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Nuclear Moments of Inertia

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The problem of nuclear moments of inertia is considered taking into account the effect of the internal motion phenomenologically. The kinetic energy of the internal motion is assumed to take the form of that of a symmetrical top. When the interactions between the irrotational and the internal motions are strong the total system has again a rotational energy spectrum whose moment of inertia is given by the sum of those of two motions. By means of the empirical data for the electric quadrupole excitations their magnitudes are estimated. In consequence the internal motion is shown to be very important. Comparison with other methods is carefully examined, especially with the work by Hayakawa and Marumori.

§ 1. Introduction

It is well known that many nuclei exhibit bands of energy levels with the spectra

$$E_I=h^2I(I+1)/2\mathcal{J} \qquad (1\cdot1)$$

where I is the spin of a level. Since these spectra resemble those of the symmetrical top, $\mathcal{J}$ is called the nuclear moment of inertia. Present paper offers some theoretical comments on the magnitude of $\mathcal{J}$.

Nowadays these energy levels are believed to be obtained by excitation of certain collective motions of nuclear particles. At first Bohr and Mottelson discussed the collective motion in the 'core' of the nucleus in terms of an irrotational motion of incompressible fluid set in motion by the action of outer particles in the unfilled shell[1]. In the strong coupling limit, the shape of the core is an ellipsoid and the low excitations are the rotational type of (1·1). Then the moment of inertia is given by

$$\mathcal{J}_{\text{ir}}=\mathcal{J}_{\text{rigid}}\,\epsilon^2 \qquad (1\cdot2)$$

where ϵ is the ratio of the difference between major and minor semi-axis of the ellipsoid to the mean radius. The deformation ϵ can be inferred directly from the quadrupole data, and it was found that $\mathcal{J}_{\text{ir}}$ is appreciably smaller than that determined from the level spacing, (1·1). Many authors have made various attempts to elucidate the above situation. Roughly speaking, those attempts may be classified into two groups. One of them has investigated the foundation of Bohr-Mottelson's

phenomenological model developing the theory of quantum-mechanical collective motion of particles and examined the origin of the above-mentioned discrepancy. The others have made a more phenomenological approach. They have remarked the fact that even on the basis of the independent particle model of the nucleus the ground state would generally be deformed by the polarizing action of the outer particles which are in the unfilled shell. Therefore the nucleus could be approximated by the independent particle system in a rotating deformed potential. Thus they have obtained a new formula of the moment of inertia.

In the former method, the collective motions of nuclear particles are assumed to be incompressible since the inter-particle force resists strongly to the compression of the system.[2] Further we assume those to be irrotational, then the displacement potential can be used which gives the particle displacement in those motions. In order to describe those motions quantum-mechanically, we take the displacement potential as the collective coordinate, and by properly defining the momentum canonically conjugate to it, we have to express the hamiltonian of the system in terms of them and the internal variables which are independent of them. When more than two modes of collective motions have to be taken into account as the surface vibration and rotation of the nucleus, canonically conjugate momenta to the displacement potentials do not exist. However, if we employ the approximately conjugate momenta, the hamiltonian can be transformed into the form expressed by the collective and internal variables, which contains the correction terms due to the approximation.[3] In such cases, we extend the degree of freedom of the system introducing new redundant coordinates and momenta canonically conjugate to each other. Instead the state vectors are imposed some subsidiary conditions relating to the new variables. Then we transform the hamiltonian so as to replace the collective variables by the new redundant ones as far as possible. If the collective coordinates and momenta were exactly canonically conjugate to each other, the replacement would be performed completely and the transformed hamiltonian would not involve the collective variables whose role would be played by the new redundant variables; so we could solve the transformed hamiltonian having nothing to do with the subsidiary conditions.[4] In the actual case the replacement cannot be performed so completely due to the approximate nature of canonical relations, and we must solve the problem taking into account the subsidiary conditions explicitly.

These attempts did not improve the situation; the resulting moment of inertia was the same as Bohr-Mottelson's phenomenological theory. This means that the assumption of irrotational collective motions is not good enough. Against our expectation they interact strongly with the internal motions, and the collective motions are not stable. Actual nuclei may also execute some other collective motions than the incompressible, irrotational ones—perhaps rotational ones. However, at present, it is not known how to treat the rotational collective motions quantum-mechanically. Thus the program to treat the collective motions quantum-mechanically has encountered with an objection.

On the other hand phenomenological approach was first made by Inglis who introduced the idea of independent particle motion in a rotating deformed potential with the fixed angular velocity Ω[5]. In the reference frame fixed to the potential, the particle system is exerted by a Coriolis force due to the rotation. Treating this force as perturbation, it is seen that the reduction in the energy of the particle system is the same with the increase in the energy of free rotation. Setting this increase as $\mathcal{J}_{\rm cr}\Omega^2/2$, we find the cranking model formula for the moment of inertia,

$$\mathcal{J}_{\rm cr}=2\sum_i|\langle 0|L|i\rangle|^2/(E_i-E_0)\,. \qquad (1\cdot3)$$

The consequences of this formula are discussed by Inglis, Bohr-Mottelson and Moszkowski.[6] Particularly if the potential were assumed to be of a deformed oscillator type, $\mathcal{J}_{\rm cr}$ would give a rigid moment of inertia at the equilibrium configuration. This value could be greatly reduced when the residual interactions between the particles were taken into account.

However, some questions remain also with this model. The first question was pointed out by Lipkin, de-Shalit and Talmi who remarked the fact that the rotation of a nucleus in Inglis' model is externally forced rotation imposed by 'cranking' the external potential, while the collective motion in the actual nucleus is free rotation resulting from the mutual interaction of the nucleons.[7] Moreover, on account of the deformation of the potential the quantum states of Inglis' model are eigenstates of the total angular momentum only in a sense of time average, while actual nuclear states are always the eigenstates of that quantity.

The first problem was discussed by Villars and Hayakawa-Marumori on the basis of quantum-mechanical many body problem.[8] Introducing a reference frame fixed to the particle system Villars expressed the hamiltonian in terms of the coordinates relative to this reference frame and the angles which indicate the orientation of the frame. Thus he obtained a form of the kinetic energy of a many body system, in which the dependence on the total angular momentum is explicitly given. Similar arguments were made by Hayakawa and Marumori who used the angular coordinate of the irrotational collective motion as a collective coordinate and the total angular momentum as the collective momentum and employed the method of canonical transformation. According to their results intrinsic motion has a coupling term with the total angular momentum through $L_{\rm in}$ which is called by them internal angular momentum. This coupling term plays the role of Coriolis force for the intrinsic motion. Hayakawa and Marumori derived the rotational spectra of the energy levels assuming the Coriolis force to be weak enough to be treated by perturbation theory and further assuming the mean square deviation of $L_{\rm in}$ to be negligibly small, the resulting moment of inertia was given by the sum of the hydrodynamical value (1·2) and the term similar to the cranking model formula (1·3). However, some criticism will be given about the consistency of above two assumptions in § 3.

With respect to the second problem about the angular momentum Peierls and Yoccoz made interesting discussions in which they remarked the degeneracy of ground state of independent particle motion in a deformed potential with the orientation of the potential.[9] Forming the linear combinations of these degenerate states properly, they found better trial wave functions which were eigenstates of the total angular momentum. However, we can use more improved trial functions, especially for the excited states, if there are some stable collective motions in the actual nuclei. As an example of the translational motion, the product of the Peierls-Yoccoz trial function for the zero momentum state and the plane wave which expresses the motion of the center-of-mass gives the improved trial function for the translating state which is lower in energy and gives no inconsistency such as the effective mass differs from the total mass. The nuclear collective motions would be under the same circumstances as the case of translational motion.

In this way the approach through the method of quantum-mechanical collective motion and that through the discussion of the phenomenological models have been related to each other and have left some questions respectively. Tomonaga, on the former standpoint, proposed to consider phenomenologically the couplings between the irrotational collective motion and the intrinsic motions.[10] Let us assume that the irrotational surface motion is coupled to one mode of the intrinsic motions. Then the coupling energy between the two motions is given only by the potential energy term and not from the kinetic energy, since the two coordinates which describe the two motions respectively are chosen to be orthogonal to each other. This coupling energy is shown to depend only on the ' relative coordinate ' between the two coordinates and approximated by expanding in its power series in the strong coupling limit. Thus the two modes move together executing relative vibration about an equilibrium point. Consequently, in a rotational motion, the rotating substance in the nucleus increases as compared with the case of surface motion alone, thus making the effective moment of inertia larger than the hydrodynamical value. However, it is not known what intrinsic motion is coupled strongly with the irrotational surface motion in the nuclei. But what motion it may be, its kinetic energy must be given by the square of the angular momentum which generates the intrinsic motion. By these discussions Tomonaga showed that the increase in the moment of inertia was given by a formula similar to that of the cranking model. At first sight this may seem to be the same as Hayakawa and Marumori's work, but they differ not only in appearance but also in substance as is shown in § 3.

The main purpose of this paper is to extend Tomonaga's idea to three dimensional cases and to derive the addition theorem of the moment of inertia in the case of coupled rotational motions. On the basis of these results the experimental data of the energy levels of the nuclei and those of the electric quadrupole excitation yields are analyzed. The results of this analysis indicate importance of the intrinsic motions. In § 2, Tomonaga's idea will be summarized in the two dimen-

sional example. In § 3, the relations with the other methods, especially with that of Hayakawa and Marumori, will be investigated. In § 4, Tomonaga's idea will be applied to separate one mode of intrinsic motions from the others in three dimensional case, and we will solve the problem of surface-internal coupled system in the strong coupling approximation in § 5, deriving the addition theorem of the moment of inertia. In § 6, Coulomb excitation phenomena will be discussed with this example inferring the magnitude of nuclear deformations ϵ and that of the moment of inertia of surface motion by the formula (1·2). Finally in § 7, the magnitude of the moment of inertia of the intrinsic motion will be inferred by means of the results in § 6 and the experimental data of energy levels.

§ 2. Illustration of the method by an example of the two dimensional nucleus

Let us begin with Tomonaga's theory since it is not published in a precise form. As Tomonaga did, we take a simple example of the two-dimensional nucleus. This example is rather simple in many respects, but still contains the very essence of the method and makes it easier to compare the discussions with other two-dimensional ones such as Hayakawa and Marumori's.

