Shell Structures and Chaos in Nuclei and Large Metallic Clusters

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Abstract

A reflection-asymmetric deformed oscillator potential is analysed from the classical and quantum mechanical point of view. The connection between occurrence of shell structures and classical periodic orbits is studied using the "removal of resonances method" in a classical analysis. In this approximation, the effective single particle potential becomes separable and the frequencies of the classical trajectories are easily determined. It turns out that the winding numbers calculated in this way are in good agreement with the ones found from the corresponding quantum mechanical spectrum using the particle number dependence of the fluctuating part of the total energy. When the octupole term is switched on it is found that prolate shapes are stable against chaos and can exhibit shells whereas spherical and oblate cases become chaotic. An attempt is made to explain this difference in the quantum mechanical context by looking at the distribution of exceptional points which results from the matrix structure of the respective Hamiltonians. In a similar way we analyse the modified Nilsson model and discuss its consequences for nuclei and metallic clusters.
1 Introduction

The development of new experimental technique in recent years has considerably increased the accuracy of the measurement of nuclear properties at low excitation energy. As a result, the superdeformed rotational bands have been discovered [1] opening new perspectives on new phenomena like the one of identical bands. Low lying negative-parity states, parity doublets, alternating parity bands with strong $E1$ - transitions in radium and nearby nuclei [4] are another interesting phenomena which could be considered as a manifestation of the octupole deformation. Possible occurrence of softness of superdeformed nuclei having the prolate shapes with respect to the octupole deformation is one of the current topics in nuclear structure physics (see for review [3]).

Ten years ago the pioneering experiments carried out by a group of W.Knight [4] (see also [4, 5]) opened a new fascinating field in study of many–body system, the atomic cluster phenomena, an intermediate form of matter between molecules and bulk systems. Experimental results on metallic clusters concerning abundance spectra, ionization potentials, photoexcitation etc was immediately interpreted in terms of electronic quantized motion in a spherical effective potential.

Phenomena observed in many–body systems like nuclei and clusters could be explained within the mean field approach based on the symmetry breaking mechanism related to quantized single–particle motion. The quantisation of a system of Fermions moving in a common potential leads to a bunching of levels in the single–particle spectrum, known as shells. The high level density around the Fermi level (large level bunching) corresponds to less stable system. When a spherical shell is only partially filled, a breaking of spherical symmetry, resulting in an energy gain, gives rise to a deformed equilibrium shape. The basic concept of the deformation in the mean field approach is the Jahn-Teller effect [7], the mechanism first time proposed for molecules, which leads to a spontaneous symmetry violation (see discussion in [8]).

On the other hand, the existence of magic numbers corresponding to spherical and deformed nuclei/clusters could be explained in terms of classical trajectories [4] based on the periodic orbit theory of Gutzwiller [10]. According to the semiclassical theory [4] the frequencies in the level density oscillations of single–particle spectra of nuclei are determined by the corresponding periods of classical closed orbits. The short periodic orbits give the
major contribution to the gross shell structure [11, 12]. Depending on the particular mean field potential a deviation from spherical symmetry can lead to chaotic motion in the corresponding classical problem, and the shell structure of the corresponding quantum spectrum is affected or even destroyed depending on the degree of chaos [13, 14, 15].

Simple interpretation of the strong peaks, which are observed in the abundance spectra of metallic clusters, in terms of the spectrum of one-particle orbits in a spherical potential, which are associated with periodic orbits of the corresponding classical problem [16, 17, 18], provide us with the important key elements. The fact that the triangular orbits play an important role for a family of quantum states with \( \Delta l = 3 \) (here \( l \) is an orbital angular momentum, see [11]) implies an importance of octupole degree of freedom for configurations with partially filled shells [19].

In the present paper we consider a reflection-asymmetric axially deformed oscillator potential and focus our analysis on the distinction between orderly and chaotic motion in many-body systems, like nuclei and metallic clusters. One major result of the classical analysis demonstrates that the prolate case including octupole deformation is still quasi-integrable. In this way the quantum mechanical shell structure found earlier [15] is given a proper theoretical foundation [20]. Similarly, we analyse the modified Nilsson model including the \( l^2 \)-term and neglecting spin-orbit coupling, and the consequences for nuclei and clusters. Quantum mechanical calculations confirm that the \( l^2 \)-term which gives rise to chaotic behaviour in the corresponding classical problem [21] may interfere with the search of shell structure.

## 2 The Model

We investigate the classical and quantum mechanical motion in an axially symmetric deformed potential which can be expanded as:

\[
V(r, \theta) = \frac{m\omega_0^2}{2} r^2 (1 + \alpha_2 P_2(\cos \theta) + \alpha_3 P_3(\cos \theta) + \ldots). \tag{1}
\]

In this expansion the terms proportional to the components of the deformation tensor (\( \alpha_i \)) are the Legendre polynomials of \( i \)-th order, respectively. In this paper we only consider terms up to, and including, the third order. Rewriting the potential in cylindrical coordinates [13]
we arrive at the form:

$$V(\varrho, z) = \frac{m\omega^2}{2} \left( \frac{\varrho^2}{b^2} + \frac{z^2}{b^2} + \frac{\lambda}{2} \frac{3z^3 - 3\varrho^2}{\sqrt{\varrho^2 + z^2}} \right),$$

(2)

where $\omega = \omega_0\sqrt{1 - \alpha^2/2}$, $b = \sqrt{(1 - \alpha^2/2)/(1 + \alpha^2)}$ and $\lambda = \alpha_3/(2 - \alpha_2)$ We will call $b$ the quadrupole deformation and $\lambda$ the octupole strength. For $b > 1$ ($b < 1$) the potential is a deformed harmonic oscillator of prolate (oblate) shape coupled to an additional octupole deformation of strength $\lambda$.

