MOTION OF NUCLEONS IN AN ANISOTROPIC OSCILLATOR POTENTIAL WITH ACCOUNT OF SPIN-ORBIT INTERACTION

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A method is proposed for the calculation of the wave function and energy levels of nucleons moving in an oscillator potential. The general case of a potential which does not possess axial symmetry but in which account is made of spin-orbit interaction is considered. An essential feature of the calculations is that use is made of smallness of the spin-orbit coupling constant. In the limiting case of a strongly deformed nucleus the solution can be obtained in a simple analytical form. Investigation of this solution indicates that the spin-orbit interaction significantly affects the axial symmetry of the nucleus. Thus the axially symmetric shape of the nucleus becomes more stable and is the cause of the discontinuous nature of the transition from axial nuclei to nonaxial ones.

1. INTRODUCTION

HE question of the motion of a particle in an anisotropic oscillator potential with account of the spin-orbit coupling (s.o.c.) plays an important role in the treatment of bound states of individual nucleons by means of a generalized model. This problem was solved by Nilsson,¹ who calculated the wave functions and the eigenvalues of the nucleon energy for the axiallysymmetrical case (two of the three oscillator frequencies coincide).

In connection with the theory of nonaxial nuclei, developed by Davydov and his co-workers, considerable interest attaches to an investigation of motion in an oscillator field in the general, nonaxial case (all three frequencies different).

Geilikman³ calculated the equilibrium deformations of the nuclei, using the anisotropic oscillator model, and showed that the equilbrium form of the nucleus has no axial symmetry if the number of nucleons in excess of the filled shell (or holes in the shell) is more than two. No account of the s.o.c. was taken in these calculations. This raises the question of the extent to which the results of Geilikman are modified by allowance for the s.o.c. It is also clear that the s.o.c. should exert a significant influence on the wave functions of the nucleons, and must therefore be taken into account in the calculation of the magnetic and quadrupole moments of the nuclei, the β -decay half lives, and other quantities that characterize the nucleus.

In the present paper we propose a method of calculating the wave functions and eigenvalues of the energies of nucleons moving in an oscillator field for the general case of absence of axial symmetry and presence of s.o.c.

It must be noted that the method proposed here differs substantially from that of Nilsson. Nilsson employs the isotropic-oscillator representation and diagonalizes both the s.o.c. and the terms due to nonsphericity. In this connection, the matrix elements which are not diagonal in N (the principal quantum number of the shell for the isotropic oscillator) are discarded. Nilsson proposes an approximate method of allowing for these discarded elements. The inaccuracy connected with this approximation is of order ϵ_{κ} (ϵ is the nonsphericity parameter and κ is the parameter of the s.o.c.) and is comparable with the value of s.o.c. at not too small deformations. In addition, this method of allowing for the discarded terms is difficult to employ in many cases of practical importance (for example, to correct the wave functions).

The method we propose is based essentially on the smallness of the s.o.c. ($\kappa \approx 0.05$), which is diagonalized in the anisotropic-oscillator representation, and only terms of order κ^2 are discarded.

2. THE HAMILTONIAN

The Hamiltonian describing the motion of nucleons in a nuclear field with allowance for the s.o.c. has the form

$$H = H_0 + \lambda s \, [\text{grad } V(\mathbf{r}) \times \mathbf{p}], \quad H_0 = \mathbf{p}^2 / 2 + V(\mathbf{r}), \quad (1)$$

where λ is the s.o.c. constant (we use a system of units in which $M = \hbar = 1$, M is the nucleon mass).

In the case of an anisotropic oscillator potential

$$V(\mathbf{r}) = \frac{1}{2} \sum_{i} \omega_i^2 x_i^2, \qquad (2)$$

where in the general case all three parameters (frequencies) ω_1 are different and satisfy the supplementary condition $\omega_X \omega_Y \omega_Z = \omega_0^3 = \text{const.}$ Substituting (2) in (1) we obtain

$$H = \frac{1}{2} \sum_{i} (p_{i}^{2} + \omega_{i}^{2} x_{i}^{2}) + \frac{1}{2} \lambda \sum_{ikl} \varepsilon_{ikl} \sigma_{i} \omega_{k}^{2} x_{k} p_{l}, \quad (3)$$

where σ_i are the Pauli matrices.

