Nuclear Shell Structure and Chaotic Dynamics in Hexadecapole Deformation

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The effect of an axially symmetric hexadecapole term is investigated in a strongly deformed quadrupole potential. While the system is nonintegrable and shows significant chaotic behaviour classically, the quantum mechanical treatment not only produces a general smoothing effect with regard to chaos but even yields a pronounced shell structure at certain hexadecapole strength parameter values for oblate and prolate deformation.

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Recently, the occurrence of shell structure has been reported for many body systems like nuclei and metallic clusters \[ [1,2] \] at strong octupole deformation. A major conclusion of \[ [2] \] is that, albeit nonintegrable, an octupole admixture to quadrupole oscillator potentials leads, for some values of the octupole strength, to a shell structure similar to a plain but more deformed quadrupole potential. This feature shows that there is a tendency of the system to restore the full original symmetry which is destroyed by the octupole term. In other words, we encounter the restoration of the original symmetry under certain conditions despite the system being nonintegrable.

In an integrable case the higher symmetry can cause a high degree of degeneracy of the eigenstates. Consequently, a spherical symmetry leads to very strong shell effects manifested in the stability of the noble gases, metallic clusters and magic nuclei. However, non-spherical shapes may be preferred by the system: shell effects associated with lesser symmetry occur. In super- and hyperdeformed nuclei deviations from the spherical shape are a consequence of strong shell closures giving rise to largest level bunching (largest degeneracy or lowest level density) for particle numbers where the spherical shell would be only partially filled. The concept of pseudo-SU(3) symmetry \[ [3,4] \] has been introduced \[ [3] \] to explain many features of superdeformed states described within a realistic nuclear potential. In the new scheme the spin-orbit splitting appears very small and the properties of the single-particle spectrum are similar to those observed in the three-dimensional harmonic oscillator with rational ratios of the frequencies \( \text{RHO} \). \[ [3,7] \]. Therefore, one can argue that the single-particle shell structure of \( \text{RHO} \) (which is an integrable system) should reflect the essential properties of super- and hyperdeformed nuclei.

The need for multipole deformations higher than the quadrupole has been recognized in nuclei and metallic clusters in numerous calculations to explain experimental data. The most important ones are the octupole and hexadecapole terms. Inclusion of either term leads to a nonintegrable problem. The hexadecapole deformation is essential for the understanding of equilibrium shapes and the fission process of super- and hyperdeformed systems \[ [8,9] \]. In the case of metallic clusters, the axial hexadecapole deformation is important for the interpretation of experimental data in simple metals \[ [10] \]. Usually the even and odd multipoles are considered together. However, obvious differences between the octupole and hexadecapole term suggests a separate study of their respective effects to shell structure phenomena. We aim at shedding more light on this old question from a new point of view. Our approach is based on the connection between shell structure phenomena in the quantum spectrum and ordered motion in the classical analogous case.

Shell structures in the quantum mechanical spectrum are associated with periodic orbits in the corresponding classical problem \[ [11–14] \]. The periodic orbits are associated with invariant tori of the Poincaré sections. If the classical problem is chaotic, the invariant tori disintegrate or disappear, and the shell structure of the quantum spectrum is affected by the degree of chaos \[ [3,10] \]. In this paper particular emphasis is placed upon strongly quadrupole deformed systems like superdeformed nuclei, and we concentrate only on the most important even multipoles, quadrupole and hexadecapole deformations. In a previous analysis of an octupole term \[ [2] \] it was demonstrated that shell structure can exist only in the super- and more deformed prolate case. In this paper we resume the study of quantum-classical correspondence for the hexadecapole term and show the occurrence of shell structure in prolate as well as oblate systems.

We investigate the classical and quantum mechanical single-particle motion in an axially symmetric harmonic oscillator potential including the hexadecapole term, \( \text{viz.} \)

\[
V(\varphi, z) = \frac{m\omega^2}{2} \left( \varphi^2 + \frac{z^2}{b^2} + \lambda \frac{8z^4 - 24z^2\varphi^2 + 3\varphi^4}{z^2 + \varphi^2} \right)
\]

(1)

where cylindrical coordinates \( (\varphi, z) \) are used. The quadrupole deformation and the hexadecapole strength are denoted by \( b \) and \( \lambda \), respectively. We use for the hexadecapole term the expression \( r^2 P_4(\cos \theta) \) to ensure a proper bound-state problem provided the hexadecapole strength is restricted to the range:
\[ \max \left( -\frac{1}{8\beta^2} ; \frac{1}{3} \right) < \lambda < \frac{(4b^2 + 3)\sqrt{5} + 2\sqrt{22b^4 + 24b^2 + 7}}{48\sqrt{5}}. \]  

Since the potential scales as \( V(\beta_0, \beta z) = \beta^2 V(\rho, z) \), only one energy value has to be considered \[15\]. The axial symmetry guarantees conservation of the \( z \)-component of the angular momentum \( p_z \), and the \( z \)-projection \( m \) of the angular momentum is therefore a good quantum number.

