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Coulomb divergence in S-matrix expansion of above-threshold ionization

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Abstract. Photoelectron spectrum of above-threshold ionization (ATI) is calculated using the first two orders of Coulomb-Volkov S-matrix series (Faisal, Phys. Rev. A 94, 031401 (2016)). Calculation shows that Coulomb divergence, due to singularity of forward scattering, still exists in the first two order terms for an unscreened Coulomb potential. This divergence can be removed by adding a decay factor into the phase of the S-matrix element which comes from depletion of the atomic ground state. We show that by using an example of hydrogen atom, the Coulomb-Volkov S-matrix series can successfully describe the energy spectrum of ATI and high-order ATI with the introduction of a deplete rate of the ground state.

Key words. above-threshold ionization, S-matrix thoery, Coulomb optential, rescattering.

1. Introduction

In the context of strong field-matter interaction, an increasing number of phenomena has been found and to be understood within the single-active-electron approximation. Such a phenomenon is above-threshold ionization (ATI) in which the ionized electron absorbs more photons than the minimum number necessary for ionization. With the discovery of ATI by Agostini et al. [1], intense-laser atom physics entered the non-perturbative regime where the force created by the strong laser field is comparable to or even larger than the Coulomb interaction between electrons and residual ion. The so-called strong field approximation (SFA) i.e., Keldysh-Faisal-Reiss (KFR) [2–4] theory has provided fruitful insights into a wide range of highly nonperturbative processes in intense fields.

The envelopes of energy spectra of ionized electron in ATI and high-order ATI(HATI) by a linearly polarized laser field typically consist of two regimes: one is a drop line with a cutoff near 2Up and a plateau extending to near 10 Up [5], with Up the electron's ponderomotive energy in the laser field. The low energy structure is attributed to those direct electrons that leave the laser focus without further interaction with their parent ion and decreases exponentially with increasing energy above 2Up. The high energy plateau, with lower yield by several orders of magnitude, is attributed to electrons that may backscatter off the parent ion and be accelerated again by the laser field reaching a kinetic energy of up to 10 Up.

Over the past several decades, however, plentiful theoretical researches mostly based on the KFR model with a plane-wave Volkov state obviously do not take into account the effect of the long-range Coulomb interaction in the ionization final state [6–10]. Therefore, originally the plane-wave KFR model has been explicitly proposed for the problem of electron detachment of negative ions [11] for which in the final state there is no Coulomb interaction between the detached electron and the residual neutral atom. The previous heuristic attempting to consider Coulomb corrections (e.g. [12–14]) had provided only a common overall enhancement factor that enlarges the total rate. Recently, a complete strong field S-matrix expansion that accounts for the final state Coulomb interaction in all orders is proposed explicitly to solve this long-standing problem [15].

The divergence of the Coulomb scattering amplitude in above-threshold ionization (ATI) is another open problem. For the long-range Coulomb potential, the forward-scattering cross section is large (actually, divergent), and this divergence is especially strong for Eret [16], where Eret denotes the return energy of electron before occurs rescattering with parent ion. This allows the low-energy-structure (LES) [17–19] to rise above the contribution of the forward rescattering electrons [20], i.e. p = k, where p, k are the final momentum and intermediate momentum in between ionization and recollision of the electron, respectively. Recently, in Ref. [21], an improved SFA-based calculation [22] in which the divergence caused by the Coulomb rescattering is removed by considering the depletion rate of the ground state in the energy denominator was presented.

A good agreement between theory and experiment of LES, demonstrated in Ref. [21], showed that the long-range Coulomb potential plays a major role on the LES, and Coulomb divergence mainly results from forward rescattering which is normally encountered in the high-order terms of the S-matrix expansion. In other words, Coulomb divergence is inevitable if we desire to obtain the structure of high energy plateau.

