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Quantum Geometry: An advanced energy approach in scattering theory

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Abstract An advanced energy-amplitude approach in a formal scattering theory is presented and based on the relativistic many-body perturbation theory and density-functional formalism

Keywords Multiphoton resonances · An advanced energy-amplitude approach · Eigen functions and energy eigen values

Mathematics Subject Classification (2000) 55R05 · 53B05

1 Introduction

Traditionally an investigation of spectra, spectral, ionization and autoionization characteristics for heavy atomic systems is of a great interest for further development of quantum theories, including quantum theory and different applications [1]–[9]. From the mathematical point of view this class of tasks is related to new branch of a geometry, namely, quantum geometry [2]. Here we present a modified energy-amplitude approach in a formal scattering theory, based on the relativistic many-body perturbation theory and and density-functional formalism and new procedure of generating basis's of the stationary and quasistationary states functions. The latter generalizes the known approach [2], [3] . Mathematical methods of calculation of the the cited parameters may be divided into a few main groups. First, the well known, classical multi-configuration Hartree-Fock method (as a rule, the relativistic effects are taken into account in the Pauli approximation or Breit hamiltonian etc.) allowed to get a great number of the useful spectral information, but in fact it provides only qualitative description of spectra of the heavy quantum systems. Second, the multi-configuration Dirac-Fock (MCDF) method is the most reliable version of calculation for multielectron

systems with a large charge. These methods can be served as an initial basis for the further studying scattering processes in quantum geometry.

2 Formal energy approach in scattering theory

We start from the formal energy approach presented in ref.[1]. The new original moment of our scheme is in using more corrected in comparison with [3], [10] gauge invariant procedure for generating the atomic functions basis's (optimized basis's) The lather includes solution of the whole differential equations systems for Dirac-like bi-spinor equations [10].

As an example, we consider the collisional de-excitation of the Ne-like ion: $((2j_{iv})^{-1}3j_{ie}[J_iM_i], \varepsilon_{in}) \to (\Phi_o, \varepsilon_{sc})$. Here Φ_o is the state of the ion with closed shells (ground state of the Ne-like ion); J_i is the total angular moment of the initial target state; indices iv, ie are related to the initial states of vacancy and electron; indices ε_{in} and ε_{sc} are the incident and scattered energies, respectively to the incident and scattered electrons.

Further it is convenient to use the second quantization representation. In particular, the initial state of the system "atom plus free electron" can be written as

$$|I\rangle = a^+_{in} \sum_{m_{iv}, m_{ie}} a^+_{ie} a_{iv} \Phi_o C^{J_i, M_i}_{m_{ie}, m_{iv}} \tag{1}$$

Here $C^{J_i, M_i}_{m_{ie}, m_{iv}}$ is the Clebsh-Gordan coefficient.

Final state is:

$$|F\rangle = a^+_{sc} \Phi_o, \tag{2}$$

where $|I\rangle$ represents three-quasiparticle (3QP) state, and $|F\rangle$ represents the one-quasiparticle (1QP) state.

The justification of the energy approach in the scattering problem is in details described in ref. [2]. For the state (1) the scattered part of energy shift $\mathrm{Im}\Delta E$ appears first in the second order of the atomic perturbation theory (fourth order of the QED perturbation theory) in the form of integral over the scattered electron energy ε_{sc} [2]:

$$\int d\varepsilon_{sc} G(\varepsilon_{iv}, \varepsilon_{ie}, \varepsilon_{in}, \varepsilon_{sc}) / (\varepsilon_{sc} - \varepsilon_{iv} - \varepsilon_{ie} - \varepsilon_{in} - i0) \tag{3}$$

with

$$\mathrm{Im}\Delta E = \pi G(\varepsilon_{iv}, \varepsilon_{ie}, \varepsilon_{in}, \varepsilon_{sc}). \tag{4}$$

Here G is a definite squired combination of the two-electron matrix elements of the interelectron interaction. The value

$$\sigma = -2\mathrm{Im}\Delta E \tag{5}$$

represents the collisional cross-section if the incident electron eigen-function is normalized by the unit flow condition and the scattered electron eigen-function is normalized by the energy δ function.

The collisional strength $\Omega(I \to F)$ is connected with the collisional cross section σ by expression [2]:

$$\sigma(I \to F) = \Omega(I \to F)\pi/\left((2J_i+1)\varepsilon_{in}\left((\alpha Z)^2\varepsilon_{in}+2\right)\right) . \tag{6}$$

Here and below the Coulomb units are used; 1 C.u.$\approx$27.054Z^2 eV, for energy; 1 C.u.$\approx 0.529 \cdot 10^{-8}/Z$ cm, for length; 1 C.u.$\approx 2.419 \cdot 10^{-17}/Z^2$ sec for time.

