Single particle shell models: spheroidal and semi-spheroidal harmonic oscillators. Influence of the term proportional to l^2 and of intermediate shapes.

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I. INTRODUCTION

The spheroidal harmonic oscillator (SHO) has been used in various branches of Physics. The famous single-particle Nilsson model [1] is very successful in Nuclear Physics. Its variants [2, 3] are of particular interest for atomic clusters [4]. Major spherical-shells $N = 2, 8, 20, 40, 58, 92$ have been found [2] in the mass spectra of sodium clusters of N atoms per cluster, and the Clemenger's shell model [3] was able to explain this sequence of spherical magic numbers.

We shall write explicitly the analytical expressions for the energy levels of SHO and derive the solutions for a semi-spheroidal harmonic oscillator (SSHO) which may be useful to study atomic clusters deposited on planar surfaces. The energy levels may be used as the input data for shell correction calculations [2, 3, 5–10]. The nanostructured coating of surfaces by cluster deposition is at present a rapidly growing field [11]. By using an atomic force microscope it is possible to observe the shapes of such clusters (see e.g. Fig. 1 of ref. [12], or Figs. 3, 4 and 9 of ref. [13]). They can be approximated in the first order by a hemispheroid. This gives us a motivation to develop the SSHO. Another argument relies on the 2D measurement [14] of the strong magicity at the number equal to 6, which can be approximated as a limiting case of an extremely large oblate deformation in our model.

In all studies using an harmonic oscillator published since 1955, the maximum degeneracy of the quantum states was reached for a spherical shape, explaining the high stability of the doubly magic nuclei or of the metal clusters with spherical closed shells. To our surprise the maximum stability of the hemispheroidal quantum harmonic oscillator occurs at a superdeformed prolate shape (semiaxes ratio $a/c = 1/2$), a shape which is also the most stable one within the LDM [15].

II. SPHEROIDAL HARMONIC OSCILLATOR

A. The wave functions and the energy levels

For spheroidal equipotential surfaces, generated by a potential with cylindrical symmetry, the states of the valence electrons were found [3] by using an effective single-particle Hamiltonian with a potential

$$V = \frac{M\omega_0^2 R_0^2}{2}\left[\rho^2\left(\frac{2+\delta}{2-\delta}\right)^{2/3} + z^2\left(\frac{2-\delta}{2+\delta}\right)^{4/3}\right] \tag{1}$$

We begin with this Hamiltonian and neglect for the moment an additional term proportional to $(\mathbf{l}^2 - \langle \mathbf{l}^2 \rangle_n)$. Then we investigate its influence in the next subsection. The deformation δ is defined by expressing the dimensionless two semiaxes (in units of the radius of a sphere with the same volume, $R_0 = r_s N^{1/3}$, where r_s is the Wigner-Seitz radius, 2.117 Å for Na [8, 16]) as

$$a = \left(\frac{2-\delta}{2+\delta}\right)^{1/3} \quad ; \quad c = \left(\frac{2+\delta}{2-\delta}\right)^{2/3} \tag{2}$$

We use dimensionless cylindrical coordinates ρ and z. Volume conservation leads to $a^2c = 1$. One can separate the variables in the Schrödinger equation, $H\Psi = E\Psi$. As a result the wave function [17, 18] may be written as

$$\Psi(\eta, \xi, \varphi) = \psi_{n_r}^{m}(\eta)\Phi_m(\varphi)Z_{n_z}(\xi) \tag{3}$$

where each component is orthonormalized, $\eta = R_0^2\rho^2/\alpha_\perp^2$, $m = (n_\perp - 2i)$ with $i = 0, 1, ...$ up to $(n_\perp - 1)/2$ for an odd $n_\perp$ or to $(n_\perp - 2)/2$ for an even $n_\perp$, $n_r = (n_\perp - |m|)/2$, $\alpha_\perp = \sqrt{\hbar/M\omega_\perp}$. We are interested in the z-component

