Super-shell structure in harmonically trapped fermionic gases and its semi-classical interpretation

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Abstract

It was recently shown in self-consistent Hartree–Fock calculations that a harmonically trapped dilute gas of fermionic atoms with a repulsive two-body interaction exhibits 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 the beating mode depends on the strength of the interaction. We give a qualitative interpretation of the beat structure in terms of a semi-classical trace formula that uniformly describes the symmetry breaking $U(3) \rightarrow SO(3)$ in a three-dimensional harmonic oscillator potential perturbed by an anharmonic term $\propto r^4$ with arbitrary strength. We show that at low Fermi energies (or particle numbers), the beating gross-shell structure of this system is dominated solely by the twofold degenerate circular and (diametrically) pendulating orbits.

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The realization of Bose–Einstein condensation in trapped dilute atom gases [1] was a milestone in quantum physics, followed by a revolutionary development of both experiment and theory. Turning from bosonic to fermionic statistics, much current interest concerns the trapping and cooling of fermionic alkalis. The focus presently often lies on pairing and the transition to a superfluid state [2].

For these ultracold atomic Fermi gases, not only is it possible to taylor the trap geometry, but also to experimentally change the value of the scattering length for two-body collisions [3]. Being able to experimentally modify the interactions from attractive to repulsive, entirely different interaction regimes can be probed: atomic finite fermion systems are a unique laboratory to study fundamental quantum phenomena.

It is apparent that these systems have much in common with atomic nuclei, with pronounced shell structures at low particle densities and a similar pairing mechanism for attractive short-range interactions [4, 5]. For weak repulsive interactions between the trapped fermionic atoms, shell structure occurs in much analogy also to other finite quantal systems, as for example electrons trapped in nanostructured semiconductor devices (so-called quantum dots [6]) or metallic clusters, in which the delocalized valence electrons are bound in the field of the metallic ions [7].

Very recently [8], we showed by self-consistent Hartree–Fock (HF) calculations that a harmonically trapped gas of fermionic atoms interacting by a weak repulsive two-body force may even exhibit a so-called super-shell structure. This means that 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. Similar super-shell structure occurs in metallic clusters [9]. Inspired by a semi-classical analysis of Balian and Bloch in terms of the periodic orbits in a spherical cavity [10], super-shell beating patterns were predicted [9] to occur in the abundance spectra of sodium clusters, and could later be observed experimentally [11].

The spherical cavity model of Balian and Bloch [10], however, cannot be applied to the present system: for a dilute atomic Fermi gas with short-range interactions trapped in a harmonic well, the semi-classical picture is different. We show that the super-shell structure originates from 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.

We confine the dilute gas of fermionic atoms by a spherical harmonic potential modelling an external trap [12], interacting through a repulsive zero-range two-body potential \( -a \sum_{j} \delta (r_j - r_i) \), where \( a \) is the s-wave scattering length. 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, \( n(r) = n^\uparrow (r) + n^\downarrow (r) = 2 n^\uparrow (r) \). In the weak-interaction regime, the interaction energy density is given by \( gn^\uparrow (r)n^\downarrow (r) = gn^2 (r)/4 \), where the coupling strength parameter \( g = 4\pi \hbar^2 a/m \) is introduced. This leads to the single-particle HF equation

\[
\left[ -\frac{\hbar^2}{2m} \Delta + gn^\uparrow (r) + V_{\text{ho}} (r) \right] \psi^\dagger_i (r) = \epsilon_i \psi^\dagger_i (r),
\]

(1)

where \( V_{\text{ho}} \) is the harmonic oscillator (HO) trap potential (for details, see [8]). In order to treat the interaction as a two-body process, diluteness of the gas requires that the interparticle spacing \( \hbar \alpha^{-1/3} \) is much larger than the range of the interaction and that \( \alpha a^3 \ll 1 \).