Classically, the trajectories [20] can be calculated using the Hamilton formalism, by integrating the following two equations of motion:

$$\ddot{\varrho} = -\frac{\partial V(\varrho, z)}{\partial \varrho},$$

$$\ddot{z} = -\frac{\partial V(\varrho, z)}{\partial z}.$$  

(3)

Two aspects are important: First, because of the axial symmetry, the $z$ component of the angular momentum ($l_z$) is conserved. As we will see in the next section, a finite value of $l_z$ will not modify the winding numbers of the orbits. For this reason we will only consider $l_z = 0$. Second, we notice that the potential scales as $V(\gamma \varrho, \gamma z) = \gamma^2 V(\varrho, z)$. This means that one value of the energy will produce the same periods and trajectories as any other energy value.

The use of the term $r^2 P_3(\cos \theta)$ instead of $r^3 P_3(\cos \theta)$ in the potential ensures a proper bound state problem for any value of the quadrupole deformation, provided $|\lambda|$ is smaller than some $\lambda_{\text{crit}}$. Here, $\lambda_{\text{crit}}$ is defined to be the least value of the octupole strength for which the potential tends to $-\infty$ along one direction in the $\varrho - z$ plane. Analytic expressions for $\lambda_{\text{crit}}$ and the directions along which the potential opens its valleys to $-\infty$ are given elsewhere [20]. There is a particular value of $b$, namely $b \approx 0.58$ for which valleys along two directions ($\varrho = 0$) and ($\varrho \approx 0.4z$) will open simultaneously when $\lambda$ approaches its corresponding critical value. We expect that this case will exhibit maximal chaotic behaviour.

3 Classical Approach

The coupling to the octupole potential renders the problem nonintegrable [15]. Despite this, it appears that in prolate situations ($b > 1$), the quantum mechanical spectrum exhibits
shells for some particular values of the octupole strength. A periodic structure which appears in the energy spectrum should be a reflection of one or more shortest classical orbits which dominate in the phase space. Here we present a method which reveals that the classical counterpart is quasi-integrable for prolate cases. It will also establish that the phase space structure is very close to that of a potential without octupole term but with a larger value of the quadrupole deformation $b$.

Our classical approach is based on the "removal of resonances" method developed in the secular perturbation theory. In the technique, the Hamiltonian written in action-angle coordinates, is averaged over the faster phase. Usually, prior to such an operation, a canonical transformation is necessary in order to remove the initial resonance from the unperturbed Hamiltonian (in our case the Hamiltonian without the octupole coupling). In the new rotating frame, one of the phases will only measure the slow variation of the variables about the original resonance which now becomes a fixed elliptic point. The problem is then treated by averaging over the remaining faster phase. In the case of a super or hyper-deformed potential though, there already appears to be a clear distinction between a slow and fast phase, therefore the canonical transformation is unnecessary.

The complete Hamilton function written in terms of the action-angle variables of the unperturbed problem reads:

$$H(J_\varrho, J_z, \theta_\varrho, \theta_z) = \omega \left( J_\varrho + \frac{1}{b} J_z + \lambda \frac{\sqrt{b} J_z \sin \theta_z (2b J_z \sin^2 \theta_z - 3J_\varrho \sin^2 \theta_\varrho)}{\sqrt{b} J_z \sin^2 \theta_z + J_\varrho \sin^2 \theta_\varrho} \right)$$

(4)

The frequencies of the two motions in $z$ and $\varrho$ can be expressed as:

$$\omega_z(J_z, \theta_z) = \frac{\partial H}{\partial J_z} = \frac{\omega}{b} \left( 1 + \lambda \frac{b \sin \theta_z (4b J_z^2 \sin^4 \theta_z + 6b J_z J_\varrho \sin^2 \theta_\varrho \sin^2 \theta_z - 3J_\varrho^2 \sin^2 \theta_\varrho)}{2 \sqrt{b} J_z (b J_z \sin^2 \theta_z + J_\varrho \sin^2 \theta_\varrho)^{3/2}} \right)$$

(5)

$$\omega_\varrho(J_\varrho, \theta_z) = \frac{\partial H}{\partial J_\varrho} = \omega \left( 1 - \lambda \frac{\sin \theta_z \sin^2 \theta_\varrho \sqrt{b} J_z (8b J_z \sin^2 \theta_z + 3J_\varrho \sin^2 \theta_\varrho)}{2 \sqrt{b} J_z (b J_z \sin^2 \theta_z + J_\varrho \sin^2 \theta_\varrho)^{3/2}} \right)$$

(6)

Obviously, the winding number of a trajectory defined as the ratio $\omega_\varrho/\omega_z$ is essentially equal to $b$ when $\lambda$ is small. This means that for $b$ sufficiently far from unity, there will always
be a fast and a slow moving phase, i.e. the averaging is performed over the corresponding fast angle.