Denoting the Cartesian coordinates of the n-th nucleon by x_n, y_n and their conjugate momenta by p_{xn}, p_{yn} respectively, the total hamiltonian of the system is given by

$$H_0=\sum_n (1/2m)\,(p_{xn}^2+p_{yn}^2)+V(x_1, y_1;\ x_2, y_2;\cdots;\ x_n, y_n) \qquad (2\cdot1)$$

where m is the nucleon mass and V is the potential depending only on relative coordinates of the particles. First we consider two modes of collective motion corresponding to an irrotational, incompressible flow inside the nucleus which are described by the set of coordinates

$$\xi_1=(AR_0^2)^{-1}\sum_n (x_n^2-y_n^2)$$
$$\xi_2=(AR_0^2)^{-1}\cdot 2\sum_n x_n y_n$$

where A is the total number of the nucleons, and R_0 is the nuclear radius. The separation of the hamiltonian (2·1) into collective and internal parts was performed by Tamura and one of the present authors (T.M.).[3] In order to avoid unnecessary complexity of finding the canonical momenta conjugate to ξ_i, they introduced a set of auxiliary variables α_i and β_i canonically conjugate to each other and the hamiltonian was transformed into the representation in which α_i and β_i play the role of the collective variables. The transformed hamiltonian was given by

$$H_0\to H=T_c+H' \qquad (2\cdot2a)$$
$$T_c=(1/mAR_0^2)\,\{2(r^2/R_0^2)\,(\beta_1^2+\beta_2^2)+l(R_0^2/r^2)\,(\alpha_1\beta_2-\alpha_2\beta_1)+\cdots\} \qquad (2\cdot2b)$$

$$H'=H_{\text{internal}}+\sum_j H_j\alpha_j+\sum_{j,k} H_{jk}\alpha_j\alpha_k+\cdots \tag{2·2c}$$

where r^2 is defined by $r^2=A^{-1}\sum_n(x_n^2+y_n^2)$ and l by $l=\sum_n(x_np_{yn}-y_np_{xn})$. H_{internal}, H_j and H_{jk} depend only on the internal variables. The first term of (2·2b) is the kinetic energy of the collective motion, while the second term is the coupling term between the internal and collective angular momenta due to the non-commutativity of the momenta taken approximately conjugate to ξ_1 and ξ_2, so this term may be neglected as small compared with the first term. The second term on the right-hand side of (2·2c) gives the coupling between the internal and the collective motions, and the third term gives the effective potential for the surface deformation α_i.

Similarly the total angular momentum was transformed under the above transformation into

$$l\to L=L_{\text{c}}+L_{\text{i}} \tag{2·3a}$$

$$L_{\text{c}}=2(\alpha_1\beta_2-\alpha_2\beta_1) \tag{2·3b}$$

$$L_{\text{i}}=l. \tag{2·3c}$$

L_{c} is the angular momentum due to the collective motion and L_{i} is that due to the internal motion.

Instead of characterizing the collective motion by the two coordinates α_1 and α_2, it may also be described by an angular coordinate θ specifying the orientation of the deformed nuclear surface and a parameter determining its shape. They are given by

$$\begin{aligned}\alpha_1&=a\cos 2\theta\\ \alpha_2&=a\sin 2\theta.\end{aligned} \tag{2·4}$$

The kinetic energy of the irrotational collective motion (2·2b) is expressed in terms of these variables and takes the form

$$T_{\text{c}}=T_{\text{rot}}+T_{\text{vib}}. \tag{2·5a}$$

The first term is the rotational kinetic energy which is given by

$$T_{\text{rot}}=L_c^2/2J \tag{2·5b}$$

with the moment of inertia

$$J=2mAR_0^2a^2,$$

while the second term is the vibrational energy independent of θ. We have neglected the second term on the right-hand side of (2·2b) and used the approximation $r^2\simeq R_0^2/2$ which was verified in heavy nuclei.[2)]

With Eq. (2·5a), we can decompose the hamiltonian (2·2a) in the form

$$H=T_{\text{rot}}+H_{\text{a}} \tag{2·6a}$$

$$H_{\text{a}}=H_{\text{internal}}+\sum_j H_j\alpha_j+\sum_{j,k} H_{jk}\alpha_j\alpha_k+\cdots+T_{\text{vib}}. \tag{2·6b}$$

As it was discussed in § 1, we cannot anticipate the collective-internal coupling, the second term on the right-hand side of (2·6b), to be negligibly small; it may be rather strong. The coupled internal motion must be of a rotational nature in order to contribute to the magnitude of the moment of inertia. This internal rotation is supposed to be described by an angular coordinate φ which satisfies the canonical commutation relation with the internal angular momentum as follows

$$[L_{\mathrm{i}}, \varphi]=-i. \tag{2·7}$$

Strictly speaking, it is not a simple matter to see if there exists in the quantum many body system such a quantity as φ that satisfies the commutation relation (2·7). However, if there takes place an internal motion which rotates together with the irrotational collective one, such an angular variable may exist, at least, approximately satisfying the relation (2·7). Moreover, if it is possible to choose φ orthogonal to any other internal coordinates, the kinetic energy of this internal rotation may be given by the square of L_{i}. The moment of inertia of the internal rotation I, being the mass parameter of the kinetic energy, will be defined by means of the following relation

$$[H_{\mathrm{a}}, \varphi]=-(i/I)L_{\mathrm{i}}. \tag{2·8}$$

In order to obtain the explicit formula of I, we make up the representations of the above two relations (2·7) and (2·8) which are diagonal in H_{a} and eliminating the matrix element of φ, I will be given by the following formula,

$$I=2\sum_{n}|(\Psi_0|L_{\mathrm{i}}|\Psi_n)|^2/(E_n-E_0), \tag{2·9}$$

where Ψ_n and E_n are the eigenstates and eigenvalues of H_{a}, respectively. In deriving this formula there seems to be some ambiguity in the choice of the state Ψ_0. However, if the separation of the mode of internal rotation from the other internal motions can be performed fairly well I does not depend on what state is chosen for Ψ_0. We will finally remark the very similarity between I and $\mathcal{J}_{\mathrm{cr}}$ which was given by the cranking model formula (1·3), since Ψ_n is the eigenfunction of the hamiltonian H_{a} which means, being phenomenologically interpreted, to be a wave function in a deformed potential.

By the use of equations (2·7) and (2·8), it can easily be derived that the quantity $H_{\mathrm{a}}-L_{\mathrm{i}}^2/2I$ commutes with the angle φ, that is to say, it does not involve the internal angular momentum L_{i} and, consequently, it is the function of φ only with respect to the internal rotational motion. The φ dependence of H_{a} can be directly inferred from equation (2·6b) in which the second term on the right-hand side, being the coupling term between the internal and the collective motions, must explicitly depend on φ. The remaining terms in (2·6b) may be also φ dependent, but their dependence must be moderate enough to be neglected as compared with that of the second term. After all, H_{a} depends on the collective and the internal rotational motions with the following form,

$$H_a=\alpha_1 H_1+\alpha_2 H_2+L_i^2/2I \qquad (2\cdot10)$$
$$+\text{terms not dependent on the rotation.}$$

Corresponding to (2·4), H_1 and H_2 can be expressed by means of the angle φ as follows:

$$\begin{aligned} H_1&=V\cos 2\varphi \\ H_2&=V\sin 2\varphi, \end{aligned} \qquad (2\cdot11)$$

the origin of the angle φ being properly adjusted. Now we shall show that the quantity V above introduced is rotation independent. As the total angular momentum is a constant of motion, it commutes with the total hamiltonian of the system

$$[H,\ L]=0. \qquad (2\cdot12)$$

According to equations (2·5b) and (2·3b), one obtains the relation

$$[T_{\text{rot}},\ L]=[T_{\text{rot}},\ L_c]=0. \qquad (2\cdot13)$$

By means of (2·6a), (2·13) and (2·10), we derive from (2·12)

$$[\alpha_1 H_1+\alpha_2 H_2,\ L_c+L_i]=0.$$

If we use the form (2·3b) for L_c, above relation gives the equation

$$\alpha_1[H_1,\ L_i]+\alpha_2[H_2,\ L_i]=2i(\alpha_2 H_1-\alpha_1 H_2).$$

Comparing the factors of α_1 and α_2 on both sides, respectively, we find

$$\begin{aligned} [H_1,\ L_i]&=-2iH_2 \\ [H_2,\ L_i]&=2iH_1. \end{aligned} \qquad (2\cdot14)$$

Making use of (2·11), we get finally

$$[V,\ L_i]=0 \qquad (2\cdot15)$$

which means that V is not dependent on the angular coordinate φ. It has already been remarked that V too does not depend on L_i, but we shall prove it again explicitly. For that purpose, we calculate the quantity

$$\begin{aligned} [\varphi,[H_a,\ L_i]]&=[\varphi,[\alpha_1 H_1+\alpha_2 H_2,\ L_i]] \\ &=[\varphi,\ -2i\alpha_1 H_2+2i\alpha_2 H_1] \\ &=(-2i\alpha_1\sin 2\varphi+2i\alpha_2\cos 2\varphi)[\varphi,\ V] \end{aligned} \qquad (2\cdot16)$$

by means of (2·10), (2·14) and (2·11). Meanwhile we can make the left-hand side of (2·16) vanish using the identity

$$[\varphi,[H_a,\ L_i]]=[H_a,[\varphi,\ L_i]]+[[\varphi,\ H_a],\ L_i]$$

and Eq. (2·7) and (2·8). Thus one obtains

$$[\varphi,\ V]=0 \qquad (2\cdot17)$$

from (2·16). Consequently we can write down the explicit angular coordinate dependence of the coupling energy between the irrotational collective motion and the internal rotation as follows,

$$\alpha_1 H_1+\alpha_2 H_2=aV\cos 2(\theta-\varphi), \tag{2·18}$$

by means of (2·4). (2·11), (2·15) and (2·17).

Finally the hamiltonian takes the form

$$\begin{aligned} H=&L_c^2/2J+aV\cos 2(\theta-\varphi)+L_i^2/2I \\ &+\text{terms not dependent on the rotation.} \end{aligned} \tag{2·19}$$

It is convenient to make the further substitution

$$\begin{aligned} \theta&=(J\theta+I\varphi)/(J+I) \\ \Omega&=\theta-\varphi, \end{aligned}$$

which means respectively the angular center of mass and the relative angle of the two rotators.

Then the total angular momentum is given by

$$L=-i\partial/\partial\theta$$

by means of (2·3a) and the hamiltonian (2·19) is written in the form

$$H=\frac{1}{2(I+J)}L^2-\frac{I+J}{2IJ}\frac{\partial^2}{\partial\Omega^2}+aV\cos 2\Omega. \tag{2·20}$$

In the case of strong coupling between the irrotational collective and the internal rotations, the absolute value of aV is large compared with the energy of the rotational excitation. In this case the angle Ω will perform small vibration around the equilibrium point where $aV\cos 2\Omega$ takes its minimum value, so we may expand the last term of the right-hand side of (2·20) in the power series in Ω. Taking the series up to the square term in Ω, the hamiltonian (2·20) may be easily diagonalized and give the energy spectrum

$$\begin{aligned} E(M,n)&=aV+M^2/2(I+J)+(n+1/2)\omega_0 \\ \omega_0^2&=-4(I+J)aV/IJ \end{aligned} \tag{2·21}$$

where M is the magnitude of the total angular momentum and n is zero or the positive integer. Now since the last term of the right-hand side of (2·21) is much larger than the second term, n must take the value zero in the low excitation of the nucleus. Then the excitation is always rotational in which the effective moment of inertia is given by the sum of those of two motions by comparing (2·21) with the expression (1·1). The effective moment of inertia deviates from the hydrodynamical value by the amount (2·9) which becomes greater, as the excited single particle levels in a deformed potential are more closely spaced and the matrix elements of L_i are larger. Therefore, considerable deviation is expected for the

nuclei which lie far from the closed shell and whose deformation are large, as was pointed out by many authors.

