ROLE OF CLOSE-COUPLING EFFECTS IN CONTINUUM FOR IONIZATION PROBLEMS

A.D.Kondorskiy

Moscow Institute of Physics and Technology (State University),
Dolgoprudny, Moscow Reg., Russia
e-mail: demokr@mail.ru

Close-coupling equations for transition amplitudes are used for investigation of the ionization of hydrogen-like atom by intense monochromatic laser field. The orthogonal and normalized basis in which the solution of the time dependent equation is expanded contains unperturbed wave functions of the discrete spectrum and generalized Coulomb wave functions of the continuum. For the investigation of the close-coupling equations the fact, that bound-free and free-free transitions are efficient in different regions of complex time plain, is used. Simplified equations are constructed. The equations for bound-free transitions are reduced to the ordinary differential equations. The equations for free-free transitions are solved by quadratures. Results are obtained for ionization of a hydrogen atom from its ground state in strong and superstrong linearly polarized fields. Energy distributions and angular momentum distributions of electrons are also presented. It is shown that in this case the ground state decays completely, and free-free transitions play a defining role in the dynamics of the process. The electron transitions from the continuum into the highest Rydberg states are also considered. The total population of all the Rydberg states is found to be less than 5%. The range of applicability of the approach is discussed. A comparison with numerical results obtained by other authors is given.

Introduction

Modern progress in the theory of non-linear ionization of atoms by intense laser fields is based on the Keldysh-Faisal-Reiss approach [1-3], its analytic developments with including classical and semiclassical models [4], and on the non-perturbative approaches [5-6]. In all the theories above, the influence of quantum free-free transitions in continuum to the ionization process has been not investigated specially. Of course, this influence accounts in the results obtained with the help of the B-spline basis [5] and R-matrix [6] calculations. Here the process of ionization of hydrogen-like atomic systems by strong and superstrong monochromatic fields is studied with the help of close-coupling equations [8] including both bound-free and free-free transitions. It is shown that the complete decay of the initial atomic state occurs due to electron redistributions in continuum. Electron transitions from the continuum into the denumerable set of the highest Rydberg states is also considered.

Basic equations

We consider ionization of the H atoms and H-like ions by a spatially homogeneous, linearly polarized, monochromatic electric field. The non-stationary Schroedinger equation

$$\left[i\frac{\partial}{\partial t}+\frac{\nabla^2}{2}+\frac{Z}{r}-i\mathbf{A}(t)\nabla\right]\Psi=0\,,\quad (1)$$

$$\mathbf{A}(t)=-\frac{\mathbf{F}}{\omega}\sin(\omega t)$$

subjects to the usual initial condition. Here Z is the nuclear charge, F and ω are the field strength and circular frequency, respectively (taken in atomic units). The close-coupling equations for transition amplitudes are obtained with the help of the orthogonal and normalized basis described earlier [7]. The complete set consist of the unperturbed wavefunctions of the discrete states and the generalized Coulomb waves with incoming wave asymptotics,

$$\Psi_{\mathbf{k}} = Q^{(-)}(\nu, \mathbf{p}(t), \mathbf{r}) \cdot \exp\left\{-\frac{i}{2}\int_0^t p^2(\tau)d\tau\right\},$$

$$\mathbf{p}(t) = \mathbf{k} - \mathbf{A}(t),\ \nu = Z/p(t). \qquad (2)$$

It should be noted that the momentum, added in this wavefunction describes an additional momentum acquired by the detached electron in the field. This orthogonal set results in Hermitian system of coupled equations. Before discussing methods of solving this system of equations for the amplitudes one should indicate the main assumptions adopted in this work. First of all only transitions between the initial 1s-state and all continuum states (bound-free coupling) and transitions inside continuum states (free-free coupling) are taken into account. The denumerable set of the highest Rydberg states is considered as a part of continuum, and for this states only interaction with continuum is considered. So the set of close-coupling equations [7] is reduced to the system:

$$i\dot{a}_0(t) = \mathbf{A}(t)\int \mathbf{U}_{0\mathbf{k}}(t)a_{\mathbf{k}}(t)d\mathbf{k}, \qquad (3)$$

$$i\dot{a}_{\mathbf{k}}(t) = \mathbf{A}(t)\left\{\mathbf{U}^*_{0\mathbf{k}}a_0(t) + \int \mathbf{U}_{\mathbf{k}\mathbf{k}'}(t)a_{\mathbf{k}'}(t)d\mathbf{k}'\right\} (4)$$

$$a_0(t_i) = 1, a_{\mathbf{k}}(t_i) = 0, \qquad (5)$$

where the matrix elements are integrals over r-space taken with ∇-operator.

The Hermitian system (5) of the CC equations for the transition amplitudes a_j and a_k is investigated and solved [8] under the condition $F/(Z\omega)>1$.

Physical model and simplified equations

The further analysis is connected to the selection rules in the $\mathbf{p}(t)$-representation. For ionization from the ground state (l=0, m=0) by linearly polarized field, the states with m=0 are populated only. Bound-free coupling results in population of the continuum states with l=1. All the states with $l \neq 1$ are populated due to free-free coupling. The bound-free transitions are the most effective in the regions of (t, $\mathbf{k}$)-space where the energy level of the ground state promotes to continuum. The set of the stationary-phase points, $t_0^j = t_0^j(\mathbf{k}, \mathbf{F}, \omega, Z)$, follows from the analytic properties of bound-free matrix elements and is given by

$$p^2(t_0^j) + 2|E_0| = 0, \qquad (6)$$
$$E_0 = -Z^2/2, \quad j=0,1,2,\ldots N.$$

In the closest vicinity of any t_0^j-point, bound-free coupling populates the states with l=1 (in the $\mathbf{p}(t)$-space) and the free-free transitions are less important. Between the t_0^j- and the t_0^{j+1}- point, probabilities of the free-free transitions predominate. In the real t-axis, we introduce the two sets of distinct intervals. The first one, $\mathrm{Re}\,t_0^j - \Delta t < t < \mathrm{Re}\,t_0^j + \Delta t$, represents the regions of bound-free transitions. The second set, $\mathrm{Re}\,t_0^j + \Delta t < t < \mathrm{Re}\,t_0^{j+1} - \Delta t$, corresponds to the regions of free-free transitions leading to electron redistributions among the continuum states with $l \neq 1$. The neighboring points, t_0^j and t_0^{j+1}, are separated in the t-axis with the halfperiod of the monochromatic field, $T/2 = \pi/\omega$. Thus, the system of close-coupling equations is splitted into the two distinct systems valid in distinct intervals,

$$i\dot{a}_{\mathbf{k}} = \mathbf{A}(t)\mathbf{U}^*_{0\mathbf{k}}a_0,\ i\dot{a}_0 = \mathbf{A}(t)\int \mathbf{U}_{0\mathbf{k}}a_{\mathbf{k}}d\mathbf{k} \quad (7)$$

in the regions of bound-free coupling and

$$i\dot{a}_{\mathbf{k}} = \mathbf{A}(t)\int \mathbf{U}_{\mathbf{k}\mathbf{k}'}a_{\mathbf{k}'}d\mathbf{k}' \qquad (8)$$

in the regions of free-free coupling.

Initial conditions in any interval result from the final values in the previous one.

Solution of the simplified equations

Further mathematical analysis of the simplified systems (7) and (8) is published in [8]. The system (7) may be reduced to two ordinary differential equations with the help of substitutions

$$a_{\mathbf{k}}(t) = c_{\mathbf{k}}(t)b(t),$$
$$\int |a_{\mathbf{k}}(t)|^2 d\mathbf{k} = |b(t)|^2, \quad (10)$$
$$\int |c_{\mathbf{k}}(t)|^2 d\mathbf{k} = 1.$$

Here the form of $c_{\mathbf{k}}$ coefficients depends on the analytic properties of the matrix elements, $\mathbf{U}_{0,\mathbf{k}}(t)$, in the vicinities of t_0^j-points.