### 3.1 Prolate Potential \((b > 1)\)

For prolate deformation the fast phase is \(\theta_\varrho\). Averaging the Hamilton function over \(\theta_\varrho\), we are led to a new averaged Hamiltonian \(H_{av}\) which is independent of \(\theta_\varrho\). This means that the corresponding action \(J_\varrho\) becomes a constant of motion in this approximation: \(J_\varrho = J_\varrho(0)\). Introducing the notation \(\xi^2 = 2J_\varrho(0)/(m\omega) = \varrho^2(0) + p_\varrho^2(0)/(m\omega)^2\), the averaged Hamiltonian reads in the original position momentum coordinates:

\[
H_{av} = \frac{p_\varrho^2 + p_z^2}{2m} + \frac{m\omega^2}{2} \left[ \varrho^2 + \frac{z^2}{b^2} + \lambda \xi^2 \text{sign}(z) \left( \frac{z^2}{\xi^2} K\left(-\xi^2\right) - 3\pi_2 F_1\left(\frac{1}{2}, \frac{3}{2}, 2, -\frac{\xi^2}{z^2}\right) \right) \right]
\]

(7)

Here, \(K\) and \(\_2 F_1\) are the complete elliptic function of the first kind and the hypergeometric function, respectively. In this way, the problem is effectively reduced to two uncoupled one dimensional cases. A remainder of the actual coupling is the fact that, through \(\xi\), the \(z\) motion still depends on the initial conditions of the \(\varrho\) motion. The frequency \(\omega_z\) is given by \(\omega_z = 2\pi/T\) where

\[
T = \sqrt{2m} \int_{z_{\min}}^{z_{\max}} \frac{dz}{\sqrt{E_z - U(z)}}
\]

(8)

with \(E_z = E - E_\varrho = E - m\omega^2\xi^2/2\) and \(U(z)\) is the effective potential of the \(z\) motion and is given by:

\[
U(z) = \frac{m\omega^2}{2} \left[ \frac{z^2}{b^2} + \lambda \xi^2 \text{sign}(z) \left( \frac{z^2}{\xi^2} K\left(-\xi^2\right) - 3\pi_2 F_1\left(\frac{1}{2}, \frac{3}{2}, 2, -\frac{\xi^2}{z^2}\right) \right) \right]
\]

(9)

The winding numbers \(\omega_\varrho/\omega_z\) can be evaluated numerically, with \(\omega_\varrho = \omega\). It turns out that for a given value of the octupole strength, the frequencies are virtually independent of \(\xi\), and most of the trajectories in the phase space will have basically the same winding number. This number can be evaluated analytically at \(\xi = 0\):

\[
\frac{\omega_\varrho}{\omega_z} = \frac{b}{2} \left( \frac{1}{\sqrt{1 + \lambda/\lambda_{\text{crit}}}} + \frac{1}{\sqrt{1 - \lambda/\lambda_{\text{crit}}}} \right)
\]

(10)

We display in Fig.1 and Fig.2 the effective potential and the variation of \(\omega_\varrho/\omega_z\) for a few values of \(\xi\), respectively. As a function of \(\lambda\) the winding number increases monotonously. It
means that for a prolate case, a superposition of quadrupole and octupole deformation is practically equivalent to a pure but larger quadrupole deformation. Of particular interest is the existence of the short periodic orbits, as they become important for the quantum-classical correspondence. For instance, in the superdeformed case ($b = 2$), according to formula (10), the winding number becomes equal to $5 : 2$ at $\lambda = 0.66\lambda_{\text{crit}}$ and should have that value for most of the orbits. As a result, the quantum mechanical spectrum is expected to exhibit a periodic structure [24] of the same kind as of a pure quadrupole deformation with winding number $b = 5 : 2$. Likewise, when $\lambda = 0.8\lambda_{\text{crit}}$, the ratio of the two frequencies becomes $3 : 1$ and, as a consequence, a shell structure very similar to the case $b = 3$ and $\lambda = 0$, is likely to occur. In Fig.3 we display the actual phase space configuration $(z - p_z)$ for $\lambda = 0.66\lambda_{\text{crit}}$ and $\lambda = 0.8\lambda_{\text{crit}}$. Of importance is the large single separatrix structure which covers most of the surface of section. The corresponding periodic orbits lying in the centre of each separatrix are displayed in Fig.4. Their winding numbers are $5 : 2$ and $3 : 1$, respectively. After having tested numerically the winding number in different regions of the phase space, it turns out that with the exception of the innermost zones, the winding numbers are very close to those given by formula (9) for about 85% of the phase space.

The expression (10) for the ratio of the winding numbers is of course valid for all values $b > 1$ for which the approximation is meaningful. It turns out that this is the case for $b \geq 1.5$. The significance of this statement is far reaching: it means that even for irrational values of $b$, where the unperturbed problem does not give rise to closed orbits, the switching on of an appropriate octupole strength will produce a situation of an unperturbed pure but larger quadrupole deformation. For instance, $b = \sqrt{3}$ and $\lambda = 0.56$ should essentially yield the situation of pure superdeformation ($b = 2$). The consequence for the quantum spectrum will be discussed at the end of the following section.

