Bogoliubov excitations of trapped superfluid Fermi gases in a BCS-BEC crossover beyond the Thomas-Fermi limit

Yong-li Ma*
Department of Physics, Fudan University, Shanghai 200433, China

Guoxiang Huang†
Department of Physics and Key Laboratory of Optical and Magnetic Resonance Spectroscopy, East China Normal University, Shanghai 200062, China

(Received 5 February 2007; revised manuscript received 28 April 2007; published 27 June 2007)

We study the Bogoliubov collective excitations of harmonically trapped superfluid Fermi gases in the crossover from Bardeen-Cooper-Schrieffer (BCS) superfluid to Bose-Einstein condensate (BEC) beyond Thomas-Fermi (TF) limit. Starting from a generalized Gross-Pitaevskii equation and an equation of state valid for the whole crossover, we derive Bogoliubov-de Gennes (BdG) equations for low-lying collective modes at zero temperature. We use a Fetter-like variational ground state wave function to remove the noncontinuity of slope at the boundary of condensate, which appears in the TF limit. We solve the BdG equations analytically and obtain explicit expressions for all eigenvalues and eigenfunctions, valid for various crossover regimes and for traps with spherical and axial symmetries. We discuss the feature of these collective excitations in the BCS-BEC crossover and show that the theoretical result obtained agrees with available experimental data near and beyond the TF limit.

DOI: 10.1103/PhysRevA.75.063629

PACS number(s): 03.75.Ss, 03.75.Kk, 67.55.Jd

I. INTRODUCTION

The crossover from Bardeen-Cooper-Schrieffer (BCS) superfluid to Bose-Einstein condensation (BEC), a topic not only of fundamental interest in condensed matter theory but also closely related to the understanding of physical mechanism for high-$T_c$ superconductivity, has received much attention in recent years [1,2]. Ultracold quantum degenerate gases of fermionic atoms (such as $^6$Li and $^{40}$K) with tunable interaction [3] offer an excellent opportunity for deep exploration on the property of BCS-BEC crossover in a controllable way. Experimentally, condensed fermionic atomic pairs in the regimes of BEC [4], BCS [5], and their crossover [6] have been observed successfully and their various superfluid properties have been investigated in detail recently by using a magnetic-field-induced Feshbach resonance technique [7].

At low temperature, collective excitations are most important quasiparticles in a superfluid system and they can be used to characterize dominant physical property of system. Since the experimental realization of the BCS-BEC crossover, considerable interest has focused on the study of collective excitations in harmonically trapped superfluid Fermi gases. By means of the Feshbach resonance, the atom-atom interaction for dilute gases, characterized by $s$-wave scattering length, can be tuned from large positive to large negative values, providing a possibility to investigate and manipulate the nature of collective excitations in various superfluid regimes. A large body of experimental works on the collective excitations in superfluid Fermi gases in the BCS-BEC crossover have been done [8–11] and a very recent precision measurement on the frequency of radial compression modes shows that the beyond-mean-field effect is crucial in strongly interacting, optically trapped Fermi gas of $^6$Li atoms [12].

Up to now there exist two theoretical treatments on the collective excitations in superfluid Fermi gases in the BCS-BEC crossover [13–25]. One of them is microscopic theory, in which single-channel (Fermi-only) or two-channel (Fermi-Boson) model Hamiltonians with Fermi or Fermi-Boson degrees of freedom are used. Because in the experiments of superfluid Fermi gases [3–7] particles are trapped in an external potential, the inhomogeneous feature of system makes the microscopic approach not easy to handle. However, notice the fact that at very low temperature the condensed fermionic atom pairs do not decay into single atoms due to the existence of energy gap in their excitation spectrum, and hence no single fermionic atoms appear by the breaking of condensed atom pairs. The dynamics of such perfect superfluid can be well described phenomenologically by an order-parameter equation, called the generalized Gross-Pitaevskii (GGP) equation [18,19,22–25]. Different superfluid regimes can be characterized by an equation of state, which can be obtained by a quantum Monte Carlo simulation [26,27] or BCS energy-gap equations [16,17]. The GGP equation captures dominant feature that the superfluid exhibits macroscopically, though its mathematical framework is simple. Thus, it is reasonable to expect that the GGP theory is a useful theoretical tool for studying macroscopically the dynamics of superfluid Fermi gases in the BCS-BEC crossover.

The GGP equation can be converted into a hydrodynamic form. In a recent work [24], we have solved relevant hydrodynamic equations by neglecting the quantum pressure term. Thus all solutions obtained in that work are valid only for the Thomas-Fermi limit, i.e., $N_0$, the particle number in condensate, is infinite. It is necessary to extend the work in Ref. [24] beyond the TF limit due to the following reasons. (i) In realistic experiments [3–11], $N_0$ is finite (typically with order of $10^3$ to $10^6$). (ii) At the boundary of condensate the Bogoliubov amplitudes obtained in the TF limit vary quickly and...
When a \[ /H20851 \] can be easily realized through tuning an applied magnetic \[ /H20851 \] both theoretical and experimental studies show that the transitions contributed by the boundary cannot be neglected. (iv) The existence of the singular points results also in a divergence for coupling matrix elements describing three-mode resonant interaction, which plays dominant role for the damping and frequency shift of collective modes in superfluid Fermi gases [28].

It the present work, we shall solve the GGP equation beyond the TF limit by extending our previous work, which is for the special case of BEC limit [29,30]. We shall give a consistent, divergence-free theoretical description for Bogoliubov excitations at zero temperature for harmonically trapped superfluid Fermi gases in the BCS-BEC crossover. The paper is arranged as follows. In Sec. II, we give a simple introduction on the time-dependent GGP equation valid for a fermionic condensate. The equation of state in various superfluid regimes is also described. In addition, the time-independent GGP equation for ground state and Bogoliubov–de Gennes (BdG) equations for collective excitations are derived by using a method of multiple scales. In Sec. III, we provide the explicit solutions of ground state wave function and eigenspectra and eigenfunctions of collective excitations for the traps of both spherical and spheroidal symmetries, which are valid for the whole BCS-BEC crossover. The result for the excitation spectrum obtained is compared with the available experimental and numerical data. Finally, the last section (Sec. IV) contains a discussion and summary of our main results.

