# S-MATRIX FORMALISM IN THE CALCULATION OF OSCILLATOR STRENGTHS, RADIATION AND AUTOIONIZATION WIDTHS FOR COMPLEX ATOMS AND MULTICHARGED IONS

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A new approach for the calculation of the oscillator strengths, radiation and autoionization widths for complex atoms and multicharged ions has been developed. The new approach is based on the S-matrix formalism and does not use any empirical information about the properties of the studied atomic systems. We have used the fundamental principle of the minimization of the gauge-dependent contribution to the radiative width for the certain class of the photon propagator calibration. The minimization criterion is tested by the calculation of the resonance radiation transition probability in the Na-like ion SVI and autoionization widths in Yb.

In the theory of radiative and non-radiative decay of the quasi-stationary states of a multielectron atom an energy approach, based on the adiabatic Gell-Mann and Low formula [1–8] for the energy shift $\delta E$ with electrodynamical scattering matrices, is well known. This approach represents the decay probability as an imaginary part of the energy shift. The method is consistently electrodynamical, allowing for the uniform consideration of a variety of induced and spontaneous processes different by their physical nature. Their contributions and interference effects are represented by successive corrections of the electrodynamical perturbation theory (EDPT). The energy approach had been applied previously in the study of the purely electronic, electron-nuclear processes in atoms and meso-atomic systems, and in the problem of the collisional electron-positron pair production [1–10].

Here we present a new approach for the calculation of the oscillator strengths, radiation and autoionization widths for complex atoms and multicharged ions. The new approach is fully *ab initio* and does not use any empirical information about atomic systems. It is based on the fundamental principle of the minimization of the gauge-dependent radiative width contribution for the certain class of the photon propagator calibration.

Consider the one-quasiparticle system. A quasiparticle is a valent electron above the core of closed electron shells or a vacancy in the core. In the lowest second order of the EDPT for the $\delta E$ there is the only one-quasi-particle Feynman diagram A (A =  ), that has a non-zeroth contribution to the imaginary part of electron energy Im $\delta E$ (the radiation decay width). In the fourth order of the EDPT there are diagrams, whose contribution into the Im$\delta$E accounts for the core polarization effects. It is on the electromagnetic potentials gauge (the gauge non-invariant contribution). Let us examine the multielectron atom with one quasi-particle in the first excited state, connected with the ground state by the radiation transition. In the zeroth EDPT approximation we, as usually (c.f.[2,3,9]),use the one electron bare potential

$$V_N(r) + V_C(r), \qquad (1)$$

with $V_N(r)$ describing the electric potential of the nucleus, $V_C(r)$, imitating the interaction of the quasi-particle with the core. The perturbation in terms of the second quantization representation reads:

$$-V_C(r)\ \psi^+(r)\psi(r) - j_\mu(x)\,A^\mu(x). \quad (2)$$

The core potential $V_C(r)$ is related to the core electron density $\rho_C(r)$ in a standard way [6]. The latter fully determines the one electron representation. Moreover, all the results of the approximate calculations are functionals of the density $\rho_C(r)$. Here the lowest-order multielectron effects, in particular, the gauge-dependent radiative contribution for the certain class of the photon propagator calibration is treated. This value is considered to be the typical representative of the electron correlation effects, whose minimization is a reasonable criterion in searching for the optimal one-electron basis of the PT. Besides, this procedure derives an undoubted profit in the routine spectroscopic calculations as it provides the way of refinement of the atomic characteristics calculations, based on the "first principles". It is well known that the closeness of the radiation probabilities calculated with the alternative forms of the transition operator is commonly used as a criterion for the multielectron calculations quality.

The imaginary part of the diagram A contribution in the case of the Lorentz calibration has been presented previously as a sum of the partial contributions of $\alpha$-$s$ transitions from the initial state $\alpha$ to the final state $s$ [3]:

$$\mathrm{Im}\delta E_\alpha\,(\mathrm{a}) = \sum_s \mathrm{Im}\ \delta E\ (\alpha\text{-}s;\ \mathrm{a}).$$

The most important diagram of the EDPT fourth order is direct polarization diagrams B ( B= ). Its contribution into $\mathrm{Im}\delta E_\alpha$ is gauge-dependent, though the results of the exact calculation of any physical quantity must be gauge-independent. All the non-invariant terms are multielectron by their nature (the particular case is the non-coincidence of the oscillator strengths values, obtained in calculations with the "length" and "velocity" transition operator forms). Let us take the photon propagator calibration as follows [3,11]:

$$D = D_T + CD_L,\ D_T = \delta_{\mu\nu}/(k_0^2 - k^2),$$
$$D_L = -k_\mu k_\nu/(k_0^2 - k^2). \quad (3)$$

