

Conspicuous QED Effects in the Positron-Impact Ionization of U^{91+} Hsiao-Ling Sun,¹ Ju-Tang Hsiao,² Sheng-Fang Lin,¹ and Keh-Ning Huang^{1,3}¹*Institute of Atomic and Molecular Sciences, Academia Sinica
P.O. Box 23-166, Taipei, Taiwan 106, Republic of China*²*Department of Natural Sciences, National Institute for Compilation and Translation,
Taipei Taiwan 106, Republic of China*³*Department of Physics, National Taiwan University
Taipei, Taiwan 106, Republic of China*

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The positron-impact ionization of U^{91+} is studied in the two-potential distorted-wave approximation in QED theory. The effects of the transverse-photon interactions between charges as well as vacuum polarization are analyzed. QED effects conspicuously enhance the cross section at all incident energies.

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I. INTRODUCTION

Impact ionization processes of atoms and ions by charged particles are fundamental for understanding the collision mechanisms and atomic structure. Knowledge of ionization cross sections has wide applications for the understanding of physical phenomena in astrophysics, plasma physics, and radiation physics. In particular, information on the ionization cross sections of highly charged ions by charged particles is important in the study of high-temperature plasmas. However, the inherent difficulties are in obtaining extensive data on the ionization cross sections of highly charged ions in both theory and experiment.

Electron-impact ionization cross sections for U^{91+} - U^{90+} were first measured by Claytor *et al.* [1] at 222 keV electron energy in the heavy-ion channeling experiment. Electron-impact ionization cross sections for some intermediate- and high- Z hydrogenlike ions were obtained by Marrs *et al.* [2, 3], O'Rourke *et al.* [4], and Watanabe *et al.* [5] in electron-beam ion trap (EBIT) experiments. Pindzola *et al.* [6] calculated the direct electron-impact-ionization cross sections for U^{91+} and U^{90+} in lowest-order quantum electrodynamics (QED), and Moores and Pindzola [7] evaluated the cross sections of electron-impact ionization for hydrogenic ions with nuclear charge Z between 26 and 92 using a relativistic distorted-wave method. Later, Pindzola *et al.* [8] calculated the electron-impact ionization for U^{91+} including exchange effects. Effects of the transverse-photon interaction were investigated by Moores and Reed [9] in relativistic distorted-wave calculations for high- Z hydrogenlike ions. The ionization cross sections of $1s$ for a variety of ions with one to four bound electrons and nuclear charge Z in the range of 10 to 92 were studied by Fontes *et al.* [10] within the relativistic distorted-wave approximation with the transverse-photon interaction. For positron-impact ionization, on the other hand, only that for U^{90+} has been

reported by Pindzola [11].

A complete relativistic kinematic formulation of the impact-ionization processes has been presented by Huang [12], in which all dynamical parameters are given in terms of reduced matrix elements. By the two-potential distorted-wave method (TPDW), relativistic cross sections of electron- and positron-impact ionizations of highly charged hydrogen- and helium-like ions and the QED cross sections of electron-impact ionization for hydrogenlike ions have been reported by Kuo and Huang [13] and Sun *et al.* [14]. In this work, we shall calculate the QED cross section for the positron-impact ionization of U^{91+} , in which exchange effects are not present to complicate the matter. In Sec. II we will present the general theory of positron-impact ionization in the two-potential distorted-wave approximation. The interaction Hamiltonians for the ionization processes and the transition matrix elements in terms of radial integrals for hydrogen-like targets are given. Present numerical results and discussions are provided in Sec. III, and a summary is made in Sec. IV.

II. THEORY

In the positron-impact ionization of hydrogen-like ions, we denote the linear momentum and total energy of the incident positron by (\mathbf{k}_i, E_i) . Before the collision, the target ion is in its ground state with only one electron. After the collision, the ion is deprived of its electron and becomes a bare nucleus. The scattered positron and ejected electron, are described by (\mathbf{k}_p, E_p) and (\mathbf{k}_e, E_e) , respectively.

