Theoretical threshold law of positron-impact ionization of He

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Single-differential and total cross sections of positron-impact ionizations of the helium atom are calculated near the ionization threshold. We investigate the threshold law of positron-impact ionization for models with various asymptotic charges in the two-potential distorted-wave approximation. The threshold power behaviors of impact-ionization cross sections depend only on the asymptotic charges experienced by the scattered positron and the ejected electron. Our numerical results agree well with experimental data and other theoretical results.

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I. INTRODUCTION

Impact ionization of atoms and ions by charged particle is a fundamental process in gas discharge and in plasmas fusion. Recent measurements of the positron-impact-ionization cross sections in the first few eV above threshold for He have been given by Ashley *et al.* [1]. The threshold power law of electron-impact ionization was first given in a classical treatment by Wannier [2] and later by Temkin [3] in the Coulomb-dipole theory. Geltman [4] studied the threshold behavior for ionization by both electrons and positrons in the Coulomb-projected-Born approximation. The positron-impact ionization cross sections of H and He^+ at near-threshold energies has been calculated by Wetmore and Olson [5] using the classical trajectory Monte Carlo method. Total cross sections for positron-impact ionization of helium have been calculated within a distorted-wave formalism by Campeanu *et al.* [6]. More recently, the positron-impact ionization of hydrogen have been calculated by Rost and Heller [7] using the semiclassical approximation of Feynman's path integral. Sil and Roy [8] analytically evaluated the positron-impact ionization of hydrogen atom near the threshold with the final-state wave function involving three Coulomb functions. Ihra *et al.* [9] used anharmonic corrections to the Wannier law for the positron-impact ionization of He. Deb and Crothers [10] used the quantum-semiclassical calculation for near-threshold ionization of helium by positron impact.

A relativistic kinematic analysis of impact-ionization processes by Huang [11] is employed in the calculation of electron- and positron-impact ionizations for hydrogenlike and heliumlike ions [12–17] in the two-potential distorted-wave approximation. Besides being a fully quantum-mechanical method, the two-potential distorted-wave approximation considers the major distorting effects arising from interactions among participating particles in computing the wave functions, while the residual interactions are also treated in a nonperturbative manner. Threshold cross section of electron-impact ionization of the hydrogen atom have been studied [18]. In the present paper, we investigate the threshold law of positron-impact ionization of ions in the two-potential distorted-wave approximation, and the results for He are given as a typical example.

In Sec. II, we review the kinematic formulation of charged-particle impact-ionization process. In Sec. III, we establish the threshold law by analyzing the wave functions near the threshold region. The two-potential distorted-wave approximation is presented in Sec. IV. In Sec. V, numerical calculations are carried out and compared with the analytically derived threshold law and with experimental results. The conclusion is discussed in Sec. VI.

II. IMPACT-IONIZATION PROCESSES

A. Kinematic formulation

We consider a charged particle with linear momentum $\mathbf{k}_i$ and total energy E_i impinging on the helium atom in its ground state. After the collision, one electron of the helium atom is ejected, and the residual hydrogenic ion is left in its ground state. The linear momentum and total energy for the scattered incident particle and ejected electron are described by $(\mathbf{k}_p E_p)$ and $(\mathbf{k}_e E_e)$, respectively. By energy conservation, we have

$$E_i + E_b = E_p + E_e , \tag{1}$$

where E_b denotes the energy of the electron originally bound in the helium atom.

We shall treat the case where both the incident charged particle and target are spin unpolarized, and no attempt is made to distinguish between the various final spin polarizations. In the relativistic formulation, the triple-differential cross section in atomic units can be expressed as [11]

$$\frac{d^3\sigma}{dE_e d\Omega_p d\Omega_e} = \frac{(2\pi)^4}{c^6}\left(\frac{k_p E_p k_e E_e E_i}{k_i}\right)\sum_{fi} |T_{fi}|^2$$

$$= \frac{\sigma}{16\pi^2} F(\Omega_p , \Omega_e), \tag{2}$$

where c is the speed of light, T_{fi} denotes the appropriate transition matrix element, and the summation over fi denotes symbolically averaging over the initial polarizations and summing over the final polarizations. After carrying out the summation over fi, we obtain the triple-differential cross

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section in terms of the total cross section σ and an angular distribution function $F(\Omega_p, \Omega_e)$.

