The effect of wave function orthogonality on the simultaneous ionization and excitation of helium*

Liu Li-Juan(刘丽娟)[a], Jia Chang-Chun(贾昌春)[a]†, Zhang Li-Min(张立民)[a], Chen Jiao-Jiao(陈姣姣)[a], and Chen Zhang-Jin(陈长进)[b]

[a] School of Physics and Material Science, Anhui University, Hefei 230601, China
[b] Department of Physics, College of Science, Shantou University, Shantou 515063, China

(Received 14 December 2012; revised manuscript received 11 April 2013)

Within the framework of the first-order Born approximation, the triple differential cross sections (TDCSs) for simultaneous ionization and excitation of helium are calculated. The wave function of the ejected electron is chosen to be orthogonal or non-orthogonal to the wave function of the bound electron before ionization. It is found that the orthogonality has a strong effect on the TDCS, especially when plane waves and Coulomb waves are used to describe the projectile and the ejected electron.

Keywords: simultaneous ionization and excitation, triple differential cross section (TDCS), first-order Born approximation, orthogonality

PACS: 34.50.Fa **DOI:** 10.1088/1674-1056/22/10/103401

1. Introduction

The (e, 2e) reaction of electron collision with atoms and molecules is one of the most effective methods to investigate the internal electronic structures of atoms and molecules and the relevant dynamic mechanisms.[1–3] Since early experiments in 1968, much effort has been devoted to studying the ionization processes in which the residual ion is left in the ground state, and the physics behind the experimental measurements has been well understood based on theoretical calculations.[4–8] In contrast, the relevant processes of simultaneous ionization and excitation which leaves the residual ion in an excited state have been much less studied. Experimentally, it is more difficult to measure the triple differential cross sections (TDCSs) for simultaneous ionization and excitation due to the fact that the count rates are two times smaller than the processes of single ionization without excitation. And only a few experiments have been carried out so far.[9–12] Theoretically, it is also a big challenge since one more active electron is involved.

The TDCSs for electron impact ionization of atoms and molecules have no analytical solutions since it is a many-body problem. As a result, the evaluation of TDCSs has to resort to some approximations. Numerous theoretical methods have been used for calculating TDCSs for the (e, 2e) processes. Particularly noteworthy is the work of Brauner, Briggs and Klar (BBK) in which a three-Coulomb product wave function for the final state that satisfies the asymptotic three-body Schrödinger equation was used to calculate the TDCS for electron–hydrogen ionization,[4] the convergent close-coupling (CCC) calculations performed by Bray and Stelbovics[5] and the second-order distorted wave Born approximation (DWB2) developed by Chen and Madison[13] who performed the TDCS calculations for the simultaneous ionization and excitation of helium with the residual ion left in the states $n = 1$ and 2. It is also worthwhile mentioning some other theoretical models, such as the time-dependent close-coupling (TDCC) theory of Pindzola and Robicheaux,[14] the R-matrix with pseudo-states (RMPS) method of Bartschat *et al.*,[15] and the B-spline R-matrix (BSR) approach of Zatsarinny and Bartschat.[16]

While the collision mechanism, polarization effect, correlation effect, and exchange effect have been well studied for the electron-impact simultaneous ionization and excitation of helium, and to the best of our knowledge, the orthogonality effect of wave function has not been addressed so far. For the process of single ionization without excitation, it has already been demonstrated that the reproduced TDCS is sensitive to the orthogonality of the wave functions of the bound and ejected electrons.[17] Therefore there is no shortage of theoretical efforts aiming at this issue for simultaneous ionization and excitation of helium by electron impact.

In this paper, we calculate the TDCS in the first-order approximation for the electron impact of ionization of helium with the residual ion left in the $n = 2$ excited state in the coplanar asymmetric geometry at intermediate incident energies. By choosing the wave function of the ejected electron to be orthogonal and non-orthogonal to that of the bound electron, the effect of the orthogonality on the TDCS is investigated.

*Project supported by the Anhui University Doctoral Research Starting Foundation, China (Grant Nos. 02303319 and 33190203) and the National Natural Science Foundation of China (Grant No. 11274219).

