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Structures in Fully Differential Cross Sections for the Single Ionization of He by 2 MeV/amu C^{6+} Ion

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Abstract: The modified coulomb born (MCB) model is applied to study the single ionization of helium by 2 MeV/amu C^{6+} ion. The fully differential cross sections are presented for a variety of momentum transfers and ejected-electron energies in the scattering plane. The MCB results are compared with the experimental data and other theoretical predictions. We find that the MCB results are similar to the 3CW (three-body coulomb wave) results and they are superior to the 3DW-EIS (three-body distorted wave-eikonal initial state) results. It turns out that the treatment of the passive electron is very important for the results and distorting effects are not obvious.

Key words: fully differential cross section; modified coulomb born model; distorting effect

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1 Introduction

The problem of atoms by charged particle impact has been of interest for several decades. But even single ionization processes are not completely understood. From one viewpoint, the most challenging type of cross section is the fully differential cross sections (FDCS) in which the momentum and angular location of all three final-state particles are determined, because it is very difficult to measure the scattered projectile momentum directly. Combining high-resolution COLTRIMS (cold-target recoil-ion momentum spectroscopy), the first measurements of the FDCS were reported by Schulz *et al.*[1], for single ionization of helium by 100 MeV/amu C^{6+} ion. In the scattering plane for small momentum transfers, the shape of the experimental data is in good agreement with theory, as would be expected for a high-energy collision. However, some significant discrepancies are found for large momentum transfer. Furthermore, the experimental data out of the scattering plane exhibited structure that was not well reproduced by theory. For 2 MeV/amu C^{6+}, theory exhibited differences comparing with experimental data even in the scattering plane. Fischer *et al.*[2] reported absolute experimental measurements for 2 MeV/amu C^{6+} single ionization of helium in the scattering plane for various momentum transfers and ejected-electron energies. Although spectacular progress in the theoretical description, So far all the published theoretical investigations, including First Born approximation (FBA), continuum distorted wave-eikonal initialstate (CDW-EIS), three-body distorted wave-eikonal initial state (3DW-EIS)[3], Coupled-pseudo state (CP)[4], three-body coulomb wave(3CW)[5] have some discrepancies between experiment and theory. For larger ejected-electron energies the shape of the experimental data was in poor agreement with theory and for smaller q all theories fail to give the correct magnitude of the experiment around the ejected electron angle $\theta_e = 0°$.

In our previous work, the 3CW model has been applied to the FDCS for 2 MeV/amu C^{6+} single ionization of helium. However compared with previous work, the modified coulomb born (MCB) model, which has been previously laid out in detail in Ref. [6], will be employed to explore distorting effects in the FDCS. In

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this model, the incident plane wave is distorted by the asymptotic forms of Coulomb wave function describing the projectile-target ion and projectile-electron interaction approximately in the initial state. The final state is approximated as a product of the He^+ ground-state wave function for the passive electron and the three-Coulomb wave. More specifically, the present MCB model establishes a proper connection between the entrance channel Coulomb asymptotic state and the pertinent perturbation potential which causes the transition in the "prior" form of the T-matrix (details are contained in the next section). The purpose of this paper is to see if the discrepancy between experiment and theory is the result of the different treatments of the passive electron and distorting effects. Atomic units are used throughout the paper unless otherwise stated.

2 Theoretical model

Let us consider the following reaction produced by the impact of a bare ion of nuclear charge Z_{P} on a He atom of nuclear charge Z_{T}

$$Z_{\mathrm{P}}+(Z_{\mathrm{T}},2\mathrm{e}^-)\rightarrow Z_{\mathrm{P}}+(Z_{\mathrm{T}},\mathrm{e}^-)+\mathrm{e}^- \ , \tag{1}$$