The single-differential cross section can be obtained by integrating over the solid angles Ω_p and Ω_e as

$$\frac{d\sigma}{dE_e} = \int\int \frac{d^3\sigma}{dE_e d\Omega_p d\Omega_e} d\Omega_p d\Omega_e . \tag{3}$$

We consider both the electron- and positron-impact ionizations and use symbols e^- and e^+ to identify them. Then the total cross sections can be calculated as

$$\sigma(e^\pm) = \int_{c^2}^{\epsilon^\pm + c^2} \frac{d\sigma}{dE_e} dE_e , \tag{4}$$

where $\epsilon^+ \equiv \epsilon$ and $\epsilon^- \equiv \epsilon/2$. Let $\epsilon \equiv E_i + E_b - 2c^2$ denote the excess energy of the colliding system, where c^2 represents the rest energy of the electron.

B. Nonrelativistic limit

We shall consider the nonrelativistic limit of the threshold behavior of impact-ionization cross sections. Relativistic effects will give rise to corrections of the order $O(\epsilon/c^2)$ relative to the leading contribution, and therefore do not modify the threshold law. In the nonrelativistic limit, the single-differential and total cross sections in Eqs. (3) and (4), respectively, reduce to

$$\frac{d\sigma}{dE_e}(e^\pm) = (2\pi)^4 \frac{k_p k_e}{k_i} \int d\Omega_p \int d\Omega_e \sum_{fi} |T_{fi}|^2, \tag{5}$$

$$\sigma(e^\pm) = \frac{(2\pi)^4}{k_i} \int_0^{\epsilon^\pm} k_p k_e d\epsilon_e \int d\Omega_p \int d\Omega_e \sum_{fi} |T_{fi}|^2, \tag{6}$$

where ϵ_e is the kinetic energy of the ejected electron.

C. Transition amplitudes

The unsymmetrized transition amplitude can be approximated by

$$T_{fi}(e^\pm) \cong \int\int\int d^3r_1 d^3r_2 d^3r_3 \phi_p^*(\mathbf{r}_1) \phi_e^*(\mathbf{r}_2) \Phi_0(\mathbf{r}_3) \times \left(\pm\frac{Z}{r_1} \mp \frac{1}{r_{12}} \mp \frac{1}{r_{13}} \right) \phi_i(\mathbf{r}_1) \Phi_b(\mathbf{r}_2) \Phi_{b'}(\mathbf{r}_3), \tag{7}$$

where the upper and lower signs are for the positron impact and electron impact, respectively, and Z is the nuclear charge of the helium atom. Here Φ_b and $\Phi_{b'}$ denote the orbital wave function with different magnetic quantum numbers for the bound electrons in the helium atom, and Φ_0 the ground-state wave function for the bound electron in the hydrogenic ion. Here $\phi(\mathbf{r})$ denotes the wave function of a charged particle with linear momentum $\mathbf{k}$ in the Coulomb potential of nuclear charge Z:

$$\phi(\mathbf{r}) = (2\pi)^{-3/2} e^{-\pi\eta/2} |\Gamma(1+i\eta)| \times e^{i\mathbf{k}\cdot\mathbf{r}} {}_1F_1(-i\eta; 1; ikr - i\mathbf{k}\cdot\mathbf{r}), \tag{8}$$

where $\eta = \pm Z/k$, and ${}_1F_1$ is the confluent hypergeometric function. Here the positive and negative signs are for positron and electron, respectively.

III. THRESHOLD LAWS

A. Threshold behaviors of wave functions

When the excess energy ϵ is sufficiently small, we consider the asymptotic behaviors of the Coulomb wave functions of the positron and electron for $kr \ll 1$ in the effective range of the ionization processes.

For the positron Coulomb wave function, we have

$$\phi(\mathbf{r}) \xrightarrow{kr\ll 1} \begin{cases} (2\pi)^{-3/2}, & Z=0 \\ (2\pi)^{-1}\sqrt{(Z/k)} e^{-\pi Z/k} I_0(2\sqrt{Z(r - \hat{\mathbf{k}}\cdot\mathbf{r})}), & Z\neq 0, \end{cases} \tag{9}$$

where $I_0(x)$ is the modified Bessel function. For the electron Coulomb wave function, we have

$$\phi(\mathbf{r}) \xrightarrow{kr\ll 1} \begin{cases} (2\pi)^{-3/2}, & Z=0 \\ (2\pi)^{-1}\sqrt{(Z/k)}\, J_0(2\sqrt{Z(r - \hat{\mathbf{k}}\cdot\mathbf{r})}), & Z\neq 0, \end{cases} \tag{10}$$

where $J_0(x)$ is the Bessel function.