†Corresponding author. E-mail: jcc@ustc.edu.cn

© 2013 Chinese Physical Society and IOP Publishing Ltd

Meanwhile, the distortion effect is also studied by using plane waves, Coulomb waves, and distorted waves for the projectile and the ejected electron, respectively.

2. Theory

The processes of simultaneous ionization and excitation of helium by electron impact can be described as follows: an incident projectile with momentum $\boldsymbol{k}_\mathrm{i}$, collides with helium atom; after an ionizing collision the scattering electron with momentum $\boldsymbol{k}_\mathrm{f}$ and the ejected electron with momentum $\boldsymbol{k}_\mathrm{e}$ are detected in coincidence; meanwhile the residual ion He^+ is left in an excited state. The TDCS for this process is given by[13]

$$\frac{\mathrm{d}^3\sigma}{\mathrm{d}E\,\mathrm{d}\Omega_\mathrm{f}\mathrm{d}\Omega_\mathrm{e}} = (2\pi)^4\frac{k_\mathrm{e}k_\mathrm{f}}{k_\mathrm{i}}|f|^2, \tag{1}$$

where $\mathrm{d}\Omega_\mathrm{f}$ $(\mathrm{d}\Omega_\mathrm{e})$ is thr solid angle, $\mathrm{d}E$ is the energy interval of scattered electron, and f is the first-order direct scattering amplitude and expressed as[13]

$$f = \left\langle \Phi_\mathrm{f}^-(0,1,2)\middle| V_\mathrm{f}(0,1,2) - U_\mathrm{f}(1,2)\middle|\Psi_\mathrm{i}^+(0,1,2)\right\rangle. \tag{2}$$

We will ignore the exchange scattering amplitude in Eq. (1), since it is negligible for intermediate and high energies in the highly asymmetric geometry considered in this paper. In Eq. (2), '0' denotes the projectile and '1' the ejected electron, and the residual ion with a bound electron '2' is left in the 2s state; Φ_f^- is the approximate final state wave function and Ψ_i^+ is the exact initial state wave function; V_f (V_i) is the final (initial) state interaction potential for the projectile and expressed as[13]

$$V_\mathrm{f} = V_\mathrm{i} = \frac{1}{r_{01}} + \frac{1}{r_{02}} - \frac{Z}{r_0}, \tag{3}$$

with Z being the charge of the target nucleus; U_f (U_i) is the distorted potential. The initial (final) state distorted wave function $\chi_\mathrm{i}(\boldsymbol{r}_0)$ $(\chi_\mathrm{f}(\boldsymbol{r}_0))$ is obtained by solving the following equation:

$$\left[T_\mathrm{p} + U_j(0) - E_j\right]\chi_j(0) = 0, \quad (j = \mathrm{i},\mathrm{f}), \tag{4}$$

where T_p (E_j) is the kinetic energy (total energy) of the projectile.

The wave function for the projectile depends on the choice of the distorting potential. In Eq. (4), if we choose

$$U_\mathrm{i} = U_\mathrm{f} = 0, \tag{5}$$

plane waves are obtained which take the following form

$$\chi(\boldsymbol{r}) = (2\pi)^{-3/2}\exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}). \tag{6}$$

In general, it is better to choose the spherical average of the initial atomic state ϕ_i to be the initial-state distorting potential

$$U_\mathrm{i} = \frac{1}{4\pi}\int\left\langle \phi_\mathrm{i}(\boldsymbol{r}_1,\boldsymbol{r}_2)\middle|\frac{1}{r_{01}} + \frac{1}{r_{02}} - \frac{Z}{r_0}\middle|\phi_\mathrm{i}(\boldsymbol{r}_1,\boldsymbol{r}_2)\right\rangle \mathrm{d}\hat{\boldsymbol{r}}_0, \tag{7}$$

since the incident electron effectively sees a neutral atom. On the other hand, the scattered electron would see an ion. Therefore, the distorting potential for the projectile in the final state is taken to be in the form of