II. ORDER PARAMETER EQUATION AND BDG FORMALISM FOR BOGOLIUBOV EXCITATIONS

A. Order parameter equation for the BCS-BEC crossover

The ground state of a superfluid fermionic atom gas of density \( \rho \) contains paired atoms with \( \rho/2 \) as pair density [1,2]. These condensed fermionic atom pairs are originated from fermionic atoms (i.e., \(^{6}\text{Li} \) or \(^{40}\text{K} \) in the present experiments [3–7]) with two different internal states. By means of Feshbach resonance the transition from BCS to BEC regimes can be easily realized through tuning an applied magnetic field, and hence changing the s-wave scattering length \( a_{sc} \). When \( a_{sc} < 0 (a_{sc} > 0) \), the system is in a BCS (BEC) regime.

By defining a dimensionless interaction parameter \( \eta = 1/(k_F a_{sc}) \), where \( k_F = (3 \pi^2 \rho)^{1/3} \) is the Fermi wave number, one can distinguish several different superfluidity regimes [19,24], i.e., BCS regime (\( \eta < -1 \)), BEC regime (\( \eta > 1 \)), and BCS-BEC crossover regime (\(-1 < \eta < 1 \)). \( \eta = -\infty (\eta = +\infty) \) is called BCS (BEC) limit and \( \eta = 0 \) is called unitarity limit. Both theoretical and experimental studies show that the transition from BCS regime to BEC regime is smooth [2], which hints that one can study the physical property of system in various superfluid regimes in a unified way.

As pointed out in the last section, at very low temperature (around \( 10^{-7} \) to \( 10^{-8} \) K) low-frequency collective modes cannot decay by formation of single fermionic excitations because of the gap in their energy spectrum. Thus thermal excitations play no significant role and the system can be taken as a perfect superfluid [31]. To describe the dynamics of such zero-temperature superfluid in the trapping potential \( V_{\text{ext}}(\mathbf{r}) \), one can use a time-dependent density-functional theory [18,19,24]. The action functional \( I[\psi] \) of the theory is

\[
I[\psi] = \int dt d\mathbf{r} \left( i \hbar \frac{\partial \psi}{\partial t} - \frac{\hbar^2}{2m} \nabla^2 \psi + V_{\text{ext}}(\mathbf{r}) \psi + \epsilon(\rho) \psi \right),
\]

where \( \psi \) is superfluid order parameter, \( C = (i \hbar/2)(\psi^\dagger \partial \psi/\partial t - \psi^* \partial \psi/\partial t) + (\hbar^2/2m) \nabla^2 \psi^2 + V_{\text{ext}}(\mathbf{r}) \rho + \epsilon(\rho) \) is the Lagrangian density. Here \( V_{\text{ext}}(\mathbf{r}) \) is trapping potential and \( \epsilon(\rho) \) represents the bulk energy per particle of the system, which is expressed as a function of the number density \( \rho = |\psi|^2 \) and has the relation \( \epsilon(\rho) = \frac{3}{2} \epsilon_F(\eta) \), where \( \epsilon_F = \hbar^2 k_F^2/(2M) \) is the Fermi energy and \( M \) is the mass of atoms. Some asymptotic expressions of \( f(\eta) \) have been obtained by fitting calculating data [26]. Interpolating these asymptotic expressions for small and large \( \eta \) one can obtain the general formula \( f(\eta) = \eta(\beta\eta + 1) / [\beta\eta + 1] \). The fitting parameters \( \beta_j (j = 1, 2, 3) \) and \( \beta_j (j = 1, 2) \) for \(^{6}\text{Li} \) have been given in Ref. [19].

The Euler-Lagrange equation for \( \psi \) is obtained by minimizing the action functional (1), which leads to a GGP equation [18,19,24]

\[
ii \hbar \frac{\partial \psi}{\partial t} = \left( -\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}}(\mathbf{r}) + U(\rho) \right) \psi,
\]

where \( U(\rho) \) is the equation of state (also called the bulk chemical potential) of the system [18,19]. Different superfluid regimes can be characterized by different \( U(\rho) \) in corresponding regimes. According to Gibbs-Duhem relation one can obtain the formula [19] \( U(\rho) = \partial \rho \epsilon(\rho) / \partial \rho \).

Because the expression of the equation of state \( U(\rho) \) is very complicated, it is hard to obtain analytical results of the GGP equation. A simple approach is to take a polytropic approximation, i.e., one assumes [16,18,19,22,24] \( \epsilon(\rho) = \epsilon_0 \rho^n \), where \( n \) is a constant [whose value depends on the values of \( \eta \) and \( \gamma \) given Eq. (18) below]. It is easy to show that the effective polytropic index takes the form \( \gamma(\eta) = \frac{2 + 2\eta/\chi}{3 + \Theta(\eta) \eta^2/\chi^2} \),

\[
\gamma(\eta) = \frac{2 + 2\eta/\chi + \eta/\chi^2}{3 + \Theta(\eta) \eta^2/\chi^2},
\]

where \( \Theta(\eta) \) is the Heaviside step function and \( \chi = \mu_m/2e_F \) is a solution of the equation \( \Ai'(-\alpha\eta)/\Ai(-\alpha\eta) = -\nabla \alpha \eta \) here \( \mu_m \) is the chemical potential of a homogeneous dimer system (i.e., in the BEC side), \( \Ai(\eta) \) is the Airy function and \( \alpha \approx 2.338 \) is the first zero point of the Ai function. The expression (3) is more convenient than that presented in Ref. [19] and we shall use it in the following calculation. In the BCS limit we have \( \gamma = 2/3 \) (corresponding to \( \eta = -\infty \)) and in the BEC limit we have \( \gamma = 1 \) (corresponding to \( \eta = +\infty \)). The minimum (\( \gamma = 0.6 \)) is at \( \eta = -0.55 \) and the maximum (\( \gamma = 1.0 \)) is at \( \eta = +\infty \). Mathematically, the polytropic approximation is a little rough but it has the advantage of allowing...
one to get an analytical expressions for the eigenfunctions and eigenfrequencies of collective modes for various superfluid regimes in a unified way. In fact, it is quite accurate because $\gamma$ is a slowly varying function of $\eta$ [16–19,22–25].

