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Positron-Impact Excitation of Hydrogen Atoms in Debye Plasmas *

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The positron-impact excitation of hydrogen atoms embedded in plasma environments is investigated using the close-coupling approximation from the low to intermediate energy region without including any positronium formation channel, and the excitation cross sections for $1s \to 2s$, $1s \to 2p$ and $2s \to 2p$ processes are calculated in a wide Debye parameter range. The screening interactions, described by the Debye–Hückel model, decrease the coupling matrix elements, resulting in the reduction of the excitation cross sections from a few percent to one magnitude of ten. This will alter remarkably the spectroscopy of hydrogen in intensity and position, which should be considered in the simulation and diagnostics under some specific plasma conditions.

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The effects of the screened Coulomb interaction between charged particles in hot, dense plasmas on the atomic structure and collision properties have been subject to extensive studies in the last 30–40 years (see, e.g., Refs. [1,2] and references therein). These studies have been motivated mainly by the researches in laser produced plasmas, extreme ultraviolet and x-ray laser development, inertial confinement fusion, and astrophysics (stellar atmospheres and interiors). The densities n and temperatures T in these plasmas span the ranges $n \sim 10^{15}$–$10^{18}\,\mathrm{cm}^{-3}$, $T \sim 0.5$–$5\,\mathrm{eV}$ (stellar atmospheres), $n \sim 10^{19}$–$10^{21}\,\mathrm{cm}^{-3}$, $T \sim 50$–$300\,\mathrm{eV}$ (laser plasmas) and $n \sim 10^{22}$–$10^{26}\,\mathrm{cm}^{-3}$, $T \sim 0.5$–$10\,\mathrm{keV}$ (inertial confinement fusion plasmas). The Coulomb interaction screening in these plasmas is a collective effect of the correlated many-particle interactions, and in the lowest particle correlation order (pairwise correlations) it reduces to the Debye–Hückel potential (for the interaction of an ion of charge Z with an electron)[1,2]

$$V(r) = -\frac{Ze^2}{r}\exp\Big(-\frac{r}{r_d}\Big), \tag{1}$$

where $r_d = (k_B T_e/4\pi e^2 n_e)^{1/2}$ is the Debye screening length, T_e and n_e are the plasma electron temperature and density, respectively, and k_B is the Boltzmann constant. The representation of charged particle interaction in a plasma by the potential (1) is adequate only if the Coulomb coupling parameter $\Gamma = e^2/(ak_BT_e)$ and plasma nonideality parameter $\gamma = e^2/(r_d k_B T_e)$ satisfy the conditions $\Gamma \le 1$, $\gamma \le 1$, where $a = [3/(4\pi n_e)]^{1/3}$ is the average interparticle distance. There is, however, a wide class of laboratory and astrophysical plasmas in which Debye plasmas conditions are fulfilled. Expressions for the screened Coulomb interaction for strongly coupled and nonideal plasmas can be found elsewhere.[1,2]

Motivated by the spectroscopy of such plasmas,[3,4] a number of works have been carried out to investigate the plasma screening effects in the electron-impact processes, including excitation,[2,5–10] ionization[11] and recombination,[12] for the hydrogen-like ions by using the Born and close-coupling approximations. However, to the best of our knowledge, except the work of Kar and Ho[13] on the low partial wave resonance effects, no others have been performed for positron-atom collision process in plasma environments, although a lot of works have been reported on the isolated-atom case.[14–20]

In the present work, the positron-hydrogen impact excitation process in plasma environments is studied by the close-coupling approximation (CCA). The plasma screening interactions are described by the Debye–Hückel potential, and the CCA is based upon an expansion of the total wave function of the system in terms of a sum of products of eigenstates of the atomic or molecular Hamiltonian and the functions (to be determined) of the projectile. This functions or 'expansion coefficients' are then determined from the solution of a set of coupled second-order integro-differential equations. The main purpose of the present work is to investigate the effects of the screening of Coulomb potential on the dynamics of positron-hydrogen impact excitation process, therefore, for simplicity, the positronium formation channel

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is not included in our calculations although it may be important in the low energy region.[21,22] Then the total wavefunction (atomic units are used throughout this study) for the positron-Hydrogen system can be expanded as

$$\psi(\boldsymbol{r}_1\sigma_1,\boldsymbol{r}_2\sigma_2)=\sum_{\Gamma}\sum_{\gamma}\langle\gamma|\Gamma\rangle\Phi_\nu(\boldsymbol{r}_1\sigma_1)Y_{l_2m_2}(\hat{r}_2)\cdot\chi_{m_{S2}}(\sigma_2)\frac{F_\Gamma(r_2)}{r_2},\tag{2}$$