The Hamiltonian (3) is conveniently rewritten in terms of the following representation for the operators x_k and p_k :

$$x_k = rac{1}{\sqrt{2\omega_k}} (a_k^+ + a_k), \qquad p_k = i \sqrt{\frac{\omega_k}{2}} (a_k^+ - a_k), \quad (4)$$

where a_k and a_k^+ are known operators with commutation relations

$$[a, a_l^+] = \delta_{kl}, \quad [a_k, a_l] = [a_k^+, a_l^+] = 0.$$
 (5)

In the representation considered here the operator H has to form

$$H = \frac{1}{2} \sum_{i} \omega_{i} (a_{i} a_{i}^{+} + a_{i}^{+} a_{i}) + i \times \sum_{ikl} \varepsilon_{ikl} \sigma_{i} f_{kl} a_{k}^{+} a_{l}$$
$$+ \frac{i \times 2}{2} \sum_{ikl} \varepsilon_{ikl} \sigma_{i} g_{kl} (a_{k} a_{l} - a_{k}^{+} a_{l}^{+}), \qquad (6)$$

where $\kappa = -\lambda \omega_0/2$ is the dimensionless s.o.c. parameter

$$f_{kl} = \frac{\omega_k + \omega_l}{2\omega_0} \sqrt{\omega_k \omega_l}, \qquad g_{kl} = \frac{\omega_k - \omega_l}{2\omega_0} \sqrt{\omega_k \omega_l}$$

We see from (6) that the s.o.c. operator breaks up into two terms, containing the operators a_i^+ and a_k , respectively, in the combinations $a_k^+a_l^$ and $a_ka_l^- - a_k^+a_l^+$.

We can use perturbation theory to estimate the role of these terms. In the second approximation of perturbation theory, terms of the type $a_I^{\dagger}a_k$ lead to energy denominators of the form $\omega_l + \omega_k$, which can vanish only in the limiting case as ω_k and $\omega_l \rightarrow 0$; but in this case, as is readily seen from (6), the numerator will also tend to 0, and much faster than the denominator at that. This difference in the behavior of the energy denominators, together with the smallness of the s.o.c. constant ($\kappa \sim 0.05$), makes it possible to neglect, with sufficiently good degree of accuracy (up to quantities of order κ^2) the terms containing $a_l a_k - a_l^{\dagger} a_k^{\dagger}$ in the s.o.c. operator. In this approximation, the Hamiltonian has the form

$$H = \frac{1}{2} \sum_{i} \omega_i \left(a_i a_i^+ + a_i^+ a_i \right) + i \times \sum_{ikl} \varepsilon_{ikl} \sigma_i f_{kl} a_k^+ a_l.$$
 (7)

Because all the operators a_i and a_k^+ enter into the Hamiltonian only in pairs of the form $a_i^+ a_k^-$, the matrix elements for states with different values of N (the principal quantum number of the shell) vanish, and the determination of the eigenvalues of the Hamiltonian (7) reduces to diagonalization of matrices with a finite number of dimensions for each specific value of N.

In the diagonalization of the Hamiltonian in the representation of the anisotropic oscillator without the s.o.c., the basis vectors will be denoted by $|n_X n_y n_Z \pm \rangle$ (the signs \pm correspond to spin projections $\pm \frac{1}{2}$). The matrix elements of the operators a_k are determined here by the relations

$$a_x | n_x n_y n_z \pm \rangle = V n_x | n_x - 1 n_y n_z \pm \rangle,$$

$$a_x^+ | n_x n_y n_z \pm \rangle = V \overline{n_x + 1} | n_x + 1 n_y n_z \pm \rangle$$

and analogously for a_y , a_y^+ , a_z , and a_z^+ . The solution of the Schrödinger equation with fixed N can be written in the form

$$\Psi_N = \sum_{n_x + n_y + n_z = N} C_{n_x n_y n_z \pm} | n_x n_y n_z \pm \rangle.$$
(8)