B. BdG formalism for collective excitations

We now begin to study the linear excitations of the superfluid gas in the BCS-BEC crossover. We assume that in the ground state of the system the superfluid wave function takes the form $\psi(t) = \psi(t) \exp(-i \mu \mathcal{G} t)$, where $\psi(r)$ is a stationary function satisfying the time-independent GGP equation

$$[\hat{H}_0 - \mu \mathcal{G} + U(\rho_{C})] \psi = 0,$$

with $\hat{H}_0 = -\hbar^2 \nabla^2 / (2M) + V_{ex}(r)$. To find an excitation we take the Bogoliubov decomposition

$$\psi(r,t) = [\psi(r) + \epsilon \phi(r,t)] \exp(-i \mu \mathcal{G} t),$$

where $\phi(r,t)$ is the component describing the excitation generated from the condensate, and $\epsilon$ is a small parameter characterizing the relative amplitude of the excitation. Then, exact to first order of $\epsilon$, Eq. (2) takes the form

$$i \hbar \frac{\partial \phi}{\partial t} = \hat{L} \phi + U'(\rho_{C}) \psi \phi^* + \epsilon \left[ U'(\rho_{C}) (2\psi \phi^2 + \psi^* \phi^2) + \frac{1}{2} U''(\rho_{C}) \psi \phi \phi^* + \psi^* \phi^2 \right] + O(\epsilon^2),$$

where $U'(\rho) = \partial U(\rho)/\partial \rho$ and the operator $\hat{L}$ is defined by $\hat{L} = -\hbar^2 \nabla^2 / (2M) + V_{ex}(r) - \mu \mathcal{G} + U(\rho_{C}) + U'(\rho_{C}) \rho_{C}$. To solve Eq. (6) we apply a method of multiple scales [33]. Letting $\phi = \phi^{(1)} + \epsilon \phi^{(2)} + \cdots$, with $\phi^{(1)} = \phi^{(1)}(r,t,\tau)$ and $\tau = \epsilon t$. Eq. (6) becomes

$$\hat{Q}^{(1)}(\phi) = \hbar \frac{\partial \phi^{(1)}}{\partial \tau} - \hat{L} \phi^{(1)} - U'(\rho_{C}) \phi^{(1)} = 0,$$

with $Q^{(1)} = i \hbar \frac{\partial \phi^{(1)}}{\partial \tau} + U'(\rho_{C}) \phi^{(1)}(2 \psi \phi^2 + \psi^* \phi^2) + \psi^* \phi^2 \phi^2$. The expressions of higher-order $Q^{(j)} (j = 3, 4, \ldots)$ are omitted here.

At the leading order ($j = 1$) one has $\hat{Q}^{(1)} = 0$. To solve this equation we make the Bogoliubov transformation

$$\phi^{(1)}(r,t) = \sum_{n \geq 0} [u_n(r)b_n(\tau) \exp(-i \omega_n t) + v_n^*(r)b_n^*(\tau) \exp(i \omega_n t)],$$

with the amplitudes $(u_n, v_n)$ being the wave functions in the real space and $b_n(\tau)$ depending on the slowly varying time $\tau$. Then the problem is converted to solve the BdG eigenvalue problem

$$\hat{L} u_n(r) + U'(\rho_{C}) \psi v_n^*(r) = + E_n u_n(r),$$

$$\hat{L} v_n(r) + U'(\rho_{C}) \psi u_n^*(r) = - E_n v_n(r),$$

where $E_n = \hbar \omega_n$ is the eigenenergy of the excitation and $(u_n, v_n)$ is the eigenfunction, also called Bogoliubov amplitude. To obtain a complete set of eigenfunctions one must solve the equation for the zero-energy $(E_0 = 0)$ mode $(u_0, v_0)$ [34,35]:

$$\hat{L} u_0(r) + U'(\rho_{C}) \psi^2 v_0(r) = \frac{\alpha_0}{2} [u_0(r) - v_0(r)],$$

$$\hat{L} v_0(r) + U'(\rho_{C}) \psi^2 u_0(r) = \frac{\alpha_0}{2} [u_0(r) - v_0(r)],$$

where the parameter $\alpha_0$ has to be determined so that the eigenfunctions $(u_n, v_n)$ $(n = 0, 1, 2, \ldots)$ constitute an orthogonal and complete set. From the BdG equations (9) and (10) it is easy to show that the eigenfunctions $(u_n, v_n)$ satisfy the following orthogonality relations:

$$\int d^3 r [u_n^*(r) u_{n'}(r) - v_n^*(r) v_{n'}(r)] = \delta_{nn'},$$

$$\int d^3 r [u_n^*(r) v_{n'}(r) - u_{n'}(r) v_n(r)] = 0.$$
\[-(1 - \rho^2) \nabla^2 \varphi_n - (1 - \rho^2) \sigma \varphi_n + \frac{\xi^2}{2 \gamma} \left[ \nabla^4 + \nabla^2 \sigma + (2 \gamma + 1) \sigma \nabla^2 \right] \varphi_n + (2 \gamma + 1) \sigma^2 \varphi_n = \frac{2}{\gamma} \bar{\omega}_n \varphi_n, \tag{17}\]

where \( \bar{\omega}_n = E_n/(\hbar \omega_1) \). We are interested in low-lying excitations in the condensate and hence \( \hbar \omega_1 \leq E_n \ll \mu_G \). It is obvious that the terms proportional to \( \xi^2 \) in the dimensionless BdG Eqs. (16) and (17) can be taken as perturbation for low-lying excitations as long as \( |\xi^2 \nabla^2 \sigma| \ll 1 \).

