Chaos in Axially Symmetric Potentials with Octupole Deformation

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Classical and quantum mechanical results are reported for the single particle motion in a harmonic oscillator potential which is characterized by a quadrupole deformation and an additional octupole deformation. The chaotic character of the motion is strongly dependent on the quadrupole deformation in that for a prolate deformation virtually no chaos is discernible while for the oblate case the motion shows strong chaos when the octupole term is turned on.

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The mean field approach is of central importance in any theoretical description of a many body system. In nuclear physics it is the basis for the shell model and its extensions such as collective states. Its success has been further demonstrated in the application to deformed nuclei and to metallic clusters where spherical symmetry is given up because of experimental evidence. Usually, quadrupole deformation is considered to be the major deviation from spherical symmetry. However, more recently a possible octupole contribution has been taken into account for a number of reasons [1,2].

Inclusion of an octupole term in addition to a quadrupole term renders the classical single particle motion nonintegrable. In fact, the system turns out to be chaotic. This has been discussed by a number of authors with various degrees of simplification [3]. A nicely systematic approach is given in [4], where the motion in a quadrupole deformed cavity is analyzed and the terms that give rise to actual chaotic behavior are clearly distinguished. In a recent investigation [5] the study of classical motion in a cavity with oscillating walls of even and odd higher order multipoles has led to interesting conclusions about elastic versus dissipative behavior of a noninteracting gas depending on the integrability or nonintegrability of the equations of motion. Surfaces of section are used to discern the onset and degree of chaotic motion.

This paper is similar in spirit in that we investigate a simplified model where we leave out terms, which, albeit physically important, are prone to blur the analysis when the interest is focused on the essentials that give rise to chaotic behavior. Since our aim is directed not only to the classical but also to the corresponding quantum mechanical motion, we leave out the spin-orbit term and the l^2 term present in the Nilsson model to render as closely as possible the analogy between the classical and quantum cases. The importance of the l^2 term is well known in nuclear physics and for metallic clusters [6]. To determine its role in the context of chaotic motion the corresponding classical case ought to be studied. We defer treatment of this term. Despite the simplifications, such a model allows one to understand the main features of shell structure effects, for example, in super (hyper) deformed nuclei [7,8]. Recent experimental data of superdeformed K isomers in nuclei [9] and electronic shell structure effects in metallic clusters [6] clearly underline the importance of oblate deformation. Therefore we investigate in the present paper the effect of the octupole term for prolate and oblate deformation; the oblate-octupole case has not been dealt with in Ref. [5]. We analyze the case of zero temperature which is good for nuclei. For metallic clusters finite temperature should be considered [10]; however, our interest is focused on shell structure whose character is unaffected by temperature except for the amplitude. Only axially symmetrical terms are taken into account which brings down to 2 the number of degrees of freedom of the motion.

The single particle motion is considered in the potential

$$V(\rho,z)=\frac{m\omega^2}{2}\left(\rho^2+\frac{z^2}{b^2}+\lambda\frac{2z^3-3z\rho^2}{\sqrt{\rho^2+z^2}}\right), \qquad (1)$$

where $\rho^2=x^2+y^2$ in Cartesian coordinates x,y,z. We recognize an axially symmetric harmonic oscillator with frequencies $\omega_x=\omega_y=b\omega_z$ with an octupole term, written in the cylindrical coordinates (ρ,z,ϕ). For the results presented the parameters are chosen such that the levels are 15 MeV apart for $b=1$ and $\lambda=0$ which corresponds to a three-dimensional isotropic harmonic oscillator. For $\lambda=0$ and $b>1$ $(b<1)$ we have the mean field potential of a prolate (oblate) nucleus. Note that choosing a suitable set of different parameters, we deal with a metallic cluster. The octupole term $(\lambda\neq0)$ is proportional to r^2Y_{30} with Y_{30} being the third order spherical harmonic and $r^2=\rho^2+z^2$.