$$Z_{n_z}(\xi) = N_{n_z} e^{-\xi^2/2} H_{n_z}(\xi) \; ; \quad N_{n_z} = \frac{1}{(\alpha_z\sqrt{\pi}2^{n_z}n_z!)^{1/2}} \tag{4}$$

where $\xi = R_0 z/\alpha_z$, $\alpha_z = \sqrt{\hbar/M\omega_z}$, and the main quantum number $n = n_\perp + n_z = 0, 1, 2, ...$ The parity of the Hermite polynomials $H_{n_z}(\xi)$ is given by $(-1)^{n_z}$.

The eigenvalues in units of $\hbar\omega_0$ are

$$\epsilon_n = \frac{E_n}{\hbar\omega_0} = \frac{2}{(2-\delta)^{1/3}(2+\delta)^{2/3}}\left[n + \frac{3}{2} + \delta\left(n_\perp - \frac{n}{2} + \frac{1}{4}\right)\right] \tag{5}$$

The low lying energy levels for the six shells (main quantum number $n = 0, 1, 2, 3, 4, 5$) can be seen in the left-hand side of figure 1. Each level, labelled by $n_\perp, n$, may accommodate $2n_\perp + 2$ particles.

One has $2\sum_{n_\perp=0}^{n}(n_\perp+1) = (n+1)(n+2)$ atoms in a completely filled shell characterized by n, and the total number of states of the low-lying $n+1$ shells is $\sum_{n=0}^{n}(n+1)(n+2) = (n+1)(n+2)(n+3)/3$ leading to the magic numbers $2, 8, 20, 40, 70, 112, 168$... for a spherical shape. Besides the important degeneracy at a spherical shape ($\delta = 0$), one also has degeneracies at some superdeformed shapes, e.g. for prolate shapes at the ratio $c/a = (2+\delta)/(2-\delta) = 2$ i.e. $\delta = 2/3$. The first four shells

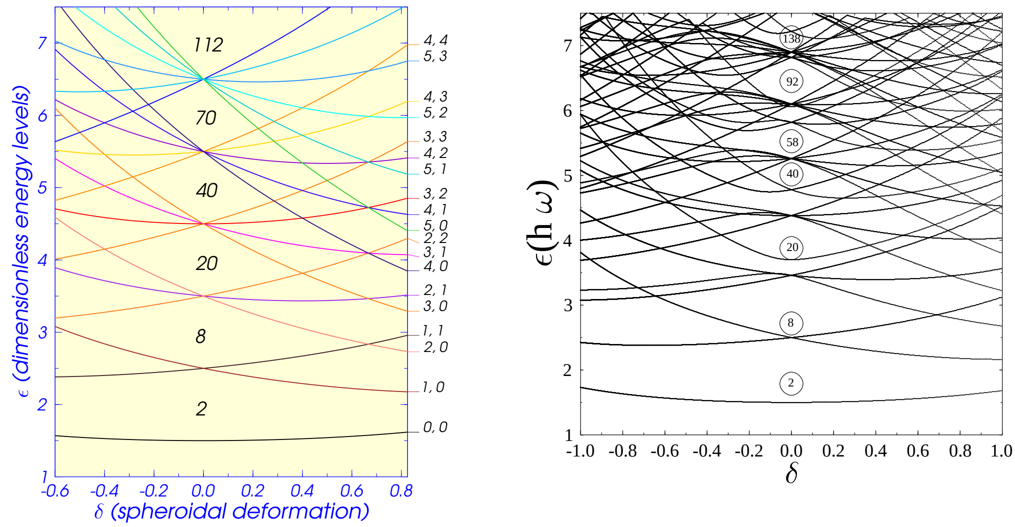

FIG. 1: Energy levels in units of $\hbar\omega_0$ vs. the deformation parameter δ of a spheroidal harmonic oscillator before (colour) and after (black and white) introducing the term proportional to l^2 in the Hamiltonian.

can reproduce the experimental magic numbers $2, 8, 20, 40$; in order to describe the other ones $(58, 92)$ one has to introduce the term proportional to $(\mathbf{l}^2 - \langle \mathbf{l}^2 \rangle_n)$ in the Hamiltonian (see the next subsection).