\section{A. Variational solution for ground state}

In order to eliminate the divergence in the solution under the TF limit, we follow the line of Fetter \cite{36} by considering a trial variational ground-state wave function, i.e., the solution of the dimensionless GGP equation (15) takes the form

\[ \psi_G = C_G (1 - \rho^2)^{\gamma + 1/2} \Phi \left( 1 - \rho \right), \tag{18}\]

with \( \rho \) being taken as variational parameter. The square of normalization coefficient \( C_G^2 = N_0 / \left[ 2 \pi R^3_B \left( 3 / 2, 1 + \beta \right) \right] \) is obtained by the condition \( N_0 = \int d^3 \mathbf{r} |\psi_G(\mathbf{r})|^2 \), where \( \beta = (q + 1)/\gamma \) and \( B(v_1, v_2) \) is beta function with arguments \( v_1 \) and \( v_2 \). In the TF limit the chemical potential in the ground state has the simple form \( \mu_G = \frac{\xi}{2} M \omega_0^2 R^3_B = U[\mu_G(0)] \). In the TF regime, the repulsive interaction between condensed pairs makes the condensate expands from the size \( a_{ho} \) to \( R \). The expansion ratio is given by \( R_{a_{ho}} \approx \xi^{1/2} \), where \( \xi = D_1 D_2^{2(3 \gamma + 2)} \), with \( D_1 = (1.695) \gamma \) and \( D_2 = \left[ \frac{3(3\pi^2/2 + 1)}{3(3\pi^2/2)} \right]^{2/3} \gamma \). Here we have used \( c = (3/2 \pi^{3/2}) \rho^2 / 10M \) and \( \xi = (9 \pi)^{-1/3} / 2 \). The ground-state energy as a function of \( \rho \) reads

\[ E_G(\rho) = \frac{1}{2} \hbar \omega_1 \left[ \frac{1}{2 \beta + 5} \frac{B(3/2, \beta \gamma + \beta + 1)}{(\gamma + 1)B(3/2, \beta + 1)} \right] \frac{1}{\xi} \]

\[ + \left[ 1 + \frac{1}{2 \lambda^2} \right] \left( \begin{array}{c} B(3/2, \beta + 1) \beta + 3/2 \beta - 1 \end{array} \right). \tag{19}\]

In the ground state \( E(\rho) \) which determines \( \rho \) as a function of \( \eta, \gamma, \lambda, \) and \( N_0 \). In the TF regime one has \( \rho \approx N_0^{3/10} \) and \( R_{a_{ho}} \approx N_0^{1/10} \). In Fig. 1(a) [Fig. 1(b)] we have shown the result for the variational parameter \( \rho \) (the dimensionless condensate radius \( R_{a_{ho}} \) as a function of \( N_0 \)) for fixed \( \lambda = 0.2 \) with different interaction parameter \( \eta = 0.5, 0 \), and 1.0. We see that \( \rho \) decreases and \( R_{a_{ho}} \) increases as \( N_0 \) increases. Note that to make the variational approximation be valid the value of \( \rho \) should not be too large.

\section{B. Solutions of BdG equations in spherically symmetric trapping potential (\( \lambda = 1 \))}

Similar to the procedure described in Refs. \cite{29,30} for the BEC limit, explicit analytic solutions of the BdG Eqs. (16) and (17) in the BCS-BEC crossover beyond the TF limit can be obtained in the following three steps.

The first step is to set the small parameter \( \xi^2 \) to zero but substitute the expression of \( \sigma \) for \( \lambda = 1 \), i.e., \( \sigma = \beta(3 - (\beta + 1)^2) / (1 - \beta^2)^2 \), into Eqs. (16) and (17). One obtains eigenfunctions of the form \( \varphi_n^R(\mathbf{r}) = C_n^R(1 - \beta^2)^{1/2} \beta P_1^R(\rho)Y_0(\theta, \phi) \), where \( Y_0(\theta, \phi) \) is the spherical harmonic function and the radial function \( P(x) \) with \( x = \rho^2 \) satisfies the hypergeometric differential equation

\[ 2x(1 - x)P''(x) + [2l + 3 - (2l + 3 + 2\beta)x]P'(x) + \left[ \gamma - (\alpha_n^R)^2 - \beta \right] P(x) = 0. \tag{20}\]

Solutions of Eq. (20) are classical \( n \)-th-order Jacobi polynomials \( P_n^{(\beta^2 - 1)}(1 - \rho^2) \), which form an orthonormal function set on the interval \( 0 \leq x \leq 1 \). The radial normalization integral with weight \( x^{l+1/2}(1 - x)^{\beta - 1} \) is given by \( I_n(\beta) \equiv \int_0^1 dx x^{l+1/2}(1 - x)^{\beta - 1} P_n^R(x) = n_n^{1/2}(l + 3/2) \Gamma(n + \beta + 1) / [(2n + l + \beta + 1/2) \Gamma(n + l + 3/2) \Gamma(n + l + \beta + 1/2)] \). Consequently, the
normalized eigensolutions that satisfy the condition
\[ \int d^3r \left( u_n^2 - v_n^2 \right) = 1 \]

\[ \varphi_n^0(r) = \sqrt{\frac{2}{n_f(r) \beta R_s}} \left( \frac{\xi \omega_n^{(0)}}{\beta} \right)^{1/2} \left( 1 - \frac{\beta^2}{4} \right)^{1/2} \times P_{n_f}(r^2) Y_{lm} (\theta, \phi), \]

(21)

where \( n = (n_r, l, m) \) are quantum numbers, with \( n_r = 0, 1, 2, \ldots, L = 0, 1, 2, \ldots, m = l, \ldots, l \). The eigenvalues of the BdG equations are given by \( (\tilde{\omega}_n^{(0)})^2 = (\tilde{\omega}_n^{(0)})^2 + 2Q_n + l/q \), where \( (\tilde{\omega}_n^{(0)})^2 = \gamma_n(2n_r + 2l + 1) + 2n_r + l \) is the result given by the TF limit. We stress that the solutions given here are different from those obtained in Refs. [29,37–40]. Because \( q > 0 \) and \( 0.6 \leq \gamma \leq 1.0 \), we have \( \beta > 1 \). The factor \( (1 - \beta^2)^{1/2} \), which reduces to 1 in the BEC and the TF limits (i.e., \( \gamma = 1 \) and \( q = 0 \) and hence \( \beta = 1 \)), takes a role for smoothing Bogoliubov amplitudes. As a result, the divergence in the integration of coupling matrix elements for three-mode resonant interaction can be eliminated completely [28].