Substituting the Coulomb wave functions $\phi(\mathbf{r})$ in Eqs. (9) and (10) into Eq. (7) and carrying out the integrations in Eqs. (5) and (6), we can obtain the threshold laws of the single-differential and total cross sections.

B. Positron-impact ionization

In the positron-impact ionization, the k_p and k_e dependences of the transition amplitude are

$$T_{fi}(e^+) \propto \begin{cases} 1, & Z_p = Z_e = 0 \\ 1/\sqrt{k_e}, & Z_p = 0, Z_e \neq 0 \\ e^{-\pi Z_p/k_p}/\sqrt{k_p k_e}, & Z_p \neq 0, Z_e \neq 0. \end{cases} \tag{11}$$

Here, Z_p and Z_e are the effective charges experienced by the scattered incident positron and the ejected electron, respectively. Hence, the single-differential cross section is a function of k_p and k_e

$$\frac{d\sigma}{dE_e}(e^+) \propto \begin{cases} k_p k_e, & Z_p = Z_e = 0 \\ k_p, & Z_p = 0, Z_e \neq 0 \\ e^{-\pi Z_p/k_p}, & Z_p \neq 0, Z_e \neq 0. \end{cases} \tag{12}$$

After integrating Eq. (12), we arrive at the threshold power law

$$\sigma(e^+) \propto \begin{cases} \epsilon^2, & Z_p = Z_e = 0 \\ \epsilon^{3/2}, & Z_p = 0, Z_e \neq 0 \\ \epsilon^{3/2} e^{-2\pi Z_p/\sqrt{2\epsilon}}, & Z_p \neq 0, Z_e \neq 0. \end{cases} \tag{13}$$

In our calculations, we have included the short-range potential experienced by the scattered positron and ejected electron in the impact-ionization processes. However, the above-threshold behaviors are not affected by the short-range potential.

Various other threshold laws for the positron-impact ionization have been given, for example, by Klar ($\sigma \propto \epsilon^{2.651}$) [19], Wetmore and Olson ($\sigma \propto \epsilon^{2.99}$) [5], Rost and Heller ($\sigma \propto \epsilon^{2.67}$) [7], Sil and Roy ($\sigma \propto \epsilon^{1.5}$) [8], and Ihra *et al.* ($\sigma \propto \epsilon^{2.64}\exp[-0.73\sqrt{\epsilon}]$) [9]. Our threshold law for $Z_p \neq 0$ and $Z_e \neq 0$ seems to account for the correct modulation factor $\exp[-2\pi Z_p/\sqrt{2\epsilon}]$, peculiar to the positron-impact ionization.

C. Electron-impact ionization

Theoretical threshold laws of electron-impact ionization have been reported by many authors [4,18–21] besides others. We present our results below for comparison with those of positron-impact ionization:

$$T_{fi}(e^-) \propto \begin{cases} 1, & Z_p = Z_e = 0 \\ 1/\sqrt{k_e}, & Z_p = 0, Z_e \neq 0 \\ 1/\sqrt{k_p k_e}, & Z_p \neq 0, Z_e \neq 0, \end{cases} \tag{14}$$

$$\frac{d\sigma}{dE_e}(e^-) \propto \begin{cases} k_p k_e\,, & Z_p = Z_e = 0 \\ k_p\,, & Z_p = 0, Z_e \neq 0 \\ 1, & Z_p \neq 0, Z_e \neq 0, \end{cases} \tag{15}$$

$$\sigma(e^-) \propto \begin{cases} \epsilon^2, & Z_p = Z_e = 0 \\ \epsilon^{3/2}, & Z_p = 0, Z_e \neq 0 \\ \epsilon, & Z_p \neq 0, Z_e \neq 0. \end{cases} \tag{16}$$