B. Influence of the term proportional to l^2

The $\mathbf{l^2}$–term must be added in order to broaden the lower part of the oscillator potential. It will lift the degeneracies for the same principal quantum number, here $n = 2n_\rho + |m|$. The term is: $V_{\mathbf{l}^2} = -U\hbar\omega_0[\mathbf{l}^2 - n(n+3)/2]$. In order to introduce the deformation dependence we employ the expression $\mathbf{l^2} = \nabla \mathbf{V_{osc}} \times \hat{\mathbf{p}}$, and by using the creation and anihilation operators one has:

$$\mathbf{l}^2 = 0.5(\mathbf{l}^+\mathbf{l}^- + \mathbf{l}^-\mathbf{l}^+) + \mathbf{l}_z^2 \tag{6}$$

The matrix elements for the calculation of the $\mathbf{l}^{+,-}$ and $\mathbf{l_z}$ are given elsewhere [19]. The completion relation leads to:

$$\langle n'_\rho m' n'_z | \mathbf{l}^+ \mathbf{l}^- | n_\rho m n_z \rangle = \sum_{''} \langle n'_\rho m' n'_z | \mathbf{l}^+ | n''_\rho m'' n''_z \rangle \langle n''_\rho m'' n''_z | \mathbf{l}^- | n_\rho m n_z \rangle \tag{7}$$

and similarly for $\mathbf{l}^-\mathbf{l}^+$. In this way we obtain the matrix elements for the $\mathbf{l^2}$–potential vs deformation. The $\mathbf{l_z}$ operator is diagonal and yields the additional energy:

$$E_{\mathbf{l}_z^2} = -\hbar\omega_0 U \frac{\omega_\rho^2}{\omega_0^2} m^2 \delta_{mm'} \delta_{n'_\rho n_\rho} \delta_{n'_z n_z} \tag{8}$$

where the dimensionless strength of interaction $U = 0.04$. As a result of the diagonalization one obtains the total deformed level energy shown in the right hand side of the fig. 1. The experimentally determined magic numbers [2] are reproduced.

III. SEMI-SPHEROIDAL HARMONIC OSCILLATOR

A. The energy levels obtained ignoring the l^2 term

The radius of the hemisphere at the deformation $\delta_s = 0$ is R_s. Volume conservation leads to $R_s = 2^{1/3} R_0$. We shall give ρ, z, a, c in units of R_s instead of R_0, so that again $a^2 c = 1$. The definition of the δ_s is the same as that of δ in eq. (2), but now a and c are expressed in terms of R_s instead of R_0. The new potential well along the symmetry axis, $V_z(z)$, has a wall of an infinitely large height at $z = 0$, and concerns only positive values of z, implying opacity of the surface. In this case the wave functions should vanish in the origin, so that only negative parity Hermite polynomials (n_z odd) should be taken into consideration. From the energy levels given in the left-hand side of the figure 1 we have to select only those corresponding to this condition. In this way the former lowest level with $n = 0, n_\perp = 0$ should be excluded. From the two levels with $n = 1$ we can retain the level with $n_\perp = 0$ i.e. $n_z = 1$. This will be the lowest level for the SSHO and will accommodate $2n_\perp + 2 = 2$ atoms. Again, each level, labelled by $n_\perp, n$, may accommodate $2n_\perp + 2$ particles.