The second step is to calculate the correction of the excitation spectrum by using of standard perturbation theory. Since for low-lying excitations \( \xi^2 \) is small, we can take a perturbation expansion for the eigenvalues and eigenfunctions to solve Eqs. (16) and (17). The solution described above is taken as a zero-order one and the first-order correction of eigenvalue can be readily obtained. As a result the eigenvalue including the zero-order one is given by

\[ \tilde{\omega}_n^{(0)} = \tilde{\omega}_n^{(0)} + \delta \tilde{\omega}_n^{(0)}, \]

\[ = \frac{\tilde{\omega}_n^{(0)}}{2L_{n_f}(\beta)} \int_0^1 dx \left[ 1 - x \right]^{-1} F_{n_f}(x) \times \left[ 1 + \frac{1}{\gamma} (1 - x)^q + \frac{2}{(1 - x)^q} \right] \times \left[ 1 + \frac{1}{\gamma} \left( (\omega_n^{(0)})^2 - 2l - 3 - 2(2 - \beta) \frac{x}{1 - x} \right) \right]. \]

(22)

In the derivation of Eq. (22), divergence terms including those such as \((\xi \omega_n^{(0)})^{-1}\) have canceled each other exactly.

The third step is to change \( 2\eta_n(\beta) \) into \( \gamma^{-1} \eta_n(\beta + q) \) in Eq. (22). This is because the correct spectrum formula returns to the result in the TF limit for \( q = 0 \). This correction is caused by the polytropic index \( \gamma \neq 1 \). We see that the first-order correction of the excitation spectrum is proportional to \( \xi^2 \sim N_0^{-2/3} \).

For the modes \( n_r = 0 \), the correction term in Eq. (22) is simplified to

\[ \frac{\delta \eta_n}{\eta_n} = \frac{\xi^2 B(l + 3/2, \beta)[(2l + 3 - \beta)B(l + 1/2, \beta - 2) - (2 - \beta)B(l + 5/2, \beta - 3)]}{\gamma^{-1} B(l + 3/2, \beta) + \gamma B(l + 1/2, \beta + q)}. \]

(23)

It seems that it is unphysical for \( \beta = 1, 2, 3 \) because the beta functions appeared in the numerator of Eq. (23) are divergent. However, notice that \( \beta = (1 + q) / \gamma \geq 1, 0.6 \leq \gamma \leq 1.0 \), and the variational approximation used in the last subsection requires \( q \) cannot be too large, we can put a constraint on \( q \) so that \( 1 < \beta < 2 \) or \( 0 < q < 2 - \gamma - 1 \). In this way there are no divergence in the expression of Eq. (23). Using the result given above it is easy to show that in the TF regime (i.e., \( N_0 \gg 1 \) and \( q > 0 \)) and at deep BEC regime (i.e., \( \gamma = 1 \)), one has \( \beta = 1 \) and hence \( \omega_0 = \sqrt{l + \text{const}} \times \xi^2 \nu_l q \) and \( \xi^2 \nu_l q \sim N_0^{-1/3} \).

This result demonstrates that the spectrum correction obtained is indeed a small quantity and it can reduce to the result in the TF limit (i.e., \( N_0 \approx \infty \)). Note that in the usual TF-like approximation, turning point \( \tilde{r} = 1 \) is at finite distance for finite radius \( R_s \). While in the TF regime we focus on in the present work, the point \( \tilde{r} = 1 \) corresponds to a very large distance for \( R_s \) \( \ll \lambda_{1/6} \). \( \psi_G \) vanishes smoothly for \( \tilde{r} \to \infty \), \( u_n \) and \( v_n \) have a divergence only below logarithms and thus remain normalizable due to the introduction of the convergent factor \((1 - \tilde{r}^2)^{1/2} \).

In Fig. 2 we have shown the result of a quadrupole mode \( n_r = 0 \) and \( l = 2 \) as a function of the interaction parameter \( \eta = 1/(k_F \alpha \omega) \) with \( N_0 = 2 \times 10^5 \) (long-dashed line), \( N_0 = 2 \times 10^7 \) (solid line), and the TF limit \( N_0 = \infty \) (short-dashed line), where \( \gamma \) as a function of \( \eta \) is given by Eq. (3). From this figure we see the following. (i) The quantum pressure has a significant contribution to the eigenfrequency with decreasing \( N_0 \). (ii) The eigenfrequency increases as \( \eta \) increases, especially in the BEC regime. The leading-order solution of the eigenfrequency of this mode is given by \( (\tilde{\omega}_n^{(0)})^2 = \gamma_n(2n_r + 2l + 1) + (2n_r + l)(1 + q) \), showing clearly the effect beyond TF limit (i.e., nonvanishing variational parameter \( q \)). This result also covers the one obtained by Baranov and Petrov [41] (also see Ref. [42]) for \( q = 0 \) (the TF limit) and \( \gamma = 2/3 \) (the BCS limit).

C. Solutions of BdG equations in axially symmetric trapping potential (\( \lambda \neq 1 \))

We now consider the solutions beyond the TF limit for an axially symmetric case (i.e., \( \lambda \neq 1 \)), which is more important because axially symmetric traps are widely used in experiments [3–11]. We solve the BdG Eqs. (16) and (17) along the line of the last subsection by taking \( \xi^2 \) as a small perturbation parameter. Noting that in this case \( \sigma = (1 + q)[(2 + \lambda^2)(1 - \tilde{r}^2) + (1 - q)(\tilde{s}^2 + \lambda^2 \tilde{z}^2)] / (1 - \tilde{r}^2)^2 \) and the axial component of an-
gular momentum \( m \) is still a good quantum number, the leading-order solution takes the form 
\( \varphi_n^s(r) = C_n^s(1 - r^2)^{\beta/2}z^{21/2} e^{im\varphi} \), where the coupled axial and radial function \( P(\bar{z}, \bar{s}) \) fulfills a two-dimensional differential equation \([29,30]\)

\[
\left\{ 1 - \bar{z}^2 - \lambda^2 \bar{z} \frac{\partial}{\partial \bar{s}} + (1 + 2|m|) \frac{\partial}{\partial \bar{s}} + \lambda^2 \frac{\partial^2}{\partial \bar{s}^2} \right\} - 2\beta \left( \frac{\partial}{\partial \bar{s}} + \lambda^2 \frac{\partial}{\partial \bar{s}^2} \right) + 2 \left[ \frac{1}{\gamma} (\omega_{n,p,m}^{(0)})^2 - \beta m \right] \right\} P(\bar{z}, \bar{s}) = 0. \tag{24}
\]

