Screening effects for transition probabilities in collisions of charged particles with an atom or stripped ion

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Screening effects for transition probabilities in collisions of charged particles with an atom or stripped ion are investigated using the modified hyperbolic-orbit path in the semiclassical approximation. Effective nuclear charges for bound electrons in many-electron atoms are determined by new screening constants [Y.-D. Jung and R. J. Gould, Phys. Rev. A **44**, 111 (1991)]. Applications were made to O, O^{4+}, and O^{7+}. For these targets, the transition probabilities are calculated for $1s \rightarrow 2p$ transitions. The results show that the maximum point of the transition probability is shifted to the nucleus with an increase of the screening effect. Moreover, the maximum amplitude of the transition probability is appreciably reduced as the screening effect increases.

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I. INTRODUCTION

Studies of screening effects of bound electrons in a target atom for the electron-atom collisional excitation or ionization has received much attention since these screening effects drastically change the cross sections. Knowledge of the screening effects in collision processes is essential for the interpretation of the behavior of target electrons and projectile particles. The behavior of the projectile is very well described by the semiclassical approximation (SCA). After Alder *et al.* [1] and Bang and Hansteen [2] used the hyperbolic-orbit (HO) method for the projectile path in the SCA for the nucleon-nucleon collisions, the SCA in excitation and ionization processes has received much attention. For ion-atom collisional excitations, the target screening effects have been investigated by McAbee [3] using the straight-line (SL) method. However, the screening effects of target electrons have not been investigated by the HO method. Recently, a symmetric modified HO method [4] was presented for electron-impact excitation processes. Also, a behavior of the trajectory of the projectile electron in electron-impact excitation for hydrogenic ions in dense plasmas was investigated recently by the modified HO method [5]. This modified HO method is, of course, much more accurate than the SL method near thresholds (see Ref. [4]). Thus, in this paper we investigate the target screening effects for transition probabilities in electron-atom collisions using the HO method for various target atoms.

In Sec. II we derive the general excitation cross sections for the charged particle–atom collision in the SCA for dipole transitions ($\Delta l = \pm 1$). The transition probabilities for the $1s \rightarrow 2p$ excitations are obtained as a function of impact parameter (b) and the $1s$ (Z_{1s}) and $2p$ (Z_{2p}) effective charges. In Sec. III we investigate the screening effects for O, O^{4+}, and O^{7+}. We obtain the transition probabilities for O, O^{4+}, and O^{7+} target atoms. The overlap effects from the passive electrons are also estimated. Finally, in Sec. IV, a summary and discussions are given.

II. EXCITATION TRANSITION PROBABILITIES

In the SCA, the cross section for excitation from an unperturbed atomic orbital n [$\equiv \psi_{nlm}(\mathbf{r})$] to an excited atomic orbital n' [$\equiv \psi_{n'l'm'}(\mathbf{r})$] becomes

$$\sigma_{n',n} = 2\pi \int P_{n',n}(b) b\, db , \tag{1}$$

where $P_{n',n}(b)$ is the transition probability

$$P_{n',n}(b) = |T_{n',n}|^2 \tag{2}$$

and b is the impact parameter. From first-order time-dependent perturbation theory, the transition amplitude $T_{n',n}$ is given by the interaction potential $V(\mathbf{r},\mathbf{R})$ (see Ref. [4])

$$T_{n',n} = -\frac{i}{\hbar} \int_{-\infty}^{\infty} dt\, e^{i(E_{n'}-E_n)t/\hbar} \langle n' | V(\mathbf{r},\mathbf{R}) | n \rangle , \tag{3}$$

where E_n and $E_{n'}$ are the energies of atomic states n and n', respectively. When the projectile and target nuclear charges are z and Z, respectively, the dipole transition ($\Delta l = \pm 1$) probability becomes

$$P_{n',n} = \frac{1}{3(2l+3)} \left[\frac{ze^2}{\hbar} \right]^2 (R_{nl}^{n'l\pm 1})^2 |V_{n',n}|^2 , \tag{4}$$

where $R_{nl}^{n'l\pm 1}$ is the radial dipole matrix element

$$R_{nl}^{n'l\pm 1} = \int_0^{\infty} r^3 dr\, R_{n'l\pm 1}(r) R_{nl}(r) ; \tag{5}$$