If $|\lambda|<\lambda_c$ we are dealing with a proper bound state problem. Here λ_c is defined to be the value for which the potential no longer binds; for $|\lambda|>\lambda_c$ the potential tends to $-\infty$ along one or two directions. The direction and the value of λ_c depend on the quadrupole deformation b. For prolate nuclei $(b>1)$, $\lambda_c=1/2b^2$ and the potential opens its valley along the positive (negative) z direction for negative (positive) λ. For oblate nuclei $(0.5\leq b<1)$

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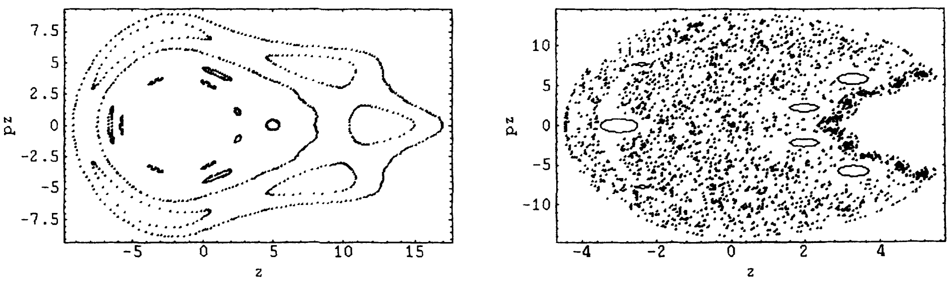

FIG. 1. Surfaces of section at $\rho=0$ for $b=2$, $\lambda=\frac{2}{3}\lambda_c$ (left) and $b=0.58$, $\lambda=\frac{1}{3}\lambda_c$ (right). In the left part stability islands are clearly discernible for winding numbers 2:5, 1:2, and 4:7. The right part is dominated by chaotic motion; some of the remaining islands are indicated by ellipses.

the other possible direction which is along the line $\rho=\mathrm{sgn}(\lambda)\alpha z$, with $\alpha\approx 0.4$, is of increasing importance. At the value $b\approx 0.58$ valleys along the two directions $\rho=0$ and $\rho=0.4z$ open simultaneously for $\lambda_c\approx 1.5$ while for a still smaller value of b, say for $b=0.5$, the valley along the direction $\rho=0.4z$ opens for $\lambda_c\approx 1.64$ while the one along the z axis now opens for a larger value of λ. (Analytic expressions for λ_c and the direction α as functions of b exist but are of little interest.) Chaotic motion is expected to become more pronounced the nearer the parameters for a bounded motion are to those for an unbounded motion. Thus increasing chaotic behavior is expected when λ approaches λ_c. Furthermore, since the geometry of the potential for $\lambda=\lambda_c(b)$ also depends on b, the chance of an escape for $\lambda\geq\lambda_c$ also depends on b. This chance reflects upon the amount of chaos, i.e., the Lyapunov exponent, for the bounded motion prevailing for values $\lambda<\lambda_c(b)$. In this way the amount of chaos is expected to be greatest for $b\approx 0.58$ where two valleys can serve as an escape route if $\lambda=\lambda_c$. In addition, at $b=2$ (superdeformed prolate nucleus) less chaos is expected than at $b=0.5$ (superdeformed oblate nucleus), since the opening of the phase space happens through a small bottle neck in the former case thus considerably reducing the chance for escape, while the chance for escape at $b=0.5$ is enhanced as the phase space opens more widely.

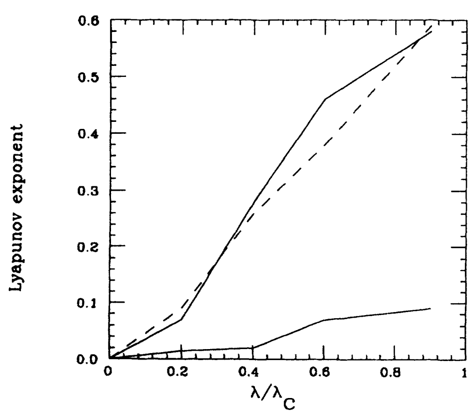

FIG. 2. Lyapunov exponent as a function of λ/λ_c. The lower solid line is for $b=1$, the upper solid line for $b=0.58$, and the dashed line for $b=0.5$. The values for $b=2$ are too small to appear on the diagram.

The results of the numerical integration of the equations of motion confirm all the expectations. Axial symmetry yields the constant of motion $p_\phi=\rho^2\dot\phi$ of the three-dimensional motion. We present results only for $p_\phi=0$. A nonzero value of the z component of the angular momentum does not produce new insights. Since the potential scales as $V(\gamma\mathbf{r})=\gamma^2V(\mathbf{r})$ it suffices to investigate one energy only [11].