Here, in this paper, we combine the Coulomb-Volkov S-matrix series and the depletion rate of the ground state to describe the energy spectra of ATI and HATI without introduction of a suitable screening constant. This paper is organized as follows: In Sec.2 we introduce the complete Coulomb-Volkov S-matrix series for the ATI and HATI process, while in Sec.3 we present calculation of the transition amplitude for the ATI and HATI process in the case of a linearly polarized, infinitely long laser pulse. The method for calculation of this amplitude also can refer to [8, 23]. In Sec.4, we show our results and discussions. Finally, conclusions and comments about the physical meaning and importance of the results obtained are presented in Sec.5. The atomic system of units ($\hbar = |e| = m = 4\pi\varepsilon_0 = 1$) is used.

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2. Coulomb-Volkov S-matrix series

The time-dependent Schrödinger equation of the laser-atom interaction for hydrogen atom in the velocity gauge is

$$\left(i\frac{\partial}{\partial t}-\frac{\hat{p}^2}{2}+\frac{1}{r}-V_i(t)-V_{sr}(r)\right)|\Psi(r,t)\rangle=0, \quad (1)$$

where $V_i(t)=\left(-\vec{A}(t)\cdot\vec{p}+\vec{A}^2(t)/2\right)$, $\vec{A}(t)=A_0\cos\omega t\vec{e_z}$ is the vector potential of the laser field, and $\vec{p}=-i\nabla$, Vsr(r) is the short-range potential. For the final state, we take account of the long-range Coulomb potential interaction. The Coulomb-Volkov final state contains stationary Coulomb wave [24]is written by

$$\Phi_{\vec{p}}(r,t)=\phi_{\vec{p}}(r)e^{-i\int^t\left[\left(\vec{p}-\vec{A}(\tau)\right)^2/2\right]d\tau}, \quad (2)$$

where stationary Coulomb wave [25]

$$\phi_p(r)=\frac{1}{(2\pi)^{3/2}}e^{\pi/2p}\Gamma(1+i/p)e^{i\vec{p}\cdot r}\times F_1\left(-i/p\,,1,-i(pr+\vec{p}\cdot\vec{r})\right), \quad (3)$$

Thus, we get the S-matrix element [9]:

$$\begin{aligned}S_{fi}&=\langle\Phi_{\vec{p}}(t)|\Psi(t)\rangle\\&=\langle\Phi_{\vec{p}}(t)|\phi_i(t_1)\rangle-i\int dt_1\langle\Phi_{\vec{p}}(t_1)|V_i(t_1)|\phi_i(t_1)\rangle\\&\quad-i\int\int dt_2dt_1\langle\Phi_{\vec{p}}(t)|V_{CV}(t_2)|G(t_2,t_1)V_i(t_1)|\phi_i(t_1)\rangle,\end{aligned} \quad (4)$$

where,$|\phi_i(t)\rangle$ is the initial state wave function of hydrogen atom, t1,t2 denote the ionization time and the rescattering time, respectively. While $V_{CV}(t)=\left[-\vec{A}\cdot\left(\hat{p}-\hat{h}\right)+V_{sr}(\boldsymbol{r})\right]$ is the corresponding rest interaction in the final state, $\hat{h}=\sum_s|\phi_s\rangle\,\vec{s}\langle\phi_s|$, where $\sum_s(\cdots)\equiv\int d^3s(\cdots)$, and $|\phi_s\rangle$ stands for the Coulomb continuum waves with momentum s. G(t1,t2) is the full propagator in terms of the Volkov propagator G_{Vol} and the intermediate interaction $V_0(\tau)$, as follows:

$$\begin{aligned}G(t_2,t_1)&=G_{Vol}(t_2,t_1)+\int d\tau\,G_{Vol}(t_2,\tau)V_0(\tau)G(\tau,t_1)\\&=G_{Vol}(t_2,t_1)+\int d\tau\,G_{Vol}(t_2,\tau)V_0(\tau)G_{Vol}(\tau,t_1)\\&\quad+\int d\tau'd\tau\,G_{Vol}(t_2,\tau')V_0(\tau')G_{Vol}(\tau',\tau)V_0(\tau)\\&\quad\times G_{Vol}(\tau,t_1)+\cdots\end{aligned} \quad (5)$$

