Stability of Pear-Shaped Nuclear Deformations*

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The possibility of stable pear-shaped deformations of nuclei is treated by a perturbation theory starting from the nucleon wave functions of a spheroidal harmonic-oscillator potential, without spin-orbit coupling. The mixing of states of opposite parity tends to stabilize the deformation, and is opposed by the cohesiveness of nuclear matter that favors a spherical shape. The former is calculated explicitly for a number of cases and the latter is estimated by imposing a constant-volume condition in a simple manner closely analogous to a more familiar treatment of spheroidal deformations. In this approximation the mixing of the states is not quite enough to overcome the competing effect, so it merely "softens" the nucleus and does not stabilize a pear-shaped deformation. The most direct effect of spin-orbit coupling is to bring states of opposite parity closer together, tending to increase the mixing and make pear-shaped nuclei stable.

THE discovery by Stephens, Asaro, and Perlman[1] of levels which appear to be odd rotational states of even nuclei, in the neighborhood of radium, raises the question whether and to what extent nuclei have pear-shaped deformations superposed on the more familiar spheroidal distortions. The original shell model[2] envisaged nucleons moving in a spherical collective potential, and important advances were made when it was realized that many nuclei could attain lower energies by taking advantage of the additional collective degrees of freedom represented by ellipsoidal distortion.[3]

Even though it is not yet practicable to compute nuclear binding energies with any accuracy from assumed two-nucleon interactions, it is possible to discuss the energy differences involved in spheroidal deformation in an apparently meaningful way in terms of nucleon energies in a three-dimensional harmonic-oscillator potential, a fictitious or zero-order potential intended to represent the average interaction of any one nucleon with all the others. The spheroidal deviation from the spherically symmetric case is accomplished by making the frequency of the oscillation in the z direction different from the other two, $\omega_1=\omega_2\neq\omega_3$. The specific question, whether a spheroidal deformation is stable, can be discussed appropriately and simply by omitting spin-orbit coupling. In this case, one fills shells at the "false magic numbers" 8, 20, 40, 70, 112, etc. The quantitative details, including settling the rather close competition between prolate and oblate shapes, may be expected to depend on inclusion of spin-orbit coupling, as has been nicely done by Nilsson.[4] In either case, the distortion becomes large when several open-shell nucleons occupy states with wave functions oriented so as to favor the same distortion, especially when the number that can be favorably oriented is increased by crossover of the levels between the open shell and the next higher unfilled shell.

It is our purpose here to discuss the stability of pear-shaped deformations in as simple a manner as possible, without taking spin-orbit coupling into account, and in close analogy with the simpler explanation of the ellipsoidal deformations. A pear-shaped deformation of an originally spheroidal nucleus mixes single-nucleon states of opposite parity, and this mixture tends to stabilize the deformation, as has recently been discussed by Strutinsky.[5] The spin-orbit coupling which we neglect has important effects on the energy separation of nucleon states of opposite parity. In making the simplified analysis, we are thus asking whether a pear shape would be stable in some nuclei without this regrouping of the states caused by spin-orbit coupling.

I. PERTURBATION PROCEDURE

We make use of the simplicity of the separability of harmonic-oscillator wave functions in Cartesian coordinates. In these coordinates a simple modification of the ellipsoidal harmonic-oscillator potential is made by adding a term of the form

$$H'=[k_1(x^2+y^2)+k_2z^2]z, \quad (1)$$

the ratio of the two constants being chosen in a simple way to avoid shifting the center of mass. The fictitious potential, intended to represent the average interaction of one nucleon with all the others, is then written

$$V=\tfrac{1}{2}K\{[(x^2+y^2)/b^2](1-gz)+[z^2/a^2](1+\tfrac{2}{3}gz)\}. \quad (2)$$

The parameter g is a measure of the pear-shaped deformation of the potential, and its coefficients are so chosen that the moment (about the x—y plane) of the volume inside an equipotential surface remains zero. That is, if the cylindrical radius (x^2+y^2) is determined as a function of z, to first order in g, by Eq. (2) with a

