Nonlinear Schrödinger equation for a superfluid Fermi gas in the BCS-BEC crossover

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We introduce a quasianalytic nonlinear Schrödinger equation with beyond mean-field corrections to describe the dynamics of a zero-temperature dilute superfluid Fermi gas in the crossover from the weak-coupling Bardeen-Cooper-Schrieffer (BCS) regime, where $k_F|a| \ll 1$ with a the s-wave scattering length and k_F the Fermi momentum, through the unitarity limit $k_F a \to \pm\infty$ to the Bose-Einstein condensation (BEC) regime where $k_F a > 0$. The energy of our model is parametrized using the known asymptotic behavior in the BCS, BEC, and the unitarity limits and is in excellent agreement with accurate Green's-function Monte Carlo calculations. The model generates good results for frequencies of collective breathing oscillations of a trapped Fermi superfluid.

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The crossover from a Bardeen-Cooper-Schrieffer (BCS) Fermi superfluid at zero temperature for weak coupling to a Bose-Einstein condensation (BEC) of dimers [1] has been an intense area of research (both experimental [2,3] and theoretical [4–10]) after the realization of a BCS to BEC crossover (BBC) in a trapped dilute Fermi superfluid near a Feshbach resonance. This allows one to change the system from the BCS regime, with small negative a ($k_F|a| \ll 1$), through the unitarity regime of divergent a ($k_F a \to \pm\infty$), to the BEC regime of dimers with positive a, with k_F the Fermi momentum. The limiting behavior of the system in the weak-coupling ($k_F|a| \ll 1$) [11–15] and unitarity limits for both positive and negative a is well known [12,13,16]. Accurate information about the BBC dynamics has recently been available from numerical fixed-node Green's-function Monte Carlo (GFMC) calculations [5,7] at zero temperature. There is also a mean-field BCS (MFBCS) calculation of the same [6].

A quasianalytical model for the BBC problem, generating a Ginzburg-Landau- (GL-) type equation for fermions for $a<0$ and a Gross-Pitaevskii- (GP-) type equation for dimers for $a>0$, both including beyond mean-field effects, so as to be valid in the unitarity limit of divergent a, should be useful. We propose such a model in three dimensions, called the BBC model (BBM), for the crossover problem of a dilute trapped Fermi superfluid at zero temperature using the known theoretical solution in the weak-coupling and unitarity limits in both the BCS and BEC regimes.

We consider a dilute superfluid Fermi gas of N spin-1/2 atoms of mass m, atomic scattering length a, and density n with singlet pairing due to an attractive atomic interaction. We assume, for a dilute gas, that the results are universal, determined solely by the scattering length a, and independent of the details of the interaction potential and its range. We present an analytical model for energy and bulk chemical potentials in the entire crossover region and hence derive a nonlinear equation for the superfluid Fermi gas. We present results for radial and axial frequencies of collective oscillation in a cigar-shaped trap and compare with GFMC and MFBCS calculations as well as experimental data.

At low densities, in the BCS regime ($k_F|a| \ll 1$), gaps are negligible [4,12] and the total energy E per particle of the superfluid Fermi gas is given by [11,13]

$$\frac{E}{N} = \frac{3}{5}E_F\left[1 + \frac{10}{9\pi}k_F a + \frac{4(11-2\ln 2)}{21\pi^2}(k_F a)^2 + 0.030\,467(k_F a)^3 - 0.062\,013(k_F a)^4 + \cdots\right], \quad (1)$$

where $E_F \equiv \hbar^2 k_F^2/(2m) = An^{2/3} \equiv \frac{\hbar^2}{2m}(3\pi^2 n)^{2/3}$ is the Fermi energy with $k_F = (3\pi^2 n)^{1/3}$ [4].

In the BEC regime ($a>0$), the paired fermions form a weakly repulsive Bose gas of dimers of mass $m' = 2m$ and density $n' = n/2$ with a dimer-dimer scattering length $a' = 0.6a$, as predicted by Petrov *et al.* [17] (valid for $a \gg R_0$, where R_0 is the typical range of interatomic potential). In this regime, the energy of the system is given by [4,5,15]

$$\frac{E}{N} + \frac{\varepsilon_B}{2} = \frac{3}{5}E_F\left[\frac{5(k_F a')}{18\pi} + \frac{64(k_F a')^{5/2}}{27\sqrt{6\pi^5}} + \cdots\right], \quad (2)$$

with $a' = 0.6a$ [17], where ε_B is the (positive) binding energy of the dimer. (Using an attractive square-well interatomic potential model, Astrakharchik *et al.* [5] calculated dimer binding energy ε_B.) The dynamics of the dimer bosons is governed by the energy $(E/N + \varepsilon_B/2)$ discounted for dimer binding. The lowest-order term in Eqs. (1) and (2) leads to the standard mean-field GL equation for Fermi superfluid and GP equation for dimer bosons, respectively, with higher-order terms leading to beyond mean-field corrections due to interaction.

