QED theory of the spectral line profile for few-electron atoms and ions

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Abstract. A review of the current status of the theoretical study of spectral line profile for systems with few electrons is presented. The line-profile approach (LPA) is introduced for the investigation of the energy levels within the framework of QED. In particular, the energy of the levels, transition probabilities and electron recombination processes are considered.

1. Introduction
The theory of the spectral line profile for the hydrogen atom has attracted renewed and broad interest due to the recent success in super-accurate resonance frequency measurements and the possibility for experimental tests of fundamental physics. Consequently, the study of the spectra of highly charged ions (HCI) has moved into the focus of experimentalists and theoreticians during the last few decades. Due to the small number of bound electrons involved, HCI appear as relatively simple systems allowing for rigorous theoretical investigations. The bound electrons move in the external electromagnetic field of the nucleus, which can become very strong for large nuclear charge number $Z$. If the total charge of electrons is small in comparison to the nuclear charge, the effect of screening is also small and binding effects dominate. Particularly, in heavy ions such as uranium the nuclear electric field exceeds in strength all other artificial electric fields accessible in laboratories. Accordingly, HCI provide a natural scenario for the study of Quantum Electrodynamics (QED) in very strong external fields.

2. Line-profile approach
The line-profile approach (LPA) is a method for description of the atomic systems (in particular, highly charged ions) within the framework of quantum electrodynamics (QED). It starts from the description of the atomic electrons as a set of noninteracting particles moving in the field of the nucleus (Furry picture) and described by the solutions of the Dirac equation. Within the framework of QED atomic electrons are interacting with each other through interaction with the quantum vacuum (the quantized electromagnetic, electron-positron fields) [1]. Accordingly, the set of electrons (together with the atomic nucleus) is not a conservative system, and the concept of the energy for this system needs to be carefully treated. Within the LPA [2] the energy levels are associated with resonances in the natural line profile for the process of resonant photon scattering. In order to keep the characteristics of the energy levels independent of the particular features of the process of scattering, the resonance approximation is employed. The resonance
approximation consists of the description of the resonance area of the natural line profile by the Lorentz contour which is characterized by two parameters: position of the resonance and its width. The energy levels are connected with the corresponding resonances. The energy and width of an energy level are determined by position of the resonance and its width within the resonance approximation.

2.1. Energy levels
For the practical implementation of the LPA the process of the elastic photon scattering on atomic electron was employed. This procedure in the lowest QED perturbation theory order is depicted in Fig. 1.

Figure 1. Feynman graph, describing the photon scattering on an atomic electron. The wavy lines with the arrows describe the absorption and emission of photons with momenta \( k \), \( k' \) and polarizations \( e, e' \), respectively. The double solid line denotes the electron in the field of the nucleus, \( a \) corresponds to the ground electron state.

According to the standard Feynman rules (see, e.g., [3]), the S-matrix element for the graph depicted in Fig. 1 reads

\[
S^{(2)} = (-ie)^2 \int d^4x_u d^4x_d \bar{\psi}_a(x_u) \gamma_{\mu u} A^{(k', \lambda')}_{\mu u}(x_u) S(x_u, x_d) \gamma_{\mu d} A^{(k, \lambda)}_{\mu d}(x_d) \psi_a(x_d),
\]  

(1)

where \( x^\mu = (t, r) \) denotes a space-time point, \( \psi_a(x) = \psi_a(r) e^{-i \omega t} \) is the one-electron wave function, \( \bar{\psi} = \psi^\dagger \gamma^0 \) is the Dirac conjugated wave function and \( A^{(k, \lambda)}_{\mu}(x) = A^{(k, \lambda)}_\mu(r) e^{-i \omega t} \) is the 4-vector of the electromagnetic field potential (photon wave function), \( k^\mu = (\omega, k) \), \( \lambda \) are the wave vector and polarization. The frequency of the absorbed and emitted photons are \( \omega = |k| \) and \( \omega' = |k'| \), respectively.