The free-free transitions (8) are investigated in strong and superstrong fields when $\mathbf{p} \approx \mathbf{A}$ (see (2)) and $|p^2 - p'^2| << p^2$. In this case, the matrix elements, $\mathbf{U}_{\mathbf{k},\mathbf{k}'}(t)$, can be taken in the asymptotic form which depends on the difference of $|p^2 - p'^2|$ only. So after expanding over eigenvalues of the angular momentum l and transformation of independent value to the energy $E = p^2/2$ can be written in the form:

$$i\dot{a}_{l,E} = \sum_{l'} \int_{-E_e}^{\infty} W_{l,l'}(E - E', t) \cdot a_{l',E'} \cdot dE'$$

$$; \; W_{l,l'}(E - E', t) = W^{*}_{l,l'}(E' - E, t). \quad (11)$$

It was found that such a system is solvable in terms of the matrix generating function, and solution can be written in the form of matrix exponent with one dimension integral as a variable.

Results and discussion

Some results are presented for ionization of H – atom (Z=1) from the ground state. First of all one should note, that the bound-free coupling by itself does not lead to complete ionization (Fig. 1) at any values of the field strength.

The free-free transitions depopulate the continuum states with l=1 that provides more effective decay of the 1s-state (Fig.2). Even medium values of the field strength, less than the atomic one, lead to almost complete decay of the initial state during a few periods of field oscillations. With the field intensity increasing, the ionization probability tends to unity. These results are found in good agreement with those of Cormier and Lambropoulos [5] at values of $F/\omega > 1$.

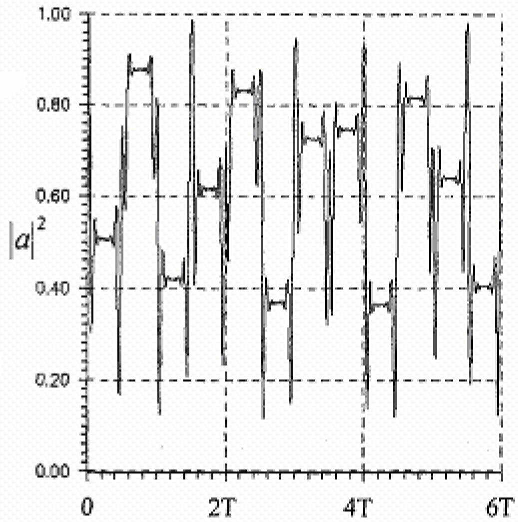

Fig. 1. Populations of the H(1s) – state against time resulting from bound-free coupling only. F=0.3 a.u.; ω = 0.1

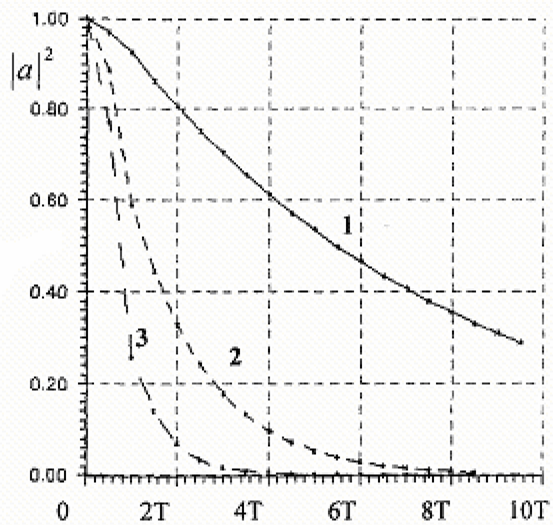

Fig. 2. Population of the H(1s) – state against time. Both bound-free and free-free coupling are included; ω = 0.1: **1**, F=0.1 a.u.; **2**, F=0.4. a.u.; **3**, F=0.6 a.u.