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[2] M. G. Mayer, Phys. Rev. **75**, 1969 (1949); Haxel, Jensen, and Suess, Naturwissenschaften **36**, 155 (1949).
[3] J. Rainwater, Phys. Rev. **79**, 432 (1950); A. Bohr, Kgl. Danske Videnskab. Selskab, Mat.-fys. Medd. **26**, No. 14 (1952); A. Bohr and B. R. Mottelson, Kgl. Danske Videnskab. Selskab, Mat.-fys. Medd. **27**, No. 16 (1953); **30**, No. 1 (1956).
[4] S. G. Nilsson, Kgl. Danske Videnskab. Selskab, Mat.-fys. Medd. **29**, No. 16 (1955).
[5] V. M. Strutinsky, J. Atomic Energy (U.S.S.R.) 4, 150 (1956).

constant V, then

$$\int(x^2+y^2)zdz=0, \tag{3}$$

the limits of integration being the values of z where $(x^2+y^2)=0$. For the spherical case $a=b$, the g-term then varies with angle as $Y_3(\cos\theta)$.

The fictitious potential gives us our wave functions, and we hope in shell-model calculations that it also gives nucleon energies whose differences are significant in calculating the total energies of the system, even though we cannot go so far as to average over interactions with these as trial functions and prove consistency. With the added complication of a pear-shaped deformation, we employ perturbation theory to obtain the crude shell-model result for the energy that the system of nucleons would have in the fictitious potential (2). With $g=0$ the energy in this approximation is simply the sum of the oscillator energies, and we treat the term in g as the perturbation

$$H_{(1)}'=\tfrac{1}{2}Kg\sum_{\text{nucleons}} z_i\left[\frac{\frac{2}{3}z_i^2}{a^2}-\frac{(x_i^2+y_i^2)}{b^2}\right]. \tag{4}$$

This has the effect of mixing those unperturbed single-nucleon wave functions of opposite parity which obey the selection rules $\Delta n=\pm1$ and either $\Delta l=0, \pm2$ with $\Delta m=0$ or vice versa, or the selection rule $n=\pm3$ with no change in l or m. Here l, m and n are the harmonic-oscillator quantum numbers in the x, y, and z directions.

Having no diagonal elements, this term contributes to the energy only in second order, through the familiar formulas

$$E_{lmn}^{(2)}=\sum_{l'm'n'}\frac{(lmn|H_{(1)}'|l'm'n')^2}{(E_{lmn}-E_{l'm'n'})}, \qquad E^{(2)}=\textstyle\sum_{lmn}E_{lmn}^{(2)}. \tag{5}$$

The first summation extends over all states obeying the selection rules and the second sum over all states insofar as they are populated by nucleons in a given nucleus. A term connecting two filled levels enters twice, pushing the upper state upward and the lower state downward by the same amount, so as to cancel in the final double summation. The net result is that the levels not too far below the highest nucleon energy are depressed by interaction with the unfilled levels and this leads to a net lowering of the energy.

Thus the mixing of states of the spheroidal nucleus induced by the collective pear-shaped deformation provides a tendency toward stabilizing such a deformation. If this were the only effect, such perturbation would be expected to grow in any nucleus. It is, of course, opposed by the cohesiveness of nuclear matter and its tendency to maintain constant density. This competing effect of the deformation raises the average single-nucleon energy in a way that amounts to "squeezing" the closed shells.

In the case of the simpler ellipsoidal deformation, a similar effect occurs. There we may put $\omega_1=\omega_2=\omega(1+\delta)^{\frac{1}{2}}$, $\omega_3=\omega(1+\delta)^{-1}$ so as to keep $\omega_1\omega_2\omega_3=\omega^3$ constant and thus the volume within an equipotential surface constant. The energy of a closed shell is then proportional to $\omega_1+\omega_2+\omega_3=3\omega(1+\frac{3}{8}\delta^2+\cdots)$. Thus in second order in δ the squeezing in two dimensions is not compensated in the energy by the greater relaxation in the third, and this term in δ^2 provides a restoring force to prevent the ellipsoidal deformations from going too far.

