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Orientation phenomena for direct s-p electron-ion collisional excitations in weakly coupled plasmas using the screened hyperbolic-orbit trajectory method

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Abstract. Orientation phenomena for direct $1s \to 2p_{\pm 1}$ electron-ion collisional excitations in weakly coupled plasmas (${n_\mathrm{e}}^{1/3}e^2/k_\mathrm{B}T \ll 1$) are investigated using the semiclassical curved trajectory method including the close-encounter effects. The results show that the orientation parameters including the close-encounter effects obtained by the hyperbolic-orbit trajectory method have maxima and minima for small impact parameter regions.

PACS. 52.20.-j Elementary processes in plasma – 34.80.Dp Atomic excitation and ionization by electron impact

1 Introduction

Atomic processes in dense and high-temperature plasmas have received much attention [1–12] in recent years because of their applications in many areas of physics and astrophysics. Moreover, the orientation and alignment phenomena in ion-atom or electron-atom collisions have been actively investigated since these phenomena provide detailed information on the mechanism of collisional excitation of target atoms and ions [7,13,14]. A recent experimental investigation [13] shows the possibility of the detection of radiative transitions from the excited $p_{\pm 1}\,(m = \pm 1)$ states to the ground state. The orientation parameter $L_\perp$ is a measure of the expectation value of the transferred orbital angular momentum to the bound electron in target atom due to the electron impact excitation. It has been known that the orientation phenomena in plasmas could provide a detailed information about the plasma parameters since the orientation parameter is connected to the relative number of coincidences for right-hand circularly (RHC) polarized and left-hand circulary (LHC) polarized photons emitting from the excited p_{+1} and p_{-1} states. The orientation phenomena for $s \to p$ electron-ion excitations in weakly coupled plasmas [6,8] have been investigated using the semiclassical straight-line (SL) approximation to visualize the behavior of the projectile electron in the excitation process. For a neutral target system, the straight-line trajectory method is quite reliable because of the weak Coulomb field. However, for an ion target system, the situation is quite different because of the strong Coulomb effect. In this case we have to consider a deflection of the projectile path due to the Coulomb interaction. Thus, in this paper we investigate the electron-ion $1s \to 2p_{\pm 1}$ oriented excitations in weakly coupled plasmas using the hyperbolic-orbit trajectory method. In dense astrophysical and laboratory plasmas, the range of the electron density (n_e) and temperature (T) are known to be around 10^{20}–10^{23} cm^{-3} and 10^7–10^8 K [4], respectively, and then the Debye length Λ is greater than ten times the first Bohr radius a_Z $(= a_0/Z)$ of hydrogenic ion with nuclear charge Z. In this situation, the Debye-Hückel model of the screened Coulomb potential is known to be quite reliable [6] to describe the interaction potential because the plasma coupling parameter Γ $(= (3/4\pi)^{1/3}{n_\mathrm{e}}^{1/3}e^2/k_\mathrm{B}T)$ is much smaller than unity, *i.e.*, pointing out weakly coupled plasmas. Using the screened hyperbolic-orbit (HO) trajectory method and the nonspherical Debye-Hückel interaction model, we investigate the orientation phenomena for direct $s \to p$ electron-ion collisional excitation including the close-encounter effects. The results show that the orientation parameters obtained by the screened HO trajectory have maxima and minima for small impact parameter regions. However, these maxima cannot be found by the SL trajectory since the Coulomb effects are significant for small impact parameters.

In Section 2, we derive a closed form of the transition amplitudes for the $1s \to 2p_{\pm 1}$ electron-impact excitations of hydrogenic ions in dense plasmas using the semiclassical screened HO trajectory method with the screened atomic wave functions. In Section 3, we obtain the orientation parameter for the $1s \to 2p_{\pm 1}$ transitions as a function

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of the impact parameter, projectile energy, and Debye length. A comparison is also given for the SL and HO trajectory methods. Finally, in Section 4, a summary and discussion are given.