$R_{nl}(r)$ and $R_{n'l\pm 1}(r)$ are, respectively, the radial wave functions of the nlth and $n'l\pm 1$th states; and $V_{n',n}$ is given by

$$V_{n',n} = \int_{-\infty}^{\infty} dt\, e^{i\omega_{n'n} t} \frac{\mathbf{R}(t)}{|\mathbf{R}(t)|^3} , \tag{6}$$

with $\omega_{n'n} \equiv (E_{n'} - E_n)/\hbar$. Under the symmetric modified HO method for the parametric representation for $\mathbf{R}(t)$, $|V_{n',n}|^2$ can be represented as (see Ref. [4])

$$|V_{n',n}|^2=\left[\frac{2\beta_{n',n}}{v_i d}\right]^2 e^{\pi\beta_{n'n}}\left[[K'_{i\beta_{n'n}}(\varepsilon\beta_{n'n})]^2+\left[\frac{\varepsilon^2-1}{\varepsilon^2}\right][K_{i\beta_{n'n}}(\varepsilon\beta_{n'n})]^2\right], \tag{7}$$

where v_i and v_f are the initial and final velocities of the projectile, $\beta_{n'n}\equiv 2\omega_{n'n}d/(v_i+v_f)$ and d $(=zZe^2/mv_iv_f)$ is half of the distance of closest approach in a head-on collision; $K_{i\beta_{n'n}}(\varepsilon\beta_{n'n})$ is the modified Bessel function [6], with order $i\beta_{n'n}$ and with argument $\varepsilon\beta_{n'n}$:

$$K_{i\bar{\beta}_{2p,1s}}(\bar{\varepsilon}\bar{\beta}_{2p,1s})=\int_0^\infty dw\, e^{-\bar{\varepsilon}\bar{\beta}_{2p,1s}\cosh w}\cos(\bar{\beta}_{2p,1s}w)\ ; \tag{8}$$

$K'_{i\beta_{n'n}}(\varepsilon\beta_{n'n})$ is a derivative of the modified Bessel function with respect to the argument $\varepsilon\beta_{n'n}$; and ε $(=\sqrt{1+b^2/d^2})$ is the eccentricity. A recent paper by Jung and Gould [7] gave prescriptions for screening constants and effective nuclear charges for bound electrons in many-electron atoms. Using this method, we can readily evaluate the radial matrix element [Eq. (5)]. Specifically, we consider the $1s\rightarrow 2p$ transition probability since it is the lowest dipole transition which has the largest magnitude. We choose the oxygen atom and its ions as targets. Then, for the electron-atom collision, the $1s\rightarrow 2p$ transition probability is given by, after some algebra,

$$P_{2p,1s}(b)=\frac{2}{3}\frac{\bar{z}_{1s}^3\bar{z}_{2p}^5}{(\bar{z}_{1s}+\bar{z}_{2p}/2)^{10}}\left[1-\frac{\xi_f}{\xi_i}\right]^2 e^{\pi(\xi_f^{-1}-\xi_i^{-1})}\times\left[[K'_{i(\xi_f^{-1}-\xi_i^{-1})}(\varepsilon(\xi_f^{-1}-\xi_i^{-1}))]^2+\left[\frac{\varepsilon^2-1}{\varepsilon^2}\right][K_{i(\xi_f^{-1}-\xi_i^{-1})}(\varepsilon(\xi_f^{-1}-\xi_i^{-1}))]^2\right], \tag{9}$$

where

$$\xi_i=\left[\frac{mv_i/2}{Z^2\mathcal{R}}\right]^{1/2},\quad \xi_f=(\xi_i^2-\xi_{2p,1s}^2)^{1/2}, \tag{10}$$