For the superdeformed prolate nucleus ($b=2$) there is hardly any chaotic behavior discernible in the classical motion for all $\lambda<\lambda_c$. When looking at surfaces of section which we have taken at $\rho=0$ (recall $p_\phi=0$) in the (p_z-z) plane there is some scattering of the dots when λ is very close to λ_c, but the Lyapunov exponent is virtually zero. There is, however, a proliferation of periodic orbits, an aspect important below when we discuss quantum mechanics. This is illustrated in Fig. 1(a) where surfaces of section are displayed for $b=2$ and $\lambda=\frac{2}{3}\lambda_c$.

For decreasing values of b the motion becomes increasingly chaotic up to the maximally chaotic case at $b\approx 0.58$. Surfaces of section are illustrated in Fig. 1(b) for $\lambda=\frac{1}{3}\lambda_c$. Note that for $b=0.58$, no structure would be discernible for $\lambda=\frac{2}{3}\lambda_c$. We have compared results for $\lambda=\beta\lambda_c(b)$ with $\beta=0.2$, 0.4, 0.6, and 0.9. The trend is uniform in that the Lyapunov exponent shows the behavior as indicated in Fig. 2. The figure presents values referring to chaotic orbits and avoids initial conditions within regions of stability. Such regions of stability gradually disappear when λ approaches λ_c if $b\leq 1$.

We find the expected proliferation of periodic orbits. However, we refrain from discussing them in great detail as the aspect of the possible retrieval [12] of periodic orbits from the quantum mechanical spectrum is discussed in a forthcoming paper.

The quantum mechanical treatment is straightforward in principle. In the spirit of previous work [13] we use for the full problem which is of the form $H_0+\lambda H_1$ a representation where H_0 is diagonal. The basis chosen is referred [7] to as the basis using the asymptotic quantum numbers $n_\perp$, n_z, and Λ, where $n_\perp = n_+ + n_-$. For a fixed value of Λ this leaves two quantum numbers (reflecting the 2 degrees of freedom) to enumerate the rows and columns of the matrix problem. For $\Lambda=0$ the diagonal entries of H_0 are thus $E_{n_\perp,n_z}=\hbar\omega[n_\perp+1+(n_z+\frac{1}{2})/b]$. The matrix elements of H_1 are obtained from those of $z\sim(a_z^\dagger+a_z)$ and $\rho^2\sim(A_+A_+^\dagger+A_-A_-^\dagger+A_+A_-+A_+^\dagger A_-^\dagger)$, where, in terms of the usual boson operators $a_{x,y}$, $A_\pm=(a_x\mp ia_y)/\sqrt{2}$. The effect of truncation was tested by looking at the variation of the lower end of the spectrum when the dimension of the matrices was increased. There is certainly a dependence on b and λ. For $\lambda\leq 0.9\lambda_c$ and $0.5\leq b\leq 2$ the variation was less than 1% for the first 300 levels obtained from 1600×1600 dimensional matrices.

For demonstration we display parts of the spectra in Fig. 3. It is obvious, and in fact quantitatively confirmed in Fig. 4 where the relevant statistical analyses are shown, that the quantum mechanical results are in line with the classical cases. The level repulsions in the superdeformed prolate case are very weak thus giving rise to a nearest neighbor distribution (NND) which appears nearer to an integrable case than to the typical Wigner distribution. Of physical interest are the pronounced new shell structures that emerge near to $\lambda=0.5\lambda_c$ and $\lambda=0.65\lambda_c$ in the superdeformed prolate case. This pattern is directly related to the periodic orbits indicated in Fig. 1(a) as will be discussed in detail in a forthcoming paper. Since we have left out terms like spin-orbit coupling and l^2 we cannot claim that such structures arise exactly where we find them. However, the essential point is the fact that such structures will always emerge. Since the situation is so close to integrability for all $\lambda<\lambda_c$, the level repulsions are always weak; as a consequence, shell structures are bound to emerge for some values of the parameters. We note that the consequent periodicity in the spectrum will produce sharp lines in the Fourier transform of the level density [14], a reflection of the many periodic orbits [15] found in the corresponding classical case as was mentioned above.