where $\Gamma = n_1l_1kl_2LSMMs$ and $\gamma = n_1l_1m_1m_{s1}kl_2m_2m_{s2}$ are the quantum numbers of the coupled and uncoupled representations of the system, respectively. The quantum numbers of the electron and incident positron are denoted by $\nu = n_1l_1m_1m_{s1}$ and $kl_2m_2m_{s2}$ respectively. Φ_ν stands for the eigenstate of the hydrogen atom, and F_Γ for the motion of the incident positron. Under the coupled-state representation Γ, we can obtain the following coupled second-order differential equations for $F_{\nu LS}(r_2)$:

$$\Big(\frac{d^2}{dr_2^2}-\frac{l_2(l_2+1)}{r_2^2}+k_\nu^2\Big)F_{\nu LS}(k,r_2)=-2\sum_{\nu'}V_{\nu,\nu'}F_{\nu' LS}(k,r_2).\tag{3}$$

In the isolated-atom case, the coupling matrix $V_{\nu,\nu'}$ is expressed as

$$V_{\nu,\nu'}(r_2)=-\frac{1}{r_2}+\sum_{\lambda}f_\lambda(l_1l_2,l_1'l_2',L)\cdot\frac{1}{r_2}y_\lambda(n_1l_1,n_1'l_1',r_2),\tag{4}$$

where $f_\lambda(l_1l_2,l_1'l_2';L)$ and $\frac{1}{r_2}y_\lambda(n_1l_1,n_1'l_1';r_2)$ can be found in Refs. [23,24], and

$$k_\nu^2=2(E-E_{n_1l_1}),\tag{5}$$

E is the total energy of the system and $E_{n_1l_1}$ is the binding energy of target state.

If the ν'th linearly independent solution for $F_{\nu LS}(r_2)$ is denoted by $F_{\nu LS}^{\nu'}(r_2)$, then the appropriate scattering boundary conditions are[23,24]

$$F_{\nu LS}^{\nu'}(0)=0,\tag{6}$$

for all channels, and

$$F_{\nu LS}^{\nu'}(r_2\to\infty)\sim\delta(\nu,\nu')\sin\Big(k_\nu r_2-\frac{l\pi}{2}\Big)+R_{\nu\nu'}^{LS}\cos\Big(k_\nu r_2-\frac{l\pi}{2}\Big),\tag{7}$$

for the open channels, and

$$F_{\nu LS}^{\nu'}(r_2\to\infty)\sim\exp(-|k_\nu|r_2).\tag{8}$$

for the remaining closed channels. Here $R_{\nu\nu'}^{LS}$ is the corresponding matrix element of the reactance matrix (or R matrix) which, in turn, is related to the scattering matrix S and transition matrix T according to

$$\boldsymbol{S}=\frac{\boldsymbol{1}+i\boldsymbol{R}}{\boldsymbol{1}-i\boldsymbol{R}},\tag{9}$$

and

$$\boldsymbol{T}=\boldsymbol{S}-\boldsymbol{1}.\tag{10}$$

The close-coupling equation in Eq. (3) can be solved by the standard method in Refs. [24,26]. Then the total excitation cross section from the state $n_1'l_1'$ to n_1l_1 is then given by (in units of πa_0^2)

$$Q(n_1'l_1'\to n_1l_1)=\sum_L\sum_{l_2l_2'}\frac{(2L+1)}{k_{\nu'}^2(2l_1'+1)}|T_{\nu\nu'}^L|^2.\tag{11}$$

In plasma environments, the eigenenergies and wave functions of hydrogen atom are calculated in the Debye screened Coulomb potential in Eq. (1) by using piecewise exact power series expansions of the radial functions.[25] The positron coupling matrix element is approximated as

$$V_{\nu,\nu'}^D(r)=V_{\nu,\nu'}(r)\exp(-r/r_d).\tag{12}$$

The resulting coupled second-order differential equations are solved numerically using the code based on that of Chandra,[26] in which the coupled equations are integrated using the De Vogelaere algorithm, and linearly independent solutions are obtained by outward integration from the origin and inward integration from the asymptotic region.