Here all notations are standard (according to [11]). The values $C$=0 and $C$=1 of the gauge constant are related to the Lorentz and Landau calibrations, respectively. The calculation of the contribution of the A, B diagrams into $\mathrm{Im}\delta E$ taking into account both the $D_T$ and $D_L$ parts, is standard. The A diagram contribution into $\mathrm{Im}\delta E$ related to the $\alpha$ -$s$ transition is determined as follows:

$$-\frac{e^2}{8\pi}\int\int dr_1\,dr_2\ \psi_\alpha^+(r_1)\ \psi_s^+(r_2)\ \frac{1-\alpha_1\alpha_2}{r_{12}}\sin(\omega_{\alpha s}r_{12})\ \psi_\alpha(r_2)\ \psi_s(r_1), \quad (4)$$

for $D = D_T$, and

$$-\frac{e^2}{8\pi}\int\int dr_1\,dr_2\ \psi_\alpha^+(r_1)\ \psi_s^+(r_2)\ \{[(1-\alpha_1 n_{12}\,\alpha_2 n_{12})/r_{12}]\sin(\omega_{\alpha s}r_{12}) + \omega_{\alpha s}\ (1+\alpha_1 n_{12}\,\alpha_2 n_{12})\times$$
$$\times\cos(\omega_{\alpha s}r_{12})\}\ \psi_\alpha(r_2)\ \psi_s(r_1), \quad (5)$$

for $D=D_L$, where $\omega_{\alpha s}$ is the $\alpha$ -$s$ transition energy. According to [12], the $D_{\mu\nu,L}$ contribution vanishes, if one-quasi-particle functions $\psi_\alpha$, $\psi_s$ satisfy the same Dirac equation. Nevertheless this term is to be retained in the distorted waves approximation. When calculating the EDPT fourth-order contribution some approximations are inevitable. Remember that the energy shifts and the transition probabilities are treated uniformly in the framework of the energy approach. Let us consider the direct polarization diagram as an example. After the linearization over the gauge constant $C$, the formal expression for Im $\delta E_{\mathrm{ninv}}$ is as follows:

$$\mathrm{Im}\,\delta E_{\mathrm{ninv}}\ (\alpha\text{-}s;\ \mathrm{b}) = -\,C \int\int\int\int dr_1\, dr_2\, dr_3\, dr_4 \sum_{\substack{n>f \\ m\le f}} \left( \frac{1}{\omega_{mn}+\omega_{\alpha s}} + \frac{1}{\omega_{mn}-\omega_{\alpha s}} \right) \psi_\alpha^{+}(r_1) \times \ \times \psi_m^{+}(r_2)$$

$$\psi_s^{+}(r_4)\ \psi_n^{+}(r_3)\ \frac{1-\alpha_1\alpha_2}{r_{12}}\ \{[\,(\alpha_3\alpha_4 - \alpha_3 n_{34}\ \alpha_4 n_{34})/r_{14}\,]\sin[\,\omega_{\alpha n}(r_{12}+r_{34})] + \qquad (6)$$

$$+\ \omega_{\alpha n}\cos[\,\omega_{\alpha n}(r_{12}+r_{34})]\,(1+\alpha_3 n_{34}\,\alpha_4 n_{34})\}\ \psi_m(r_3)\ \psi_\alpha(r_4)\ \psi_n(r_2)\ \psi_s(r_1).$$

