Collective Behavior of the Closed-Shell Fermi Gas

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We propose an unconventional description for the ground state and collective oscillations of the two-component normal Fermi gas with two-body zero-range interactions. The many-body problem can be accurately reduced to a linear, one-dimensional Schrödinger equation in a single collective coordinate, the hyperradius $R$ of the $N$-atom system which is the root mean square radius. The calculated properties of the Fermi gas ground state are shown to agree accurately with results from the Hartree-Fock (HF) approximation over a wide range of interspecies scattering lengths. The breathing mode excitation frequency deviates qualitatively from HF predictions, but we show that this reflects a failure of the HF approach for this observable.

Tremendous excitement has ensued in the ultracold physics community since dilute 2-component Fermi gases have recently been shown to exhibit BCS-like pairing physics. This pairing occurs at sufficiently low temperature $T << T_f$, sufficiently attractive interatomic scattering length $a$, and sufficiently high density $\rho \equiv k_F^3/(\pi^2)$, where $k_F$ is the Fermi wavenumber. This intriguing physical regime of the BEC-BCS crossover arises in the range $k_F a < -1$. The DFG currently studied in this region experimentally are in a metastable state whose decay to a more compact geometry in a different region of configuration space is inhibited by a multiparticle tunnelling barrier. Comparatively little attention has been given to the behavior of the low-temperature normal Fermi fluid with attractive interactions. In this Letter we discuss the behavior of this normal Fermi fluid from a viewpoint that departs from conventional mean-field theory. This theoretical framework and subsequent improvements may prove useful for analyzing other many-body systems, because in contrast to the familiar mean-field theories that require the solution of inherently non-linear differential or integro-differential equations, the present treatment utilizes only linear Schrödinger equations throughout.

Our treatment is related to the hyperspherical coordinate treatments that have been applied to finite nuclei, as in the “K-harmonic” method reviewed by Smirnov and Shitikova. The formulation is a rigorous variational many-body calculation, aside from the usual limitations of the assumed pairwise Hamiltonian with zero-range interactions. As was found in a similar study for bosons, the resulting hyperspherical coordinate description again provides a linear, one-dimensional, effective Schrödinger equation in the hyperradius. In this initial study of the usefulness of this methodology, we restrict ourselves to the study of fermionic systems with completely filled shells. This is done for analytical and computational simplification; the same approach should be equally applicable to open-shell fermi systems, with modest extensions.

Consider $N$ identical fermions confined either magnetically or optically in a spherically symmetric harmonic oscillator trap with angular frequency $\omega$. Half of the fermions are in one spin substate, while the other half are in a second spin substate. The full $N$-body time-independent Schrödinger equation for this system reads

$$H = \sum_{i=1}^{N} \left( -\frac{\hbar^2}{2m} \nabla_i^2 + \frac{1}{2} m\omega a_i^2 \right) + \sum_{i>j} U_{int} (\vec{r}_i - \vec{r}_j).$$

Here $m$ is the mass of the fermions under consideration and $U_{int}$ is the pairwise atomic interaction potential. We adopt the Fermi pseudopotential $U_{int} (\vec{r}_i - \vec{r}_j) = 4\pi\hbar^2 a \delta (\vec{r}_i - \vec{r}_j)$ where $a$ is the two body $s$ wave scattering length. Next we transform to a set of hyperspherical coordinates. The hyperradius for this system of equal mass particles is the root mean square distance of the atoms from the trap center, $R = \left( \sum r_i^2 / N \right)^{1/2}$. The remaining $3N-1$ dimensions are described by a set of angular coordinates collectively denoted by $\Omega$. In addition to the ordinary set of $2N$ spherical polar coordinates for each particle $\{ (\theta_i, \phi_i) \}_{i=1}^{N}$, we follow Ref. in defining $N-1$ hyperangles $\alpha_i$, $i = 1, 2, 3, ..., N-1$, as:

$$\tan \alpha_i \equiv \left( \sum_{j=1}^{i} r_j^2 \right)^{1/2} / r_{i+1}.$$

In this coordinate system the kinetic energy becomes

$$-\frac{\hbar^2}{2M} \left( \frac{1}{R^{3N-1}} \frac{\partial}{\partial R} R^{3N-1} \frac{\partial}{\partial R} - \frac{\Lambda^2}{R^2} \right)$$

