Supershell structure in trapped dilute Fermi gases

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We show that a dilute harmonically trapped two-component gas of fermionic atoms with a weak repulsive interaction has a pronounced super-shell structure: the shell fillings due to the spherical harmonic trapping potential are modulated by a beat mode. This changes the "magic numbers" occurring between the beat nodes by half a period. The length and amplitude of this beating mode depend on the strength of the interaction. We give a simple interpretation of the beat structure in terms of a semiclassical trace formula for the symmetry breaking $U(3) \to SO(3)$.

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In finite systems of fermions, quantum effects lead to bunching of energy levels resulting in shell structure. Well-known examples are the shell structures in atoms or nuclei $^1$, determining their chemical properties and stability. In fact, shell effects and the so-called "magic numbers", corresponding to spherical shell closings, have been discovered in a variety of other finite fermion systems. Metal clusters in which the delocalized valence electrons are bound in the field of the metallic ions $^2$, or quantum dots in semiconductor heterostructures $^3$ are famous examples. More recent experimental progress makes it possible to study yet another species of finite quantal systems: atomic gases, often weakly interacting, confined e.g. by an optical dipole trap $^4$.

In this paper, we show that a harmonically trapped gas of fermionic atoms interacting by a weak repulsive two-body force may exhibit super-shell structure: the shell oscillations of the spherical harmonic oscillator are modulated by a beat structure, whereby the positions of the magic numbers are shifted by half a period between successive beats. We can explain this surprising result semiclassically by the interference of diameter and circle orbits surviving the breaking of the $U(3)$ symmetry of the harmonic oscillator by the leading anharmonicity term in the mean field.

Similar super-shell structure was predicted for metallic clusters $^5$, inspired by a semiclassical analysis of Balian and Bloch in terms of the periodic orbits in a spherical cavity $^6$, and observed experimentally $^7$. Analogous ideas could be applied to the description of shell structure in transport properties of quantum wires $^8$.

Let us consider a dilute gas of fermionic atoms, confined by a spherical harmonic potential modeling an external trap $^9$, interacting through a repulsive zero-range two-body potential. The many-body Hamiltonian is

$$H = \sum_{i=1}^{N} \left( \frac{P_i^2}{2m} + \frac{m\omega^2 r_i^2}{2} \right) + \frac{4\pi\hbar^2 a}{m} \sum_{i<j} \delta^3(r_i - r_j),$$

where $a$ is the $s$-wave scattering length. The value and the sign of $a$ can be varied either by changing the type of atoms or by applying a magnetic field: Feshbach resonances $^9$ allow to tune the scattering length from a large positive to a large negative value. (Here, we focus on the repulsive case.)

Due to the Pauli principle the $\delta$ interaction only applies to fermions of pairwise opposite spin. We consider a fully unpolarized two-component system with two spin states, so that the total particle density is composed of two different densities of equal magnitude, $\rho(\mathbf{r}) = n^\uparrow(\mathbf{r}) + n^\downarrow(\mathbf{r}) = n^\uparrow(\mathbf{r}) = n^\downarrow(\mathbf{r})$. In the weak-interaction regime, the interaction energy density is given by $g n^\uparrow(\mathbf{r}) n^\downarrow(\mathbf{r}) = g n^2(\mathbf{r})/4$, where the coupling strength parameter $g$ is introduced by

$$g = 4\pi\hbar^2 a/m. \quad (1)$$

This leads to the single-particle Hartree-Fock equation

$$\left[ -\frac{\hbar^2}{2m} \Delta + g n^\uparrow(\mathbf{r}) + V_{ho}(\mathbf{r}) \right] \psi_i^\uparrow(\mathbf{r}) = \epsilon_i \psi_i^\uparrow(\mathbf{r}), \quad (2)$$

where $V_{ho}$ is the harmonic oscillator (HO) trap potential.

The diluteness condition necessary to treat the interaction as a two-body process is that the interparticle spacing $\bar{n}^{-1/3}$ is much larger than the range of the interaction and that $\bar{n}a^3 \ll 1$. This dimensionless parameter also limits the life time of the two-component atomic fermion gas due to dimer formation, which is a three-body process $^11$. To guarantee that this condition is fulfilled, we calculate the central density $n(0)$ in the Thomas-Fermi approximation and plot level curves of $\log(a^3 n(0))$ in a $g-N$ landscape seen in Fig. 1. The diluteness condition is seen to be fulfilled for all considered combinations of particle numbers and interaction strengths. This also rules out the possibility of phase separation discussed in $^10$. Assuming spherical symmetry, Eq. 2 reduces to its radial part

$$\left[ -\frac{\hbar^2}{2m} \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) + \frac{\hbar^2 l(l+1)}{2m r^2} + U(r) \right] \psi_i^\uparrow = \epsilon_i \psi_i^\uparrow, \quad (3)$$

where $\psi_i^\uparrow(\mathbf{r}) = \psi_i^\uparrow(r)$ and $U(r)$ is the central potential.
with $U(r) = gn^\dagger(r) + \frac{1}{2}m\omega^2 r^2$ being the effective mean-field potential. Each state has a $(2l + 1)$-fold angular momentum degeneracy. We solve Eq. (4) self-consistently on a grid. The interaction term is updated (with some weight factors) in each iteration according to $gn^\dagger(r) = g\sum_i |\psi_i^\dagger(r)|^2$.