where one of the electrons is ionized and the other one remains bound to the target nucleus. The orthogonal Jacobi coordinate system $\{\boldsymbol{x}_2,\ \boldsymbol{X}_1,\ \boldsymbol{r}\}$is chosen for the four particles in this work that is include the projectile mass (M_{P}) , the target core mass (M_{T}), and m the corresponding electron mass (which is equal to unity). Here, $\boldsymbol{x}_2$ is the position of the second electron relative to the target nucleus, $\boldsymbol{X}_1$ represents the relative position of the first electron relative to the center of mass of the nucleus-second electron subsystem, and $\boldsymbol{r}$ is the relative position of the projectile to the atomic center of mass. When the target nucleus is considered as infinitively massive compared to the electrons, the Jacobi coordinates $\boldsymbol{X}_1$ and $\boldsymbol{r}$ are approximately equal to $\boldsymbol{x}_1$ and $\boldsymbol{R}$. Here $\boldsymbol{s}_i=\boldsymbol{x}_i-\boldsymbol{R}$ with $i=1,\ 2$ are the electron-projectile relative positions and $\boldsymbol{x}_{12}=\boldsymbol{x}_1-\boldsymbol{x}_2$ is the interelectronic position vector. The total Hamiltonian for this system can be written as

$$H=H_i+V_i=H_f+V_f \ . \tag{2}$$

Where $H_{i,f}$ represent the Hamiltonian in the entrance and exit channels, respectively, and $V_{i,f}$ are the corresponding perturbation potentials, respectively. In the initial channel, one may write

$$H_i=-\frac{1}{2\mu}\nabla^2_R-\frac{1}{2b}\nabla^2_{x_1}-\frac{1}{2b}\nabla^2_{x_2}-\frac{Z_{\mathrm{T}}}{x_1}-\frac{Z_{\mathrm{T}}}{x_2}+\frac{1}{x_{12}} \ , \tag{3}$$

$$V_i=-\frac{Z_{\mathrm{P}}}{s_1}-\frac{Z_{\mathrm{P}}}{s_2}+\frac{Z_{\mathrm{P}}Z_{\mathrm{T}}}{R} \ , \tag{4}$$

In the exit channel, H_f and V_f can be written as

$$H_f=-\frac{1}{2\mu}\nabla^2_R-\frac{1}{2b}\nabla^2_{x_1}-\frac{1}{2b}\nabla^2_{x_2}-\frac{Z_{\mathrm{T}}}{x_2} \ , \tag{5}$$

$$V_f=-\frac{Z_{\mathrm{P}}}{s_1}-\frac{Z_{\mathrm{P}}}{s_2}-\frac{Z_{\mathrm{T}}}{x_1}+\frac{1}{x_{12}}+\frac{Z_{\mathrm{P}}Z_{\mathrm{T}}}{R} \ . \tag{6}$$

The quantity $b=(M_{\mathrm{T}}+1)/(M_{\mathrm{T}}+2)\approx 1$ is the reduced mass of each electron relative to the atomic core. The reduced mass between the projectile and the target core is

$$\mu=\frac{M_{\mathrm{P}}(M_{\mathrm{T}}+2)}{M_{\mathrm{P}}+M_{\mathrm{T}}+2}\approx\frac{M_{\mathrm{P}}M_{\mathrm{T}}}{M_{\mathrm{P}}+M_{\mathrm{T}}} \ .$$

The prior form of the exact transition T-matrix in the distorted wave formalism is given by

$$\begin{aligned}T^-_{fi}=&\langle\Psi^-_f|V'_i|\chi^+_i\rangle=\langle\Psi^-_f|V_i|\chi^+_i\rangle-\langle\Psi^-_f|V_id|\chi^+_i\rangle\\ \equiv&T^-_{vi}+T^-_{vd} \ .\end{aligned} \tag{7}$$

$$V'_i=V_i-V_{id} \ , \tag{8}$$

V_{id} ought to be connected with χ^+_i, but otherwise is temporarily considered as being an arbitrary distorting potential operator, and T^-_{vi} and T^-_{id} stem from the perturbation potential V_i and the distorting potential V_{id} respectively. ψ^-_f is the exact final-state four-body wavefunction. The initial distorted wave χ^+_i, is defined by

$$(H_i+V_{id}-E)\chi^+_i=0 \ . \tag{9}$$

Here, E is the total energy of the whole system. Much better approximations can be made for χ^+_i, such as eikonal-initial-state approximation (EIS) introduced by Belkić[6]. He showed that in order to preserve a proper asymptotic behavior in the asymptotic scattering region, the asymptotic forms of Coulomb wave must be used