$$U_\mathrm{f} = \frac{1}{4\pi}\int\left\langle \varphi_\mathrm{f}(\boldsymbol{r}_2)\middle|-\frac{Z}{r_0} + \frac{1}{r_{02}}\middle|\varphi_\mathrm{f}(\boldsymbol{r}_2)\right\rangle \mathrm{d}\hat{\boldsymbol{r}}_0, \tag{8}$$

where $\varphi_\mathrm{f}(\boldsymbol{r}_2)$ is the final wave function of He^+. Here for the final 2s state,[13]

$$\varphi_\mathrm{f}(\boldsymbol{r}_2) = 2(1-r_2)\exp(-r_2)Y_{00}(\hat{\boldsymbol{r}}_2). \tag{9}$$

The distorted wave function χ_e of the ejected electron satisfies the following equation:[13]

$$\left[T_\mathrm{e} + U_\mathrm{ion}(1) - E_\mathrm{e}\right]\chi_\mathrm{e}(1) = 0, \tag{10}$$

where T_e (E_e) denotes the kinetic energy (total energy) of ejected electron and U_ion is the distorting potential, which is given by

$$U_\mathrm{ion}(r_1) = \frac{1}{4\pi}\int\langle\varphi_\mathrm{f}(\boldsymbol{r}_2)|-\frac{Z}{r_1} + \frac{1}{r_{12}}|\phi_\mathrm{f}(\boldsymbol{r}_2)\rangle\,\mathrm{d}\hat{\boldsymbol{r}}_1. \tag{11}$$

The distortion effect on the two outgoing electrons can be tested if the pure Coulomb potential is used for both of them

$$U_\mathrm{ion} = U_\mathrm{f} = -\frac{Z-1}{r}. \tag{12}$$

Consequently, the wave function takes the form[4]

$$\chi(\boldsymbol{r}) = (2\pi)^{-3/2}\exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r})C(\alpha,\boldsymbol{k},\boldsymbol{r}), \tag{13}$$

where

$$\begin{aligned} C(\alpha,\boldsymbol{k},\boldsymbol{r}) \equiv\ & \Gamma(1-\mathrm{i}\alpha)\exp(-\pi\alpha/2) \\ & \times {}_1\mathrm{F}_1(\mathrm{i}\alpha;1;-\mathrm{i}(kr+\boldsymbol{k}\cdot\boldsymbol{r})). \end{aligned} \tag{14}$$

The final target wave function can be expressed as a symmetric product of the He^+ wave function φ_f and the distorted wave χ_e for the ejected electron,[13]

$$\phi_\mathrm{f}(1,2) = 2^{-1/2}\left[\varphi_\mathrm{f}(1)\chi_\mathrm{e}(2) + \phi_\mathrm{f}(2)\chi_\mathrm{e}(1)\right]. \tag{15}$$

So the direct scattering amplitude can be expressed as

$$\begin{aligned} f &= \left\langle \Phi_\mathrm{f}^-(0,1,2)\middle|V_\mathrm{f}(0,1,2) - U_\mathrm{f}(1,2)\middle|\Psi_\mathrm{i}^+(0,1,2)\right\rangle \\ &= \left\langle \chi_\mathrm{f}^-(0)\,\phi_\mathrm{f}^-(1,2)\middle|V_\mathrm{f}(0,1,2) - U_\mathrm{f}(1,2)\middle|\phi_\mathrm{i}(1,2)\,\chi_\mathrm{i}^+(0)\right\rangle \\ &= \langle\chi_\mathrm{f}^-(0)\,2^{-1/2}\left[\varphi_\mathrm{f}(2)\,\chi_\mathrm{e}^-(1) + \varphi_\mathrm{f}(1)\,\chi_\mathrm{e}^-(2)\right]| \\ &\quad \times V_\mathrm{f}(0,1,2) - U_\mathrm{f}(1,2)\left|\phi_\mathrm{i}(1,2)\,\chi_\mathrm{i}^+(0)\right\rangle. \end{aligned} \tag{16}$$