If we take into account the invariance of the Hamiltonian under rotation through an angle π about the principal axes of the ellipsoid (symmetry group D₂) and under the transformation $x_i \rightarrow x_i$, $p_i \rightarrow -p_i$, $\sigma_i \rightarrow -\sigma_i$, connected with time inversion, we find that each energy level corresponds to two solutions $\Psi_N^{(+)}$ and $\Psi_N^{(-)}$. Here the functions $\Psi_N^{(+)}$ contain only the basis vectors corresponding to the eigenvalues of the operator $U_Z =$ $\sigma_Z (-1)^{n_X + n_Y}$ of rotation through an angle π about the z axis, equal to +1, while the function $\Psi_N^{(-)}$ contains vectors corresponding to the eigenvalue -1. In addition, it is found that the coefficients C, which determine these functions, are connected by the relation

$$C_{n_x n_y n_z \pm}^{(+)} = \pm (-1)^{N - n_y} C_{n_x n_y n_z \pm}^{(-)}$$
(9)

and have the form

$$C_{n_x n_y n_z \pm}^{(+)} = i^{n_y} A_{n_x n_y n_z \pm}, \qquad (10)$$

where $A_{n_x n_y n_z}$ are real numbers.

Thus, each solution is characterized by a definite number N (N = 0, 1, 2, ...). For a given N, there are (N + 1)(N + 2) basis vectors $|n_x n_v n_z \pm >$. The diagonalization of the Hamiltonian in this representation makes it possible to construct the same number of solutions. Since the solutions of type $\Psi_N^{(+)}$ and $\Psi_N^{(-)}$ correspond to different eigenvalues of the operator U_Z , which commutes with the Hamiltonian, these functions can be obtained independently, and the corresponding secular equation will be of degree not (N + 1)(N + 2), but $\binom{1}{2}(N + 1)(N + 2)$. In addition, it is clear that there is no need for solving the equation for both $\Psi_N^{(+)}$ and $\Psi_N^{(-)}$. By obtaining $\Psi_N^{(+)}$ we can directly construct $\Psi_N^{(-)}$ from (9). Finally, relation (10) shows that each coefficient C⁽⁺⁾ is expressed through only one real number.

3. LIMITING CASES

We assume that $\omega_x \ge \omega_y \ge \omega_z$ (which obviously does not limit the generality) and consider several limiting cases.

a) Case of a strongly nonspherical with large degree of nonaxiality: $\omega_{\rm X} - \omega_{\rm Z} \gg \kappa$, $\omega_{\rm y} \gg \kappa$, $\omega_{\rm X} - \omega_{\rm y} \gg \kappa$. In this case the s.o.c. makes a contribution of order κ^2 and can be disregarded.

b) Case of strongly nonspherical nucleus with arbitrary nonaxiality: $\omega_{\rm X} - \omega_{\rm Z} \gg \kappa$, $\omega_{\rm y} - \omega_{\rm Z} \gg \kappa$, $\omega_{\rm X} - \omega_{\rm Z}$ arbitrary.

In this case, which is of great practical interest, we can discard in the s.o.c. the terms which are not diagonal in n_Z , since they give corrections of order κ^2 . We then obtain

$$H = A(N, n_{z}) + \frac{1}{2} (\omega_{x} - \omega_{y}) (a_{x}^{+} a_{x} - a_{y}^{+} a_{y})$$

+ $i \times f_{xy} (a_{x}^{+} a_{y} - a_{y}^{+} a_{x}) \sigma_{z},$
$$A(N, n_{z}) = \frac{1}{2} (\omega_{x} + \omega_{y}) (N - n_{z})$$

+ $n_{z} \omega_{z} + \frac{1}{2} (\omega_{x} + \omega_{y} + \omega_{z}).$ (11)