The limiting energies (1) and (2), valid for small $|a|$, drastically fail as one approaches the unitarity limit $a \to \pm\infty$. For a dilute Fermi superfluid, the unitarity limit is supposed to be universal and the relevant energy scale is the energy of the noninteracting Fermi gas $3E_F/5$ [14,18], so that the energy of the system is given by [12,13] $E/N = 3E_F\xi/5$ with ξ a universal factor. By using the Padé approximant Baker [13] estimated two values for $\xi = 0.326$ and 0.568, and Heiselberg [12] obtained $\xi = 0.326$. Later, from experimental results the following values for ξ have been obtained $\xi = 0.51 \pm 0.04$ [19], 0.7 [20], $0.27^{+0.12}_{-0.09}$ [21], 0.41 ± 0.15 [22], 0.46 ± 0.05 [23], and $0.46^{+0.05}_{-0.12}$ [24]. The accurate theoretical estimates for the factor ξ are $\xi = 0.44 \pm 0.01$ [7] and 0.437 ± 0.009

(GFMC) [14] and 0.59 (MFBCS) [6]. Bulgac and Bertsch [16] suggested the following approximate behavior of energy per particle near the $(k_F|a|)^{-1}\to 0$ limit:

$$\frac{E}{N}=\frac{3}{5}E_F\left[\xi-\zeta(k_Fa)^{-1}-\frac{5}{3}v(k_Fa)^{-2}+\cdots\right] \tag{3}$$

in both BCS ($a<0$) and BEC ($a>0$) regimes with $\zeta\approx v\approx 1$. In the BEC regime ($a>0$), one should replace $\frac{E}{N}$ by $\frac{E}{N}+\frac{\varepsilon_B}{2}$.

We write a simple expression for energy E/N combining the limiting behaviors (1) and (3) in fermion ($a<0$) and dimer boson ($a>0$) regimes. We suggest the following expression for the fermion energy for $a<0$:

$$\frac{E}{N}=\frac{3}{5}E_F\left[1+\frac{\frac{10k_Fa}{9\pi}}{1-\frac{10k_Fa}{9\pi(1-\xi)}}\right]. \tag{4}$$

This expression has the constant $10/(9\pi)$ taken from the limit (1) and the constant ξ from the limit (3). Expression (4) reproduces the first two terms in Eq. (1) exactly for small $|a|$. It also reproduces the first term in Eq. (3) for large $|a|$; for the second term, it yields $\zeta=0.9186$ in place of the approximate value $\zeta\approx 1$

For $a>0$, we use the asymptotic behaviors of energy for large and small a, Eqs. (2) and (3), to propose the following expression for the energy:

$$\frac{E}{N}+\frac{\varepsilon_B}{2}=\frac{3}{5}E_F\left[\frac{\frac{5}{18\pi}(k_Fa')+\frac{64}{27\sqrt{6\pi^5}}(k_Fa')^{5/2}}{1+\frac{64(a'/a)(k_Fa')^{3/2}}{27\xi^2\sqrt{6\pi^5}}+\frac{64(k_Fa')^{5/2}}{27\xi\sqrt{6\pi^5}}}\right]. \tag{5}$$

For large a', by construction, expression (5) satisfies Eq. (3) with $\zeta=1$. For small a it reproduces the first term of expansion (2) exactly and the next terms closely.

The only free parameter in the model, Eqs. (4) and (5) (termed BBM), is the universal factor ξ, for which we use $\xi=0.44$ [5,7,14]. The k_Fa dependence of BBM (4) and (5) is consistent with the behavior for small and large $k_F|a|$. Kim and Zubarev [9] considered two different [2/2] Padé approximants to parametrize energy in the Fermi superfluid and BEC regimes. Manini and Salasnich [8] considered an energy function with arctan dependence on scattering length in both the Fermi superfluid and dimer BEC regimes.

Next, we plot in Fig. 1, for $a<0$, the energy from Eq. (4), in addition to those from limits (1) and (3). We also plot the results of GFMC calculations of Refs. [7,14] and parametrizations of Refs. [8,9]. Next we plot, for $a>0$, in Fig. 2, the results for energy from Eq. (5), the asymptotic limits (2) and (3), the GFMC results of Refs. [7,14], and the parametrizations of Refs. [8,9].