2 Hyperbolic orbital semiclassical 1s → 2p$_{\pm 1}$ transition amplitudes

For simplicity, we assume that the target is a hydrogenic ion with nuclear charge Z. Using the nonspherical Debye-Hückel model, the interaction potential for the electron-impact excitation for the hydrogenic ion in weakly coupled plasmas is given by [8,10,11]

$$V(\mathbf{R},\mathbf{r}) = -\frac{Ze^2}{R}\mathrm{e}^{-R/\Lambda} + \frac{e^2}{|\mathbf{R}-\mathbf{r}|}\mathrm{e}^{-|\mathbf{R}-\mathbf{r}|/\Lambda}, \quad (1)$$

where Λ, $\mathbf{r}$, and $\mathbf{R}$ are the Debye length, the position vectors of the bound electron, and the projectile electron, respectively. Using the semiclassical approximation, the cross section for excitation from the unperturbed atomic state $|n\rangle[\equiv \psi_{n,l,m}(\mathbf{r})]$ to a state $|n'\rangle[\equiv \psi_{n',l',m'}(\mathbf{r})]$ can be found [15]

$$\sigma_{n',n} = 2\pi \int b\,\mathrm{d}b\,|T_{n',n}(b)|^2, \quad (2)$$

where $T_{n',n}(b)$ is the transition amplitude for excitation from an atomic state n to a state n' and b is the impact parameter. From the first-order time dependent perturbation theory [6,16], the transition amplitude $T_{n',n}(b)$ is given by the interaction potential $V(\mathbf{R},\mathbf{r})$,

$$T_{n',n}(b) = -\frac{\mathrm{i}}{\hbar}\int_{-\infty}^{\infty}\mathrm{d}t\,\mathrm{e}^{\mathrm{i}\omega_{n',n}t}\langle n'|V(\mathbf{R},\mathbf{r})|n\rangle, \quad (3)$$

where $\omega_{n',n} \equiv (E_{n'} - E_n)/\hbar$, and E_n and $E_{n'}$ are the energies of atomic states n and n', respectively. Using the nonspherical Debye-Hückel potential (Eq. (1)), the matrix elements for inelastic scattering processes ($n' \neq n$) are given by [6]

$$\langle n'|V(\mathbf{R},\mathbf{r})|n\rangle = e^2\left\langle n'\left|\frac{\exp(-|\mathbf{R}-\mathbf{r}|/\Lambda)}{|\mathbf{R}-\mathbf{r}|}\right|n\right\rangle, \quad (4a)$$

$$\equiv e^2\bar{V}_{n',n}. \quad (4b)$$

For the $1s \to 2p_{\pm 1}$ excitations, the transition matrix elements are given by

$$\bar{V}_{2p_{\pm 1},1s} \equiv \int \mathrm{d}^3\mathbf{r}\,\Psi_{2p_{\pm 1}}(\mathbf{r})\,\frac{\mathrm{e}^{-|\mathbf{R}-\mathbf{r}|/\Lambda}}{|\mathbf{R}-\mathbf{r}|}\,\Psi_{1s}(\mathbf{r}). \quad (5)$$

Using the addition theorem with the spherical harmonics $Y_{l,m}$, the nonspherical electron-electron interaction term can be expanded in a form [17]

$$\frac{\mathrm{e}^{-|\mathbf{R}-\mathbf{r}|/\Lambda}}{|\mathbf{R}-\mathbf{r}|} = \frac{4\pi}{\Lambda}\sum_{l=0}^{\infty}\sum_{m=-l}^{l} i_l\left(\frac{r_<}{\Lambda}\right)k_l\left(\frac{r_>}{\Lambda}\right)Y_{l,m}(\hat{r})Y^*_{l,m}(\hat{R}), \quad (6)$$

where i_l and k_l are the spherical modified Bessel functions and $r_<(r_>)$ is the smaller(larger) of r and R. Then, the transition matrix elements are found to be

$$\bar{V}_{2p_{\pm 1},1s} = \frac{\sqrt{4\pi}}{\Lambda}Y^*_{1,\pm 1}(\hat{R})\left[k_1\left(\frac{R}{\Lambda}\right)J_<(R,\Lambda) + i_1\left(\frac{R}{\Lambda}\right)J_>(R,\Lambda)\right]. \quad (7)$$

