Shell structure and pairing for interacting fermions in a trap

Henning Heiselberg and Ben Mottelson
NORDITA, Blegdamsvej 17, DK-2100 Copenhagen Ø, Denmark

Dilute systems of cold degenerate fermionic atoms have been trapped and cooled down to a fraction of the Fermi temperature [1]. Collective modes are studied and the superfluid gap is actively searched for. At low particle densities the shell structures in traps are pronounced as they are in nuclei and the level degeneracies are important for the size of the gaps which can differ substantially from those known from homogeneous systems [2] and systems with continuous level densities. The atomic traps have the advantage as compared to, e.g., nuclei, that one can study almost any number of particles and vary their density, interaction strength (by tuning Feshbach resonances [3]), and the number of spin states, e.g. 18 for $^{40}$K atoms. The object of this paper is to study the novel shell structures for weakly interacting fermions in harmonic oscillator traps at zero temperature $T_F=0$. We shall mainly discuss a spherically symmetric trap and a dilute gas (i.e. where the density $\rho$ obeys $\rho|a|^3 \ll 1$) of particles with two spin states with equal population. The Hamiltonian is then given by

$$H = \sum_{i=1}^{N} \left( \frac{\mathbf{p}_i^2}{2m} + \frac{1}{2} m \omega^2 r_i^2 + 4\pi \frac{\hbar^2 a}{m} \sum_{i<j} \delta^3(\mathbf{r}_i - \mathbf{r}_j) \right).$$

(1)

For a large number of particles $N$ at zero temperature the Fermi energy is for a non-interacting system

$$E_F = (n_F + 3/2) \hbar \omega \simeq (3N)^{1/3} \hbar \omega,$$

(2)

where $n_F$ is the h.o. quantum number at the Fermi surface. The h.o. levels are highly degenerate with states having angular momenta $l = n_F, n_F - 2, ..., 1$ or 0 due to the $U(3)$ symmetry of the 3D spherically symmetric h.o. potential. However, interactions split this degeneracy. In the Thomas-Fermi (TF) approximation the mean-field potential is

$$U(r) = 2\pi \frac{\hbar^2 a}{m} \rho(r),$$

(3)

the Fermi energy $E_F = \hbar^2 k_F(r)/2m + (1/2)m\omega^2 r^2 + U(r)$, and the density

$$\rho(r) = k_F^3(r)/3\pi^2 \simeq \rho_0 \left(1 - r^2/R_F^2\right)^{3/2},$$

(4)

inside the cloud $r \leq R_F = a_{osc}\sqrt{2n_F + 1}$, where $a_{osc} = (\hbar/m\omega)^{1/2}$ is the oscillator length, and $\rho_0 = (2n_F)^{3/2}/3\pi^2 a_{osc}^3$ the central density [4]. These equations constitute the energy density functionals which now can be solved self-consistently. The latter expression in Eq. (4) is valid for dilute systems where the interactions contribute a mean-field weak compared to the confining potential.

The system is dilute when the Fermi energy is large compared to the mean-field energy, $E_F \gg |U|$, or equivalently $k_F|a|^3 \simeq \rho^{1/3}|a| \simeq n_F^{1/2}|a|/a_{osc} \ll 1$. Dense Fermi and Bose systems are studied in Refs. [5] and [6]. We shall be particularly interested in very dilute systems where also the h.o. energy exceeds the mean-field potentials, $\hbar \omega \gg |U|$, or equivalently $n_F^{3/2}|a|/a_{osc} \ll 1$ (see Fig. 3).

The splitting of the degenerate $l = n_F, n_F - 2, ..., 1$ or 0 states by the mean-field potential can be calculated perturbatively in the very dilute limit. From the radial h.o. wave function $R_{nl}(r)$ for the state with angular momentum $l$ and $n$ radial nodes in the h.o. shell $n_F = 2n + l$, we obtain the single particle energies

$$\epsilon_{n_F,l} = \left(n_F + \frac{3}{2}\right) \hbar \omega = \int U(r)|R_{nl}(r)|^2 r^2 dr$$

$$= \frac{4\sqrt{2}}{3\pi} \frac{a}{a_{osc}} n_F^{3/2} \hbar \omega F(n_F,l),$$

(5)

where the mean-field and wave function overlap is

$$F(n_F,l) = \int_{0}^{R_F} |R_{nl}(r)|^2 \left(1 - \frac{r^2}{R_F^2}\right)^{3/2} r^2 dr$$

$$\simeq \frac{4}{3\pi} - \frac{1}{4\pi} \frac{l(l+1)}{n_F^2} + O(n_F^{-1}).$$

(6)

(7)
The latter result is obtained using the WKB approximation which compares well to numerical results for all \( n_F \) when \( n_F \gg 1 \) as shown in Fig. 1. The mean-field energies are proportional to the coupling and \( n_F^{3/2} \) and are split like rotational bands with a prefactor that is smaller than the average mean-field energy by a factor \( \sim 3/16 \). The relative small splitting reflects the fact that the mean-field potential is almost quadratic in \( r \) and the anharmonic terms therefore small. For attractive interactions \( (a < 0) \) the lowest-lying states have small angular momentum, which is opposite to nuclei.