As mentioned in the previous section, we restrict ourselves only to zero value for the $z$ component of the angular momentum. A finite value of $l_z$ does not change the result of the averaging procedure. This implies that if at some value of $\lambda$ the quantum spectrum exhibits a shell like structure for one value of the angular momentum, it will exhibit the same type of structure for any angular momentum and therefore produce genuine shells. We return to this point in the next section.
3.2 Spherical and Oblate Potential \((b \leq 1)\)

In these cases, the approximation procedure described above does not achieve any decoupling between \(\rho\) and \(z\) motion. For an oblate potential, the faster phase is \(\theta_z\). Since the octupole part of the potential is an odd function of \(\theta_z\), the result of the averaging now vanishes. If higher order terms in the Fourier expansion of the octupole are considered, the coupling between the two degrees of freedom is still maintained; the attempt to obtain an analytic expression for the effective potential seems to stop here. The fact that the problem remains coupled even perturbatively indicates that chaotic behaviour may occur with increasing \(\lambda\).

In the spherical case, one could in principle perform a canonical transformation enforcing one of the two frequencies to become faster and then averages over the faster phase. However, the slower frequency turns out to be a complicated function of time, in other words, the ratio \(\omega_\rho/\omega_z\) fails to remain constant even for an individual orbit. Like in the oblate case, the spherical potential is expected to yield chaos for sufficiently large values of \(\lambda\). For comparison, we display surfaces of sections in Fig. (5) for the spherical and oblate case where the onset of chaos is obvious. We mention here that the special case \(b \approx 0.58\) requires the smallest octupole strength to become chaotic. The onset of chaos is associated with the disappearance of periodic (shell) structure in the corresponding quantum mechanical spectrum. This feature will be dealt with in the next section.

4 Quantum Mechanical Approach

We write the Hamilton operator in the form \(H_0 + \lambda H_1\) in a representation where \(H_0\) is diagonal. The basis chosen is referred to as the basis using the asymptotic quantum numbers \(n_\perp, n_z\) and \(\Lambda\) where \(n_\perp = n_+ + n_-\) and \(\Lambda = n_+ - n_-\). Here the quantum numbers \(n_+\) and \(n_-\) are the eigenvalues of \((A_+)^\dagger A_+\) and \((A_-)^\dagger A_-\), respectively, where, in terms of the usual boson operators \(a_x\) and \(a_y\), we use \(A_\pm = (a_x \mp ia_y)/\sqrt{2}\). For a fixed value of \(\Lambda\) this leaves two quantum numbers (reflecting the two degrees of freedom) to enumerate the rows and columns of the matrix problem. For \(\Lambda = 0\) the diagonal entries of \(H_0\) are thus \(\varepsilon^0_{n_\perp,n_z} = \hbar \omega(n_\perp + 1 + (n_z + 1/2)/b)\). The matrix elements of \(H_1\) are obtained from those of \(z \sim (a_\perp^\dagger + a_z)\) and \(\rho^2 \sim (A_+ (A_+)^\dagger + A_- (A_-)^\dagger + A_+ A_- + (A_-)^\dagger (A_+)^\dagger)\). To get the matrix elements of \(1/\sqrt{\rho^2 + z^2}\) in a numerically consistent way, we first calculate the
matrix elements $S_{m,n}$ of $g^2 + z^2$ from which the inverse square root is obtained using $S^{-1/2} = U \cdot D^{-1/2} \cdot U^\dagger$ where $D = U^\dagger \cdot S \cdot U$ is the diagonal form of the positive definite matrix $S$ and $U$ is the orthogonal matrix which diagonalises $S$. To ensure also numerically that $S$ has only positive eigenvalues it is important that the matrix for $z^2$ is obtained by squaring $z$ and not by evaluating analytically the matrix elements from $(a_z^+ + a_z)^2$; inconsistencies are otherwise introduced due to truncation. In this way, we also ensure that the truncated matrices $S^{-1/2}$ and the representation of $2z^3 - 3zg^2$ commute.

4.1 Energy Levels

In Fig.(6a) we illustrate the spectrum so obtained as a function of $\lambda$ for $b = 2$. The shell structure at about $\lambda = 0.63\lambda_{\text{crit}}$ and $\lambda = 0.76\lambda_{\text{crit}}$ is clearly discernible. The fact that the structures do not occur exactly at those values of $\lambda$ as calculated in section 3.1 is a consequence of the approximation introduced by the "removal of resonances" method. However, the agreement is very good, with an error of only 5%. While Fig.(6a) presents the spectrum for $\Lambda = 0$, we illustrate in Fig.(6b) the whole spectrum which is a superposition of all possible $\Lambda$-values. The shell structure is then more pronounced which is expected since, according to the discussion in section 3.1, the orbits will have the same winding numbers independent of the angular momentum; as a consequence, the quantum spectra will have shell structures similar to an unperturbed oscillator. To contrast with the case $b = 2$, we also display spectra for $b = 1$ (spherical) and $b = 1/2$ (oblate superdeformed). As predicted by the classical analysis, there are no obvious regions where periodic structures such as shells would occur. The level statistics shows that such cases are actually chaotic, in that their nearest neighbour distribution approaches the Wigner surmise [15].