From Figs. 1 and 2, we realize that the limits (1) and (3), essentially, determine the energy for $k_F|a|<1$ and $k_F|a|>10$. The correct energy over the entire crossover should be a smooth interpolation between these limits. This

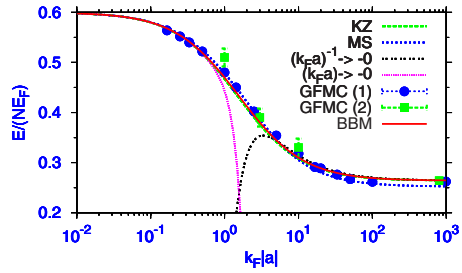

FIG. 1. (Color online) $E/(NE_F)$ vs $k_F|a|$ for $a<0$: BBM, Eq. (4); KZ from Ref. [9]; MS from Ref. [8]; limiting value $(k_Fa)^{-1}\to -0$ of Eq. (3); limiting value $k_Fa\to -0$ of Eq. (1); GFMC (1) [14]; GFMC (2) [7].

is what has been done to obtain the present results for $a<0$ and $a>0$, in very good agreement with the accurate GFMC calculations [7,14] and asymptotic limits.

To study the collective and bulk properties of the superfluid Fermi gas, we write convenient mean-field equations. They are, essentially, the Schrödinger equation with a nonlinear term equal to the bulk chemical potential $\mu(n,a)=\partial\mathcal{E}/\partial n$, with $\mathcal{E}\equiv(E/N)n$ the energy density. A straightforward calculation with the leading two terms of energy of Eq. (1) yields the following bulk chemical potential for $a\to -0$ [4]:

$$\mu(n,a)=An^{2/3}+2\pi\hbar^2an/m, \tag{6}$$

to be used in the nonlinear Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\Psi=\left[-\frac{\hbar^2}{2m^*}\nabla_{\mathbf{r}}^2+U(\mathbf{r})+\mu(n,a)\right]\Psi, \tag{7}$$

where $U(\mathbf{r})$ is a trap, $(\mathbf{r},t)$ are space and time variables, the density n is related to the order parameter Ψ by $n=|\Psi|^2$, such that $\int n\,d\mathbf{r}=N$, and $m^*\approx 2m$ is the effective mass of pairs. This equation can also be interpreted to be the Euler-Lagrange equation of a time-dependent density functional theory [8,25]. Also, for a large number of atoms, N, for a description of collective properties Eq. (6) is completely equivalent to the quantum hydrodynamic equations [4]. The first term on the right-hand side of Eq. (6) is the standard nonlinearity in the three-dimensional GL equation of a Fermi superfluid (equal to Fermi energy) with the last term appearing due to atomic interaction. This last term is reduced by a

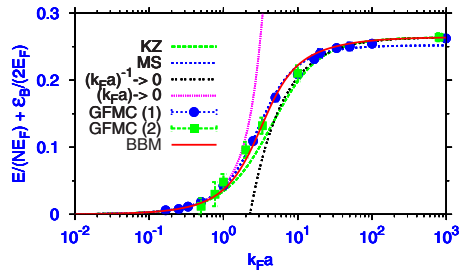

FIG. 2. (Color online) $E/(NE_F)+\epsilon_B/(2E_F)$ vs k_Fa for $a>0$: BBM, Eq. (5); KZ from Ref. [9]; MS from Ref. [8]; limiting value $(k_Fa)^{-1}\to +0$ of Eq. (3); limiting value $k_Fa\to +0$ of Eq. (2); GFMC (1) [14]; GFMC (2) [7].

factor of 2 compared to the GP nonlinearity for bosons $(4\pi\hbar^2 an/m)$, as, in the present case, half of the atomic interactions, those between spin-parallel fermions, are inoperative.

The bulk chemical potential $\mu(n,a)$ corresponding to the BBM energy (4),

$$\mu(n,a) = An^{2/3}\frac{1-\dfrac{4(3\pi^2 n)^{1/3}}{9\pi}a\dfrac{2+3\xi}{1-\xi}+\dfrac{100(3\pi^2 n)^{2/3}\xi}{81\pi^2(1-\xi)^2}a^2}{\left(1-\dfrac{10(3\pi^2 n)^{1/3}}{9\pi(1-\xi)}a\right)^2}, \tag{8}$$

is to be used in Eq. (7). A simpler expression for bulk chemical potential can be obtained if we recall that, in the unitarity limit $(a\to-\infty)$, the energy is given by $E/N=3E_F\xi/5$ corresponding to a bulk chemical potential [13]

