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ENERGY APPROACH TO COLLISIONAL IONIZATION OF THE RYDBERG ATOMS: QUANTUM DEFECT APPROXIMATION

T. N. Zelentsova[1], Yu. M. Lopatkin[3], L. V. Nikola[2], T. B. Tkach[1], S. S. Seredenko[1]

[1] Odessa National Polytechnical University, Odessa
[2] I. I. Mechnikov Odessa National University, Odessa
[3] Sumy State University, Sumy

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Abstract. Within the energy approach (S-matrix formalism) it is presented a new approach to collisional ionization of the Rydberg atoms in the quantum defect approximation. The Rydberg systems theory is a basis for creation of new class of the atomic sensors.

Keywords: sensing Rydberg atoms, collisional ionization, energy approach

ЕНЕРГЕТИЧНИЙ ПІДХІД ДО ОПИСУ ІОНІЗАЦІЇ ЗА РАХУНОК ЗІТКНЕНЬ РІДБЕРГІВСЬКИХ АТОМІВ: НАБЛИЖЕННЯ КВАНТОВОГО ДЕФЕКТУ

Т. М. Зеленцова, Ю. М. Лопаткін, Л. В. Нікола, Т. Б. Ткач, С. С. Середенко

Анотація. В межах енергетичного підходу (S-матричний формалізм) запропонований новий підхід до опису іонізації рідбергівських атомів за рахунок зіткнень у наближенні квантового дефекту. Теорія рідбергівських систем є базою для створення відповідних атомних сенсорів нового класу.

Ключові слова: детектування рідбергівських атомів, іонізація за рахунок зіткнень, енергетичний підхід

ЭНЕРГЕТИЧЕСКИЙ ПОДХОД К ОПИСАНИЮ СТОЛКНОВИТЕЛЬНОЙ ИОНИЗАЦИИ РИДБЕРГОВСКИХ АТОМОВ: ПРИБЛИЖЕНИЕ КВАНТОВОГО ДЕФЕКТА

Т. Н. Зеленцова, Ю. М. Лопаткин, Л. В. Никола, Т. Б. Ткач, С. С. Середенко

Аннотация. На основе энергетического подхода (S-матричный формализм) предложен новый подход к описанию столкновительной ионизации ридберговских атомов в приближении квантового дефекта. Теория ридберговских атомов является основой для создания атомных сенсоров нового класса.

Ключевые слова: детектирование ридберговских атомов, столкновительная ионизации, энергетический подход

1. Introduction

The modern quantum theory of atomic systems can be considered as a fundamental basis for treating a wide cycle of phenomena, including the excitation, photoionization, radiation and autoionization decay etc. [1-21]. In the last years a great success has been achieved in the applied atomic physics, laser physics, atomic sensors electronics. One could mention very perspective papers devoting to engineering so called Rydberg atoms with different mechanisms of ionization processes [5-9]. New schemes of the different atomic sensor devices are proposed. One could mention here so called atomic watches etc [1]. Naturally, for more than 80 years, the theory of collisional ionization was developing and considering mainly the ground states and lowest excited states in usual neutral atoms, beginning from the hydrogen one. But a great progress in experimental laser physics and appearance of the so called tunable lasers allow to get the highly excited Rydberg states of atoms. In fact this is a beginning of a new epoch in the atomic physics regarding the Rydberg atoms [1-9]. The experiments with Rydberg atoms had very soon resulted in the discovery of an important ionization mechanism, provided by unique features of the Rydberg atoms. Relatively new topic of the modern theory is connected with consistent treating the electron-collisional ionization of the Rydberg atoms [1]. From the theoretical point of view, the low energy electron collisions could essentially affect on the Rydberg states in atoms. Its role was estimated theoretically and observed in the tunable lasers experiments (look for example, [1-3]). The account for fast redistribution of the atomic levels' population, excitation and further and ionization caused by the collisions is of a great importance for successfully handling atoms in their Rydberg states. In the last years there is appearing a sufficiently great number of papers devoted to the collisional ionization of the Rydberg atoms within the on-relativistic and relativistic approaches (look refs. [1-20]). Usually the standard methods of atomic physics, including the Hartree-Fock, Dirac-Fock, different model potential schemes, R-matrix and energy approaches etc [1-4] were used in order to define the electron-collisional ionization characteristics of neutral and even Rydberg atoms. In our opinion the significant advantage of the simple model potential and quantum defect approached (non-relativistic schemes) in comparison with other methods and, particularly, other model potentials is the possibility of presenting analytically, in terms of the hypergeometric functions, the quantitative characteristics for arbitrarily high orders, related to both bound–bound and bound–free transitions. From the other side, the heavy Rydberg atomic systems and corresponding collisional phenomena should be considered within strictly relativistic theory. Here we present new combined quantum defect method and energy approach to definition of the electron-collisional excitation and ionization characteristics of the Rydberg atoms. The important feature of new theory is implementation of the quantum defect approximation to the S-matrix energy formalism. This provides sufficiently correct and simultaneously simplified numerical procedure to definition of the corresponding collisional ionization properties. Naturally, the similar information is of a great importance for carrying out the new schemes of different atomic sensor devices

