Collective Excitations of Strongly Interacting Fermi Gases of Atoms in a Harmonic Trap

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The zero-temperature properties of a dilute two-component Fermi gas in the BCS-BEC crossover are investigated. On the basis of a generalization of the Hylleraas-Undheim method, we construct rigorous upper bounds to the collective frequencies for the radial and the axial breathing mode of the Fermi gas under harmonic confinement in the framework of the hydrodynamic theory. The bounds are compared to experimental data for trapped vapors of $^6$Li atoms.

PACS numbers: 03.75.-b, 03.75.Ss, 67.40.Db

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The recently reported ultracold trapped Fermi gases with tunable atomic scattering length [1-19] in the vicinity of a Feshbach resonance stimulated a large number of theoretical investigations. In this letter the dynamics of strongly interacting dilute Fermi gases (dilute in the sense that the range of interatomic potential is small compared with inter-particle spacing) is investigated in the framework of the hydrodynamic theory [20-29].

Instead of using the scaling approximation of Refs[20-22,25,27], the polytropic approximation of Refs.[24,28] or the perturbative approximation of Ref.[26], we will construct a rigorous upper bounds to the collective frequencies.

Our starting point is the variational formulation of the Kohn-Sham time-dependent theory for a dilute two-component Fermi gas in a trap potential \( V_{\text{ext}}(\vec{r}) = (m/2)(\omega_{\perp}^2(x^2 + y^2) + \omega_{z}^2 z^2) \)

\[
\delta \int dt < \Psi |i\hbar \partial_t - H|\Psi > = 0, \tag{1}
\]

where \( |\Psi > \) is a product of two Slater determinants, one for each internal state built up by the Kohn-Sham orbitals \( \psi_i \), and \( H = T + U \) is Hamiltonian in the local density approximation (LDA).

We consider two approximations:

(i) local transform \( \psi_i \approx \phi_i \exp(i\chi) \), where \( \psi_i \) and \( \chi \) are real functions, and

(ii) \( < \phi|T|\phi > \approx (1/N) \int (t_{TF}(n) + t_W(n))n(\vec{r}, t)d^3r \),

where \( n \) is the density, normalized to the total number of atoms \( N, \int n d^3r = N, |\phi > \) is the product of two Slater determinants built on \( \phi_i \) alone, \( t_{TF}(n) = (3\pi^2)^{2/3}(3h^2/(10m))n(\vec{r}, t)^{2/3} \) is the Thomas-Fermi (TF) kinetic energy density, and \( t_W(n) = (\hbar^2/(8m))(\nabla n)^2/n \) is the von Weizsäcker kinetic energy density.

Using the approximations (i) and (ii), we obtain from Eq.(1) [20-22]

\[
i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + V_{\text{ext}} \psi + V_{\text{xc}} \psi, \tag{2}
\]

where \( \psi = \sqrt{n} \exp(i\chi) \), \( V_{\text{xc}}(\vec{r}, t) = [\frac{d\epsilon(n)}{dn}]_{n=n(\vec{r}, t)} \) and \( \epsilon(n) \) is the ground state energy per particle of a uniform system. The only difference from equations holding for bosons [30,31] is given by density dependence of \( \epsilon(n) \).

It is useful to rewrite Eq.(2) in a form

\[
\frac{\partial n}{\partial t} + \nabla(n\vec{v}) = 0, \tag{3}
\]
\[
\frac{\partial \vec{v}}{\partial t} + \frac{1}{m} \nabla (V_{\text{ext}} + \frac{d(n\epsilon(n))}{dn}) + \frac{1}{2}mv^2 - \frac{\hbar^2}{2m\sqrt{n}} \nabla^2 \sqrt{n} = 0,
\]
where \( \vec{v} = (\hbar/m) \nabla \chi \) is the velocity field.

It was shown in Refs.[20,21] that for experimental conditions of Refs.[14,16,17] the quantum pressure term in Eq.(4) can be neglected. For the reminder of this Letter we will use this hydrodynamic approximation.