$$\chi^+_i=\phi_i\exp[-\mathrm{i}\alpha_0\ln(vs_1+\boldsymbol{v}\cdot\boldsymbol{s}_1)+\mathrm{i}\alpha'_0\ln(vR-\boldsymbol{v}\cdot\boldsymbol{R})] \tag{10}$$

where $\alpha_0=Z_{\mathrm{P}}/v$, $\alpha'_0=Z_{\mathrm{P}}Z'_{\mathrm{T}}/v$, and $Z'_{\mathrm{T}}=Z_{\mathrm{T}}-1$. The initial wave vector labeled by $\boldsymbol{k}_i$ is defined via $\boldsymbol{k}_i=\mu\boldsymbol{\nu}$, where $\boldsymbol{\nu}$ is the velocity of the incident projectile with respect to the target. This state thus includes the projectile-target ion and projectile-electron interaction approximately in the initial channel.

The Schrödinger equation defining in the entrance channel is given by $(H_i-E)\phi_i=0$. The unperturbed state ϕ_i reads as

$$\phi_i=(2\pi)^{-3/2}\exp(\mathrm{i}\boldsymbol{k}_i\cdot\boldsymbol{r})\phi(x_1,\ x_2) \ . \tag{11}$$

Further, $\phi(x_1,\ x_2)$ is the initial wave function of the helium target introduced by $(H_i-\varepsilon)\phi(x_1,\ x_2)=0$, where ε is the corresponding binding energy of the helium obeying law $E=\varepsilon+k_i/2\mu$. For the initial state of He, we have chosen the analytical fit to the Hartree-Fock wave function given by Byron and Joachain[7]

$$\phi(x_1,\ x_2)=U(x_1)U(x_2)\ , \tag{12}$$

where $U(x) = (4\pi)^{-1/2}(2.60505\mathrm{e}^{-1.41x} + 2.08144 \times \mathrm{e}^{-2.61x})$. With the help of Eqs. (2) and (8), we can rewrite Eq. (9) in the equivalent form

$$(H-E)|\chi_i^+\rangle = V_i'|\chi_i^+\rangle\ . \tag{13}$$

Inserting Eqs. (8), (9) and (10) into Eq. (13) and resorting to the usual mass limit $\mu \gg 1$, one readily identifies the additional distorting potential V_{id} as

$$V_{id}=\frac{\alpha_0' v}{R}-\frac{\alpha_0 v}{s_1}-\frac{\alpha_0 Z_\mathrm{P}}{s_1}\frac{1}{vs_1+\boldsymbol{v}\cdot\boldsymbol{s}_1}-\frac{i\alpha_0}{s_1}\frac{1}{vs_1+\boldsymbol{v}\cdot\boldsymbol{s}_1}\nabla_{x_1}(\ln\phi)\cdot[v\boldsymbol{s}_1+s_1\boldsymbol{v}] \tag{14}$$

so that the prior form of the distorted wave T-matrix (7) can be expressed as the nine-dimensional overlap integral between Ψ_f^- and $V_i'\chi_i^+$ in the configuration space of variables $\{R,\ x_1,\ x_2\}$.

The wavefunction Ψ_f^- should be an exact solution of the four body problem in the final channel, so we are constrained to find an appropriate approximation for Ψ_f^-. Let $H_\mathrm{core}=-1/(2b)\nabla^2_{x_2}-Z_\mathrm{T}/x_2$ be Hamiltonian of He^+ in the final channel and $\phi_f(x_2)$ an eigenfunction of H_core, *i.e.* $H_\mathrm{core}\phi_f(x_2)=\varepsilon\phi_f(x_2)$. Then an approximate Hamiltonian for the system in the final channel can be written as

$$H\approx H_\mathrm{core}+(-\frac{1}{2\mu}\nabla^2_R-\frac{1}{2b}\nabla^2_{x_1}-\frac{Z_\infty}{x_1}+\frac{Z_\infty Z_\mathrm{P}}{R}-\frac{Z_\mathrm{P}}{s_1})\ , \tag{15}$$