where $M = Nm$ is the total mass of the system and the squared grand angular momentum operator $\Lambda^2$ is defined in the standard fashion. The trap potential is purely hyperradial, i.e. $\sum_{i=1}^{N} \frac{1}{2} m\omega a_i^2 r_i^2 = \frac{1}{2} M \omega^2 R^2$. Multiplying $\psi$ by $R^{(3N-1)/2}$ allows us to eliminate first derivative terms. One can view the rest of the calculation as the simplest approximation to Macek’s adiabatic hyperspherical description or as a one-term truncation of
an expansion of the exact $\psi(R,\Omega)$ into the complete, orthonormal set of eigenfunctions of the operator $A^2$, multiplied by unknown radial functions that are optimized variationally. These eigenfunctions, or “hyperspherical harmonics” (HHs, see [2, 3]) can be expressed analytically in terms of Jacobi polynomials, for any number of particles. Their eigenvalue equation is

$$A^2Y_{\lambda\nu}(\Omega) = \lambda(\lambda + 3N - 2)Y_{\lambda\nu}(\Omega)$$

where $\lambda = 0, 1, 2, \ldots$ is the order of the harmonic. The second index, $\nu$, stands for the further set of $N-2$ quantum numbers required to distinguish the (usually quite large) set of degenerate states having any chosen value of $\lambda$. This allows for the choice of a trial wave function $\psi(R,\Omega) = G(R)\Phi_\lambda(\Omega)$ where $\Phi_\lambda(\Omega)$ is a linear combination of HHs (multiplied by appropriate spinors) with grand angular momentum $\lambda$, which satisfies the antisymmetry requirements of this fermionic system. Generally the coefficients of this expansion are very difficult to obtain; in previous studies they have usually been calculated recursively using a coefficient of fractional parentage (cfp) expansion. To eliminate the need for a demanding cfp calculation with hundreds or thousands of particles, we restrict our treatment here to only magic numbers of particles, i.e., to filled energy shells of the noninteracting spherical harmonic oscillator. Because the $N$-particle oscillator has a separable Schrödinger equation in either independent particle coordinates or hyperspherical coordinates, any nondegenerate, normalized, antisymmetric $N$-body state must be identical in the two coordinate systems. The nondegenerate wavefunction for $n$ completely filled shells ($n = 1, 2, \ldots$) can thus be written as a Slater determinant of the independent particle states, which allows us to construct $\Phi_\lambda(\Omega)$ as:

$$\frac{1}{\sqrt{N!F_\lambda(R)}} \sum_P (-1)^P P \prod_{j=1}^N R_{n,\ell_j}(r_j) y_\ell_m(\omega_j)|m_{s_j}|.$$

Here $R_{n,\ell_j}(r_j)$ is the radial solution to the independent particle harmonic oscillator for the $i$th particle given by $rR_{n,\ell}(r) = N_{nl} \exp(-r^2/2l^2) (r/l)^{\ell+1/2}(r/l^2)$ where $L_\ell^n(r)$ is a modified Laguerre polynomial with $l = \sqrt{\hbar^2/m\omega}$. $y_\ell_m(\omega)$ is an ordinary 3D spherical harmonic with $\omega_j$ as the spatial solid angle for the $i$th particle, $|m_{s_i}|$ is a spin ket that allows for two spin species of atoms, $|\uparrow\rangle$ and $|\downarrow\rangle$. $R^{(3N-1)/2}F_\lambda(R) = A_\lambda \exp(-R^2/2L^2) (R/L)^{\lambda+3/2}$ is the nodeless hyperradial solution for $N$ noninteracting particles in an oscillator with hyperangular momentum $\lambda$ where $A_\lambda$ is a normalization factor and $L = \lambda/\sqrt{N}$. With this trial wavefunction, the expectation value of the Fermi pseudopotential yields an $R$-dependent effective potential for the function $G(R)$. From known properties of the $\delta$ function and the standard properties of matrix elements of two-body operators between two Slater determinant wave functions, the desired diagonal potential matrix elements can be shown to have the form (in harmonic oscillator units for both energy and radius)

$$\left\langle \Phi_\lambda(\Omega) \right| 4\pi a C_\lambda \sum_{i\neq j} \delta(\vec{r}_i - \vec{r}_j) \left| \Phi_\lambda(\Omega) \right\rangle = \frac{4\pi a C_\lambda}{N^{3/2}R^3}. \quad (2)$$

The constant $C_\lambda$ only depends on the number of atoms in the system, and is found by examining the diagonal matrix element of this hyperradial potential in the state $F_\lambda(R)$. Integration over the hyperradius allows us to solve for $C_\lambda$:

$$C_\lambda = \frac{N(N-1)^{7/2}(K+3/2)}{2^{7/2}(K)} \times \left\langle F_\lambda(R) \left| \Phi_\lambda(\Omega) \right| \delta(\vec{r}_1 - \vec{r}_2) \left| F_\lambda(R) \Phi_\lambda(\Omega) \right\rangle. \quad (3)$$