With a fixed elliptical deformation, that is, with ω_2/ω_3 or a/b of Eq. (2) fixed, the introduction of the term in g has a similar effect which comes in through readjustment of K. We write $K=(1+f)K'$, with K' constant. For the sake of simplicity we again adopt the constancy of the volume within an equipotential as the criterion for constant over-all density of nuclear matter, and obtain the volume inside an equipotential of constant V by integrating:

$$I\equiv(\text{vol})a^2/\pi b^2=\int(x^2+y^2)dz, \tag{6}$$

with (x^2+y^2) a function of z, from Eq. (2):

$$(x^2+y^2)=(b^2/a^2)[Z_0^2-z^2(1+\tfrac{2}{3}gz)]/(1-gz), \tag{7}$$

where $Z_0^2=2Va^2/K'$, the limits of integration Z_2 and Z_1 being similar to those for Eq. (3), i.e.,

$$Z_{2,1}\approx\pm Z_0(1\mp\tfrac{1}{3}gZ_0). \tag{8}$$

After expanding the denominator of Eq. (7), integrating, and keeping terms in g^2, one obtains an expression for I which remains constant to this order if

$$f=(1/9)g^2Z_0^2/(1+f)\approx(2/9)(Va^2/K')g^2, \tag{9}$$

f here being treated as a small quantity of order g^2. This correction term f is different for each equipotential and is thus a function of position,

$$f=f(x,y,z)=(g^2/9)[(a^2/b^2)(x^2+y^2)+z^2]. \tag{10}$$

The perturbation term in the Hamiltonian, the difference between V and V with $g=0$, is then

$$H'=\tfrac{1}{2}K'\left\{g\left[\frac{\frac{2}{3}z^2}{a^2}-\frac{(x^2+y^2)}{b^2}\right]+g^2\left(\frac{a}{3}\right)^2\left[\frac{(x^2+y^2)}{b^2}+\frac{z^2}{a^2}\right]^2\right\}=H_{(1)}'+H_{(2)}'. \tag{11}$$

Here $H_{(1)}'$ is proportional to g and enters in second order to give an effect proportional to g^2, according to Eqs. (4) and (5) but with K replaced by K'. $H_{(2)}'$ is proportional to g^2 and because it enters in first order makes comparable contributions which, in fact, compete with those of $H_{(1)}'$ in determining the stability of the pear-shaped deformation.

Repeated application of the recursion formula for the normalized Hermite polynomials,

$$2^{\frac{1}{2}}\zeta H_n(\zeta)=(n+1)^{\frac{1}{2}}H_{n+1}(\zeta)+n^{\frac{1}{2}}H_n(\zeta), \tag{12}$$

gives

$$\begin{aligned}
(n|\zeta^2|n)&=\tfrac{1}{2}(2n+1),\\
(n|\zeta^4|n)&=\tfrac{3}{4}[(n+1)^2+n^2],\\
(n|\zeta|n+1)&=2^{-\frac{1}{2}}(n+1)^{\frac{1}{2}},\\
(n|\zeta|n-1)&=2^{-\frac{1}{2}}n^{\frac{1}{2}},\\
(n|\zeta^3|n+1)&=3^{-\frac{3}{2}}[(n+1)/2]^{\frac{3}{2}},\\
(n|\zeta^3|n-1)&=3(n/2)^{\frac{3}{2}},\\
(n|\zeta^3|n+3)&=2^{-\frac{3}{2}}(n+3)^{\frac{1}{2}}(n+2)^{\frac{1}{2}}(n+1)^{\frac{1}{2}},\\
(n|\zeta^3|n-3)&=2^{-\frac{3}{2}}(n-2)^{\frac{1}{2}}(n-1)^{\frac{1}{2}}n^{\frac{1}{2}}.
\end{aligned} \tag{13}$$

Products of these one-dimensional matrix elements provide the three-dimensional matrix elements needed, such as

$$(lmn|\xi^2\eta^2|lmn)=\tfrac{1}{4}(2l+1)(2m+1), \tag{14}$$

for the evaluation of $H_{(2)}'$ and

$$(lmn|\xi^2\zeta|l-2,m,n-1)=2^{-\frac{3}{2}}(l-1)^{\frac{1}{2}}l^{\frac{1}{2}}n^{\frac{1}{2}} \tag{15}$$

used in evaluating $H_{(1)}'$.