with the asymptotic charge $Z_\infty=1$. For the eigenfunction of H we assume the form

$$\Psi_f^-(\boldsymbol{x}_1,\boldsymbol{x}_2,\boldsymbol{R})=\phi_f(x_2)\Psi_{3c}^-(\boldsymbol{x}_1,\boldsymbol{R})\ , \tag{16}$$

where Ψ_{3c}^- is the solution of the three-body Schrodinger equation

$$\Big(-\frac{1}{2\mu}\nabla^2_R-\frac{1}{2b}\nabla^2_{x_1}-\frac{Z_\infty}{x_1}+\frac{Z_\infty Z_\mathrm{P}}{R}-\frac{Z_\mathrm{P}}{s_1}\Big)\times \Psi_{3c}^-(\boldsymbol{x}_1,\boldsymbol{R})=E\Psi_{3c}^-(\boldsymbol{x}_1,\boldsymbol{R}) \tag{17}$$

with the energy $E=p^2/(2b)+k_f^2/(2\mu)$. An approximate expression for the wave function reads[8–9]

$$\Psi_{3c}^-(\boldsymbol{x}_1,\boldsymbol{R})\approx(2\pi)^{-3}\mathrm{e}^{\mathrm{i}(\boldsymbol{k}_f\cdot\boldsymbol{R}+\boldsymbol{p}\cdot\boldsymbol{x}_1)}\chi_f(\alpha_\mathrm{PT},\ k_f,\ R)\times \chi_\mathrm{e}(\alpha_\mathrm{Te},\ p,\ x_1)\chi(\alpha_\mathrm{Pe},\ K,\ s_1)\ . \tag{18}$$

The projectile's final momentum is $\boldsymbol{k}_f$ and the ejected-electron's momentum is given by $\boldsymbol{p}$. The momentum $\boldsymbol{K}$ of the ejected-electron with respect to the projectile is defined in (18) as $\boldsymbol{K}=\boldsymbol{p}-b\boldsymbol{k}_f/\mu$. χ_f and χ_e are distorted wave for the scattered projectile and ejected electron respectively. $\chi(\alpha_\mathrm{Pe},\ K,\ s_1)$ is the Coulomb interaction which is often referred to as post-collision interaction (PCI). The Coulomb distorted factor is given by

$$\chi(\alpha,k,r)=\mathrm{e}^{(-\pi\alpha/2)}\Gamma(1-\mathrm{i}\alpha)\,{}_1F_1\left[\mathrm{i}\alpha,1,-\mathrm{i}(kr+\boldsymbol{k}\cdot\boldsymbol{r})\right]\ . \tag{19}$$

The symbols Γ and ${}_1F_1$ represent the gamma function and the confluent hypergeometric function, respectively. The Sommerfeld parameters have the form

$$\alpha_\mathrm{PT}=\frac{\mu Z_\mathrm{P}Z_\infty}{k_f},\ \alpha_\mathrm{Pe}=-\frac{Z_\mathrm{P}}{K},\ \alpha_\mathrm{Te}=-\frac{Z_\infty}{p}\ . \tag{20}$$

The wave function Ψ_{3c}^- represents interactions between twobody subsystems since the distortion effects of each twobody Coulomb potential have been treated exactly. An uncertain point of this model represents the use of the asymptotic charge $Z_\infty=1$. It is showed that the wave function (18) is asymptotically correct in all asymptotic domains of coordinate space, as detailed in Refs. [10-12]. This means that the above wave function is the leading term of the exact scattering wave function if any two particles are far apart. This completes the derivation necessary for the formulation of the present model called hereafter the MCB approximation[6]. Of course it represents a four-body model.

Due to the steady increase in computational power, it is possible now to treat all the interactions between particles pairs in a single collision process on an equal footing. In this model, the interaction between the projectile and the residual-target-ion (PI interaction) is taken into account by a Coulomb wavefunction for the final state and an eikonal phase for the initial one.