The bound-electron propagator is represented in terms of an eigenmode decomposition with respect to one-electron eigenstates of the Dirac equation:

\[
S(x_u, x_d) = \frac{i}{2\pi} \int d\omega_n e^{-i\omega(t_u - t_d)} \sum_n \frac{\psi_n(r_u) \bar{\psi}_n(r_d)}{\omega_n - \epsilon_n (1 - i0)}.
\]  

(2)

The sum over \( n \) runs over the entire Dirac spectrum, \( \epsilon \) denotes the corresponding Dirac energy.

Inserting the expressions for the propagator and wave functions in Eq. (1) and integrating over time and frequency variables we arrive at

\[
S^{(2)} = (-2\pi i) \delta(\omega' - \omega) e^{2} \sum_n \frac{A^{(k', \lambda')}_{\alpha \beta} A^{(k, \lambda)}_{\beta \alpha}}{\omega + \epsilon_a - \epsilon_n}.
\]  

(3)
Here we employed the shorthand notation

$$A^{(k,\lambda)}_{ab} = \int d^3r \bar{\psi}_a(r) \gamma^\mu A^{(k,\lambda)}_{\mu}(r) \psi_b(r). \quad (4)$$

The amplitude \((U)\) of the process of elastic photon scattering is related to the S-matrix element via

$$S = (-2\pi i)\delta(E_F - E_I)U,$$

where \(E_I\) and \(E_F\) represent the energies of the initial and final states, respectively.

The resonance scattering means that the photon frequency \(\omega\) is close to the energy difference between two atomic levels \(\omega = \varepsilon_n - \varepsilon_a + O(\alpha)\), where \(\alpha\) is the fine-structure constant. Accordingly, we have to retain only one term in the sum over \(n\) in Eq. \((3)\). Then the resonance amplitude looks like

$$U^{(0)} = e^2 A^{(k',\lambda')}_{an} \frac{1}{\omega + \varepsilon_a - \varepsilon_n} A^{(k,\lambda)}_{na}. \quad (6)$$

This amplitude has a singularity at \(\omega = -\varepsilon_a + \varepsilon_n\). To avoid this singularity and to obtain the Lorentz profile for the photon absorption and photon emission processes we have to consider the radiative insertions into the internal electron line in Fig. 1. The insertion of the electron self-energy is depicted in Fig. 2. In the resonance approximation the corresponding amplitude looks like

$$U^{(1)} = e^2 A^{(k',\lambda')}_{an} \frac{1}{\omega + \varepsilon_a - \varepsilon_n} \tilde{\Sigma}_{nn}(\omega + \varepsilon_a) \frac{1}{\omega + \varepsilon_a - \varepsilon_n} A^{(k,\lambda)}_{na}. \quad (7)$$

Here we introduced the energy-dependent matrix element of the electron self-energy

$$\Sigma_{ud}(\tilde{\xi}) = e^2 \sum_n \frac{i}{2\pi} \int d\Omega \frac{I_{unnd}([\Omega])}{\tilde{\xi} - \Omega - \varepsilon_n(1 - i\delta)} \quad \text{(8)}$$

together with the shorthand notation

$$I_{u1u2d1d2}(\Omega) = \sum_{\mu_1\mu_2} \int d\mathbf{r}_1 d\mathbf{r}_2 \bar{\psi}_{u1}(\mathbf{r}_1) \psi_{u2}(\mathbf{r}_2) \gamma^\mu_1 \gamma^\mu_2 I_{\mu_1\mu_2}(\Omega, r_{12}) \psi_{d1}(\mathbf{r}_1) \psi_{d2}(\mathbf{r}_2). \quad (9)$$

It is assumed that the ultraviolet divergent matrix element \((8)\) are renormalized in a standard way for the tightly bound electrons in atoms (see, e.g., [3]).