4.2 Total Energy Method

To analyse the quantum spectrum we proceed in the orthodox fashion in that the total energy $E_{\text{tot}}(N, \lambda) = \sum_i^N \epsilon_i(\lambda)$ is approximated by a smooth average function $S(z, \lambda)$ and the fluctuating difference

$$\delta E(N, \lambda) = E_{\text{tot}}(N, \lambda) - S(N, \lambda)$$

is then subjected to further investigation. The finding of a suitable form for the average function $S(z, \lambda)$ is facilitated in our case as it is well known that the leading term of $E_{\text{tot}}(N, \lambda)$,
as a function of $N$, is proportional to $N^{4/3}$. We determine the five constants $a_0(\lambda), \ldots, a_4(\lambda)$ in $S(z, \lambda) = \sum_{k=0}^{4} a_k(\lambda) z^{k/3}$ by a least square fit which turns out to be perfectly satisfactory for all values of $0 \leq \lambda < \lambda_{\text{crit}}$.

In Fig.(7a) the fluctuating part $\delta E(N, \lambda)$ is presented as a contour plot and refers to $b = 2$. It displays the ranges $100 \leq N \leq 700$ and $0 \leq \lambda < \lambda_{\text{crit}}$. For $\lambda = 0$ (the bottom horizontal line) we clearly discern the shell structure of the plain deformed oscillator. Note that the sharp minima (dark shadowing) occur at the positions $N$ where a shell is closed; the distances are proportional to $N^3$. When $\lambda$ is switched on the shell structure persists to a great extent; only when $\lambda$ approaches its critical value (top horizontal line) the structure begins to be washed out. There are local minima discernible at $\lambda/\lambda_{\text{crit}} \approx 0.76$. This is a reflection of the enhanced shell structure discussed in the previous section. For comparison we also display contour plots for $b = 1.5, 1, 0.58$ and 0.5. As expected, the ordered formation of local minima along a line $\lambda = \text{const}$ becomes lesser pronounced and eventually disappears as the spherical and oblate region is approached. The greatest extent of disorder is obtained for $b = 0.58$ where the classical case is maximally chaotic.

4.3 Magic Numbers

The detailed shell structure is obtained from the second derivative of $\delta E(N, \lambda)$ to which we turn next. For $b = 2$, we have plotted in Figs.(8) the function $g(E) = \delta E(N + 1, \lambda) + \delta E(N - 1, \lambda) - 2\delta E(N, \lambda)$ versus $N^{1/3}$ for a few characteristic values of $\lambda$. The peaks of the plots represent the magic numbers which characterise the shells, and the heights of the peaks reflect the energy distance from one shell to the next. In Fig.(8a) the essentially unperturbed result ($\lambda/\lambda_{\text{crit}} = 0.15$) is presented for demonstration. The second row displays the results for the particular values of $\lambda$ for which the winding numbers are 5:2 ($\lambda/\lambda_{\text{crit}} = 0.63$) and 3:1 ($\lambda/\lambda_{\text{crit}} = 0.76$), respectively. The magic numbers and the heights of the peaks agree well with those which are obtained from the unperturbed ($\lambda = 0$) quadrupole deformed oscillators (third row in Fig.(8)) with $b = 5/2$ and $b = 3$, respectively, at least for $N \leq 700$, $N^{1/3} \leq 8.88$. The agreement extends in particular to the respective occupation numbers, i.e. the degeneracies; of course, the heights of the peaks do not show the same regularity as the corresponding unperturbed problem; nevertheless, even for the heights an overall agreement prevails when comparing with Figs.(8e) and (8f) where the respective
unperturbed structures are displayed. For higher values of $N$ we do get deviations which reflect upon the fact that the system is nonintegrable and cannot give complete order in all its results. While the agreement for lower values of $N$ was to be expected from the discussion in the previous section, the extent of the agreement is rather remarkable, especially for $\lambda \approx 0.76\lambda_{\text{crit}}$ where an astoundingly clean shell structure reoccurs after it partially disappeared for a somewhat smaller value of $\lambda$. It is this recurrence of shell structure which gives rise to the local minima in Fig.(7) as pointed out above.

One of the questions addressed in this paper is also the possible occurrence of supershell effects when a quadrupole deformed harmonic oscillator is perturbed by an anharmonic term, i.e. the octupole deformation. Of particular interest in this respect is Fig.(8b) which refers to the intermediate value $\lambda = 0.7\lambda_{\text{crit}}$ where the genuinely different orbits with winding numbers 5:2 and 3:1 coexist. The long wave length fluctuation could well be interpreted as a supershell structure, even though that it is not as clearly pronounced as in a more transparent integrable case [17]. Yet the difference to Fig.(8d) which refers to a larger value of $\lambda$ is striking.