The FDCS for the process (1) may be written as

$$\frac{\mathrm{d}^3\sigma}{\mathrm{d}\Omega_\mathrm{p}\mathrm{d}\Omega_\mathrm{e}\mathrm{d}E_\mathrm{e}}=N_\mathrm{e}(2\pi)^4\mu^2p\frac{k_f}{k_i}|T_{fi}^-|^2\ . \tag{21}$$

Where N_e is the number of electrons in the atomic shell and E_e is the ejected electron's energy. The solid angles $\mathrm{d}\Omega_\mathrm{p}$ and $\mathrm{d}\Omega_\mathrm{e}$ represent the direction of scattering of the projectile and the ejected electron, respectively.

3　Results and discussion

In order to check the accuracy of the MCB model, we have computed the FDCS for C^{6+} impact ionization of helium at incident energy of 2 MeV/amu in the coplanar geometry, which corresponds to the measurements of Fischer *et al*[2]. Our results are compared with the absolute experiment[2] and 3DW-EIS theoretical data of Foster *et al*[3]. and 3CW theoretical data of Lixia *et al.*[5]

From the Figs. 1∼3 with the ejected electrons being emitted into the scattering plane with energies of 1 eV (Fig. 1), 4 eV (Fig. 2), or 10 eV (Fig. 3) and momentum transfers of 0.45, 0.65, 1.0, and 1.5 a.u.. We find that in the case of all momentum transfers, the MCB results are in good agreement with experimental data in the shape and magnitude in the recoil region. The 3DW-EIS results are found to give smaller results of the recoil peak in all the case studied and are inferior to the MCB results. The 3DW-EIS results show some superiority over the MCB results in the binary peak position at small momentum transfer. The magnitudes of binary peak of the MCB results in the case of $E_e = 1.0$ eV and $E_e = 4.0$ eV are in better agreement with the absolute experiment measurements than the 3DW-EIS results. In the case of the ejected electron energy are 10.0 eV, the MCB results overestimate the binary peak of the experiment. The results are surprisingly larger than the measured data by a factor of about 1.5, except for small momentum transfer 0.45 a.u., whereas 3DW-EIS results are in better agreement with experiment than the MCB results, especially for

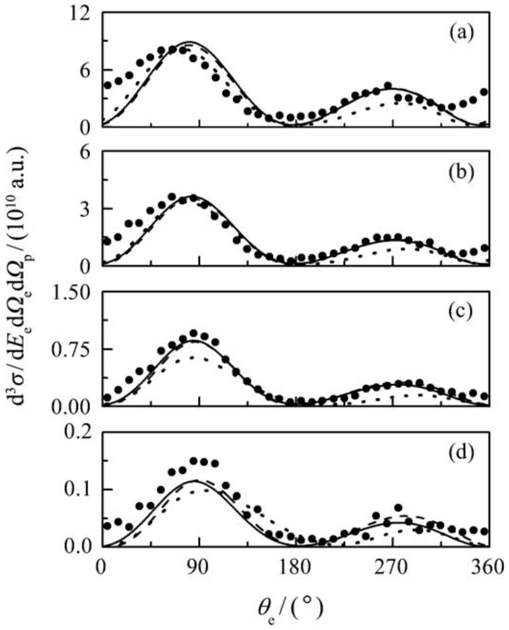

Fig. 1　FDCS in the scattering plane for 2 MeV/amu C^{6+} single ionization of helium. the ejected electron energy is 1.0 eV and the momentum transfers are (a) 0.45, (b) 0.65, (c) 1.0, and (d) 1.5 a.u., respectively. The angle θ_e is the emission angle of the electron. The solid circles represent the experiment measurement[4]. The MCB (solid), 3DW-EIS[5] (dot) 3CW[6] (dash), results are also shown.