$$\mu(n,a) = \hbar^2(3\pi^2 n)^{2/3}\xi/(2m). \tag{9}$$

In the full crossover problem, combining the limiting values (6) and (9), we suggest the following bulk chemical potential in BBM valid for all negative a:

$$\mu(n,a) = An^{2/3}\left(1+\frac{\dfrac{4\pi}{(3\pi^2)^{2/3}}an^{1/3}}{1-\dfrac{4\pi}{(1-\xi)(3\pi^2)^{2/3}}an^{1/3}}\right), \tag{10}$$

to be used in Eq. (7). This is the simplest minimal bulk chemical potential consistent with limits (6) and (9). Expression (8) also satisfies these limits and is consistent with the accurate GFMC calculations. We have checked through numerical calculation that expressions (8) and (10) agree with each other within an error of less than 1%. We suggest here the GL-type BBM, Eqs. (7) and (10), including beyond mean-field corrections valid for $a<0$ and especially in the unitarity limit $a\to-\infty$.

For $a>0$, from Eq. (2), in the small-a' limit, the leading terms in energy density can be written as

$$\mathcal{E}' = \frac{2\pi\hbar^2 n'^2 a'}{m'}+\frac{256\sqrt{\pi}}{15}\frac{\hbar^2}{m'}(n'a')^{5/2}. \tag{11}$$

This result, applicable to dimers, is written in terms of dimer variables denoted by prime and is obtained for a uniform hard-sphere Bose gas (here composite bosonic dimers) in a perturbation calculation for small $n'a'^3$ [26]. This leads to a bulk chemical potential [4,15]

$$\mu'(n',a') = \frac{4\pi\hbar^2 a' n'}{m'}+128\sqrt{\pi}\frac{\hbar^2 a'^{5/2} n'^{3/2}}{3m'} \tag{12}$$

in the mean-field equation (7), however now with mass, trap, scattering length, particle number, etc., appropriate for dimers. We have recovered in Eq. (12) the proper beyond mean-field generalization of the GP equation for small a [26]. In the large-a limit, from Eq. (9), the leading term in the bulk chemical potential is given by [4]

$$\mu'(n',a') = \xi\hbar^2(6\pi^2)^{2/3}n'^{2/3}/m'. \tag{13}$$

Equations (12) and (13) can be combined to form the following chemical potential valid for small and large a:

$$\mu'(n',a') = \frac{\dfrac{4\pi\hbar^2 a' n'}{m'}\left(1+\dfrac{64}{3\sqrt{\pi}}a'^{3/2}\sqrt{n'}\right)}{1+\dfrac{32}{3\sqrt{\pi}}a'^{3/2}\sqrt{n'}+\dfrac{64}{3\sqrt{\pi}}\dfrac{2\pi}{(6\pi^2)^{2/3}\xi}a'^{5/2}n'^{5/6}}. \tag{14}$$

This bulk chemical potential has been constructed to satisfy Eq. (13) for large a' and Eq. (12) for small a'. [After a simple algebra it can be shown that Eq. (14) satisfies limit (3) for large a' with $\zeta\approx 1$.] Expression (14) is much simpler than that obtained directly from Eq. (5). Equations (7) and (14) are the present GP-type BBM equations for the bosonic dimers including beyond mean-field corrections valid for $a>0$ and especially in the unitarity limit. For $\xi=0.44$, Eq. (14) produces the following unitarity limit for composite bosonic dimers: $\mu'(n',a')=\kappa\hbar^2 n'^{2/3}/m'$, $\kappa\approx 7$. For fundamental bosons a similar relation is obtained with a different coefficient κ [18]. Equations (7) and (14) with a different numerical coefficient ξ appropriate for the study of a fundamental-boson superfluid have recently been suggested [27].

Next we subject bulk chemical potential (14) to the stringent test by calculating the radial and axial frequencies ν_ρ and ν_z of collective oscillations in a cigar-shaped trap, where $\mathbf{r}\equiv(\rho,z)$ are the radial (ρ) and axial (z) coordinates. Cozzini and Stringari [4,28] showed that for a power-law politropic dependence of bulk chemical potential on density $\mu'\propto n'^\Gamma$, ν_ρ and ν_z are given by $\nu_\rho^2=2(\Gamma+1)$ [8] $\nu_z^2=3-1/\Gamma(\Gamma+1)$, respectively, with $\Gamma=\frac{n'}{\mu'}\frac{\partial\mu'}{\partial n'}$. To test the BBM, we plot, in Figs. 3(a) and 3(b), ν_ρ^2 and ν_z^2 vs $\arctan(1/k_F a)$, respectively, and compare them with the GFMC and MFBCS calculations and experimental data of Refs. [3,29], as quoted in Refs. [8,30,31]. The end points of the present BBM plot in Fig. 3 are determined by the value of $\Gamma=2/3$ and 1 at $a=+\infty$ and 0, respectively. However, as ν^2 is related to the derivative $\partial\mu'/\partial n'$, bulk chemical potential (14) provides a good fit of the derivative of the μ'-n' curve to theoretical models [6,31] and experiment [3,31] in addition to the μ'-n' curve as can be seen from Fig. 3. In this figure the difference between different curves is small (of the order of 2%–3%) and by slightly altering the constants in Eq. (14) we can obtain a result close to either the GFMC or MFBCS plot. We did not do so, and the present result is obtained only from asymptotic conditions without any fitting.