The motion of our system may be pictured in the following manner. Suppose that the system is in a configuration corresponding to the lowest value of the coupling energy $aV\cos 2\Omega$, that is a configuration with $\theta=\varphi$ or $\theta=\varphi+\pi/2$ according to the sign of V. Then let us imagine that θ is increased by a small amount δ. This means that our drop of nuclear matter is deformed irrotationally, the change of the drop shape being a tidal rotation of the angle δ. This deformation then causes the increase of energy by the amount $2aV\delta^2$, so that it should be followed by the change of φ of the same angle δ which compensates the increase of energy. Physically this change of φ means the rearrangement of the particles in such a way that the inner stress is eliminated and the lowest value of the coupling energy is restored, the drop shape being kept unchanged. Thus our motion will be, roughly speaking, a succession of deformation and rearrangement, resulting in a rotation of the drop not purely tidal, but, on the other hand, not necessarily rigid because the rearrangement does not necessarily mean the persistence of a fixed relative position of particles in the drop.

§ 3. The connexion with other methods

In order to discuss the connexions between the other methods and that by Tomonaga, we will consider the work by Hayakawa and Marumori[8] which is most suitable for our purpose as an example because their work is very similar to others such as Villars', and is closely related with the idea of cranking model and, in addition, they employed the mathematical methods in common with ours.

They decomposed the hamiltonian of two dimensional particle system in the form:

$$H=H_{\rm rot}+H_{\rm part}\,, \tag{3·1a}$$

$$H_{\rm rot}=1/(2J)\cdot\{(M-\langle L_{\rm i}\rangle)^2+2(M-\langle L_{\rm i}\rangle)\langle L_{\rm i}\rangle+(L_{\rm i}-\langle L_{\rm i}\rangle)^2\}, \tag{3·1b}$$

$$H_{\rm part}=H_{\rm a}-\omega L_{\rm i} \tag{3·1c}$$

where $\omega=J^{-1}(M-\langle L_{\rm i}\rangle)$ and $\langle L_{\rm i}\rangle$ is the expectation value of $L_{\rm i}$ by the eigenfunction of $H_{\rm part}$. This decomposition involves no approximation. In order to solve the Schrödinger equation

$$H_{\rm part}\psi=\epsilon\psi, \tag{3·2}$$

it was assumed that the last term of the right-hand side of (3·1c) could be treated as a perturbation as in the case of cranking model. As a result of the approximation, one obtains

$$\langle L_{\rm i}\rangle=MI/(I+J). \tag{3·3}$$

Finally, making the expectation value of $H_{\rm rot}$ in ψ they showed the possibility to derive the rotational spectrum in which the effective moment of inertia was given

by the sum of I and J, if the last term of (3·1b) could be neglected compared with the preceding two terms. Quantitatively the first assumption may be formulated as

$$\sum_{m\neq 0}\left|\frac{\omega}{E_0-E_m}(\Psi_m|L_i|\Psi_0)\right|^2\ll 1, \tag{3·4}$$

where Ψ_m and E_m are the eigenfunction and eigenvalue of H_a respectively, as defined below Eq. (2·9). Meanwhile the second assumption means

$$\begin{aligned}\langle(L_i-\langle L_i\rangle)^2\rangle&=\langle L_i^2\rangle-\langle L_i\rangle^2\ll|(M-\langle L_i\rangle)^2+2(M-\langle L_i\rangle)\langle L_i\rangle|\\&=|M^2-\langle L_i\rangle^2|=M^2-\langle L_i\rangle^2,\end{aligned}$$

by means of (3·3). We may thus write

$$\langle L_i^2\rangle\ll M^2. \tag{3·5}$$

We shall now examine the validity of these two conditions on the basis of the phenomenological model given in § 2. The hamiltonian H_a takes the form

$$\begin{aligned}H_a=L_i^2/2I+aV-2aV(\varphi-\theta)^2+\cdots\\+\text{terms not dependent on the rotation}\end{aligned}$$

from (2·10) and (2·18) in the strong coupling approximation. Therefore E_m is given by

$$E_m=aV+(m+1/2)(\alpha^2/I), \tag{3·6}$$

with $\alpha^4=-4aVI$ which is large compared with unity in the strong coupling and m non-negative integer. And Ψ_m now takes the form

$$\begin{aligned}&\Psi_m=N_mH_m[\alpha(\varphi-\theta)]\exp\{-\alpha^2(\varphi-\theta)^2/2\},\\&N_m=\left(\frac{\alpha}{\sqrt{\pi}\,2^m m!}\right)^{1/2}\end{aligned} \tag{3·7}$$

where H_m is the Hermite polynomial of order m.

By means of the definition of ω, (3·3), (3·6) and (3·7), one is able to calculate the left-hand side of (3·4) and the result is given by

$$\sum_{m\neq 0}\left|\frac{\omega}{E_0-E_m}(\Psi_m|L_i|\Psi_0)\right|^2=\left(\frac{IM}{I+J}\right)^2\frac{1}{2\alpha^2},$$

which is small compared with unity in the strong coupling. Thus the condition (3·4) is satisfied by the model in § 2. In the same way, the left-hand side of (3·5) may be shown to be

$$\begin{aligned}\langle L_i^2\rangle&\simeq(\Psi_0|L_i^2|\Psi_0)-2Re\sum_{m\neq 0}\frac{\omega}{E_0-E_m}(\Psi_0|L_i^2|\Psi_m)(\Psi_m|L_i|\Psi_0)\\&=\frac{1}{2}\alpha^2+\frac{3}{4}\left(\frac{IM}{I+J}\right)^2.\end{aligned} \tag{3·8}$$

Since this is large compared with unity, the condition (3·5) cannot be satisfied by the model. This indicates the fundamental difference between the two methods. Moreover, it seems to suggest the inconsistency between the two assumptions (3·4) and (3·5).

By the condition (3·4), it may be expected that the ratio of the two terms on the right-hand side of (3·8) is appreciably small compared with unity which we shall designate by δ. It can be interpreted as an expansion parameter of the perturbation series in the problem of (3·2). Then Eq. (3·8) takes the form

$$\begin{aligned}\langle L_i^2\rangle &\simeq (1+\delta)\,(\Psi_0|L_i^2|\Psi_0)\\ &=(1+\delta)\sum_{n\neq 0}|(\Psi_n|L_i|\Psi_0)|^2\\ &=(1+\delta)\,(E_1-E_0)\sum_{n\neq 0}|(\Psi_n|L_i|\Psi_0)|^2/(E_1-E_0)\\ &\geqq(1+\delta)\,(E_1-E_0)\sum_{n\neq 0}|(\Psi_n|L_i|\Psi_0)|^2/(E_n-E_0)\\ &=(1+\delta)\,(E_1-E_0)\,(I/2),\end{aligned}\tag{3·9}$$

by means of (2·9); E_1 is the energy of the first excited state of H_a. Meanwhile, the second order perturbation energy of H_{part} is given by $-I\omega^2/2$, therefore we may set

$$\delta^2(E_1-E_0)\simeq I\omega^2/2.\tag{3·10}$$

By means of (3·9) and (3·10) one obtains

$$\langle L_i^2\rangle\geqq\frac{1+\delta}{\delta^2}\left(\frac{I\omega}{2}\right)^2=\frac{1+\delta}{4\delta^2}\left(\frac{IM}{I+J}\right)^2.$$

Imposing on $\langle L_i^2\rangle$ the condition (3·5) and assuming the relation $I\simeq 4J$ which may be expected from the experimental data, we find the condition for the magnitude of δ

$$25\delta^2-4\delta-4\geqslant 0.$$

Thus one obtains the result

$$\delta\geqslant 0.5$$

which explicitly contradicts our expectation $\delta\ll 1$. Even if δ takes a value between 0.5 and 1, one must give up the application of perturbation theory to solve Eq. (3·2). Then the discussion to derive the rotational spectra may be entirely changed. This seems to mean that it is rather difficult to obtain the rotational spectrum in the case of weak coupling between the irrotational collective and the internal motion.

§ 4. Application to the three dimensional nucleus

In the case of the three dimensional nucleus the total hamiltonian H_0 is given by

$$H_0=(1/2m)\sum_n\sum_\nu p_{\nu n}p_{\nu n}^*+V(\mathbf{r}_1,\ \mathbf{r}_2,\ \cdots,\ \mathbf{r}_A),\tag{4·1}$$

with

$$p_0=p_z,\qquad p_\pm=\mp\frac{1}{\sqrt{2}}(p_x\pm ip_y).$$

To describe the irrotational collective motion we use the set of coordinates

$$\xi_m=(4\pi/3AR_0^2)\sum_n Y_{2m}(\mathbf{r}_n),$$

where $Y_{2m}(\mathbf{r}_n)$ is the solid harmonics of the second order. The separation of the hamiltonian (4·1) into collective and internal parts gives the result, according to Tamura and one of present authors,[3)]

$$H_0\to H=T_c+H',\tag{4·2a}$$

$$T_c=(4\pi/3mAR_0^4)\sum_{\mu=-2}^{2}\beta_\mu^*R^2\beta_\mu,\tag{4·2b}$$

$$H'=\sum_{\mu=-2}^{2}\alpha_\mu H_\mu+H_I,\tag{4·2c}$$

small correction terms in the kinetic energy of the collective motion T_c being neglected. In these expression R is defined by $R^2=(5/3A)\sum_{n=1}^{A}\mathbf{r}_n^2$ and approximately equal to R_0, the nuclear radius. The first term on the right-hand side of (4·2c) gives the coupling between the irrotational collective and the internal motions, the second term contains the energy of internal motion, the potential energy of the collective motion and so on. α_μ are the coordinates of the irrotational collective motion in this transformed representation, and β_μ are the momenta canonically conjugate to α_μ. And H_μ depends only on the internal variables. The total angular momentum takes the form

$$L_m=L_m^c+L_m^i\ ;\ m=-1,\ 0,\ +1,\tag{4·3}$$

where the angular momentum of irrotational collective motion L_m^c is given by

$$L_m^c=\sqrt{10}\,i\sum_{\lambda,\mu=-2}^{2}(2\lambda 2\mu|1m)\alpha_\lambda\beta_\mu^*,\tag{4·4}$$

and L_m^i is that of the internal rotation.

