7] E. Timmermans, K. Furuya, P. W. Milonni, and A. K. Kerman, Phys. Lett. A **285**, 228 (2001); H. Heiselberg, Phys. Rev. A **63**, 043606 (2001); Y. Ohashi and A. Griffin, Phys. Rev. Lett. **89**, 130402 (2002); A. Perali, P. Pieri, and G. C. Strinati, Phys. Rev. A **68**, 031601(R) (2003); J. Stajic *et al.*, *ibid.* **69**, 063610 (2004).

[8] H. Heiselberg, Phys. Rev. A **63**, 043606 (2001); M. Holland, S. J. J. M. F. Kokkelmans, M. L. Chiofalo, and R. Walser, Phys. Rev. Lett. **87**, 120406 (2001); T.-L. Ho, *ibid.* **92**, 090402 (2004).

[9] L. Pitaevski and S. Stringari, *Bose-Einstein Condensation* (Clarendon, Oxford, 2003).

[10] C. Chin *et al.*, Science **305**, 1128 (2004).

[11] M. Greiner, C. A. Regal, and D. S. Jin, Phys. Rev. Lett. **94**, 070403 (2005).

[12] J. Carlson, S.-Y. Chang, V. R. Pandharipande, and K. E. Schmidt, Phys. Rev. Lett. **91**, 050401 (2003).

[13] G. E. Astrakharchik, J. Boronat, J. Casulleras, and S. Giorgini, Phys. Rev. Lett. **93**, 200404 (2004).

[14] D. S. Petrov, C. Salomon, and G. V. Shlyapnikov, Phys. Rev. Lett. **93**, 090404 (2004); D. S. Petrov, C. Salomon, and G. V. Shlyapnikov, Phys. Rev. A **71**, 012708 (2005).

[15] N. Andrenacci, P. Pieri, and G. C. Strinati, Eur. Phys. J. B **13**, 637 (2000).

[16] A. Fetter and J. D. Walecka, *Quantum Theory of Many-Particle Systems* (Dover, New York, 2003).

[17] K. M. O'Hara *et al.*, Science **298**, 2179 (2002); M. E. Gehm *et al.*, Phys. Rev. A **68**, 011401(R) (2003); T. Bourdel *et al.*, Phys. Rev. Lett. **93**, 050401 (2004).

[18] H. Heiselberg, Phys. Rev. Lett. **93**, 040402 (2004)

[19] H. Hu *et al.*, Phys. Rev. Lett. **93**, 190403 (2004).

[20] N. Manini and L. Salasnich, Phys. Rev. A **71**, 033625 (2005).

[21] C. Chin and P. S. Julienne, Phys. Rev. A **71**, 012713 (2005).

[22] C. A. Regal, C. Ticknor, J. L. Bohn, D. S. Jin, Nature (London) **424**, 47 (2003).

[23] J. Kinnunen, M. Rodrguez, and P. Törmä, Science **305**, 1131 (2004).