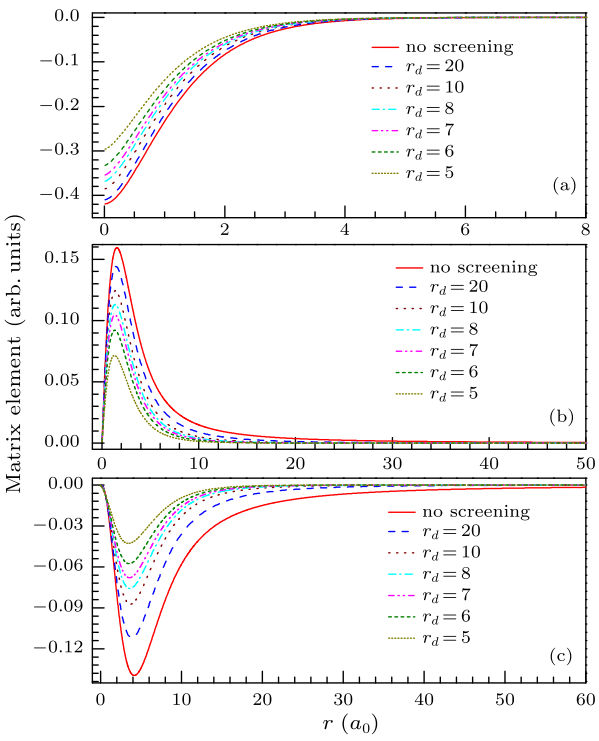

Fig. 1. Matrix elements for various scaled Debye length r_d: (a) $1s\to 2s$ excitation, (b) $1s\to 2p$ excitation; and (c) $2s\to 2p$ excitation.

The coupling matrix elements of the $1s\to 2s$, $1s\to 2p$ and $2s\to 2p$ excitations in unscreened and

screened cases with various Debye lengths are shown in Fig. 1. A rapid decrease of absolute values of these coupling matrix elements is observed with decreasing r_d, since the plasma screening effects decrease the interactions. In fact, the change of the wave functions will also affect the matrix elements, because the wave functions become broader with r_d decreasing. However, this effect is not as obvious as the interactions, and the screening effects make matrix elements more compact. The significant change of coupling matrix elements will alter the positron-impact excitation cross sections.

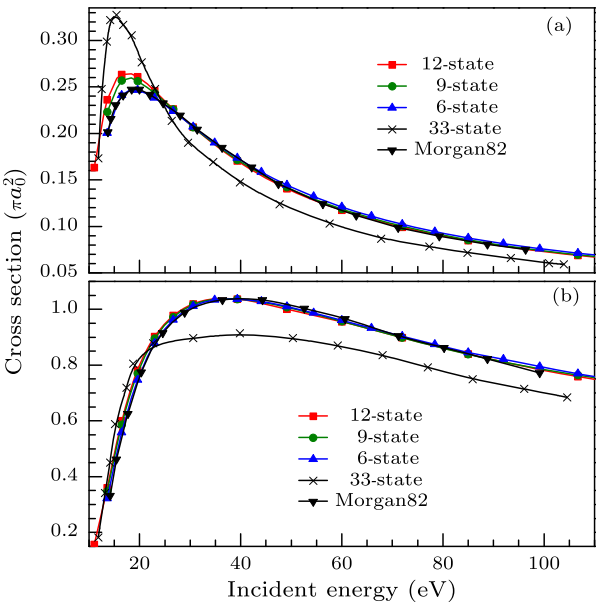

Fig. 2. Excitation cross sections for the unscreened cases in various basis: (a): $1s \to 2s$ excitation, and (b) $1s \to 2p$ excitation. Cross: 33-state calculation of Kernoghan *et al.*,[18] downtriangle: 6-state calculation of Morgan,[14] and for 12-, 9- and 6-state calculations (present results).

The unscreened $1s \to 2s$, $1s \to 2p$ excitation cross sections for different bases are shown in Fig. 2. The 12-, 9- and 6-state close-coupling calculations include the $(1s, 2s, 2p, 3l, 4l,$ and $5l)$, $(1s, 2s, 2p, 3l$ and $4l)$, $(1s, 2s, 2p$ and $3l)$ ($l = s, p$ and d) states, respectively. The pseudo-states and the positronium formation channels are not included in our calculations.[3] It can be seen that the $1s \to 2s$ excitation is slightly sensitive to various bases in the energy region 15–25 eV, but 12-state calculation gives the convergent results. The $1s \to 2p$ excitation process is insensitive to various basis, and 6-state basis can produce the convergent results. In the following, we present the 12-state CCA results, except for the highly excited states merging into the continuum states that are not included in the screened cases.

Our results are compared with Kernoghan's 33-state CCA calculations, which include the pseudo-states and positronium formation channels.[18] Our results underestimate the cross section up to 25% below 25 eV, and overestimate the cross section to 20% above 25 eV. In the low energy region, the inclusion of positronium formation channels is important, especially for the $1s \to 2s$ excitation process, as shown in Fig. 2. The pseudo-states may induce the discrepancy in the higher energy region. Our results are in good agreement with Morgan's 6-state CCA calculations without including the pseudo-states and positronium formation channels.[14] This tests our calculations.

Then our calculations are extended to the screened cases with various Debye lengths and all the results to be represented in the following are converged. For the screened cases, a basis smaller than the unscreened cases is needed, because the long-range Coulumb potential becomes the short-range Debye one. Meanwhile, the number of bound state to construct the basis becomes less as the plasma screening interactions increase.