### 4.4 Quantum-Classical Correspondence

In Figs.(9) we display the square of the modulus of the Fourier transform of the level density, i.e. the function

$$F(t) = |\sum_n e^{i\varepsilon_n t}|^2.$$  \hspace{1cm} (12)

The spectrum is taken for $b = 2$ at $\lambda = 0.63\lambda_{\text{crit}}$ (Fig.(9a)) and at $\lambda = 0.76\lambda_{\text{crit}}$ (Fig(9b)), both spectra refer to $\Lambda = 0$ only. The pronounced peaks can be directly associated with the periods of the classical 5:2 and 3:1 orbit, respectively, the periods obtained from Figs.(9) are in perfect agreement with those of the corresponding classical orbits which are found numerically by integrating Eqs.(3). This is a beautiful demonstration of Gutzwiller’s trace formula [10]. As expected the frequencies deviate considerably from the unperturbed values, i.e. from the frequency associated with $b = 2, \lambda = 0$, but also from the frequencies associated with $b = 5/2$ or $b = 3$. In units of the unperturbed value ($b = 2$) we find $T_{5:2} = 1.2$ and $T_{3:1} = 1.4$; the values are larger than unity in accordance with Fig.(2). We mention that a similar situation is encountered also in the hyperdeformed prolate case. There the two main orbits have the winding numbers $b = 7 : 2$ (occurring at $\lambda = 0.6\lambda_{\text{crit}}$) and $b = 4 : 1$.
(occurring at $\lambda = 0.72\lambda_{\text{crit}}$), respectively. In a similar vein, as was emphasised towards the end of Section 3.1, a shell structure just like that of a pure superdeformed prolate case must occur for, say, $b = \sqrt{3}$ and $\lambda \leq 0.56$ [23]. These findings make it quite clear that, as far as the model is concerned, the spectrum alone cannot distinguish between an additional octupole deformation and an unperturbed but larger quadrupole deformation; additional experimental information is needed to settle this point.

Again we stress that the high degree of order which prevails in the superdeformed and hyperdeformed prolate case when the octupole term is turned on, does not exist in the corresponding oblate, in fact, not even in the spherical case. There, chaotic behaviour becomes manifest for much lesser octupole strength, which results in a complete disappearance of shell structure in the quantum spectrum.

5 Exceptional Points

The spectra displayed in Figs.(6) exhibit avoided level crossings which are related to the singularities [24] of the energy in the complex $\lambda$ plane. These singularities are known as exceptional points [28]. They represent the values of $\lambda$ where two energy levels coalesce when continued into the complex plane. The connection between the occurrence of avoided level crossings and exceptional points is similar in nature to the connection between the poles of a scattering function and the resonance structure of a cross section. In the same way as the poles of the scattering function give rise to the shape of the cross section, the exceptional points bring about the shape of the spectrum. Their interplay alone [28] provides the mechanism for the signature of chaos in a quantum system. With the aid of exceptional points, criteria for quantum chaos can be found even when the classical counterpart does not exist [28].

The levels are obtained by solving the secular equation:

$$\det(E - H_0 - \lambda H_1) = 0$$

To enforce coalescence of the roots of Eq. (12) the additional algebraic equation

$$\frac{d}{dE}\det(E - H_0 - \lambda H_1) = 0$$

must be solved simultaneously. Since the Hamilton operator is irreducible with respect to symmetries, the fulfilment of the two equations simultaneously is generically excluded for
real finite $\lambda$, as this would mean a genuine crossing for two levels. It has previously been established that a high density of exceptional points is a prerequisite for the occurrence of chaos in the energy spectrum [28]. Also, it is known that the statistical distribution of the real parts of exceptional points is close to the distribution of avoided level crossings. It means that for the particular values of $\lambda$ where the density of avoided level crossings is high the energy spectrum generically obeys the same level statistics as that ascribed to quantum chaos. We have analysed the eigenvalue problem of the operator $H_0 + \lambda H_1$ beyond the $\lambda_{\text{crit}}$ value. Although the region $\lambda > \lambda_{\text{crit}}$ is of no physical significance, it gives information about the distribution of avoided level crossings. To exclude genuine crossings between levels we display the $\Lambda = 0$ subspace of the energy spectrum in Fig.(10). The spectrum is extended into the physically forbidden region for the prolate superdeformed ($b = 2$) potential. It appears that the maximum of the distribution of level repulsions occurs in the unphysical region for the prolate case in contrast to the spherical and oblate case (see Figs.(6c,d)). This can be understood since, unlike in the spherical and the oblate situation, the first order perturbation term of the prolate problem vanishes. As a result, the spectrum has a zero derivative at $\lambda = 0$, and the exceptional points cannot occur near to the $\lambda = 0$ axis, in fact most occur beyond $\lambda_{\text{crit}}$. In turn, the occurrence of avoided level crossings in the physical region for oblate and spherical potentials indicates the onset of chaos for $\lambda < \lambda_{\text{crit}}$. While this was expected from the classical behaviour, we see here the corresponding mechanism of the quantum mechanical matrix problem at work. It is interesting to note the connection between the symmetry breaking mechanism and the distribution of level repulsions: the system aspires to break the spherical symmetry where the density of avoided level crossings is high, so as to keep order and stability. The conclusion that the prolate case exhibits less chaos for small values of $\lambda$ than the spherical and oblate case, can in fact be drawn from the matrix structure alone, which in turn is directly related to the gross distribution of exceptional points [28].

