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1991 J. Phys. A: Math. Gen. 24 5665

(http://iopscience.iop.org/0305-4470/24/23/028)

J. Phys. A: Math. Gen. 24 (1991) 5665–5674. Printed in the UK

Quantum electrodynamical theory for the natural shape of the spectral line

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Received 18 February 1991, in final form 9 July 1991

Abstract. In order to study the natural spectral line shape in the framework of quantum electrodynamics the resonance photon scattering on the relativistic few-electron atom is considered. The general case of the few overlapping levels is studied. In the resonance approximation the calculation formulae for the differential and total scattering cross-sections are obtained. The equations allowing improvement of the resonance approximation are also derived.

1. Introduction

For the first time the shape of the spectral lines corresponding to transitions between the levels of a non-relativistic atom has been considered by Weisskopf and Wigner [1] with the use of quantum mechanics. A consistent theory of the spectral line shape can be developed, however, only in the framework of quantum electrodynamics (QED). Such a theory has been constructed by Low [2] for the one-electron atom. Low considered the resonance photon scattering on the atom in its ground state. This avoided difficulties in the choice of the initial conditions. The Low method is renormalizable and it allows improvement of the resonance approximation.

In recent years interest in the QED theory of the spectral line shape has greatly increased [3–7] in connection with the astrophysical and laboratorial investigations of the multiply charged ions in which the QED effects can be considerable. Investigations of the spectral line shape of the multiply charged ions are especially interesting in connection with the fact that in the spectra of such ions the two overlapping levels with equal quantum numbers can be found [4, 5, 7].

The natural shape of the atomic spectral lines of the relativistic few-electron atom was studied in [3–7]. So the decay of the system prepared at the time $t = 0$ was studied with the use of the adiabatic formalism of Gell-Mann and Low in [3–5]. The time development of quasistationary atomic levels was considered by using the technique of Green functions in [6]. The spectral line shape was also considered with the help of the method based on an expansion in the number of the particles [7].

Since in these works [3–7] the decay of the atomic state produced at the time $t = 0$ is considered, the problem of the correct choice of the initial conditions arises. This problem, to my mind, is especially relevant in the case of the overlapping levels with equal quantum numbers. In order to avoid this problem, in the present work the whole process, starting from the formation of the excited atom and finishing with its decay to the stable products, is studied, i.e. the scattering of the stable particles with formation

0305-4470/91/235665+10$03.50

of the intermediate unstable ones is considered. In such a process we consider the resonance photon scattering on the relativistic few-electron atom, i.e. the Low results are generalized in the case of the few-electron atoms. In principle, our approach is also applicable for the other possible cases of the formation of the excited atom.

In QED, as is known, the transition from the one-electron atom to the few-electron atom is not trivial and requires special methods. The present work is based on the Green function method version proposed in [8, 9].

In section 2 of the present paper, perturbation theory for the calculation of the relativistic few-electron atom is formulated. In section 3, the reduction formulae for the amplitude of the photon scattering on the few-electron atom are derived. The resonance scattering and the natural spectral line shape are considered in section 4.

2. Perturbation theory for the calculation of the relativistic few-electron atom

For simplicity, we shall suppose that in the zeroth approximation the electrons of the atom considered in the framework of QED interact only with the Coulomb field of the nucleus (the Furry picture). This corresponds to the case of the multiply charged ions (the relativistic few-electron atoms). In the case of the heavy atoms the Dirac–Fock approximation can be used as zeroth order [10]. This leads to the appearance in the Feynman diagrams of the vertices corresponding to the interaction of the electrons with the additional external field $-V_{\mathrm{HF}}$.

For the description of the relativistic few-electron atom we consider the Green function of the N-electron system in the external field of the nucleus

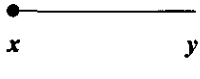
$$G(x'_1,\ldots,x'_N;x_1,\ldots,x_N)=\langle 0|T\psi(x'_1)\ldots\psi(x'_N)\bar{\psi}(x_1)\ldots\bar{\psi}(x_N)|0\rangle \tag{1}$$

where $\psi(x)$ are Heisenberg field operators for the electrons, $\bar{\psi}=\psi^{+}\gamma^{0}$, T is the time-ordered product. In what follows, we shall work with the Green function in the mixed representation

$$\begin{aligned}G(p'^{0}_1,\ldots,p'^{0}_N;p^{0}_1,\ldots,p^{0}_N)=(2\pi)^{-2N}\int_{-\infty}^{\infty}\mathrm{d}x^{0}_1\ldots\mathrm{d}x^{0}_N\,\mathrm{d}x'^{0}_1\ldots\mathrm{d}x'^{0}_N\\ \times\exp(\mathrm{i}p'^{0}_1x'^{0}_1\ldots+\mathrm{i}p'^{0}_Nx'^{0}_N-\mathrm{i}p^{0}_1x^{0}_1\ldots-\mathrm{i}p^{0}_Nx^{0}_N)\\ \times G(x'^{0}_1,\ldots,x'^{0}_N;x^{0}_1,\ldots,x^{0}_N).\end{aligned} \tag{2}$$

