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COLLECTIVE EXCITATIONS OF EVEN-EVEN NUCLEI

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Collective excitations of axially symmetric even-even nuclei are investigated. It is shown that such excitations can be divided into two classes: those which are accompanied by appreciable changes in the nuclear quadrupole moment, and those which are not. The energy of the collective oscillations is expressed in terms of two parameters.

IN a paper of Scharff-Goldhaber and Weneser[1] it was pointed out that there is a large class of even-even nuclei in the mass number region $66 < A < 150$ for which the first excited state has spin 2^+ and excitation energy of 300 kev or more, while the second excited state has spin 2^+, 4^+, 0^+. The ratio of the energy of the second excited state to that of the first had a value between 2 and 2.5. This showed that these are not purely rotational states. Apparently in such nuclei an excited state cannot be rigorously assigned to pure rotation or vibration.

In the present paper, we investigate the collective excitations of axially-symmetric even-even nuclei, using the generalized nuclear model developed by A. Bohr.[2] We shall show that the collective excited states of such nuclei can be classified into two types: excitations which do not involve an appreciable change in the nuclear quadrupole moment, and excitations in which the quadrupole moment changes considerably. Excitations of the second type may occur in nuclei which do not deviate strongly from spherical shape. In nuclei which deviate markedly from spherical shape, excitations of the second type play no part in transitions involving small changes in the energy.

1. FUNDAMENTAL EQUATIONS FOR DETERMINING COLLECTIVE NUCLEAR EXCITATIONS

In the generalized nuclear model developed by A. Bohr,[2] it is assumed that the states of nucleons outside of closed shells can be described by using the one-particle approximation, while the nucleons in filled shells (i.e., in the core) manifest themselves only through their collective properties. For collective coordinates we use the three Euler angles, characterizing the spatial orientation of the nucleus, and the parameters β and γ which determine the deviation of the nucleus from spherical shape.

In the adiabatic (strong coupling) approximation, we may treat the motion of the outer nucleons in the field of a core of fixed shape. By averaging the interaction energy of core and outer nucleons and the rotational energy of the core over a state of motion with total angular momentum J, and over all states of the outer nucleons which have quantum numbers $n_i \ell_i j_i m_i$ such that the projection on the nuclear symmetry axis of $J_3 = \sum_i m_i = 0$, we can find the nuclear energy as a function of the collective coordinates β, γ:

$$E = \frac{B}{2}(\dot{\beta}^2 + \beta^2\dot{\gamma}^2) + \frac{C}{2}\beta^2 + \frac{\hbar^2}{4}\left(\frac{1}{I_1} + \frac{1}{I_2}\right)[J(J+1) + D] + A\beta\cos\gamma, \tag{1.1}$$

where the first term represents the kinetic energy of the surface oscillations, the second is the potential energy exclusive of interaction with the outer nucleons, the third is the rotational energy of the nucleus, and the fourth is the interaction of the outer nucleons with the core. The quantities A and D depend on the number of outer nucleons and their states of motion; the explicit form of the dependence can be found in a paper of Ford[3] (formula 18). The moments of inertia I_1 and I_2 with respect to axes perpendicular to the nuclear symmetry axis, are given, in the hydrodynamic approximation which is used in the model to describe the collective motion, by:

$$I_\lambda = 4B\beta^2 \sin^2(\gamma - \lambda 2\pi/3), \quad \lambda = 1.2. \tag{1.2}$$

If we use the explicit form (1.2) for the dependence of the moments of inertia on β and γ, we find that the total potential energy of surface oscillation (which does not depend on J)

$$V(\beta\gamma) = \frac{C}{2}\beta^2 + A\beta\cos\gamma + \frac{\hbar^2 D}{4}\left(\frac{1}{I_1} + \frac{1}{I_2}\right) \tag{1.3}$$

has its minimum, for fixed β, at $\gamma = 0$ or $\gamma = \pi$, corresponding to nuclei with axial symmetry; the position of this minimum does not depend on the values of the parameters in (1.3). The function $V(\beta\gamma)$ becomes infinite for $\gamma = \pm\pi/3$, $\pm 2\pi/3$. It should be noted that (1.1) was obtained on the assumption that the nucleus has axial symmetry, so that the values $\gamma = 0$, π are the "self-consistent" values.

We shall assume that the surface oscillations do not destroy the axial symmetry of the nucleus,* which is observed for the ground states of all nonspherical nuclei, and shall consider the two values $\gamma = 0$ and $\gamma = \pi$ separately.