Combining three terms of the form ζ^4 and three like Eq. (14), we have

$$\begin{aligned}
(lmn|H_{(2)}'|lmn)
&=\frac{\alpha^4\omega_3 g^2}{36\beta^2}\{\rho^2[3(l^2+m^2)+4lm+5(l+m)+4]\\
&\quad+2\rho(l+m+1)(2n+1)+3(n^2+n)+\tfrac{3}{2}\}.
\end{aligned} \tag{16}$$

Similarly, combining twelve terms of the sum in Eq. (5) from terms of the form $\xi^2\zeta$ and four from terms involving ζ^3, one obtains

$$\begin{aligned}
E^{(2)}=\frac{\alpha^4\omega_3 g^2}{36\times 8\beta^2}\sum_{lmn}\Bigg\{&-\rho^2\left[\frac{9\lambda}{2\rho+1}-\frac{9\nu}{2\rho-1}+36(l+m+1)^2\right]\\
&+72\rho(l+m+1)(2n+1)-120(n^2+n)-44\Bigg\}.
\end{aligned} \tag{17}$$

Here

$$\begin{aligned}
&\rho=\omega_2/\omega_3,\quad \alpha=\rho^{1/6},\quad \beta=(KM/\hbar^2)^{1/4},\\
&\lambda=(l^2+m^2)+(l+m)(4n+3)+4(n+1),\\
&\nu=(l^2+m^2)-[(l+m)(4n+1)+4n].
\end{aligned}$$

Thus

$$\begin{aligned}
\Delta E=(\alpha^4\omega_3 g^2/36\beta^2)\{&11\rho(l+m+1)(2n+1)\\
&-\rho^2[1.5(l^2+m^2)+5lm+4(l+m)+\tfrac{1}{2}\\
&+(9/8)\lambda/(2\rho+1)-(9/8)\nu/(2\rho-1)]\\
&-12(n^2+n)-40\}.
\end{aligned} \tag{18}$$

II. SPHEROIDAL DEFORMATION

As in a previous paper,[6] we put

$$E=\sum_{\text{nucleons}}E_{lmn}=\hbar[2\omega_2\sum_m(m+\tfrac{1}{2})+\omega_3\sum_n(n+\tfrac{1}{2})], \tag{19}$$

and, on keeping volume constant by the condition $\omega_2{}^2\omega_3=$ constant, find the energy minimized when

$$\rho=\omega_2/\omega_3=\sum(n+\tfrac{1}{2})/\sum(m+\tfrac{1}{2}). \tag{20}$$

The individual-nucleon levels E_{lmn} are plotted as functions of ρ for prolate deformations in Fig. 1. The numbers along the left edge represent $N=l+m+n$. The numbers along the right edge are values of n. On the lowest line, having $N=n=1$, for example, there is a circle marked 8. This represents the equilibrium deformation of a nucleus having $A=8$, obtained by putting four nucleons (two neutrons and two protons) in the s-shell, $N=0$, and four in this level $N=n=1$. Equilibrium deformations are similarly indicated for heavier nuclei having the values as A shown, always with equal numbers of neutrons and protons. These deformations indicated by circles assume the normal order of populating the states, as for small deformations, not taking advantage of any crossing-over of the levels. The usual tendency is apparent for the deformations to be largest in the vicinity of half-filled shells. It will

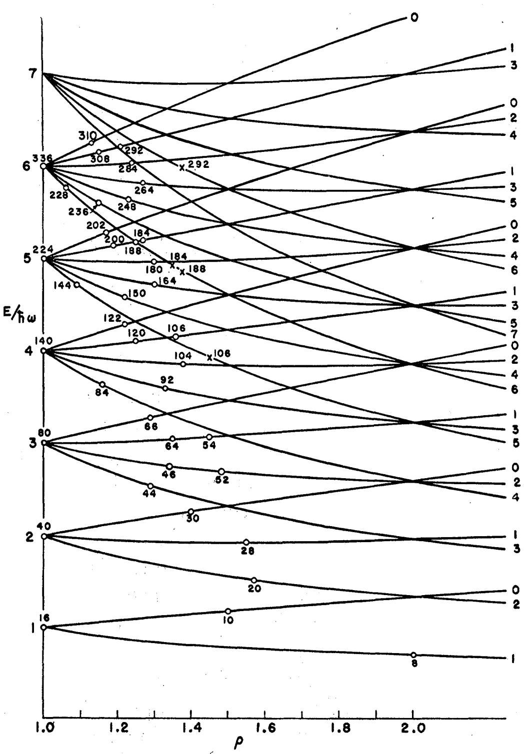

FIG. 1. Levels and deformations in spheroidal nucleus. The numbers along the left edge represent $N=l+m+n$. The numbers along the right edge are values of n. The numbers adjacent to the open circles represent A.