For the Green function $G(p'^{0}_1,\ldots,p'^{0}_N;p^{0}_1,\ldots,p^{0}_N)$ the following Feynman rules take place:

(i) External electron line



$$\left(\frac{\mathrm{i}}{2\pi}\right)S(\omega,x,y)$$

where

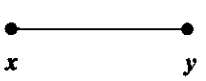
$$S(\omega,x,y)=\sum_n\frac{\psi_n(x)\bar{\psi}_n(y)}{\omega-\varepsilon_n(1-\mathrm{i}0)}$$

$\psi_n(x)$ are solutions of the Dirac equation

$$\left(\boldsymbol{\alpha}\boldsymbol{p}+\beta m-\frac{\alpha Z}{r}\right)\psi_n=\varepsilon_n\psi_n$$

(We use relativistic units $\hbar=c=1$.)

(ii) Internal electron line

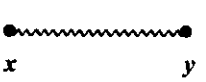


$$\left(\frac{\mathrm{i}}{2\pi}\right)\int_{-\infty}^{\infty} \mathrm{d}\omega\, S(\omega, x, y).$$

(iii) Separate electron line, which is not connected with the others

$$\left(\frac{\mathrm{i}}{2\pi}\right) S(\omega, x, y)\delta(\omega-\omega').$$

(iv) Internal photon line



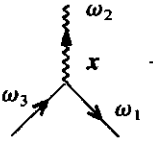
$$\left(\frac{\mathrm{i}}{2\pi}\right)\int_{-\infty}^{\infty} \mathrm{d}\omega\, D_{\mu\nu}(\omega, x-y)$$

where $D_{\mu\nu}(w, x-y)$ is given by

$$D_{\mu\nu}(\omega, x-y) = -g_{\mu\nu}\int \frac{\exp(\mathrm{i}k(x-y))}{\omega^2-k^2+\mathrm{i}0}\,\frac{\mathrm{d}k}{(2\pi)^3}$$

in Feynman gauge.

(v) Vertex



$$-\mathrm{i}e\gamma_\mu 2\pi\delta(\omega_3-\omega_2-\omega_1)\int \mathrm{d}x.$$

(vi) Symmetry factor $(-1)^P$, where P is the parity of the permutation of the outgoing electrons with respect to the incoming ones. Minus sign for every closed fermion loop.

We note that we are constructing the perturbation theory with the usual QED vacuum. The transition to the hole formalism in which the closed shells are considered as the vacuum can be carried out by changing the sign of i0 in the electron propagator denominators corresponding to the closed shells.

Let us consider the atomic energy levels $E^{(1)}, \ldots, E^{(m)}$ coming from the m-multiply degenerate unperturbed level with the energy $E^{(0)}$ (the case of the quasidegenerate levels can be considered in the same way). We assume, as usual, that the value of the splitting of the level $E^{(0)}$ due to the interaction is much smaller than the distance from the other levels. The unperturbed states corresponding to the level $E^{(0)}$ form the m-dimensional space Ω, the projector on which we designate by $P_0 = \Sigma_{k=1}^{m} u_k u_k^+$, where u_k are the unperturbed wavefunctions.

To exclude the variables of the relative energies in the Green function we introduce, following the idea of quasipotential approach [11], the Green function g

$$g(E)\delta(E-E') = \frac{2\pi}{\mathrm{i}}\frac{1}{N!}\int_{-\infty}^{\infty} \mathrm{d}p_1^0 \ldots \mathrm{d}p_N^0\, \mathrm{d}p_1'^0 \ldots \mathrm{d}p_N'^0\, \delta(E-p_1^0 \ldots -p_N^0)\delta(E'-p_1'^0 \ldots -p_N'^0)$$
$$\times P_0 G(p_1'^0, \ldots, p_N'^0; p_1^0, \ldots, p_N^0)\gamma_1^0 \ldots \gamma_N^0 P_0. \tag{3}$$

In the zeroth approximation one can obtain

$$g_0(E) = \frac{P_0}{(E-E^{(0)})}.$$

The spectral representation of the Green function $g(E)$ gives

$$g(E)=\sum_{k=1}^{m}\frac{\varphi_k\varphi_k^{+}}{E-E^{(k)}}+\text{terms that are regular by } E\sim E^{(0)}. \tag{4}$$

It is clear from the definition of $g(E)$ that the vectors $\{\varphi_k\}_{k=1}^{m}$ belong to the space Ω.