Here,

$$J_<(R,\Lambda) = \int_0^R r^2\mathrm{d}rR_{2p}(r)i_1\left(\frac{r}{\Lambda}\right)R_{1s}(r), \quad (8)$$

$$J_>(R,\Lambda) = \int_R^{\infty} r^2\mathrm{d}rR_{2p}(r)k_1\left(\frac{r}{\Lambda}\right)R_{1s}(r), \quad (9)$$

where R_{1s} and R_{2p} are the screened $1s$ and $2p$ radial wave functions including the plasma screening effects [3] in weakly coupled plasmas, respectively,

$$R_{1s}(r) = 2\alpha_{1s}^{-3/2}\mathrm{e}^{-r/\alpha_{1s}}, \quad (10)$$

$$R_{2p}(r) = \frac{1}{2\sqrt{6}}\alpha_{2p}^{-5/2}r\mathrm{e}^{-r/2\alpha_{2p}}, \quad (11)$$

with

$$\alpha_{1s} \cong \frac{a_Z}{[1-(3/4)(a_Z/\Lambda)^2 + (a_Z/\Lambda)^3]}, \quad (12)$$

$$\alpha_{2p} \cong \frac{a_Z}{[1-10(a_Z/\Lambda)^2 + 40(a_Z/\Lambda)^3]}. \quad (13)$$

Here, α_{1s} and α_{2p} are the screened Bohr radii for the $1s$ and $2p$ states and $\alpha \to a_Z\,(= a_0/Z)$ for vanishing plasma screening effects ($\Lambda \to \infty$). The expressions of equations (12, 13) are known to be quite reliable for the domain of our interest, namely, the Debye length $\Lambda \geq 10a_Z$ [4]. Here, the function $J_>$ (Eq. (9)) vanishes in the long range dipole approximation [13] ($R \gg r$). However, we shall keep this function to investigate the close-encounter effects on the transition probabilities and orientation parameters for small impact parameters since $J_>$ would be expected to make some contribution to the transition matrix elements for small impact parameters. We thus obtain the $1s \to 2p_{\pm 1}$ transition matrix elements as

$$\bar{V}_{2p_{\pm 1},1s} = 8\sqrt{\frac{2\pi}{3}}\frac{\eta_{1s}^{3/2}\eta_{2p}^{5/2}}{a_Z}Y^*_{1,\pm 1}(\hat{R})\frac{\bar{N}}{(\bar{N}^2 - a_\Lambda^2)^3} \times\left[\left(\frac{1}{\bar{R}^2} + \frac{a_\Lambda}{\bar{R}}\right)\mathrm{e}^{-a_\Lambda\bar{R}} - \left\{\frac{1}{\bar{R}^2} + \frac{\bar{N}}{\bar{R}} + \frac{1}{2}(\bar{N}^2 - a_\Lambda^2) + \frac{1}{8}(\bar{N}^3 - 2\bar{N}a_\Lambda^2 + \frac{a_\Lambda^4}{\bar{N}})\bar{R}\right\}\mathrm{e}^{-\bar{N}\bar{R}}\right], \quad (14)$$

where $a_Z \equiv a_0/Z$ (a_0 is the Bohr radius of the hydrogen atom), $a_\Lambda \equiv a_Z/\Lambda$, $\bar{R} \equiv R/a_Z$, and $\bar{N} \equiv (\eta_{1s} + \eta_{2p}/2)$ with

$$\eta_{1s} \cong 1 - \frac{3}{4}\left(\frac{a_Z}{\Lambda}\right)^2 + \left(\frac{a_Z}{\Lambda}\right)^3, \quad (15)$$

$$\eta_{2p} \cong 1 - 10\left(\frac{a_Z}{\Lambda}\right)^2 + 40\left(\frac{a_Z}{\Lambda}\right)^3. \quad (16)$$

If we apply the dipole approximation, the terms proportional to $e^{-\bar{N}\bar{R}}$ in equation (14) would be neglected. However, these terms would play a very important role for small impact parameters. Since the SL path approximation is not reliable for low projectile energies and for small impact parameters, we use the curved trajectory method called the HO path approximation to investigate the $s \to p$ orientation parameters. The convenient parametric representation [15,18] of the HO trajectory $\mathbf{R}(t)$, for the attractive case, in the $x-y$ plane, is given by

$$\begin{aligned} R_x &= d(\epsilon^2-1)^{1/2}\sinh w, \\ R_y &= d(-\cosh w + \epsilon), \\ R(t) \equiv |\mathbf{R}(t)| &= d(\epsilon\cosh w - 1), \\ t &= \frac{d}{v}(\epsilon\sinh w - w), \quad -\infty < w < \infty, \end{aligned} \tag{17}$$

where d, $\epsilon(= 1 + b^2/d^2)^{1/2}$, and v are the half of the distance of closest approach in a head-on collision, the eccentricity, and the initial velocity of the projectile electron, respectively. Including the plasma screening effects, the parameter d can be obtained by a simple perturbation calculation with the nonspherical screened interaction potential (Eq. (1)):

