MAGNETIC DIPOLE TRANSITION OPERATOR ACCURATE TO α^2 TERMS FOR ONE- AND TWO-ELECTRON ATOMS

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The customary expansion of atomic functions in powers of α^2 ($\alpha = e^2/\hbar c$) is insufficiently complete for the calculation of forbidden transition probabilities. Terms $\sim\alpha^2$ in the expansion of the relativistic transition operator should also be taken into account. An expression accurate to these terms is obtained for the magnetic dipole transition operator in one- and two-electron systems. Probabilities of the single-photon transitions $2s^3S-1s^1S$ and $2s^1S-2s^3S$ are calculated on the basis of his expression for hydrogen-like and helium-like ions [Eqs. (13) and (14)]. A similar expansion is also obtained for electric dipole transitions; the additional terms $\sim\alpha^2$ remove the intercombination forbiddenness for pure LS coupling.

It is known that either one or two photons can be emitted in 2s–1s transitions of H-like ions. The probability of a single-photon (magnetic dipole) transition[1)] is zero in the nonrelativistic approximation. Due to the extra $Z^4\alpha^3$ factor ($\alpha = e^2/\hbar c$ is the fine-structure constant) relativistic calculations[1,2] yield a result that is considerably smaller than for a two-photon transition.[3] A different situation exists for $2s^3S-1s^1S$ transitions in He-like ions; here two-photon transitions are considerably less probable because of additional spin forbiddenness.[4] Moreover, several previously unknown lines in experimental spectra of the solar corona[6–9] have been identified in [5] with the $2s^3S-1s^1S$ transition in He-like ions (C V, O VII, Ne IX, Si XIII, S XV, and Fe XXV). This interpretation requires that the single-photon transition probability exceed the two-photon probability. This condition is fulfilled according to a calculation of the $2s^3S-1s^1S$ single-photon decay probability in the hydrogen-like approximation,[10] although Griem's final equation is incorrect.

In the customary procedure for calculating the probabilities of transitions that are forbidden in the nonrelativistic approximation terms of the order of α^2, which take magnetic interactions into account, are added to the nonrelativistic wave function. However, this procedure yields zero probability for the aforementioned s–s transitions. (For this reason exact Dirac functions were used in [1,2].) We shall show here that this result is due to neglect of the additional α^2 term that appears when the relativistic transition operator is replaced with the corresponding nonrelativistic approximation, and we shall present expressions for additional terms $\sim\alpha^2$ in the operators for magnetic and electric dipole transitions.

We first consider one-electron atoms, for which the probability of a magnetic dipole transition from state 1 to state 0 can be written as (see Sec. 47 of [11])

$$W = \frac{4}{3}\frac{\omega^3}{\hbar c^3}\frac{1}{2J_1+1}\sum_m |\mu_{01}|^2,$$

$$\mu_{01} = \frac{e}{2c}\langle 0|g(kr)[\mathbf{rj}]|1\rangle = \frac{e\hbar}{2}[\langle\varphi_0|g(kr)[\mathbf{r\sigma}]|\chi_1\rangle - \langle\chi_0|[\boldsymbol{\sigma}\mathbf{r}]g(kr)|\varphi_1\rangle], \qquad (1)^*$$

where $\boldsymbol{\mu}$ is the magnetic dipole moment operator, $\mathbf{J}_1$ is the angular momentum of the initial state, ω is the transition frequency, $\mathbf{j}$ is the current density, $\mathbf{k}$ is the photon wave vector, φ and χ are the respective large and small components of the Dirac functions, and $\boldsymbol{\sigma}$ represents the Pauli matrices. The function g(kr) is expressed in terms of Bessel functions:

$$g(kr) = \frac{2^{3/2}\Gamma(5/2)}{(kr)^{3/2}}J_{3/2}(kr) \approx 1 - \frac{(kr)^2}{10}. \qquad (2)$$

We are not interested in other terms of (2), which are of a higher order of smallness than α^2. We note that in the widely known Breit–Teller equation[1] the term $(kr)^2/10$ is omitted; this error was corrected in [2].