We can consider insertion of two self-energy matrix elements into the internal electron line, see Fig. 3. Retaining in the electron propagators Eq. \((2)\) only one term we get the following expression for the amplitude

$$U^{(2)} = e^2 A^{(k',\lambda')}_{an} \frac{1}{\omega + \varepsilon_a - \varepsilon_n} \tilde{\Sigma}_{nn}(\omega + \varepsilon_a) \frac{1}{\omega + \varepsilon_a - \varepsilon_n} \tilde{\Sigma}_{nn}(\omega + \varepsilon_a) \frac{1}{\omega + \varepsilon_a - \varepsilon_n} A^{(k,\lambda)}_{na}. \quad (10)$$

Comparing Eqs. \((6)\), \((7)\), \((10)\) we can see that the corrections to the amplitude corresponding to the insertion of the self-energy matrix elements compose a geometric progression. Applying the formula for convergent geometric progression we get

$$U = \sum_{l=0}^{\infty} U^{(l)} = e^2 A^{(k',\lambda')}_{an} \frac{1}{\omega + \varepsilon_a - \varepsilon_n - \tilde{\Sigma}_{nn}(\omega + \varepsilon_a)} A^{(k,\lambda)}_{na}. \quad (11)$$
Figure 3. Feynman graph representing the higher-order electron self-energy correction within the line profile approach (SESE, loop-after-loop, irreducible).

Figure 4. The Feynman graphs representing multiple insertions of the self-energy operator into the lower outer electron line.

We note that the insertion of the self-energy graphs into the outer lines in Fig. 2 leads to singularities. In the paper [4] it was shown that within the adiabatic formalism of Gell-Mann and Low [5] the contributions of the insertion of the self-energy graphs into the outer lines (see Fig. 4) compose a geometric progression. Accordingly, the expression for the adiabatic S-matrix corresponding to graphs in Fig. 4 yields

$$\sum_{l=0}^{\infty} S_{\lambda}^{(l)} = (-2\pi i)\delta(\omega - \omega')e^{2}\left[\sum_{n} \frac{A_{an}^* A_{na}}{\omega + \varepsilon_a + \Sigma_{aa}(\varepsilon_a) - \varepsilon_n} + R_{\lambda}\right] \exp\left(\frac{\Sigma_{aa}(\varepsilon_a)}{2i\lambda}\right).$$

(12)

Here, $\varepsilon$ are the Dirac energies, $\lambda$ is the adiabatic parameter ($\lambda \to 0$), $R_{\lambda}$ represents the terms for which $\lim_{\lambda \to 0} R_{\lambda} = 0$. As the self-energy matrix element for the ground state has no imaginary part, then all the singularities compose an imaginary exponent, and the absolute value of the amplitude reads

$$|U| = e^{2}\left|\sum_{n} \frac{A_{an}^* A_{na}}{\omega + \varepsilon_a + \Sigma_{aa}(\varepsilon_a) - \varepsilon_n}\right|.$$  \hspace{1cm} (13)

Accordingly, the insertions to the outer lines lead to corrections to the energy of the ground state.

In the general case for one- or many-electron system the amplitude of the process

$$A \xrightarrow{\omega} N \xrightarrow{\omega'} A,$$

(14)

where $A$ is the ground state of the system, $N$ is the excited state, $\omega = \omega'$ are the photons, in the resonance approximation can be written as

$$U = T^+ \frac{1}{\omega + E_a - V(\omega)} T.$$  \hspace{1cm} (15)
Here, the matrices $T$ describe complicated vertices, the matrix $V$ is defined by the operator $\hat{V}$ which is built within the framework of the standard QED perturbation theory [2]. These operators are defined by their action on many-electron wave functions of noninteracting electrons.

$$V(\omega) = V^{(0)} + \Delta V(\omega).$$  \hspace{1cm} (16)

The matrix $V^{(0)}$ is a diagonal matrix, its eigenvalues are the sums of Dirac energies. The matrix $\Delta V$ describes various corrections: electron self-energy, vacuum polarization, one-photon exchange etc.