[6] D. R. Inglis, Phys. Rev. 103, 1786 (1956).

TABLE I. Contributions to the energy induced by a pear-shaped deformation.

A	Last level in orig. shell l, m, n	No. of nucleons in it	Crossover level l, m, n	No. of nucleons in it	$\Sigma(lmn\|H_{(2)}'\|lmn)$ (in units of $\hbar\omega g^2\beta^{-2}$)	$E^{(2)}$ (in units of $\hbar\omega g^2\beta^{-2}$)	ΔE (in units of $\hbar\omega g^2\beta^{-2}$)
180	3 0 2	4			465.0	−388.9	+76.1
184	2 2 1	4			466.7	−390.3	+76.4
			0 0 6	4	522.8	−468.3	+54.5
188	3 1 1	4			473.6	−394.6	+79.4
			0 1 5 0 0 6	4 4	573.9	−518.6	+55.3
192	3 1 1	4			479.4	−396.7	+82.7
			0 0 6 0 1 5 1 0 5	4 4 4	615.3	−570.0	+45.3
264	0 3 3	4			844.4	−769.4	+75.0
268	2 2 2	4			857.5	−775.0	+82.5
			0 0 7	4	924.2	−885.3	+38.9
272	1 3 2	4			867.5	−773.9	+93.6
			0 0 7 2 2 2	4 4	935.6	−885.6	+50.0
284	2 2 2	4			922.8	−791.7	+131.1
292	2 3 1	4			932.5	−798.3	+134.2
			0 0 7 0 1 6	4 4	1115.0	−1042.8	+72.2

be noted, however, that under the population condition here imposed, the larger shells are less easily deformed because of the greater number of filled shells involved.

The large deformations of certain heavy nuclei are, of course, known[4,7] to be the result of repopulation of the states to best energetic advantage made possible by the crossover of the levels from different originally degenerate groups. Transferring a nucleon from a level sloping upward (toward the right) in Fig. 1, to a level sloping downward, provides a force tending to distort the nucleus further. Deformations obtained, for some sample values of atomic number A, after repopulation, are indicated by crosses (×) in Fig. 1. All levels below the level on which the (×) is drawn are considered filled, and enough nucleons are in the level indicated to make up A (proton and neutron numbers being again equal). It is seen that one does indeed obtain considerably larger deformations in this way, and these examples provide cases in which to examine the stability of a further pear-shaped deformation.

III. PERTURBATION PROCEDURE APPLIED TO SPECIFIC CASES

Application of the perturbation procedure described above to various examples of nuclei in their equilibrium spheroidal deformations shows that they are stable against a further pear-shaped deformation. The positive contribution to the energy from $H_{(2)}'$ is in each case greater in magnitude than the negative contribution from $H_{(1)}'$, as shown in Table I.

IV. INTERPRETATIONS OF ODD ROTATIONAL STATES OF EVEN NUCLEI

Odd rotational states could occur at low energy in even nuclei either because a pear-shaped deformation is stable or because the nucleus is "soft" to pear-shaped deformation about a stable spheroidal shape, making possible a low-energy surface vibration of this symmetry.

If the pear shape is stable, the situation is similar to one in the molecular spectroscopy of methane, for example. An inversion of the ends of the pear is possible by passage through a potential barrier represented by the higher energy of the spheroidal shape. This is illustrated by the potential curve on the left side of Fig. 2. We assume, as usual, that the wave function is factorable:

$$\psi(\theta,\rho,g,x_i)=\psi_{\mathrm{rot}}(\theta)\psi_{\mathrm{shape}}(\rho,g)\psi_{\mathrm{int}}(x_i),$$

the rotation function ψ_{rot} depending on the angles θ giving the direction of the positive z-axis, and the shape factor depending on the spheroidal parameter ρ and the pear-shape parameter g. The sign of g determines which end of the pear is toward the positive z-axis. The wave function is invariant to simultaneous rotation through π and reflection in the x—y plane. Thus even rotational states go with shape functions even in g, odd with odd.