We solve equation (1) self-consistently on a grid under the assumption of spherical SO(3) symmetry, which leads to states with \( (2l+1) \)-fold angular momentum degeneracy. The HF interaction term is updated (with some weight factors) in each iteration according to \( gn^\uparrow (r) = g \sum_{i} |\psi^\dagger_i (r)|^2 \).

After convergence is obtained, the HF ground-state energy of the \( N \)-particle system is summed up. 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, \( E_{\text{tot}} = E_{\text{av}} + E_{\text{osc}} \). 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 three-dimensional (3D) harmonic trap, the leading-order term for the average energy is found in the Thomas–Fermi approximation to be \[ E_{\text{av}} = (3N)^{1/3} \hbar \omega (N/3) \omega/4. \] For the repulsive interacting case, we find \( E_{\text{av}} (g > 0) \propto N^{2/3} \) with a larger exponent \( \alpha > 4/3 \). However, equation (1) with an interaction term linear in the density is only valid for moderate \( g \) values and in practice we are close to \( \alpha = 4/3 \) (e.g., \( \alpha \approx 1.35 \) for \( g = 2 \)). 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 total HF energy over the particle number \( N \) in order to extract its oscillating part.

In the non-interacting case \( (g = 0) \), the shell energy \( E_{\text{osc}} \) 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 [13] for \( E_{\text{osc}} \) of the 3D harmonic oscillator, whose leading-order term is given by

\[
E_{\text{osc}}^{\text{ho}} \simeq (3N)^{2/3} \hbar \omega \sum_{k=1}^{\infty} \frac{(-1)^k}{k^2} \cos (2\pi k (3N)^{1/3}).
\]

(2)

Here \( k \) 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 equation (2) 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 figure 1, 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 very close to that of the non-interacting system, given by equation (2). 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 \( 80^{3} \approx 500,000 \), the amplitude of the shell energy is about \( 400 \hbar \omega \), 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 \( 2\pi 3^{1/3} \approx 9.06 \). The super-shell features appear when the contribution to the effective potential from the interaction, \( gn^1 \), 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 figure 1 (lower curve), 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 figure 2, 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 describe the major tools in an ongoing semi-classical interpretation of these features [14]. The U(3) symmetry of the unperturbed HO system is broken by the term \( \delta U = gn^1 \) in (1), 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 including the centrifugal term. These two orbits lead to the observed super-shell beating [14]. The above symmetry breaking had not been discussed in the semi-classical literature before. In a perturbative approach [15], it can be accounted for by a group average of the lowest-order action shift $\Delta S(o)$ brought about by the perturbation of the system: $\langle e^{i/2}\Delta S(o)\rangle_{o\in U(3)}$. Here $o$ 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 4D manifold $\mathbb{CP}^2$ [16], which for a perturbation $\delta U(r) = \epsilon r^4$ can be done analytically [14]. We therefore model the self-consistent numerical HF field by the following perturbed HO potential:

$$V(r) = V_{ho}(r) + \frac{\epsilon}{4} r^4,$$

(3)

where the anharmonic term simulates the symmetry breaking effect of the part $g n^4(r)$ in (1). For small interaction strenghts $g$, $\epsilon$ is proportional to $g$.

In the perturbative regime ($\epsilon \ll 1$), we have found the following perturbed trace formula for the level density:

$$\delta g_{pert}(E) = \frac{\omega^2}{2\pi \hbar^2} \sum_{k=1}^{\infty} (-1)^k \left[ \sin \left(\frac{k S_d}{\hbar}\right) - \sin \left(\frac{k S_c}{\hbar}\right) \right].$$

(4)

where $k S_d$ and $k S_c$ are the classical actions of the diameter and circle orbits, respectively. In the limit $\epsilon \rightarrow 0$, their difference goes as $k(S_d - S_c) \rightarrow k \pi \hbar^2 / \sqrt{N} / \omega^2$, so that (4) tends to the level density of the pure HO limit corresponding to (2).