We now construct the perturbation theory in the Rayleigh–Schrödinger form in a manner similar to what was done in the operator theory by Nagy and Kato [12–14]. Choosing the integration contour Γ so that it surrounds the levels $E^{(1)},\dots,E^{(m)}$ and does not surround the other levels, we obtain the equation [8, 9]

$$HPv_k=E^{(k)}Pv_k \tag{5}$$

where

$$HP\equiv\frac{1}{2\pi i}\oint_{\Gamma}dE\,Eg(E)\qquad P\equiv\frac{1}{2\pi i}\oint_{\Gamma}dE\,g(E)$$

$\{v_k\}_{k=1}^{m}$ is the set of the vectors that are biorthogonal to the set $\{\varphi_k\}_{k=1}^{m}$, i.e.

$$\varphi_k^{+}v_{k'}=\delta_{k,k'}.$$

From this we obtain the normalization condition for v_k

$$v_k^{+}Pv_{k'}=\delta_{k,k'}. \tag{6}$$

The condition of solvability of (5) gives the equation for the determination of the energy levels of the atom

$$\det(HP-EP)=0. \tag{7}$$

Introducing $\Delta g\equiv g-g_0$ we obtain

$$\det\left\{(E-E^{(0)})\left(\delta_{ik}+\frac{1}{2\pi i}\oint_{\Gamma}dE\,\Delta g_{ik}(E)\right)-\frac{1}{2\pi i}\oint_{\Gamma}dE(E-E^{(0)})\Delta g_{ik}(E)\right\}=0 \tag{8}$$

where $\Delta g_{ik}=u_i^{+}\Delta g u_k$. For an undegenerate state n (8) gives

$$\Delta E_n\equiv E_n-E_n^{(0)}=\frac{1}{2\pi i}\oint_{\Gamma}dE(E-E_n^{(0)})\Delta g_{nn}(E)\left(1+\frac{1}{2\pi i}\oint_{\Gamma}dE\,\Delta g_{nn}(E)\right)^{-1}. \tag{9}$$

Equation (5) with the normalization condition (6) can be transformed to the Schrödinger-like equation

$$H\psi_k=E^{(k)}\psi_k \tag{10}$$

with the normalization condition

$$\psi_k^{+}\psi_{k'}=\delta_{k,k'} \tag{11}$$

where

$$\psi_k\equiv P^{1/2}v_k\qquad H\equiv P^{-1/2}(HP)P^{-1/2}.$$

The calculation according to formulae (3), (8) and (9) can be simplified in the case of the diagrams in which the N-electron states out of Ω are not encountered as intermediate states. We shall call this diagram irreducible. It is clear that the contribution in Δg from this diagram can be written in the form

$$\Delta g_{ir}(E)=g_0(E)\tilde{T}(E)g_0(E)$$

where $\tilde{T}(E)$ is an operator that is regular by $E\sim E^{(0)}$. From this it follows that a

non-zero contribution to the integral

$$\frac{1}{2\pi i}\oint_{\Gamma} dE(E-E^{(0)})\Delta g_{ir}(E)$$

can be obtained only from those terms in which by integration over the variables $p_1^0,\ldots,p_N^0, p_1'^0,\ldots,p_N'^0$ after the disappearance of all the δ-functions only the residuals in poles coming from the states out of Ω are taken into account. In reality, the same simplification can also be made in the case of the reducible diagrams.

By the derivation of formulae (5)-(11) we assumed that the Green function has the isolated poles corresponding to discrete states of the atom. In reality, because of zero photon mass the Green function $g(E)$ is regular in the complex plane E with the cuts beginning from the discrete energy levels. To make our formulae (5)-(11) correct we introduce a photon mass μ. We suppose that the photon mass μ is much larger than the distance between the considered levels and much smaller than the distance from the other levels. In every order of the perturbation theory after taking into account the whole gauge-invariant diagram set both the energy levels $E^{(k)}$ and the operator H in (10) will be regular by $\mu\to 0$. It follows that at the end of the calculations we can set $\mu=0$.

In concluding this section we note that (5)-(7), (10) and (11) are also suitable for the case of quasidegenerate levels.