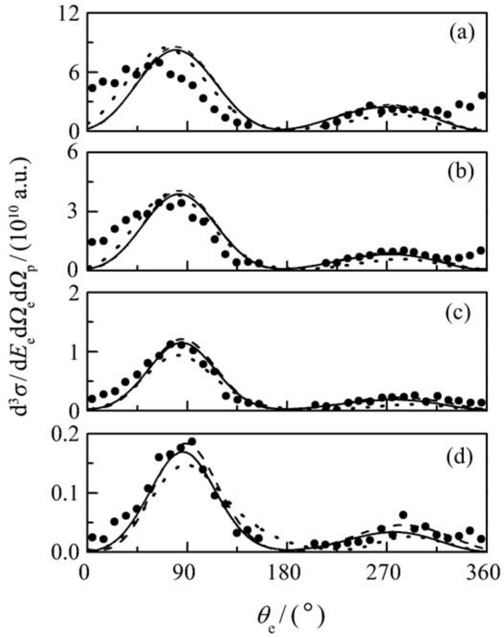

Fig. 2　Same as Fig. 1 except that the ejected electron energy is 4.0 eV.

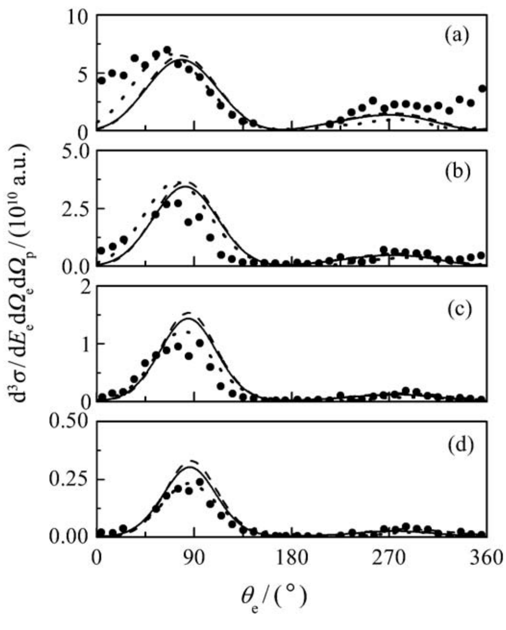

Fig. 3　Same as Fig. 1 except that the ejected electron energy is 10.0 eV.

the momentum transfer of 1.5 a.u..

Both the 3DW-EIS method and the MCB method contain the distorting effects, but they are different in the way they deal with the passive electron. In the MCB method the standard approximation used for the single ionization of helium target is to model the four body problem, while in the 3DW-EIS method the model is an effective three body problem. In detail, for the initial state of He, the MCB calculation has chosen the analytical fit to the hertree-Fock wave function like $\phi(x_1, x_2) = U(x_1)U(x_2)$, whereas the 3DW-EIS calculation chosen wave function like $\phi(x_1, x_2) = U(x_1)$ which the role of the passive electron is to partially screen the nucleus of the ion. In the present calculations the perturbation contains all the interaction between the projectile and target atom (*i.e.* the sum of the projectile -target nucleus, projectile -ejected electron and projectile-passive electron interactions). However, the 3DW-EIS model does not consider the projectile-passive electron interaction. The last difference is that the present model treats the final state as a four-body model which contains the wave function for the passive electron and the three-coulomb wave, whereas the 3DW-EIS model uses a three-body final-state wave function much like that in Eq. (18). This demonstrates that the role of the passive electron is important in the recoil peak and may be overestimated in our calculation in the binary peak.

In order to explore the influence of distorting effects, we compare the MCB model and the 3CW model. We also find out contributions of the distorting potential and the perturbation potential in the MCB model. The important distinction between the MCB model and the 3CW model is that the previous 3CW model calculates only first term of Eq. (7), whereas we count both terms. The other disparity is that the initial wave function in the MCB calculation is a distorted wave, but in the 3CW calculation the initial wave function is much like Eq. (11).