After convergence is obtained, the ground-state energy of the $N$-particle system is given by ($E_F =$ Fermi energy)

$$E_{tot}(g, N) = \sum_{\epsilon_i \leq E_F, \sigma = \uparrow, \downarrow} \epsilon_i - g \int n_{\uparrow}^2(r) d^3r. \quad (4)$$

In general, the ground-state energy as a function of $N$ can be written as the sum of a smooth average part and an oscillating part, $E_{tot} = E_{av} + E_{osc}$. The oscillating part, referred to as the shell-correction energy, or shell energy in short, reflects the quantized level spectrum $\{\epsilon_i\}$. For a non-interacting Fermi gas in a spherically symmetric 3D harmonic trap, the leading-order term for the average energy is found in the Thomas-Fermi approximation to be $E_{av} = (3N)^{1/3}/4$. For the repulsive interacting case, we find $E_{av}(g > 0) \propto N^{\alpha}$ with a larger exponent $\alpha > 4/3$. However, Eq. (4) with an interaction term linear in the density is only valid for moderate $\alpha > 4/3$. Contrary to the non-interacting case, and also to self-saturating fermion systems (such as nuclei and metal clusters) with a nearly constant particle density, it is not possible here to obtain the smooth part of the energy by a simple expansion in volume, surface and higher-order terms. We therefore perform a numerical averaging of the energy over the particle number $N$ in order to extract its oscillating part.

In the non-interacting case ($g = 0$) the shell energy $E_{osc}$ oscillates with a frequency $2\pi 3^{1/3} \approx 9.06$ as a function of $N^{1/3}$ and has a smoothly growing amplitude $\propto N^{2/3}$. This follows from the exact trace formula for $E_{osc}$ of the 3D harmonic oscillator, whose leading-order term is given by

$$E_{osc}^{\text{ho}} \approx (3N)^{2} \frac{\hbar \omega}{2\pi} \sum_{k=1}^{\infty} \frac{(-1)^k}{k^2} \cos \left(2\pi k (3N)^{1/3}\right). \quad (5)$$

Hereby $k$ is the repetition number of the primitive classical periodic orbit of the system with action $S_0(E) = 2\pi E/\omega$. The argument of the cosine function in Eq. (5) is simply $k$ times $S_0(E)/\hbar$, taken at the Thomas-Fermi value of the Fermi energy $E_F(N) = (3N)^{1/3}/\hbar \omega$. The gross-shell structure is governed by the lowest harmonic with $k = 1$.

Switching on the interaction, this scenario changes. A beating modulation of the rapid oscillations is found. In Fig. 3 we show the shell energy versus $N^{1/3}$ for three values of the interaction strength, $g = 0.2$, $0.4$ and $2$. A beating modulation of the amplitude of the shell energy, i.e., a super-shell structure, is clearly seen to appear for all cases. At small particle numbers and particularly for small $g$ values, the shell energy is that of the non-interacting system, given by Eq. (5). For larger interaction strengths the super-shell structure is more clearly seen, and several beating nodes appear for $g = 2$. With increasing interaction strength the amplitude of the shell energy oscillations becomes smaller. For example, for particle numbers around $80^{1/3} \approx 500000$, the amplitude of the shell energy is about $40\hbar\omega$, which is only about $10^{-6}$ of the total ground-state energy.

Through Fourier analysis of the calculated shell energy, two frequencies are seen to smoothly appear with increasing $g$ value around the HO frequency (9.06), see Fig. 3. The exact values of the two frequencies depend on the range of particle numbers included in the analysis. The super-shell features appear when the contribution to the effective potential from the interaction, $gn^\dagger$, is sufficiently large, i.e., at large values of $g$ and $N$. We also observe that (almost) until the first super-node, i.e., $N^{1/3} \approx 28$ in Fig. 3 the magic numbers agree with the HO ones ($g = 0$). Between the first two super-nodes, i.e., $28 \leq N^{1/3} \leq 49$ in Fig. 4 the magic numbers for the interacting system are situated in the middle of two HO magic numbers, i.e., they appear at the maxima of the fast shell oscillations. Then, after the second super-node they roughly agree with the unperturbed HO ones again.