Taking squared absolute value of the amplitude Eq. (15) and integrating over the momentum and polarization of the absorbed photon we can get the absorption probability

$$dW_{A\rightarrow n}(\omega) = \frac{1}{2\pi} \frac{\Gamma_{A\rightarrow N}(\omega)}{[\omega + E_A - V_N^{(0)} - \text{Re}\Delta V_N(\omega)]^2 + [\text{Im}\Delta V_N(\omega)]^2} d\omega. \hspace{1cm} (17)$$

Condition of the resonance reads

$$\omega_{\text{res}} + E_A - V_N^{(0)} - \text{Re}\Delta V_N(\omega_{\text{res}}) = 0. \hspace{1cm} (18)$$

Interpolation of the line profile Eq. (17) by the Lorentz contour yields

$$dW_{A\rightarrow N}(\omega) = \frac{1}{2\pi} \frac{\Gamma_{A\rightarrow N}(\omega_{\text{res}})}{[\omega + E_A - E_N^0]^2 + \frac{4}{\Gamma_N^2}} d\omega, \hspace{1cm} (19)$$

where we introduced the energy of the level

$$E_N = \omega_{\text{res}} + E_A - V_N^{(0)} = V_N^{(0)} + \text{Re}\Delta V_N(\omega_{\text{res}}) \hspace{1cm} (20)$$

and the width of the level

$$\Gamma_N = -2\text{Im}\Delta V_N(\omega_{\text{res}}). \hspace{1cm} (21)$$

We note that the resonance approximation is plausible only either for the cases of one isolated energy level or a small group of energy levels. If we go beyond the resonance approximation, the energy level can not be describe by two parameters (the energy and the width). The corresponding corrections are called nonresonant corrections [6, 2]. Calculations of the energy levels (including quasidegenerate levels) for low-lying two-electron configurations within the framework of QED are presented in [7, 8, 9]. In these three works the covariant-evolution-operator method [10], the LPA [2] and the two-time Green’s function method [11] were employed, respectively.

2.2. Transition probabilities

For consideration of transition from the initial state (I) to the final state (F) with emission of a photon ($\omega$) within the framework of the LPA, we have to consider process of scattering

$$A \xrightarrow{\omega} I \xrightarrow{\omega_0} F \xrightarrow{\omega'} A. \hspace{1cm} (22)$$

In the resonance approximation the amplitude of this process can be written as

$$U = T^+ \frac{1}{\omega + E_A - V(\omega')} \Xi(\omega_0) \frac{1}{\omega + E_A - V(\omega)} T. \hspace{1cm} (23)$$
The operator $\Xi(\omega_0)$ is derived within the framework of standard QED perturbation theory [4]. The resonance determined by the left denominator defines the initial state, the resonance caused by the right denominator defines the final state. The transition amplitude from the initial state ($I$) to the final state ($F$) is defined as

$$U_{I \rightarrow F} = \Xi(\omega_0)_{FI}. \quad (24)$$

The calculations of the transition probabilities for the two-electron states were performed by Drake [12] with the unified method (UM) and by Johnson [13] within the relativistic many-body perturbation theory (RMBPT). The QED calculation of the transition probabilities for the nondegenerate two-electron states is presented in [14], the calculations are performed within the two-time Green’s function method [11]. The QED calculation of the transition probabilities for low-lying two-electron states (including quasidegenerate levels) within the framework of the QED is presented in [4].

2.3. One-electron capture
We consider process of electron recombination with a one-electron heavy ion. The process of electron recombination can be presented as

$$e(E_e) + U^{91+}(1s) \rightarrow \cdots \rightarrow U^{90+}(1s, 1s) + n\gamma(\omega). \quad (25)$$