These findings nicely contrast with the oblate case where the spectrum and in particular the NND all have signatures of chaos. For sufficiently large values of the

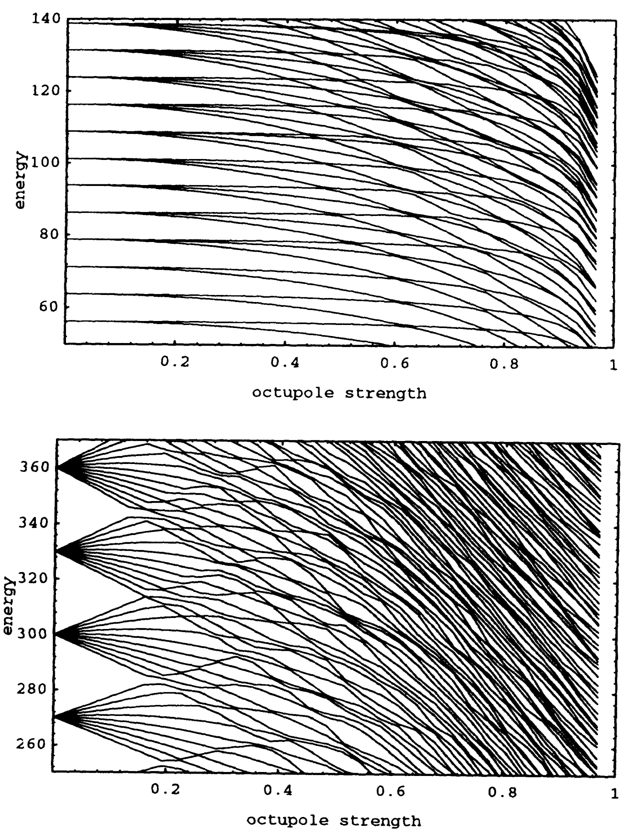

FIG. 3. A section of energy levels as a function of λ/λ_c for $b=2$ (top) and $b=0.5$ (bottom). For greater clarity volume conservation is not taken into account.

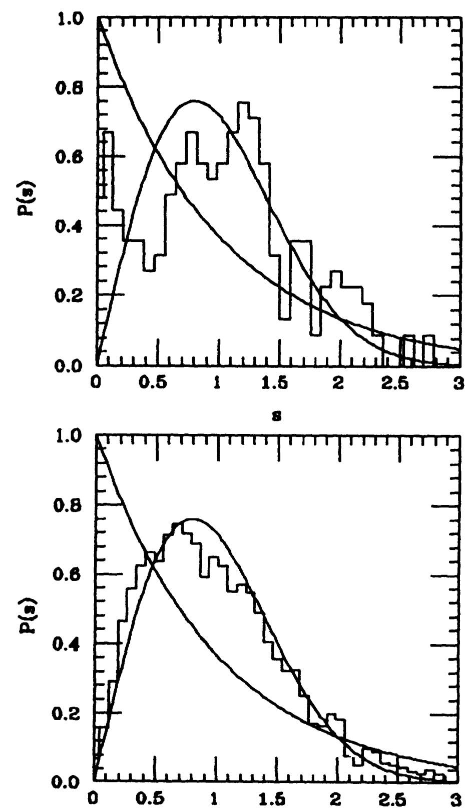

FIG. 4. Nearest neighbor distribution of the spectra shown in Fig. 3 for $\lambda/\lambda_c=0.5$ as a function of the unfolded energy. For the top ($b=2$) 200 levels and for the bottom ($b=0.5$) 600 levels have been used.

octupole strength λ all periodic structure is destroyed and there is no scope for new magic numbers. We mention that the NND best approaches the Wigner surmise for $b \approx 0.58$.

In summary, we have found for a problem typical for nuclear physics and for metallic clusters that chaotic behavior should be expected in principle even for the single particle motion if deformations of higher order than quadrupole are taken into account. Moreover, for the prolate and in particular the superdeformed prolate case, there is a remarkable stability against chaos when octupole deformation is switched on. This result is in agreement with a prediction of an octupole instability of super- and hyperdeformed nuclei [16], based on realistic calculations. We conjecture that this pattern prevails also when axial symmetry is broken, i.e., when terms of the form Y_{3m}, $m \neq 0$ are taken into account. To what extent stability against chaos can be associated with stability in general terms—it is a well known fact that there are more prolate than oblate nuclei—is subject to further investigation. In the spirit of Ref. [5] we should expect prolate nuclei to behave rather elastically in contrast to oblate nuclei where more dissipative behavior is anticipated. We may speculate that the absence of shell structure for the oblate-octupole case could prevent the existence of stable oblate-octupole deformed clusters.

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