By energy conservation, we have

$$E_i + E_b = E_p + E_e, \quad (1)$$

where E_b is the binding energy of the electron in the target ion. In collision theory, we obtain the single-differential cross section for hydrogen-like targets,

$$\frac{d\sigma}{dE_e} = \frac{\pi^3}{k_i^2} \sum_{\alpha} d_{\alpha}^2. \quad (2)$$

Here the summation is over all possible channels $\alpha \equiv (\kappa_i, \kappa_p, \kappa_e, j, J)$ with $\kappa_i \equiv (j_i, l_i)$, etc., and the real amplitude d_{α} is defined as the reduced matrix element of the partial-wave amplitude in channel α ,

$$d_{\alpha} \exp(i\delta_{\alpha}) = i^{l_i - (l_p + l_s)} \exp[i(\sigma_{\kappa_p} + \sigma_{\kappa_s})] \times \langle \alpha^- [J_{\alpha}(j_p j_s) j] J \| H_I \| (j_b j_i) J \rangle, \quad (3)$$

where H_I denotes symbolically the appropriate interaction operator, $j_b = 1/2$, and the coupling schemes adopted are indicated.

In our case, the unperturbed Hamiltonian H_i and the interaction potential V_i are written as

$$H_i = (c\alpha_1 \cdot \mathbf{p}_1 + c^2\beta_1) + (c\alpha_2 \cdot \mathbf{p}_2 + c^2\beta_2) - \frac{Z}{r_2}, \quad (4)$$

$$V_i = \frac{Z}{r_1} + V(r_{12}), \quad (5)$$

where α_i and β_i are Dirac matrices, and Z is the nuclear charge of the ion. The indices 1 and 2 refer to, respectively, the incident positron and bound electron before the collision as well as the scattered positron and ejected electron after the collision. Here $V(r_{12})$ stands for potentials arising from electron-positron interactions in QED theory at various levels of approximation, e.g., the Coulomb interaction, or the Coulomb interaction plus the Breit interaction, etc. These interactions between charges are due to the exchange of four types of photons, namely, one time-like photon, one longitudinal photon, and two transverse photons. The exchange of a time-like photon and a longitudinal photon together leads to the instantaneous Coulomb interaction. The transverse-photon interaction [15, 16] is due to the exchange of two types of transverse photons and may be approximated in the lowest order by the Breit interaction. In addition, processes involving the creation of virtual electron-positron pairs by the photon fields produce the vacuum-polarization potential between charges.

In collision theory, the transition matrix element may be written exactly in the prior form as

$$T_{fi} = \left\langle \Psi_f^{(-)} \left| V_i \right| \Psi_i \right\rangle, \quad (6)$$

where Ψ_i is the eigenstate of H_i , and $\Psi_f^{(-)}$ is the eigenstate of the total Hamiltonian H with the incoming-wave boundary condition.

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

$$V_i = U_i + W_i. \quad (7)$$

Since in the initial state the incident positron is generally screened by the bound electron, we may choose

$$U_i = \frac{Z}{r_1} + v_i(r_1), \quad (8)$$

$$W_i = V(r_{12}) - v_i(r_1). \quad (9)$$

Here the average potential $v_i(r_1)$ is due to the wave function $\Phi_0(\mathbf{r}_2)$ of the bound electron of the hydrogen-like target,

$$v_i(r_1) = - \left\langle \Phi_0(\mathbf{r}_2) \left| \frac{1}{r_{12}} \right| \Phi_0(\mathbf{r}_2) \right\rangle. \quad (10)$$

The transition matrix element in the two-potential formulation assumes the form

$$T_{fi} = \left\langle \Psi_f^{(-)} \left| W_i \right| \psi_i^{(+)} \right\rangle, \quad (11)$$

where $\psi_i^{(+)}$ denotes the distorted wave function in the distorting potential U_i which can be expressed as

$$\psi_i^{(+)} = \chi_i^{(+)}(\mathbf{r}_1) \Phi_0(\mathbf{r}_2). \quad (12)$$

Here the distorted wave function $\chi_i^{(+)}(r_1)$ for the incident positron with the outgoing-wave boundary condition satisfies the equation

$$(c\alpha_1 \cdot \mathbf{p}_1 + c^2\beta_1 + U_i - E_i) \chi_i^{(+)}(\mathbf{r}_1) = 0. \quad (13)$$