For the negative S-wave scattering length between the two fermionic species, \( a < 0 \), in the low-density regime, \( k_F | a | \ll 1 \), the ground state energy per particle, \( \epsilon(n) \), is well represented by an expansion in power of \( k_F | a | \) \[32\]
\[
\epsilon(n) = 2E_F[\frac{3}{10} - \frac{1}{3\pi}k_F | a | + 0.055661(k_F | a |)^2 - 0.00914(k_F | a |)^3 + ...],
\]
where \( E_F = \hbar^2k_F^2/(2m) \) and \( k_F = (3\pi^2n)^{1/3} \). In the opposite regime, \( a \to -\infty \) (the Bertsch many-body problem, quoted in Refs.[33]), \( \epsilon(n) \) is proportional to that of the non-interacting Fermi gas
\[
\epsilon(n) = (1 + \beta) \frac{3}{10} \frac{\hbar^2k_F^2}{m},
\]
where the universal parameter \( \beta \) \[10\] is estimated to be \( \beta = -0.56 \) \[34\]. The universal limit \[10,34-38\] is valid at least in the case where the width of the Feshbach resonance is large compared to the Fermi energy as in the cases of \(^6\)Li and \(^{40}\)K.

In the \( a \to +0 \) limit the system reduces to the dilute Bose gas of dimers \[39\]
\[
\epsilon(n) = E_F(-1/(k_Fa)^2 + a_mk_F/(6\pi) + ...),
\]
where \( a_m \) is the boson-boson scattering length, \( a_m \approx 0.6a \) \[40\].

A simple interpolation of the form \( \epsilon(n) \approx E_FP(k_Fa) \) with a smooth function \( P(x) \) was considered in several papers. In Ref.[20] it has been proposed a \([2/2]\) Padé approximant for the function \( P(x) \) for the the case of negative \( a \)
\[
P(x) = \frac{3}{5} - 2 \frac{\delta_1 | x | + \delta_2x^2}{1 + \delta_3 | x | + \delta_4x^2},
\]
where \( \delta_1 = 0.106103, \delta_2 = 0.187515, \delta_3 = 2.29188, \delta_4 = 1.11616 \). Eq.(8) is constructed to reproduce the first four terms of the expansion (5) in the low-density regime and also to exactly reproduce results of the recent Monte Carlo calculations \[34\], \( \beta = -0.56 \), in the unitary limit, \( k_Fa \to -\infty \).
For the positive case (the interaction is strong enough to form bound molecules with energy $E_{\text{mol}}$) we have considered in Ref.[21] a [2/2] Padé approximant

$$P(x) = \frac{E_{\text{mol}}}{2E_F} + \frac{\alpha_1 x + \alpha_2 x^2}{1 + \alpha_3 x + \alpha_4 x^2},$$

(9)

where parameters $\alpha$ are fixed by two continuity conditions at large $x$, $1/x \to 0$, and by two continuity conditions at small $x$, $\alpha_1 = 0.0316621$, $\alpha_2 = 0.0111816$, $\alpha_3 = 0.200149$, and $\alpha_4 = 0.0423545$.

In Ref.[41] a Padé approximation has been considered for the chemical potential. Authors of Ref.[28] have used a model for $P(x)$, interpolating the Monte Carlo results of Ref.[36] across the unitary limit and limiting behaviors for small $|x|$. We note here also the BCS mean-field calculations of Ref.[27]

The hydrodynamic equations after linearization take the form

$$\frac{\partial^2}{\partial t^2} \delta n + \frac{1}{m} \nabla (n \nabla (\frac{d^2(n\epsilon(n))}{dn^2} \delta n)) = 0,$$

(10)

where $\delta n(\vec{r},t)$ is the change in the density profile with respect to the equilibrium configuration. If we consider oscillations with time dependence $\delta n \propto \exp(i\omega t)$, Eq.(10) can be reduced to a Hermitian equation [26]

$$-\omega^2 \left[ \frac{d^2(n\epsilon(n))}{dn^2} \right]^{-1} f = \frac{1}{m} \nabla (n \nabla f),$$

(11)

where $f = \frac{d^2(n\epsilon(n))}{dn^2} \delta n$, and the equilibrium density, $n$, is given by equation

$$\mu = V_{\text{ext}} + \frac{d(n\epsilon(n))}{dn},$$

(12)

where $\mu$ is the chemical potential, in the region where $n(\vec{r})$ is positive and $n(\vec{r}) = 0$ outside this region.

The Hilleraas-Undheim method [42] for upper bounds to eigenenergies of excited states of atoms can be generalized to the case of Eq.(11). Defining the functional $I[\chi]$ by

$$I[\chi] = -(1/m) \int \chi \nabla (n \nabla \chi) d^3r / \int \chi [\frac{d^2(n\epsilon(n))}{dn^2}]^{-1} \chi d^3r,$$

we get $I[f] = \omega^2$, where $f$ is the solution of Eq.(11).