The classical perturbative treatment follows the secular perturbation theory \[18\] using the removal of resonances method (RRM); the application to quadrupole deformed systems including an octupole term is described in detail in \[8\]. Notice, that the RRM is particularly effective in the case of a two-dimensional problem. The main task is to find the values of the parameters \( b \) and \( \lambda \) for which the nonintegrable problem reduces effectively to an integrable case, which is in our case the two-dimensional oscillator with new effective frequencies. In this way we obtain good estimates for the winding numbers of the classical orbits and find the conditions where the original symmetry is restored. In contrast to the octupole case the hexadecapole deformation evokes more chaotic behaviour and involves resonances of higher order, hence the method may not produce results of comparable accuracy. However, without major efforts the approach turns out to give reliable guide lines as to what to expect quantum mechanically.

In the oblate case, the perturbative method yields an unperturbed motion in the \( z \)-coordinate with a frequency \( \omega_z = \omega/b \). The motion in \( \rho \) is described by the effective potential:

\[ V_{\text{eff}}(\rho, \xi_z) = \frac{m\omega_z^2}{2} \left( 1 - 32\lambda \rho^2 + 35\lambda \frac{\rho^3 \text{sign}(\rho)}{\sqrt{\rho^2 + \xi_z^2}} + 4\lambda \xi_z^2 \right) + \frac{p_z^2}{2m\rho^2}. \]

where \( \xi_z = \sqrt{2bE_z/(m\omega_z^2)} \) reminds us of the actually coupled motion in \( \rho \) and \( z \); it represents the portion \( E_z \) residing in the \( z \)-motion of the total energy. From Eq.(3) the frequencies of the anharmonic oscillations \( \omega_z \) can be evaluated. It turns out that, if the quadrupole deformation is sufficiently large, for instance \( b = 2/5 \), the winding number defined as \( \omega_0/\omega_z \) is independent of \( \xi_z \) for about 65% of its allowed range. In fact, for \( 0 \leq \xi_z \leq 0.65\xi_z^{\text{max}} \) and \( p_z = 0 \) it is close to \( \omega_0/\omega_z = \sqrt{1 + 3\lambda} \) which is the exact expression for \( \xi_z = 0 \). For \( b = 2/5 \) and \( \lambda = 0.18 \), we obtain \( \omega_0/\omega_z = 1 : 2 \) which applies for about two thirds of the \( \xi_z \) range. For these values of the deformation parameters we therefore expect in the quantum spectrum a sequence of levels which have virtually the same pattern as the shell structure of a pure oblate superdeformed \((b = 1/2)\) system. A slight \( p_z \)-dependence of the winding number decreases the actual value of \( \lambda \) (see below).

A Strutinsky-type analysis has been carried out for levels comprising values of \( m \) from 0 to 15. The total energy \( E_{\text{tot}}(\lambda, N) \) which is the sum over all single particle levels up to \( N \) is fitted by a polynomial \( E_{\text{smooth}}(\lambda, N) = \sum_{\lambda=0}^{N} c_\lambda(\lambda) N^{1/3} \), and the fluctuation \( \delta E(\lambda, N) = E_{\text{tot}}(\lambda, N) - E_{\text{smooth}}(\lambda, N) \) is plotted versus \( \lambda \) and \( N \). The resulting contour plot is displayed in Fig.(1a).

We discern significant alternating minima and maxima along the line \( \lambda \approx 0.09 \) clearly indicating shell structure. The \( p_z \)-dependence of the winding number is reflected in a slight \( m \)-dependence of the spectrum. This is, however, sufficiently weak so as not to disturb the bunching of the levels when all \( m \)-values are considered. The \( m \)-dependence is noted in a decrease of the effective \( \lambda \)-value where shell structure occurs and in a slight broadening of the peaks in Fig.(2); we find bunching of levels for \( m = 0 \) at \( \lambda \approx 0.12 \) and for \( m = 15 \) at \( \lambda \approx 0.07 \).

Apart from the shell structure there are some remarkable stability islands for \( \lambda \approx 0.25, 0.22, 0.21 \) corresponding to the particle number \( N \) (or \( Z \)) \approx 56, 86 and 126, respectively. Their physical significance should be subjected to further experimental investigation. From the quantity \( \Delta E(\lambda, N) = \delta E(\lambda, N + 1) + \delta E(\lambda, N - 1) - 2\delta E(\lambda, N) \) which is displayed in Fig.(2a) we obtain the precise location of the magic numbers. The pronounced peaks coincide with the magic numbers of the oblate superdeformed \((b = 1/2)\) system.

While the quantum spectrum shows a fair degree of order, the analogous classical problem reveals a significant amount of chaos. In Fig.(3) we display surfaces of section in the \((\rho, p_\rho)\)-plane for \( p_z = 0 \); \( p_z > 0 \) does not lead to further insight. The phase space accommodates the coexistence of chaotic and regular motion. It is dominated by a large fourfold separatrix which contains in its four outer centres the four stability islands of the stable periodic orbit with winding number 1:2. It is this orbit which is responsible for the shell structure in the quantum spectrum. Note that the separatrix occupies about two thirds of phase space. The decay of the separatrix is clearly discernible. In the centre, additional short periodic orbits with winding numbers 2:5, 1:3, 2:1 are found. They can be associated with minor peaks in the power spectrum of the levels at \( \lambda = 0.12 \) shown in Fig.(4). Yet, their contribution to the level density of the low lying levels \((N \leq 150)\) is less pronounced than the contribution of the main orbit with its winding number 1:2. Note the oscillatory envelope of the major peak which is in line with general expectations \[19\].