6 Modified Nilsson Model

Used with a great deal of success in the description of deformed nuclei, the modified Nilsson model has recently been extended to metallic clusters [25] (see for review [5, 6]). In practical applications the Woods–Saxon potential, also used successfully for the investigation of
metallic clusters, has the disadvantage that it can not be solved analytically, in contrast to the modified oscillator potential \[26, 27\]. The level ordering in the Woods-Saxon case falls between the soft-surface harmonic oscillator (HO) and the hard-surface square well. The same level ordering is obtained in HO by the addition of a term and reads in cylindrical coordinates

\[
H = \frac{\vec{p}^2}{2m} + \frac{m\omega^2}{2} \left( \varrho^2 + \frac{z^2}{b^2} \right) - v_{ll}\hbar \omega \vec{l}^2
\]  

(15)

Here, \( \vec{l}^2 \) is the square of the dimensionless angular momentum operator and \( v_{ll} \) is a constant. To avoid a general compression of the shells produced by \( \vec{l}^2 \) alone, the average value of \( < \vec{l}^2 >_{N} \) is usually subtracted. However, while in nuclear structure the interest is focused on the lower lying levels in the single particle potential, the relevant energy range extends higher up for clusters. This necessitates a re-discussion of the possible usefulness in the application of this model to metallic clusters. For the present discussion we leave out the term \( < \vec{l}^2 >_{N} \) \[29\]. The classical Hamilton function can then be defined:

\[
H(\vec{p}, \vec{r}) = \frac{p_{\varrho}^2 + p_z^2}{2m} + \frac{m\omega^2}{2} \left( \varrho^2 + \frac{z^2}{b^2} \right) - U \left( (qp_z - zp_{\varrho})^2 + l_z^2 \right) + \frac{l_z^2}{\varrho^2}
\]  

(16)

Because of the axial symmetry, \( l_z \) is conserved. Again, the zero value of \( l_z \) is sufficient for all relevant aspects of our analysis. The classical problem is nonintegrable and gives rise to chaotic motion \[21\] if \( U > 0 \) and \( b \neq 1 \). We also note that the Hamilton function scales as: \( H(\alpha\vec{p}, \alpha\vec{r}) = \alpha^2 H(\vec{p}, \vec{r}) \), provided the product \( EU \) remains constant (\( E \) is the energy). Since the connection between \( U \) and \( v_{ll} \) is given by:

\[
U = \frac{\omega}{\hbar} v_{ll},
\]  

(17)

the classical behaviour for \( EU = \text{const} \) will be reflected in the quantum counterpart along the invariant lines \( Ev_{ll} = \text{const} \). To get an idea for which energy and coupling strength signatures of chaos can be expected in the quantum spectrum, a brief discussion of the classical phase space is appropriate \[21\]. In Fig.11 a section of the \( \varrho - p_z \) plane with the \( \varrho = 0 \) plane is displayed. The phase space is noncompact as can be seen from the figure where the allowed regions are shaded. The parameter \( EU \) determines the structure of the phase space; if it is larger than \( \omega^2/4 \) the two lines \( z = \pm 1/\sqrt{2mU} \) intersect the ellipse. In this case, chaos is clearly discernible inside the ellipse for the classical motion even for small
deviations from unity of $b$. If $EU < \omega^2/4$ chaos occurs inside the ellipse only for $b \gtrsim 1.5$. For $E \leq 0$ the ellipse is absent and the motion appears regular. Using the expression (17) this translates for the quantum levels $E_N$ into $E_N \sim N\omega^2v_\|$ which means that, for $v_\| = 0.07$, chaotic behaviour is expected for $N \geq 3$ if $b = 2$, while for, say, $b = 1.05$ its onset should occur only as high as $N \gtrsim 20$. Actual calculations fully confirm these expectations. The fact that an arbitrary large negative energy is allowed classically, is reflected also in the quantum spectrum; however, if the matrix problem is truncated, there is a limitation on the eigenvalues of $\vec{l}^2$; in any case, this part of the spectrum is virtually uncoupled to positive energies and has no part in avoided level crossings.