In this paper, the helium ground state wave function is taken from Silverman *et al.*[18] It includes radial and angular correlations, and is expressed as

$$\phi_\mathrm{i}(1,2) = \phi_\mathrm{i}^s(1,2) + \varphi_\mathrm{i}^\mathrm{p}(1,2), \tag{17}$$

where

$$\phi_{\rm i}^{s}(1,2) = n_s\left[\varphi_{1s}(1)\,\varphi'_{1s}(2)+\varphi_{1s}(2)\,\varphi'_{1s}(1)\right],$$
$$\phi_{\rm i}^{p}(1,2) = n_p\sum_{m=-1}^{+1}\tilde{\varphi}_{2p,m}(1)\,\tilde{\varphi}'_{2p,m}(2), \tag{18}$$

and

$$n_s = \left(1+\lambda^2\right)^{-1/2}N,\ \ n_p = \lambda\left(1+\lambda^2\right)^{-1/2}/\sqrt{3}, \tag{19}$$

with N being the normalization constant of the $1s1s'$ function which is given by

$$N = \left\{2\left[1+64(ab)^3(a+b)^{-6}\right]\right\}^{-1/2}. \tag{20}$$

And

$$\begin{aligned}
\varphi_{1s}(\boldsymbol{r}) &= R_{10}(r)\,Y_{00}(\hat{\boldsymbol{r}}),\\
\varphi'_{1s}(\boldsymbol{r}) &= R'_{10}(r)\,Y_{00}(\hat{\boldsymbol{r}}),\\
\tilde{\varphi}_{2p,m}(\boldsymbol{r}) &= R_{21}(r)\,Y_{1m}(\hat{\boldsymbol{r}}),\\
\tilde{\varphi}'_{2p,m}(\boldsymbol{r}) &= R_{21}(r)\,Y^{*}_{1m}(\hat{\boldsymbol{r}}),
\end{aligned} \tag{21}$$

where

$$\begin{aligned}
R_{10}(r) &= 2a^{3/2}\exp(-ar),\\
R'_{10}(r) &= 2b^{3/2}\exp(-br),\\
R_{21}(r) &= \left(2/\sqrt{3}\right)c^{5/2}r\exp(-cr).
\end{aligned} \tag{22}$$

The constants are given by

$$\begin{aligned}
a &= 2.17621,\ \ b = 1.20152,\\
c &= 2.47547,\ \ \lambda = -0.0617557.
\end{aligned} \tag{23}$$

The partial wave expansion of the distorted wave function can be expressed as[19]

$$\left[\chi_j^{-}(\boldsymbol{r}_j)\right]^{*} = \sqrt{\frac{2}{\pi}}\frac{1}{k_j r_j}\sum_{l_j\mu_j}{\rm i}^{-l_j}\chi_{l_j}(k_j,r_j)\,Y_{l_j\mu_j}(\hat{\boldsymbol{r}}_j)\,Y^{*}_{l_j\mu_j}(\hat{\boldsymbol{k}}_j), \quad (j=i,e,f) \tag{24}$$

which will be used to calculate the TDCS.

It should be noted that the wave functions for the ejected electron and the bound electron that will be ionized are assumed to be orthogonal since they are eigen-functions of the same Hamiltonian. However, in the numerical calculations, it is not necessary to be true since the potential used to obtain the ejected electron wave function is not exactly the same as that used to obtain the bound state wave function, especially when a pure Coulomb potential or a neutral potential is used, i.e.,

$$\langle\chi_{\rm e}|\phi_{\rm i}\rangle \neq 0. \tag{25}$$

In our calculations, the orthogonality

$$\langle\chi_{\rm e}|\phi_{\rm i}\rangle = 0 \tag{26}$$

is obtained by using the Schmidt orthogonalization procedure.