Here $K = \lambda + (3N-1)/2$ and $F_\lambda(R) \Phi_\lambda(\Omega)$ is the fully anti-symmetrized, non-interacting atom wave function. Thus the matrix element $\left\langle F_\lambda(R) \Phi_\lambda(\Omega) \right| \delta(\vec{r}_1 - \vec{r}_2) \left| F_\lambda(R) \Phi_\lambda(\Omega) \right\rangle$ is a sum of integrals over products of Laguerre polynomials in independent particle coordinates. Every diagonal matrix element coefficient $C_\lambda$ for the $n$-th complete filled shell can be written as a rational number multiplied by $\sqrt{2}/\pi^2$. For instance, the $n = 2$ filled shell state has $N = 8$ particles, and in its ground state, grand angular momentum $\lambda = 6$, and $C_8$ has the value (134217728/570285)$\sqrt{2}/\pi^2$. For the $n = 3$ filled shell with 20 particles, $C_\lambda$ involves the ratio of two integers, the larger of which is in the numerator with 34 digits. In view of the rapid increase as the number of particles is increased, we focus on the asymptotics in the large $N$ limit. The following functional form is found to be reasonably accurate for all $N$ beyond about $N = 20$ particles, namely $C_\lambda(N) \to 0.168022N^{7/2}/\sqrt{2}/\pi^2$. The fractional error in this approximation is smaller than 1% for $N = 20$ particles, and smaller than 0.1% for the 30th filled shell with 9920 particles, and beyond. The computational strategy has enabled us to carry out explicit calculations for as high as the 50th magic number, which is a degenerate fermi gas with 44,200 atoms. This is high enough to extract the leading behavior in the high-$N$ limit.

This effective potential now gives a linear, one-dimensional Schrödinger equation in the hyperradius $h[R^{(3N-2)/2}G(R)] = E[R^{(3N-2)/2}G(R)]$ where $h$ (in oscillator units) is given by

$$-\frac{1}{2N} \frac{d^2}{dR^2} + \frac{K(K+1)}{2N R^2} + \frac{1}{2} N R^2 + \frac{4\pi a C_\lambda}{N^{3/2}R^3}. \quad (4)$$

It is informative to recast this radial Schrödinger equation into dimensionless form with $E = EN_1 E'$ and $R = \sqrt{(R^2/N_1)R'}$, where $E_{N1} = (\lambda + 3N/2)$ and $(R^2/N_1) = (3/2 + \lambda/N)$ are the energy and expectation values of
The resulting linear effective one-dimensional Schrödinger equation is given by

\[ \left( -\frac{1}{2m} \frac{d^2}{dR^2} + V_{\text{eff}}(R') - E \right) R^{(3N-1)/2} G(R') = 0 \]

(5)

where \( m^* \equiv (\lambda + 3N/2)^2 \), and, in the large \( N \) limit, \( V_{\text{eff}}(R) \) is given by

\[ V_{\text{eff}}(R') = \frac{1}{2R'^2} + \frac{1}{2} R'^2 + \frac{4\pi aC_\lambda}{l(\lambda + 3N/2)^{3/2}} R'^3. \]

The value of \( \lambda \) for each filled shell ground state can be ascertained by comparing the energy of \( N \) noninteracting particles in a harmonic oscillator potential, written in each coordinate system. In the independent atom representation the energy is given by \( E = \hbar \omega \left[ \sum_{i=1}^{N} (l_i + 2n_i) + 3N/2 \right] \). The energy of \( N \) noninteracting particles, described using hyperspherical quantum numbers, with grand angular momentum \( \lambda \) and \( \chi = 0, 1, 2, \ldots \) hyperradial nodes in \( F_\lambda(R) \), is given by \( E = \hbar \omega \left( \lambda + 2\chi + \frac{3N}{2} \right) \). The ground state has \( \chi = 0 \), while the first breathing mode excited state has \( \chi = 1 \). After we equate the two expressions for the ground state energy, we obtain \( \lambda = \sum_{i=1}^{N} (l_i + 2n_i) \). In terms of the number of complete filled shells, \( n \), namely \( N(n) = n(n+1)(n+2)/3 \), and \( \lambda(n) = (n-1)n(n+1)(n+2)/4 \). To a good approximation at all \( N \), \( \lambda(N) \approx (3N)^{4/3}/4 - 3N/2 + N^{2/3}/1921^{1/3} \), which becomes exact in the limit \( N \to \infty \). Similarly, the Fermi wave number, \( k_f \), may be shown to be \( k_f = \sqrt{2(n+1)/l} \to \sqrt{2(3^{1/6}) N^{1/6}}/l. \) This all shows that in the large-\( N \) limit

