Nonlinear Schrödinger equation for a superfluid Fermi gas from BCS to Bose crossover

S. K. Adhikari
Instituto de Física Teórica, UNESP - São Paulo State University, 01.405-900 São Paulo, São Paulo, Brazil

We introduce a quasi-analytic 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, $k_Fa \to \pm \infty$, to the Bose regime where $k_Fa > 0$. The energy of our model is parametrized using the known asymptotic behavior in the BCS, Bose, and the unitarity limits and is in excellent agreement with accurate Green function Monte Carlo calculations. The model generates good results for frequencies of collective breathing oscillation of a trapped Fermi superfluid.

PACS numbers: 71.10.Ay, 03.75.Ss, 67.85.Lm, 05.30.Fk

The crossover from a Bardeen-Cooper-Schrieffer (BCS) Fermi superfluid at zero temperature for weak coupling to a Bose condensate of dimers has been an intense area of research (both experimental [2,3] and theoretical [4,5,6,7,8,9,10]) after the realization of a BCS to Bose crossover (BBC) in a trapped dilute Fermi superfluid near a Feshbach resonance. This allows to change the system from the BCS regime, with small negative $a$ ($k_F|a| \ll 1$), through the unitarity regime of divergent $a$ ($k_Fa \to \pm \infty$), to the Bose regime of dimers with positive $a$, with $k_F$ the Fermi momentum. The limiting behavior of the system in the weak-coupling ($k_F|a| \ll 1$) [11,12,13,14,15] and unitarity limits for both positive and negative $a$ are 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 mean-field BCS (MFBCS) calculation of the same [6].

A quasi-analytical 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 Bose regimes.

We consider a dilute superfluid Fermi gas of $N$ spin-half 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 detail of the interaction potential and its range. We present an analytical model for energy and bulk chemical potential 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 $E/N$ per particle of the superfluid Fermi gas is given by [11,13]

$$E/N = \frac{3}{5} E_F \left[ 1 + \frac{10}{9\pi} k_F a + \frac{4(11 - 2\ln 2)}{21\pi^2} (k_F a)^2 + 0.030467(k_F a)^3 - 0.062013(k_F a)^4 + \cdots \right],$$

(1)

where $E_F \equiv \hbar^2 k_F^2/(2m) = \pi^2 a^2 / (2m) (3\pi^2 n)^{2/3}$ is the Fermi energy with $k_F = (3\pi^2 n)^{1/3}$. In the Bose 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]. In this regime, the energy of the system is given by [4,5,15]

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

(2)

with $a' = 0.6a$ [17], where $\varepsilon_B$ is the (positive) binding energy of the dimer. 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 $E/N = 3E_F\xi/5$ with $\xi$ a universal factor. By using Padè 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 $\xi$ have been obtained $\xi = 0.51 \pm 0.04$ [19], 0.7 [20], 0.27 [21], 0.41 ± 0.15 [22], 0.46 ± 0.05 [23], and 0.46 ± 0.12 [24]. The accurate theoretical estimates for the factor $\xi$ are $\xi = 0.44 \pm 0.01$ [7] and 0.437 ± 0.009 (GFMC)
Bulgac and Bertsch\cite{BBM} suggested the following approximate behavior of energy per particle near the \((k_F|a|)^{-1} \to 0\) limit
\[
\frac{E}{N} = \frac{3}{5} E_F [\xi - \frac{5}{3} \nu (k_F a)^{-2} + \ldots] \tag{3}
\]
in both BCS \((a < 0)\) and Bose \((a > 0)\) regime with \(\xi \approx \nu \approx 1\). In the Bose regime \((a > 0)\), one should replace \(\frac{\xi}{\nu}\) by \(\frac{\xi + \nu}{2}\).