Instead of characterizing the collective motion by the set of coordinates α_μ, we can use three angular coordinates θ_i specifying the orientation of the deformed nuclear surface and two parameters a_μ determining its shape. The latter coordinates are related to α_μ by the following formula

$$\alpha_\lambda=\sum_{\mu=-2}^{2}D_{\lambda\mu}(\theta_i)a_\mu\tag{4·5}$$

with $a_2=a_{-2}$ and $a_1=a_{-1}=0$, $D_{\lambda\mu}(\theta_i)$ being the transformation functions for the spherical harmonics of order two. Denoting the unit vectors along the each axis

of the frame of reference fixed in space by $(\mathbf{f}_x, \mathbf{f}_y, \mathbf{f}_z)$ and those fixed to the nuclear surface by $(\mathbf{k}^c_x, \mathbf{k}^c_y, \mathbf{k}^c_z)$, we define the transformation coefficients which are the functions of θ_i by

$$K_{uv}(\theta_i) = (\mathbf{f}_u \cdot \mathbf{k}^c_v) \; ; \quad u, \; v = x, \; y, \; z, \tag{4·6}$$

the functional form of $K_{uv}(\theta_i)$ was derived, for example, by Casimir.[11] By means of (4·6) one obtains the component of the collective angular momentum along $\mathbf{k}^c_u$ axis as follows,

$$P_u = \sum_v K_{vu}(\theta_i) L^c_v \; ; \quad u = x, \; y, \; z.$$

Then T_c written in terms of θ_i and a_λ takes the form

$$\begin{aligned} &T_c = T_{rot} + T_{vib} \, , \\ &T_{rot} = (1/2J_x) P_x^2 + (1/2J_y) P_y^2 + (1/2J_z) P_z^2, \end{aligned} \tag{4·7}$$

where T_{vib} is the kinetic energy of surface vibration and J_u are the moments of inertia of surface rotation which are given by

$$\begin{aligned} &J_x = J_y = 9mAR_0^2\beta^2/8\pi = \mathcal{J}_{rigid}\epsilon^2 = \mathcal{J}_{irr} \, , \\ &J_z = 0, \end{aligned} \tag{4·8}$$

where β defined by

$$\beta^2 = a_0^2 + 2a_2^2$$

gives a measure of the degree of deformation of the nuclear surface and is proportional to ϵ. These relations were first derived by Bohr.[1]

With Eq. (4·7), we can decompose the hamiltonian (4·2a) into the form

$$H = T_{rot} + H_a, \tag{4·9a}$$

$$H_a = \sum_{\mu=-2}^{2} \alpha_\mu H_\mu + H_I + T_{vib} \, . \tag{4·9b}$$

Now we shall separate phenomenologically the internal rotation coupled with the collective motion. As in the two dimensional example, it may be described by three eulerian angles, φ_1, φ_2, φ_3, which specify the orientation of the principal axes $\mathbf{k}^i_u$ (u=x, y, z) characteristic of the internal rotation. Instead of the angles the transformation coefficients may be used which are defined by

$$K_{uv}(\varphi_i) = (\mathbf{f}_u \cdot \mathbf{k}^i_v) \; ; \quad u, \; v = x, \; y, \; z. \tag{4·10}$$

Since this rotation is generated by the internal angular momentum they must satisfy the set of commutation relations

$$L^i_x K_{yu}(\varphi_i) - K_{yu}(\varphi_i) L^i_x = K_{xu}(\varphi_i) L^i_y - L^i_y K_{xu}(\varphi_i) = iK_{zu}(\varphi_i),$$

.....

u=x, y, z.

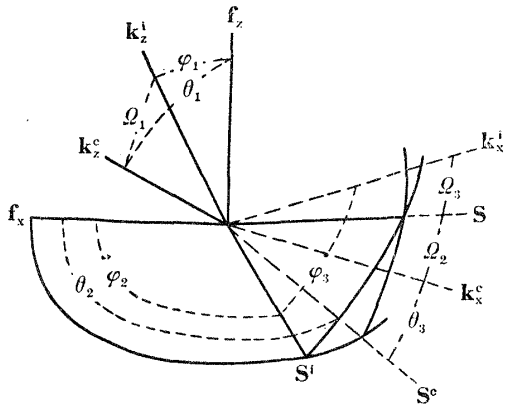

Fig. 1. Eulerian angles of three kinds. θ_1, θ_2, θ_3 denote the orientation of the nuclear surface ($\mathbf{k}_x^c$, $\mathbf{k}_y^c$, $\mathbf{k}_z^c$) relative to the frame of reference ($\mathbf{f}_x$, $\mathbf{f}_y$, $\mathbf{f}_z$) fixed in space. φ_1, φ_2, φ_3 give the directions of the principal axes ($\mathbf{k}_x^i$, $\mathbf{k}_y^i$, ($\mathbf{k}_z^i$,) characteristic of the internal motion. Finally Ω_1, Ω_2, Ω_3 determine the relative orientation of ($\mathbf{k}_x^c$, $\mathbf{k}_y^c$, $\mathbf{k}_z^c$) and ($\mathbf{k}_x^i$, $\mathbf{k}_y^i$, $\mathbf{k}_z^i$) systems. $\mathbf{S}^c$ is the nodal line, the line of intersection of the $\mathbf{f}_x$, $\mathbf{f}_y$ and the $\mathbf{k}_x^c$, $\mathbf{k}_y^c$ plane. $\mathbf{S}^i$ is that of the $\mathbf{f}$ and $\mathbf{k}^i$ systems and $\mathbf{S}$ is that between $\mathbf{k}^c$ and $\mathbf{k}^i$ systems. The definitions of quantities are the same as those given in the textbook by Casimir[11].

By means of (4·10) the component of internal angular momentum along $\mathbf{k}_u^i$ axis is given by

$$Q_u = \sum_v K_{vu}(\varphi_i) L_v^i .$$

Now, we suppose that the moment of inertia I_u of the internal rotation exists and can be defined by the relations

$$[H_a, K_{uz}(\varphi_i)] = (i/2I_x)\{Q_x K_{uy}(\varphi_i) + K_{uy}(\varphi_i) Q_x\} - (i/2I_y)\{Q_y K_{ux}(\varphi_i) + K_{ux}(\varphi_i) Q_y\}, \qquad (4\cdot11)$$

.....

$$u = x,\ y,\ z,$$

which express our expectation that the internal kinetic energy takes the form of that of an asymmetrical top whose moments of inertia are I_x, I_y and I_z. In order to gain the explicit form of I_u we multiply the first equation in (4·11) by $K_{uy}(\varphi_i)$ from left and sum them up with respect to the index u. Then by means of the relations

$$\sum_u K_{uv}(\varphi_i) K_{uw}(\varphi_i) = \delta_{vw}$$

one obtains

$$(2i/I_x) Q_x = \sum_u \{K_{uy}(\varphi_i) H_a K_{uz}(\varphi_i) - K_{uz}(\varphi_i) H_a K_{uy}(\varphi_i)\} . \qquad (4\cdot12)$$

Making use of the eigenvalues E_n and eigenfunctions Ψ_n of H_a, I_x may be expressed from (4·12) as

$$I_x = \frac{(\Psi_0 | Q_x | \Psi_0)}{\mathrm{Im} \sum_{un} E_n (\Psi_0 | K_{uy}(\varphi_i) | \Psi_n)(\Psi_n | K_{uz}(\varphi_i) | \Psi_0)} .$$

Similar expressions are valid for I_y and I_z. They are the three dimensional version of the moments of inertia corresponding to (2·9) of the two-dimensional case.

Since $H_a - \sum_u (1/2I_u) Q_u^2$ commutes with $K_{uv}(\varphi_i)$ by means of (4·11), it does

not contain the internal angular momentum, which means that it is a function of angles only with respect to the internal rotational motion. The angular dependence may be inferred from Eq. (4·9b) in which the first term on the right-hand side is most effective as compared with the others. It may therefore be expected that H_a now takes the form

$$H_a=\sum_{\mu}\alpha_\mu H_\mu+\sum_{u}(1/2I_u)Q_u^2 \\ +\text{terms independent of the rotation.} \qquad (4\cdot13)$$

In order to visualize the mechanism of the motions, we will put

$$H_\mu=\sum_{\lambda=-2}^{2}D^*_{\mu\lambda}(\varphi_i)V_\lambda\,. \qquad (4\cdot14)$$

Then it is easy to see the rotational invariance of the quantity V_λ above introduced by the discussion similar to that given in § 2. Finally, by means of (4·9a), (4·7), (4·13), (4·5) and (4·14), the hamiltonian takes the form

$$H=\sum_{u}(1/2J_u)P_u^2+\sum_{\lambda\mu\nu}a_\lambda V_\mu D_{\nu\lambda}(\theta_i)D^*_{\nu\mu}(\varphi_i)+\sum_{u}(1/2I_u)Q_u^2 \\ +\text{terms independent of the rotation.} \qquad (4\cdot15)$$

Now what sort of energy spectrum will this system have in the case of strong coupling? It is too difficult to treat the problem of coupled asymmetrical tops, but fortunately many nuclei seem to have the spheroidal deformation. We shall therefore assume the rotational symmetry of the system from the beginning, that is to say, we put

$$J_x=J_y \quad\text{and}\quad I_x=I_y\,. \qquad (4\cdot16)$$

Although J_z vanishes in this case as shown in (4·8), it will be treated as if it were not zero, since $J_z=0$ is a special case which can be considered more easily.

To solve the problem under the condition of strong coupling, the hamiltonian (4·15) is still inconvenient in two points. One of them is the fact that the interaction term between the two "tops" is too complicated. The other is that, since the nuclear spin does not appear explicitly in the hamiltonian, it is not easy to obtain the rotational spectrum. Thus it is more convenient to use three eulerian angles θ_i specifying the orientation of the system as a whole and three angles Ω_i determining the relative orientation of two tops. It may be natural to define Ω_i as the eulerian angles between $\mathbf{k}_u^c$- and $\mathbf{k}_u^i$, systems; explicitly, they are given by

$$K_{uv}(\Omega_i)=(\mathbf{k}_u^c\cdot\mathbf{k}_v^i)=\sum_{w}K_{wu}(\theta_i)K_{wv}(\varphi_i)\,. \qquad (4\cdot17)$$

Meanwhile it is desirable to define θ_i so as to separate the kinetic energy of the system into two parts as far as possible, one of which represents the motion of the system as a whole and the other represents the relative motion of the two tops If it is possible, θ_i will be chosen as the eulerian angles specifying the orientations of the principal axes of momental ellipsoid of the total system. According to the

above anticipation, θ_i will be defined by the solution of equations

$$\sum_{w}(A_{uw}-A_v\delta_{uw})K_{wv}(\theta_i)=0, \qquad u,\ v=x,\ y,\ z, \tag{4·18}$$

where A_{uw} is given by

$$A_{uw}=\sum_{v}(K_{uv}(\theta_i)K_{wv}(\theta_i)J_v+K_{uv}(\varphi_i)K_{wv}(\varphi_i)I_v), \qquad u,\ w=x,\ y,\ z,$$

and A_v is determined from Eq. (4·18).