The expression for the small components in terms of the large components is

$$\chi = \frac{1}{2mc}\left[\left(1+\frac{e\Phi}{2mc^2}\right)\boldsymbol{\sigma}\mathbf{p} - \boldsymbol{\sigma}\mathbf{p}\frac{H_0}{2mc^2}\right]\varphi, \qquad (3)$$

where H_0 is the nonrelativistic Hamiltonian, $e\Phi$ is the potential energy of the system, and $\mathbf{p}$ is the momentum operator. Inserting (3) into (1) and omitting terms of higher order than α^2, we obtain

$$\mu_{01} = \frac{e}{2mc}\Big[\langle\varphi_0|F[\mathbf{rp}]|\varphi_1\rangle + {}^1/_2\langle\varphi_0|iF[\mathbf{r}[\mathbf{p}\boldsymbol{\sigma}]]|\varphi_1\rangle - \frac{1}{2}\langle\varphi_0|[[\boldsymbol{\sigma}\mathbf{p}]\mathbf{r}]iF|\varphi_1\rangle - \frac{1}{2}\left\langle\varphi_0\left|i\frac{\{[\mathbf{r}[\mathbf{p}\boldsymbol{\sigma}]],H_0\}}{2mc^2}\right|\varphi_1\right\rangle\Big],$$

$$F = 1 + \frac{e\Phi-\varepsilon_0}{2mc^2} - \frac{1}{10}(kr)^2, \qquad (4)$$

where ϵ_0 is the energy of state 0 and $\{A, B\}$ is the commutator of the operators A and B. We have thus far assumed that φ_0, φ_1 are the "large" components of the exact Dirac functions. The transition to nonrelativistic functions ψ follows the rule $\varphi \to (1 - p^2/8m^2c^2)\psi$ [Sec. 33 of [11]], where ψ satisfies the ordinary Schrö-

[1)] The electric dipole transition is parity forbidden, while transitions of higher multipolarities conflict with angular momentum conservation.

*$[\mathbf{rj}] \equiv \mathbf{r}\times\mathbf{j}$.

dinger equation. Relativistic α^2 corrections to ψ will be discussed below.

For the operator $\boldsymbol{\mu}$ we finally obtain

$$\boldsymbol{\mu}=\frac{e\hbar}{2mc}\mathbf{l}\left[1+\frac{e\Phi-\varepsilon_0}{2mc^2}-\frac{1}{10}(kr)^2-\frac{p^2}{4m^2c^2}\right]+\frac{e\hbar}{mc}\mathbf{s}\left[1+\frac{1}{2mc^2}\left(e\Phi+\frac{e}{3}\mathbf{r}\nabla\Phi-\frac{1}{3}\left\{\frac{p^2}{m}-\mathbf{r}\nabla\Phi\right\}\right)-\frac{1}{6}(kr)^2-\frac{p^2}{4m^2c^2}\right]+\frac{e\hbar}{mc}\frac{1}{6}\left[\mathbf{s}(\mathbf{r}\nabla f)-3(\mathbf{rs})\nabla f-\frac{1}{2mc^2}\left(\mathbf{s}\frac{p^2}{m}-3\frac{\mathbf{p}}{m}(\mathbf{ps})\right)\right],\tag{5}$$

$$f=\frac{e\Phi}{mc^2}-\frac{1}{10}(kr)^2.$$

It is reasonable to divide $\boldsymbol{\mu}$ into two parts, $\boldsymbol{\mu}'=(e\hbar/2mc)(\mathbf{l}+2\mathbf{s})$ and $\boldsymbol{\mu}''$, which is proportional to α^2. We shall discuss in some detail the physical meanings of the different terms in $\boldsymbol{\mu}''$. The operator $p^2/4mc^2$ is associated with the "pure" nonorthogonality of the large components of the Dirac functions; the terms containing (kr) arise by taking into account a "retardation" effect; the remaining terms are determined by the ratio between the Coulomb interaction energy and the rest energy of an electron [compare with Eq. (3)].

We note that $\boldsymbol{\mu}''$ contains a quadrupole term[2)] in addition to the terms with vector properties similar to the properties of the orbital angular momentum $\mathbf{l}$ and spin $\mathbf{s}$ operators in $\boldsymbol{\mu}'$.

