EFFECT OF DEFORMATION OF THE NUCLEUS ON THE ELECTRONIC WAVE FUNCTIONS. APPLICATION TO BETA DECAY

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The effect of the quadrupole interaction on the wave functions of an electron-nucleus system is studied. In the case of a nonspherical nucleus the electron and nuclear variables cannot be separated. This has the result that there are "satellite" nuclear and electronic angular momenta I and j, which satisfy the inequalities $|I-I_0| \leq 2$ and $|j-j_0| \leq 2$, where I_0 and j_0 are the total nuclear and electronic angular momenta in the absence of quadrupole interaction. The wave function of an electron-nucleus system for a nucleus with axial symmetry is determined by a perturbation calculation. An explicit expression is given for the wave functions in the region $r \leq R$ (R is the radius of the nucleus). The "satellite" states cause the appearance of new matrix elements, which in some cases can greatly change the value of the probability of the corresponding transitions. In the case of beta decay, for $Z \sim 70$ and $Q_0 \sim 5 \cdot 10^{-24}$ cm^2, with $\Delta I \geq 3$, where ΔI is the difference of the nuclear spins of the initial and final states, the new matrix elements can exceed by one to two orders of magnitude the values calculated without taking the nuclear-deformation effect into account.

INTRODUCTION

ELECTRONIC wave functions (e.w.f.) play an important part not only in atomic transitions but also in all nuclear processes in which electrons take part, such as β decay, internal conversion, and so on. Since in these latter phenomena the electron density in the region of the nucleus is important, the probability of such transitions must depend to a considerable degree on the finite dimensions of the nucleus. The effects of the finite size of the nucleus on the e.w.f. have been studied in a number of papers, both in connection with β decay (cf., e.g., references 1, 2) and also with internal conversion.[3,4] These treatments, however, dealt only with the nonsingular charge distribution of the nucleus and did not take into account effects of the shape of the nucleus on the e.w.f. and on nuclear transitions. To speak more exactly, in these papers it was always assumed that the nucleus is spherical. There exists in nature, however, a rather extensive class of nonspherical nuclei, for which a number of specific properties are observed, and special models must be devised to explain these properties.

It can be expected that also the e.w.f., in particular in their behavior near the nucleus, are sensitive to the shape of the nucleus, and that there are resulting effects on nuclear transitions (the influence of the form of the nucleus on nuclear transitions by means of nuclear wave functions was studied in a number of papers devoted to deformed nuclei;[5-8] a paper by Smorodinskiĭ[9] predicts an increase of the probabilities of forbidden β-decay transitions owing to effects of the dependence of the interaction constant on the shape of the nucleus). Indeed, the form of the e.w.f. is determined by the interaction of the electron with the nucleus. For spherically symmetrical nuclei this interaction is characterized by the fact that the total angular momenta of the nucleus and the electron are exact quantum numbers, in terms of which selection rules hold for the nuclear transitions.

The situation is different in the case of deformed nuclei. For example, the existence of an electric quadrupole moment destroys the spherical symmetry of the electric field of the nucleus; in this case it is already impossible to separate the electronic and nuclear variables, and we can no longer speak of electronic and nuclear states separately, but only of the state of the nucleus-electron system. In other words, instead of exactly defined electronic and nuclear angular momenta we must consider their superposition. This effect can change the selection rules, and thus also the probabilities of nuclear transitions. Under some circum-

stances these changes can be large.

In the present paper we determine, in the framework of perturbation theory, the wave functions of a system consisting of one electron and a deformed axially symmetrical nucleus. We have confined ourselves to the first approximation in the deformation parameter. We give a formula for the new functions which is suitable for the calculation of matrix elements for electron capture and β decay.