Finding the explicit relations between θ_i, Ω_i and θ_i, φ_i, we can express the nuclear spin (4·3) and the total hamiltonian (4·15) in terms of θ_i and Ω_i. Though the calculation is tedius and lengthy, it can be performed completely without using any approximations.

The components of the spin along the principal axes of whole system defined by

$$R_u=\sum_{v}K_{vu}(\theta_i)L_v$$

take the form

$$\begin{aligned}
R_x&=-i\left[\cos\theta_3\frac{\partial}{\partial\theta_1}+\frac{\sin\theta_3}{\sin\theta_1}\frac{\partial}{\partial\theta_2}-\frac{\cos\theta_1\sin\theta_3}{\sin\theta_1}\frac{\partial}{\partial\theta_3}\right],\\
R_y&=-i\left[-\sin\theta_3\frac{\partial}{\partial\theta_1}+\frac{\cos\theta_3}{\sin\theta_1}\frac{\partial}{\partial\theta_2}-\frac{\cos\theta_1\cos\theta_3}{\sin\theta_1}\frac{\partial}{\partial\theta_3}\right],\\
R_z&=-i\frac{\partial}{\partial\theta_3}.
\end{aligned} \tag{4·19}$$

Thus it becomes apparent that θ_i satisfy the relations between the eulerian angles and the angular momentum.[11] Similarly by means of (4·16) and (4·19) the hamiltonian (4·15) may be written in terms of R_u and Ω_i, whose explicit form will be given in the Appendix.

§ 5. Strong coupling approximation and rotational spectrum

In the case of strong coupling between the two tops, they may execute small relative vibrations about the equilibrium point at which both principal axes coincide. We shall show in this section that the energy spectrum of the coupled system approximately reduces to that of a symmetrical top.

Such vibrations as mentioned above are characterized by

$$\Omega_1\ll 1 \quad\text{and}\quad |\tan\tfrac{1}{2}(\Omega_2+\Omega_3)|\ll 1. \tag{5·1}$$

Therefore it is convenient to make use of three variables

$$\Omega_1, \quad s=\tan\tfrac{1}{2}(\Omega_2+\Omega_3), \quad \vartheta=\Omega_2-\Omega_3, \tag{5·2}$$

instead of eulerian angles Ω_i to describe the relative motions. In terms of these variables the Schrödinger equation is given by

$$H\Psi=E\Psi \tag{5·3}$$

where H is the sum of (A·1) and (A·2) in which variables are transformed by means of (5·2), while the normalization condition for the wave function Ψ now takes the form

$$\int_0^{\pi}\sin\Omega_1 d\Omega_1\int_{-\infty}^{\infty}\frac{ds}{1+s^2}\int_{-2\pi}^{2\pi}d\vartheta\langle\Psi^*\Psi\rangle_{\Theta}=1 \tag{5·4}$$

where $\langle\cdots\rangle_{\Theta}$ is the inner product with respect to θ_i angles. In order to remove the weight function in Eq. (5·4), we make a similarity transformation

$$\Psi\to\Phi=\sqrt{\frac{\sin\Omega_1}{1+s^2}}\,\Psi,$$

$$H\to\mathfrak{H}=\sqrt{\frac{\sin\Omega_1}{1+s^2}}\,H\sqrt{\frac{1+s^2}{\sin\Omega_1}},$$

which gives the Schrödinger equation and the normalization condition

$$\mathfrak{H}\Phi=E\Phi,$$

$$\int_0^{\pi}d\Omega_1\int_{-\infty}^{\infty}ds\int_{-2\pi}^{2\pi}d\vartheta\langle\Phi^*\Phi\rangle_{\Theta}=1,$$

from (5·3) and (5·4) respectively. In conformity with the anticipation (5·1), hamiltonian $\mathfrak{H}$ may be expanded in power series in Ω_1 and s. Then it is shown that in the interaction term (A·2) appear linear terms in Ω_1 and s, unless $U_1=U_1'=U_2'=0$. This means the fact that our choice of eulerian angles φ_i was not adequate in general. Therefore we have rather to determine the angles φ_i so that the linear terms of Ω_1 and s vanish in the interaction energy (A·2). The condition is given by

$$U_1=U_1'=U_2'=0,$$

or, by means of (A·3),

$$V_2=V_{-2},\quad V_1=V_{-1}=0.$$

Now the interaction term may be expanded up to the fourth order in Ω_1 and s except those proportional to $\cos\vartheta$ which are taken only up to the second order. These terms must be small enough under the present circumstances because they give the interaction energy variable with the orientation of nodal line S (Fig. 1), which is physically meaningless. Though Ω_1 is restricted on the range

$$0\leq\Omega_1\leq\pi,$$

it may be approximately extended, in the case of strong coupling, over the whole positive value

$$0\leq\Omega_1<\infty.$$

The expanded form of the hamiltonian now becomes

$$\mathfrak{H}=\mathfrak{H}_0+\mathfrak{H}_1+\mathfrak{H}_2+\mathfrak{H}_3,$$

$$\mathfrak{H}_0=-\frac{1}{2}\left[\frac{1}{L}\frac{\partial^2}{\partial\Omega_1^2}+\frac{1}{4L\Omega_1^2}+\frac{1}{4D}\frac{\partial^2}{\partial s^2}+\frac{4}{L\Omega_1^2}\frac{\partial^2}{\partial\vartheta^2}+\left(\frac{1}{B}-\frac{1}{C}\right)\frac{\partial^2}{\partial s\partial\vartheta}\right]$$
$$-\frac{i}{2}R_z\left\{\frac{1}{2B}\frac{\partial}{\partial s}+\frac{4}{L\Omega_1^2}\frac{\partial}{\partial\vartheta}\right\}+\frac{1}{2L\Omega_1^2}R_z^2$$
$$+a_0V_0+2a_2U_2-\left(\tfrac{3}{2}a_0V_0+a_2U_2\right)\Omega_1^2-16a_2U_2s^2,$$

$$\mathfrak{H}_1=-\frac{1}{2}\left[\frac{1}{3L}+\frac{\Omega_1^2}{16L}\frac{\partial^2}{\partial s^2}+\frac{1}{D}\left(s\frac{\partial}{\partial s}+\frac{1}{2}s^2\frac{\partial^2}{\partial s^2}+\frac{1}{4}\right)+\left(\frac{1}{D}-\frac{2}{3L}\right)\frac{\partial^2}{\partial\vartheta^2}\right]$$
$$-\frac{i}{2}\left(\frac{1}{3L}-2b\right)R_z\frac{\partial}{\partial\vartheta}+\frac{b}{2}(R_x^2+R_y^2)+\frac{1}{2}\left(\frac{1}{3L}-b\right)R_z^2$$
$$+\left(\frac{1}{2}a_0V_0+\frac{5}{24}a_2U_2\right)\Omega_1^4+8a_2U_2s^2\Omega_1^2+32a_2U_2s^4,$$

$$\mathfrak{H}_2=-\frac{ic}{2}\left(R_x\frac{\partial}{\partial\Omega_1}+\frac{2R_y}{\Omega_1}\frac{\partial}{\partial\vartheta}\right)+\frac{c}{4\Omega_1}(R_yR_z+R_zR_y)$$
$$-\sqrt{\frac{3}{2}}(a_0U_2+a_2V_0)\Omega_1^2\cos\vartheta,$$

$\mathfrak{H}_3$=the remainders,

where the following notations are employed

$$1/B=1/I_x-1/J_x,\quad 1/C=1/I_z-1/J_z,\quad 1/D=1/I_z+1/J_z,$$
$$b=\frac{1}{(\Delta I+\Delta J)^2}\left\{\frac{(\Delta I)^2}{I_x}+\frac{(\Delta J)^2}{J_x}\right\},\qquad c=\frac{2}{\Delta I+\Delta J}\left(\frac{\Delta I}{I_x}-\frac{\Delta J}{J_x}\right).$$

$\mathfrak{H}_0$ is the lowest order term in Ω_1 and s, $\mathfrak{H}_1$ and $\mathfrak{H}_2$ are the correction terms being of higher order in these variables. $\mathfrak{H}_3$ contains the terms all of which are of higher order than $\mathfrak{H}_1$ and $\mathfrak{H}_2$, and may be seen to be negligible. It is clear that $\mathfrak{H}_0$ and $\mathfrak{H}_1$ commute with the quantities $\partial/\partial\vartheta$, $\sum_u R_u^2$, L_z and R_z which makes it convenient to use the symbols of eigenfunctions defined by

$$\left(\sum_u R_u^2\right)|IMK\rangle=I(I+1)|IMK\rangle,$$
$$L_z|IMK\rangle=M|IMK\rangle,$$
$$R_z|IMK\rangle=K|IMK\rangle.$$

Now the equation of the lowest order approximation

$$\mathfrak{H}_0\Phi_0=E_0\Phi_0$$

may be solved by putting

$$\Phi_0=(1/\sqrt{4\pi})f(\Omega_1)g(s)\exp(ik\vartheta/2)|IMK\rangle,$$
$$k=0,\ \pm1,\ \cdots, \tag{5·5}$$

with f and g obeying the equations

$$\left[-\frac{1}{2L}\frac{d^2}{d\Omega_1^2}+\frac{4\rho^2-1}{8L\Omega_1^2}-(\tfrac{3}{2}a_0V_0+a_2U_2)\Omega_1^2-\epsilon_1\right]f(\Omega_1)=0, \tag{5·6}$$

and

$$\left[-\frac{1}{8D}\frac{d^2}{ds^2}-\frac{i}{4}\left(\frac{\rho}{B}-\frac{k}{C}\right)\frac{d}{ds}-16a_2U_2s^2-\epsilon_2\right]g(s)=0, \tag{5·7}$$

respectively, where

$$\rho=K+k,\quad E_0=a_0V_0+2a_2U_2+\epsilon_1+\epsilon_2.$$

(1) Equation (5·6) for $f(\Omega_1)$ is solved easily and gives the result

$$\epsilon_1(mk\,;\ IMK)=\frac{2\sigma}{L}(2m+1+|\rho|),$$
$$f_m^\rho(\Omega_1)=c_m^\rho\Omega_1^{(1/2)+|\rho|}\exp(-\sigma\Omega_1^2)\cdot\sum_{n=0}^{m}\binom{m}{n}\frac{(-2\sigma\Omega_1^2)^n}{(n+|\rho|)!},$$
$$(c_m^\rho)^{-2}=\frac{1}{2(2\sigma)^{|\rho|+1}}\sum_{r,s=0}^{m}\binom{m}{r}\binom{m}{s}\frac{(-1)^{r+s}}{(r+|\rho|)!(s+|\rho|)!}(s+r+|\rho|)\,!, \tag{5·8}$$
$$\sigma=\left[-\frac{L}{2}(\tfrac{3}{2}a_0V_0+a_2U_2)\right]^{1/2},$$
$$m=0,\ 1,\ 2,\cdots.$$