For weak fields or, more exactly, for values of F/ω <<1, our approach should be properly modified.

The energy spectrum of photoelectrons is given in Fig. 3. The total probability of transitions into the highest Rydberg states is less than 0.05 in the intense fields (Fig. 4).

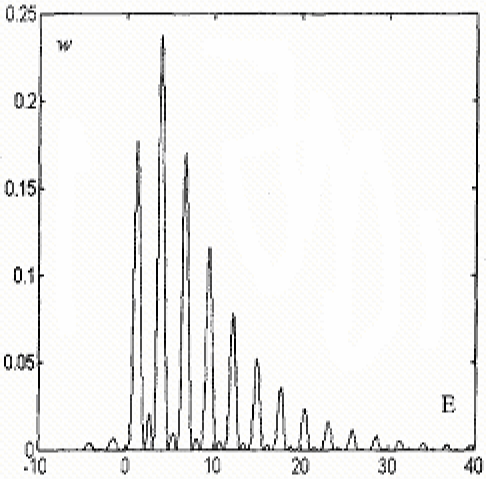

Fig. 3. Ionization probability of the H(1s) – state versus field intensity; $w = 1 - |a_0(t_f)|^2$, t_f =25 fs and ω=2 eV. Solid curve represents the results of present work and quadrates are taken from ref. [9].

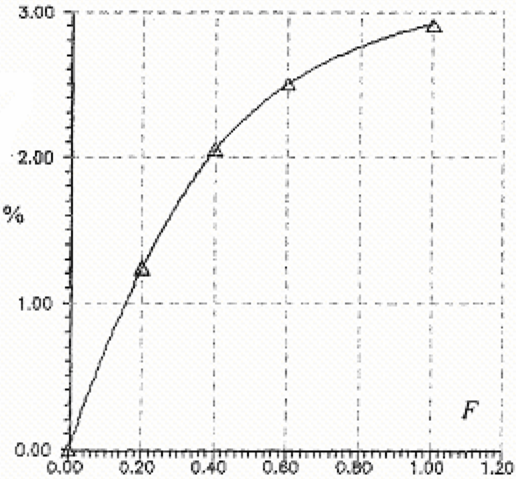

Fig. 4. Ratios, R, of Rydberg states populations to populations of all continuum states versus the field strength in atomic units; ω = 0.1.

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РОЛЬ ЕФЕКТІВ СИЛЬНОГО ЗВ'ЯЗКУ В КОНТИНУУМІ У ЗАДАЧАХ ІОНІЗАЦІЇ

А.Д.Кондорський

Московський фізико-технічний інститут (державний університет),
Долгопрудний, Московська обл., Росія
e-mail: demokr@mail.ru

Рівняння сильного зв'язку для амплітуд переходів використано для дослідження іонізації водневоподібних атомів інтенсивним монохроматичним лазерним полем. Ортогональний нормалізований базис, в якому розв'язок залежного від часу рівняння є розширеним, містить незбурені хвильові функції дискретного спектру та узагальнені кулонівські хвильові функції континууму. При дослідженні рівнянь сильного зв'язку використано той факт, що зв'язано-вільні та вільно-вільні переходи є ефективними у різних областях комплексної площини часу. Сформульовано спрощені рівняння, а рівняння для зв'язано-вільних преходів зведено до звичайних диференціальних рівнянь. Рівняння для вільно-вільних переходів розв'язуються з використанням квадратур. Отримано результати з іонізації атома водню з основного стану у сильному та надсильному лінійно поляризованому полях. Представлено також енергетичні розподіли електронів та їх розподіли за кутовими моментами. Показано, що у цьому випадку основний стан повністю розпадається, а вільно-вільні переходи грають визначальну роль у динаміці процесу. Враховано також електронні переходи з континууму на вищі рідбергівські стани. Знайдено, що загальне заселення всіх рідбергівських станів є меншим від 5%. Обговорюється область застосовності підходу. Наведено порівняння з чисельними результатами, отриманими іншими авторами.