

Quantum Geometry: Generalized version of an energy approach in scattering theory and its application to electron-collisional excitation of multi-charged ions

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Abstract Within quantum geometry it is presented an Generalized version of an energy approach in scattering theory and its application to electron-collisional excitation of multicharged ions. The reestimated numerical data for electron-collisional excitation cross-sections are presented for barium.

Keywords Scattering theory · An advanced energy approach · Eigen functions and energy eigen values

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1 Introduction

This paper goes on our investigations of the energy, spectral and geometric features of electron-collisional parameters of atomic (ionic) systems. The main attention is devoted to quantitative studying the eigen energy values and eigen function of electrons in the scattering processes. The different algorithms of an energy amplitude approach have been presented in [1]–[12]. Let us remind that at present time a great progress can be noted in development of a quantum geometry and quantum dynamics, that is mainly provided due to the carrying out more correct and effective mathematical methods of solving eigen function and eigen values tasks for multi-body complex quantum systems in relativistic

approximation and new algorithms of accounting for the complex exchange-correlation effects. Nevertheless in many calculations there is a serious problem of the gauge invariance, connected with using non-optimized one-electron representation. In fact it means uncorrect accounting for the complex exchange-correlation effects (such as polarization and screening effects, a continuum pressure etc.). In this paper, which goes on our studying [4]–[12], we present an generalized version of an energy approach in scattering theory and its application to calculation of cross-sections for some complex atomic systems. It is based on the relativistic many-body perturbation theory (PT) with the Dirac-Kohn-Sham zeroth approximation and more correct numerical accounting for the complex polarization, screening effects and continuum pressure. As application of generalized version of energy approach, the numerical data for electron-collisional excitation cross-sections are presented for some complex atomic ions.

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 latter includes solution of the whole differential equations systems for Dirac-like bi-spinor equations [10]. More exactly, we use the Dirac-Kohn-Sham zeroth approximation in a formally exact relativistic perturbation theory. As an exchange potential we use the known-Kohn-Sham one in the consistent relativistic form. Besides, the correct Gunnarsson-Lundqvist correlation potential in a relativistic form is also used (look details regarding the used potentials, for example, in ref.[13]).

Besides using this effective one-quasiparticle representation in relativistic perturbation theory the rest computational scheme remains the same [4]–[10].

Following to [4], as an example, we consider the collisional de-excitation of the Ne-like ion: $((2j_{iv})^{-1}3j_{ie}[J_i M_i], \varepsilon_{in}) \rightarrow (\Phi_o, \varepsilon_{sc})$. 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

$$|I\rangle = a_{in}^+ \sum_{m_{iv}, m_{ie}} a_{ie}^+ a_{iv} \Phi_o C_{m_{ie}, m_{iv}}^{J_i, M_i} \quad (1)$$

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

Final state is:

$$|F\rangle = a_{sc}^+ \Phi_o, \quad (2)$$

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 $\text{Im}\Delta E$ 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]:

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

with

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

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

$$\sigma = -2\text{Im}\Delta E \quad (5)$$

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

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

Here and below the Coulomb units are used; 1 C.u. $\approx 27.054 Z^2$ 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]:

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

Here $B_{ie,iv}^{IK}$ 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:

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

Here values Q_{λ}^{Qul} and Q_{λ}^{Br} 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

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

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

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

with

$$\langle j_{fe}, j_{fv}, J_f | j_{in}, j_{sc} | 0 \rangle = \text{sqr}t(2j_{fe} + 1)(2j_{fv} + 1)(-1)^{j_{fe}+1/2} \sum_{\lambda} (-1)^{\lambda+J_f} \times \\ \times \left(\delta_{\lambda, J_f} (1/(2J_f + 1)) Q_{\lambda}(sc, ie; iv, in) \begin{pmatrix} j_{in} & j_{sc} & J_f \\ j_{fe} & j_{fv} & \lambda \end{pmatrix} Q_{\lambda}(fe, sc; fv, in) \right) \quad (11)$$

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 we use the basis of the one-particle relativistic functions as eigen functions of the Dirac-Kohn-Sham-Gunnarsson-Lundqvist effective hamiltonian. Simulteniously, the check of gauge invariance principle fulfilling is performed. In result the last procedure provides more effective account of the complex exchange-correlation effects and increases the accuracy of computed collisional parameters.

Table 1 Comparison of measured and calculated electron-collisional excitation cross-sections (σ) for Ne-like barium for two values of incident electron energy 5.69 keV and 8.20 keV (Units are 10^{-21} cm^2).

Level Calculated	J	Measured	Calculated	Calculated	Calculated	Calculated
		Marrs et al.	Ivanov et al.	Zhang et al.	Glushkov et al	Svinarenko
present paper		[2]	[4]	[2]	[7]	[11]
			$E_{el} = 5.69 \text{ keV}$			
$2p_{3/2}3d_{5/2}$ 3.74	1	3.98 ± 0.56	3.20	3.44	3.25	3.62
$2p_{1/2}3d_{3/2}$ 2.09	1	2.12 ± 0.30	1.78	2.42	1.84	2.06
			$E_{el} = 8.20 \text{ keV}$			
$2p_{3/2}3d_{5/2}$ 3.28	1	3.30 ± 0.46	2.87	2.99	2.93	3.25
$2p_{1/2}3d_{3/2}$ 1.83	1	1.82 ± 0.25	1.64	2.10	1.64	1.81

3 Some examples and conclusions

We applied our approach to estimate of the electron collisional excitation cross-sections, strengths and rate coefficients for electron-collisional excitation for Ne- and Ar-like ions. To test our theory we compare our calculations on collisional cross-sections for Ne-like iron with known calculations [2], [12]. Table 1 compares the experimental results with our calculations and with those of other theoretical works [2], [5], [7], [11].

It should be noted that the experimental information about the electron-collisional cross-sections for high-charged Ne-like ions is very scarce and is extracted from indirect observations. In any case implementation of such new elements as indicated above, allows to meet more fine agreement between theoretical relativistic energy-approach data and empirical results. An analysis of theoretical results accuracy shows that a gauge invariance principle fulfilling in collisional processes, more exact account of the complex exchange-correlation effects can lead to increasing accuracy of computed collisional parameters.

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