2. Collisional ionization of the Rydberg atoms: Energy approach

As starting basis for formulation of a new approach to collisional ionization of the Rydberg atoms we use an energy approach [4,11-14], which is based on the S-matrix formalism and relativistic many-body perturbation theory. As in refs. [13,14], for definiteness, we consider the highly excited Rydberg states $1s^22s^22p^5nl$ ($n>>3$) of the Ne-like ion, which can be treated as two-quasi-particle (2QP) states. It is usually accepted, as the bare potential, a potential including the electric nuclear potential V_N and some parameterized potential V_C, that imitates the interaction of closed-shell electrons with quasi-particles. The parameters of the model bare potential are chosen so as to generate accurate eigen-energies of all one-quasi-particle (1QP) states, i.e. $2s2p^6$, $2s^22p^5$ states of the F-like ion and $2s^22p^6nl$ states of Na-like ions, with the same nucleus. Usually the experimental one-quasi-particle energies are used for determination of parameters of the model potential (look refs. [4,10,11]). Naturally (look below) the quantum defect approximation is very effective here as it provides the hydrogen-like approximation for the corresponding wave functions.

Further we briefly discuss the energy approach in scattering theory [11,12] and give main formulas. We briefly outline the main idea using, as an example, the collisional de-excitation of the Rydberg Ne-like ion: $((2j_{iv})^{-1}3j_{ie}[J_iM_i],\ \varepsilon_{in}) \rightarrow (\Phi_o, \varepsilon_{sc})$.

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. 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

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

Here $C_{m_{ie},m_{iv}}^{J_i,M_i}$ is the Clebsh-Gordan coefficient. Final state is: $|F>=a_{sc}^{+}\Phi_o$, where Φ_o is the state of an ion with closed electron shells (ground state of Ne-like ion), $|I>$ represents three-quasiparticle (3QP) state , and $|F>$ represents the one-quasiparticle (1QP) state. For the state (1) the scattered part of energy shift *Im* ΔE appears first in the PT second order in the form of integral over the scattered electron energy ε_{sc}:

$$\int d\varepsilon_{sc} G(\varepsilon_{iv},\varepsilon_{ie},\varepsilon_{in},\varepsilon_{sc})/(\varepsilon_{sc}-\varepsilon_{iv}-\varepsilon_{ie}-\varepsilon_{in}-i0)\ , \qquad (2)$$

with

$$Im\Delta E=\pi\, G(\varepsilon_{iv},\varepsilon_{ie},\varepsilon_{in},\varepsilon_{sc})\ . \qquad (3)$$

Here G is a definite squired combination of the two-electron matrix elements (2). The value $\sigma=-2\ Im\Delta E$ 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 (c.f. [4,14]):

$$\sigma(I\to F)= =\Omega(I\to F)\cdot\pi/\{(2J_i+1)\varepsilon_{in}[(\alpha Z)^2\varepsilon_{in}+2]\}\ . \qquad (4)$$