$$\xi_{2p,1s}=\left[\frac{E_{2p,1s}}{Z^2\mathcal{R}}\right]^{1/2} \tag{11}$$

$$\varepsilon=[1+(b/a_Z^2)(\xi_f\xi_i)^2]^{1/2}, \tag{12}$$

$\bar{z}_{1s}\equiv Z_{1s}/Z$, $\bar{z}_{2p}\equiv Z_{2p}/Z$ and $\mathcal{R}=1$ Ry. Here, Z_{1s} and Z_{2p} are the $1s$ and $2p$ effective charges, and $E_{2p,1s}$ is the $1s\rightarrow 2p$ excitation threshold energy. From Eq. (9), the leading charge dependence of $P_{2p,1s}(b)$ is found to be

$$Z_{1s}^3 Z_{2p}^5/(Z_{1s}+Z_{2p}/2)^{10}\ .$$

This also was verified by MacAbee [3] for ion-atom excitation using the SL method. If we use the SL path, i.e., $R_x(t)=0$, $R_y(t)=b$, $R_z(t)=v_it$, the transition probability $P_{2p,1s}(b)$ is proportional to the product of the zeroth- and first-order modified Bessel functions. In a recent investigation [4], the SL cross section approaches the Born-Bethe cross section with a finite cutoff in the momentum transfer. In high-energy limit, the Born-Bethe approximation without a finite cutoff in the momentum transfer overestimates the cross section by factor of 2 (see Refs. [8] and [9]) due to an excessive contribution from large momentum transfer. The equivalence of the semiclassical and quantum-mechanical Born approximations in the calculation of the inelastic cross section was demonstrated by Bethe and Jackiw [10].

Since the impact parameter is roughly conjugate to the momentum transfer, the dependence of the transition probability on the impact parameter contains the same physics seen in the dependence of the generalized oscillator strength (GOS) on the momentum transfer. Therefore, the maximum of the transition probability $bP_{2p,1s}(b)$ corresponds to the minimum of the GOS, $F_{2s,1s}(qa_Z)$. Here, $\mathbf{q}$ $(=\hbar\mathbf{k}_i-\hbar\mathbf{k}_f)$ is the momentum transfer, and $\mathbf{k}_i$ and $\mathbf{k}_f$ are the relative wave vectors before and after the collision. A general discussion of the behavior of the GOS $F_{n'n}$ in the first-order plane-wave Born approximation (PWBA) has been given by Iwai, Shimamura, and Watanabe [11].

III. SCREENING EFFECTS FOR $P_{2p,1s}(b)$

In this section we shall discuss the screening effects for the target atoms; O, O^{4+}, and O^{7+}. Table I shows the $1s$, $2s$, and $2p$ effective charges and $\xi_{2p,1s}$ for O, O^{4+}, and O^{7+}. The first values in each column are the initial effective charges, i.e., before $1s\rightarrow 2p$ excitation. The values in parentheses are the final effective charges, i.e., after $1s\rightarrow 2p$ excitation. These effective charges and excitation threshold energies are obtained by new screening constants [7]. To account for the effects of the hole in the K shell left by the excited electron on the other electrons, the transition probability [Eq. (9)] must be multiplied by the *overlap factor C*. Then the atomic transition probability is then given by

TABLE I. The effective charges and dimensionless excitation energies for target atoms: O, O^{4+}, and O^{7+}. Z_{1s}, Z_{2s}, and Z_{2p} refer to the $1s$, $2s$, and $2p$ effective charges, respectively. $\xi_{2p,1s}^2$ is given by Eq. (11).