We have thus far neglected relativistic corrections of the order of α^2 in the wave functions.[3)] When these corrections are included we have for the transition matrix element accurate to α^2 terms (with V representing the perturbation of α^2 order and H_0 as the nonrelativistic Hamiltonian)

$$\tilde{\psi}=\psi-\frac{1}{H_0-\varepsilon}V\psi,\tag{6}$$

$$\langle\tilde{\psi}_0|\boldsymbol{\mu}|\tilde{\psi}_1\rangle=\langle\psi_0|\boldsymbol{\mu}|\psi_1\rangle-\left\langle\psi_0\left|V\frac{1}{H_0-\varepsilon_0}\boldsymbol{\mu}'+\boldsymbol{\mu}'\frac{1}{H_0-\varepsilon_1}V\right|\psi_1\right\rangle.$$

Utilizing $\boldsymbol{\mu}'=(e\hbar/mc)(\mathbf{J}-\mathbf{l})$ (where $\mathbf{J}$ is the total angular momentum) and the vanishing of the commutators $\{\boldsymbol{\mu}', H_0\}$ and $\{\mathbf{J}, V\}$, we transform the second term into

$$\frac{e\hbar}{mc}\frac{1}{\varepsilon_0-\varepsilon_1}\langle\psi_0|\{V,\mathbf{l}\}|\psi_1\rangle.$$

This expression vanishes identically for s–s transitions. Thus the probability of a 2s–1s single-photon transition is nonvanishing only because of the term $\langle\psi_0|\boldsymbol{\mu}''|\psi_1\rangle$.

A calculation based on (5), with only the term proportional to the spin operator $\mathbf{s}$ remaining, yields

$$W(2s-1s)=\frac{\alpha^9Z^{10}}{972}\frac{me^4}{\hbar^3}.\tag{7}$$

This result agrees with the calculations in [3].

[2)] It is easily seen that for s–s transitions this term, like the term proportional to $\mathbf{l}$, does not contribute to the transition matrix element.

[3)] The difference between the foregoing corrections and corrections made directly to the nonrelativistic function actually consists in the fact that corrections such as (3) and (5) are corrections to χ. The operator changes because the ordinary nonrelativistic theory contains nothing analogous to the small components of the relativistic functions.

We now consider two-electron atoms, writing the Hamiltonian in the form

$$H=c\boldsymbol{\alpha}_1\mathbf{p}_1+\beta_1m_1c^2+c\boldsymbol{\alpha}_2\mathbf{p}_2+\beta_2m_2c^2+e\Phi+V.\tag{8}$$

Here $\boldsymbol{\alpha}_1$, $\boldsymbol{\alpha}_2$, β_1, β_2 are the Dirac matrices operating on the coordinates of the first and second electrons,

$$e\Phi=-\frac{Ze^2}{r_1}-\frac{Ze^2}{r_2}+\frac{e^2}{r_{12}}$$

is the nonrelativistic potential energy, and V is the operator of magnetic and delayed interelectronic interactions. The specific form of V is not required, but only that its order of magnitude be $\sim\alpha^2$. We introduce the following notation for the large and small components of the 16-component function ψ:

$$\psi_{ik}=\begin{cases}\varphi, & i\leqslant 2,\ k\leqslant 2,\\ \chi^{(1)}, & i>2,\ k\leqslant 2,\\ \chi^{(2)}, & i\leqslant 2,\ k>2,\\ \chi, & i>2,\ k>2.\end{cases}\tag{9}$$

Regarding the φ components as "large," the customary expansion in powers of α gives the other components:

$$\chi^{(1)}=\frac{1}{2mc}\left[\left(1+\frac{1}{2mc^2}\left\{e\Phi+\frac{p_2^2}{2m}\right\}\right)(\boldsymbol{\sigma}_1\mathbf{p}_1)-(\boldsymbol{\sigma}_1\mathbf{p}_1)\frac{H_0}{2mc^2}\right]\varphi,$$

$$\chi^{(2)}=\frac{1}{2mc}\left[\left(1+\frac{1}{2mc^2}\left\{e\Phi+\frac{p_1^2}{2m}\right\}\right)(\boldsymbol{\sigma}_2\mathbf{p}_2)-(\boldsymbol{\sigma}_2\mathbf{p}_2)\frac{H_0}{2mc^2}\right]\varphi,$$

$$\chi=\frac{(\boldsymbol{\sigma}_1\mathbf{p}_1)(\boldsymbol{\sigma}_2\mathbf{p}_2)}{4(mc)^2}\varphi.\tag{10}$$