3. Results and discussion

The TDCSs for electron-impact simultaneous ionization and excitation of helium in coplanar asymmetric geometry are presented for orthogonal and non-orthogonal cases in which plane waves, Coulomb waves, and distorted waves are used for the projectile and the ejected electron, respectively. The positive direction of the scattering electron angle is denoted anticlockwise and that of ejected electron angle is indicated clockwise. The scattering angle has been fixed to be 4.0°. All of the theoretical results are compared with the experimental data of Avaldi *et al.*[10]

Figure 1 exhibits the TDCSs at an incident energy of 675.4 eV and ejected electron energy of 40 eV. The theoretical results obtained by using distorted wave are presented in Fig. 1(a). It can be seen that obvious differences exist in the magnitude of both the binary and recoil peaks between orthogonal and non-orthogonal situations. It is interesting that better overall agreement with experiment is achieved if the non-orthogonal wave functions are used although the predicted binary peak position shifts toward smaller angle and the recoil peak is overestimated. On the other hand, the calculated results obtained with an orthogonalized wave function reproduce a recoil peak that is about a half smaller than the experimental one.

Figures 1(b) and 1(c) show the corresponding results obtained using Coulomb wave and plane wave, respectively. In contrast to the case in Fig. 1(a), the calculations obtained with non-orthogonalized wave function reproduce the TDCSs which are more than 10 times higher than experimental results (Note that the theoretical results in Figs. 1(b) and 1(c) for non-orthogonal case are divided by 10 and 20, respectively.), which indicates that the theory completely fails so that the orthogonalization procedure is highly desired. It is demonstrated that the measured recoil peak can be well predicted by the calculations in which the ejected electron wave function is set to be orthogonal to the bound state wave function in the initial state although the binary peak is more overestimated compared with the distorted wave calculations.

Similarly, in Fig. 2 we show the results at the energy pair of 645.4 eV and 10 eV. Again, the theoretical results in the non-orthogonal case are divided by 100 in Figs. 2(b) and 2(c). It can be seen that the discrepancy in both the magnitude and the shape of the TDCS between orthogonal and non-orthogonal cases increases comparing with that in Fig. 1, especially when plane waves and Coulomb waves are used. This indicates that the orthogonality effect on the TDCS is enhanced as the ejected electron energy decreases. Again, it can be seen from Figs. 2(b) and 2(c) that the Coulomb wave and plane wave calculations with non-orthogonalized ejected electron wave function completely fail in reproducing both the magnitude and the angular distributions of the TDCS.

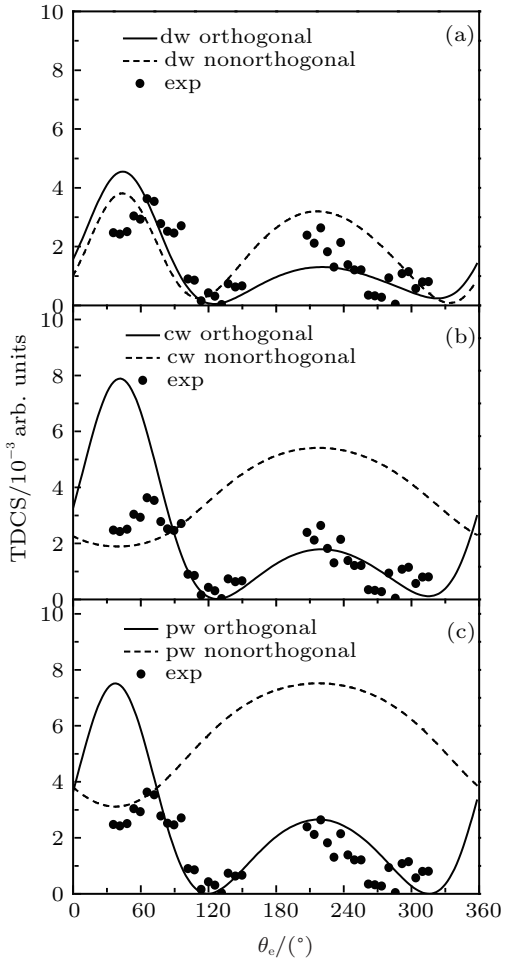


Fig. 1. TDCSs for electron-impact simultaneous ionization and excitation of helium at incident energy of 675.4 eV in coplanar asymmetric geometry, using (a) distorted wave (dw), (b) Coulomb wave (cw), and (c) plane wave (pw). In panels (b) and (c), the non-orthogonal data are reduced by 10 and 20 times, respectively. The solid circle data are taken from Avaldi *et al.*[10]