IV. TWO-POTENTIAL DISTORTED-WAVE APPROXIMATION

A. Total Hamiltonian

The total Hamiltonian H of the projectile-target system can be separated into two parts,

$$H = H_i + V_i\,, \tag{17}$$

where H_i is the unperturbed Hamiltonian before the collision and V_i is the interaction potential between the projectile and target during the collision:

$$H_i = (c\alpha_1 \cdot \mathbf{p}_1 + c^2\beta_1) + (c\alpha_2 \cdot \mathbf{p}_2 + c^2\beta_2) + (c\alpha_3 \cdot \mathbf{p}_3 + c^2\beta_3) - \frac{Z}{r_2} - \frac{Z}{r_3} + \frac{1}{r_{23}}, \tag{18}$$

$$V_i = \frac{Z}{r_1} - \frac{1}{r_{12}} - \frac{1}{r_{13}}. \tag{19}$$

where α_i and β_i are Dirac matrices. Here $r_1 \equiv |\mathbf{r}_1|$, $r_2 \equiv |\mathbf{r}_2|$, and $r_3 \equiv |\mathbf{r}_3|$ refer, respectively, to the radial coordinates of the incident positron and bound electrons of the helium atom before the collision, and r_{ij} indicates the interparticle distance between $\mathbf{r}_i$ and $\mathbf{r}_j$.

By collision theory, the transition amplitudes of impact ionization have the general form [22]

$$T_{fi} = \langle \Psi_f^{(-)} | V_i | \Phi_i \rangle - \langle P\Psi_f^{(-)} | V_i | \Phi_i \rangle, \tag{20}$$

where the first and second terms are the direct and exchange terms, respectively, Φ_i is the eigenstate of H_i, and $\Psi_f^{(-)}$ is the eigenstate of H with the incoming-wave boundary condition. Here the symbol P denotes the permutation between electrons.

B. Two-potential formulation

In the two-potential formulation, we separate the interaction potential V_i into the distorting potential U_i and the residual potential W_i as

$$V_i = U_i + W_i\,. \tag{21}$$

We can therefore reduce the transition amplitudes (20) into the two-potential form as

$$T_{fi} = \langle \Psi_f^{(-)} | W_i | \psi_i^{(+)} \rangle - \langle P\Psi_f^{(-)} | W_i | \psi_i^{(+)} \rangle, \tag{22}$$

where $\psi_i^{(+)}$ denotes the distorted wave function in the distorting potential U_i.

Taking the electrostatic polarization potential into account, the distorting potential U_i and residual potential W_i can be chosen as

$$U_i = \frac{Z}{r_1} + \nu_i(r_1) + 2V_{pol}(r_1), \tag{23}$$

$$W_i = -\frac{1}{r_{12}} - \frac{1}{r_{13}} - \nu_i(r_1) - 2V_{pol}(r_1). \tag{24}$$

Here the average potentials $\nu_i(r_1)$ are due to the bound electrons of the helium atom,

$$\nu_i(r_1) = -2\left\langle \Phi_b(\mathbf{r}_3) \left| \frac{1}{r_{13}} \right| \Phi_b(\mathbf{r}_3) \right\rangle, \tag{25}$$

and the polarization potentials are approximated by the hydrogenic value $V_{pol}(r_1)$ with $x = Zr_1$ [23],

$$V_{pol}(r_1) = -\frac{9}{4x^4}\left[1 - e^{-2x}\left(1 + 2x + 2x^2 + \frac{4}{3}x^3 + \frac{2}{3}x^4 + \frac{4}{27}x^5\right)\right]. \tag{26}$$

C. Distorted waves

The distorted-wave functions $\psi_i^{(+)}$ in Eq. (22) can be expressed as

$$\psi_i^{(+)} = \chi_i^{(+)}(\mathbf{r}_1)\Phi_b(\mathbf{r}_2)\Phi_{b'}(\mathbf{r}_3). \tag{27}$$

TABLE I. Distorting potentials U_p and U_e for the scattered positron and ejected electron in the positron-impact ionization.