Atom-ion	Z_{1s}	Z_{2s}	Z_{2p}	$\xi_{2p,1s}^2$
O	7.69(8)	4.59(5.15)	4.58(5.19)	0.6070
O^{4+}	7.69(8)	5.95(6.51)	0(6.55)	0.6259
O^{7+}	8(8)	0(0)	0(8)	0.7500

TABLE II. The overlap factors for O, O^{4+}, and O^{7+}. C_{1s}, C_{2s}, C_{2p}, and C refer to the 1s, 2s, 2p, and total overlap factors, respectively.

Atom-ion	C_{1s}	C_{2s}	C_{2p}	C
O	0.9994	0.9915	0.9903	0.9449
O^{4+}	0.9994	0.9984		0.9962
O^{7+}				1

$$P_a = P_{2p,1s}(b)C \ . \tag{13}$$

The factor C is represented as a product of squared overlap integrals involving the initial and final states of the *passive* electrons. Because of the hole left in the K shell and the active electron that exists in the L shell, these integrals are not unity, but can be evaluated easily using the screening-constant orthogonal basis-set wave functions. The core relaxation factors are summarized in Table II. In the present paper, we do not consider the secondary excitation or ionization processes. C_{1s}, C_{2s}, and C_{2p} are the overlap factors for the 1s, 2s, and 2p electrons, respectively, and C is the total overlap factor. For example, the $1s \rightarrow 2p$ transition probability for an O atom without considering these overlap factors is in error by about 6%. These overlap factors were neglected in McAbee [3] for the ion-atom excitation. Thus, from Eq. (12), we can investigate the screening effects of the target atoms and the variation of the *proper* impact parameter (b_p). Since the *proper* impact parameter is determined by the maximum of $bP_a(b)$, we can understand that b_p corresponds to the position at which the excitation process take places. Figure 1 shows the $1s \rightarrow 2p$ transition probabilities for O, O^{4+}, and O^{7+} at $\xi_i = 1$. As we see in this figure, the *proper* impact parameter corresponds to the mean shell radius of the final electron state. The results show that the *proper* impact parameter is shifted to the nucleus with an increase of the screening effect, and the maximum amplitude of $bP_a(b)$ is appreciably reduced as the screening effect increases. For low-energy projectiles, the SL and the PWBA are not appropriate to evaluate the transition probability. However, our formulation of the transition probability [Eq. (9)] using the modified HO method is very reliable in every energy domain. The accuracy of the modified HO method can be obtained from Ref. [9].

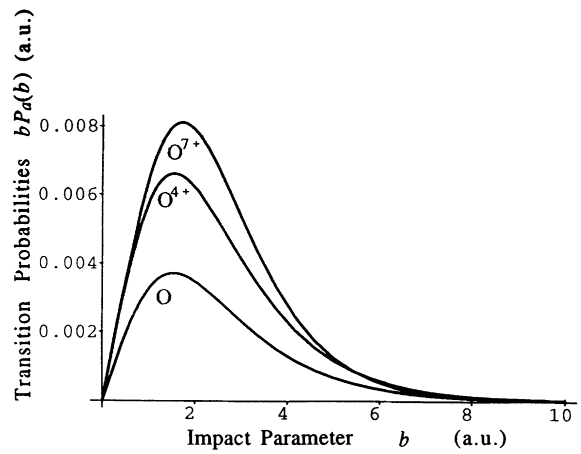

FIG. 1. Transition probabilities as a function of the impact parameter (b) in atomic units for O, O^{4+}, and O^{7+} at $\xi_i = 1$.

IV. SUMMARY AND DISCUSSION

In this paper we investigate the target screening effects for the transition probabilities in electron-atom collisions using the hyperbolic-orbit method in the semiclassical approximation for various targets: O, O^{4+}, and O^{7+}. The overlap factors are obtained by the screening-constant method which is based on the orthogonal Slater orbitals [7]. From these results we can understand the behavior of target electrons and the variation of the proper impact parameter at which $bP_{2p,1s}(b)$ is maximized for the excitation process. The maximum amplitude of $bP_a(b)$ is appreciably reduced as the screening effect increases. These results provide a general description for the screening effects for charged particle impact excitation for many-electron atoms.

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