$$d \cong (d_0^{-1} + \Lambda^{-1})^{-1}, \tag{18}$$

where $d_0 \equiv Ze^2/mv^2$. For positive low energy projectiles, the motion of the projectile electron in the electron-ion collisions can be dealt with on the basis of hyperbolic orbits. However, for the motion of trapped electrons, *i.e.*, negative energies, the electron motion can be described by the elliptical or circular orbits with the eccentricity $(0 \le \epsilon < 1)$. For the $1s \to 2p_{\pm1}$ excitations, the spherical harmonics $Y^*_{1,\pm1}(\hat{R})$ become

$$\begin{aligned} Y^*_{1,\pm1}(\hat{R}) = &\mp\sqrt{\frac{3}{8\pi}}\frac{\bar{d}}{\bar{R}} \\ &\times\Big[(\epsilon^2-1)^{1/2}\sinh w \mp \mathrm{i}(-\cosh w + \epsilon)\Big], \end{aligned} \tag{19}$$

where $\bar{d} \equiv d/a_Z$. After some straightforward manipulations, we obtain the closed forms of the transition amplitudes for the $1s \to 2p_{\pm1}$ excitations using the screened HO trajectory method:

$$\begin{aligned} T_{2p_{\pm1},1s} = &\pm\mathrm{i}\frac{4}{Z\sqrt{\varepsilon_i}}\frac{\eta_{1s}^{3/2}\eta_{2p}^{5/2}\bar{N}\bar{d}}{(\bar{N}^2 - a_\Lambda^2)^3}\int_{-\infty}^{\infty}\mathrm{d}w\,\mathrm{e}^{\mathrm{i}\gamma(\epsilon\sinh w - w)} \\ &\times\Big[(\epsilon^2-1)^{1/2}\sinh w \mp \mathrm{i}(-\cosh w+\epsilon)\Big] \\ &\times\Big[\Big(\frac{1}{\bar{R}^2}+\frac{a_\Lambda}{\bar{R}}\Big)\mathrm{e}^{-a_\Lambda\bar{R}} - \Big\{\frac{1}{\bar{R}^2}+\frac{\bar{N}}{\bar{R}}+\frac{1}{2}(\bar{N}^2-a_\Lambda^2) \\ &+\frac{1}{8}(\bar{N}^3 - 2\bar{N}a_\Lambda^2 + \frac{a_\Lambda^4}{\bar{N}})\bar{R}\Big\}\mathrm{e}^{-\bar{N}\bar{R}}\Big], \end{aligned} \tag{20}$$

where γ $(\equiv \omega_{2p_{\pm1},1s}d/v) = (1 - 4a_\Lambda^2/3 + 12a_\Lambda^3)\beta/(\varepsilon_i + a_\Lambda)$, $\omega_{2p_{\pm1},1s} = (E_{2p_{\pm1}} - E_{1s})/\hbar$, $\beta = 3/8\sqrt{\varepsilon_i}$, ε_i $(\equiv \frac{1}{2}mv^2/Z^2Ry)$ is the scaled projectile energy, and Ry $(= me^4/2\hbar^2 \cong 13.6$ eV) is the Rydberg constant.

3 Orientation parameter

The orientation parameter [14] for the electron-impact excitations is defined as

$$L_\perp = \frac{\left|T_{2p_{+1},1s}(\bar{b})\right|^2 - \left|T_{2p_{-1},1s}(\bar{b})\right|^2}{\left|T_{2p_{+1},1s}(\bar{b})\right|^2 + \left|T_{2p_{-1},1s}(\bar{b})\right|^2}, \tag{21}$$

where $T_{2p_{\pm1},1s}$ are given by equation (20) and $\bar{b}$ $(\equiv b/a_Z)$ is the scaled impact parameter. The quantity $L_\perp$ is a measure of the expectation value of the transferred orbital angular momentum to the bound electron in target system due to the direct $1s \to 2p_{\pm1}$ excitations including the plasma screening effect a_Λ. From the relationship between the orientation parameter and the degree of polarization of the emitted radiation, the relative number of coincidences for the RHC and LHC photons is related to the orientation parameter. The orientation parameter $L_\perp$ using the HO trajectory method with the close-encounter and plasma screening effects can be obtained by equations (20, 21). The orientation parameter using the SL trajectory method can also be obtained by changing the parameters as $R_x = vt$ and $R_y = b$ in equation (17). Hence, we can readily verify that the transition amplitudes obtained by the SL and HO trajectory methods are almost identical in high energy domain from equation (20):

$$\left(T_{2p_{\pm1},1s}\right)_{\mathrm{SL}} \cong \lim_{\substack{\bar{d}\to0\\ \gamma\to0\\ \epsilon\bar{d}\to\bar{b}}}\left(T_{2p_{\pm1},1s}\right)_{\mathrm{HO}}. \tag{22}$$