By means of the canonical transformation

 $a_{x}^{+'} = \cos \varphi a_{x}^{+} - i \sin \varphi a_{y}^{+}, \quad a_{x}^{'} = \cos \varphi a_{x} + i \sin \varphi a_{y},$ $a_{y}^{+'} = -i \sin \varphi a_{x}^{+} + \cos \varphi a_{y}^{+}, \quad a_{y}^{'} = i \sin \varphi a_{x} + \cos \varphi a_{y}; \quad (12)$

 $\sin \varphi = \sigma_z \sqrt{(1 - \cos 2\varphi)/2}, \qquad \cos \varphi = \sqrt{(1 + \cos 2\varphi)/2}, \\ \cos 2\varphi = \Delta/\sqrt{\Delta^2 + (2\varkappa')^2}, \qquad \Delta = (\omega_x - \omega_y)/\omega_0, \quad \varkappa' = \varkappa f_{xy}/\omega_0$ (13)

the Hamiltonian (11) assumes the form

$$H = A(N, n_z) + \frac{1}{2} \omega_0 \sqrt{\Delta^2 + (2x')^2} (a_x^+ a_x - a_y^+ a_y).$$
(14)

Since the transformation (12) is canonical, the spectrum of eigenvalues of the operators $a_X^+ a_X'$ and $a_y^+ a_y' a_y'$ will be the same as for the operators $a_X^+ a_X$ and $a_y^+ a_y$ (their eigenvalues and n_X' and n_y' are integers, including zero). Comparing (14) and (11) we reach the conclusion that an account of the

s.o.c. reduces in this case the problem of the energy levels to the problem of the oscillator without s.o.c. but with other frequencies: ω_x and ω_i are replaced by frequencies ω'_x and ω'_y such that

$$\Delta' \equiv (\omega_x - \omega_y) / \omega_0 = \sqrt{\Delta^2 + (2x')^2}. \tag{15}$$

It follows therefore that if the solution of the problem of minimum energy of the nucleus without account of the s.o.c. leads to an equilibrium value of the parameter $\Delta' = \Delta'_0$, then allowance for the s.o.c. leads to a reduction of Δ , i.e., to an increase in the nonaxiality, in accordance with the relations

$$\Delta_{0} = \sqrt[]{\Delta_{0}^{'2} - (2\mathbf{x}')^{2}}, \qquad \Delta_{0}^{'} \geqslant 2\mathbf{x}', \Delta_{0} = 0, \qquad \qquad \Delta_{0}^{'} \leqslant 2\mathbf{x}',$$
(16)

which follow from (15) and from the fact that Δ' is defined only in the region $\Delta' \ge 2\kappa'$. If Δ'_0 is found to be in the region $0 \le \Delta'_0 \le 2\kappa'$, this means, as shown in Fig. 1, that we must disregard this "nonphysical" region. The minimum energy will correspond here to the value $\Delta'_0 = 2\kappa'$ or, according to (16), $\Delta_0 = 0$.

It is seen from Fig. 1 that if a small perturbation of the nucleus changes the position of the energy minimum (dotted curve), but does not take it out of the nonspherical region, then $\Delta_0 = 0$ as before. We conclude thus that the s.o.c. stabilizes the axial form of the nucleus, making it stable with respect to small perturbations.

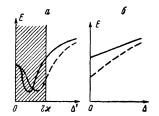


FIG. 1. Dependence of the energy of the nucleus on the nonaxiality; a – effective oscillator without s.o.c., b – real oscillator. The shaded (nonphysical) region on Fig. a corresponds to the point $\Delta = 0$ on Fig. b. The solid curve on Fig. a and the corresponding solid curve on Fig. b show the dependence of the nuclear energy on the nonaxiality; the dotted line represents the same dependence in the presence of a small perturbation.