As an approximation to the final-state wave function $\Psi_f^{(-)}$, we choose the distorted final-state wave function as

$$\Psi_f^{(-)} \approx \chi_p^{(-)}(\mathbf{r}_1) \chi_e^{(-)}(\mathbf{r}_2), \quad (14)$$

where $\chi_p^{(-)}(\mathbf{r}_1)$ and $\chi_e^{(-)}(\mathbf{r}_2)$ satisfy the following equations:

$$(c\alpha_1 \cdot \mathbf{p}_1 + c^2\beta_1 + U_p - E_p) \chi_p^{(-)}(\mathbf{r}_1) = 0, \quad (15)$$

$$(c\alpha_2 \cdot \mathbf{p}_2 + c^2\beta_2 + U_e - E_e) \chi_e^{(-)}(\mathbf{r}_2) = 0. \quad (16)$$

Here the distorting potentials U_p and U_e are for the positron and electron, respectively. We choose the model in the present calculation such that the scattered positron is completely screened by the ejected electron in the asymptotic region, while the ejected electron is affected only by the Coulomb potential of the nucleus. The distorting potentials U_p and U_e are given explicitly as

$$U_p(r_1) = \frac{Z}{r_1} + v_i(r_1), \quad (17)$$

$$U_e(r_2) = -\frac{Z}{r_2}. \quad (18)$$

By using a graphical method [17], we obtain an expression for the real transition matrix elements d_α of Eq. (3) in terms of $3n - j$ coefficients and radial integrals. Numerical calculations are then carried out for the transition matrix elements.

The electron-positron interaction between two-particle configurations in the jm scheme has the general form [17]

$$\langle ab | V(r_{12}) | cd \rangle = \int d^3r_1 \int d^3r_2 u_a^\dagger(1) u_b^\dagger(2) V(r_{12}) u_c(1) u_d(2), \quad (19)$$

where $a, b, c,$ and d indicate generally different Dirac orbitals with the form

$$u_{n\kappa m}(\mathbf{r}) = \frac{1}{r} \begin{pmatrix} G_{n\kappa}(r) \Omega_{\kappa m} \\ iF_{n\kappa}(r) \Omega_{-\kappa m} \end{pmatrix}. \quad (20)$$

Here the radial functions $G_{n\kappa}$ and $F_{n\kappa}$ are the large and small components, respectively, and $\Omega_{\kappa m}$ are normalized two-component Dirac spinors. Using the techniques of the vector-spherical-harmonics expansion, we reduce the matrix element of the electron-positron interaction to a linear combination of radial integrals, suitable for numerical computations [17]:

$$\langle ab | V(r_{12}) | cd \rangle = \sum_j G_j(ab; cd) X_j(ab; cd). \quad (21)$$

Here the coefficient $G_j(ab; cd)$ relates to angular-momentum couplings of the interacting particles and is defined in terms of 3- j m symbols as

$$G_j(ab; cd) = \begin{pmatrix} j_a & j & m_c \\ m_a & m_c - m_a & j_c \end{pmatrix} \begin{pmatrix} j_b & m_d & m_c - m_a \\ m_b & j_d & j \end{pmatrix}. \quad (22)$$

The expression $X_j(ab; cd)$ is called the interaction strength with the general form

$$X_j(ab; cd) = C_j(ab; cd) I_j(ab; cd), \quad (23)$$

$$C_j(ab; cd) = (-)^{j_a + j_d} [(2j_a + 1)(2j_b + 1)(2j_c + 1)(2j_d + 1)]^{1/2} \begin{pmatrix} j_a & j & j_c \\ \frac{1}{2} & 0 & -\frac{1}{2} \end{pmatrix} \begin{pmatrix} j_b & j & j_d \\ \frac{1}{2} & 0 & -\frac{1}{2} \end{pmatrix}, \quad (24)$$

where $I_j(ab; cd)$ is defined in terms of radial integrals, depending on the specific form of $V(r_{12})$. We summarize the results for various interactions:

(i) Coulomb interaction: $-1/r_{12}$

$$I_j(ab; cd) = - \langle W_{ac} R_j W_{bd} \rangle^{\text{even}}, \quad (25)$$

which has the explicit form

$$\langle W_{ac} R_j W_{bd} \rangle^{\text{even}} = \int_0^\infty dr_1 \int_0^\infty dr_2 W_{ac}(r_1) R_j W_{bd}(r_2) \quad (26)$$

with

$$W_{\alpha\beta}(r) = G_\alpha(r) G_\beta(r) + F_\alpha(r) F_\beta(r),$$

$$R_j = r_{<}^j / r_{>}^{j+1}.$$

Here the notation $\langle \rangle^{\text{even (odd)}}$ denotes the selection rule that both $(l_a + j + l_c)$ and $(l_b + j + l_d)$ have to be even (odd).

$$\begin{aligned}
(ii) \text{ Breit interaction: } & \frac{1}{2r_{12}} \left[(\alpha_1 \cdot \alpha_2) + \frac{(\alpha_1 \cdot \mathbf{r}_{12})(\alpha_2 \cdot \mathbf{r}_{12})}{r_{12}^2} \right] \\
I_j(ab; cd) = & (1 - \delta_{jo}) (\kappa_a + \kappa_c) (\kappa_b + \kappa_d) \frac{1}{j(j+1)} \langle V_{ac} R_j V_{bd} \rangle^{\text{odd}} \\
& - \frac{j(j+1)}{2j+1} \left[\frac{1}{2j-1} \langle P_{ac} R_{j-1} P_{bd} \rangle^{\text{even}} + \frac{1}{2j+3} \langle Q_{ac} R_{j+1} Q_{bd} \rangle^{\text{even}} \right. \\
& \left. + \frac{1}{2} \langle Q_{ac} v_j P_{bd} \rangle^{\text{even}} + \frac{1}{2} \langle P_{ac} v_j Q_{bd} \rangle^{\text{even}} \right], \tag{27}
\end{aligned}$$

where

$$v_j = \epsilon(r_1 - r_2) [R_{j+1}(r_1 r_2) - R_{j-1}(r_1 r_2)] \tag{28}$$

with the Heaviside step function $\epsilon(r_1 - r_2)$ defined as

$$\epsilon(x) = \begin{cases} 1 & x \geq 0, \\ 0 & x < 0. \end{cases} \tag{29}$$

In (27) the different combinations of radial functions are defined as

$$\begin{aligned}
V_{\alpha\beta}(r) &= G_\alpha(r) F_\beta(r) + F_\alpha(r) G_\beta(r), \\
P_{\alpha\beta}(r) &= G_\alpha(r) F_\beta(r) - F_\alpha(r) G_\beta(r) + V_{\alpha\beta}(r) (\kappa_\beta - \kappa_\alpha) / j, \\
Q_{\alpha\beta}(r) &= -G_\alpha(r) F_\beta(r) + F_\alpha(r) G_\beta(r) + V_{\alpha\beta}(r) (\kappa_\beta - \kappa_\alpha) / (j+1). \tag{30}
\end{aligned}$$

$$(iii) \text{ Transverse-photon interaction: } (\alpha_1 \cdot \alpha_2) \frac{e^{i\omega r_{12}}}{r_{12}} - (\alpha_1 \cdot \nabla_1) (\alpha_2 \cdot \nabla_2) \left[\frac{e^{i\omega r_{12}} - 1}{\omega^2 r_{12}} \right]$$

$$\begin{aligned}
I_j(ab; cd) = & (1 - \delta_{jo}) (\kappa_a + \kappa_c) (\kappa_b + \kappa_d) \frac{2j+1}{j(j+1)} \langle V_{ac} g_j V_{bd} \rangle^{\text{odd}} \\
& - (\kappa_c - \kappa_a) [\langle V_{ac} g_{j-1} P_{bd} \rangle^{\text{even}} + \langle V_{ac} g_{j+1} Q_{bd} \rangle^{\text{even}}] \\
& - j(j+1) [\langle P_{ac} s_j Q_{bd} \rangle^{\text{even}} + \langle Q_{ac} t_j P_{bd} \rangle^{\text{even}}], \tag{31}
\end{aligned}$$