Let the sequence of eigenvalues of Eq.(11) be denoted by $\omega_1^2 \leq \omega_2^2 \leq ...$ and let $\chi_1, \chi_2, ..., \chi_q$ form a set of $q$ linear independent functions. Introducing the function $\chi = \sum_{r=1}^{q} c_r \chi_r$, where
\(c_1, c_2, ... c_q\) are \(q\) variable parameters, we see that the functional \(I\) is stationary if \(\partial I/\partial c_r = 0\). Then the values of the \(q\) roots, \(\tilde{\omega}_1^2 \leq \tilde{\omega}_2^2 \leq \tilde{\omega}_3^2 \leq ... \leq \tilde{\omega}_q^2\), of the secular equations

\[
det[-\frac{1}{m} \int \chi_p \nabla (n \nabla \chi_s) d^3 r - \tilde{\omega}^2 \int \chi_p [\frac{d^2 (n \epsilon(n))}{dn^2}]^{-1} \chi_s d^3 r] = 0
\]

provide upper bounds to the \(q\) lowest eigenvalues of Eq. (11) \(\tilde{\omega}_r^2 \geq \omega_r^2\) for \(r = 1, 2, ..., q\). It follows that as extra terms are added to the expansion of \(\chi\), a given root of the secular equation \(\tilde{\omega}_r\) is decreased.

For the most interested case of \(M = 0\) modes, we can put in Eq. (13) \(q = 3, \chi_1 = 1, \chi_2 = (x^2 + y^2)\) and \(\chi_3 = z^2\), which give

\[
\omega_{\pm}^2 \overline{\omega}_\perp^2 = \eta \pm \sqrt{\eta^2 - 8 \lambda^2 \zeta (5 \zeta - 9)} \overline{(5 \zeta - 9)},
\]

where \(\eta = (3 + 4 \lambda^2) \zeta - (3 + 6 \lambda^2)\), \(\zeta = I_0 I_4 / I_2^2\), \(I_t = \int \bar{x} n(\bar{x}) d\bar{x}, \bar{x} = \sqrt{x^2 + y^2 + \lambda^2 z^2}\), \(\lambda = \omega_\perp / \omega_\perp\), and \(\pm\) signs refer to the transverse and axial mode, respectively.

To calculate \(\zeta\), we have used the following expansion

\[
n(\vec{r}) \approx (1 - \beta V_{ext}(\vec{r}))^{1/(2-p)} \sum_{i=0}^{l-1} c_i [V_{ext}(\vec{r})]^i,
\]

where parameters \(\beta, p\) and \(c_i\) are fixed by requiring that \(n(\vec{r})\) must satisfy a variational principle \(\delta \int n(V_{ext} + \epsilon(n)) d^3 r = 0\) with a subsidiary condition \(\int nd^3 r = N\).

From the Table 1 one can see a very fast convergence for \(\zeta\) and consequently for \(\omega_{\pm}\), the first term of the expansion (15) has accuracy \(10^{-3}\) [43], while the sum of the first three terms has accuracy \(10^{-4}\).

It is easy to show that our upper bounds, Eq. (14), give exact solutions for frequencies of the breathing modes for the polytropic equation of state, \(\epsilon(n) \approx n^\gamma\).

The hydrodynamic equation is expected to be applicable for describing the macroscopic excitations of the system up to energies of the order of the energy gap, \(\Delta\), needed to break-up a Cooper pair. But for the trapped gas, \(\Delta\) is a function of \(\vec{r}\) (\(\Delta\) decreasing when we go away from the center). It is natural to assume that the condition of the applicability of hydrodynamics to describe the macroscopic excitations of the system at \(T = 0\) is [22,44]

\[
\frac{\hbar \Omega}{\Delta} \ll 1,
\]

where \(\Omega\) is the frequency of the macroscopic excitations and the mean energy gap is given by \(\bar{\Delta} = \int n(\vec{r}) \Delta(\vec{r}) d\vec{r} / N\). To calculate \(\bar{\Delta}\) we have used results of Refs.[45,46]. The predictions of
Eq. (14) for the radial breathing mode frequency of the cloud of $^6Li$ atoms are shown in Fig. 1. For $\epsilon(n)$ we have used two approximations, the Padé [2/2] approximation of Refs. [20,21] and the parameterization of Ref. [28]. It can be seen a very small difference between these two approximations.