Figure 2 shows, by way of illustration of the influence of the s.o.c. on the axiality, the dependence of nonaxiality parameter γ on the number of nucleons in the shell N = 3, obtained by Geilikman without accounting for the s.o.c., and the dependence calculated from (16) with $\kappa' = \kappa = 0.05$ and $\beta = 0.4$. The parameters β and γ are

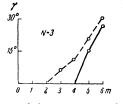


FIG. 2. Dependence of the parameter of nonaxiality of the nucleus y on the number of nucleons m in the unfilled shell (N = 3). The dotted line shows the same dependence in the absence of s.o.c., while the solid one corresponds to the presence of s.o.c.

related with the frequencies ω_X , ω_y , ω_z by equations that correspond to the usual definition of β and γ :

$$\omega_{x} = (1 + s_{0} + s_{1}) \omega (s_{0}, s_{1}), \quad \omega_{y} = (1 + s_{0} - s_{1}) \omega (s_{0}, s_{1}),$$
$$\omega_{z} = (1 - 2s_{0}) \omega (s_{0}, s_{1}),$$
$$s_{0} = \frac{1}{2} \sqrt{5/4\pi} \beta \cos \gamma, \quad s_{1} = \sqrt{15/4\pi} \beta \sin \gamma, \quad (17)$$

 ω (s₀, s₁) is determined from the requirement $\omega_X \omega_V \omega_Z = \omega_0^3$.

It is seen from Fig. 2 that the s.o.c. leads to greater stability of the axial form of the nucleus (in this case the nucleus becomes nonaxial with five external nucleons, and not with three as in the absence of s.o.c.). In addition, the transition from the axial to the nonaxial form becomes sharper — the minimum and nonaxiality amounts to $\gamma = 15^{\circ}$ and not 6.5°.

In conclusion, we determine the wave functions for this limiting case. The wave function of the state characterized by the quantum numbers n'_X , n'_Y , n_Z , and $\Sigma (\Sigma = \pm \frac{1}{2}$ is the spin projection) can obviously be written in the form Ψ^{\pm} , $= (n' + n' + n')^{-\frac{1}{2}} (n' + n'')^{\frac{n}{2}} (n'' + n'')^{\frac{n}{2}} (n' + n'')^{\frac{n}{2}} (n'' + n'')^{\frac{n}{2}} (n' + n'')^{\frac{n}{2}} (n' + n'')^{\frac{n}{2}} (n' + n'')^{\frac{n}{2}} (n'')^{\frac{n}{2}} ($

$$\Psi_{x_{x}n_{y}n_{z}}^{\mu'} = (n_{x}^{\prime}! \ n_{y}^{\prime}! \ n_{z}!)^{-l_{z}} (a_{x}^{+\prime})^{n_{x}} (a_{y}^{+\prime})^{n_{y}} (a_{z}^{+\prime})^{n_{z}} | \ 000 \pm \rangle. (18)$$

Substituting in (18) the expressions $a_X^{+\prime}$ and $a_V^{+\prime}$, according to (12), we obtain finally

$$I_{n_{x}n_{y}n_{z}}^{i_{\pm}} = (n_{x}'! \ n_{y}'! \ n_{z}!)^{-1/2} (\cos \varphi a_{\pm}^{+} - i \sin \varphi a_{\pm}^{+})^{n_{x}} \\ \times (-i \sin \varphi a_{\pm}^{+} + \cos \varphi a_{\pm}^{+})^{n_{y}'} (a_{\pm}^{+})^{n_{z}} |000 \pm \rangle.$$
(19)

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¹S. G. Nilsson, Kgl. Danske Videnskab. Selsk., Mat.-Fys. Medd., 29, No. 16 (1955).

²A. S. Davydov and G. F. Filippov, JETP **35**, 440 (1958) and **36**, 1497 (1959), Soviet Phys. JETP **8**, 303 (1959) and **9**, 1061 (1959). A. S. Davydov and V. S. Rostovskiĭ, JETP **36**, 1788 (1959), Soviet Phys. JETP **9**, 1275 (1959).

³B. T. Geĭlikman, JETP **35**, 989 (1958), Soviet Phys. JETP **8**, 690 (1959).

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