3. Photon scattering on the atom

In the framework of the formalism considered in the present work we shall derive the reduction formula for the amplitude of the photon scattering on the atom.

In order to avoid difficulty in studying the external lines in the S-matrix we shall suppose, following [15], that the interaction with the Coulomb field of the nucleus is not included in the unperturbed action. Thus, in the Feynman diagrams the vertices in which the line corresponding to the Coulomb field joins with the electron line appear. Since in our case the Coulomb field is strong we shall sum up over all insertions of the vertices with the Coulomb field in the electron lines. In that way we replace the propagators and the wavefunctions of the free electron with the propagators and the wavefunctions of the electron in the Coulomb field. The constants of the renormalization, Z_2 and Z_3, will be the same as for the theory without the external field.

Let us consider the scattering of a photon with the momentum k_i and the polarization ε_i on the relativistic few-electron atom in the state m. As the result of the scattering the photon with the moment k_f and the polarization ε_f arises, and the atom comes to the state n. The transition amplitude is [16]

$$\begin{aligned}
S_{n,\gamma_f;m,\gamma_i} &= \langle n|a_{\text{out}}(k_f,\varepsilon_f)a_{\text{in}}^{+}(k_i,\varepsilon_i)|m\rangle \\
&= \text{Discon. term} - Z_3^{-1}\int d^4y\, d^4z \frac{\varepsilon_f^{\mu} e^{ik_f\cdot y}}{\sqrt{2k_f^0(2\pi)^3}} \\
&\quad \times \frac{\varepsilon_i^{\nu} e^{-ik_i\cdot z}}{\sqrt{2k_i^0(2\pi)^3}} \langle n|T(j_\mu(y)j_\nu(z))|m\rangle = \text{Discon. term} \\
&\quad - Z_3^{-1} 2\pi\delta(k_f^0+E_n-k_i^0-E_m)\int dy\, dz\, dt \frac{\varepsilon_f^{\mu} e^{-ik_f y}}{\sqrt{2k_f^0(2\pi)^3}} \\
&\quad \times \frac{\varepsilon_i^{\nu} e^{ik_i z}}{\sqrt{2k_i^0(2\pi)^3}} e^{ik_f^0 t}\langle n|T(j_\mu(y,t)j_\nu(z,0))|m\rangle
\end{aligned} \tag{12}$$

where $j_\mu(x)=(e/2)[\bar\psi(x)\gamma_\mu,\psi(x)]$ is the electron current operator, $|m\rangle$, $|n\rangle$ are vectors of the initial and final states in the Heisenberg representation. The first term in the right-hand side of (12) corresponds to the case when the photon does not interact with the atom. We are interested in the second term, which corresponds exactly to the photon scattering on the atom. Let us designate it by $S^{\rm scat}_{n,\gamma_f;m,\gamma_i}$.

In order to derive the formulae for $S^{\rm scat}_{n,\gamma_f;m,\gamma_i}$ we pick out in the scattering amplitude the term corresponding to the photon scattering only by external field. With this in mind we write

$$\langle n|Tj(y)j(z)|m\rangle=\langle n|(Tj(y)j(z)-\langle 0|Tj(y)j(z)|0\rangle)|m\rangle+\delta_{nm}\langle 0|Tj(y)j(z)|0\rangle. \tag{13}$$

Here the second term corresponds to the photon scattering only by the external field, and the first term corresponds to the scattering by the atomic electrons. For the calculation of the contribution in the scattering amplitude from the first term which we designate by $\langle n|Tj(y)j(z)|m\rangle_{\rm con}$ we introduce the Green function

$$\begin{aligned}
&\delta(E+k_i^0-E'-k_f^0)g^{\rm con}_{\gamma_f,\gamma_i}(E',E,k_f^0)\\
&\quad=\frac{1}{N!}P_0^{(n)}\int_{-\infty}^{\infty}{\rm d}p_1^0\ldots{\rm d}p_N^0\,{\rm d}p_1'^0\ldots{\rm d}p_N'^0\\
&\quad\times\delta(E-p_1^0\ldots-p_N^0)\delta(E'-p_1'^0\ldots-p_N'^0)\\
&\quad\times G^{\rm con}_{\gamma_f,\gamma_i}(p_1'^0,\ldots,p_N'^0,k_f^0,k_i^0,p_1^0,\ldots,p_N^0)\gamma_1^0\ldots\gamma_N^0P_0^{(m)}
\end{aligned}\tag{14}$$