By using the method similar to that in Refs. \([24,39]\), we look for the solution of Eq. (24) with the form

\[
P_{n_p}^{(2n)}(\bar{z}, \bar{s}) = \sum_{k=0}^{n_p} \sum_{n=0}^{\text{int}(k/2)} b_{k,n} \bar{z}^{2k-2n} \bar{s}^n, \tag{25}
\]

where \( n_p \) is a principal quantum number \([29,30,39]\) and the coefficient \( b_{k,n} \) fulfills the relation

\[
g_n = \frac{-4\lambda^2(n+1)(n+|m|+1)(n_p-2n-1)}{D_3(2(\omega_{n,p,m}^{(0)})^2/\gamma - 2|m|\beta - 4n(n+|m|+\beta) - \lambda^2(n_p-2n)(n_p-2n-1+2\beta)},
\]

where \( D_3 = 2\gamma - 2|m|\beta - 4(n+1)(n+|m|+1+\beta) - \lambda^2(n_p-2n-2)(n_p-2n-3+2\beta) \). The polynomials \( P_{n_p}^{(2n)}(\bar{z}, \bar{s}) \) form an orthonormal set on the interval \( 0 \leq \bar{s} \leq 1 \), and the normalization integral with weight \( \bar{z}^{2m}(1 - \bar{z}^2)^{\beta-1} \) is given by \( I_{n,p,m}(\beta) = 2(1^{1/2} \tilde{d} \tilde{s})^{1/2} \tilde{d} \tilde{z}^{2m}(1 - \bar{z}^2 - \lambda^2 \bar{z})^{\beta-1}/[P_{n_p}^{(2n)}(\bar{z}, \bar{s})]^2 \). Consequently, the normalized eigenfunctions read

\[
\varphi_n^s(r) = \frac{(\omega_{n,p,m}^{(0)})^{1/2}}{\sqrt{4\pi n_p^{1/2} \gamma I_{n,p,m}(\beta)}} \left(1 - \bar{z}^2 - \lambda^2 \bar{z}\right)^{(\beta-1)/2} \bar{z}^{1/2} e^{im\varphi}.
\tag{28}
\]

With the zero-order solutions obtained we can go to the next order of perturbation expansion. It is easy to get the first-order correction of eigenvalues

\[
\frac{\delta \omega_{n,p,m}}{\omega_{n,p,m}} = \xi^2 \int_{\bar{z}, \bar{s}, \bar{r}} \int_{\bar{z}, \bar{s}, \bar{r}} \left(1 - \bar{z}^2 - \lambda^2 \bar{z}\right)^{(\beta-1)/2} \bar{z}^{1/2} e^{im\varphi} \times [P_{n_p}^{(2n)}(\bar{z}, \bar{s})]^2 \left[ \frac{1}{\gamma} (\omega_{n,p,m}^{(0)})^2 - 2 - \lambda^2 - 2|m| \right] - 2(2-\beta) \bar{z} + \lambda^2 \bar{z} \frac{\partial}{\partial \bar{s}} + 2 \left( \frac{\partial}{\partial \ln \bar{s}} + \lambda^2 \frac{\partial}{\partial \ln \bar{z}} \right)
\]

\[
\times \ln P_{n_p}^{(2n)}(\bar{z}, \bar{s}) \right]. \tag{29}
\]

From this equation, one can show that zero-order eigenvalues \( (\omega_{n,p,m}^{(0)})^2 \) are the solution of the standard continued fraction equation

\[
-1 = \frac{g_0}{1 + \frac{g_1}{1 + \cdots + \frac{g_{2n-2}}{1 + \frac{g_{2n-1}}{1 + \frac{g_{2n-2}}{1 + g_{2n-2}}}}}}, \tag{27}
\]

for \( n = (n_z, n_r, m) \) modes with \( Z = 1 + \text{int}(|n_r|/2) \) and

\[
J_{n,p,m} = \gamma^{-1} I_{n,p,m}(\beta) + \gamma I_{n,p,m}(\beta + g).
\]

For illustration we discuss the collective modes with \( n_p = 0, 1 \). Then one has \( n_z = 0 \) and \( n_r = 0 \) and 1, respectively. The zero-order eigenvalues are \( (\omega_{n,p,m}^{(0)})^2 = \beta \gamma (|m| + \lambda^2 n_z) \). Their corrections to \( \xi^2 \) order are given by

\[
\frac{\delta \omega_{n,p,m}^{(0)}}{\omega_{n,p,m}^{(0)}} = \frac{\xi^2}{\gamma I_{n,p,m}(\beta)} \int_{\bar{z}, \bar{s}, \bar{r}} \int_{\bar{z}, \bar{s}, \bar{r}} \left(1 - \bar{z}^2 - \lambda^2 \bar{z}\right)^{(\beta-1)/2} \bar{z}^{1/2} e^{im\varphi} \times [P_{n_p}^{(2n)}(\bar{z}, \bar{s})]^2 \left[ \frac{1}{\gamma} (\omega_{n,p,m}^{(0)})^2 - 2 - \lambda^2 - 2|m| \right] - 2(2-\beta) \bar{z} + \lambda^2 \bar{z} \frac{\partial}{\partial \bar{s}} + 2 \left( \frac{\partial}{\partial \ln \bar{s}} + \lambda^2 \frac{\partial}{\partial \ln \bar{z}} \right)
\]

\[
\times \ln P_{n_p}^{(2n)}(\bar{z}, \bar{s}) \right]. \tag{29}
\]