Model	Distorting potential		Asymptotic charges	
	U_p	U_e	Z_p	Z_e
TPDW01	$\frac{Z}{r_1}+\nu_i(r_1)+2V_{pol}(r_1)$	$-\frac{Z}{r_2}-\nu_f(r_2)-V_{pol}(r_2)$	0	1
TPDW11	$\frac{Z}{r_1}+\nu_f(r_1)+V_{pol}(r_1)$	$-\frac{Z}{r_2}-\nu_f(r_2)-V_{pol}(r_2)$	1	1

Here the distorted-wave function $\chi_i^{(+)}(\mathbf{r}_1)$ with the outgoing-wave boundary condition for the incident positron satisfies the equation

$$(c\alpha_1\cdot\mathbf{p}_1+c^2\beta_1+U_i-E_i)\chi_i^{(+)}(\mathbf{r}_1)=0. \tag{28}$$

We approximate the unsymmetrized distorted final-state wave functions $\Psi_f^{(-)}$ in Eq. (22) as

$$\Psi_f^{(-)}\simeq\chi_p^{(-)}(\mathbf{r}_1)\chi_e^{(-)}(\mathbf{r}_2)\Phi_0(\mathbf{r}_3). \tag{29}$$

Here the distorted-wave functions $\chi_p^{(-)}$ and $\chi_e^{(-)}$ for the scattered positron and ejected electron, respectively, satisfy the following equations:

$$(c\alpha_1\cdot\mathbf{p}_1+c^2\beta_1+U_p-E_p)\chi_p^{(-)}(\mathbf{r}_1)=0, \tag{30}$$

$$(c\alpha_2\cdot\mathbf{p}_2+c^2\beta_2+U_e-E_e)\chi_e^{(-)}(\mathbf{r}_2)=0. \tag{31}$$

The distorting potentials including the polarization effects U_p and U_e for the scattered positron and ejected electron, respectively, are summarized in Table I. Here, TPDW approximation stands for the relativistic two-potential distorted-wave approximation. The TPDW models are used to account for the mutual screening of the scattered positron and the ejected electron. For the neutral atom, the asymptotic charges (Z_pZ_e) are (01) and (11) in models TPDW01 and TPDW11, respectively. In Table I, ν_f denotes the average potential due to the bound electron of the residual hydrogenic ion,

$$\nu_f(r_k)=-\left\langle \Phi_0(\mathbf{r}_3)\left|\frac{1}{r_{k3}}\right|\Phi_0(\mathbf{r}_3)\right\rangle. \tag{32}$$

D. Transition amplitudes

By considering antisymmetrization, we arrive at expressions for the transition amplitude T_{fi} of positron-impact ionization of the helium atom,

$$T_{fi}\cong D_{fi}-E_{fi}, \tag{33}$$

where the direct term D_{fi} and exchange term E_{fi} are given as

$$D_{fi}=\sqrt{2}\langle\chi_p^{(-)}(\mathbf{r}_1)\chi_e^{(-)}(\mathbf{r}_2)\Phi_0(\mathbf{r}_3)|W_i| \times\chi_i^{(+)}(\mathbf{r}_1)\Phi_b(\mathbf{r}_2)\Phi_{b'}(\mathbf{r}_3)\rangle, \tag{34}$$

$$E_{fi}=\sqrt{2}\langle\chi_p^{(-)}(\mathbf{r}_1)\chi_e^{(-)}(\mathbf{r}_3)\Phi_0(\mathbf{r}_2)|W_i| \times\chi_i^{(+)}(\mathbf{r}_1)\Phi_b(\mathbf{r}_2)\Phi_{b'}(\mathbf{r}_3)\rangle. \tag{35}$$

By using a graphical method [24], we can express the transition amplitude T_{fi} in terms of $3n$-j coefficients and radial integrals [17].

V. RESULTS AND DISCUSSION

We have calculated the single-differential and total cross sections of positron-impact ionization of He near the ionization threshold in the two-potential distorted-wave approximation in models TPDW01 and TPDW11. To present the ionization cross sections, we use the threshold-energy units $u_i=(E_i-c^2)/I$, $u_p=(E_p-c^2)/I$, and $u_e=(E_e-c^2)/I$, measured with respect to the rest energy of the electron, and where $I=c^2-E_b$ denotes the ionization potential of the helium atom. The ionization cross sections are given in units of πa_0^2 throughout, where a_0 is the Bohr radius.