Specifically we consider three cases of the projectile energy $\varepsilon_i = 1$ (low energy), 9 (intermediate energy), and 25 (high energy). In Figure 1, the orientation parameters for $a_\Lambda = 0.1$ are plotted as functions of the scaled impact parameter $\bar{b}$ for various projectile energies. A comparison is also given for the SL and HO trajectory methods. As we see in these figures, the orientation parameters obtained by the screened HO trajectory method show the maxima and minima for small impact parameters. These maximum phenomena have not been found using the SL trajectory method since the Coulomb effects are quite significant for small impact parameters. The maxima correspond to the complete $1s \to 2p_{+1}$ transitions at small impact parameters. However, the minima correspond to the complete $1s \to 2p_{-1}$ transitions. These minimum phenomena [8] have been also found using the SL trajectory method. Hence, it is known that the elaborate trajectory method such as the screened HO trajectory method rather than the SL trajectory method gives more correct informations on collisional excitation processes since the HO trajectory method includes the Coulomb deflection effects which are important for small impact parameters. It is also found that the plasma screening effects on the atomic wave functions slightly increase the tendency of the $1s \to 2p_{-1}$ transitions for impact parameters near to the minimum positions and also increase the $1s \to 2p_{+1}$ tendency for impact parameters near to the maximum positions. Both the maximum and minimum positions approach to the target nucleus with the increase of the projectile energy.

