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NONADIABATIC CORRECTIONS TO THE ROTATIONAL SPECTRUM OF ATOMIC NUCLEI

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We have used a consistent microscopic description to evaluate the $BI^2(I+1)^2$ term in the energy of a rotating system of particles, without taking pair correlations into account. The calculated coefficient B agrees qualitatively with the experimental value.

It is well known that in the regions $150 < A < 190$ and $A > 226$ the atomic nuclei are deformed and possess rotational excitations along with single-particle and "vibrational" excitations.

In that region, the energies E_I of the rotational states are much smaller than the single-particle and vibrational excitation energies and have the simple form

$$E_I = h^2 I(I+1)/2J + E_0\,, \tag{1}$$

where I is the spin of the nucleus, J the moment of inertia, and E_0 a constant. Equation (1) corresponds to the energy of a rotating system calculated up to terms of the order Ω^2, where Ω is the angular rotational velocity.

It is of interest to study the corrections to the energy of the system of higher order in the rotational velocity. One usually obtains such corrections by considering phenomenologically the influence of vibrations on the rotation. They are then of the form

$$E_v = -2I^2(I+1)^2/(h\omega_v)^2 J^3\,, \tag{2}$$

where $h\omega_v$ is the average vibrational frequency in the nucleus.

In deformed nuclei, however, the collective excitations with energies of 0.7 – 1.2 Mev can be called vibrational only under very special conditions, for they are not connected with the vibrations of the surface of the nucleus and are, apparently, bound states of two quasi-particles, as is the case in a spherical nucleus. There is thus no sufficient basis for applying Eq. (2) in this case.

It is of interest to calculate the corrections to the rotational energy of the system, using a consistent microscopic description. To do this we consider particles moving in a self-consistent potential. We shall then neglect the residual interaction between the particles which leads to "pairing off."

We can write the Hamiltonian of a rotating nucleus in the form

$$H = H^0 - \mathbf{M}\Omega\,, \tag{3}$$

where H is the Hamiltonian in a rotating coordinate system, **M** the angular momentum, and Ω the angular velocity.

To evaluate the energy of the system we need to know the density matrix which one can easily find from the Green function

$$G(x_1, x_2) = -i\,\langle\Phi_0|\,T\psi(x_1)\psi^+(x_2)\,|\Phi_0\rangle\,,$$

where T is the chronological operator, Φ_0 the ground state wave function, and ψ and ψ^+ are annihilation and creation operators for the particles. The equation for the Green's function is of the form

$$(i\partial/\partial t - H)G = \delta(\mathbf{r}_1 - \mathbf{r}_2)\,. \tag{4}$$

In particular, it is for a rotating system of the form

$$(i\partial/\partial t - H^0 + M^x\Omega)\,G = \delta\,(\mathbf{r}_1 - \mathbf{r}_2). \tag{5}$$

If we consider $M^x\Omega$ to be a perturbation, we can easily find G in zeroth approximation. The component $G^0_\lambda(\omega)$ of the expansion of the function G in terms of the eigenfunctions of the Hamiltonian H^0 is of the form[1]

$$G^0_\lambda(\omega) = 1/[\omega - \varepsilon_\lambda + i\delta\theta(\varepsilon_\lambda)], \tag{6}$$

where ϵ_λ are the eigenvalues of the Hamiltonian H^0, and

$$\theta(\varepsilon_\lambda) = \begin{cases} +1, \text{ if } \varepsilon_\lambda - \varepsilon_{\lambda_0} > 0 \\ -1, \text{ if } \varepsilon_\lambda - \varepsilon_{\lambda_0} < 0\,, \end{cases}$$

where ϵ_0 is the energy of the Fermi surface.

In successive orders of perturbation theory the corrections to the Green function are of the form

$$G'_{\lambda\lambda'} = G^0_\lambda H'_{\lambda\lambda'} G^0_{\lambda'},$$

$$G''_{\lambda\lambda'} = G^0_\lambda H'_{\lambda\lambda_1} G^0_{\lambda_1} H'_{\lambda_1\lambda'} G^0_{\lambda'},$$

$$\cdots\cdots\cdots\cdots\cdots\cdots$$

$$G^{(4)}_{\lambda\lambda'} = G^0_\lambda H'_{\lambda\lambda_1} G^0_{\lambda_1} H'_{\lambda_1\lambda_2} G^0_{\lambda_2} H'_{\lambda_2\lambda_3} G^0_{\lambda_3} H'_{\lambda_3\lambda'} G^0_{\lambda'} \tag{7}$$

(summation is understood to occur over repeated indices and $H' = M^x\Omega$).

