THE ELECTRIC MULTIPOLE RADIATION OPERATOR

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Emission by a multipole of the electric type is considered without utilizing the long wavelength approximation. The analysis is carried out for quantum transitions of charged particles of spin ½ described by the Dirac equation. Using the example of x-ray radiation from heavy atoms corrections are calculated to the long wavelength approximation, and for Z = 92 these corrections turn out to be quite substantial.

IN the long wavelength approximation the operator for the interaction between an electromagnetic field of the electric type and a charged particle can be reduced[1,2] to the operator for the electric multipole moment

$$A_{\lambda\mu} = er^{\lambda} Y_{\lambda\mu}(\theta, \varphi). \tag{1}$$

This form of the operator is always utilized for considering the emission and absorption of photons both in atomic and in nuclear systems, and in the latter case the form of writing (1) expresses the content of the so-called Siegert theorem[2,3] according to which the operator for the electric multiple radiation is independent of the nature of the nuclear interaction.

However, the long wavelength approximation defined by the inequality $\omega R \ll 1$ (here ω is the frequency of the electromagnetic field, R is the size of the system), is not always applicable. For example, for electromagnetic transitions in heavy atoms this approximation is not valid in the x-ray region of the spectrum (thus, for U^{92} the wavelength of the K_{α_1} line is equal to 0.126 Å[4], and for the K- and L-shells we have respectively $\omega R_K \approx 0.3$ and $\omega R_L \approx 1$). For nuclei the inequality $\omega R \ll 1$ is of little use for the microdescription of the "giant resonances" in the region of heavy nuclei. Moreover, the use of the long wavelength approximation can turn out to be incorrect in considering certain strongly forbidden nuclear gamma-transitions, if the degree of forbiddenness is reduced for terms not taken into account in such an approximation (cf., also[5]). All this makes it of interest to go beyond the framework of the long wavelength approximation.

We consider the interaction between an electromagnetic field and charged particles of spin ½ described by the Dirac equation. The matrix element for the transition between stationary states ψ_1 and ψ_2 has the form[1]

$$U_{21} = ie\sqrt{4\pi}\int \bar{\psi}_2(\mathbf{r})\gamma_\nu A_\nu \psi_1(\mathbf{r})\, d\mathbf{r}, \tag{2}$$

where γ_ν are the Dirac matrixes (ν = 1, 2, 3, 4), A_ν are the potentials of the electromagnetic field. The specific form of A_ν for a photon of electric type of angular momentum λ and its projection μ is given, for example, in[1] (cf., the same reference for the notation not defined here).

Utilizing the equations (cf., for example,[1]) connecting the longitudinal and the transverse components of the vector potential and the scalar potential of the photon one can obtain (cf., also[5])

$$U_{21} = C\left\{\int \psi_2^+(\mathbf{r}) j_\lambda(\omega r) Y_{\lambda\mu}^* \psi_1(\mathbf{r})\, d\mathbf{r} + i\sqrt{\frac{2\lambda+1}{\lambda+1}}\int \mathbf{J}_{21} j_{\lambda+1}(\omega r)\mathbf{Y}^*_{\lambda,\lambda+1,\mu} d\mathbf{r}\right\} \tag{3}$$

where j_λ and $j_{\lambda+1}$ are the spherical Bessel functions, $\mathbf{Y}_{\lambda,\lambda+1,\mu}$ are the vector spherical harmonics[1], the current $\mathbf{J}_{21}$ is equal to

$$\mathbf{J}_{21} = \psi_2^+ \boldsymbol{\alpha} \psi_1, \tag{4a}$$

$\boldsymbol{\alpha}$ is the Dirac matrix vector,

$$C = (-)^{\lambda+1} i^\lambda e \sqrt{\frac{4\pi\omega}{R_N}}\sqrt{\frac{\lambda+1}{\lambda}}, \tag{4b}$$

R_N is the radius of the normalization sphere.

Expression (3) is rigorous. By neglecting in (3) the second term and restricting ourselves to the principal term in the expansion of $j_\lambda(\omega r)$ in powers of ωr we obtain the usual result of the long wavelength approximation with the multipole moment operator given in the form (1).

