DOI: http://dx.doi.org/10.15673/2072-9812.4/2014.42029
Proc. Intern. Geom. Center 2014 **7**(4) 72–76 $d\omega$

Quantum Geometry: Application of an advanced energy approach in scattering theory to multi-charged ions

Andrey A. Svinarenko

Abstract Within quantum geometry it is presented an advanced energy approach in scattering theory and its application to calculation of cross-sections for some complex atomic systems. The improved numerical data for electron-collisional excitation cross-sections are presented for barium.

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

Mathematics Subject Classification (2000) 55R05 · 53B05

1 Introduction

At present time a great progress can be noted in development of a quantum geometry and quantum mechanics [1]–[12], 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 sustems in relativistic approximation and new algorythms 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]–[10], we present an advanced 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) and more correct numerical accounting for the complex polarization, screening effects and continuum pressure. The improved numerical data for electron-collisional excitation cross-sections are presented for sodium-like barium.

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

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

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

Final state is:

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

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:

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

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

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 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 three other theoretical works [2], [5], [7].

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.

Acknowledgement. The author would like to thank Prof. A.Glushkov for useful advices and critical comments.

References

1. Grant, I.: Relativistic Quantum Theory of Atoms and Molecules –Oxford (2008), 650p
2. Glushkov, A. : Relativistic quantum theory. Quantum mechanics of atomic systems – Odessa, Astroprint (2008), 700p.
3. Glushkov, A., Ivanov, L.: Radiation decay of atomic states: Atomic residue and gauge non-invariant contributions – Phys. Lett.A., **170** (1992), P.33-37.
4. Ivanov, L.N., Ivanova, E.P., Knight, L.: Energy Approach to consistent QED theory for calculation of electron-collision strengths– Phys.Rev.A., **48** (1993), P.4365-4374.
5. Glushkov, A.V., Ivanova, E.P., Ivanov, L.N.: Generalized energy approach in a theroy of decaying atomic state – Autoionization phenomena in atoms – Moscow, Moscow State University (1986), P.58-160.
6. Glushkov, A., Khetselius, O., Prepelitsa G., Svinarenko, A.: Energy approach to atoms in a laser field and quantum dynamics with laser pulses of different shape – Coherence and Ultrashort Pulsed Emission, Ed. Duarte F. J. – Vienna, Intech (2011), P.159-186.
7. Glushkov, A., Malinovskaya, S., Loboda, A., etal: Diagnostics of the collisionally pumped plasma and search of the optimal plasma parameters of x-ray lasing – Jpurnal of Physics: C Ser. (IOP, UK), **11** (2005), P.188-198.
8. Glushkov, A., Khetselius, O., Svinarenko, A.: Relativistic theory of cooperative muon-gamma-nuclear processes: Negative muon capture and metastable nucleus discharge – Advances in the Theory of Quantum Systems in Chemistry and Physics. Series: Frontiers in Theoretical Physics and Chemistry, Eds. P.Hoggan, E.Brandas, G. Delgado-Barrio, P.Piecuch – Berlin, Springer, **22** (2011), P.51-70.
9. Glushkov, A., Khetselius, O., Svinarenko, A.: QED approach to atoms in a laser field: Multi-photon resonances and above threshold ionization – Frontiers in Quantum Systems in Chemistry and Physics, Eds. S.Wilson, P.Grout, J. Maruani, G. Delgado-Barrio, P.Piecuch – Berlin, Springer, **18** (2008), P.541-558.
10. Svinarenko, A.: Quantum Geometry: Energy-amplitude approach to multiphoton resonances and above threshold ionization – Proc. of Int. Geometry Center., **6** (2013), N3, P.54-59.
11. Svinarenko, A.: Quantum Geometry: An advanced energy approach in scattering theory – Proc. of Int.Geometry Center., **7** (2014), N1, P.30-34.
12. Glushkov, A., Svinarenko, A., Khetselius, O. et al : Relativistic Quantum Chemistry: Advanced Approach to Construction of the Green's Function of the Dirac Equation with Complex Energy and Mean-Field Nuclear Potential – Frontiers in Quantum Methods and Applications in Chemistry and Physics – Berlin, Springer, **29** (2015), P.197-218.

Andrey A. Svinarenko

Odessa State Environmental University, Odessa, Ukraine.

E-mail: quantsvi@mail.ru