Semiclassical theory of melting of shell effects in nuclei with temperature

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Introduction

Semiclassical trace formulae establish a connection of the density of energy levels and classical periodic orbits [1]. Unfortunately, this formula diverges for harmonic oscillator potentials, which are very important in the context of nuclear physics. Nearly twenty five years later, the analytically exact trace formula was found [2] for harmonic oscillator potentials. This formula has been used extensively in literature in understanding many important features of a many-body Fermionic system in general. Specifically, there has been much development in the specific areas [3] on nuclear ground-state deformations, double-humped fission barrier, mass asymmetry in nuclear fission, shells and supershells in metal clusters, conductance oscillations in quantum dots, and so on. The level density is a sum of an average form and an oscillating component added to it. The average density is, in fact, related to the zero-length periodic orbits. Alternatively, it can also be obtained within a Thomas-Fermi formalism. In this work, we present calculations of the level density for prolate deformed nuclei, showing the effect of temperature. The aim of the work is to bring out the theoretical expectation, and the hope is to eventually include spin-orbit interaction and relate to the experimental work.

Semiclassical trace formula for level density

Considering the simplest case of harmonic mean-field with no spin-orbit interaction, the Hamiltonian is

$$H = \frac{1}{2}(p_x^2 + p_y^2 + p_z^2) + \frac{1}{2}(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2) \tag{1}$$

where we have set mass to unity. The density of energy levels is given by

$$g(E) = \sum_{n=1}^{\infty} \delta(E - E_n). \tag{2}$$

There is a well-known connection of this quantity with the canonical partition function:

$$\begin{aligned} Z(\beta) &= \mathcal{L}_\beta[g(E)] = \int_0^\infty e^{-\beta E} g(E) dE \\ &= \sum_{n=1}^{\infty} e^{-\beta E_n}. \end{aligned} \tag{3}$$

It is very important to keep in mind that β is just a mathematical variable (which could even be complex). The level density is the inverse Laplace transform of the partition function. Furthermore, there is an important connection between the zero-temperature partition function, $Z_0(\beta)$ and non-zero temperature one, $Z_T(\beta)$. Setting the Boltzmann constant to unity and measuring the temperature in the units of energy, the level density at temperature T is

$$g^T(E) = \mathcal{L}_E^{-1}\left[Z_0(\beta)\frac{\pi\beta T}{\sin(\pi\beta T)}\right]. \tag{4}$$

For the axially symmetric case, $\omega_x = \omega_y = \omega_\perp = p\omega_0$, $\omega_z = n\omega_0$ where n, p are co-prime, the average part of the Z_0 is

$$Z_0^{av} = \frac{\eta^3}{2(2\pi)^3 p^2 n}\left\{\frac{2}{\beta^2} - \frac{1}{12}[(\hbar\omega_0)^2(2p^2 + n^2)]\right\}. \tag{5}$$

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The oscillating part of the level density will give corresponding partition function (calling $2\pi/\hbar\omega_0$ by η, $\eta^2+\beta^2$ by F):

$$\delta Z_0(\beta) = \frac{\eta^3}{(2\pi)^3 p^2 n}\sum_{k=1}^{\infty}(-1)^{kn} \frac{(-6\beta\eta^2+2\beta^3)12\eta^2 - 4\pi^2\beta(2p^2+n^2)F^2}{12\eta^2 F^3}$$
$$+ \frac{\eta^2}{4\pi^2 p^2}\sum_{k\neq lp}^{\infty}\frac{2\beta\eta(k/p)}{\sin(\pi nk/p)((k\eta/p)^2+\beta^2)^2}$$
$$+ \frac{\beta\eta n}{4\pi p^2}\sum_{k\neq lp}^{\infty}\frac{\cos(k\pi n/p)}{\sin^2(k\pi n/p)[\beta^2+(k\eta/p)^2]}$$
$$+ \frac{\beta\eta}{4\pi n}\sum_{k\neq ln}^{\infty}\frac{(-1)^{k+1}}{\sin(k\pi p/n)[\beta^2+(\eta k/n)^2]}. \quad (6)$$

With this result, multiplying by $\pi\beta T/\sin\pi\beta T$, we get the partition function for non-zero temperature. The next step involves performing the inverse Laplace transform of $Z_0^{av}+\delta Z_0$. It is useful to employ the identity:

$$\frac{\pi\beta T}{\sin(\pi\beta T)} = \beta\sum_{s=-\infty}^{\infty}\frac{(-1)^s}{\beta - s/T}. \quad (7)$$

The inverse Laplace transform then involves a contour integration accounting for an infinite number of poles appearing due to (7). Fortunately, the entire calculation can be performed analytically. For a representative case, the level density has been plotted in Fig. 1. It is remarkable that the average trend is also correctly found even in this case when $T\neq 0$. The association of the oscillations with classical periodic orbits is one of the deepest remarks on the semiclassical understanding of the subject, we do not pursue it here any further.

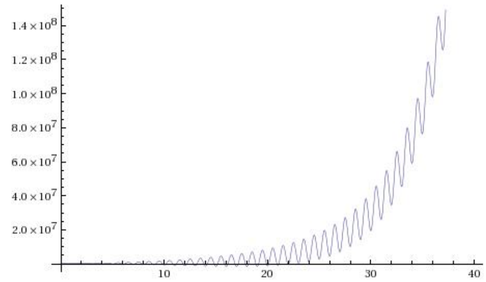

FIG. 1: For the case of $\omega_\perp/\omega_z = 1/2$, and, on considering large number of periodic orbits and their repetitions, we see here the level density as a function of energy in arbitrary units. The average trend follows exactly the Thomas-Fermi formula or even the trace formula with zero path length-orbits.

Conclusion

Quite expectedly, we have found that the semiclassical trace formula for axially symmetric (prolate deformed) systems can be developed even when the temperature is nonzero. The case of doubly magic nuclei (without spin-orbit interaction) has been dealt with in the past. In that case, the shell effects are clearly seen washed off [3]. Using the formula obtained by inverse Laplace transform, for higher temperatures, we do not observe as much suppression of shell effects as in the spherically symmetric case. But this will have to be quantified in a proper manner. Finally, the incorporation of spin-orbit interaction is important, and currently in progress.

Acknowledgments

More than ten years ago, during my visit to Panjab University, Chandigarh, Raj K. Gupta had asked me if I knew how to account for temperature and excitation in shell model. Recent experimental results by the group at BARC have re-kindled my interest in this problem, I thank Vivek Datar and Prakash Rout for discussions.

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