THE WAVE FUNCTIONS OF THE NUCLEUS-ELECTRON SYSTEM

The Hamiltonian of a system consisting of one electron and a nucleus is

$$H = H_n + H_e + H_{en}, \tag{1}$$

where H_n is the Hamiltonian of the nucleus, which depends only on the nuclear variables; H_e is the electron Hamiltonian, containing only the electronic variables; and H_{en} is the interaction term, depending on both the nuclear and the electronic variables.

In the calculation of the wave functions the electrostatic part of the interaction is the most important. Let us consider deformed axially symmetrical nuclei. In first approximation we can confine ourselves to a treatment of the quadrupole term (we include the monopole term, the part of the interaction independent of the angles, in H_e)

$$H_{en} = -\tfrac{1}{2} Q_0 \alpha f(r) P_2(\cos\theta_{en}), \tag{2}$$

where Q_0 is the intrinsic quadrupole moment of the nucleus, α is the fine-structure constant, and $f(r)$ is a radial function determined by the distribution of the electric charge of the nucleus (r is the distance between the electron and the center of mass of the nucleus). In the case of a distribution uniform throughout the volume of the nucleus $f(r)$ has the following form:

$$f(r) = \begin{cases} r^2/R^5 & \text{for } r \leqslant R, \\ r^{-3} & \text{for } r > R, \end{cases} \tag{3}$$

where R is the radius of the corresponding spherical nucleus; θ_{en} is the angle between the radius vector of the electron and the axis of symmetry of the nucleus.

Since H_{en} is the Hamiltonian for the interaction of the electron with the nucleus as a whole, we shall be interested in only that part of H_n that determines the orientation of the nucleus.[10] The eigenfunctions of H_n will be the symmetrical-top functions:

$$\psi_{I\mu K} = [(2I+1)/8\pi^2]^{1/2} D^{I*}_{\mu K}(\theta_n), \tag{4}$$

where θ_n are the three Euler angles of the axes of the nucleus, I is the spin of the nucleus, and K and μ are its projections on the axis of symmetry and the z axis, respectively. The phases of the $D^I_{\mu K}$ are defined as in reference 11.

H_e is the ordinary Dirac Hamiltonian[12]

$$H_e = \alpha \mathbf{p} + \beta m - eA_0(r), \tag{5}$$

where $A_0(r)$ is the monopole electrostatic potential of the nucleus. The solutions of the equations

$$H_e \varphi^0 = \varepsilon_e \varphi^0, \tag{6}$$

in the representation of j^2, j_z, ϵ_e, and the parity $(-1)^l$ have the form

$$\varphi^0_{jlj_z} = \begin{pmatrix} i g_{jl}(r) Y^{j_z}_{jl\,1/2} \\ f_{jl}(r) \frac{\sigma r}{r} Y^{j_z}_{jl\,1/2} \end{pmatrix} \equiv \begin{pmatrix} i r^{-1} \Phi^{0+}_{jl}(r) Y^{j_z}_{jl\,1/2} \\ r^{-1} \Phi^{0-}_{jl}(r) \frac{\sigma r}{r} Y^{j_z}_{jl\,1/2} \end{pmatrix}, \tag{7}$$

(we shall always omit the index ϵ_e from wave functions), where the spinors $Y^{jz}_{jl\,1/2}$ are defined as in the book of Blatt and Weisskopf.[13]

Our problem is that of solving the equation

$$H\Psi = \varepsilon\Psi, \tag{8}$$

with H_{en} playing the part of a perturbation. The unperturbed wave functions are products of the $\psi_{I\mu K}$ and $\varphi^0_{jlj_z}$. Instead of these products it is convenient to choose the linear combinations

$$\Psi^0_{FM\ldots} = \sum_{\mu + j_z = M} C(I j_0 F;\ \mu j_z)\, \psi_{I_0 \mu K} \varphi^0_{j_0 l_0 j_z}, \tag{9}$$

where F is the total angular momentum, M is its projection along the z axis, and $C(\ldots)$ are Clebsch-Gordan coefficients.[11] Since H_{en} is invariant under rotations, F and M are also exact quantum numbers for Eq. (8). Therefore we shall look for the solution of Eq. (8) in the form