The further transformations are analogous to those which are carried out in reducing the expressions for the internal conversion coefficients to the radial integrals[1,2]. The wave function for a relativistic particle in a central field has the form[1,2]

$$\psi_{jlm} = \begin{pmatrix} ig_\kappa \Omega_{jlm} \\ f_\kappa\left(\frac{\boldsymbol{\sigma}\mathbf{r}}{r}\right)\Omega_{jlm} \end{pmatrix}, \tag{5}$$

where $g_\kappa(r)$ and $f_\kappa(r)$ are the radial wave functions, Ω_{jlm} is a spherical spinor, $\boldsymbol{\sigma}$ are the Pauli matrixes, $\kappa = \pm(j + ½)$ for $j = l \mp ½$.

Utilizing the equation

$$(\boldsymbol{\sigma}\mathbf{n})\boldsymbol{\sigma}\mathbf{Y}_{\lambda,\lambda+1,\mu} = -\sqrt{\frac{\lambda+1}{2\lambda+1}}\, Y_{\lambda\mu} - \frac{\boldsymbol{\sigma}\mathbf{L}}{\sqrt{(2\lambda+1)(\lambda+1)}} Y_{\lambda\mu} \tag{6}$$

and the properties of the functions Ω_{jlm}, we obtain

$$U_{21} = C\left\{R_1 + \frac{\varkappa_1+\lambda+2}{\lambda+1}R_2 + \frac{\varkappa_1-\lambda}{\lambda+1}R_3 + R_4\right\} \times \int \Omega^+_{j_2 l_2 m_2} Y_{\lambda\mu}^* \Omega_{j_1 l_1 m_1} \sin\theta\, d\theta\, d\varphi, \tag{7}$$

where

$$R_1 = \int g_{\varkappa_1} g_{\varkappa_2} j_\lambda r^2 dr, \qquad R_2 = \int g_{\varkappa_1} f_{\varkappa_2} j_{\lambda+1} r^2 dr,$$
$$R_3 = \int f_{\varkappa_1} g_{\varkappa_2} j_{\lambda+1} r^2 dr, \qquad R_4 = \int f_{\varkappa_1} f_{\varkappa_2} j_\lambda r^2 dr. \tag{8}$$

Utilizing (7) and carrying out the summation over the magnetic quantum numbers we obtain for the probability of the electric multipole radiation per unit time

$$\frac{1}{\tau}=2e^2\omega\,\frac{\lambda+1}{\lambda}\,(2l_1+1)\,(2l_2+1)\,(2j_2+1)\,(l_2l_1\lambda|00)^2$$
$$\times W^2\left(l_2j_2l_1j_1|\frac{1}{2},\lambda\right)\left\{R_1+\frac{\varkappa_1+\lambda+2}{\lambda+1}R_2+\frac{\varkappa_1-\lambda}{\lambda+1}R_3+R_4\right\}^2, \quad (9)$$

where $(l_2l_1\lambda\,|\,00)$ and W are respectively the Clebsch and the Racah coefficients.

If we neglect the integrals R_2, R_3, R_4, and restrict ourselves in R_1 to the first term in the expansion of $j_\lambda(\omega r)$, then we obtain the usual formula for the electric multipole radiation (the Moszkowski formula in the case of nucleons).

The ratio of the small (f_K) to the large (g_K) component of the radial wave functions depends on the choice of the field, but, generally speaking, this ratio is of order of magnitude v/c. Thus, in the nonrelativistic approximation only the integral R_1 differs from zero. However, such estimates of orders of magnitude are too rough, and the domains of applicability of strong inequalities of the type $\omega R \ll 1$ are quite indefinite. Formulas (3) and (9) give us the possibility of utilizing that approximation which is preferable in a specific case, or of avoiding the use of any approximation at all.

We consider the possible magnitude of the corrections to the long wavelength approximation on the example of x-ray transitions in heavy atoms. In Table I we give for Z = 92 the results of the calculations of the ratios of the radial integrals $R_{i=1,2,3,4}$ from (9) to the integral R_1 in the long wavelength approximation (we denote it by R_1^{lw}), i.e., the one obtained from R_1 by the replacement of $j_\lambda(\omega r)$ by the first term of the expansion $(\omega r)^\lambda/(2\lambda+1)!!$ In doing this we have taken for the electron wave functions the hydrogenlike functions taking screening into account according to Slater (the values of the effective charges Z_{eff} were chosen in the same way as in reference[6] equal to 91.7 for the K-shell, 88.7 for the L_{II}-, L_{III}-shells and 71.85 for the MV-shell). We note that we are here interested only in the magnitude of the error in the long wavelength approximation, and, therefore, the inexactness of the wave functions utilized by us does not play an essential role. For each transition the calculations were carried out for two values of ω: one was taken from the difference in the energies of the initial and the final states of the electron (the corresponding wavelength is indicated on the left) and one was taken from experiment[4] (the wavelength is given on the right hand side).

