Quantum Geometry: An advanced energy-amplitude approach to multiphoton resonances in atomic spectra

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Abstract An advanced energy-amplitude approach to calculation of the characteristics of multi-photon and autoionization resonances in spectra of atomic systems is presented and based on the many-body perturbation theory. The improved numerical data are listed for magnesium and caesium.

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 atomic quantum and nuclear theories 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]. 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 about light and not heavy systems, 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 multi-photon and autoionization resonances properties. Among existed approaches to the last problem it should be mentioned the Green function method (the imaginary part of the Green function pole for atomic quasienergetic state), the density - matrix formalism (the stochastic equation of motion for density - matrix operator and its correlation functions), a time-dependent density functional formalism, direct numerical solution of the Schrödinger (Dirac) equation, multi-body multi-photon approach etc. [1]–[8]. In [2],[4] authors extended the non-Hermitian multi-state Floquet dynamics approach by Day to treat one-electron atomic system to the case of general multi-electron ones. The approach based on the eigenchannel R-matrix method and multichannel quantum-defect theory , introduced by Robicheaux and Gao to calculate two-photon processes in light alkaline-earth atoms has been implemented by Luc-Koenig et al [4] in j-j coupling introducing explicitly spin-orbit effects and employing both the length and velocity forms of the electric dipole transition operator. Nevertheless in many calculations there is a serious problem of the gauge invariance, connected with using non-optimized one-electron representation. In this paper, which goes on our studying [5]–[10], we present an advanced version of an amplitude approach to calculation of the characteristics of resonances in atomic systems. It is based on the many-body perturbation theory (PT) and applied to numerical calculating two atomic systems. In particular, the improved numerical data are listed for magnesium and caesium.

2 An advanced energy relativistic approach to resonances

Let us briefly consider earlier presented formally exact approach based on the QED perturbation theory [5]–[12], which allow to calculate the characteristics of resonances in atomic spectra. As usually [10], We start from the two-photon amplitude for the transition from an initial state Ψ_0 with energy E_0 to a final state $|Psi_f$ with energy $E_f = E_0 + 2\omega$ is:

$$T_{f0}^{(2)} = \lim_{n \to 0_+} \int d\epsilon \langle \Psi_f | D \times e | \epsilon \rangle (E_0 + \omega - \epsilon + in)^{-1} \langle \epsilon | d \times e | \Psi_0 \rangle. \qquad (1)$$

Here D is the electric dipole transition operator (in the length r form), e is the electric field polarization and ω is a laser frequency. The integration in equation 1 is meant to include a discrete summation over bound states and integration over continuum states. Usually an explicit summation is avoided by using the Dalgarno-Lewis by means the setting [3]:

$$T_{f0}^{(2)} = C_f \langle \| D \times e \| \Lambda_p \rangle, \tag{2}$$

where $\langle \| ... \| \rangle$ is a reduced matrix element and C_f is an angular factor depending on the symmetry of the Ψ_f, Λ_p, Ψ_0 states. Λ_p can be founded from solution of the following inhomogeneous equation [3]

$$(E_0 + \omega \times H | \Lambda_p \rangle = (D \times e) | \Psi_0 \rangle \tag{3}$$

at energy $E_0 + \omega$, satisfying outgoing-wave boundary condition in the open channels and decreasing exponentially in the closed channels. The total cross section (in $\mathrm{cm}^4\ \mathrm{W}^{-1}$) is defined as

$$\sigma / I = \sum_J \sigma_J / I = 5.7466 \times 10^{-35} \omega_{\mathrm{au}} \sum_J |T_{J,0}^{(2)}|^2, \tag{4}$$

where I (in $\mathrm{W/cm}^2$) is a laser intensity. To describe two-photon processes there can be used different quantities [9]: the generalized cross section $\sigma^{(2)}$, given in units of $\mathrm{cm}^4\mathrm{s}$, by

$$\sigma_{\mathrm{cm}^4\mathrm{s}}^{(2)} = 4.3598 \times 10^{-18} \omega_{\mathrm{au}} \sigma / I_{\mathrm{cm}^4\mathrm{W}^{-1}} \tag{5}$$

and the generalized ionization rate $\Gamma^{(2)}/I^2$, (and probability of to-photon detachment) given in atomic units, by the following expression

$$\sigma / I_{\mathrm{cm}^4\mathrm{W}^{-1}} = 9.1462 \times 10^{-36} \omega_{\mathrm{au}} \Gamma_{\mathrm{au}}^{(2)} / I_{\mathrm{au}}^2 \tag{6}$$