The density matrix is obtained from the relation

$$\rho_{\lambda\lambda'} = \int\limits_C G_{\lambda\lambda'} \frac{d\omega}{2\pi i}, \qquad (8)$$

where the contour C consists of the real axis and a semicircle in the upper half-plane. Once we know the density matrix we can easily evaluate the energy of the system, using the formula

$$E = \mathrm{Sp}\, H\rho = \sum_{\lambda\lambda'} H_{\lambda\lambda'}\rho_{\lambda'\lambda}. \qquad (9)$$

In the expansion of the energy in terms of the perturbation, odd terms in Ω vanish and we get from (9)

$$E = \sum_{\lambda} \varepsilon_\lambda \rho_\lambda^0 + \sum_{\lambda} \varepsilon_\lambda \rho''_{\lambda\lambda} + \sum_{\lambda\lambda'} \varepsilon'_{\lambda\lambda'} \rho'_{\lambda'\lambda} + \sum_{\lambda\lambda'} \varepsilon'_{\lambda\lambda'} \rho^{(3)}_{\lambda'\lambda} + \sum_{\lambda} \varepsilon_\lambda \rho^{(4)}_{\lambda\lambda}. \qquad (10)$$

Using Eqs. (6), (7), and (8) we get after simple calculations

$$E = E_0 + \frac{\Omega^2}{2} \sum_{\lambda\lambda'} \frac{|M^x_{\lambda\lambda'}|^2 (n_\lambda - n_{\lambda'})}{\varepsilon_\lambda - \varepsilon_{\lambda'}}$$

$$- \Omega^4 \Bigg[\sum_{\lambda, \lambda_1, \lambda'} \frac{M^x_{\lambda\lambda'} M^x_{\lambda'\lambda} M^x_{\lambda\lambda_1} M^x_{\lambda_1\lambda} n_\lambda}{(\varepsilon_\lambda - \varepsilon_{\lambda_1})^2 (\varepsilon_\lambda - \varepsilon_{\lambda'})}$$

$$- \sum_{\substack{\lambda \\ \lambda_1 \neq \lambda'}} \frac{M^x_{\lambda\lambda'} M^x_{\lambda'\lambda} M^x_{\lambda\lambda_1} M^x_{\lambda_1\lambda} n_{\lambda_1}}{(\varepsilon_\lambda - \varepsilon_{\lambda_1})^2 (\varepsilon_{\lambda_1} - \varepsilon_{\lambda'})} \Bigg], \qquad (11)$$

where

$$n_\lambda = \begin{cases} 1, & \varepsilon_\lambda - \varepsilon_0 < 0 \\ 0, & \varepsilon_\lambda - \varepsilon_0 > 0 \end{cases}.$$

Equation (11) gives a general expression for the corrections to the energy of the system arising from the rotation. The quantity E_0 is the internal energy which is independent of the rotation. The term proportional to Ω^2 corresponds to the rotational energy of a rigid body, as we have not taken pair correlations into account.

It has been shown by Migdal[2] that the first sum in (11) is equal to the moment of inertia of a rigid body. The term proportional to Ω^4 is the correction we are looking for. To evaluate it we use a simple model of a deformed axially-symmetric oscillating nuclear potential

$$U = \tfrac{1}{2} m \left[\omega_x^2 (x^2 + y^2) + \omega_z^2 z^2\right].$$

Then the operator $\dot{M}^x = m(\omega_y^2 - \omega_z^2)yz$. The matrix element $\dot{M}^x_{\lambda\lambda'}$ is different from zero for the transitions $n'_x = n_x \pm 1$, $n'_y = n_y \pm 1$. In the semiclassical approximation all possible values of $\dot{M}^x_{\lambda\lambda'}$ are the same.

One sees easily that

$$\sum_{\lambda\lambda'} |f_{\lambda\lambda'}|^2 \frac{(n_\lambda - n_{\lambda'})}{(\varepsilon_\lambda - \varepsilon_{\lambda'})} = \sum_{\lambda\lambda'} |f_{\lambda\lambda'}|^2 \delta(\varepsilon_\lambda), \qquad (12)$$

as long as $|f_{\lambda\lambda'}|^2$ changes little in the interval $(\epsilon_\lambda - \epsilon_{\lambda'})$.

By evaluating the sum over the intermediate states λ_1 and λ' one can then show that in the semiclassical approximation the first sum within the square brackets in (11) is equal to

$$\frac{1}{8d_1^6} \sum_{\lambda} [(\dot{M}^2)_{\lambda\lambda}]^2 \, \delta(\varepsilon_\lambda), \qquad (13)$$

where $d_1 = \omega_x - \omega_z = \omega_0\beta$, where ω_0 is the average oscillator frequency and β the deformation.