The existence of even and odd functions $\psi_{\mathrm{shape}}=\psi_\rho(g)$ is very similar to the familiar situation in the hydrogen

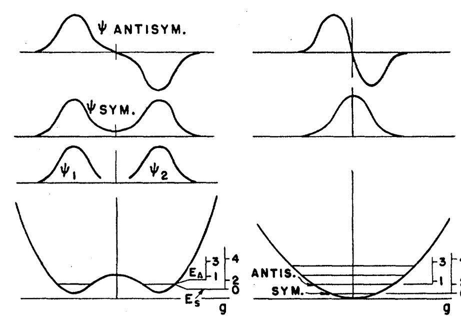

FIG. 2. Rotational levels with stable or unstable asymmetry.

[7] S. Gallone and C. Salvetti, Nuovo cimento 10, 145 (1953).

molecule ion wherein the electron may, in a Heitler-London perturbation treatment, have an initial wave function concentrated on either ion, the two combining into odd and even functions. With fixed-axis, a nucleus so stably pear-shaped as to have a high potential barrier at the symmetric shape may have a solution $\psi_p(g)$ with the fat end of the pear either along the positive or the negative z-axis, as suggested in Fig. 2. With an easily penetrable barrier, these combine to make the two functions similar to "molecular orbitals," one even and one odd in g. As usual, the odd function has the higher energy, the energy difference being proportional to the frequency of oscillation between the two positions by penetration of the barrier.

In this picture, one expects a ladder of even rotational states, $J=0, 2, 4\cdots$, and another ladder of odd states $J=1, 3, \cdots$ not in their normal positions between even states, but displaced upward by an amount that becomes small only if the pear shape is made quite stable by a rather high potential barrier. Presumably, then, the pear shape becomes most stable in the neighborhood of radium, where the displacement is observed to be least.

The alternative interpretation is based on the nucleus being merely "soft" to pear-shaped deformation, as represented on the right side of Fig. 2. The potential function is of course symmetric in g, and initially parabolic for small g. The strength of the restoring force helps determine the frequency of oscillation, and the displacement between successive vibrational levels, which are of course alternately even and odd in g. The frequency also depends on the inertial behavior of the nucleons in readjusting to the change of shape[8] which makes quantitative comparison with experiment difficult. On the zero-vibrational level is built a band $J=0, 2, 4, \cdots$ and on the first vibrational level the odd band $J=1, 3, \cdots$, just as in the previous discussion, but now there is also an even band built on the second vibrational level, etc., providing the possibility of experimentally distinguishing between the two interpretations. The present experimental situation does not appear to be decisive. The mechanism by which the moment of inertia appears different for the odd and even bands is not clear in either picture.

[8] D. L. Hill and J. A. Wheeler, Phys. Rev. **89**, 1102 (1953); D. R. Inglis, Phys. Rev. **97**, 701 (1955); A. Bohr and B. R. Mottelson, Kgl. Danske Videnskab. Selskab, Mat.-fys. Medd. **30**, No. 1 (1956); S. Moskowski, Phys. Rev. **103**, 1328 (1956).

V. CONCLUSION

The result of our second-order perturbation treatment is thus to be interpreted as providing merely a softening of the nucleus to pear-shaped deformation, which, however, might still account for the existence of the fairly low odd bands observed.

Because this calculation avoids the complexity of spin-orbit coupling, it provides what may be considered a lower limit to the amount the total energy is depressed in second order by the mixing of the states. Spin-orbit coupling brings single nucleon states of opposite parity closer together (thus establishing the "magic numbers"). This decreases some of the relevant energy denominators and increases the amount of depression of the total energy. We have shown that the depression calculated without spin-orbit coupling is not quite equal to the competing positive contribution to the energy, but in some cases almost. It is thus entirely possible that a more complete calculation would show that certain nuclei have a stable pear-shaped deformation, and that the odd rotational states of even nuclei are to be interpreted accordingly. This also leaves it not implausible that fission should proceed by asymmetric passage of the "saddle."