In model TPDW01 for the positron-impact ionization of He, only the ejected electron experiences the long-range Coulomb potential, while the scattered positron is screened by both electrons. According to Eq. (15), the single-differential cross section is a linear function of k_p. But in

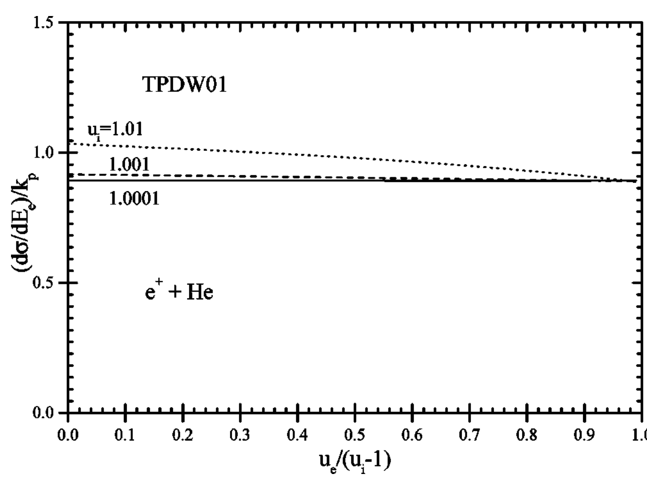

FIG. 1. Single-differential cross sections $d\sigma/dE_e$ (in units of πa_0^2) divided by k_p for the positron-impact ionization of He in the model TPDW01 at $u_i=1.01$, 1.001, and 1.0001 threshold-energy units.

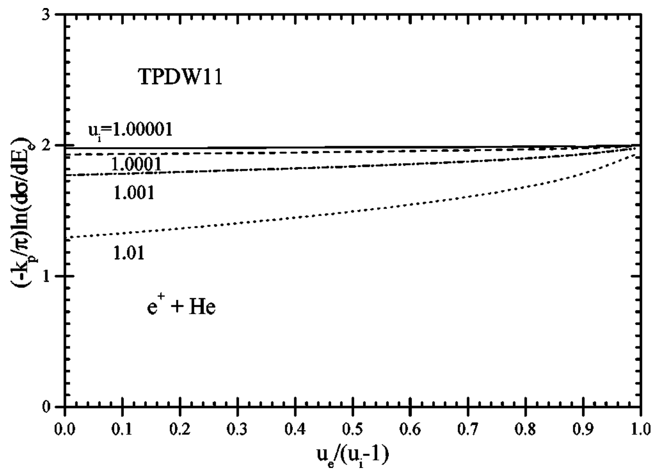

FIG. 2. Logarithm of single-differential cross sections $d\sigma/dE_e$ (in units of πa_0^2) multiplied by $(-k_p/\pi)$ for the positron-impact ionization of He in the model TPDW11 at $u_i = 1.01$, 1.001, 1.0001, and 1.000 01 threshold-energy units.

model TPDW11, both outgoing positron and electron move in the Coulomb potential, the single-differential cross section is an exponential function of k_p. In Fig. 1, we present the single-differential cross sections $d\sigma/dE_e$ divided by k_p in the model TPDW01 at $u_i = 1.01, 1.001$, and 1.0001 to show the energy dependence of the cross sections. In Fig. 2, we present the logarithm of the single-differential cross sections multiplied by $(-k_p/\pi)$ in the model TPDW11 at $u_i = 1.01, 1.001, 1.0001$, and 1.000 01. In both Figs. 1 and 2, the curves approach constant horizontal lines as the incident energy u_i decreases. By Eq. (16), the total cross section in model TPDW01 is a power function of the excess energy ϵ and the near-threshold power factor is 1.5. In model TPDW11, the total cross section is a compound function with power and exponential of the excess energy ϵ. In Fig. 3, we present the near-threshold power factor of the total cross section, $d(\ln \sigma)/d(\ln \epsilon)$, in the model TPDW01. In Fig. 4, we present the scaled total cross section $-(1/\pi)\sqrt{\epsilon/2}\ln \sigma$ in the

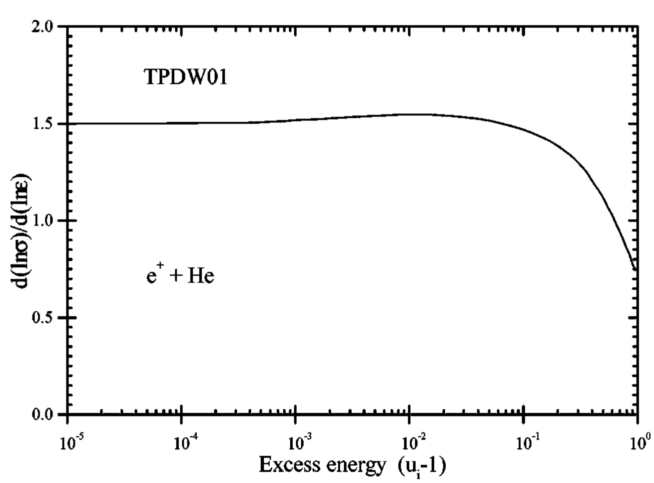

FIG. 3. The near-threshold power factor of the total cross section, $d(\ln \sigma)/d(\ln \epsilon)$, for the positron-impact ionization of He in the model TPDW01.