Finally, we solve, numerically, for a spherical harmonic trap, Eqs. (7) and (10) for fermions $(a<0)$ and Eqs. (7) and (14) for dimer bosons $(a>0)$, by the method of imaginary time propagation after discretizing it with the semi-implicit Crank-Nicholson rule. We employ the length scale $l=\sqrt{\hbar/m\omega}$ and time scale $(\tau=\omega^{-1})$ with ω the angular frequency of the trap and 2000 fermionic atoms (1000 dimers). In numerical simulation we use $l=0.025$ and $\tau=0.001$. The calculated densities plotted in Fig. 4 show interesting behav-

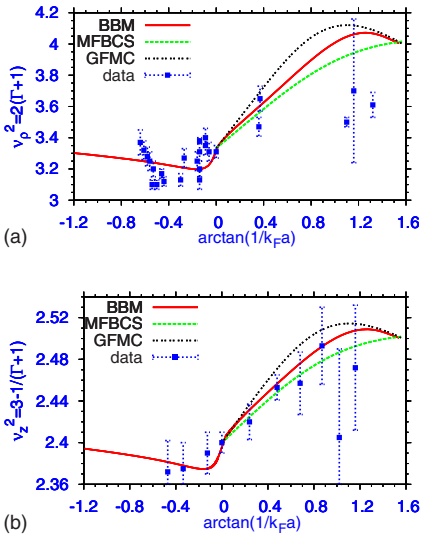

FIG. 3. (Color online) Square of the radial and axial frequencies (a) ν_ρ^2 and (b) ν_z^2 in a cigar-shaped trap vs $k_F a$, for BBM (14), GFMC, and MFBCS as quoted in [31]. Data for radial frequency taken from Refs. [8,29] and those for axial frequency taken from Refs. [3,30,31].

ior. The rms radius r_{rms} in different regimes obeys the inequalities $r_{rms}^{a\to-0} > r_{rms}^{|a|\to\infty} > r_{rms}^{a\to+0}$ with numerical values 4.74 μm, 3.85 μm, and 1.25 μm, respectively. The size depends on the respective nonlinearity, increasing as the nonlinearity increases. In the BCS limit ($a\to-0$) the Fermi gas extends to a greater distance than at unitarity due to an increased repulsion. The ideal dimer Bose gas with $a'=0$ has the most compact structure due to no repulsion.

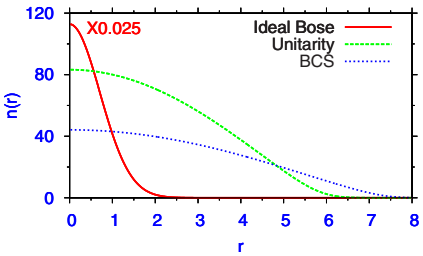

FIG. 4. (Color online) Density $n(r)$ vs r in units of oscillator length ($l=\sqrt{\hbar/m\omega}$) in BCS and BEC regimes normalized to $4\pi\int n(r)r^2dr=N=2000$: Unitarity $|a|\to\infty$, ideal BEC $a\to+0$, and BCS $a\to-0$.

To conclude, we proposed and solved numerically a quasianalytic nonlinear Eq. (7) for BCS-BEC crossover of a dilute Fermi gas with beyond mean-field correction so that it is valid in the unitarity region with divergent scattering length a. This model produces the known analytic behavior of the energy and bulk chemical potential of the system (dependence on scattering length) in the BCS ($a\to-0$), BEC ($a\to+0$), and unitarity $a\to\pm\infty$ limits. For $a<0$ (Fermi regime), the equations are GL-type equations (7) and (10), and for $a>0$ (dimer BEC regime), they are the GP-type equations (7) and (14). The calculated radial and axial frequencies of collective breathing oscillation of a system in a cigar-shaped trap are found to be in good agreement with experiment and GFMC and MFBCS calculations.

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