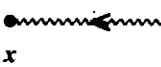
$$\begin{aligned}
&G^{\rm con}_{\gamma_f,\gamma_i}(p_1'^0,\ldots,p_N'^0,k_f^0,k_i^0,p_1^0,\ldots,p_N^0)\\
&\quad=-\frac{1}{(2\pi)^{2N}}\int{\rm d}x_1^0\ldots{\rm d}x_N^0\,{\rm d}x_1'^0\ldots{\rm d}x_N'^0\,{\rm d}y\,{\rm d}z\frac{\varepsilon_f^\nu\,{\rm e}^{-{\rm i}k_fy}}{\sqrt{2k_f^0(2\pi)^3}}\frac{\varepsilon_i^\mu\,{\rm e}^{{\rm i}k_iz}}{\sqrt{2k_i^0(2\pi)^3}}\\
&\quad\times\exp({\rm i}\,p_1'^0x_1'^0\ldots+{\rm i}p_N'^0x_N'^0-{\rm i}p_1^0x_1^0\ldots-{\rm i}p_N^0x_N^0+{\rm i}k_f^0y^0-{\rm i}k_i^0z^0)\\
&\quad\times\{\langle 0|T\psi(x_1')\ldots\psi(x_N')j_\nu(y)j_\mu(z)\bar\psi(x_1)\ldots\bar\psi(x_N)|0\rangle\\
&\quad-\langle 0|T\psi(x_1')\ldots\psi(x_N')\bar\psi(x_1)\ldots\bar\psi(x_N)|0\rangle\langle 0|Tj_\nu(y)j_\mu(z)|0\rangle\}.
\end{aligned}\tag{15}$$

From the spectral representation of $g^{\rm con}_{\gamma_f,\gamma_i}(E',E,k_f^0)$ we obtain

$$\begin{aligned}
S^{\rm con}_{\gamma_f,n;\gamma_i,m}&\equiv-Z_3^{-1}\int{\rm d}^4y\,{\rm d}^4z\frac{\varepsilon_f^\mu\,{\rm e}^{{\rm i}k_f\cdot y}}{\sqrt{2k_f^0(2\pi)^3}}\frac{\varepsilon_i^\nu\,{\rm e}^{-{\rm i}k_i^0\cdot z}}{\sqrt{2k_i^0(2\pi)^3}}\langle n|T(j_\mu(y)j_\nu(z))|m\rangle_{\rm con}\\
&=Z_3^{-1}\delta(k_f^0+E_n-k_i^0-E_m)\oint_{\Gamma_n}{\rm d}E'\oint_{\Gamma_m}{\rm d}E\,v_n^+g^{\rm con}_{\gamma_f,\gamma_i}(E',E,k_f^0)v_m.
\end{aligned}\tag{16}$$

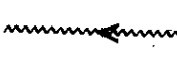
Here v_m, v_n are the vectors of the initial and final states of the atom, respectively. They are determined by (5) and (6). When constructing the Green function $g^{\rm con}_{\gamma_f,\gamma_i}$ according to the perturbation theory the external photon line has to join at least with one of the atomic electrons; therefore, the residual calculation in formula (16) is quite correct.

The diagram technics rules for $G^{\rm con}_{\gamma_f,\gamma_i}$ are different from the rules for G by the presence of the incoming photon



$$\frac{\varepsilon_i^\nu\,{\rm e}^{{\rm i}k_ix}}{\sqrt{2k_i^0(2\pi)^3}}$$

and the outgoing photon



$$\frac{\varepsilon_f^{\nu} e^{-ik_f x}}{\sqrt{2k_f^0(2\pi)^3}}.$$

The contribution to the scattering amplitude from the second term in (13) can be calculated separately. It is

$$S^{\text{discon}}_{\gamma_f n;\gamma_i m} = -Z_3^{-1}\delta_{nm}\int dy\, dz \frac{\varepsilon_f^{\nu} e^{ik_f\cdot y}}{\sqrt{2k_f^0(2\pi)^3}} \frac{\varepsilon_i^{\mu} e^{-ik_i\cdot z}}{\sqrt{2k_i^0(2\pi)^3}} \langle 0|Tj_{\nu}(y)j_{\mu}(z)|0\rangle. \tag{17}$$