$$\Psi_{FM} = \Psi^0_{FM} + \Psi^c_{FM}. \tag{10}$$

In first approximation in Q_0 the correction function Ψ^c_{FM} satisfies the equation

$$(H_n + H_e - \varepsilon_{I_0} - \varepsilon_e)\Psi^c_{FM} = (\varepsilon_c - H_{en})\Psi^0_{FM}, \tag{11}$$

where ϵ_{I_0} is the rotational energy of the nucleus and ϵ_c is the correction to the total energy of the unperturbed system. These quantities are connected by the relation

$$\varepsilon = \varepsilon_{I_0} + \varepsilon_e + \varepsilon_c. \tag{12}$$

Let us expand the function Ψ^c_{FM} in the orthonormal system

$$\chi_{FMIKjl} = \sum_{\mu + j_z = M} C(IjF;\ \mu j_z)\, \psi_{I\mu K} Y^{j_z}_{jl\,1/2}. \tag{13}$$

Then

$$\Psi^{c}_{FM..} = \begin{pmatrix} \sum_{Ijl} ir^{-1}\Phi^{+}_{Ijl}(r)\,\chi_{FMIKjl} \\ \sum_{Ijl} r^{-1}\Phi^{-}_{Ijl}(r)\,(\sigma r/r)\,\chi_{FMIKjl} \end{pmatrix}, \tag{14}$$

where the expansion coefficients $\Phi^{\pm}_{Ijl}(r)$ are radial "electronic" correction functions. To determine them, we substitute Eqs. (14) and (9) in Eq. (11). Using the properties of the functions χ_{FMIKjl}, after some simple calculations we get the following equation for $\Phi^{\pm}_{Ijl}$:

$$[d/dr \pm r^{-1}\varkappa_{jl}]\,\Phi^{\pm}_{Ijl} \mp [\bar{\varepsilon} \pm m + eA_0(r)]\,\Phi^{\mp}_{Ijl} = \pm[\varepsilon_c \delta_{II_0}\delta_{jj_0}\delta_{ll_0} + A_{Ijl;\,I_0j_0l_0} f(r)]\,\Phi^{0\mp}_{j_0l_0}; \tag{15}$$

here

$$A_{Ijl;\,I_0j_0l_0} = \tfrac{1}{2} Q_0 \alpha (-1)^{I_0+j_0-F}[(2I_0+1)(2j_0+1)(2l_0+1)(2j+1)]^{1/2} C(2I_0I;\,0K)\,C(2l_0l;\,00) \times W(II_0jj_0;\,2F)\,W(2lj_0{}^1\!/_2;\,l_0j); \tag{16}$$

$$\varkappa_{jl} = \begin{cases} -(l+1) & \text{for } j = l + 1/2, \\ l & \text{for } j = l - 1/2; \end{cases} \tag{17}$$

$$\bar{\varepsilon} = \varepsilon_e + \varepsilon_{I_0} - \varepsilon_I; \tag{18}$$

The W's are the well known Racah coefficients (cf., e.g., reference 11). From the properties of the Clebsch-Gordan and Racah coefficients in Eq. (16) it follows that the "satellite" angular momenta I, j, l are connected with the basic angular momenta by the relations

$$|I - I_0| \leqslant 2, \qquad |j - j_0| \leqslant 2, \quad l = l_0, \qquad l_0 \pm 2. \tag{19}$$

From the equations (15) one can calculate both the energy correction ϵ_c caused by the quadrupole moment and the corrections $\Phi^{\pm}_{Ijl}(r)$ to the wave functions. The calculation of ϵ_c essentially means the determination of the hyperfine splitting of the atomic levels. We shall not concern ourselves with this problem, which has been sufficiently thoroughly studied. Moreover, we shall not go into the calculation of the wave-function corrections $\Phi^{\pm}_{I_0j_0l_0}(r)$ that correspond to the basic angular momenta I_0, j_0, l_0, since they do not give new matrix elements. Accordingly, the quantity ϵ_c will always be omitted hereafter.