Here and below the Coulomb units are used; 1 C.u. $\approx$27,054Z^2 eV, for energy; 1 C.u.$\approx0{,}529\cdot10^{-8}/Z$ cm, for length; 1 C.u. $\approx2{,}419\cdot10^{-17}/Z^2$ sec for time. The collisional de-excitation cross section is:

$$\sigma(IK\to 0)=2\pi\sum_{j_{in},j_{sc}}\Big[(2j_{sc}+1)\times \times\{\sum_{j_{ie},j_{iv}}<0\,|\,j_{in},j_{sc}\,|\,j_{ie},j_{iv},J_i>B_{ie,iv}^{IK}\}^2\Big]\ . \qquad (5)$$

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 (8) has the following form:

$$<0\,|\,j_{in},j_{sc}\,|\,j_{ie},j_{iv},J_i>= =\sqrt{(2j_{ie}+1)(2j_{iv}+1)}(-1)^{j_{ie}+1/2}\times\sum_{\lambda}(-1)^{\lambda+J_i}\times \times\{\delta_{\lambda,J_i}/(2J_i+1)Q_\lambda(sc,ie;iv,in)+ +\begin{bmatrix} j_{in}\ldots j_{sc}\ldots J_i \\ j_{ie}\ldots j_{iv}\ldots\ldots\lambda\end{bmatrix}Q_\lambda(ie;in;iv,sc)\}\ . \qquad (6)$$

In (6) values Q_λ^{Qul} and Q_λ^{Br} are defined in ref. [4]. For the collisional excitations from ground state (inverse process) one must consider $a_{in}^{+}\Phi_0$ as the initial state and

$$|F>=a_{sc}^{+}\sum_{m_{fe},m_{fv}} a_{fe}^{+}a_{fv}\Phi_o\tilde{C}_{m_{fe},m_{fv}}^{J_f,M_f} \qquad (7)$$

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

$$\sigma(0\to IF)=2\pi(2J_f+1)\sum_{j_{in},j_{sc}}(2j_{sc}+1)\cdot \cdot\{\sum_{j_{fe},j_{fv}}B_{fe,fv}^{FK}<j_{fe},j_{fv}J_f\,|\,j_{in},j_{sc}\,|\,0>\}^2\ . \qquad (8)$$

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 (11). The expression for the cross-section of the collisional excited-excited *IK-IF* transition can be found in [13]. To calculate the corresponding parameters, one should use the relativistic expressions for quantum defect approximation wave functions. As it was indicated, the heavy Rydberg atomic systems should be considered within strictly relativistic theory.

3. Quantum defect approximation for Rydberg atoms

As an energy approach provides an effective scheme for calculation the collisional ionization cross-sections [11-13], the important question here is implementation of the relativistic quantum defect approximation to the cited scheme. The general expression for the wave function can be presented in a standard form as follows:

$$\Psi(\Gamma PJM)=\sum_{r}^{NCF}c_r\Phi(\gamma_r PJM)\ , \qquad (9)$$

which should be received from the self-consistent solutions of the Dirac type quantum-defect equations. Configuration mixing coefficients c_r are usually obtained through diagonalization of the Dirac-Coulomb Hamiltonian, which is chosen by us in the following form [4]:

$$H_{DC}=\Sigma_i\,[c\alpha_i p_i + (\beta_i - 1)c^2 - V(r|nlj)] +$$

$$+ \Sigma_{i>j} \exp(i\omega r_{ij})(1-\alpha_1\alpha_2)/r_{ij}, \qquad (10)$$

where α_i,,β are the Dirac matrices. The potential in H_{DC} contains the electrical potential of a nucleus, the electron self-consistent potential and the potential of exchange inter-electron interaction. In the quantum defect approximation the one-particle wave functions are found from solution of the relativistic Dirac equation, which can be written in the central field in a two-component form:

$$\frac{\partial F}{\partial r}+(1+\chi)\frac{F}{r}-(\varepsilon+m-v)G=0,$$

$$\frac{\partial G}{\partial r}+(1-\chi)\frac{G}{r}+(\varepsilon-m-v)F=0. \qquad (11)$$