(2) The solutions for the equation (5·7) are given by

$$\epsilon_2(nk\,;\ IMK)=(n+\tfrac{1}{2})\frac{\tau}{4D}-\frac{D}{8}\left(\frac{\rho}{B}-\frac{k}{C}\right)^2,$$
$$g_n^{k\rho}(s)=c_nH_n(\sqrt{\tau}\,s)\exp\left\{-iD\left(\frac{\rho}{B}-\frac{k}{C}\right)s-\tfrac{1}{2}\tau s^2\right\},$$
$$c_n=\left(\frac{\sqrt{\tau}}{\sqrt{\pi}\,2^n n!}\right)^{1/2},\quad \tau=8(-2a_2U_2D)^{1/2},$$
$$n=0,\ 1,\ 2,\cdots.$$

In this way we find the eigenvalues of the hamiltonian $\mathfrak{H}_0$ to be

$$E_0(mnk\,;\ IMK)=a_0V_0+2a_2U_2+(2m+1+|\rho|)\frac{2\sigma}{L}$$
$$+(n+\tfrac{1}{2})\frac{\tau}{4D}-\frac{D}{8}\left(\frac{\rho}{B}-\frac{k}{C}\right)^2, \tag{5·9}$$

and the eigenfunction belonging to the eigenvalue from (5·5)

$$\Phi_0(\Omega_1 s\vartheta:\ mnk;\ IMK)=(1/\sqrt{4\pi})f^{\rho}_{m}(\Omega_1)g^{k\rho}_{n}(s)\exp(ik\vartheta/2)\,|IMK\rangle. \qquad (5\cdot10)$$

Since the conditions of strong coupling are quantitatively given by $\sigma\gg1$ and $\tau\gg1$, the relative motions are not excited in the low lying states of actual nuclei. The low lying excited states consist of the rotational states corresponding to $m=n=\rho=0$. In order to find them we consider the effect of the correction terms $\mathfrak{H}_1$ and $\mathfrak{H}_2$ by means of the perturbation theory.

We will use the following simple notation

$$|K\rangle=\Phi_0(\Omega_1 s\vartheta:\ 0\ 0\ -K;\ IMK)$$

to denote a state with $m=n=0$, $k=-K$ (or $\rho=0$). In this notation the parameters to specify the values of I and M are omitted since they are exact constants of motion. Among the states with the definite common values for these quantities, $2I+1$ states

$$|-I\rangle,\quad |-I+1\rangle,\cdots,\ |I\rangle,$$

have almost the same energy values which are given by (5·9) and, further, $2I$ of which are composed of I sets of doubly degenerate states. Therefore, it seems necessary to use the perturbation theory for the degenerate system in order to find the rotational spectrum. But, fortunately, this is not the case for the reason which we shall presently account for.

It is sufficient to determine the energy up to the order $1/L$, the higher orders being no concern of ours, since they give a small correction to the resulting moment of inertia. Then we may neglect the effect of $\mathfrak{H}_3$ and apply the perturbation theory with $\mathfrak{H}_1+\mathfrak{H}_2$ only up to the second order. In these calculations one gets no matrix element of the perturbation energy which connects the different states among $|K\rangle$, and we can use the perturbation formula for the nondegenerate system.

The first order energy is given by

$$\begin{aligned}E_1(K)&\cong\langle K|\mathfrak{H}_1+\mathfrak{H}_2|K\rangle=\langle K|\mathfrak{H}_1|K\rangle\\&=-\frac{1}{6L}+\frac{1}{16D}+\frac{\tau}{128L\sigma}+\frac{b}{2}\{I(I+1)-K^2\}\\&\quad+\frac{K^2}{8D}+\frac{1}{4\sigma^2}\left(a_0V_0+\frac{5}{12}a_2U_2\right)+\frac{2a_2U_2}{\tau}\left(\frac{1}{\sigma}+\frac{12}{\tau}\right).\end{aligned}$$

In the second order calculation $\mathfrak{H}_1$ may be neglected. Further neglecting the terms in the matrix elements of $\mathfrak{H}_2$ which are smaller than $\sqrt{\sigma}/L$ or $\sqrt{\tau}/L$, we obtain

$$\langle\Phi_0(\Omega_1 s\vartheta:\ mn-K;\ IMK+1)\,|\mathfrak{H}_2|K\rangle=$$

$$\begin{cases}=0; & \text{if}\quad m\geq1,\\ =(ic/16\sigma)c_0^0c_0^1c_n(\pi/\tau)^{1/4}\sqrt{(I-K)(I+K+1)}\,(iD/\sqrt{\tau}\,B)^n\exp(-D^2/4\tau B^2); & \\ & \text{if}\quad m=0,\end{cases}$$

$$\begin{cases} \simeq 0\,; & \text{if} \quad m=0, \quad n\geq 1, \\ \simeq ic\sqrt{(I-K)(I+K+1)\sigma/8}\,; & \text{if} \quad m=n=0, \end{cases}$$

$$\langle \Phi_0(\Omega_1 s\vartheta:\ mn-K;\ IMK-1)\,|\mathfrak{H}_2|K\rangle =$$

$$\begin{cases} =0\,; & \text{if} \quad m\geq 1, \\ \simeq 0\,; & \text{if} \quad m=0,\ n\geq 1, \\ \simeq ic\sqrt{(I+K)(I-K+1)\sigma/8}\,; & \text{if} \quad m=n=0, \end{cases}$$

and

$$\langle \Phi_0(\Omega_1 s\vartheta:\ mn-K\pm 2;\ IMK)\,|\mathfrak{H}_2|K\rangle =$$

$$\begin{cases} =0\,; & \text{if} \quad m\geq 1, \\ \simeq 0\,; & \text{if} \quad m=0,\ n\geq 1, \\ \simeq -(1/16)\sqrt{3/2}\,(a_0U_2+a_2V_0)\,c_0{}^0c_0{}^2/\sigma^3\,; & \text{if} \quad m=n=0, \end{cases}$$

other matrix elements vanish. Using the energy difference

$$E_0(00\ -K;\ IMK)-E_0(00\ -K;\ IMK\pm 1)\simeq -2\sigma/L,$$

$$E_0(00\ -K;\ IMK)-E_0(00\ -K\pm 2;\ IMK)\simeq -4\sigma/L,$$

the second order energy may be estimated as

$$E_2(K)\simeq -(Lc^2/8)\,\{I(I+1)-K^2\}-(3L/32\sigma^3)\,(a_0U_2+a_2V_0)^2.$$

Finally we will summarize the result. The energy of the system is given up to the order of $1/L$ by

$$\begin{aligned} E(IMK) &= E_0(00\ -K;\ IMK)+E_1(K)+E_2(K) \\ &= \mathfrak{E}_0+\frac{1}{2}\left(b-\frac{Lc^2}{4}\right)\{I(I+1)-K^2\}+\left(\frac{1}{D}-\frac{D}{C^2}\right)\frac{K^2}{8} \qquad (5\ 11) \\ &= \mathfrak{E}_0+\frac{1}{2(I_x+J_x)}\{I(I+1)-K^2\}+\frac{1}{2(I_z+J_z)}K^2, \end{aligned}$$

with

$$\mathfrak{E}_0=a_0V_0+2a_2U_2+\left(2\sigma-\frac{1}{6}+\frac{\tau}{128\sigma}\right)\frac{1}{L}+\left(\tau-1-\frac{\tau}{8\sigma}\right)\frac{1}{8D}$$

$$+\frac{1}{4\sigma^2}\left(a_0V_0+\frac{5}{12}a_2U_2\right)-\frac{3L}{32\sigma^3}(a_0U_2+a_2V_0)^2.$$

The wave function takes, up to the order of $1/\sqrt{\sigma}$ or $1/\sqrt{\tau}$, the form

$$\begin{aligned} \Phi = |K\rangle & \\ -(iLc/4\sqrt{2\sigma})\,\{ & \sqrt{(I-K)(I+K+1)}\,\Phi_0(\Omega_1 s\vartheta:\ 00\ -K;\ IMK+1) \\ & +\sqrt{(I+K)(I-K+1)}\,\Phi_0(\Omega_1 s\vartheta:\ 00\ -K;\ IMK-1)\} \end{aligned}$$

$$+(\sqrt{3}\,L/16\sigma^2)\,(a_0U_2+a_2V_0)\,\{\Phi_0(\Omega_1 s\vartheta:\ 00\ -K+2\,;\ IMK)$$
$$+\Phi_0(\Omega_1 s\vartheta:\ 00\ -K-2\,;\ IMK)\}.$$

It is now known from (5·11) that a pair of the symmetrical tops strongly coupled with each other shows a rotational spectrum as if it were a symmetrical top whose moments of inertia are the sum of those of each ones.

§ 6. Discussion of Coulomb excitation

When a charged nuclear particle impinges upon the nucleus with its energy well below the Coulomb barrier, the nucleus may be excited through the electromagnetic interaction between the particle and the nucleus. Since all excitations identified so far have been found to be of electric quadrupole type, we shall now consider E2 transitions.

In the classical treatment of the impinging particle of the charge Z_1e and velocity v moving along a hyperbolic orbit in the repulsive Coulomb field of the target nucleus with the charge Z_2e, the differential excitation cross section is given by[12]

$$d\sigma_{E2}=(Z_1e/v)^2a^{-2}B(E2)\,df_{E2}(\vartheta,\,\xi), \tag{6·1}$$

with $a=Z_1Z_2e^2/m_0v^2$, $\xi=Z_1Z_2e^2\Delta E/2vE$, m_0 reduced mass, $E=m_0v^2/2$, ΔE the excitation energy and ϑ being the scattering angle. $f_{E2}(\vartheta,\,\xi)$ is a definite function of the variables explicitly defined by K. Alder et al.[12] They used the notation $B(E2)$ for the square sum of the matrix elements of electric quadrupole moment between the initial and the final states of the target nucleus

$$B(E2\,;\ I_i\to I_f)=\sum_{M_f,\,\mu}|\langle I_iM_i|\mathfrak{M}_0(E2,\,\mu)\,|I_fM_f\rangle|^2 \tag{6·2}$$

with

$$\mathfrak{M}_0(E2,\,\mu)=\sum_k e_kr_k^2Y_{2\mu}(\theta_k,\,\phi_k). \tag{6·3}$$

By means of (6·1), $B(E2)$ may be estimated from the experimental information for $d\sigma_{E2}$, the results for various nuclei being tabulated in the review work by K. Alder et al.