Described approach is realized as computer program block in atomic numeric code "Super-atom" (c.f. [2]–[7], which includes a numeric solution of the Dirac equation and calculation of the matrix elements of the Eqs. 1–5 type. The new original moment of the advanced scheme is in using more corrected in comparison with [9], [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 [2].

3 Some results and conclusion

Let us present the results of calculating the multi-photon resonances spectra characteristics for atoms of magnesium (new data) and caesium in a laser field. It is worth to list the data of different methods for comparison: relativistic R-matrix method (R-method; Robicheaux-Gao, 1993; Luc-Koenig E. etal, 1997),

Table 1 Characteristics for $3p^2{}^1S_0$ resonance of atom of the magnesium: E- energy, counted from ground state (cm^{-1}), Γ- autoionization width (cm^{-1}), σ/I- maximum value of generalized cross-section (cm^4W^{-1}).

Methods	E	Γ	σ/I
Luc-Koenig E. etal, 1997	without	account	SE
Length form	68492	374	$1{,}96\ 10^{-27}$
Velocity form	68492	376	$2{,}10\ 10^{-27}$
Luc-Koenig E. etal, 1997	With	Account	SE
Length form	68455	414	$1{,}88\ 10^{-27}$
Velocity form	68456	412	$1{,}98\ 10^{-27}$
Moccia and Spizzo (1989)	68320	377	$2{,}8\ 10^{-27}$
Robicheaux and Gao (1993)	68600	376	$2{,}4\ 10^{-27}$
Mengali and Moccia(1996)	68130	362	$2{,}2\ 10^{-27}$
Karapanagioti et al (1996)	68470	375	$2{,}2\ 10^{-27}$
Svinarenko (2012)	68281	323	$2{,}0\ 10^{-27}$
This paper	68395	386	$1{,}9\ 10^{-27}$

added by multi-channel defect method, K-matrix method (K-method; Mengali-Moccia,1996), different versions of the finite L^2 method (L^2 method) with account of polarization and screening effects (SE) (Moccia-Spizzo, 1989; Karapanagioti et al, 1996), Hartree-Fock configuration interaction method (CIHF), operator QED PT (Glushkov-Ivanov, 1992; Glushkov et al; 2004), energy amplitude approach (Svinarenko, 2012) etc.(c.f.[2,10]. In table 1 we list results of calculating characteristics for $3p^2{}^1S_0$ resonance of Mg; E- energy, counted from ground state (cm^{-1}), Γ-autoionization width (cm^{-1}), σ/I- maximum value of generalized cross-section (cm^4W^{-1}). R-matrix calculation with using length and velocity formula led to results, which differ on 5-15% , that is evidence of non-optimality of atomic basis's.

Let us consider further the numerical data for the three-photon (k=3) resonance 6S-6F in the caesium (wavelength 105,9 nm). The detailed experimental study of the multi-photon processes in the caesium has been earlier carried out in details (look refs. [2],[11]). According to [12], the 6S-6F resonance line shift is linear to respect to the laser intensity (laser intensity is increased from $1,4$ to $5,7\ \cdot 10^7\ W/cm^2$) and is equal (the gaussian multi-mode pulse): bI. Here I is a laser pulse intensity and coefficient b is expressed in terms of energy of the three-photon transition 6S-6F: $b = (5,6 \pm 0,3)\ cm^{-1}/GW \times cm^{-2}$.

For comparison let us present the analogous theoretical value, obtained in the S-matrix formalism calculation [2]: b=5,63. Our theoretical values, obtained with using the non-optimized and optimized basis's, are as follows: i). for the gaussian multi-mode pulse (non-optimized basis): b=5,84; ii). for the gaussian multi-mode pulse (optimized basis): b=5,62.

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