In the following we outline a semiclassical interpretation of these features. The $U(3)$ symmetry of the unperturbed HO system is broken by the term $\delta U = gn^\dagger$ in (2), resulting in the $SO(3)$ symmetry of the interacting system. The shortest periodic orbits in this system are the pendulating diameter orbits and the circular orbits with a radius corresponding to the minimum of the effective potential in (2), including the centrifugal term. These two orbits lead to the observed supershell beating. The above symmetry breaking has so far not been discussed in the semiclassical literature. In a perturbative approach it can be accounted for by a group average of the lowest-order action shift $\Delta S(\alpha)$ brought about by the perturbation of the system: $\langle e^{\frac{i}{\hbar} \Delta S(\alpha)} \rangle_{\alpha \in U(3)}$. Hereby

FIG. 1: (Color online)Level curves of $\log(a^3 n(0))$ calculated within the Thomas-Fermi approximation. $g = 4\pi \hbar^2 a/m$ ($h = \omega = m = 1$).
$o$ is an element of the group $U(3)$ characterizing a member of the unperturbed HO orbit family (ellipses or circles). For the average it is sufficient to integrate over the 4-dimensional manifold $\mathbb{CP}^2$, which for a perturbation $\delta U(r) = \varepsilon r^4$ can be done analytically.

In the perturbative regime ($\varepsilon \ll 1$) we find the following perturbed trace formula:

$$E_{\text{osc}}^{\text{pert}}(N) = \frac{m^2 \omega^4}{2\varepsilon \pi^3} \sum_{k=1}^\infty \frac{(-1)^k}{k^3} \left[ \sin \left( \frac{kS_c}{\hbar} \right) - \sin \left( \frac{kS_d}{\hbar} \right) \right],$$

where $kS_d$ and $kS_c$ are the classical actions of the diameter and circle orbits, respectively. In the limit $\varepsilon \to 0$, their difference goes as $k(S_c - S_d) \to k\varepsilon \pi E^S_P(N)/m^2 \omega^5$, so that $E_{\text{osc}}^{\text{pert}}$ tends to the pure HO limit $E_{\text{osc}}^{\text{HO}}$. Extracting $\varepsilon$ from a polynomial fit to the numerical potential $U(r)$ in $U$, one can qualitatively describe the beating of the shell energy $E_{\text{osc}}(N)$. With $\varepsilon$ of order $\sim 5 \times 10^{-4} g$, Eq. $E_{\text{osc}}^{\text{pert}}$ approximately reproduces the curves seen in Fig. 2 up to the beginning of the second supershell. It explains, in particular, also the phase change in the position of the magic numbers $N_{\text{mag}}$ shown in Fig. 4.

To cover larger values of $\varepsilon$ (and $N$), we have developed an analytical uniform trace formula for the potential $U(r) = m\omega^2 r^2/2 + \varepsilon r^4$, which contains the contributions...
of the 2-fold degenerate families of diameter and circular orbits to all orders in \( \varepsilon \). This is analogous to uniform trace formulae obtained earlier for U(1) [16] and U(2) symmetry breaking [17].

As mentioned above, in a Fermi gas of atoms with repulsive interaction \((a > 0)\), atoms can be lost through three-body recombination events. Two atoms with opposite spin form a molecule while the third takes up energy. Having a low recombination rate, and thus a long life time of the system, is desired. Petrov [11] made an estimate of the loss rate of particles, \( \dot{n}/n \approx 111 (na^3)^2 \bar{\varepsilon}/\hbar \) where \( \bar{\varepsilon} \) is the average kinetic energy of atoms. Taking \( \bar{\varepsilon} \approx 10\mu K \), a realistic energy scale in current experiments, we estimate the life time of atoms in the trap to be \( 10^{-6}s, 10^{-5}s, 10^{-2}s \) for \( g = 2, 0.4, 0.2 \) respectively, when the number of particles is so large that the first node of the super-shell is reached. Hence the life time is longer when \( g \) (or \( a \)) is smaller, reflecting that the loss rate is proportional to \( a^6 \). The temperature regime of this super-shell structure is below \( 0.1\mu K \).

In conclusion, we have seen that the shell structure of fermions with weak, repulsive interactions in a harmonic trap shows a pronounced beating pattern, with the single shell positions changing by half a period length between the different beat nodes. A Fourier analysis of the oscillating shell-correction part of the Hartree-Fock energy shows clear peaks at two slightly different frequencies. This is interpreted semiclassically by the interference of the shortest periodic orbit families generated by the breaking of the U(3) symmetry of the non-interacting HO system, which are the families of diameter and circle orbits, through a uniform trace formula given fully in [13] and, in the perturbative limit, in Eq. 9.

For very weak interactions, the splittings of the highly degenerate HO levels have earlier been calculated perturbatively within the WKB approximation [21]. However, the perturbative results do not apply for the interaction strengths where super-shell structure appears visible.

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