To cover larger values of $g$ and $N$, we have also developed an analytical uniform trace formula [14]. Uniform here means that it reproduces the HO trace formula for the U(3) (higher symmetry) limit $\epsilon = 0$ in a smooth way, analogously to those derived earlier for U(1) [17] and U(2) symmetry breaking [18]. In the large-energy (or large-$N$) limit, it yields the correct trace formula for the diameter and circular orbits, forming twofold degenerate families, valid for all strengths $\epsilon$:

$$\delta g(\epsilon) \simeq \sum_{k=1}^{\infty} [A^d_k(\epsilon) \sin(k S_d(\epsilon)/\hbar) + A^c_k(\epsilon) \sin(k S_c(\epsilon)/\hbar)].$$

(5)

Analytical expressions for the amplitudes and actions (in terms of elliptic integrals) are given in [14]. Equation (5) goes over into the perturbative trace formula (4) in the limit $\epsilon \rightarrow 0$. This confirms the statement made in [8] that only the diameter and circle orbits are important in this limit.

In the upper panel of figure 2, we compare the level density for the potential (3) obtained with the perturbative trace formula (4) (dashed line) and the uniform trace formula (5) (solid line) for the value $\epsilon = 0.005$, using only the lowest harmonics ($k = 1$). While, there is good agreement up to the first super-shell maximum for this small value of $\epsilon$, for larger perturbations the two formulae only agree for very small energies. In the lower panel of figure 2, we compare the coarse-grained result of the uniform trace formula (5) (solid line) with the exact quantum-mechanical result (dashed line) for $\epsilon = 0.01$, demonstrating that the semi-classical interpretation of the super-shell beat in terms of circular and diameter orbits is perfect.

At sufficiently high energies and perturbation strengths $\epsilon$, threefold degenerate families of tori with rational ratios $\omega_r : \omega_q = n : m \geq 7 : 3$ of radial and angular frequency bifurcate from higher repetitions ($k \geq 3$) of the circle orbit$^3$.

$^3$ This situation persists in the limit $\epsilon \rightarrow \infty$, which corresponds to a pure quartic oscillator potential, and is consistent with a general result obtained for homogeneous potentials $V(r) = cr^a$ with $a \geq 2$, see [19].
The shortest of them, a star-like orbit with \( n : m = 7 : 3 \), is approximately 10 times longer than the shortest diameter and circle orbits. Therefore, all the tori only contribute to finer quantum structures at higher energies. They can be included in the semiclassical trace formula using standard techniques [20–22].

The beat structure in \( E_{osc} \) has some similarities with that found in nuclei [23] and metal clusters [7]. There are, however, two essential differences. (i) Those systems are self-saturating and have steep mean-field potentials that can be modelled by a spherical cavity [10]. The present system, in contrast, has a mean field with much smoother walls that are dominated at large distances by the confining harmonic potential. (ii) The super-shells in the cavity model come from the interference of the shortest periodic orbit families with threefold degeneracy, as is usual in spherical systems [20, 21]. Here, however, the gross-shell structure comes uniquely from the diameter and circle orbits which are only twofold degenerate, whereas the fully threefold degenerate tori are so much longer that they only affect the finer quantum structures at higher energies.

In conclusion, we have seen that the shell structure of weakly interacting fermions 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 HF energy shows clear peaks at two slightly different frequencies. This we have interpreted semiclassically by the interference of the shortest periodic orbits generated by the breaking of the U(3) symmetry of the non-interacting HO system, which are the families of diameter and circle orbits. A more detailed quantitative interpretation using the uniform trace formula (5) derived in [14] is in progress. After extracting \( \epsilon \) and \( \omega_{eff} \) from a polynomial fit to the numerical HF potential, we expect to describe the beat structure in the numerically obtained HF shell energies \( E_{osc}(N) \) quantitatively in terms of classical periodic orbits.

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