In Fig. 1, we have also compared the hydrodynamic predictions with experimental data [17]. We have used Ref. [47] to convert $a$ to the magnetic field $B$. Near the unitary limit there is a very good agreement with experimental data [17]. We note here that two experimental results [14,17] and [16] for $\omega_+$ are still about 10% in disagreement with each other, which is not fully understood yet. At $[N^{1/6}a/a_{ho}]^{-1} = -1.26$ the hydrodynamic upper bound begins to be below the sharp increased measured frequency that confirms a breakdown of hydrodynamic theory [17].

In Fig. 2, the calculated hydrodynamic upper bounds to the axial breathing mode frequency of the cloud of $^6Li$ is compared with experimental data [16] in the BCS-BEC crossover region. It can be seen that the difference between the two approximations for $\epsilon(n)$ is practically negligible and both approximations give a very good agreement between calculations and experimental data [16] for $[N^{1/6}a/a_{ho}]^{-1} \geq -1.14$. However at $[N^{1/6}a/a_{ho}]^{-1} = -1.31$ the hydrodynamic upper bound begins to be below the measured frequency that indicates, as in the radial mode case, breakdown of hydrodynamics, even though for the axial mode case the ratio between the collective energy and the gap energy, Eq. (16), is very small, $\hbar\omega_-/\tilde{\Delta} \approx 0.01$, at $[N^{1/6}a/a_{ho}]^{-1} = -1.31$ [48]. This breakdown of hydrodynamic theory may be related to the finite-temperature effects.

In summary, we have constructed the rigorous upper bounds to the collective frequencies of the Fermi gas under harmonic confinement in the framework of the hydrodynamic theory. The bounds are compared to experimental data on confined vapors of $^6Li$ atoms. It is shown that the hydrodynamic upper bound begins to be below the measured frequency at $[N^{1/6}a/a_{ho}]^{-1} \approx -1.3$, although the ratio between the collective energy and the gap energy, Eq. (16), for the axial mode is very small.

We thank J. Thomas for stimulating this work and for sharing with us the experimental results prior to publication. We also thank R. Grim and M. Bartenstein for providing us with the updated experimental data.
Table 1. $\zeta$ in the BCS region as a function of the dimensional parameter $X = (N^{1/6}a/a_{ho})^{-1}$ and the number of terms, $l$, in the expansion (15). The [2/2] Padé approximation of Refs.[20,21] is used for the energy per particle $\epsilon(n)$.

| $X$   | $l = 1$ | $l = 2$ | $l = 3$ | $l = 4$ | $l = 5$ |
|-------|---------|---------|---------|---------|---------|
| -0.1  | 2.2587  | 2.2572  | 2.2577  | 2.2575  | 2.2576  |
| -0.2  | 2.2658  | 2.2637  | 2.2642  | 2.2640  | 2.2641  |
| -0.4  | 2.2753  | 2.2732  | 2.2735  | 2.2735  | 2.2735  |
| -0.6  | 2.2801  | 2.2789  | 2.2787  | 2.2789  | 2.2788  |
| -0.8  | 2.2821  | 2.2818  | 2.2814  | 2.2816  | 2.2815  |
| -1.1  | 2.2822  | 2.2830  | 2.2825  | 2.2827  | 2.2826  |
| -1.4  | 2.2810  | 2.2825  | 2.2819  | 2.2821  | 2.2820  |
| -1.7  | 2.2792  | 2.2811  | 2.2805  | 2.2807  | 2.2806  |
| -2.0  | 2.2774  | 2.2795  | 2.2789  | 2.2791  | 2.2790  |
| -3.0  | 2.2720  | 2.2742  | 2.2738  | 2.2739  | 2.2739  |
Fig. 1. Radial breathing mode frequency $\omega_+$ in units of $\omega_\perp$ as a function of the dimensional parameter $X = (N^{1/6}a/a_{ho})^{-1}$. In the unitary limit, $a \to -\infty$, one expect $\omega/\omega_\perp = \sqrt{10/3} \approx 1.826$. The solid line and the dashed line represent the hydrodynamical upper bounds calculated using for the energy per particle the [2/2] Padé approximation of Refs.[20,21] and the parameterization of Ref.[28], respectively. The circular dots with error bars are the experimental results given by the Duke University group [17].
Fig. 2. Axial breathing mode frequency $\omega_\bot$ in units of $\omega_z$ as a function of the dimensional parameter $X = (N^{1/6}a/a_{ho})^{-1}$. The circular dots and diamonds represent the hydrodynamical upper bounds calculated using for the energy per particle the $[2/2]$ Padé approximation of Refs. [20,21] and the parameterization of Ref. [28], respectively. The triangles with error bars are the experimental results given by the Innsbruck group [16].
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