In order to estimate the right-hand side of (6·2) we now transform (6·3) to the representation in which α_μ and β_μ play the role of the irrotational collective variables, by means of the method given by Tamura and one of present authors.[3] Then the electric quadrupole operator takes the form

$$\mathfrak{M}_0(E2,\,\mu)\to\mathfrak{M}(E2,\,\mu)=\mathfrak{M}_0(E2,\,\mu)+(5R_0^2\alpha_\mu/4\pi R^2)\sum_k e_kr_k^2$$
$$-(dR_0^2/R^2)\sum_{\lambda\nu}(2\lambda 2\nu|2\mu)\,\mathfrak{M}_0(E2,\,\lambda)\,\alpha_\nu, \tag{6·4}$$

with $d=\sqrt{35/8\pi}$, up to the linear order in α_μ. The second term of (6·4) may be interpreted as the irrotational collective part of the electric quadrupole moment and the third term, being due to the approximately conjugate relations between the

collective coordinates and momenta, may be neglected. Assuming that the density of the particle is uniform within the nucleus one may write

$$\mathfrak{M}(E2,\ \mu)=\mathfrak{M}_0(E2,\ \mu)+3Z_2eR_0^2\alpha_\mu/4\pi. \tag{6·5}$$

Since we have not discussed the detailed nature of the internal motion, it is now hard to say something about the electromagnetic excitations of nucleus by means of the internal motion. Therefore, we shall first assume that it has rather smaller effect for the transitions than the irrotational collective motion does. When the mechanism of the internal motion becomes clear, the correction may be easily taken into account.

We obtain from (6·5)

$$\begin{aligned}\langle I_iM_iK_i|\mathfrak{M}(E2,\ \mu)|I_fM_fK_f\rangle&=(3Z_2eR_0^2/4\pi)\langle I_iM_iK_i|\alpha_\mu|I_fM_fK_f\rangle\\&=(3Z_2eR_0^2\beta/4\pi)\langle I_iM_iK_i|D_{\mu0}(\theta_i)|I_fM_fK_f\rangle\end{aligned} \tag{6·6}$$

by means of (4·5) and the condition of rotational symmetry $a_2=0$. Further we may write

$$\langle I_iM_iK_i|D_{\mu0}(\theta_i)|I_fM_fK_f\rangle=(I_iK_i\|D_0(\theta_i)\|I_fK_f)\ (I_fM_f2\mu|I_iM_i)/\sqrt{2I_i+1}\ . \tag{6·7}$$

In order to know the magnitude of $(I_iK_i\|D_0(\theta_i)\|I_fK_f)$, matrix elements of $D_{00}(\theta_i)$ between the states $M_i=0$ and $M_f=0$ are now to be calculated.

$D_{00}(\theta_i)$ is given by

$$\begin{aligned}D_{00}(\theta_i)&=(1/2)\ (3\cos^2\theta_1-1)\\&=\frac{3}{4}\left(\frac{\Delta J+\Delta I\cos 2\Omega_1}{\sqrt{Z(\Omega_1)}}+1\right)\cos^2\theta_1-\frac{3}{4}\left(\frac{\Delta J+\Delta I\cos 2\Omega_1}{\sqrt{Z(\Omega_1)}}-1\right)\sin^2\theta_1\cos^2\theta_3\\&\quad+\frac{3\Delta I}{\sqrt{Z(\Omega_1)}}\sin\Omega_1\cos\Omega_1\sin\theta_1\cos\theta_1\cos\theta_3-\frac{1}{2}\\&\simeq(1/2)\ (3\cos^2\theta_1-1),\end{aligned}$$

up to the lowest order in Ω_1.

Meanwhile the wave functions of the system are slightly changed from (5·10) on account of the symmetry conditions $J_z=0$ and $a_2=0$ and take, in the lowest order approximation, the form

$$\begin{aligned}&\Phi(\Omega_1\Omega_2\Omega_3:\ nm\ ;\ IMK)=(1/2\pi)f_n^\rho(\Omega_1)\exp(im\Omega_3)|IMK\rangle,\\&n=0,\ 1,\ 2,\cdots;\quad m=0,\ \pm1,\ \pm2,\cdots,\end{aligned}$$

where $f_n^\rho(\Omega_1)$ is defined in (5·8) and $\rho=|K-m|$. Within the energy region of the rotational excitation, n and ρ vanish. The initial state of the target nucleus, being the ground state, is characterized by $I_i=M_i=K_i=0$, the final state by $I_f=2$. Thus we obtain

$$(\Phi(\Omega_i:\ 00\ ;000)|D_{00}(\theta_i)|\Phi(\Omega_i:\ 0K\ ;\ 20K))=\delta_{K0}/\sqrt{5}\ ,$$

which gives the result, from (6·7)

$$(00\|D_0(\theta_i)\|2K)=\delta_{K0}. \tag{6·8}$$

Finally, by means of (6·2), (6·6), (6·7) and (6·8), we get

$$B(E2\,;\ 0\to 2)=9e^2Z_2^2R_0^4\beta^2/16\pi^2 \tag{6·9}$$

which coincides with the result given phenomenologically by Bohr and Mottelson.[1] Consequently if the internal rotation makes little contribution to the electric quadrupole transition, we can estimate magnitude of J_x by means of (6·9) and (4·8). The results are tabulated in the Table.

§ 7. Discussions

According to our model, the effective moment of inertia $\mathcal{J}$ is given by the sum I_x+J_x. As shown in § 6, J_x is related to the nuclear deformation and experimentally determined by using the Coulomb excitation. On the other hand, $\mathcal{J}=I_x+J_x$ is calculated from the empirical data for the rotational excitation energy. In this way I_x and J_x are determined separately. The results are listed in the Table and drawn in Fig. 2 as a function of the neutron number of the nucleus.

Table. Irrotational and internal moments of inertia J_x and I_x. The energy of the first excited state $3/(I_x+J_x)$ and the reduced transition probability $B(E2)$ give the magnitudes of I_x and J_x according to the formulas (4·8), (5·11) and (6·9). Empirical data are given in the work by K. Alder et al.[12] in which the isotope separation is insufficient for Er and Yb.

Nucleus	$3\hbar^2/(I_x+J_x)$ (kev)	I_x+J_x (10^{-47} gr cm^2)	β	J_x (10^{-47} gr cm^2)	I_x (10^{-47} gr cm^2)	I_x/J_x
Nd^{150}	130	1.60	0.25	0.23	1.37	5.96
Sm^{152}	122	1.71	0.28	0.30	1.42	4.73
Sm^{154}	83	2.50	0.33	0.42	2.08	4.95
Gd^{154}	123	1.69	0.30	0.35	1.34	3.86
Gd^{156}	89	2.34	0.41	0.66	1.68	2.55
Gd^{158}	79	2.64	0.46	0.85	1.79	2.12
Gd^{160}	76	2.73	0.47	0.90	1.83	2.03
Dy^{162}	82	2.54	0.36	0.54	2.00	3.71
Dy^{164}	73	2.84	0.41	0.72	2.12	2.96
Er	80	2.60	0.33	0.48	2.12	4.42
Yb	78	2.66	0.31	0.45	2.21	4.92
Hf^{176}	89	2.34	0.29	0.40	1.94	4.85
Hf^{178}	91	2.28	0.31	0.47	1.81	3.85
Hf^{180}	93	2.23	0.27	0.36	1.87	5.20
W^{182}	100	2.08	0.26	0.34	1.74	5.12
W^{184}	112	1.86	0.24	0.30	1.56	5.22
W^{186}	124	1.67	0.24	0.30	1.37	4.57
Th^{232}	52	4.01	0.25	0.48	3.53	7.36
U^{238}	44	4.75	0.28	0.63	4.12	6.54

In general I_x is four or five times as large as J_x, especially for heavy nuclei with the neutron number larger than 140, the rotational excitations are mainly due to the internal rotation. We thus find that the internal rotation is important. However, there seems to be, at present, little experimental indication which suggests what is the internal motion. We know only that the internal motion may be something of rotational nature but different from the rigid rotation. In our treatment of the internal rotation, we did not assume that the internal hamiltonian has exactly a quadratic term with respect to the internal angular momentum L_i. We only assumed that the internal motion cranked up by the surface rotation may be a rotational one with a definite moment of inertia I when the rotation follows the crank (the surface rotation) with a small phase lag, $\theta-\varphi=\Omega$. The relations (2·7) and (2·8) defining φ are only valid for a range of φ small compared with 2π. Only in this approximation the formula (2·9) is valid too. These relations have no meaning when interpreted too literally, since the quantity I defined by the operator relation (2·8) is not constant strictly. In this connection, it may be worth-while to notice that, when the same procedure as mentioned above is applied to a hamiltonian H which commutes with the total angular momentum L (see eg. Bohr and Mottelson[13]), the formula corresponding to (2·9) has no meaning, because L has no off-diagonal elements. Considering the case of a mechanical top, it is clear that, although such quantities as $\cos\varphi$, $\sin\varphi$, can be defined without any ambiguity, exact definition of the matrix element of the angle φ is impossible. We must be careful in applying such formulas.

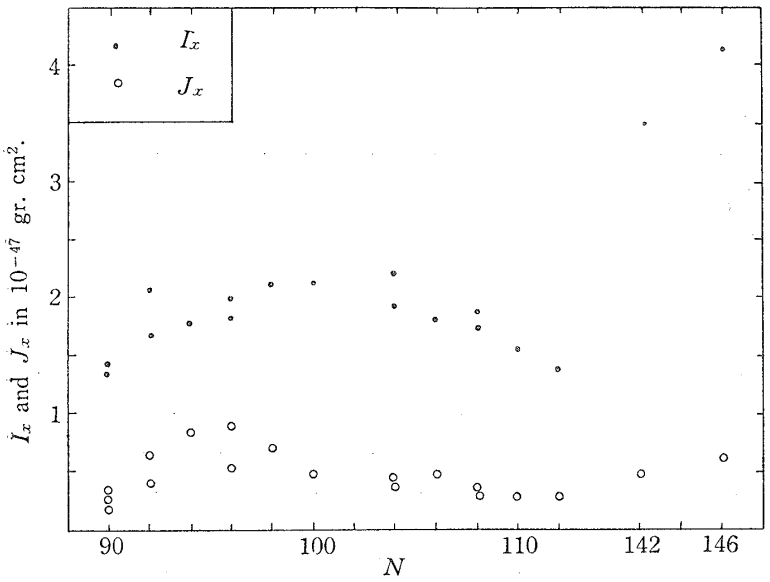

Fig. 2. Irrotational and internal moments of inertia. The figure shows the irrotational moment of inertia J_x (circle) and that of internal one I_x (point) with the neutron number $90\leqq N\leqq 112$ and $142\leqq N\leqq 146$. They are determined by means of the quadrupole and the spectral data. The experimental data are taken from the compilation in the review work by K. Alder et al[12].

Consideration about the nature of the internal motion was made by S. Nagata et al. basing upon the analyses of the unsatisfactory points in the usual quantum theory of irrotational collective motions.[14] They showed the necessity of introduction of the rotational collective mode. However, their discussion is a kinematical one having nothing to do with the interaction potential between nucleons. In addition, it contains ambiguity with respect to the nature of the rotational motion.

Thus the discussion seems to be insufficient to clarify the mechanism of the internal motions.