As can be seen from Table I the corrections turn out to be considerable for Z = 92. They should all the more be taken into account considering that in the calculations of the x-ray transitions (cf., for example, the classical paper by Massey and Burhop[6]) relativistic wave functions are utilized. However, in this case the long wavelength approximation has been utilized for the electric multipole operator, so that in the final analysis the quantity $R_1^{lw} + R_4^{lw}$ is calculated. But, as can be seen from Table I, such a calculation is incorrect since in carrying it out terms (R_2, R_3) are omitted which are not smaller than the term R_4^{lw} that has been taken into account, and also the approximation in the principal term (the replacement of R_1 by R_1^{lw}) leads to a greater error than the quantity R_4^{lw} that has been taken into account. Thus, the available relativistic calculations of x-ray transitions (the same also applies to the calculations based on them of the fluorescence yield[7]) are not consistently relativistic due to the use of the long wavelength approximation.

We note that in the K_{α_1} and K_{β_5} transitions considered above the values of R_i and the numbers κ_1 and λ are such that in the total matrix element

$$R=R_1+\frac{\varkappa_1+\lambda+2}{\lambda+1}R_2+\frac{\varkappa_1-\lambda}{\lambda+1}R_3+R_4$$

the corrections are to a large extent compensated (this is not the case for K_{α_2}). Without reference to the combination of the quantities R_i the deviation from the long wavelength approximation can be illustrated in calculations with nonrelativistic wave functions, when only one radial integral is present. The results of calculations with nonrelativistic functions (with the same values of Z_{eff}, as given above) are given in the second line of Table II, where we have given the ratio of the matrix elements using the operator $j_\lambda Y_{\lambda\mu}$ (the quantity R_{nr}) and using the operator $(\omega r)^\lambda Y_{\lambda\mu}/(2+1)!!$ (the quantity R_{nr}^{lw}). We note that we ascribe to these calculations a meaning only in the illustrative sense. Indeed, in accordance with (9) in the nonrelativistic approximation irrespectively of the ratio between the wavelength and the dimensions of the system one can use the operator $ej_\lambda Y_{\lambda\mu}$ instead of the operator $e(\omega r)^\lambda Y_{\lambda\mu}/(2\lambda+1)!!$. However, for atomic electrons the quantities ωR and v turns out to be of the same order of magnitude[1] and, consequently, in this case the domains of applicability of the long wavelength and the nonrelativistic approximations coincide. Therefore, for $\omega R \sim 1$ in calculations intended for a comparison with experiment one should utilize the relativistic wave functions for the atomic electrons. The ratios of the matrix elements and of the intensities of the x-ray radiation with relativistic functions without utilizing the long wavelength approximation to the corresponding quantities in the long wavelength and the nonrelativistic approximations are given in Table II (the primes denote the matrix elements and the intensities calculated using the experimental values of ω).

Table I

Transition	K_{α_1}		K_{α_2}		K_{β_5}	
Wavelength Å	0.117	0.126	0.117	0.131	0.0962	0.111
R_1/R_1^{lw}	0.81	0.87	0.91	0.97	0.73	0.92
R_2/R_1^{lw}	−0.06	−0.06	−0.05	−0.05	−0.12	−0.10
R_3/R_1^{lw}	−0.03	−0.03	0.02	0.02	−0.03	−0.02
R_4/R_1^{lw}	0.05	0.06	−0.08	−0.07	0.02	0.03

Table II

Transition	K_{α_1}	K_{α_2}	K_{β_5}
R_{nr}/R_{nr}^{lw}	0.86	0.86	0.76
R/R_{nr}^{lw}	0.75	0.70	0.74
I/I_{nr}^{lw}	0.73	0.64	0.72
R'/R'^{lw}_{nr}	0.73	0.68	0.63
I'/I'^{lw}_{nr}	0.53	0.47	0.40

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