We write a simple expression for energy \(E/N\) combining the limiting behaviors\cite{BF} and \cite{S} in fermion \((a < 0)\) and dimer boson \((a > 0)\) regime. We suggest the following expression for fermion energy for \(a < 0\)
\[
\frac{E}{N} = \frac{3}{5} E_F \left[ 1 + \frac{10 k_F a}{9 \pi} \right]. \tag{4}
\]
This expression has the constant \(10/(9\pi)\) taken from limit\cite{BF} and the constant \(\xi\) from limit\cite{S}. Expression\cite{SBF} reproduces the first two terms in Eq. \cite{BF} exactly for small \(|a|\). It also reproduces the first term in Eq. \cite{S} for large \(|a|\), for the second term it yields \(\xi = 0.9186\) in place of the approximate value \(\xi \approx 1\).

For \(a > 0\), we use the asymptotic behaviors of energy for large and small \(a\), Eqs. \cite{KZ} and \cite{MS}, to propose the following expression for energy
\[
\frac{E}{N} + \frac{\varepsilon_B}{2} = \frac{3}{5} E_F \left[ \frac{5}{12} (k_F a') + \frac{64}{27 \sqrt{6} \pi^2} (k_F a')^{5/2} \right] \ldots \tag{5}
\]
For large \(a'\), by construction, expression\cite{SBF} satisfies Eq. \cite{S} with \(\xi = 1\). For small \(a\) it reproduces the first term of expansion\cite{KZ} exactly and the next terms closely.

The only free parameter in model Eqs. \cite{BF} and \cite{SBF} (termed BBM) is the universal factor \(\xi\), for which we use \(\xi = 0.44\).\cite{BF, S, BBM}. The \(k_F a\) dependence of BBM\cite{BF} and \cite{SBF} is consistent with the behavior for small and large \(k_F|a|\). Kim and Zubarev\cite{KZ} considered two different[2/2] Padé approximants to parametrize energy in the Fermi superfluid and Bose dimer regimes. Manini and Salasnich\cite{MS} considered an energy function with arctan dependence on scattering length both in the Fermi superfluid and Bose dimer regimes.

Next we plot in Fig. \ref{fig1} for \(a < 0\), the energy from Eq. \cite{BF}, in addition to those from limits \cite{KZ} and \cite{MS}. We also plot the results of GFMC calculations of Refs. \cite{BBM, BF} and parametrizations of Refs. \cite{KZ, MS}. Next we plot, for \(a > 0\), in Fig. \ref{fig2} the results for energy from Eq. \cite{SBF}, the asymptotic limits \cite{KZ} and \cite{MS}, the GFMC results of Refs. \cite{BBM, BF} and the parametrizations of Ref. \cite{KZ, MS}.

From Figs. \ref{fig1} and \ref{fig2} we realize that limits\cite{KZ} and \cite{MS}, essentially, determine the energy for \(k_F|a| < 1\) and \(k_F|a| > 1\). The correct energy over the entire crossover should be a smooth interpolation between these limits. This 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 \cite{BBM, BF} and asymptotic limits.
action. This last term is reduced by a 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 BBM energy \(\mathbb{H}\)

\[
\mu(n, a) = An^{2/3} \left(1 - \frac{4(3n^2)^{1/3} - \frac{2\sqrt{2\pi}}{\sqrt{3}} + \frac{100(3n^2)^{2/3}}{8\pi^2(1-\xi^2)a^2}}{(1 - \frac{100(3n^2)^{1/3}}{8\pi^2(1-\xi^2)a^2})^2} \right)
\]

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 \[13\]

\[
\mu(n, a) = \hbar^2(3n^2)^{2/3}\xi/(2m).
\]