One can show similarly that the second sum within the square brackets in (11) is equal to

$$\frac{1}{16d_1^6} \sum_{\lambda} [(\dot{M}^2)_{\lambda\lambda}]^2 \, \delta(\varepsilon_\lambda). \qquad (14)$$

One verifies easily by a direct calculation that in the same semiclassical approximation

$$\sum_{\lambda'} (\dot{M}^2)_{\lambda\lambda'} (\dot{M}^2)_{\lambda'\lambda} = (\dot{M}^4)_{\lambda\lambda} = 4(\dot{M}^2)^2_{\lambda\lambda}. \qquad (15)$$

Using Eqs. (13), (14), and (15) we get then

$$E^{(4)} = -\frac{\Omega^4}{2^6 d_1^6} \sum_{\lambda} (\dot{M}^4)_{\lambda\lambda} \, \delta(\varepsilon_\lambda). \qquad (16)$$

On the other hand,

$$\sum_{\lambda} (\dot{M}^4)_{\lambda\lambda} \, \delta(\varepsilon_\lambda) = (\omega_x^2 - \omega_z^2) \int \rho(\varepsilon_0, \mathbf{r}) (yz)^4 \, dV, \qquad (17)$$

where

$$\rho(\varepsilon_0, \mathbf{r}) = \sum_{\lambda} \varphi^*_\lambda(\mathbf{r}) \varphi_\lambda(\mathbf{r}) \delta(\varepsilon_\lambda)$$

is the density of particles with energy ϵ_0. In the semiclassical approximation the particle density is

$$\rho(\varepsilon_0, \mathbf{r}) = 3mC\sqrt{2m(\varepsilon_0 - U)}, \qquad (18)$$

where C is a constant.

We express the sum (17) in terms of the moment of inertia and the total level density at the Fermi surface $\rho_0(\epsilon_0) = \int \rho(\epsilon_0, \mathbf{r})\, dV$. Evaluating the density and the moment of inertia, we get

$$\rho_0 = 3C\pi^2\varepsilon_0^2/\omega_0^3, \qquad J_0 = C\pi^2\varepsilon_0^4/2\omega_0^5, \qquad (19)$$

$$\sum_{\lambda} (\dot{M}^4)_{\lambda\lambda} \, \delta(\varepsilon_\lambda) = \frac{2^3 \cdot 3^3 \cdot d_1^4 J_0^2}{5\rho_0}. \qquad (20)$$

Substituting Eq. (20) into (16), and taking into account that $\Omega^2 = I(I+1)J_0^2$ we find

$$E^{(4)} = -\frac{9}{40\rho_0 J_0^2 d_1^2} I^2 (I+1)^2. \qquad (21)$$

The coefficient in front of $I^2(I+1)^2$ in the expansion of the energy of the system is usually denoted by B. Comparing the coefficient B obtained from Eq. (21) with B_V from (2), we get

$$B/B_v \sim (h\omega_v)^2 J_0/\rho_0 d_1^2. \tag{22}$$

The energy of the "vibrational" levels in a deformed nucleus is about 0.7 — 1 Mev, i.e., of the order of the energy required to break up a pair amounts to $\sim \epsilon_0 A^{-2/3}$. Since $J_0 \sim A^{5/3}/\epsilon_0$, $\rho_0 \sim A/\epsilon_0$, and $d_1 \sim \epsilon_0 A^{-2/3}$, we have $B/B_V \sim A^{2/3}$.

The formula thus yields for the energy correction arising from the coupling of the rotation to the single-particle motion an appreciably larger value than the phenomenological correction connected with the vibrations. Numerically, they turn out to be very close to one another.

When the deformation decreases, B increases, as in this model $B \sim \beta^{-2}$. A similar tendency is observed experimentally. The criterion for the applicability of perturbation theory is the condition $\beta \gg A^{-2/3}$. The theory developed here is thus applicable in the region of stable deformations where $\beta \sim A^{-1/3}$.

Let us estimate the average numerical value of the coefficients B. For the rare-earth region $h^2/J_0 \approx 13$ kev, d = 2 Mev, and $\rho_0 = 3A/2\epsilon_0 \approx 7$ Mev^{-1}. It follows then from Eq. (21) that $B_{\text{theor}} \sim 2 \times 10^{-3}$ kev, while $B_{\text{exp}} \sim 10 \times 10^{-3}$ kev. For the region of the heavy elements $h^2/J_0 = 7.4$ kev, d = 1.7 Mev, $\rho_0 \approx 10$ Mev^{-1}, and $B_{\text{theor}} \sim 0.5 \times 10^{-3}$ kev, $B_{\text{exp}} \sim 4 \times 10^{-3}$ kev.

To obtain quantitative agreement between theory and experiment it is necessary to take into account the effects of pair correlation and for small deformation also the presence of collective excitations; this will be done in subsequent papers.

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[1] V. M. Galitskii and A. B. Migdal, JETP **34**, 139 (1958), Soviet Phys. JETP **7**, 96 (1958).

[2] A. B. Migdal, JETP **37**, 249 (1959), Soviet Phys. JETP **10**, 176 (1960).

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