The relations (15) are a system of inhomogeneous equations which are to be solved with the following boundary conditions:[14]

$$\lim_{r\to 0} \Phi^{\pm} = 0, \qquad \lim_{r\to\infty} \Phi^{\pm} \neq \infty. \tag{20}$$

For $|\bar{\epsilon}| > m$ we must also impose the radiation condition.[14,15] The solution that satisfies the boundary conditions is of the form

$$\Phi^{\pm} = \frac{1}{\Phi_1^+\Phi_2^- - \Phi_1^-\Phi_2^+}\Big[\Phi_1^{\pm}\int_{\infty}^{r}(\mathcal{A}^-\Phi_2^- + \mathcal{A}^+\Phi_2^+)\,dr - \Phi_2^{\pm}\int_{0}^{r}(\mathcal{A}^-\Phi_1^- + \mathcal{A}^+\Phi_1^+)dr\Big], \tag{21}$$

$$\mathcal{A}^{\pm} = A_{Ijl;I_0j_0l_0} f(r)\,\Phi^{0\pm}_{j_0l_0}; \tag{22}$$

$\Phi_1^{\pm}$ and $\Phi_2^{\pm}$ are the two linearly independent solutions of the homogeneous equation

$$(d/dr \pm r^{-1}\varkappa_{jl})\,\Phi^{\pm} \mp (\bar{\varepsilon} \pm m + eA_0(r))\,\Phi^{\mp} = 0, \tag{23}$$

which satisfy the following boundary conditions:

$$\lim_{r\to 0}\Phi_1^{\pm} = 0, \qquad \lim_{r\to\infty}\Phi_2^{\pm} \neq \infty \qquad (\text{for } |\bar{\varepsilon}| < m); \tag{24}$$

$$\lim_{r\to\infty}\Phi_2^{\pm} \sim e^{i(pr+\delta)} \qquad (\text{for } |\bar{\varepsilon}| > m). \tag{25}$$

Here $p = (\bar{\epsilon}^2 - m^2)^{1/2}$ and δ is a radial function whose form depends on $A_0(r)$.

To get a concrete solution, we must know the spherically symmetrical potential $A_0(r)$, which determines the form of the functions $\Phi_1^{\pm}$ and $\Phi_2^{\pm}$, and the unperturbed functions $\Phi^{0\pm}$. In the choice of $A_0(r)$ the finite dimensions of the spherical nucleus should be taken into account. For simplicity we shall omit this refinement, however; this is quite permissible in determining the order of magnitude of the effect for β-decay transitions.

Thus we take A_0 to be the Coulomb potential of a point nucleus:

$$eA_0(r) = Z\alpha/r. \tag{26}$$

The corresponding functions $\Phi_1^{\pm}$ and $\Phi_2^{\pm}$ are

$$\Phi_1^{\pm} = \sqrt{1 \pm \bar{\varepsilon}/m}\,\rho^{-1/2}[(\varkappa + N_0)\,M_{N-1/2,\gamma} \mp (\gamma + N)\,M_{N+1/2,\gamma}],$$
$$\Phi_2^{\pm} = \sqrt{1 \pm \bar{\varepsilon}/m}\,\rho^{-1/2}[(\varkappa + N_0)\,W_{N-1/2,\gamma} \pm W_{N+1/2,\gamma}], \tag{27}$$
$$\rho = 2\lambda r, \qquad \lambda = \sqrt{m^2 - \bar{\varepsilon}^2} \qquad (\text{for } |\bar{\varepsilon}| < m);$$
$$\Phi_1^{\pm} = a_{\pm}\rho^{-1/2}[(\varkappa - i\nu_0)\,M_{-i\nu-1/2,\gamma} \mp (\gamma - i\nu)\,M_{-i\nu+1/2,\gamma}],$$
$$\Phi_2^{\pm} = F(\gamma) + F(-\gamma), \quad \lambda = i\sqrt{\bar{\varepsilon}^2 - m^2} \quad (\text{for } |\bar{\varepsilon}| > m), \tag{28}$$