In the full crossover problem, combining the limiting values \(\mathbb{H}\) and \(\mathbb{H}^\prime\), we suggest the following bulk chemical potential in BBM valid for all negative \(a\)

\[
\mu(n, a) = An^{2/3} \left(1 + \frac{4\pi}{(3n^2)^{1/3}an^{1/3}} \right).
\]

to be used in Eq. (7). This is the simplest minimal bulk chemical potential consistent with limits \(\mathbb{H}\) and \(\mathbb{H}^\prime\). Expression \(\mathbb{H}\) also satisfies these limits and is consistent with the accurate GFMC calculations. We have checked through numerical calculation that expressions \(\mathbb{H}\) and \(\mathbb{H}^\prime\) agree to 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 specially 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

\[
\mathcal{E}' = \frac{2\pi\hbar^2n'^2a'}{m'} + \frac{256\sqrt{\pi} \hbar^2}{15} \frac{n'(a')^{3/2}}{m'(n'a')^{3/2}}.
\]

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 \(n'a'^3\). This leads to a bulk chemical potential \(\mu' = \mathbb{H}'\)

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

in the mean-field Eq. (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 \(a\).

In the large \(a\) limit, from Eq. (9), the leading term in the bulk chemical potential is given by \(\mu\)

\[
\mu'(n', a') = \xi^2(6\pi^2)^{2/3}n'^{2/3}/m'.
\]

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. (13) satisfies limit \(\mathbb{H}\) for large \(a'\) with \(\zeta \approx 1\).) Expression (13) is much simpler than that obtained directly from Eq. (5). Equations (7) and (13) 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. (13) produces the following unitarity limit for composite bosonic dimers \(\mu'(n', a') = \kappa\hbar^2n'^{2/3}/m', \kappa \approx 7\). For fundamental bosons a similar relation is obtained with a different coefficient \(\kappa [18]\). Equations (7) and (13) with a different numerical coefficient \(\xi\) appropriate for the study of a fundamental-boson superfluid has recently been suggested [27].

Next we subject bulk chemical potential (13) to the stringent test by calculating the radial and axial frequencies \(\nu_\rho\) and \(\nu_z\) of collective oscillation in a cigar shaped trap, where \(r = (p, z)\) are the radial \(p\) and axial \(z\) coordinates. Cozzi and Stringari [11, 28] showed that for a power-law poltropic dependence of bulk chemical potential on density \(\mu' \propto n'^3\), \(\nu_\rho\) and \(\nu_z\) are given by \(\nu_\rho^2 = 2(\Gamma + 1)\) \(\nu_z^2 = 3 - 1/\Gamma(\Gamma + 1)\), respectively, with \(\Gamma = \frac{n'}{\mu'} \frac{\partial \mu'}{\partial n'}\). To test the BBM, we plot, in Fig. 3 (a) and (b), \(\nu_\rho^2\) and \(\nu_z^2\) vs. \(\text{atan}(1/k_Fa)\), respectively, and

![Image](https://via.placeholder.com/150)
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 $\nu^2$ is related to the derivative $\partial\mu/\partial\nu^2$, bulk chemical potential [11] provides a good fit of the derivative of the $\mu - n'$ curve to theoretical models [3, 31] and experiment [3, 31] in addition to the $\mu - n'$ curve as can be seen from Fig. 3. In this figure the difference between different curves is small (order of 2% to 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 condition without any fitting.

Finally, we solve, numerically, for a spherical harmonic trap, Eqs. (17) and (10) for fermions ($a < 0$) and Eqs. (17) 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 length scale $l = (\hbar/m\omega)^{1/2}$ and time scale $(\tau = \omega^{-1})$ with $\omega$ the angular frequency of 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 behavior. The rms radius $r_{\text{rms}}$ in different regimes obey inequalities $r_{\text{rms}}^a \rightarrow 0 = r_{\text{rms}}^{|a| \rightarrow \infty} > r_{\text{rms}}^a \rightarrow +0$ with numerical values 4.74\mu m, 3.89\mu m, and 1.25\mu m, respectively. The size depends on the respective nonlinearity, increasing as the nonlinearity increases. In the BCS limit ($a \rightarrow -0$) 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.