FIG. 2. Dimensionless oscillating frequencies of \( \omega_{02} \) mode vs dimensionless interaction parameter \( 1/(k_F a_{BC}) \) for a spherical symmetrical trap (\( \lambda = 1 \)). The long-dashed line, solid line, and short-dashed line correspond to \( N_0 = 2 \times 10^5, 2 \times 10^7, \) and \( \infty \), respectively.
\[ \frac{\delta \omega_{0m}}{\omega_{0m}} = \frac{\xi^2}{3} \left[ \frac{\beta}{|m| + \beta - 1 - \lambda^2} \right] \]
\[ \times B(1/2, \beta + |m| - 1)B(|m| + 1, \beta - 2) \]
\[ - 2(2 - \beta)B(1/2, \beta + |m| - 2)B(|m| + 1, \beta - 3) \}
\] (30)

with \( I_{0m}(\beta) = B(1/2, \beta + |m| + 1)B(|m| + 1, \beta/2\lambda) \).

\[ \frac{\delta \omega_{10m}}{\omega_{10m}} = \frac{\xi^2}{3} \left[ \left( \frac{\beta}{|m| + \lambda^2} - 2(\lambda^2 - 3\lambda^2) \right) \right] \]
\[ \times B(3/2, \beta + |m| - 1)B(|m| + 1, \beta - 2) \]
\[ - 2(2 - \beta)B(3/2, \beta + |m| - 2)B(|m| + 1, \beta - 3) \}
\] (31)

with \( I_{10m}(\beta) = B(3/2, \beta + |m| + 1)B(|m| + 1, \beta/2\lambda^3) \). In Fig. 3 we have plotted the result of the quadrupole (002) and (102) modes for \( m = \pm 2 \) and \( \lambda = \sqrt{3} \). The curves in the figure show the dependence of the eigenfrequencies for azimuthal [Fig. 3(a)] and axial [Fig. 3(b)] excitations. The contribution to the eigenfrequency by quantum pressure has a similar behavior as shown in Fig. 2.

For breathing modes with \( n_z = 2, n_x = 0 \) and \( m = 0 \), and \( n_z = 0, n_x = 1 \) and \( m = 0 \), we have \( \hat{P}(\vec{r}, \vec{s}) = \hat{b}_1 \hat{z}^2 + \hat{b}_2 \hat{s}^2 \) with \( \hat{b}_2 = -[(\bar{\omega}_{n, n, m}^{(0)})^2 - \beta \gamma |m|]/[(\bar{\omega}_{n, n, m}^{(0)})^2 - \beta \gamma |m| + 2] \) and \( \hat{b}_1 = -[2|m| + 2 - \bar{\omega}_{n, n, m}^{(0)}]/\beta \gamma |m| + 2] \). Equation (29) is simplified to

\[ \frac{\delta \bar{\omega}_{n, n, 0}}{\bar{\omega}_{n, n, 0}} = \frac{\xi^2 B(1/2, \beta + 1)}{2\beta(\beta - 1)(\beta - 2)I_{n, n, 0}} \left[ \frac{1}{\gamma} \bar{\omega}_{n, n, 0}^{(0)} - 2 - \lambda^2 \right] \]
\[ \times \left[ \beta - \frac{1}{4} + \frac{\beta \hat{b}_1}{\lambda^2} \left( 1 + \frac{3b_1/4\lambda^2}{\beta + 1/2} \right) + \left( 2\beta + 1 \right) \right. \]
\[ + \frac{\hat{b}_1}{\lambda^2} \left( b_2 + 2b_2^2 \right) - 2 \left( \frac{\beta + 1/2}{b_1 + 2b_2} \right) + \frac{3b_1}{2\lambda^2} \]
\[ + \left( 1 + \frac{1}{\lambda^2} \right) b_1 b_2 + 2b_2 \right] + 2 \left( \beta - \frac{2}{3} \right) \left( 3\beta^2 - \frac{1}{2\lambda^2} - \frac{1}{2} \right) \]
\[ + \frac{\beta \hat{b}_1}{\lambda^2} \left( 5 + \frac{21b_1/4\lambda^2}{\beta + 1/2} \right) + \left( 10\beta + 5 + \frac{7b_1}{\lambda^2} \right) \]
\[ + 14b_2 \right] \}
\] (32)

where \( (\bar{\omega}_{n, n, m}^{(0)})^2 = \gamma |m| + 1 + \frac{1}{2}\lambda^2 + (|m| + \lambda^2)\beta \gamma \pm \sqrt{\gamma |m| + 1 + \beta^2 - 3\beta |m| - 1 + 2(\lambda^2 + \beta \gamma |m| + \lambda^2)^{1/2}} \) and \( I_{n, n, 0}(\beta) = \frac{\beta^{1/2}(\beta + 1)}{\beta} \left[ \frac{1}{\beta} + \frac{b_1/2(\beta + 1/2)}{\beta + 3/2} \right] \). In Eqs. (29)–(32) the condition of \( 1 < \beta < 2 \) (see in the last subsection) guarantees the validity of the correction for the eigenvalues in the TF regime. In particular, for \( \beta = 1 \) (deep BEC regime in the TF limit) \( \xi^2 \approx q \) has a finite value although \( q \rightarrow 0 \). Notice that our solutions presented here cover the special solutions found by Heiselberg [16] and Cozzini and Stringari [43] for the \( m = 0 \) breathing modes, observed in recent experiments by Grimm’s group and Thomas’s group [8,9,11].