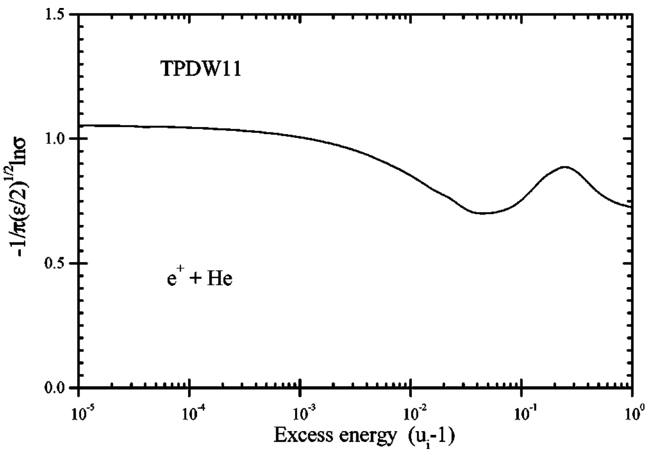

FIG. 4. The scaled total cross section $-(1/\pi)\sqrt{\epsilon/2}\ln \sigma$ for the positron-impact ionization of He in the model TPDW11 near threshold.

model TPDW11 near the threshold. Finally, we display the total cross section of positron-impact ionization for He in Fig. 5 and compare with the experimental data of Ashley *et al.* [1] and with the theoretical results of Ihra *et al.* [9] and Deb and Crothers [10] who used different threshold forms. Our curve offers a reasonable agreement at excess energy higher than 3 eV.

VI. CONCLUSION

The threshold law of positron-impact ionization is discussed by analyzing the threshold behaviors of the wave functions near the threshold region in the two-potential distorted-wave approximation. The threshold law depends only on the asymptotic behaviors of the distorting potentials experienced by the scattered positron and the ejected electron. Different asymptotic charges are used in models TPDW01 and TPDW11 for the distorting potentials. We find that the near-threshold ionization cross section depends only on whether the scattered positron experiences a long-range Coulomb interaction. We have demonstrated numerically that

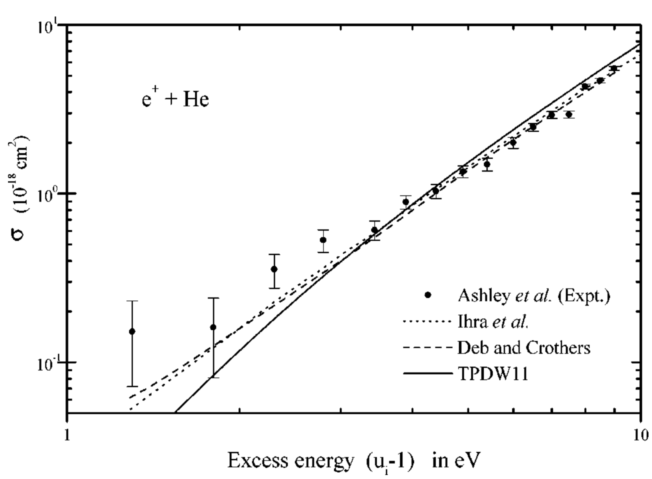

FIG. 5. Comparison of total cross sections for the positron-impact ionization of He.

the near-threshold ionization cross sections agree well with the analytically derived threshold law that accounts for the correct modulation factor $\exp[-2\pi Z_p/\sqrt{2\epsilon}]$ peculiar to the positron-impact ionization. Various other threshold laws have also been suggested [3–5,7–10,19]. Our results arising from an *ab initio* calculation seem to agree reasonably well with experiment; however, it is difficult to discern different theoretical models by available experimental results within a small range of the excess energy ϵ. More experimental data of the cross section for positron-impact ionization of ions near the threshold region are certainly needed for comparison.

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