4. Spectral line shape

Let us consider the photon scattering on the few-electron relativistic ($Z \sim 70 \div 110$, where Z is the nucleus charge) atom in its ground state in the case $E_1 + k_i^0 \approx E_l^{(0)}$, where E_1 is the ground state energy, k_i^0 is the energy of the initial photon, $E_l^{(0)}$ is the unperturbed energy of the excited level which under the effect of the perturbation is split into the levels $E_l^{(1)} \ldots E_l^{(s)}$. For the photon scattering amplitude on the atom we have reduction formulae (14)–(17). In the non-resonant case ($E_1 + k_i^0 \neq E_l^{(0)}$) the Green function $G^{\text{con}}_{\gamma_f,\gamma_i}$ in these formulae can be calculated using the perturbation theory according to the diagram technics rules. In the resonant case this calculation leads to singularities which follow from the fact that the energy denominator coming from the intermediate green function is equal to zero in zeroth order. We must, therefore, calculate the intermediate Green function more exactly. For this purpose let us assume

$$\begin{aligned} g^{\text{con}}_{\gamma_f,\gamma_i}(E', E, k_f^0) &= \hat{g}_1(E') R^{(-)}_{\gamma_f}(E', k_f^0, E + k_i^0)\hat{g}_l(E + k_i^0) R^{(+)}_{\gamma_i}(E + k_i^0; k_i^0, E) \\ &\quad \times \hat{g}_1(E) + \Delta g^{\text{con}}(E', E, k_f^0) \end{aligned} \tag{18}$$

where $\hat{g}_{1,l} \equiv (i/2\pi) g_{1,l}$, $g_{1,l}$ is determined from (3) with the corresponding projectors $P_0^{(1)}$, $P_0^{(l)}$; $k_i^0 + E = k_f^0 + E'$; $\Delta g^{\text{con}}(E', E, k_f^0)$ is the Green function part that is regular by $E + k_i^0 = E_i$. The operators $R^{(-)}_{\gamma_f}$, $R^{(+)}_{\gamma_i}$ are constructed according to (18) by using perturbation theory. By using the spectra representation for g_1 we obtain

$$\begin{aligned} S^{\text{con}}_{\gamma_f,\gamma_i} &= Z_3^{-1}\delta(k_f^0 - k_i^0)\varphi_1^{+} R^{(-)}_{\gamma_f}(E_1, k_f^0, E_1 + k_i^0)\hat{g}_l(E_1 + k_i^0) \\ &\quad \times R^{(+)}_{\gamma_i}(E_1 + k_i^0, k_i^0, E_1)\varphi_1 + Z_3^{-1}\delta(k_f^0 - k_i^0) \\ &\quad \times \oint_{\Gamma_l} dE' \oint_{\Gamma_1} dE\, v_1^{+} \Delta g^{\text{con}}(E', E, k_f^0) v_1. \end{aligned} \tag{19}$$

We now consider separately how the Green function $\hat{g}_l(E_1 + k_i^0)$ in (19) can be calculated. Let us introduce the quasipotential $V(E)$ by

$$g_l(E) = g_l^{(0)}(E) + g_l^{(0)}(E) V(E) g_l(E) \tag{20}$$

where $g_l^{(0)}(E) = P_l^{(0)}/(E - E_l^{(0)})$. The quasipotential $V(E)$ is constructed by using perturbation theory according to (20). We shall calculate the Green function $\hat{g}_l$ in (19) by

$$\hat{g}_l(E) = \frac{i}{2\pi}(E - E_l^{(0)} - V(E))^{-1}. \tag{21}$$

It has poles in the second sheet of the Riemann surface some lower than the right real semi-axis and does not have singularities by a real E. Thus if in formula (21) we do not neglect the quasipotential and take it into account at least at the lowest approximation ($V(E) \simeq V(E_l^{(0)})$), the calculation of the resonance scattering amplitude is quite correct.

We now consider the calculation of the resonance scattering amplitude in the lowest, resonant, approximation. Let us introduce $\mathscr{H}$ by

$$\mathscr{H} \equiv E_l^{(0)} + V(E_l^{(0)}). \tag{22}$$

It is clear that $\mathscr{H}$ is not Hermitian and thus it has complex eigenvalues. We assume that $\mathscr{H}$ is a simple matrix, i.e. its eigenvectors form the full basis in the space Ω_l. Let us designate its eigenvalues by $E_l^{(i)}$, right eigenvectors by φ_{R_i}, left eigenvectors by φ_{L_i}:

$$\mathscr{H}\varphi_{\mathrm{R}_i} = E_l^{(i)}\varphi_{\mathrm{R}_i} \qquad \varphi_{\mathrm{L}_i}^{+}\mathscr{H} = E_l^{(i)}\varphi_{\mathrm{L}_i}^{+}. \tag{23}$$