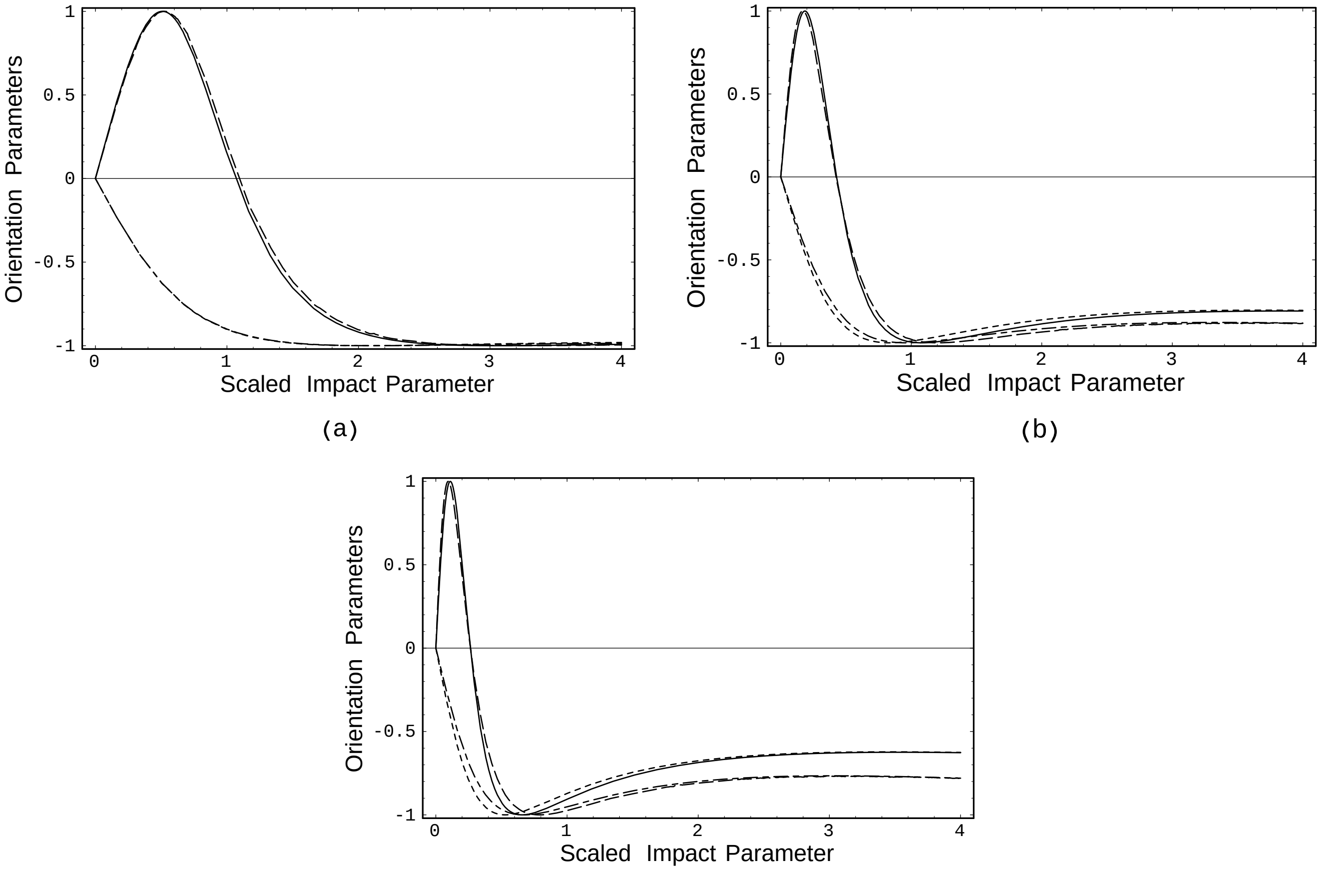

Fig. 1. The $1s \rightarrow 2p_{\pm 1}$ orientation parameters for $a_\Lambda = 0.1$. The solid lines represent the orientation parameters obtained by the screened hyperbolic-orbit trajectory method including the plasma screening effects on the atomic wave functions. The dotted lines represent the orientation parameters obtained by the straight-line trajectory method including the plasma screening effects on the atomic wave functions. The dashed lines represent the orientation parameters obtained by the screened hyperbolic-orbit trajectory method neglecting the plasma screening effects on the atomic wave functions. The dot-dashed lines represent the orientation parameters obtained by the straight-line trajectory method neglecting the plasma screening effects on the atomic wave functions; (a) $\varepsilon_i = 1$; (b) $\varepsilon_i = 9$; (c) $\varepsilon_i = 25$.

The maximum and minimum positions have receded from the target nucleus as the plasma screening effects on the atomic wave functions are included. If the screening term $\mathrm{e}^{-|\mathbf{R}-\mathbf{r}|/\Lambda}$ in equation (1) is replaced by the static one $\mathrm{e}^{-R/\Lambda}$, the amplitude of the transition probability is found to be smaller than that of the transition probability obtained by equation (1) due to the extra exponential factor $\mathrm{e}^{-r/\Lambda}$ since the main contribution position of the projectile electron is close to the position of the bound electron, *i.e.*, $\langle \mathbf{R} \rangle \approx \langle \mathbf{r} \rangle$ [10].

4 Summary and discussion

In this paper we investigate the orientation phenomena for direct $1s \rightarrow 2p_{\pm 1}$ electron-ion collisional excitations in weakly coupled plasma using the screened hyperbolic-orbit trajectory method including the close-encounter and plasma screening effects. The electron-ion interaction potential including the plasma screening is given by the nonspherical Debye-Hückel model. The semiclassical orientation parameters for the direct $1s \rightarrow 2p_{\pm 1}$ excitations are obtained for various Debye lengths and projectile energies. A comparison is also given for the orientation parameters obtained by the straight-line and screened hyperbolic-orbit trajectory methods. The results show that the orientation parameters obtained by the screened hyperbolic-orbit trajectory method, including the close-encounter effects, have maxima and minima for small impact parameters. The maximum phenomena have not been found using the straight-line trajectory method since the Coulomb effects are quite significant for small impact parameters. The plasma screening effects on the atomic wave functions increase the $1s \rightarrow 2p_{-1}$ tendency for impact parameters near to the minimum positions. For impact parameters near to the maximum positions, the plasma screening effects slightly increase the $1s \rightarrow 2p_{+1}$ tendency. The plasma screening effects on the atomic wave function near to the maximum positions ($1s \rightarrow 2p_{+1}$ transitions) are found to be quite small; however, these effects are very significant near to the minimum positions ($1s \rightarrow 2p_{-1}$ transitions). These results will provide a useful information on the orientation phenomena in atomic collision processes in weakly coupled plasmas.

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