The equation (5) from the harmonic oscillator, in units of $\hbar\omega_0$ is still valid, but one should only allow the values of n and $n_\perp$ for which $n_z = n - n_\perp \geq 1$ are odd numbers. The energy levels are plotted in the left hand side of fig. 2. *The striking result is that the maximum degeneracy is obtained at a superdeformed prolate shape ($\delta_s = 2/3$). The magic numbers (MN) of SSHO are those of spherical shape ($\delta = 0$) SHO.* The MN of oblate, $\delta_s = -0.4$, SSHO are identical to those of hyperdeformed oblate, $\delta = -1$, SHO. The MN of hemispherical, $\delta_s = 0$, SSHO are the same as of the superdeformed oblate, $\delta = -2/3$, SHO, etc.

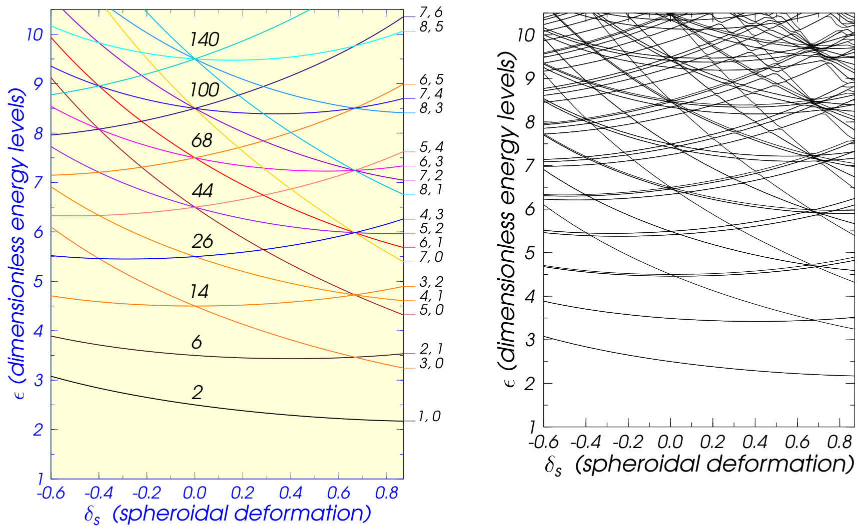

FIG. 2: Energy levels in units of $\hbar\omega_0$ vs. the deformation parameter δ of a semi-spheroidal harmonic oscillator before (colour) and after (black and white) introducing the term proportional to l^2 in the Hamiltonian.

B. Influence of the term proportional to l^2

By including a term proportional to $(\mathbf{l}^2 - \langle \mathbf{l}^2 \rangle_n)$ in the Hamiltonian

$$H = -\frac{\hbar^2 \Delta}{2M} + \frac{M\omega_0^2 R_0^2}{2}\left(\frac{\rho^2}{a^2} + \frac{z^2}{c^2}\right) - \hbar\omega_0 U(\mathbf{l}^2 - \langle \mathbf{l}^2 \rangle_n) \tag{9}$$

with the dimensionless quantity $U = 0.04$ and $\langle \mathbf{l}^2 \rangle_n = n(n+3)/2$ like in Ref. [3] for the spheroidal oscillator, we obtained again an analytical relationship for the energy levels

$$\epsilon_n = \frac{E_n}{\hbar\omega_0} = \frac{n_\perp + 1}{a} + \frac{n_z + 1/2}{c} - \frac{Um^2}{4a^4} + \frac{Un(n+3)}{2} \tag{10}$$

The terms proportional to U are both diagonal, the first one $-Um^2/(4a^4)$ representing the contribution of the $\hat{l}_z^2$ part of the angular momentum operator. The possible nondiagonal terms coming from $(\hat{l}^+\hat{l}^- + \hat{l}^-\hat{l}^+)/2$ are not present since their contribution vanishes due to the selection rules excluding even values of the quantum number n_z. As we mentioned above the quantum number $m = (n_\perp - 2i)$ with $i = 0, 1, ...$, so that for $n_\perp = 0$ one has $m = 0$ — the energy level is not changed. When $n_\perp = 1$, $m = \pm 1$ and the energy is changed but the degeneracy of 4 remains unlifted. For

TABLE I: TOP: Deformed magic numbers of the spheroidal harmonic oscillator. BOTTOM: Deformed magic numbers of the hemispheroidal harmonic oscillator.