For $\gamma = 0$, the potential energy (1.3) is given by

$$V_0(\beta) = C\beta^2/2 + A\beta + \hbar^2 D/6B\beta^2, \tag{1.4}$$

while the energy (1.1) is rewritten as

$$E = B\dot{\beta}^2/2 + V_0(\beta) + M^2/6B\beta^2. \tag{1.5}$$

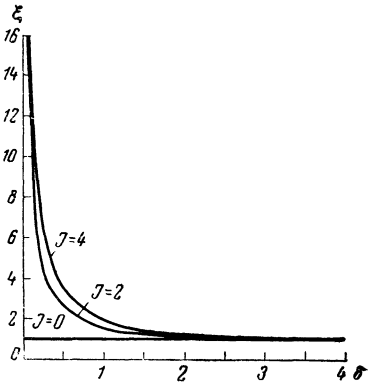

FIG. 1

The potential energy (1.4) has a pole at $\beta = 0$. The presence of this pole corresponds to the fact that the moment of inertia of the nucleus tends to zero for $\beta \to 0$. If there are nucleons outside of closed shells, then even if the total angular momentum of the nucleus is zero, the angular momentum of the core and the angular momentum of the extra-core nucleons are not integrals of the motion and are not separately equal to zero. Expanding $V_0(\beta)$ in powers of the deviation from the value β_0 corresponding to the minimum of (1.4), which is given by

$$\beta_0 = -A/C + \hbar^2 D/3CB\beta_0^2,$$

and keeping only quadratic terms, we rewrite (1.5) as

$$\varepsilon \equiv E - V_0(\beta_0) = \frac{B}{2}\dot{\beta}^2 + \frac{M^2}{6B\beta^2} + \frac{C_0}{2}(\beta - \beta_0)^2,$$

where

$$C_0 = C + \hbar^2 D/B\beta_\theta^4.$$

To make the transition to a quantum equation, we note that the square of the angular momentum in the coordinate system, β, θ, φ, for mass coefficient B, is

$$M^2 = B^2\beta^4(\dot{\theta}^2 + \dot{\varphi}^2\sin^2\theta).$$

If T is the kinetic energy of collective motion, then

$$2T dt^2 = B d\beta^2 + \frac{B}{3}\beta^2 d\theta^2 + \frac{B}{3}\beta^2\sin^2\theta\cdot d\varphi^2,$$

so that the operator for the kinetic energy of the collective motion is

$$\hat{T} = -\frac{\hbar^2}{2B\beta^2}\left\{\frac{\partial}{\partial\beta}\left(\beta^2\frac{\partial}{\partial\beta}\right) + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right\},$$

and the Schrödinger equation which determines the energy of the collective motion is

$$[\hat{T} + {}^1\!/_2\, C_0(\beta - \beta_0)^2 - \varepsilon]\,\Psi(\beta\theta\varphi) = 0. \tag{1.6}$$

We shall look for a solution of (1.6) of the form

$$\Psi(\beta\theta\varphi) = \sum_J \frac{U_J(\beta)}{\beta} Y_{JM}(\theta\varphi)$$

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*The question of possible deviations from axial symmetry requires investigation of the conditions for breakdown of the "self-consistent" values of γ, and cannot be solved on the basis of (1.1), which was obtained on the assumption that the nucleus has this symmetry.

where J takes on only even values, since the function should not depend on the choice of the direction of the symmetry axis. The functions $U_J(\beta)$ satisfy the equation

$$-\frac{\hbar^2}{2B}\frac{d^2U_J(\beta)}{d\beta^2}+V_J(\beta)U_J-\varepsilon U_J=0, \qquad U^J(0)=0, \tag{1.7}$$

where

$$V_J(\beta)=\frac{C_0}{2}(\beta-\beta_0)^2+\frac{\hbar^2}{6B\beta^2}J(J+1)\approx V_J(\beta_J)+\frac{C_J}{2}(\beta-\beta_J)^2; \tag{1.8}$$

$$\beta_J=\beta_0+\frac{\hbar^2J(J+1)}{3BC_0\beta_J^3}, \quad C_J=C_0\left(1+\frac{\hbar^2J(J+1)}{B\beta_J^4}\right). \tag{1.9}$$

Introducing the dimensionless parameter $\delta=\beta_0(BC/\hbar^2)^{1/4}$ and $\xi=\beta_J/\beta_0\geq 1$, Eq. (1.9) becomes

$$\xi^3(\xi-1)=J(J+1)/3\delta^4. \tag{1.10}$$

The solutions of (1.10) for J = 0, 2, 4 are shown in Fig. 1.