\[ V_{\text{eff}}(R') \to \frac{1}{2R'^2} + \frac{1}{2} R'^2 + \frac{\zeta k_f a}{R'^3}, \]

where \( \zeta \approx 0.16802 (64\sqrt{12}/81\pi) \). Note that the only parameter in this asymptotic large-\( N \) potential curve is in fact \( k_f a \). At \( N \to \infty \) we see that \( m^* \to N^{8/3} \), whereby the second derivative term in equation (5) is negligible. This means the squared zero-order ground state wave function in the large \( N \) limit is approximated by \( [R^{(3N-1)/2} G(R')]^2 \approx \delta(R' - R_{\text{min}}) \) where \( R_{\text{min}} \) is the location of the minimum of \( V_{\text{eff}}(R') \), if it exists. This recognition of the strong hyperradial localization for infinite dimensional systems is also used extensively in dimensional perturbation theory. Ground state expectation values of quantities involving the hyperradius can be extracted by simply evaluating them at \( R_{\text{min}} \) (e.g. \( \langle R^2 \rangle = R_{\text{min}}^2 \), and \( E = V_{\text{eff}}(R_{\text{min}}) \)).

The effective potential in equation (5) is similar in form to the analogous hyperradial potential obtained for the Bose-Einstein condensate (BEC) in Ref. [9]. The main differences between these two potentials stem from the antisymmetry requirements; whereas the constant in the interaction potential [9] acted as \( N^{3/2} \) for a BEC, we find for the DFG an \( N^{7/2} \) behavior for \( N >> 1 \). On the other hand, the coefficient of the \( R^{-2} \) effective centrifugal repulsion increases as \( N^{5/3} \), as opposed to \( N \) for the BEC case, which is a manifestation of the Fermi pressure in the DFG. The hyperspherical results for the ground state energy and expectation value of \( R^2 \) are very close to the HF predictions, for both repulsive and attractive interactions, as is evident from Fig. 1.

![Figure 1](#)
bosons. BECs formed with \( a < a_c \) were predicted to collapse by a number of studies \[9, 11, 12, 13\], and the corresponding phenomenon of the bosonova was observed experimentally. \[14, 15\]

![FIG. 2: The effective potential for five values of \( k_f a \) spaced evenly from \( k_f a_c = 0.5 \) to \( k_f a_c + 0.5 \). The bold curve is at \( k_f a = k_f a_c \), and the dotted curve is the non-interacting potential. Moreover, as \( k_f a \) is lowered, the local minimum of \( V_{eff}(R) \) becomes “softer”, as the curvature at the local minimum decreases. This suggests that the lowest excitation frequency (the frequency of the breathing mode) should decrease as \( a \) is made increasingly negative. Figure 3 compares the excitation frequency calculated in our hyperspherical method with the lowest one predicted using the sum rule method, \[16\], in which the desired moments were calculated using the Hartree-Fock ground state. The calculated HF frequencies for the lowest 8 excitations caused by the same \( R^2 \) breathing mode operator are also shown. The hyperspherical frequencies are in excellent agreement with the sum rule predictions, but the Hartree-Fock frequencies are qualitatively different and apparently erroneous. Our hyperspherical description allows for the calculation of collective monopole excitations in which every particle in the cloud oscillates in and out at the characteristic frequency, while Hartree-Fock predicts only single-particle excitations in which just one orbital of the DGF gets excited.

In summary, we have developed a fully antisymmetrized, variational description of \( N \) fermionic atoms, with zero-range interactions in a spherical harmonic trap. Truncation to the lowest antisymmetric hyperspherical harmonic reduces the problem to a linear, one-dimensional Schrödinger equation in the hyperradius with an effective potential. In the large atom number limit, it only depends on the quantity \( k_f a \). The ground state energy and radius predicted from this linear quantum mechanical treatment map accurately onto those predicted with the Hartree-Fock method, while the breathing mode frequencies agree with the sum rule and are a qualitative improvement over the calculated HF frequencies. This picture predicts a ground state energy that collapses to \(-\infty\) at \( k_f a < -1.21 \), in a manner identical to the physics of the “bosonova”. But the full interrelationship between this phenomenon and the physics of pairing in the BEC-BCS crossover region goes beyond the scope of the present study and will be explored in a subsequent publication.

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