where

$$\begin{aligned}
s_j &= \begin{cases} -(i/r_1) j_{j+1}(\omega r_2) h_j(\omega r_1), & r_1 > r_2 \\ r_1^{j-1} / \omega^2 r_2^{j+2} - (i/r_1) j_j(\omega r_1) h_{j+1}(\omega r_2), & r_1 < r_2, \end{cases} \\
t_j &= \begin{cases} r_2^{j-1} / \omega^2 r_1^{j+2} - (i/r_1) j_{j-1}(\omega r_2) h_j(\omega r_1), & r_1 > r_2, \\ -(i/r_1) j_j(\omega r_1) h_{j-1}(\omega r_2), & r_1 < r_2, \end{cases} \tag{32}
\end{aligned}$$

with j_j and h_j being the spherical Bessel and Hankel functions, respectively.

The lowest-order vacuum-polarization potential, known as the Uehling potential, may be expanded for a spherical charge distribution in a convergent form valid for all distances [18]. The ratios of vacuum-polarization potentials of various orders to the Coulomb potential for a point nucleus have been evaluated by Huang [18] for $r \leq 1351.6$ fm, where the Uehling potential falls to less than 0.1 ppm of the Coulomb potential. In this work, cross sections are calculated with and without the vacuum-polarization potential to demonstrate the effects of the creation of virtual electron-positron pairs.

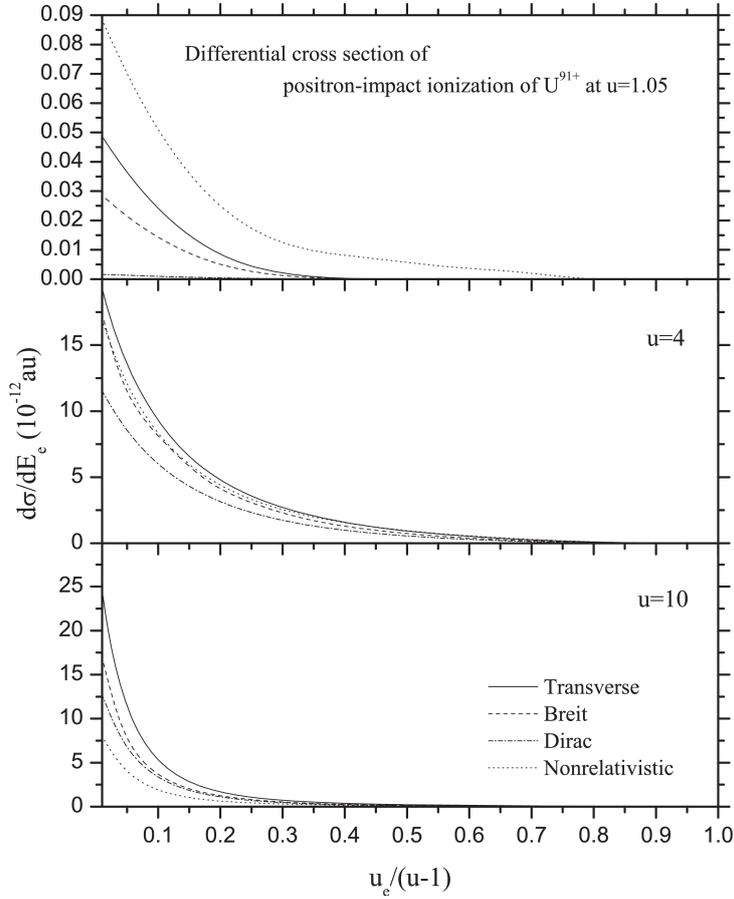


FIG. 1: Single-differential cross section of positron-impact ionization for U^{91+} at incident energies $u = 1.05, 4$, and 10 , where $u = (E_i - c^2)/I$ is the threshold-energy unit.