In terms of the variables ξ, δ, and $\omega_0=\sqrt{C_0/B}$, the energy $V_J(\beta_J)$ has the form

$$V_J(\beta_J)/\hbar\omega_0=\delta^2(\xi-1)^2+J(J+1)/6\delta^2\xi^2, \tag{1.11}$$

and

$$C_J=C_0(1+J(J+1)/\delta^4\xi^4).$$

Substituting (1.8) in (1.7), we have

$$-(\hbar^2/2B)\,d^2U_J/d\beta^2+{}^1\!/_2C_J(\beta-\beta_J)^2U_J-[\varepsilon-V_J(\beta_J)]\,U_J=0. \tag{1.12}$$

Equation (1.12) coincides with the equation for a one-dimensional harmonic oscillator. However, because of the conditions $\beta\geq 0$ and $U_J(0)=0$, the solutions of (1.12) are not Hermite polynomials.

To determine the eigenfunctions and eigenvalues of (1.12), we introduce the new variable $\zeta=\xi\delta\times(\beta-\beta_J)/\beta_J$ which varies between the limits $-\xi\delta\leq\zeta<\infty$ and the new function $v(\zeta)$ defined by

$$U(\beta)=v(\zeta)\exp\{-\zeta^2/2\}.$$

The function $v(\zeta)$ will satisfy the differential equation

$$v''(\zeta)-2\zeta v'(\zeta)+2\nu v(\zeta)=0 \tag{1.13}$$

and the boundary conditions

$$v(-\xi\delta)=0 \text{ and } e^{-\zeta^2/2}v(\zeta)\to 0, \quad \text{for} \quad \zeta\to\infty. \tag{1.14}$$

The eigenvalue of (1.13) is related to the energy ϵ by:

$$\nu=\frac{\varepsilon-V_J(\beta_J)}{\hbar\omega_J}-\frac{1}{2}, \quad \omega_J=\sqrt{\frac{C_J}{B}}=\omega_0\sqrt{1+\frac{J(J+1)}{\delta^4\xi^4}}.$$

The general solution of (1.13) for non-integral ν is given in terms of Hermite functions[4] of the first kind:

$$v_\nu(\zeta)=aH_\nu(\zeta)+bH_\nu(\zeta),$$

which can be represented by the series

$$H_\nu(\zeta)\equiv\frac{1}{2\Gamma(-\nu)}\sum_{k=0}^{\infty}\frac{(-1)^k}{k!}\Gamma\left(\frac{k-\nu}{2}\right)(2\zeta)^k.$$

By examining the asymptotic behavior of the Hermite functions for large ζ, we can verify that we must set b = 0 in order to satisfy the boundary condition (1.14) at $\zeta\to\infty$. Then the eigenvalues ν, and consequently the energy

$$\varepsilon-V_J(\beta_J)=\hbar\omega_J(\nu+{}^1\!/_2), \tag{1.15}$$

are determined by the condition

$$v(-\xi\delta)=aH_\nu(-\xi\delta)=0.$$

For $\gamma = \pi$, the potential energy (1.4) becomes

$$V_\pi(\beta) = C\beta^2/2 - A\beta + \hbar^2 D/6B\beta^2,$$

where $0 \leq \beta < \infty$. It is easy to check that the replacement of β by $-\beta$ enables us to keep all the results for the previous case of $\gamma = 0$ [including Eq. (1.13)], if we merely note that now the domain of variation of β is $-\infty < \beta \leq 0$, and consequently ζ varies between the limits $-\infty < \zeta \leq -\xi\delta$. Then β_0, δ, and ξ will have the same meaning and values as for the case of $\gamma = 0$. The function $v(\zeta)$ must satisfy the differential equation (1.13) with the boundary conditions

$$v(\zeta)e^{-\zeta^2/2} \to 0 \text{ for } \zeta \to -\infty; \; v(-\xi\delta) = 0. \qquad (1.16)$$

The requirement that the boundary conditions (1.16) be satisfied gives us

$$v_\nu(\zeta) = bH_\nu(-\zeta)$$

and a transcendental equation

$$H_\nu(\delta\xi) = 0.$$

which determines the eigenvalue.