Here H_0 is the ordinary nonrelativistic Hamiltonian for a two-electron atom. The matrix element of the magnetic moment is

$$\boldsymbol{\mu}_{01}=\frac{e}{2c}\langle 0|g(kr_1)[\mathbf{r}_1\mathbf{j}_1]+g(kr_2)[\mathbf{r}_2\mathbf{j}_2]|1\rangle.\tag{11}$$

The subsequent calculations are performed like those for one-electron systems. For the relation between the φ components and the nonrelativistic wave function ψ we have

$$\varphi\to(1-(p_1^2+p_2^2)/8m^2c^2)\psi.$$

Finally, for the operator $\boldsymbol{\mu}$ we obtain

$$\boldsymbol{\mu}=\boldsymbol{\mu}^{(1)}+\boldsymbol{\mu}^{(2)},$$

$$\boldsymbol{\mu}^{(1)}=\frac{e\hbar}{2mc}\mathbf{l}_1\left[1+\frac{e\Phi-\varepsilon_0}{2mc^2}-\frac{1}{10}(kr_1)^2-\frac{p_1^2-p_2^2}{4m^2c^2}\right]+\frac{e\hbar}{mc}\mathbf{s}_1\left(1+\frac{1}{2mc^2}\left\{e\Phi+\frac{1}{3}\mathbf{r}_1\nabla_1e\Phi-\frac{1}{3}\left(\frac{p_1^2}{m}-\mathbf{r}_1\nabla_1e\Phi\right)\right\}-\frac{1}{6}(kr_1)^2-\frac{1}{4m^2c^2}(p_1^2-p_2^2)\right)+\frac{e\hbar}{mc}\frac{1}{6}\left[(\mathbf{s}_1(\mathbf{r}_1\nabla_1f)-3(\mathbf{r}_1\mathbf{s}_1)\nabla_1f)-\frac{1}{2mc^2}\left(\mathbf{s}_1\frac{p_1^2}{m}-3\frac{\mathbf{p}_1}{m}(\mathbf{p}_1\mathbf{s}_1)\right)\right].\tag{12}$$

The expression for $\boldsymbol{\mu}^{(2)}$ is obtained simply by changing the indices in (12). As in the case of a one-electron atom [see Eq. (6)], the operator V makes no contribution to the transition matrix element.

We used (12) to calculate the probabilities of $2s\,^3S-1s\,^1S$ and $2s\,^1S-2s\,^3S$ single-photon transitions in He-like ions. Since we are interested mainly in atoms that are in a high stage of ionization, it is feasible to construct the nonrelativistic wave functions by means of perturbation theory in terms of the interelectronic interaction term $1/r_{12}$.[12] For the $2s^3S-1s^1S$ transition probability we obtain

$$W(2s^3S-1s^1S)=\frac{2^5}{3^9}\alpha^9 Z^{10}\left(\frac{\Delta E}{Z^2\mathrm{Ry}}\right)^3\left\{1+\frac{1}{Z}0.28\right\}^2\frac{me^4}{\hbar^3}. \quad (13)$$

This probability is about four orders greater than that of two-photon decay;[4] therefore the $2s^3S-1s^1S$ line should be extremely intense in the case of a highly rarefied plasma.

We obtain, similarly,

$$W(2s^1S-2s^3S)=\frac{3}{2^7}\alpha^9 Z^{10}\left(\frac{\Delta E}{Z^2\mathrm{Ry}}\right)^3\frac{me^4}{\hbar^3}. \quad (14)$$

Unlike the $2s^3S-1s^1S$ line, this line is very weak even in a rarefied plasma, because the probability (14) is considerably smaller than that of $2s^1S-1s^1S$ two-photon decay.[4]

The lifetime of the $2s^3S$ level of Ar XVII was measured in recent work.[13] The value 172 ± 30 nsec that was obtained is consistent with (13), which yields 196 nsec.

We note, in conclusion, that a similar expansion for the electric dipole transition operator leads to replacement of the operator $\mathbf{r}$ by

$$\mathbf{r}\to\mathbf{r}+[\mathbf{ps}]/8m^2c^2. \quad (15)$$

When in (14) the term added to $\mathbf{r}$ is taken into account along with the usual magnetic interactions we find that intercombination transitions are possible even in the case of "pure" LS coupling. The power of $Z\alpha$ is then the same as for the spin-spin and spin-other orbit interactions, but is Z^2 times smaller than for the spin-(same) orbit interaction.

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