Here we put the fine structure constant $\alpha=1$. The moment number

$$\chi=\begin{cases}-(l+1), & j>1\\ l, & j<l\end{cases}.$$

To prevent the integration step becoming too small it is convenient to turn to new functions isolating the main power dependence: $f=Fr^{1-|\chi|}$, $g=Gr^{1-|\chi|}$. The Dirac equation for F and G components are transformed as:

$$f'=-(\chi+|\chi|)f/r-\alpha ZVg-(\alpha ZE_{n\chi}+2/\alpha Z)g, \qquad (12)$$

$$g'==(\chi-|\chi|)g/r-\alpha ZVf+\alpha ZE_{n\chi}f.$$

Here the Coulomb units (C.u.) are used; $E_{n\chi}$ is one-electron energy without the rest energy.

In the quantum defect approximation to describe a spectrum of the Rydberg atom it is usually used the simple formula:

$$E_{alk}=-\frac{1}{2n_{eff}^2}=-\frac{1}{2(n-\delta_l)^2},\ n\in N, \qquad (13)$$

where n_{eff} — effective quantum number, δ_l — quantum defect, which is dependent upon the orbital quantum number. Usually to reach a high accuracy in definition of the quantum defect it is used an expansion (the known Ritzs formula):

$$\delta_l=\delta_l^{(0)}+\sum_{i=1}^{M}\delta_l^i E^i. \qquad (14)$$

From the physical point of view, for the bound states a quantum defect defines an effect of the non-Coulomb part of the atomic potential. For the scattering states a role of the quantum defect belongs to the asymptotic phase shift τ. According to the Siton theorem , a link between phase shift and quantum defect is given by [1]:

$$\tau=\delta_l\cdot\pi. \qquad (15)$$

Further it is non-difficult to present the Dirac equations (11) or (12) in the quantum defect approximation. Really, in this case the potential $V_{at}=-1/r$ for $r>r_0>0$ (r_0 is a radius of the atomic core, for example in the F-,Ne-,Na-like ions). Naturally for the bound states the corresponding components, for example, $F(r)\to 0$ under $r\to\infty$. For large values of r the corresponding functions are satisfying to the asymptotics as follows:

$$f(E,l,r)\to u(m.l.r)\sin(\pi m)-v(m,l,r)e^{i\pi m}, \qquad (16a)$$

$$g(E,l,r)\to -u(m.l.r)\sin(\pi m)+$$
$$+v(m,l,r)e^{i\pi(m+1/2)}, \qquad (16b)$$

where u,v are respectively exponentially increasing and decreasing functions. Naturally to get asymptotically exponentially decreasing function a multiplier u in (16) must reach to zero, i.e. it is correct a condition:

$$\sin(\tau+\pi m)=\sin(\tau+\pi\sqrt{-1/2E})=0. \qquad (17)$$

Finally for the bound state, the correctly normalized solution is as follows:

$$F_{l,E_{alk}}(r)=\cos(\pi\delta_l)s_l(E_{alk},r)+$$
$$+\sin(\pi\delta_l)c_l(E_{alk},r), \qquad (18)$$

where $E_{alk}=E$ and the functions s_l, c_l represent the normalized (on energy) regular and non-regular Coulomb functions. Further using the quantum defect approximation functions in the energy approach scheme to calculating the electron-collisional ionization of the Rydberg atoms is the same as in the initial version of the method [4] (see also [21]).

4. Conclusions

So, we have presented a new combined quantum defect method and energy approach to definition of the electron-collisional excitation and ionization characteristics of the Rydberg atoms. The important feature of new theory is implementation of the quantum defect approximation to the S-matrix energy formalism. This provides sufficiently correct and simultaneously simplified numerical procedure to definition of the corresponding collisional ionization properties and thus it is represented significantly more advantagable in comparison with the

standard Hartree-Fock approximation approach and even Dirac-Fock method when the latter is used in the Rydberg atoms calculations. This circumstance is to be very important because of a great necessity the corresponding data about the electron-collisional parameters of the Rydberg atoms under creation and construction of new classes of the Rydberg-atomic sensors. In conclusion the authors would like to thank Professors V.D.Rusov, A.V.Glushkov, V.N.Vysotsky and V.N. Pavlovich for useful comments.

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