where

$$N = Z\alpha\bar{\varepsilon}/\sqrt{m^2 - \bar{\varepsilon}^2}, \qquad N_0 = Z\alpha m/\sqrt{m^2 - \bar{\varepsilon}^2},$$
$$\gamma = \sqrt{\varkappa^2 - Z^2\alpha^2}, \qquad a_+ = \sqrt{\bar{\varepsilon}/m + 1},$$
$$a_- = i\sqrt{\bar{\varepsilon}/m - 1}, \tag{29}$$
$$\nu = Z\alpha\bar{\varepsilon}/\sqrt{\bar{\varepsilon}^2 - m^2}, \qquad \nu_0 = Z\alpha m/\sqrt{\bar{\varepsilon}^2 - m^2};$$
$$F(\gamma) = e^{i\pi\gamma}\Gamma(\gamma - i\nu)\,\Gamma(-2\gamma)\,\Phi_1^{\pm} \quad (|\bar{\varepsilon}| > m), \tag{30}$$

and $M(\rho)$ and $W(\rho)$ are the well known solutions of the Whittaker equation.[16]

As for the functions $\Phi^{0\pm}$, they are solutions of

the unperturbed equation. Here we must distinguish bound states ($\epsilon_e < m$) from unbound states ($\epsilon_e > m$). In the former case the $\Phi^{0\pm}$ are the well known electronic functions of the hydrogenlike atom, and in the latter case they are continuous-spectrum Coulomb functions.[12] The $\Phi^{0\pm}$ are normalized, and here in the determination of the normalization constants we can also take screening into account, as is usually done in the derivation of formulas for β decay.

APPLICATION TO BETA DECAY

Let us now return to the solutions (21). In the general case $\Phi^{\pm}_{1,2}$ and $\Phi^{0\pm}$ have simple forms only at very small or very large values of the argument. For β decay, however, we are interested in the behavior of the electronic functions only for $r < R$. We note that ρ, the argument of the functions $\Phi^{\pm}_{1,2}$, defined in Eq. (27), has a parametric dependence on the relation between $\bar{\epsilon}$ and m, whereas the argument of $\Phi^{0\pm}$ depends on ϵ_0/m. For strongly deformed nuclei the difference $\epsilon_{I_0} - \epsilon_I$ with $|I - I_0| \leq 2$ ordinarily does not exceed 2m (1 Mev). As for the electron's energy ϵ_e, in β decay it is limited by the energy of the transition. If we consider β-decay transitions with energies not exceeding 1 Mev (which is always the case for transitions between rotational levels), then $\bar{\epsilon} \leq 5m$ (2.5 Mev). From the relation $\rho = 2\lambda r$ for $R \sim 6 \times 10^{-13}$ cm (rare earths) and $\bar{\epsilon} = 5m$ we have $\rho(r = R) \approx 1/6$. The smaller $\bar{\epsilon}$, the smaller the error in expanding $\Phi^{\pm}$ in powers of ρ. There is another simplifying circumstance for $\rho(r = R) \leq 1$; this is that the integral

$$\int_{\infty}^{r} (\mathcal{A}^{-}\Phi_2^{-} + \mathcal{A}^{+}\Phi_2^{+})\, dr$$

in Eq. (21) is determined by the behavior of the integrand for small ρ.