In Fig. 4 we have shown the experimental and theoretical results on \( 1/(k_F\alpha_{BC}) \) dependence of the radial breathing mode (010) [Fig. 4(a)] with \( \lambda = 0.20 \) and axial breathing mode (200) [Fig. 4(b) with \( \lambda = 0.05 \)] for different \( N_0 \). The dotted lines are taken from experimental data [8,9], the long-dashed lines, thick solid lines, and short-dashed lines are our calculating results for \( N_0 = 2 \times 10^5, 2 \times 10^7, \) and \( \infty \), respectively, and the thin solid lines are taken from theoretical results [19]. From the figure we see that (i) in the BCS side, our theoretical results on the collective-mode frequencies agree well with the available experimental data [8,9] and theoretical curves [19] near and beyond the TF limit. (ii) In the BEC side, our theoretical results are larger than the experimental data even in the TF limit. This may be due to the reason of
plane for obtain that the zero-order solution for the divergence-free density distribution zero-energy mode. By taking potential, and the beyond mean-field effect the finite temperature \(\zeta=2\). The long-dashed lines, thick solid lines, and short-dashed lines are for \(N_0=2 \times 10^5, 2 \times 10^7\), and \(\infty\), respectively. This means that the finite-size effects are not important only when \(N_0 \approx 1 \times 10^7\).

D. Solutions of BdG equations for zero-energy mode

In a similar way we may solve Eqs. (11) and (12) for the zero-energy mode. By taking \(\psi_0^+(\mathbf{r})=u_0 \pm v_0\) it is easy to show that \(\psi_0^-\) satisfies Eq. (4) and hence \(\psi_0^-=\psi_G = C_G \sqrt{\lambda/(1-\bar{r}^2)^{3/2}} \Theta(1-\bar{r})\). By a simple calculation one can obtain that the zero-order solution for \(\psi_0^+\) has the form \(\psi_0^+ = (\bar{a}_0/2\gamma)(1-\bar{r}^2)^{-3/2} \Theta(1-\bar{r})\), where \(\bar{a}_0 = a_0 \sqrt{\rho_G(0)/(\gamma +1)c_0^2} \). This is determined by the normalization condition 1 \(=\int d^3\mathbf{r} (u_0^2-v_0^2)=\bar{a}_0 \rho_G(0) B(3/2,\beta)/\lambda \gamma\). By defining the dimensionless density \(\rho_0 = (10a_0)^2(u_0^2-v_0^2)\), one has the divergence-free density distribution \(\rho_0(r)=\bar{\rho}_0(0) \times (1-\bar{r}^2)^{-\beta-1} \Theta(1-\bar{r})\) with \(\bar{\rho}_0(0)=2 \times 10^3 / B(3/2,\beta)\) being the value at the center of the trapping potential and \(\zeta\) being the small value defined below Eq. (18).

As an example, in Fig. 5 we have plotted the density distribution of the zero-energy mode as a function of \(1/(k_F a_\text{sc})\) for \(\lambda=1\). We see that the values of \(\eta, \gamma, \lambda, N_0\) contribute obvious effects on the density distribution of the zero-energy mode. Especially, there is a kinklike change of the density in the trap center when \(1/(k_F a_\text{sc})\) passes through the unitarity point (i.e., \(a_\text{sc} \to \pm \infty\)) of the BCS-BEC crossover.

IV. SUMMARY

Ground state and elementary excitations are two key issues in the physics of the BCS-BEC crossover. Because of the existence of the trapping potential, it is hard to get the ground state solution and all eigenvalues and eigenfunctions

FIG. 4. Dimensionless breathing mode frequencies vs the dimensionless interaction parameter \(1/(k_F a_\text{sc})\). (a) \(\bar{a}_{000}\) in the \(xy\) plane for \(\lambda=0.02\). (b) \(\bar{a}_{000}\) along the \(z\) axis for \(\lambda=0.05\). In both panels, the large solid circles are taken from experimental data [8,9]. The thin solid lines are taken from theoretical result [19]. The long-dashed lines, thick solid lines, and short-dashed lines are for \(N_0=2 \times 10^5, 2 \times 10^7\), and \(\infty\), respectively.

FIG. 5. Dimensionless density distribution of the zero-energy mode for \(\lambda=1\). (a) Density distribution as a function of radial distance (in the unit of \(a_\text{sc}\)) for \(N_0=2 \times 10^5\). The long-dashed line, solid line, and short-dashed line are for the interaction parameter \(1/(k_F a_\text{sc})=-0.5, 0, \text{and } 1.0\), respectively. (b) Maximum density at \(r=0\) as a function of the dimensionless interaction parameter \(1/(k_F a_\text{sc})\). The long-dashed line, solid line, and short-dashed line are for \(N_0=2 \times 10^5, 2 \times 10^7, \text{and } 2 \times 10^8\), respectively.

063629-8
for excitations in a consistent way. In the present work, we have made a detailed investigation on the Bogoliubov collective excitations of trapped superfluid Fermi gases in the BCS-BEC crossover beyond the TF limit. Starting from the GGP equation and the simplified equation of state, valid for the whole crossover, we have derived the time-independent GGP equation for the ground state of the condensate and the BdG equations for low-lying collective modes at zero temperature. By introducing a variational parameter \( q \) in the ground state wave function we have removed the noncontinuity of its slope at the boundary of the condensate, which appears in the TF limit. We have solved the BdG equations analytically for the trapping potentials of spherical and axial symmetries. The explicit expressions for all eigenvalues and eigenfunctions, which are valid for various crossover regimes, have been provided. We have discussed the features of various collective modes in the BCS-BEC crossover and made a comparison with available experimental data near and beyond the TF limit. The results presented in this work may be useful for understanding the physical property of superfluid Fermi gases in the BCS-BEC crossover and guiding experimental findings for observing new collective modes predicted here. In addition, our results may be used to consider the interaction between collective excitations in superfluid Fermi gases and study the damping and frequency shift of collective modes in various superfluid regimes.

**ACKNOWLEDGMENTS**

This work was supported by the National Natural Science Foundation of China under Grant Nos. 10574028, 10321003, 90403008, 10434060, and 10674060, and by the State Key Development Program for Basic Research of China under Grant Nos. 2005CB724508 and 2006CB921104.


The damping and frequency shift of collective modes in superfluid Fermi gases has been observed in recent experiments [8,9,11]. However, their theoretical explanation remains a problem but beyond the scope of the present work.

[28] It has been shown that the collective-mode frequency in the BEC side decreases as temperature increases, see S. Giorgini, Phys. Rev. A 61, 063615 (2000).

[44] It has been shown that the collective-mode frequency in the BEC side decreases as temperature increases, see S. Giorgini, Phys. Rev. A 61, 063615 (2000).