The vectors φ_{R_i}, φ_{L_i} are normalized by the condition

$$\varphi_{\mathrm{L}_i}^{+}\varphi_{\mathrm{R}_k} = \delta_{ik} \tag{24}$$

and satisfied the completeness condition

$$\sum_{i=1}^{s} \varphi_{\mathrm{R}_i}\varphi_{\mathrm{L}_i}^{+} = I. \tag{25}$$

For $\hat{g}_l$ we obtain

$$\hat{g}_l \simeq \frac{\mathrm{i}}{2\pi}(E-\mathscr{H})^{-1} = \frac{\mathrm{i}}{2\pi}\sum_{i=1}^{s}\frac{\varphi_{\mathrm{R}_i}\varphi_{\mathrm{L}_i}^{+}}{E-E_l^{(i)}}. \tag{26}$$

In fact, due to T-invariance $\mathscr{H}_{ik} = \mathscr{H}_{ki}$. It leads to orthogonality of $\{\varphi_{\mathrm{R}_i}\}_{i=1}^{s}$ in the symmetric metrics (without conjugation) $\Sigma_{q=1}^{s}\varphi_{\mathrm{R}_i}^{(q)}\varphi_{\mathrm{R}_k}^{(q)} = \delta_{ik}$ [6]. In this metrics the relations of orthonormality and completeness have the form

$$\sum_{q-\mathrm{i}}^{s}\varphi_i^{(q)}\varphi_k^{(q)} = \delta_{ik} \qquad \sum_{i=\mathrm{i}}^{s}\varphi_i^{(q)}\varphi_i^{(q')} = \delta_{qq'}. \tag{27}$$

However, in what follows we shall use the right and left vectors keeping in mind that $\varphi_{\mathrm{L}_i}^{(q)} = \varphi_{\mathrm{R}_i}^{(q)*}$.

Substituting (26) in (19) in the lowest (resonant) approximation we obtain

$$S_{\gamma_f\gamma_i} \simeq \frac{\mathrm{i}}{2\pi}\delta(k_f^0 - k_i^0)\sum_{r=1}^{s}\frac{u_1^{+}R_{\gamma_{f,0}}^{(-)}\varphi_{\mathrm{R}_r}\varphi_{\mathrm{L}_r}^{+}R_{\gamma_{i,0}}^{(+)}u_1}{E_1 + k_i^0 - E_l^{(r)}} \tag{28}$$

where u_1 is the ground state wavefunction of the atom in zeroth order, the operators $R_{\gamma_{f,0}}^{(-)}$, $R_{\gamma_{i,0}}^{(+)}$, calculated by using (18), in the lowest approximation are

$$R_{\gamma_{f,0}}^{(-)} = -e\frac{2\pi}{\mathrm{i}}\sum_{n=1}^{N}\frac{(\boldsymbol{\alpha}\boldsymbol{\varepsilon}_f)\,\mathrm{e}^{-\mathrm{i}\mathbf{k}_f\mathbf{x}_n}}{\sqrt{2k_f^0(2\pi)^3}} \tag{29}$$

$$R_{\gamma_{i,0}}^{(+)} = -e\frac{2\pi}{\mathrm{i}}\sum_{n=1}^{N}\frac{(\boldsymbol{\alpha}\boldsymbol{\varepsilon}_i)\,\mathrm{e}^{\mathrm{i}\mathbf{k}_i\mathbf{x}_n}}{\sqrt{2k_f^0(2\pi)^3}}. \tag{30}$$

Finally, we write the formulae for the cross-sections in the resonant approximation.

for the differential cross-section we obtain

$$d\sigma = (2\pi)^4 \delta(k_i^0 - k_f^0)\left\{ \sum_{r=1}^{s} \frac{|\langle 1|\hat{R}_0^+(k_f, \varepsilon_f)|R_r\rangle\langle L_r|\hat{R}_0(k_i, \varepsilon_i)|1\rangle|^2}{(E_1 + k_i^0 - \varepsilon_r)^2 + (\Gamma_r^2/4)} \right.$$
$$+ 2\,\mathrm{Re} \sum_{r<r'} \left[\frac{\langle 1|\hat{R}_0^+(k_f, \varepsilon_f)|R_r\rangle\langle L_r|\hat{R}_0(k_i, \varepsilon_i)|1\rangle}{(E_1 + k_i^0 - \varepsilon_r + i(\Gamma_r/2)} \right.$$
$$\left.\left. \times \frac{\langle 1|\hat{R}_0^+(k_f, \varepsilon_f)|R_{r'}\rangle^*\langle L_{r'}|R_0(k_i, \varepsilon_i)|1\rangle^*}{(E_1 + k_i^0 - \varepsilon_{r'} - i(\Gamma_{r'}/2))} \right] \right\} dk_f \tag{31}$$