where (for details see ref. [15]):

$$G_{Vol}(t_2,t_1)=-ie^{-i\int_{t_1}^{t_2}[(\vec{p}-\vec{A}(\tau)^2)/2]d\tau}\int d\vec{p}\,|\,p\rangle\langle\,p\,| \quad (6)$$

where, $|\vec{p}\rangle=\frac{1}{(2\pi)^{3/2}}e^{i\vec{p}\cdot\vec{r}}$ is plane wave function, and the rest interaction is:

$$V_0(t)=H(t)-H_{Vol}(t)=[-\frac{1}{r}+V_{sr}(\mathbf{r})]. \quad (7)$$

Finally, collecting the resulting terms from Eq.(4) explicitly, we obtain the all-order Coulomb-Volkov S-matrix series of ATI:

$$\begin{aligned}S_{fi}&=S_{fi}^{(1)}+S_{fi}^{(2)}+\cdots\\&=-i\int dt_1\langle\Phi_{\vec{p}}(\vec{r}_1,t_1)|-\vec{A}(t_1)\cdot\vec{p}+\vec{A}^2(t_1/2)|\phi_i(\vec{r}_1,t_1)\rangle\\&\quad-i\iint dt_2dt_1\langle\Phi_{\vec{p}}(\vec{r}_2,t_2)|-\vec{A}(t_2)\cdot\left(\hat{p}-\hat{h}\right)+V_{sr}(\vec{r})\,|\\&\quad G_{Vol}(\vec{r}_2,t_2,\vec{r}_1,t_1)\times\left(-\vec{A}(t_1)\cdot\vec{p}+\vec{A}^2(t_1/2)\right)|\phi_i(\vec{r}_1,t_1)\rangle\\&\quad+\cdots\end{aligned} \quad (8)$$

It should be noted that the S-matrix series introduced above, like most other well-known S-matrix series, have not been proven to be convergent [15]. Then we demonstrate that $|S_{fi}^{(2)}|^2$ is larger than $|S_{fi}^{(1)}|^2$ by calculating the first two orders of Coulomb-Volkov S-matrix series of ATI for hydrogen atom in the infrared laser field. It can be seen easily from Eq.(8) that the first two terms of the Coulomb-Volkov S-matrix series take into account both the "direct" electron that departs from the atom without any further interaction with the binding potential as well as those electrons rescattering with the ionic core.

3. Calculation of the transition amplitude

The first term of the Coulomb-Volkov S-matrix series does not contain the forward scattering, so there is no Coulomb divergence.

$$\begin{aligned}S_{fi}^{(1)}&=-i\int dt_1\langle\Phi_{\vec{p}}(\vec{r}_1,t_1)\left|\left(-\vec{A}(t_1)\cdot\vec{p}+\vec{A}^2(t_1/2)\right)\right|\phi_i(\vec{r}_1,t_1)\rangle\\&=-i\int dt_1\langle\Phi_{\vec{p}}(\vec{r}_1,t_1)\left|\left(-\vec{A}(t_1)\cdot\vec{p}\right)\right|\phi_i(\vec{r}_1,t_1)\rangle\\&=i\sum_{n=n_0}^{\infty}\int dt_1A_0e^{i(p^2/2+U_p+I_p-n\omega)}J_n\left(\frac{\vec{p}\cdot\vec{E}_0}{\omega^2},-\frac{z}{2}\right)\\&\quad\times\langle\phi_{\vec{p}}(\vec{r}_1)|(\vec{e}_z\cdot\vec{p})|\phi_i(\vec{r}_1)\rangle\\&=2\pi i\sum_{n=n_0}^{\infty}A_0J_n\left(\frac{\vec{p}\cdot\vec{E}_0}{\omega^2},-\frac{z}{2}\right)\langle\phi_{\vec{p}}(\vec{r}_1)|(\vec{e}_z\cdot\vec{p})|\phi_i(\vec{r}_1)\rangle\\&\quad\times\delta\left(p^2/2+U_p+I_p-n\omega\right),\end{aligned} \quad (9)$$