2. THE TWO CLASSES OF COLLECTIVE EXCITATIONS OF AXIALLY-SYMMETRIC NUCLEI

According to (1.15) the rotation-vibration energy of the nucleus can be written as

$$\varepsilon_J/\hbar\omega_0 = (\nu + 1/2)\sqrt{1 + J(J+1)/\delta^4\xi^4} + 1/2\,\delta^2(\xi - 1)^2 + J(J+1)/6\delta^2\xi^2, \qquad (2.1)$$

where ν is determined from the transcendental equation $H_\nu(-\xi\delta) = 0$ if $\gamma = 0$ and from the equation $H_\nu(\xi\delta) = 0$ if $\gamma = \pi$. Since ξ is uniquely determined by the values of J and the parameter δ, $\epsilon_J/\hbar\omega_0$ will be a function only of J and δ, so that the latter should be regarded as the parameter of the theory.

Figure 2 shows the dependence of (2.1) on δ as computed by Filippov[5] for nuclei having a positive quadrupole moment in the ground state. In this case, the ground state is an s-state with $\gamma = 0$. The excited states for each spin value J = 0, 2, 4 are shown for the case of $\gamma = 0$ by the solid lines, and for the case of $\gamma = \pi$ by the dashed lines. As we have already pointed out in a separate communication,[6] for $\delta > 0$, the case of $\gamma = 0$ corresponds to positive quadrupole moments, while for the case of $\gamma = \pi$, the quadrupole moments are small and negative. With increasing δ, the energy of excited states with positive quadrupole moment decreases, while the energy of excited states with negative quadrupole moment increases.

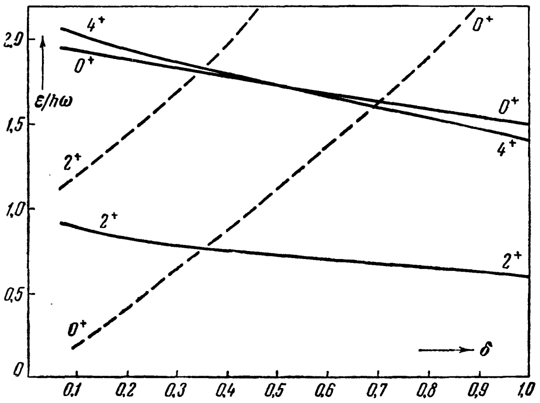

FIG. 2

A transition of the nucleus from the ground state (which has a positive quadrupole moment) to excited states corresponding to $\gamma = \pi$ (the dotted lines), is accompanied by a change in the sign as well as the absolute value of the quadrupole moment. A transition of the nucleus from the ground state to a state with $\gamma = 0$ (the solid lines) does not involve a change in the sign of the quadrupole moment. Thus the collective excitations of axially-symmetric nuclei can be of two types: (1) excitations without any essential change in the quadrupole moment; (2) excitations with a considerable change in the quadrupole moment. As we see from Fig. 2, excitations of the second type can occur in nuclei with low values of δ. We should, of course, remember that for low values of δ the adiabatic approximation is not fulfilled, and that the curves have only a qualitative meaning in this region.

Because of the small quadrupole moments in the excited states of the second type (cf. Fig. 2, dotted lines), gamma transitions between them should have very low probability.

In Table I we give experimental values (the references are given in the last column of the table) for

TABLE I

Nucleus	Level energy		Spin		δ	Literature
	exptl.	theoret	exptl.	theoret		
Sn^{116}	—	0.40	—	[0]	0.16	[7]
	1.00	1.00	2	2		
	1.65	1,65	2	[2]		
	1.86	2.28	4	4; 0		
Ba^{134}	—	0,50	—	[0]	0.2	[8]
	1.00	1.00	2	2		
	1,72	1,72	2	[2]		
	1.95	2,26	4	4; 0		
Pt^{192}	—	0.65	—	[0]	0.25	[9]
	1.00	1.00	2	2		
	1.93	1,93	2	[2]		
	2.48	2.32	4	4; 0		
Ge^{72}	0,82	0.82	0	[0]	0,29	[10]
	1,00	1.00	2	2		
	1.74	2.15	2	[2]		
Se^{76}	—	0.86	—	[0]	0.3	[11]
	1.00	1.00	2	2		
	2,18	2,2	2	[2]		
	—	2.30	—	0		
	2	2,33	—	4		
Xe^{128}	—	0,86	2	[0]	0,3	[12]
	1,00	1,00	2	2		
	2.18	2,18	2	[2]		
	—	2.30	—	0		
	—	2.33	—	4		
Cd^{114}	—	0,86	—	[0]	0.3	[13]
	1,00	1.00	2	2		
	2.17	2.18	2	[2]		
	2,30	2,30	4	0		
	2.34	2,34	0	4		
Pd^{106}	1.00	1,00	2	2	0,66	[14]
	2,2	2.35	0	[0]; 0; 4		
	3.02	4	2	[2]		

the ratio of the energy of the first few excited states to the energy of the first excited state (which has spin 2), and the spin values. We also give the corresponding values obtained from Fig. 2 with a suitably chosen value of δ (which is given in the next-to-last column). All the states given in Table I have positive parity. For levels which according to the theory are of the second type, the spin value is put in square brackets.