From Fig. 4 we notice that the MCB results for the FDCS are only marginally different from that of

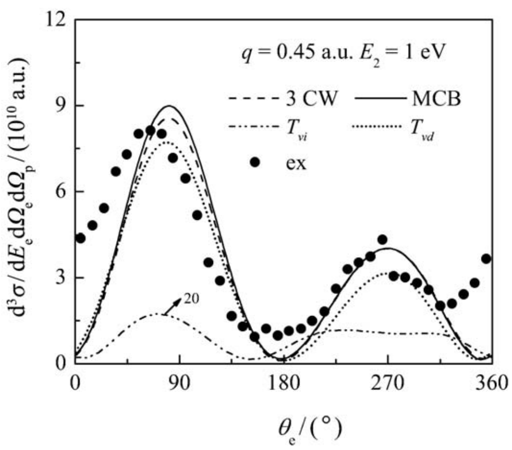

Fig. 4　FCDS in the scattering plane for 2 MeV/amu C^{6+} single ionization of helium. the ejected electron energy is 1.0 eV and the momentum transfer is 0.45 a.u. The angle θ_e is the emission angle of the electron. The solid circles represent the experiment measurement. The MCB (solid), 3CW (dash), T^-_{id} multiplied by 20 (dash dot), T^-_{vi} (dot) results are also shown.

the 3CW results. Thus the distorting effects have not eliminated or decreased the difference between the experiment and the theory. T^-_{vi} shows the main features of the experimental data. Comparing (only the initial wave function is distorted wave) with the 3CW results, the magnitude of T^-_{vi} is smaller than that of the 3CW results. When the distorting potential is switched on, the interference effect of the perturbation potential and the distorting potential makes the magnitudes larger than the peak due to the perturbation potential. But the distorting potential effect is very small, comparing with the perturbation potential effect. It demonstrates that the distorted wave in initial state wave makes the magnitude of FDCS small and the distorting potential makes FDCS large.

All theories fail to give the correct magnitudes of the experiment around the ejected electron angle $\theta_e = 0°$ especially for smaller q. Based on the results of Wang[13], this difference may be explained that the C^{6+} beam is incoherent or partial coherence. They pointed out that the projectile coherence can also significantly affect FDCS for atomic targets. In our calculation, the projectile is treated as completely coherent. It is currently not clear whether the projectile beam is completely coherent in the experiment. The projectile beam is only coherent if the transverse coherence length is larger than the separation in the impact parameter. We can see a correlation between the scattering angle and the impact parameter, namely, the larger the scattering angle, the smaller the impact parameter. Generally, a relatively large scattering angle corresponds to large q. It is evident that the impact parameter becomes smaller as q increases. So we find that as q increases, both calculations get better agreement with the experimental data.

4　Conclusions

We have carried out the MCB calculation of FDCS for single ionization of helium by 2 MeV/amu C^{6+} impact. Comparing the 3CW theory with the MCB theory, the distorting effects are not obvious and do not improve the agreement between the present results and the experiment. The other primary objective of the present paper was to determine the role of the passive electron in the collision process. The important outcome of this work lies in the fact that the FDCS result are extremely sensitive to how this interaction is treated and that the passive electron seems to play an important role, especially in recoil peak. We find that there is a qualitative agreement between our calculations and the measurements. However, the agreement between experiment and theory is still not as good as expected. The projectile beam is not complete coherent may be the reason of the discrepancies between experiment and theory. These improvements, however, within the physical picture provided by the MCB model, might be insufficient to provide substantial changes in the description of ionization events, at the FDCS level. A more definitive interpretation of projectile-residual-target-ion interaction needs to be further studied.

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2 MeV/amu裸碳离子碰撞氦离子单电离的全微分截面的结构

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摘要： 用修饰的库仑波(MCB)模型计算入射能量2 MeV/amu裸碳离子碰撞氦单电离的全微分截面,并将计算结果与相应的实验数据和其他理论结果进行比较，发现MCB理论在较小的电离电子能量和较大的动量转移条件下与实验结果符合得很好，在动量转移比较小时MCB理论结果binary峰的位置向大角方向发生了偏移。MCB理论和3CW(三体库仑波)理论相似，他们都比3DW-EIS(三体扭曲波程函初态近似)理论符合的好，说明了在微扰势中被动离子与入射粒子的相互作用是不可忽略的。与3CW理论相比，MCB模型在初态波函数和相互作用势中加入扭曲效应，比较发现扭曲效应会影响全微分截面的大小，但影响不是很明显。

关键词： 全微分截面；修正的库仑波模型；扭曲效应

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