The wave function for a pair of particles each with angular momentum \( l \) adding up to total angular momentum \( L \) is a sum of time-reversed two-particle states

\[
\phi_L(n_F, l) = \sum_m \langle ml - m|L0\rangle \psi_{lm}(r_1)\psi_{-m}(r_2),
\]

for \( M = 0 \). Here \( \psi_{lm}(r) = R_{nl}(r)Y_{lm}(\theta, \phi) \) is the single particle wave function normalized to unity and \( m = -l, ..., l \). As the spin wave function is always in a singlet state, since otherwise the interactions vanish, it has been excluded in Eq. (5). The corresponding gap equal to half the pairing energy between two particles, is

\[
\Delta_L(n_F, l) = \frac{1}{2} \langle \phi_L(n_F, l)|4\pi \hbar^2|\delta^3(r_1 - r_2)|\phi_L(n_F, l)\rangle
\]

\[
= \frac{\hbar^2|a|}{2m} (2l + 1)^2 \frac{\langle 00|L0\rangle^2}{2L + 1} \int |R_{nl}(r)|^4 r^2 dr,
\]

for even \( L \) and zero otherwise. The gap is largest when pairs of particles are coupled to total angular moment \( L = 0 \) for which the Clebsch-Gordan coefficient is \( \langle 00|00\rangle^2 = (2l + 1)^{-1} \).

The overlap integrals can be calculated for \( n_F \gg 1 \) within the WKB approximation

\[
\Delta_0(n_F, l) = \left( \frac{1}{\pi^{1/2} \omega_s L}, l = n_F, 1 \ll l, 1 \ll n_F - l \right).
\]

Here, the function \( L(n_F, l) \approx \ln(l) \), to leading logarithmic accuracy. Numerical calculations of the gaps are shown in Fig. 2.

For two or more particles in a shell, it is known from nuclear pairing theory that it is generally energetically favorable for the particles to pair in states with \( L = 0 \) where their spatial overlap is maximum. In the degenerate pairing model with interactions only in the \( L = 0 \) pair state the pairing energy between \( n_v \) particles in a shell is

\[
\Delta(n_v, v) = \frac{(n_v - v)(2n_v - n_v - v + 2)}{4n_v} \Delta_0,
\]

where the seniority \( v \) is the number of unpaired particles. The number of available states in the multiplet is \( \Omega = 2(2l + 1) \) for the multiplet \( l \) with pairing gaps \( \Delta_0 = \Delta_0(n_F, l) \). In the ground state for even \( n_v \) all particles are paired i.e. \( v = 0 \), and the lowest excitations are reached by breaking pairs.

When \( n_F \) (or \( l \)) is sufficiently small, however, the mean-field splitting of Eq. (5) is smaller than the pairing gaps and the pairing acts between all states in an oscillator shell and not just in a single \( l \) multiplet, i.e. the full \( SU(3) \) symmetry is effectively restored as compared to the \( SU(2) \) symmetry of the single \( l \) multiplet. We shall refer to this enhanced pairing as “\( SU(3) \)-pairing” or “super-pairing”. We shall calculate the gap first by writing down the “super”-pair wave function and secondly by solving the gap equation.
Assuming $SU(3)$ symmetry the pairing can be calculated variationally with a pair wave function that is a generalization of Eq. (8) to a sum over $l = n_F, n_F - 2, ..., 1$ or 0

$$\Phi_0(n_F) = \sum_i \alpha_i \phi_0(n_F, l) \left/ \left| \sum_i \alpha_i^2 \right|^{1/2} \right..$$

(12)

The weights $\alpha_i$ can be found by a variational method with the overlap integrals $\int \mathcal{R}^2 m_1^2 \mathcal{R}^2 m_2^2 dr$ calculated numerically. For large $n_F$ we find $\alpha_i \sim \sqrt{2l+1}$ very accurately. The sums then reduce to the h.o. level density:

$$\sum_{lm} |\psi_{lm}(r)|^2 = (4\pi)^{-1} \int (2l+1)\mathcal{R}^2 = (1/2)\rho(r)/dn_F, \text{ and the supergap becomes}$$

$$G = \frac{1}{2} \left( \Phi_0(n_F) [4\pi \hbar^2/m] \delta^3(r_1 - r_2) |\Phi_0(n_F)| \right)$$

$$\approx \frac{\pi \hbar^2}{m} \int |d\rho(r)/dn_F|^2 d^3r$$

$$= \frac{32\sqrt{2}}{15\pi^2} a_{osc}^2 \hbar \omega,$$

(13)

(14)

with the particle density $\rho(r)$ from Eq. (3). The gap is a factor $n_F$ larger than that for a single $l$ value because the level degeneracy is larger by $n_F$.