7 Summary

In the present paper we thoroughly investigated a simplified model to analyse the nature of shell effects at quadrupole/octupole axial deformations. We left out terms in the Nilsson model, which, albeit physically important, are prone to blur the analysis when the interest is focussed on the essentials, in particular a distinction between orderly and chaotic motion in many body systems, like nuclei and metallic clusters. Contrary to the case of spherical potentials our Hamiltonian is nonintegrable. Using the method based on the 'removal of resonances' approach [22], we established a connection between shell structures in the quantum mechanical spectrum and periodic orbits in the corresponding classical problem. In the prolate case the classical problem can effectively be reduced to an integrable set of equations, since the motion in the two coordinates becomes uncoupled. This is in contrast to the spherical and oblate cases, where the motion becomes chaotic when the octupole term is switched on. In the prolate case, at particular values of the strength parameter $\lambda$ the octupole term produces a motion which resembles to a great extent that of a pure but more enhanced prolate oscillator. A superposition of quadrupole and octupole deformations is practically equivalent to a pure but larger quadrupole deformation. This provides the classical explanation for the existence of quantum shell structure for prolate/octupole deformed system within the model [15, 20]. The fluctuating part of the energy has been extracted from the quantum mechanical single particle spectrum using the procedure which is a variant of the method discussed in [14]. We have found remarkable agreement between manifestations of shell structure for the same values of $\lambda/\lambda_{\text{crit}}$ and the ones which give rise to large stability
islands in the Poincaré surfaces of sections relating to the classical short orbits with winding numbers 2:1 \((\lambda \approx 0)\), 5:2 \((\lambda/\lambda_{\text{crit}} = 0.63)\), 3:1 \((\lambda/\lambda_{\text{crit}} = 0.76)\). In the intermediate case \((\lambda/\lambda_{\text{crit}} = 0.7)\) when the orbits with winding numbers 5:2 and 3:1 coexist the long wavelength fluctuation could be interpreted as a supershell structure. But due to the narrowness of these orbits the supershell structure is not as clearly pronounced as in a more transparent integrable case [16]. We placed our emphasis on the superdeformed case which is the most interesting situation when the octupole term is switched on. Shell structure is destroyed for smaller values of the octupole strength for lesser quadrupole deformation or even more so for the spherical case. Our results imply that the shell structure is supported by the superdeformed prolate/octupole in contrast to the oblate/octupole case. This conclusion was confirmed by the analysis of exceptional points connected with the occurrence of avoided level crossings in quantum spectra. It appeared that in the spherical and oblate case, the distribution of level repulsions, which provide the mechanism for the signature of chaos in a quantum system, occurs to a much greater extent in the physically relevant region than in the prolate case. The analysis of the modified Nilsson model without spin–orbit coupling leads to the conclusion that using the \(l^2\)-term in models for metallic clusters with the coupling strength similar to that in nuclear physics would conflict, at least for larger deformations \(b\), with the experimental finding of shell structure. Only if the deformation \(b\) is very close to unity can the regular motion associated with shells prevail, provided the shell number \(N\) is not too large. In turn, only a much smaller coupling can yield shell structure for larger deformations \(b\). Since the \(l^2\)-term has only a phenomenological meaning, this finding simply calls for caution when transferring models from nuclear to cluster physics.
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Figure captions

**Fig.1** The potential $U(z)$ in units of $m\omega^2/2$ for a few values of $\lambda$ and an intermediate value of $\xi$. Variation of $\xi$ produces similar shapes.

**Fig.2** The ratio $\omega_p/\omega_z$ as a function of $\lambda$ for various values of $\xi$. A genuine $\xi$ dependence is discernible only for $\xi > 0.8\xi_{\text{max}}$.

**Fig.3** Surfaces of section ($b = 2$) for $\lambda = 0.63\lambda_{\text{cr}}$ (top) and $\lambda = 0.76\lambda_{\text{cr}}$ (bottom).

**Fig.4** The major orbits with winding numbers $5:2$ ($\lambda/\lambda_{\text{cr}} = 0.63$) and $3:1$ ($\lambda/\lambda_{\text{cr}} = 0.76$).

**Fig.5** Surfaces of section for $b = 1$ (top) and $b = 1/2$ (bottom) for $\lambda = 0.5\lambda_{\text{cr}}$.

**Fig.6** Spectrum ($b = 2$) for $\Lambda = 0$ (a) and for all $\Lambda$ (b) as a function of $\lambda$. (c) and (d) are the $\Lambda = 0$ spectra for $b = 1$ and $b = 1/2$, respectively.

**Fig.7** a.) Contours of $\delta E(N, \lambda)$ with $100 < N < 700$ as abscissa and $0 < \lambda/\lambda_{\text{cr}} < 1$ as ordinate. Dark areas represent minima. Volume conservation is taken into account in Figs.(7) and (8). In b),c),d) and e) the same quantity is displayed for $b = 1.5$, $b = 1$, $b = 0.5$ and $b = 0.58$, respectively.

**Fig.8** Shell structure for fixed values of $\lambda$ and $b = 2$. The second derivative of $\delta E(N, \lambda)$ is illustrated versus $N^{1/3}$ for $\lambda/\lambda_{\text{cr}} = 0$, $0.7$, $0.63$ and $0.76$ in (a), (b), (c), and (d), respectively. In (e) and (f) the unperturbed ($\lambda = 0$) structure is displayed for $b = 2.5$ and $b = 3$, respectively.

**Fig.9** Fourier transform of the modulus square of the level density for $\Lambda = 0$, $b = 2$ for $\lambda/\lambda_{\text{cr}} = 0.63$ (top) and $\lambda/\lambda_{\text{cr}} = 0.76$ (bottom).

**Fig.10** Spectrum ($b = 2$) for $\Lambda = 0$ extended beyond $\lambda_{\text{cr}} = 0.125$. Note that the distribution of the avoided level crossings occurs largely for $\lambda > \lambda_{\text{cr}}$.

**Fig.11** Surfaces of section for the modified Nilsson model. Two situations of accessible phase space (shaded) are displayed; left: $|\lambda| < \omega^2/(4E)$, right: $|\lambda| > \omega^2/(4E)$