If the process of electron recombination is registered by detection of a photon with frequency $\omega \approx E_e + E_{1s} - E(r)$, where $E(r)$ is the energy of a two-electron single-excited configuration ($r = (1s, 2s)$, $(1s, 2p)$), then the electron recombination is determined by two particular processes,

$$e(E_e) + U^{91+}(1s) \rightarrow U^{90+}(r) + \gamma(\omega) \rightarrow \cdots \quad (26)$$

and the dielectronic recombination (DR)

$$e(E_e) + U^{91+}(1s) \rightarrow U^{90+}(d) \rightarrow U^{90+}(r)\gamma(\omega) \rightarrow \cdots, \quad (27)$$

where $d$ denotes the double-excited configurations $(2s, 2s)$, $(2s, 2p)$, $(2p2p)$. The cross section of electron recombination considered as a function of the incident electron energy ($E_e$) reveals resonances in the area where sum of the incident electron and 1s-electron energies ($E_{1s} = E_e + E_{1s}$) is close to the energies of the double excited two-electron configurations. The DR process is the dominant process contributing to the cross-section in the resonance areas. The RR process is nonresonant. The frequency ($\omega$) of emitted photon is defined by the energy conservation law. The RR and DR processes compose a single process of electron recombination, the RR and DR contributions to the cross-section can be separated only in the lowest order of the perturbation theory. Accordingly, in the general case the contributions of the RR and DR processes to the total cross-section become inseparable.

For calculation of the cross-section for the process of electron recombination within the LPA we introduce an auxiliary bound electron system which properties are explicitly related to the original system. We introduce a function

$$\psi_{eR}^{aux}(r) = \psi_e(r)\theta(R - |r|), \quad (28)$$

where $\psi_e(r)$ is the wave function of the incident electron, $\theta(R - |r|)$ is the Heaviside step function, $R$ is a radius of the large sphere. The function $\psi_{eR}^{aux}(r)$ can be normalized to unity with the normalization factor $N_R$

$$\psi_{eR}(r) = N_R^{-1}\psi_{eR}^{aux}(r), \quad \|\psi_{eR}\| = 1. \quad (29)$$
We can introduce an artificial bound electron state $e_R$ described by the wave function $\psi_{e_R}$. The energies and angular quantum numbers of the continuum electron state $\psi_e$ and the bound electron state $\psi_{e_R}$ are equal. Consider now two processes of transition from the initial state $\{I\}$ to the final state $\{F\}$ which differ by the initial states. The first initial state is $1s$ electron and the continuum electron $e$. The second initial state is $1s$ electron and the artificial bound electron $e_R$. The amplitudes of the first process ($U$) and the second one ($U_R$) are related like

$$U = \lim_{R \rightarrow \infty} N_R U_R. \quad (30)$$

The LPA can be applied for the bound electron system ($1s, e_R$) in the way it was performed for calculation of the transition probabilities [4]. The limit ($R \rightarrow \infty$) can be evaluated numerically.

Calculations of the electron recombination with one-electron uranium are presented in [15, 16]. These calculations are performed within various approximations. The first ab initio QED calculation of the electron recombination with one-electron uranium and gadolinium is presented in [17, 18]. The measurement of the cross-section is presented in [19]. In the work [19] there is also presented QED calculation of the cross-section.

3. Conclusion

Summarizing, we have presented the complete and consequent formulation of QED theory of the line profile and applied it for describing dynamic processes in atomic systems. One of the important features of this approach is that it provides a most general way for the evaluation of all observable quantities of physical interest: energy levels, transition frequencies, all kinds of cross-sections, etc. Moreover, it allows for the exact description of the interelectronic interaction for both in- and out-states with the accuracy accepted in the Relativistic Many-Body Theory (RMBT); hence, QED and RMBT can be partly merged.

Our studies have been continued by going beyond the Lorentz (resonance) approximation. We have shown [2] that the nonresonant (NR) corrections to the Lorentz profile will set an absolute theoretical limit to the accuracy of the possible frequency measurements. This is closely related to the fact, that the concept of atomic levels, characterized by a level energy and width, becomes inadequate as soon as the distortions due to nonresonant corrections can no longer be neglected. Under such circumstances only the line profile remains as the quantum-mechanical observable that can be measured and compared with experimental data.

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