To conclude, we proposed and solved numerically a quasi-analytic nonlinear Eq. (7) for Bose to BCS 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 ($a \rightarrow -0$), Bose ($a \rightarrow +0$), and unitarity $a \rightarrow \pm \infty$ limits. For $a < 0$ (Fermi regime), the equations are GL-type Eqs. (7) and (10), and for $a > 0$ (dimer Bose regime), they are the GP-type Eqs. (17) 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.

We thank Luca Salasnich for valuable discussion, Stefano Giorgini for additional results [14] and FAPESP and CNPq (Brazil) for partial support.

[1] D. M. Eagles, Phys. Rev. 186, 456 (1969); A. J. Leggett, J. Phys. (Paris) Colloq. 41, C7-19 (1980).
[2] M. Greiner et al., Nature (London) 426, 537 (2003); T. Bourdel et al., Phys. Rev. Lett. 93, 050401 (2004).
[3] M. Bartenstein et al., Phys. Rev. Lett. 92, 203201 (2004).
[4] S. Giorgini et al., Rev. Mod. Phys. in press (2008).
[5] G. E. Astrakharchik et al., Phys. Rev. Lett. 93, 200404 (2004); J. Carlson et al., ibid. 91, 050401 (2003).
[6] J. R. Engelbrecht, M. Randeria, and C. A. R. Sá de Melo, Phys. Rev. B 55, 15153 (1997).
[7] S. Y. Chang et al., Phys. Rev. A 70, 043602 (2004).
[8] N. Manini and L. Salasnich, Phys. Rev. A 71, 033625 (2005).
[9] Y. E. Kim, and A. L. Zubarev, Phys. Rev. A 70, 033612 (2004).
[10] P. Pieri and G. C. Strinati, Phys. Rev. Lett. 91, 030401 (2003); G. C. Strinati and P. Pieri, Phys. Rev. A 69, 011601(R) (2004).
[11] T. D. Lee and C. N. Yang, Phys. Rev. 105, 1119 (1957).
[12] H. Heiselberg, Phys. Rev. A 63, 043606 (2001).
[13] G. A. Baker, Jr., Phys. Rev. C 60, 054311 (1999); Int. J. Mod. Phys. B 15, 1314 (2001).
[14] S. Giorgini, private communication (2008).
[15] T. D. Lee et al., Phys. Rev. 106, 1135 (1957).
[16] A. Bulgac and G. F. Bertsch, Phys. Rev. Lett. 94, 070401 (2005).
[17] D. S. Petrov et al., Phys. Rev. Lett. 93, 090404 (2004).
[18] S. Cowell et al., Phys. Rev. Lett. 88, 210403 (2002).
[19] M. E. Gehm et al., Phys. Rev. A 68, 011401(R) (2003); J. Kinast et al., Science 307, 1296 (2005).
[20] T. Bourdel et al., Phys. Rev. Lett. 91, 020402 (2003).
[21] M. Bartenstein et al., Phys. Rev. Lett. 92, 120401 (2004).
[22] L. Tarruell et al., e-print [cond-mat/0701151].
[23] G. B. Partridge et al., Science 311, 503 (2006).
[24] J. T. Stewart et al., Phys. Rev. Lett. 97, 220406 (2006).
[25] H. Hu et al., Phys. Rev. Lett. 93, 190403 (2004).
[26] A. Fabrocini and A. Polls, Phys. Rev. A 60, 2319 (1999).
[27] S. K. Arthikarla and L. Salasnich, e-print arXiv:0801.4302.
[28] M. Cozzini and S. Stringari, Phys. Rev. Lett. 91, 070401 (2003).
[29] J. Kinast et al., Phys. Rev. A 70, 051401(R) (2004).
[30] R. Combescot and X. Leyronas, Phys. Rev. Lett. 93, 130401 (2004).
[31] G. E. Astrakharchik et al., Phys. Rev. Lett. 95, 030404.
(2005).