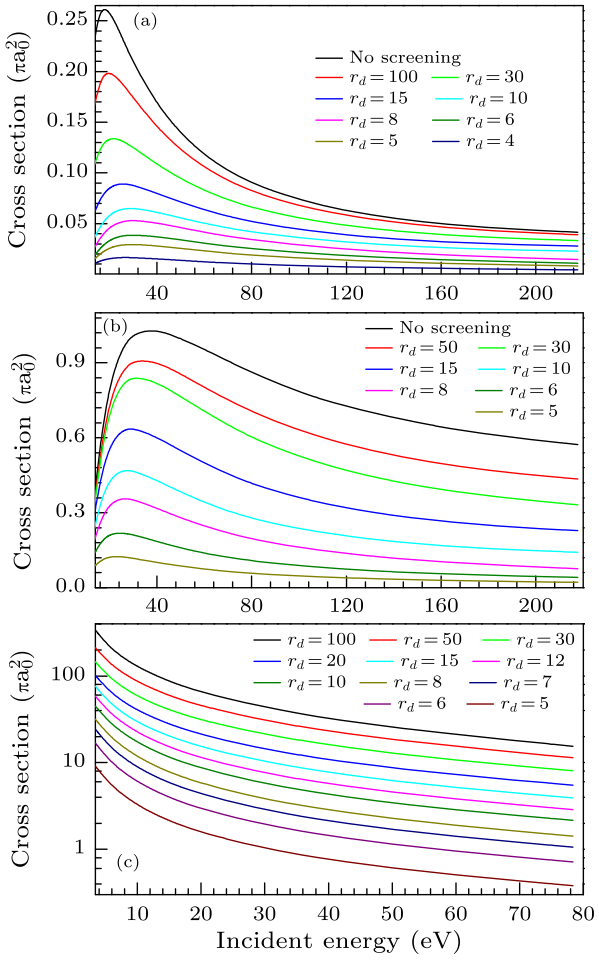

Fig. 3. Excitation cross sections for various Debye length r_d: (a) $1s \to 2s$ excitation, (b) $1s \to 2p$ excitation, and (c) $2s \to 2p$ excitation.

In Figs. 3(a) and 3(b), the positron-impact excitation cross sections from the $1s$ ground state to $2s$ and $2p$ excitation states are plotted for the unscreened and screened cases with various Debye lengths. The cross sections increase from the threshold with the increasing incident energy, reach to a maximum at about 25 eV, and then decrease gradually. For the screened cases, the cross sections significantly decrease from

a few percent to a magnitude of ten as the plasma screening interactions increase (or r_d decrease). Furthermore, as the Debye length r_d decreases, the cross section maximum for $1s \rightarrow 2s$ process slightly shifts towards to the higher energy, while the maximum for $1s \rightarrow 2p$ process shifts towards to the lower energy.

The $2s \rightarrow 2p$ excitation cross sections for screened cases with various Debye lengths are shown in Fig. 3(c). Since $2s$ and $2p$ states of hydrogen atoms are degenerate in the unscreened cases, the excitation cross section is very large and it is very difficult to obtain the converged cross section, therefore, the unscreened cross section is not presented here. It can be seen that the cross sections decrease as the incident energy increases in the calculated energy region (3.4–70 eV). The cross sections remarkably decrease from a few percentages to tens of times with the plasma screening interactions increasing. Compared with the $1s \rightarrow 2s$ and $1s \rightarrow 2p$ excitation processes, we can find that the $2s \rightarrow 2p$ excitation process is more sensitive than the $1s \rightarrow 2s$ and $1s \rightarrow 2p$ processes. For example, at energy of 3.4 eV, the cross section for $r_d = 100a_0$ is 30 times greater than that for $r_d = 5a_0$. The reason is that the $2s \rightarrow 2p$ excitation process is a big impact parameter process, and the screening effects are more obvious than the small impact parameter processes for the $1s \rightarrow 2s$ and $1s \rightarrow 2p$ excitations.

In summary, the eigenenergies and wave functions of hydrogen atoms in the plasma environments have been calculated using a power series expansion method,[25] and then the plasma effects on the positron-hydrogen collision processes have been studied using the close-coupling approximation without including the positronium formation channel. The excitation cross sections for the $1s \rightarrow 2s$, $1s \rightarrow 2p$ and $2s \rightarrow 2p$ processes for the unscreened and screened cases with various Debye lengths are presented. Our work demonstrates that the screening interactions decrease the matrix elements, resulting in the reduction of excitation cross sections from a few percentages to one magnitude of ten. This will change the spectroscopy of plasma both in intensity (reduced) and line position (red shifted),[27,28] affecting the simulation and diagnostics of plasmas.

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