The collisional de-excitation cross section is defined as follows [2]:

$$\sigma(IK \to 0) = -\pi \sum_{j_{in},j_{sc}} (2j_{sc}+1) \left(\sum_{j_{ie},j_{iv}} \langle 0|j_{in},j_{sc}|j_{ie},j_{iv},J_i\rangle \, B^{IK}_{ie,iv} \right)^2 . \tag{7}$$

Here $B^{IK}_{ie,iv}$ is a real matrix of eigen-vectors coefficients, which is obtained after diagonalization of the secular energy matrix. The amplitude like combination in the above expression has the following form:

$$\langle|j_{in},j_{sc}|j_{ie},j_{iv},J_i\rangle = sqrt(2j_{ie}+1)(2j_{iv}+1)(-1)^{j_{ie}+1/2)} \sum_{\lambda} (-1)^{\lambda+J_i} \times$$
$$\times \left(\delta_{\lambda,J_i}/(2J_i+1) Q_\lambda(sc,ie;iv,in) + \begin{pmatrix} j_{in} & j_{sc} & J_i \\ j_{ie} & j_{iv} & \lambda \end{pmatrix} Q_\lambda(ie,in;iv,sc) \right) . \tag{8}$$

Here values Q^{Qul}_λ and Q^{Br}_λ are defined by the standard Coulomb and Breit expressions [2]. For the collisional excitations from the ground state (inverse process) one must consider $a^+_{in}\Phi_o$ as the initial state and

$$|F\rangle = a^+_{sc} \sum_{m_{fe},m_{fv}} a^+_{fe} a_{fv} \Phi_o \tilde{C}^{J_f,M_f}_{m_{fe},m_{fv}} \tag{9}$$

as a final state. The cross-section is as follows:

$$\sigma(0 \to IF) = 2\pi(2J_f+1) \sum_{j_{in},j_{sc}} (2j_{sc}+1) \left(\sum_{j_{fe},j_{fv}} B^{FK}_{fe,fv} \langle j_{fe},j_{fv}J_f|j_{in},j_{sc}|0\rangle \right)^2 \tag{10}$$

with

$$\langle j_{fe}, j_{fv}, J_f | j_{in}, j_{sc} 0 | \rangle = sqrt(2j_{fe}+1)(2j_{fv}+1)(-1)^{j_{fe}+1/2} \sum_{\lambda} (-1)^{\lambda+J_f} \times$$

$$\times \left(\delta_{\lambda,J_f} (1/(2J_f+1)) Q_\lambda(sc, ie; iv, in) \begin{pmatrix} j_{in} & j_{sc} & J_f \\ j_{fe} & j_{fv} & \lambda \end{pmatrix} Q_\lambda(fe, sc; fv, in) \right) (11)$$

The different normalization conditions are used for the incident and for the scattered electron wave functions. Upon the normalization multipliers one gets symmetrical expressions for the excitation and de-excitation, saving the weight multiplier $(2J_f+1)$ in (17). To calculate all necessary matrix elements one must use the basis's of the one-particle relativistic functions. In next section we briefly consider our idea to generalize an approach and give some conclusions.

3 Concluding comments

In ref.[3] it has been proposed *ab initio* optimization principle for construction of cited basis's. There is used the minimization of the gauge dependent multielectron contribution of the lowest QED PT corrections to the radiation widths of atomic levels. In the fourth order of QED PT there appear diagrams, whose contribution into the $\mathrm{Im}\Delta E$ accounts for the core polarization effects (polarization of the closed shell core by the quasi-particle). This contribution describes collective effects and it is dependent upon the electromagnetic potentials gauge (the gauge non-invariant contribution). Following [3] let us also consider the multi-electron atom with 1QP in the first excited state, connected with the ground state by the radiation transition. In the zeroth order of QED PT we will use the one-electron bare potential $V_N(r) + V_C(r) + V_X C(r)$. Here the written terms are corresponding to the standard nuclear, Coulomb and exchange-correlation potentials. This is a key difference of the original approach [3] and many other versions (c.f. [3]–[10]) as in the cited versions there is absent $V_X C(r)$ potential. It is easily to understand that in fact our version is based on the density-functional formalism. In ref.[7]–[9]this formalism has been used in order to develop a new theory of the autoionization and multiphoton phenomena in atomic systems. From theoretical point of view using formalism in a scattering problem looks very naturally and logistically. In this light the fact that all the results of the approximate calculations are the functionals of the density $\rho_C(r)$ looks as very comprehensive. All the gauge non-invariant terms are multielectron by their nature (the particular case of the gauge non-invariance manifestation is non-coincidence of the oscillator strengths values, obtained in the approximate calculations with the 'length'

and 'velocity' transition operator forms) are the density functionals too. To realize the described scheme we have used the modified version of the standard atomic code "Superatom" [2]. The preliminary estimates show that new version is practically identical to original ones from the accuracy point of view, however, it is significantly simplified from the computational point of view.

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