Turning the mean-field splitting back on, the condition for superpairing is that the pairing field $2G$ exceeds the mean-field splitting of the single particle levels, $\epsilon_{n_F,l} = -\epsilon_{n_F,l} = 0$. Using Eqs. (3), (4), and (14) the condition for superpairing becomes

$$n_F \gtrsim \frac{64}{5},$$

(15)

corresponding to $N \lesssim 10^5$ trapped particles. For $n_F > 64/5$ we find that only the lower lying states $l \lesssim 64/5$ superpair. The seniority scheme of Eq. (1) also applies to many superpairs replacing $\Delta_0 = G$ and the level degeneracy for a full h.o. shell $\Omega = (n_F + 1)(n_F + 2)$.

The transition from pairing within a single $(n_F, l)$ level to many levels can be calculated by solving the gap equation

$$\Delta(n_F, l) = -\frac{1}{2} \sum_{l'} \sqrt{\Delta^2(n_F', l')} + (\epsilon_{n_F,l} - \mu)^2 \sqrt{2l' + 1}$$

$$\langle \phi_0(n_F', l') | \hbar^2/2m \delta^3(r_1 - r_2) | \phi_0(n_F, l) \rangle. $$

(16)

within the same shell, i.e., $n_F' = n_F$. Here, the single particle energies are given by Eq. (3) in the very dilute limit and the number of particles is such that the Fermi level is positioned at $\mu = \epsilon_{n_F, l}$. When $n_F \lesssim 64/5$ the gap equation reproduces Eq. (13), which is followed by a transition region as shown in Fig. 3. When $n_F \gtrsim (64/5) \ln(n_F)$, equivalent to $n_F \gtrsim 50$, the pairing gap approach for a single $l$ level as given by Eq. (10).

When the interaction becomes sufficiently strong pairing also takes place between different h.o. shells. The pair wave function can still be expressed as a sum over time-reversed single particle wave functions $|\Psi_0(n_F)|$. For interaction strengths $G \ln(n_F) \lesssim h \omega$, Eq. (3) is still a good approximation and the generalized gap equation is then simply Eq. (10), but also summed over $n_F \neq n_F$ [1]. For strong interactions, $2G \ln(n_F) \gtrsim h \omega$, the radial wave functions differ substantially from the h.o. ones due to the strong pair field [14]. The coherence length $\xi \gtrsim R_{TF} h \omega/\Delta$ is smaller than the system size and bulk superfluidity sets in (see Fig. 3). The finite system behaves like an irrotational fluid and exhibits collective oscillations with frequencies of order $\sim h \omega$ [12].

![FIG. 3. Diagram displaying the transitions of the level structures and pairing gaps $\Delta$ (in units of $h \omega$) in traps as a function of the number of particles $N = n_F^3/3$ and the scaled interaction strength $G/h \omega = (32/15\pi^2)(2n_F)^{1/2}/a_{osc}$. The dashed lines separate the dense, dilute and very dilute trapped gases. The region between the dash-dotted lines indicates the transition between superpairing, $\Delta = G$, and pairing in a single $l$-level, $\Delta \approx (G/n_F) \ln(l)$. Above the full line $G = h \omega/2\ln(2n_F)$ inter-shell pairing enhances the gap $\Delta$ above $h \omega$.](image-url)

Whereas nuclei with partially filled shells generally are quite deformed, $\delta = (r_2^2)/(r_1^2) - 1 \sim 1/n_F \gtrsim 1$, the atomic mean-field does not deform in bulk in a spherically symmetric h.o. trap. The h.o. shell at the Fermi surface does not deform either because the energy of the superfluid state is always lower than that of the deformed state, and the atoms will be a spherically symmetric fluid.