By comparing the orthogonal results in Figs. 2(a) and 2(b) with those in Figs. 1(a) and 1(b) respectively, one can see that when the distorted wave and Coulomb wave are used, they are in better agreement with experimental results for smaller ejected electron energy. This is due to the fact that the exchange amplitude which is ignored in this work plays a more important role for less asymmetric geometry. However, the Coulomb potential and distortion effect become more crucial as ejected electron energy decreases. This is why the plane wave calculations for ejected electron energy of 10 eV in Fig. 2(c) deviate from experimental results much more than those for 40 eV in Fig. 1(c).

To examine the Coulomb potential and distortion effect directly, in Fig. 3 we present a comparison between different wave functions in orthogonal situation, where the theoretical results and experimental data are taken from Fig. 1. One can see that all the calculations obtained using different wave functions predict the same positions for both binary and recoil peaks. While the observed recoil peak position can be well predicted by all the calculations, the reproduced binary peak shifts toward smaller angle. The comparison between the TDCSs obtained from distorted wave and those obtained from the Coulomb wave reveals the distortion effect of the short range potential while the comparison between the results by using the Coulomb wave and those by using the plane wave reflects the effect of Coulomb potential. It can be seen from Fig. 3 that the binary peak is dramatically overestimated by both the Coulomb wave and plane wave calculations, which indicates that the distortion effect is essentially important. The better agreement in magnitude of the recoil peaks reproduced by the Coulomb wave and plane wave calculations with the experimental one could be misleading. It does not imply that a plane wave or a Coulomb wave should be used instead of distorted wave. As a matter of fact, for the simultaneous ionization–excitation processes, it has already been well established that the second Born term may dominate the first Born amplitude. By taking into account the second Born term, the agreement of the distorted wave results with the experimental TDCS will be improved.[13]

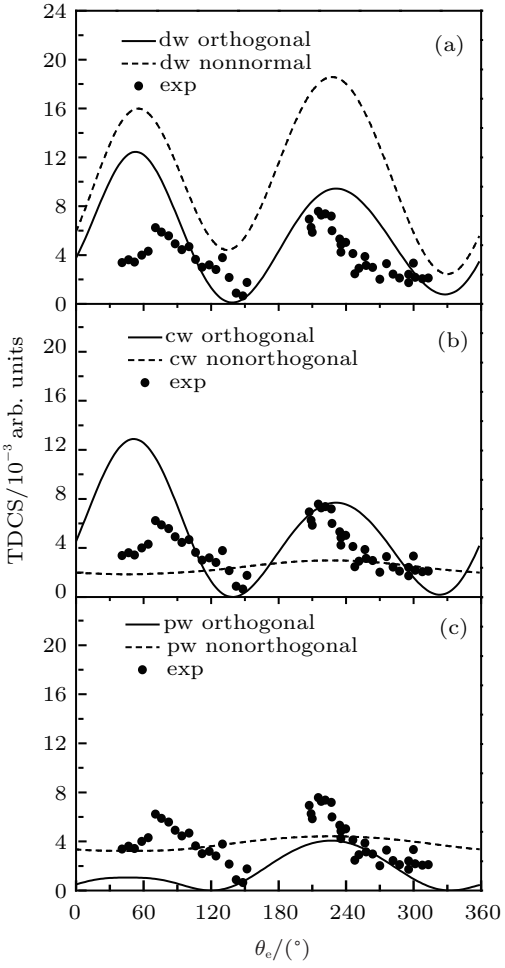


Fig. 2. TDCSs for electron-impact simultaneous ionization and excitation of helium TDCS at incident energy of 645.4 eV in coplanar asymmetric geometry using (a) distorted wave, (b) Coulomb wave, and (c) plane wave. In panels (b) and (c), the non-orthogonal data were reduced by 100 times. The solid circle data are taken from Avaldi *et al.*[10]