In summary, we find that neither the chaotic orbits nor the abundance of periodic orbits are significantly reflected in the quantum spectrum except for the shortest one dominating the phase space. The model constitutes a fine example of quantum suppression of classical chaos.
The same analysis can be carried out for prolate systems. The estimated winding number $\omega_\phi/\omega_z$, which is now a function of $\xi_\phi = \sqrt{2E_\phi/(m\omega^2)}$, is equal to its value at $\xi_\phi = 0$ for about 85% of the allowed range for $\xi_\phi$, provided the quadrupole deformation $b$ is sufficiently large. At $\xi_\phi = 0$, the winding number becomes $\omega_\phi/\omega_z = b/\sqrt{1 + 8\lambda^2}$. For $b = 5/2$ and $\lambda = 0.011$ this yields the winding number 2:1. The Strutinsky-type analysis displayed in Figs.(1b) and (2b) nicely confirms the quantum mechanical expectation, in fact, this time the RRM gives a very accurate prediction of $\lambda$ for the occurrence of superdeformed shell structure. There is no noticeable angular momentum dependence in the prolate case, since the $g$-motion is virtually unperturbed. The hexadecapole strength considered is much smaller than in the oblate case and the shell structure occurs over a relatively wider range of $\lambda$ values with magic numbers for $N$ (or $Z$) $\approx 40, 80, 140$. This result agrees with a prediction of superdeformed shell structure for prolate nuclei [2], which confirms the physical relevance of our analysis. The numerical integration of the equations of motion reveals the same kind of structure as in the oblate case. The major orbit with the winding number 2 : 1 lies in the outer centres of the four-fold separatrix that occupies a large portion of the phase space. Other short periodic orbits which are insignificant for the quantum-classical correspondence ($N \leq 150$) again occur in the surface of sections. This time the onset of chaos along the four-fold separatrix is less pronounced.

One of the major results of this work is the occurrence of shell structure in an oblate deformed potential when a hexadecapole term is added. This is not an obvious result in view of the nonintegrability of the problem. Also, the occurrence of shell structure in the oblate case is of particular interest as the adding of an octupole term produces chaos without structure. The explanation for the latter result is found in the RRM which excludes, within the model considered, the possibility of decoupling the two degrees of freedom for odd multipoles in the oblate case; only the addition of even multipoles can restore the original symmetry and give rise to shell structure.

The Strutinsky-type analysis indicates stable energy configurations for oblate and prolate deformation; it appears that for particular magic numbers the oblate configuration is favoured as the respective minima in Fig.(1) are more pronounced. For positive values of $\lambda$ the net effect for the spectrum lies in its resemblance to that of a lesser quadrupole deformation. We mention that a negative value of $\lambda$ leads to the opposite effect in that a spectrum similar to that of a hyperdeformed system is found. Note that for prolate deformation the hexadecapole term is much weaker than that in the oblate case, i.e. a $\lambda$-value as large as the one used in the oblate case would produce hard chaos in the prolate case with all shell structure destroyed. In fact, a minute admixture of a hexadecapole deformation in the prolate case changes the pure $b = 5/2$ deformation into a $b = 2$ situation for the lower part of the energy spectrum relevant for nuclei. This means, that shell structure manifested experimentally by specific magic numbers cannot be directly associated with a definite type of deformation of the system. For instance, within our model similar superdeformed shell patterns can be reproduced in the prolate case with a combination of less quadrupole + octupole deformations or with more deformed quadrupole system and a hexadecapole admixture. Experimental information extracted from electromagnetic transitions could clarify as to whether we are faced with the plain superdeformed Hamiltonian is restored even though the problem becomes nonintegrable due to the additional term.

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Figure Captions

Fig.1 Contour plots of the fluctuating part of the total energy $\delta E$ as a function of particle number $N$ and hexadecapole strength $\lambda$ for (a) the oblate ($b = 2/5$) and (b) the prolate ($b = 5/2$) case. Dark regions correspond to energy minima which are associated to shell closures. Volume conservation is taken into account.

Fig.2 The quantity $\Delta E(\lambda, N)$ (see in the text) for (a) the oblate ($b = 2/5, \lambda = 0.09$) and (b) the prolate case ($b = 5/2, \lambda = 0.011$). The highest peaks occur at magic numbers which coincide with those of the oblate superdeformed and the prolate superdeformed systems, respectively.

Fig.3 Surface of sections indicating the phase space structure in the oblate situation for $p_\phi = 0$ and $\lambda = 0.12$.

Fig.4 Power spectrum of the level density for $\lambda = 0.12, m = 0$ and $b = 2/5$. The period of the peaks marked by a diamond agrees perfectly with that of the classical 1:2 periodic orbit. It is the orbit associated with the magic numbers of Fig.(2a) and its shape is displayed in the insert.