OBLATE			PROLATE		
δ	a/c	Magic numbers	δ	a/c	Magic numbers
$-0.8/3$	17/13	2, 8, 18, 20, 34, 38, 58, 64, 92, 100, 136, 148, ...	0.8/3	13/17	2, 8, 20, 22, 42, 46, 76, 82, 124, 134 ...
-0.4	1.5	2, 6, 8, 14, 18, 28, 34, 48, 58, 76, 90, 114, 132, ...	0.4	2/3	2, 8, 10, 22, 26, 46, 54, 66, 84, 96, 114, 138, 156, ...
$-2/3$	2	2, 6, 14, 26, 44, 68, 100, 140, ...	2/3	0.5	2, 4, 10, 16, 28, 40, 60, 80, 110, 140, ...
-1	3	2, 6, 12, 22, 36, 54, 78, 108, 144, ...	1	1/3	4, 12, 18, 24, 36, 48, 60, 80, 100, 120, 150, ...
$-0.8/3$	17/13	2, 6, 12, 22, 26, 36, 42, 56, 64, 82, 92, 114, 126, 154, ...	0.8/3	13/17	2, 6, 8, 14, 18, 28, 34, 48, 58, 76, 90, 114, 132, ...
-0.4	1.5	2, 6, 12, 22, 36, 54, 78, 108, 144, ...	0.4	2/3	2, 8, 18, 20, 34, 38, 50, 58, 64, 80, 92, 100, ...
$-2/3$	2	2, 6, 12, 20, 32, 48, 68, 92, 122, 158, ...	2/3	0.5	2, 8, 20, 40, 70, 112, 168, ...
-1	3	2, 6, 12, 20, 30, 42, 58, 78, 102, 130, ...	1	1/3	2, 8, 10, 14, 22, 26, 46, 54, 66, 84, 96, 114, 138, 156, ...

$n_\perp = 2$, $m = \pm 2, 0$ so that one has a split leading to one level with $m = 0$ and the degeneracy 2, and another with $m = \pm 2$ and the degeneracy 4, etc. In this way we obtain the level scheme in the right hand side of fig. 2. For the lower levels (say up to 10 closed shells), the sequence of the magic numbers at the maximum degeneracy, taking place at the superdeformed prolate shape $\delta = 2/3$, remain the same: $N = 2, 8, 20, 40, 70, 112, 168$. Another remarkable fact is that for very large oblate deformations, leading to "pan-cake" shapes approximating a 2D situation, one of the magic number is 6, in agreement with the experiments performed by Chiu et al. [14].

C. Influence of the intermediate shapes

As may be seen from figures 1 an 2, the nuclear shape is extremely important: the magic numbers obtained at some oblate and prolate deformations are different from those obtained at the spherical shape in case of the spheroidal harmonic oscillator (SHO) or at the hemispherical shape in case of semi-spheroidal harmonic oscillator (SSHO).

As an example we give the table 1 in which the remarkable properties of symmetry can be also seen. *The magic numbers (MN) of the oblate ($\delta = -0.4$) semi-spheroidal harmonic oscillator (SSHO) are identical to those of the hyperdeformed oblate ($\delta = -1$) spheroidal harmonic oscillator (SHO). MN of a semi-spherical ($\delta = 0$) SSHO are identical to MN of superdeformed oblate ($\delta = -2/3$) SHO. MN of the superdeformed prolate ($\delta = 2/3$) SSHO are the same as MN of spherical ($\delta = 0$) SHO (maximum degeneracy).*

Acknowledgments

This work was partly supported within the IDEI programme under contract 123/01.10.2007 with UEFISCSU, Bucharest, by Deutsche Forschungsgemeinschaft (DFG), Bonn, and by the network of excellence EXCELL of the European Commission, Brussels. One of us (DNP) is grateful to DFG for the Mercator Guest Professorship.

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