III. RESULTS AND DISCUSSION

We use the threshold-energy units $u = (E_i - c^2)/I$ and $u_e = (E_e - c^2)/I$, where $I = c^2[1 - \sqrt{1 - (Z\alpha)^2}]$ denotes the ionization potential of U^{91+} . As examples, the single-differential cross sections at $u = 1.05, 4$, and 10 are presented in Fig. 1. “Breit” and “Transverse” mean that the interactions between the electron and positron include the Coulomb interaction plus the Breit and transverse-photon interactions, respectively. Relativistic and nonrelativistic cross sections including the Coulomb interaction only are denoted respectively by “Dirac” and “Nonrelativistic”. The Dirac curve is generally lower than the nonrelativistic curve at low incident energies and becomes higher at high incident energies. The QED curves are always significantly higher than the Dirac curve.

Total cross sections for the positron-impact ionization of U^{91+} are presented in Fig. 2. At higher incident energies, the Dirac cross section goes up gradually while the nonrela-

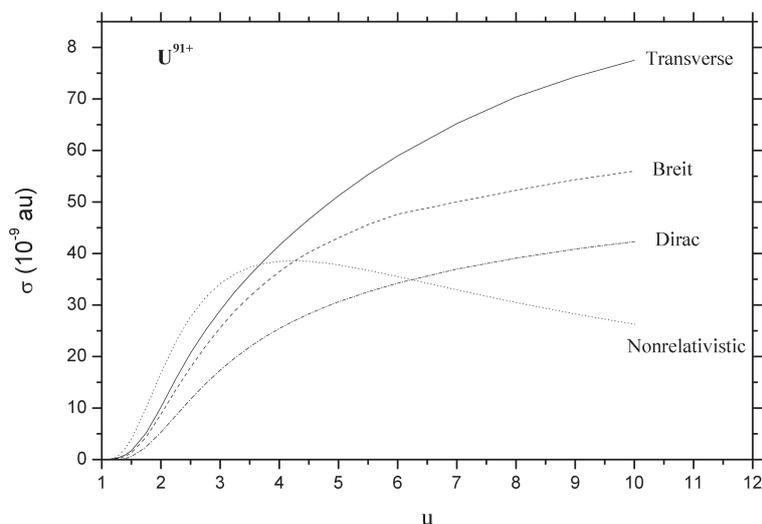


FIG. 2: The positron-impact ionization cross sections of U^{91+} at various levels of approximation.

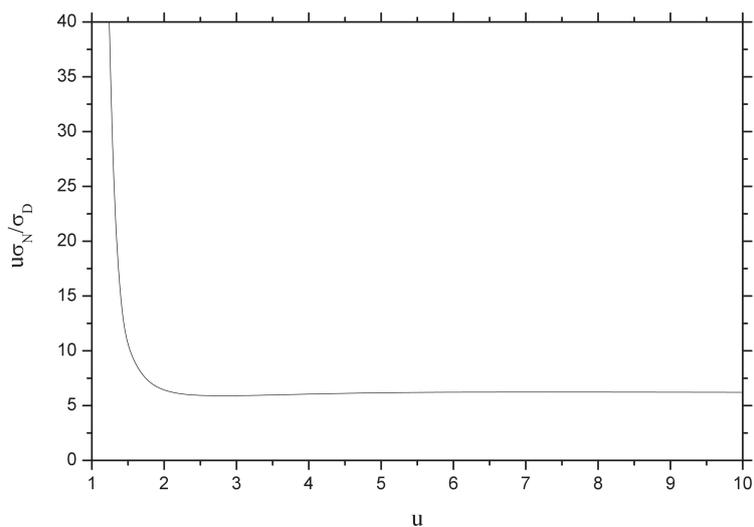


FIG. 3: Nonrelativistic cross section multiplied by u and divided by Dirac cross section for U^{91+} .

tivistic one decreases. This phenomenon can be explained as being due to the fact that the nonrelativistic cross section σ_N is proportional to $(u - 2)/u^2$ and the Dirac cross section σ_D is proportional to $(u - 2)/u$ at high incident energies for high- Z ions.