In what follows we confine ourselves to the first term of the expansion in powers of ρ. Then the quantities $\Phi^{0\pm}$ have the same form both for the discrete spectrum $\epsilon_e < m$ (capture) and for the continuous spectrum $\epsilon_e > m$ (β decay):

$$\Phi^{0\pm} \underset{r\to 0}{\approx} C^{\pm}(\varepsilon_e)\, r^{\gamma_0}, \tag{31}$$

where γ_0 is the value of γ for the unperturbed state j_0, l_0. Owing to this the functions $\Phi^{\pm}$ will also be the same in this approximation for the bound and free states. As the result of calculation we get for $r \leq R$:

$$\Phi^{+}_{jl}(r) = \frac{A_{jl;l_0j_0l_0}}{R^2}\,\bar{\Phi}^{0+}_{j_0l_0}(r)\left\{\left(\frac{r}{R}\right)^{\gamma-\gamma_0}\frac{5Z\alpha\,[1 + (\varkappa - \gamma)/(\varkappa_0 - \gamma_0)]}{2\gamma(\gamma_0 + 3 - \gamma)(\gamma + 2 - \gamma_0)} - \left(\frac{r}{R}\right)^{3}\frac{Z\alpha}{(\gamma_0 + 3)^2 - \gamma^2}\left(1 + \frac{\varkappa - \gamma_0 - 3}{\varkappa_0 - \gamma_0}\right)\right\}; \tag{32}$$

$$\Phi^{-}_{jl}(r) = \frac{A_{jl;l_0j_0l_0}}{R^2}\,\Phi^{0+}_{j_0l_0}(r)\left\{\left(\frac{r}{R}\right)^{\gamma-\gamma_0}\frac{5\,[\varkappa + \gamma + Z^2\alpha^2/(\varkappa_0 - \gamma_0)]}{2\gamma(\gamma_0 + 3 - \gamma)(\gamma + 2 - \gamma_0)} - \left(\frac{r}{R}\right)^{3}\frac{1}{(\gamma_0 + 3)^2 - \gamma^2}\left(\varkappa + \gamma_0 + 3 + \frac{Z^2\alpha^2}{\varkappa_0 - \gamma_0}\right)\right\}. \tag{33}$$

It can be seen from Eqs. (32) and (33) that the correction functions depend only on ϵ_e (but not on $\bar{\epsilon}$), through the unperturbed functions. This fact is essential in applications. The proportionality between $\Phi^{\pm}$ and $\Phi^{0\pm}$ also has another consequence; namely, since in the region of the nucleus the $\Phi^{0\pm}$ have appreciable values only for small angular momenta of the electron, in practice the only important corrections will be those to states with small j_0, l_0.

It is easy to see that for β decay inclusion of the new "satellite" states can change the order of magnitude of the probabilities of forbidden transitions. In fact, for a given type of β interaction the value of the matrix element is determined by the difference ΔI of the nuclear spins of the initial and final states, and in the case of electron capture also by the electronic states j_0, l_0. The correction functions (14) contain new nuclear and electronic states, which leads to an effective decrease of the order of forbiddenness. The quantitative calculation of this effect of course depends on the type of interaction. It will be presented in another paper, in which we shall also examine the influence of the "satellite" states on the shape of the β-ray spectrum, and in which the results of calculations will be compared with the experimental data. We here mention only that at energies up to 1 Mev and with $\Delta I \geq 3$, for $Z \sim 70$ and $Q_0 \sim 5 \times 10^{-24}$ cm^2 (both for β decay and for capture) the transition probabilities can be increased by several orders of magnitude. Moreover, the matrix elements of transitions with $\Delta I = 3, 4, 5$ are of the same order of magnitude, which is not so in the case of spherical nuclei. Similar results can also be expected in the case of internal conversion.

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Note added in proof (February 13, 1960). It has recently become known to us [private communication from J. M. Pearson; see also Bull. Am. Phys. Soc. **4**, No. 4, 229 (1959)] that Pearson is now studying the influence of the nuclear quadrupole moment on the relative intensities of first-forbidden β transitions for Np^{236}. For this purpose the appropriate Dirac equations are being solved numerically. Pearson's preliminary results are negative (corrections ~ 4 percent), which agrees with the conclusion of the present paper.

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