Here $f$ is the boundary of the closed shells; $n \ge f$ indicating the unoccupied bound and the upper continuum electron states; $m \le f$ indicates the finite number of states in the core and the states of the negative continuum (accounting for the electron vacuum polarization). All the vacuum polarization and self-energy corrections to the sought values are omitted because of the known reasons [3]. The sum $\sum_{n>f,\ m<f}$ can be calculated numerically. Its calculation leads to solving of the system of ordinary differential equations (a one-dimensional procedure) [8–10]. The minimization of the density functional Im $\delta E_{\mathrm{ninv}}$ (b+c) leads to the integral differential equation for $\rho_c$ that can be solved using one of the standard numerical codes. In [3] the authors treated the function $\rho_c$ in the simple analytic form with the only variable parameter $b$ and substituted it into (6). More accurate calculation requires the solution of the integral differential equation for $\rho_c$. This program has been realized by us within our atomic code [3,4,6–10]. As an example, we consider the resonance $3p_{1/2}$ - $3s_{1/2}$ transition in the Na-like multicharged ion SVI. It is one of the most studied ions of the very popular Na-like sequence for which the core polarization effects are known to be of great importance. The results of calculations are presented in Table.1. One should note the smallness of the gauge non-invariant contribution into the value of the oscillator strength. In [3] it is ~$10^{-3}$, in our calculation – $10^{-5}$. This means that the results of the calculations with the "length" and "velocity" transition operator forms are practically equal. As the accurate calculations show this is true for all other transitions between the states with one electron above the same core $1s^2 2s^2 2p^6$ . In Table 2 we present the results of calculation of the energies and autoionization widths for the low-lying states of Yb atom. At first the similar states were experimentally studied by Letokhov *et al.* [13]. We consider the states of 6s(2), 6s6p, 6s5d,6p(2),6p5d,5d(2),7s6p which can be treated as the two-quasiparticles states above the core $(...4f^{14})$.The numerical procedure is the same as in the relativistic PT method with zeroth model potential approximation [2-4]. The main difference is related to the use of the above described minimization procedure. In conclusion we note that the abnormal smallness of the 5d...5d level is connected with the relativistic channel of decay for these states.

Table 1. The oscillator strength (OS) for the dipole transition in SVI ion: a) gauge non-invariant contribution (polarization part); b) the OS with the account of the fourth-order core polarization effect, c) the OS without the polarization effect, d) experimental value ($b$ -adjustable parameter of the $\rho_c$ – function in Glushkov-Ivanov model [3]).

| B | (a) ($10^{-2}$) | (b) | (c) | (d) | This paper (a) | This paper gf |
|---|---|---|---|---|---|---|
| 0.56 | 0.1052 | 0.652 | | | | |
| 0.58 | 0.1035 | 0.665 | 0.690 | 0.66±0.02 | $10^{-5}$ | 0.658 |
| 0.60 | 0.1040 | 0.678 | | | | |
| 0.62 | 0.1051 | 0.691 | | | | |
| 0.64 | 0.1063 | 0.705 | | | | |

Table 2. Energies ($cm^{-1}$) and autoionization widths ($cm^{-1}$) of low-lying states for Yb atom

| Conf. | J | -E,cal. [7,13] | -E, this work | G, [7,13] | G, this work |
|---|---|---|---|---|---|
| $6p_{3/2}6p_{3/2}$ | 0 | 92000 | 91800 | 5.4 | 5.5 |
| $6p_{3/2}5d_{3/2}$ | 2 | 91400 | 91280 | 0.2 | 0.28 |
| $6p_{3/2}5d_{5/2}$ | 1 | 94900 | 94760 | 5.7 | 5.58 |
| $6p_{3/2}5d_{5/2}$ | 3 | 96300 | 96240 | 1.6 | 1.65 |
| $5d_{3/2}5d_{3/2}$ | 0 | [98100] | 98230 | [0.01] | [0.008] |
| $5d_{3/2}5d_{5/2}$ | 1 | [98000] | 98150 | $[10^{-4}]$ | $[10^{-4}]$ |
| $7s_{1/2}6p_{1/2}$ | 0 | 88900 | 88640 | 0.7 | 0.85 |
| $7s_{1/2}6p_{1/2}$ | 1 | 88700 | 88590 | 3.0 | 3.2 |

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# S-МАТРИЧНИЙ ФОРМАЛІЗМ У РОЗРАХУНКАХ СИЛ ОСЦИЛЯТОРІВ, РАДІАЦІЙНИХ ТА АВТОІОНІЗАЦІЙНИХ ШИРИН ДЛЯ СКЛАДНИХ АТОМІВ ТА БАГАТОЗАРЯДНИХ ІОНІВ


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Розвинуто новий підхід до розрахунку сил осциляторів, радіаційних та автоіонізаційних ширин складних атомів та багатозарядних іонів. Новий підхід грунтується на S-матричному формалізмі і не використовує емпіричної інформації про властивості досліджуваних систем. Використано фундаментальний принцип мінімізації калібровочно залежного внеску в радіаційну ширину для визначеного класу калібровок фотонних пропагаторів. Проведено розрахунок сил осциляторів для Na-подібних іонів і енергій та ширин автоіонізаційних станів для атома Yb.