On the other hand Elliott made an interesting study taking into account the correlations of nuclear particles.[15]. He found the level structure of a set of particles occupying levels which are degenerate in harmonic oscillator potential and subject to an internucleon interaction. His interaction takes the form

$$G\sum_{m}\xi^{*}_{m}\xi_{m}$$

in our notations and it is restricted to be effective among the particles in a set of degenerate levels. Since the irrotational collective motion would be generated mainly by the particles in the unfilled shell, the restriction does not seem to be so effective. Elliott's interaction will in the main give couplings among the irrotational motions, which act as the potential energy of the surface vibrations that serves to determine the equilibrium shape of the nuclear surface. Therefore in his model the interactions between the irrotational and internal motions are not so essential. Consequently it may be open to question if it can give the correct order of magnitude for the moment of inertia when we use the value of G determined from the quadrupole data. Hence, it would be necessary to take into account more complicated correlations among the particles in order to explain the deviation of $\mathcal{J}$ from the irrotational value.

There are other arguments[5,9] on the moment of inertia. They are probably more closely connected with the cranking model than with ours, and it may not be easy to say more than that the former corresponds, in a sense, to the introduction of rotating deformed potential (a model wave function) in place of the internal hamiltonian (the internal wave function).

In this paper we discussed only the case of strong coupling between the irrotational and internal rotations. When the coupling is not strong, the spectra will not be rotational in general. It may be of some interest to see if deviation from the rotational spectra can be interpreted in terms of the intermediate coupling.

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Appendix

The hamiltonian of the coupled symmetrical tops (4·15) can be written in terms of the nuclear spin $\mathbf{R}$ (4·19) and the relative eulerian angles Ω_i between the two tops. The kinetic energy now takes the form

$$
\begin{aligned}
&(P_x^2+P_y^2)/2J_x+P_z^2/2J+(Q_x^2+Q_y^2)/2I_x+Q_z^2/2I_z= \\
&=-\frac{1}{2}\Big[\frac{1}{J_x}\Big(\frac{\partial^2}{\partial\theta_1^2}+\frac{\cos\theta_1}{\sin\theta_1}\frac{\partial}{\partial\theta_1}+\frac{1}{\sin^2\theta_1}\frac{\partial^2}{\partial\theta_2^2}-\frac{2\cos\theta_1}{\sin^2\theta_1}\frac{\partial^2}{\partial\theta_3\partial\theta_2} \\
&\quad+\frac{\cos^2\theta_1}{\sin^2\theta_1}\frac{\partial^2}{\partial\theta_3^2}\Big)+\frac{1}{J_z}\frac{\partial^2}{\partial\theta_3^2}\Big] \\
&\quad-\frac{1}{2}\Big[\frac{1}{I_x}\Big(\frac{\partial^2}{\partial\varphi_1^2}+\frac{\cos\varphi_1}{\sin\varphi_1}\frac{\partial}{\partial\varphi_1}+\frac{1}{\sin^2\varphi_1}\frac{\partial^2}{\partial\varphi_2^2}-\frac{2\cos\varphi_1}{\sin^2\varphi_1}\frac{\partial^2}{\partial\varphi_3\partial\varphi_2} \\
&\quad+\frac{\cos^2\varphi_1}{\sin^2\varphi_1}\frac{\partial^2}{\partial\varphi_3^2}\Big)+\frac{1}{I_z}\frac{\partial^2}{\partial\varphi_3^2}\Big] \\
&=-\frac{1}{2}\Big[\frac{1}{L}\frac{\partial^2}{\partial\Omega_1^2}+\frac{1}{L}\frac{\cos\Omega_1}{\sin\Omega_1}\frac{\partial}{\partial\Omega_1}+\Big(\frac{1}{L\sin^2\Omega_1}-\frac{1}{J_x}+\frac{1}{J_z}\Big)\frac{\partial^2}{\partial\Omega_2^2} \\
&\quad-\frac{2\cos\Omega_1}{L\sin^2\Omega_1}\frac{\partial^2}{\partial\Omega_2\partial\Omega_3}+\Big(\frac{1}{L\sin^2\Omega_1}-\frac{1}{I_x}+\frac{1}{I_z}\Big)\frac{\partial^2}{\partial\Omega_3^2}\Big] \\
&\quad-\frac{i}{2}\Big[W_1(\Omega_1)R_x\frac{\partial}{\partial\Omega_1}+S_1(\Omega_1)R_x-R_y\Big\{W_2(\Omega_1)\frac{\partial}{\partial\Omega_2}+W_3(\Omega_1)\frac{\partial}{\partial\Omega_3}\Big\} \\
&\quad+R_z\Big\{S_2(\Omega_1)\frac{\partial}{\partial\Omega_2}+S_3(\Omega_1)\frac{\partial}{\partial\Omega_3}\Big\}\Big] \\
&\quad+\tfrac{1}{2}[T_1(\Omega_1)R_x^2+T_2(\Omega_1)R_y^2+T_3(\Omega_1)\{R_yR_z+R_zR_y\}+T_4(\Omega_1)R_z^2],
\end{aligned}
\tag{A·1}
$$

where following notations are used:

$$1/L=1/I_x+1/J_x,$$

$$W_1(\Omega_1)=\frac{2}{Z(\Omega_1)}\Big[\frac{\Delta I}{I_x}(\Delta I+\Delta J\cos 2\Omega_1)-\frac{\Delta J}{J_x}(\Delta I\cos 2\Omega_1+\Delta J)\Big],$$

$$W_2(\Omega_1)=2\sqrt{2}\cot\Omega_1\Big[-\frac{\Delta I}{I_x\{Z(\Omega_1)+(\Delta J+\Delta I\cos 2\Omega_1)\sqrt{Z(\Omega_1)}\}^{1/2}} +\frac{\Delta J\cos\Omega_1}{J_x\{Z(\Omega_1)+(\Delta I+\Delta J\cos 2\Omega_1)\sqrt{Z(\Omega_1)}\}^{1/2}}\Big],$$

$W_3(\Omega_1)=W_2(\Omega_1)$ in which I_x and J_x, ΔI and ΔJ are exchanged respectively,

$$S_1(\Omega_1)=\frac{\cot\Omega_1}{Z(\Omega_1)}\Big[\frac{\Delta I}{I_x}(\Delta I+\Delta J\cos 2\Omega_1)-\frac{\Delta J}{J_x}(\Delta J+\Delta I\cos 2\Omega_1)\Big] +2\Delta I\Delta J\frac{(\Delta I)^2-(\Delta J)^2}{LZ(\Omega_1)^2}\sin 2\Omega_1,$$

$$S_2(\Omega_1)=\frac{\sqrt{2}}{Z(\Omega_1)^{1/4}\sin^2\Omega_1}\Big[\frac{1}{I_x}\{\Delta J+\Delta I\cos 2\Omega_1+\sqrt{Z(\Omega_1)}\}^{1/2} +\frac{1}{J_x}\{\Delta I+\Delta J\cos 2\Omega_1+\sqrt{Z(\Omega_1)}\}^{1/2}\cos\Omega_1\Big],$$

$S_3(\Omega_1)=-S_2(\Omega_1)$ in which I_x and J_x, ΔI and ΔJ are exchanged respectively,

$$T_1(\Omega_1)=\frac{1}{Z(\Omega_1)^2}\left[\frac{(\Delta I)^2}{I_x}(\Delta I+\Delta J\cos 2\Omega_1)^2+\frac{(\Delta J)^2}{J_x}(\Delta J+\Delta I\cos 2\Omega_1)^2\right],$$

$$T_2(\Omega_1)=\frac{1}{I_xZ(\Omega_1)+(\Delta J+\Delta I\cos 2\Omega_1)\sqrt{Z(\Omega_1)}}\,2(\Delta I)^2\cos^2\Omega_1$$

$$+\frac{1}{J_xZ(\Omega_1)+(\Delta I+\Delta J\cos 2\Omega_1)\sqrt{Z(\Omega_1)}}\,2(\Delta J)^2\cos^2\Omega_1,$$

$$T_3(\Omega_1)=\left(\frac{\Delta I}{I_x}-\frac{\Delta J}{J_x}\right)\frac{\cot\Omega_1}{\sqrt{Z(\Omega_1)}},$$

$$T_4(\Omega_1)=\frac{(\Delta J+\Delta I\cos 2\Omega_1+\sqrt{Z(\Omega_1)})/I_x+(\Delta I+\Delta J\cos 2\Omega_1+\sqrt{Z(\Omega_1)})/J_x}{2\sin^2\Omega_1\sqrt{Z(\Omega_1)}},$$

$$Z(\Omega_1)=(\Delta I)^2+2\Delta I\Delta J\cos 2\Omega_1+(\Delta J)^2,$$

$$\Delta I=I_x-I_z,\quad \Delta J=J_x-J_z.$$

The first term on the right-hand side of (A·1) is the kinetic energy of the relative motion, the second term gives the coupling between the relative motion and the rotation of the system as a whole, and the last term is the kinetic energy of the rotation.

Meanwhile the interaction energy between two tops now takes the form

$$\sum_{\lambda\mu\nu}a_\lambda V_\mu D_{\nu\lambda}(\theta_i)\,D^*_{\nu\mu}(\varphi_i)=$$

$$\begin{aligned}
&=(a_0V_0/2)\,(3\cos^2\Omega_1-1)-a_0U_2\sqrt{3/2}\,\sin^2\Omega_1\cos 2\Omega_3-a_2V_0\sqrt{3/2}\,\sin^2\Omega_1\cos 2\Omega_2\\
&\quad+a_2U_2\{\cos 2\Omega_2\cos 2\Omega_3(1+\cos^2\Omega_1)-2\cos\Omega_1\sin 2\Omega_2\sin 2\Omega_3\}\\
&\quad+\sqrt{6}\,a_0U_1\sin\Omega_1\cos\Omega_1\cos\Omega_3-\sqrt{6}\,a_0U_1'\sin\Omega_1\cos\Omega_1\sin\Omega_3\\
&\quad-(\sqrt{6}/2)\,a_0U_2'\sin 2\Omega_3\sin^2\Omega_1 \qquad\qquad (A\cdot 2)\\
&\quad-2a_2U_1\{\sin\Omega_1\sin 2\Omega_2\sin\Omega_3-\sin\Omega_1\cos\Omega_1\cos 2\Omega_2\cos\Omega_3\}\\
&\quad-2a_2U_1'\{\sin\Omega_1\sin 2\Omega_2\cos\Omega_3+\sin\Omega_1\cos\Omega_1\cos 2\Omega_2\sin\Omega_3\}\\
&\quad+a_2U_2'\{(1+\cos^2\Omega_1)\cos 2\Omega_2\sin 2\Omega_3+2\cos\Omega_1\sin 2\Omega_2\cos 2\Omega_3\},
\end{aligned}$$

where the hermitian quantities U_μ and U'_μ are defined by

$$V_2=V^*_{-2}=U_2+iU_2',\quad V_1=-V^*_{-1}=U_1'+iU_1. \qquad (A\cdot 3)$$

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