3. ROTATIONAL ENERGY OF NUCLEI

For large deviations from spherical symmetry, the excited states of the second type have considerable excitation energy. Thus the first few levels will all correspond to excitations of the first type and will go over into a pure rotational spectrum with increasing δ.

For $\delta > 1$, the function $\xi = F[J(J+1)/3\delta^4]$ in (1.10) is very close to unity. Expanding this function in series and stopping with the linear terms, we can rewrite (2.1) in the form

$$\varepsilon_J / \hbar\omega_0 \approx \varepsilon_0 / \hbar\omega_0 + J(J+1)/6\delta^2 - aJ^2(J+1)^2/\delta^6. \tag{3.1}$$

Using the fact that $\delta = \beta_0 (BC/\hbar^2)^{1/4}$, and introducing the moment of inertia $I = 3B\beta_0^2$ we can rewrite (3.1) as

$$\varepsilon_J = \varepsilon_0 + AJ(J+1) - BJ^2(J+1)^2, \tag{3.2}$$

where

$$A = \hbar^2/2I, \quad B = a(\hbar\omega_0)^{-2}(\hbar/I)^3.$$

It is known that formula (3.2) gives good agreement with experiment if A and B are regarded as adjustable parameters. Table II gives the values of A and B obtained from the energy spectra of a few nuclei.

Using (1.16) and $I = 3B\beta_0^2$, we can express the parameter δ in terms of the moment of inertia and $\hbar\omega_0$:

$$\delta^2 = \hbar\omega_0 I / 3\hbar^2 = \hbar\omega_0 / 6A. \tag{3.3}$$

In the third column of Table II we give the values of δ obtained from (3.3) by setting $\hbar\omega_0 \sim 1$ Mev and using the experimentally determined value of A. These are typical values of δ for nuclei having a well defined rotational spectrum.

TABLE II

Nucleus	A (kev)	B (kev)	δ
Hf^{180}	15.58	0.0703	3.3
Th^{226}	12.16	0.043	3.7
Pu^{238}	7.37	0.0033	4.7

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ON THE THEORY OF THE INTERACTION OF "EXCESS" CHARGES IN IONIC CRYSTALS

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Interaction between polarons is considered. It is shown that the formation of "bipolarons," two polarons separated by a finite distance R and bound by a common polarization, is energetically feasible in crystals with parameters satisfying the condition $n^2/\epsilon \leq 0.05$.

THE interaction of an "excess" electron, introduced into an ionic dielectric, with the crystal polarization oscillations leads, as is known, to the appearance of polaron states.[1] Polarons are majority carriers in ionic crystals; they determine the electrical, photoelectrical, and optical properties of these crystals. Interaction between polarons reduces to electrostatic repulsion and attraction caused by the influence of the inertial polarizational potential well of each electron on the remaining ones (such an attraction will be called hereinafter polarizational in the interests of brevity). Interaction between polarons was not taken into account in polaron theory[1] since it was assumed that the polaron concentration was small enough. The interaction of two electrons in a common polarizational potential well was considered in Refs. 2 and 3. It has been found that such compounds (called bipolarons) do not exist independently of the crystal parameter values. Physically, this means that the Coulomb repulsion force is dominant in this case. However, the electrostatic repulsion and polarizational attraction forces depend differently on the distance between the centers of gravity of the polarizational potential wells and, in general, it cannot be stated beforehand that a stable state of a complex of polarons is impossible when this distance is not zero.

The simplest of such complexes, two interacting polarons, is considered below. The purpose of this work is to explain the possibility of the existence of such a formation. We shall henceforth call it a bipolaron, thus ascribing to this concept a more general meaning than in Refs. 2 and 3. Moreover, our analysis permits an estimate of the influence of polaron interaction on the energy of each polaron and serves therefore as a criterion of whether it is permissible to neglect this interaction for the purpose of formulating a multielectron theory.

The interaction of an "excess" electron with vacancies has also been analyzed; the interaction potential obtained can be used to analyze scattering of carriers by impurities in ionic crystals.

Using the methods developed by Pekar,[1] the Hamiltonian of a system consisting of a crystal with two