where,$n_0=[(U_P+I_P)/\omega]$ is the minimum necessary number of absorbed photons required for ionization, UP is the electron's ponderomotive energy and IP is the ionization energy. $\vec{E}_0=\vec{A}_0\omega$, $J_n\left(\vec{p}\cdot\vec{E}_0/\omega^2\,,-z/2\right)$ is the generalized Bessel function of three arguments [4, 14], and $z=U_P/\omega$. $|\phi_i(\vec{r}_1)\rangle$ is initial ground state of the hydrogen atom. And the remaining matrix element:

$$\begin{aligned}&\langle\phi_{\vec{p}}(\vec{r}_1)\left|(\vec{e}_z\cdot\vec{p})\right|\phi_i(\vec{r}_1)\rangle\\&=\frac{1}{\sqrt{2\pi}}e^{\pi/2p}\Gamma(1-i/p)\\&\quad\times\int e^{-i\vec{p}\cdot r_1}F_1\left(-i/p\,,1,-i(pr+\vec{p}\cdot\vec{r})\right)(\vec{e}_z\cdot\vec{p})e^{-r}d^3r\\&=4\sqrt{2}e^{\pi/2p}\Gamma(1-i/p)(\vec{e}_z\cdot\vec{p})(1+i/p)\frac{(1-ip)^{-2-i/p}}{(1+ip)^{-2-i/p}}\end{aligned} \quad (10)$$

Next, we calculate the second term of the Coulomb-Volkov S-matrix series $|S_{fi}^{(2)}|^2$. The hydrogen atom only has a long-range Coulomb potential. So

$$\begin{aligned}S_{fi}^{(2)}&=\frac{A_0}{(2\pi)^{4.5}}\int_{-\infty}^{\infty}dt_2\int_{-\infty}^{t_2}dt_1\int d\vec{k}\left\langle\phi_{\vec{p}}(\vec{r}_2)\right|\left(\vec{e}_z\cdot\left(\hat{p}-\hat{h}\right)\right)\left|\vec{k}\right\rangle\\&\quad\times\langle\vec{k}|\left(-\vec{A}(t_1)\cdot\vec{p}+\vec{A}^2(t_1)/2\right)|\phi_i(\vec{r}_1)\rangle\\&\quad\times e^{i\int_{-\infty}^{t_2}[(\vec{p}-\vec{A}(\tau)^2)/2]d\tau}e^{-i\int_{-\infty}^{t_2}[(\vec{k}-\vec{A}(\tau)^2)/2]d\tau}\\&\quad\times e^{i\int_{-\infty}^{t_1}[(\vec{k}-\vec{A}(\tau)^2)/2]d\tau+iI_pt_1}\\&=\frac{A_0}{(2\pi)^{4.5}}\sum_N\sum_{n=n_0}^{\infty}\int dt_2\int d\vec{k}\,\frac{e^{i(p^2/2-\varepsilon_N)}}{\vec{k}^2/2-\varepsilon_n}\left(U_p-n\omega\right)\\&\quad\times J_N\left(\frac{\vec{q}\cdot\vec{E}_0}{\omega^2}\right)J_n\left(\frac{\vec{k}\cdot\vec{E}_0}{\omega^2},-\frac{z}{2}\right)\frac{8/\sqrt{\pi}}{(1+k^2)^2}\\&\quad\times\left\langle\phi_{\vec{p}}(\vec{r}_2)\right|\vec{e}_z\cdot\left(\hat{p}-\hat{h}\right)|\vec{k}\rangle\end{aligned} \quad (11)$$

where, $\varepsilon_n=n\omega-U_p-I_p$ and $\varepsilon_N=N\omega-U_p-I_p$. **k** is the intermediate momentum, and **q** = **p**–**k** is the remaining matrix element.

In the current context, from Eq.(12), the transition amplitude is logarithmically divergent for forward scattering, i.e., p = k. For the Coulomb potential, numerical evaluation indicates that for low