Periodic Orbit Theory for Trapped Fermi Gases

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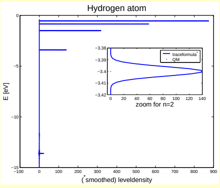
Introduction

One can obtain information about a quantum mechanical spectrum from certain classical orbits (trajectories). This is called periodic orbit theory, which we abbreviate here with *POT*.

An early example of POT with connection to the house!

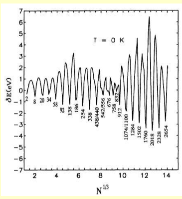
The famous model by Bohr which led to the formula for the hydrogen spectrum [1] was an early example of *POT*. Even though Bohr's assumption about (only) circular orbits and his assumption about the quantization of the angular momentum were incorrect, the errors canceled and he obtained the same spectrum as the one given by the Schrödinger equation.

This whim of fate might have been an important historical coincidence for the development of quantum mechanics, which then proceeded through the successful comparison with experimental spectra. The success of Bohr's model shows that quantum mechanical properties can sometimes be well described by only a few important classical periodic orbits, the circular orbits in Bohr's case.



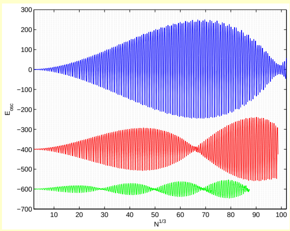
POT for metal clusters

After theoretical developments of *POT*, especially in the 70's, *POT* could successfully explain the super shell structure seen in metal clusters [2]. In this case, where the mean-field potential for the valence electrons is close to a spherical hard wall potential, the major components in the gross shell structure are determined by two classical periodic orbits the triangular and square.



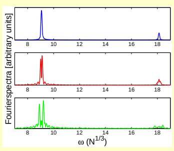
POT for trapped Fermi gases

Inspired by the analysis of metal clusters, we have investigated the recently developed systems of ultracold trapped atomic Fermi gases. To be more specific we have investigated the shell structure of spherical three-dimensional harmonically trapped weakly repulsive Fermi gases. The Hamiltonian for short-range two body interaction is



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

where due to the Pauli principle the s-wave interaction only occurs between two different spin-states, spin up and down, say. By introducing an effective coupling strength parameter $g=4\pi\hbar^2 a/m$ and assuming two equally populated spin-states, we are led to the following Hartree-Fock equations, which we solve self-consistently



$$\left[-\frac{\hbar^2}{2m}\Delta+gn^{\uparrow}(\mathbf{r})+V_{HO}(\mathbf{r})\right]\psi_i^{\downarrow}(\mathbf{r})=\epsilon_i\psi_i^{\downarrow}(\mathbf{r})\,,\quad n^{\uparrow}=\sum_{i=1}^{N/2}\left|\psi_i^{\uparrow}\right|^2. \qquad (2)$$

Within the Hartree-Fock framework we have observed a clear super shell structure [3] in the oscillating part of the total energy as a function of the cubic root of the number of particles. The Fourier spectra indicates that the structure is dominated by two frequencies. We have shown that they correspond to diameter and circle orbits.

Trace formulae for broken SU(3)-symmetry

We have modelled the HF mean-field potential by a quartic perturbed harmonic oscillator (*HO*)

$$V_{model}=\frac{1}{2}m\omega^2 r^2+\frac{\epsilon}{4}r^4,\ \epsilon>0. \qquad (3)$$

We first explained the super shell structure from the HF calculations qualitatively [3] with semi-classical perturbation theory due to Creagh [4], applied to the potential V_{model}. We have calculated a modulation factor $\mathcal{M}$ for the trace formula describing the oscillating part of the level density g_{osc} of the unperturbed HO system, corresponding to non-interacting fermions

$$g_{osc}^{pert.}(E)=\frac{E^2}{2(\hbar\omega)^3}Re\left(\sum_{k=-\infty}^{\infty}(-1)^k\mathcal{M}(k\sigma/\hbar)\,e^{i2\pi kE/\hbar\omega}\right). \qquad (4)$$

We have also developed a uniform trace formula which is valid for arbitrary values of ϵ [5]

$$g_{osc}^{uni.}(e)=\sum_{k=1}^{\infty}\left[\mathcal{A}_k^{diam.}(e)\sin(kS_{diam.}(e)/\hbar)+\mathcal{A}_k^{circ.}(e)\sin(kS_{circ.}(e)/\hbar)\right], \qquad (5)$$

where the $\mathcal{A}_k$'s and S's can be given in terms of elliptic integrals.

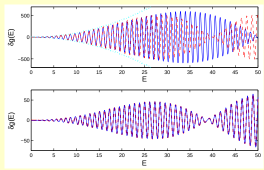
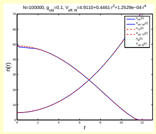


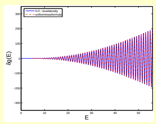
Figure caption: The upper figure shows the perturbed trace formula Eq. (4), dashed red, the uniform trace formula Eq. (5), solid blue, for the case of $\epsilon=0.005$. The dotted cyan curve is the amplitude of the unperturbed system. In the lower figure we can see a comparison between the uniform trace formula Eq. (5), solid blue, and the numerically calculated quantum mechanical level density, dashed red.

HF mean-field potential vs Model potential

To make contact between the HF (2) results and the model potential (3), we use an analytical g-dependent Thomas-Fermi particle density and then fit ω and ϵ in (3) to a mean-field model potential.



We have managed to reproduce the HF level density for weakly interacting fermions. This leads to a qualitative understanding of the super shell structure seen in the oscillating part of the total energy.



Conclusion

The gross shell structure of a perturbed three-dimensional harmonic oscillator has super shells. The super shell structure is to a high accuracy reproduced by only two classical periodic orbits, the diameter and circle [5]. The super shells in the level density of the quartic perturbed harmonic oscillator explains qualitatively the super shells in the oscillating part of the total energy from a Hartree-Fock calculation. More details can be found in [6].

References

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