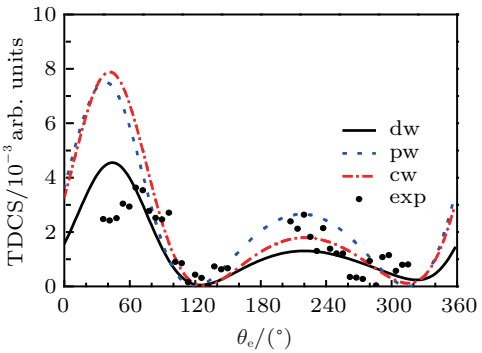


Fig. 3. (color online) Orthogonalized TDCSs for simultaneous ionization excitation of helium in coplanar asymmetric geometry (the same as in Fig. 1).

4. Conclusions

To summarize, the first-order Born approximation for calculating the TDCSs of simultaneous ionization and excitation of helium by electron impact has been presented and the results compared with the experimental measurements in coplanar asymmetric geometry. The influences of orthogonality of ejected and bound electron wave functions are investigated. It is demonstrated that the orthogonality effect is crucial so that the Schmidt orthogonalization procedure should be used to make the wave function of the ejected electron orthogonal to that of the bound electron before ionization. By comparing the theoretical results of the distorted wave, the Coulomb wave, and the plane wave with experimental data, we find that the distorted wave is the optimal choice.

References

[1] Weigold E, Hood S T and P J O 1973 *Phys. Rev. Lett.* **30** 475
[2] Madison D H and Al-Hagan O 2010 *J. At. Mol. Opt. Phys.* **2010** 367180
[3] Andersen N and Bartschat K 2001 *Polarization, Alignment, Orientation in Atomic Collisions* (New York: Springer)
[4] Brauner M, Briggs J S and Klar H 1989 *J. Phys. B: At. Mol. Opt. Phys.* **22** 2265
[5] Bray I and Stelbovics A T 1992 *Phys. Rev. A* **46** 6995
[6] Zhang S M, Chen Z J and Xu K Z 1999 *Acta Phys. Sin.* **48** 453 (in Chinese)
[7] Sun S Y, Jia X F, Miao X Y, Zhang J F, Xie Y, Li X W and Shi W Q 2009 *Chin. Phys. B* **18** 2744
[8] Wang Y, Zhou Y J and Jiao L G 2012 *Chin. Phys. B* **21** 083401
[9] Dupré C, Lahmam-Bennani A, Duguet A, Mota-Furtado F, O'Mahony P F and Cappello C Dal 1992 *J. Phys. B: At. Mol. Opt. Phys.* **25** 259
[10] Avaldi L, Camilloniy R, Multariy R, Stefani G, Langlois J, Robaux O, Tweed R J and Nguyen Vien G 1998 *J. Phys. B: At. Mol. Opt. Phys.* **31** 2981
[11] Dogan M and Crowe A 2000 *J. Phys. B: At. Mol. Opt. Phys.* **33** L461
[12] Rouvellou B, Rioual S, Pochat A, Tweed R J, Langlois J, Nguyen Vien G and Robaux O 2000 *J. Phys. B: At. Mol. Opt. Phys.* **33** L599
[13] Chen Z J and Madison D H 2005 *J. Phys. B: At. Mol. Opt. Phys.* **38** 4195
[14] Pindzola M S and Robicheaux F 1996 *Phys. Rev. A* **54** 2142
[15] Bartschat K, Hudsonz E T, Tweed R J, Langlois J, Nguyen Vien G and Robaux O 1996 *J. Phys. B: At. Mol. Opt. Phys.* **29** 115
[16] Zatsarinny O and Bartschat K 2011 *Phys. Rev. Lett.* **107** 023203
[17] Li J, Xu S C, Wang L, Liu M and Li H B 2007 *Journal of Tonghua Teachers College* **28** 25 (in Chinese)
[18] Silverman J N, Platas O and Matsen F A 1960 *J. Chem. Phys.* **32** 1402
[19] Chen Z J, Madison D H, Whelan Colm T and Walters H R J 2004 *J. Phys. B: At. Mol. Opt. Phys.* **37** 981