where

$$\varepsilon_r \equiv \mathrm{Re}\, E_l^{(r)} \qquad \Gamma_r \equiv -2\,\mathrm{Im}\, E_l^{(r)}$$
$$\hat{R}_0(k, \varepsilon) = -e \sum_{n=1}^{N} \frac{(\boldsymbol{\alpha}\boldsymbol{\varepsilon})e^{i\mathbf{k}\mathbf{x}_n}}{\sqrt{2k^0(2\pi)^3}}$$
$$\langle 1|\hat{R}_0^+|R_r\rangle = u_1^+ \hat{R}_0^+ \varphi_{R_r} \qquad \langle L_r|\hat{R}_0|1\rangle = \varphi_{L_r}^+ \hat{R}_0 u_1 .$$

For the total cross-section by using the optical theorem we obtain

$$\sigma_{\mathrm{tot}} = 2(2\pi)^3 \sum_{r=1}^{s} \left\{ \frac{\mathrm{Re}(\langle 1|\hat{R}_0^+(k_i, \varepsilon_i)|R_r\rangle\langle L_r|\hat{R}_0(k_i, \varepsilon_i)|1\rangle)(\Gamma_r/2)}{(E_1 + k_i^0 - \varepsilon_r)^2 + (\Gamma_r^2/4)} \right.$$
$$\left. + \frac{\mathrm{Im}(\langle 1|\hat{R}_0^+(k_i, \varepsilon_i)|R_r\rangle\langle L_r|\hat{R}_0(k_i, \varepsilon_i)|1\rangle)(\varepsilon_r - E_1 - k_i^0)}{(E_1 + k_i^0 + \varepsilon_r)^2 + (\Gamma_r^2/4)} \right\}. \tag{32}$$

Let us discuss, for simplicity, the case of two overlapping levels ($s = 2$). The second term in formula (32) is not equal to zero only in the case of the overlapping levels with equal quantum numbers, i.e. in the case when the states corresponding to the overlapping levels are not mutually orthogonal in the usual metrics (with conjugation). In the contrary case $\mathrm{Im}(\langle 1|\hat{R}_0^+(k_i, \varepsilon_i)|R_r\rangle\langle L_r|\hat{R}_0(k_i, \varepsilon_i)|1\rangle) = 0$ and the total cross-section is the sum of the Weisskopf–Wigner type terms. In the differential cross-section (31) the second term, generally speaking, is not zero in both cases.

In the case when the one quantum transition to the ground state is the main channel of the decay of the excited state of the atom formula (32) gives the spectral line shape corresponding to this transition. In this case formula (32) can also be obtained by integrating the differential cross-section $d\sigma$, given by (31), over the final states of the emitted photon.

5. Conclusion

We derived our formulae (31) and (32) in the general case of the few overlapping levels including the case of the levels with equal quantum numbers. But, in fact, among the single excited states of the multiply charged ion there are no overlapping levels with equal quantum numbers. Thus, the second term in the right-hand side of formula (32) is equal to zero. Overlapping levels with equal quantum numbers can arise in the case of double excited states, for example, $(2s_{1/2}2s_{1/2})$, $(2p_{1/2}2p_{1/2})$ [5]. In order to study the spectral line shape of these states one can consider a process of the capture of an electron by an one-electron ion with the formation of the double excited states and the following decay of these states. Such processes were studied before in the

framework of the quantum mechanical scattering theory [17, 18]. The total cross-section of this process is the sum of the dielectronic recombination and the radiative recombination cross-sections and the interference term. The dielectronic recombination cross-section for the process of the capture of an electron by Pb^{80+} as a function of the energy of the electron was calculated recently [19]. According to these calculations the levels with equal quantum number $((2s_{1/2}2s_{1/2}), (2p_{1/2}2p_{1/2}))$ in Pb^{80+} are not overlapping. But, according to preliminary calculations for U^{90+} [20] one can expect that the relative magntidue of the difference between the common line shape of these states and the sum of two Lorentz contours reaches 20%. In this connection it seems important to consider this process in the framework of QED. The formalism proposed in the present paper is quite suitable for this purpose. The detailed analysis of this process will be considered in a forthcoming paper.

Acknowledgments

The author wishes to thank Professor M A Braun, Professor L N Labzovsky, Professor J Kaniauskas and Dr A A Sultanaev for fruitful discussion.

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