The values of $u\sigma_N/\sigma_D$ are constant at high incident energies and are also plotted in Fig. 3. In Fig. 3 we also found that the values of $u\sigma_N/\sigma_D$ are very large near the threshold energy and decreases rapidly as u increases. By the threshold law of positron-impact ionization [19], the cross section is proportional to $\varepsilon^3 e^{-2\pi Z_p/\sqrt{2\varepsilon}}$ near the threshold

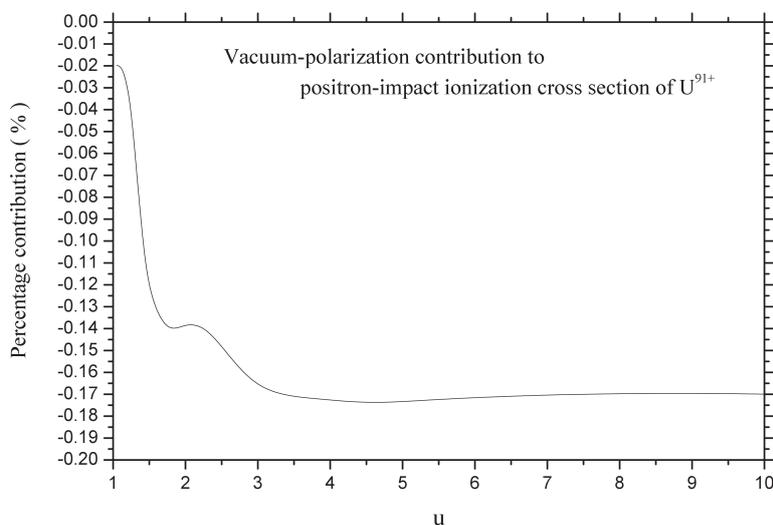


FIG. 4: The percentage contribution of the vacuum polarization to the total cross section for U^{91+} in the positron-impact ionization.

energy, where ε is the excess energy of the colliding system and Z_p is the effective charge experienced by the scattered incident positron. Because of using the relativistic ionization potential for the incident energy unit, the excess energy $\varepsilon_D = (E_i - c^2 - I)$ in the Dirac case is less than the excess energy $\varepsilon_N = (E_i - c^2 - I_N)$ in the nonrelativistic case, where $I_N = Z^2/2$. Therefore the Dirac cross sections are much less than the nonrelativistic cross sections at low incident energies. In Fig. 2 the QED cross sections are always conspicuously larger than the Dirac cross sections. The transverse-photon interaction can be expanded in powers of ωr_{12} and written in the form

$$V_{trans} = \frac{1}{2r_{12}} [(\alpha_1 \cdot \alpha_2) + (\alpha_1 \cdot \mathbf{r}_{12})(\alpha_2 \cdot \mathbf{r}_{12})/r_{12}^2] + i\frac{2}{3}\omega(\alpha_1 \cdot \alpha_2) + O(\alpha_1)(\alpha_2)(\omega r_{12})^2. \quad (33)$$

By a simple argument we can show that the matrix elements of the operators α and ωr_{12} are both of order $(Z^*\alpha)$, with Z^* being a certain effective charge. The first term on the right-hand side in (33) is the Breit interaction; it has the order of $(Z^*\alpha)^2$ relative to the Coulomb interaction. The leading imaginary term and the high-order correction term are of order $(Z^*\alpha)^3$ and $(Z^*\alpha)^4$ relative to the Coulomb interaction, respectively. In order to understand the QED effects in the positron-impact ionization of U^{91+} , the ratios of transverse cross sections to Dirac cross sections were evaluated and are about 72 at $u = 1.05$ and about 1.8 at $u = 10$.

The cross sections were also calculated in the transverse case with and without the vacuum-polarization potential between the positron and the nucleus. The percentage contribution of the vacuum-polarization potential to the cross section varies from -0.02% to about -0.17% , which is plotted in Fig. 4. The vacuum-polarization potential reduces the cross section at all incident energies.

IV. SUMMARY

In this paper, a fully relativistic calculation of positron-impact ionization including Coulomb, Breit, and transverse-photon interactions as well as the vacuum polarization potential for highly charged U^{91+} ion is performed. As might be expected, QED effects increase the cross sections substantially at high incident energies, and the contribution of the vacuum-polarization potential is negligibly small. In the future, we plan to apply our methods to study the total and differential ionization cross sections for few-body relativistic systems.

Acknowledgements

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