Deformed traps such as the oblate ones with $\omega_\perp \equiv \omega_1 = \omega_3 > \omega_\parallel$ will only have $SU(2)$ symmetry and correspondingly lower level degeneracies except when ratios of the trap frequencies are rational numbers. The Fermi energy for the deformed h.o. potential is $E^2_F \approx n_F h \omega_\perp + n_F h \omega_3$, where $n_F$ now is the h.o. quantum number in two dimensions which has degenerate single particle states of angular momentum projected along the symmetry axis: $m = -n_F, -n_F + 2, ..., n_F$. 

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For very deformed traps such that \( \omega_\perp \ll \omega_3 N^{-1/2} \), the h.o. potential is effectively two-dimensional, \( U(r) \propto (1 - r^2/R_\perp^2) \theta(R_\perp - r) \), inside the cloud. Such a quadratic mean-field potential does not destroy the \( SU(2) \) symmetry or split the h.o. shells, except for the states with lowest angular momentum whose wave functions extend slightly outside \( R_\perp \). The pairing gaps can be calculated for two particles in shell \( n_F \) exploiting the \( SO(2,1) \) symmetry \([14]\) of a two-dimensional trap for particles with delta-function interactions

\[
\Delta^{2D}(S,M) = \frac{1}{2} \left( SM |\frac{\hbar}{2m} a |^2 \delta^3(r_1 - r_2)|SM\right) = \frac{|a|}{a_3} \frac{1}{2^{2S}} \frac{m}{(m_3^2/2\hbar)} \left( |S - M|!(S + M)!\right),
\]

where \( M = -S, -S + 2, \ldots, S - 2, S \), is half the total angular momentum projected along the symmetry axis, and \( S = 0, 1, 2, \ldots, n_F \), is a quantum number similar to seniority. The spatial extent of the particles along the symmetry axis enters through \( a_3^{-1} = \int |\psi_{n_F,S}(r_3)|^2 dr_3 \), and it is a remarkable feature that the pairing energies are independent of \( n_F \) in two dimensions. In the supershell \( n_F \), pair energies of the states with \( S \leq n_F - 1 \) equal those of the previous supershell \( n_F - 1 \), recursively. Thus, for example, the energy spectrum corresponding to Eq. (17) always has states with excitation \( 2\hbar \omega_\perp \), which follows from the \( SO(2,1) \) symmetry \([14]\) also for strong interactions. For more than two particles in a shell the low lying excitations will be dominated by paired states with the seniority quantum number describing the number of unpaired particles.

We now turn to experimental observation of superfluidity and gaps which requires temperatures below \( T \lesssim \Delta/k_B \). For temperatures \( T \sim 0.2 E_F \) as reached in \([1]\) this would require strongly interacting atoms (e.g. near a Feshbach resonance) with inter-shell pairing so that \( h_\omega \lesssim \Delta E_F = n_F \hbar \omega_\perp \). Alternatively, a cloud of \( \sim 10^{10} \) \(^6\)Li atoms, which have a very large and negative natural scattering length, the supergap is \( \Delta = G \approx 10^{-2} E_F \) and cooling below that would be required in order to measure the gap.

Superfluid gaps can be determined in experiments with cold trapped Fermions from response functions for multipole modes \([12]\) or from the scissors mode \([15]\) in a deformed trap. Alternatively, we suggest rotating the deformed trap slowly around an axis perpendicular to the symmetry axis. When \( \Delta \lesssim \hbar \omega \) superfluidity reduces the moment of inertia from the rigid-body one to that of an irrotational fluid, which is smaller by a factor \( \delta^2 \) for small deformations. As for rapidly rotating nuclei \([8]\) several interesting phenomena such as superdeformation, backbending, fission, etc. may occur in deformed traps. Optical lattices in current experiments \([16]\) have few atoms in each local trap and we thus expect superpairing which favors the insulator vs. conductor state.

In summary, we have calculated the shell structure for a dilute system of interacting fermions as a function of the interaction strength and number of particles in a h.o. trap. For weak interactions, \( G \lesssim \hbar \omega/2 \ln(n_F) \), and few particles \( N \lesssim 10^3 \) in the trap, the \( U(3) \) symmetry of the h.o. leads to larger degeneracy and superpairing occurs with supergaps \( \Delta = G \). For a larger number of particles \( N \gtrsim 10^4 - 10^5 \), the mean-field energy generally dominates and splits the \( U(3) \) symmetry of the h.o. into multiplets by an energy that is large compared with the gaps. For two dimensional traps, however, the mean-field does not split the \( U(2) \) degeneracy and the gaps display a remarkable regularity as given by Eq. (17). Atoms with more than two spins have larger level degeneracies for spin independent interactions, and the gaps are correspondingly larger as is also the case for uniform density \([13]\].

We thank G. Bruun and C. J. Pethick for valuable discussions.

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