Classical ionization and charge-transfer cross sections for $H^+ + He$ and $H^+ + Li^+$ collisions with consideration of model interactions

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The three-body system is analyzed in relation to the calculation of atomic scattering cross sections. A method is presented to generate the initial electronic conditions for the classical-trajectory Monte Carlo method in the case where the active electron is subject to non-Coulomb interactions. The method is then applied to study the collisions of H^+ with He and Li^+ targets in the intermediate- to high-energy range. Single-electron capture and single-ionization total cross sections are presented for both collision systems. In the case of He targets, total cross sections for double ionization and singly differential cross sections for free-electron production are also calculated. Cross sections and initial electronic distributions are obtained with both Coulomb and model interactions and compared. Good agreement is found between theoretical and experimental results, except for the double ionization of He.

I. INTRODUCTION

The classical-trajectory Monte Carlo method (CTMC) proposed by Abrines and Percival[1,2] has been largely employed in the intermediate to high projectile velocity range to treat electron-capture and ionization processes in ion-atom collisions. The method is based on the numerical integration of a three-body system subject to Coulomb interactions. For completely stripped ions colliding with hydrogenlike targets, all the interactions are exactly taken into account. For such systems the method has been successful in predicting either total cross sections[2-4] or differential cross sections.[5,6] The calculation of differential cross sections demands a greater numerical effort than that required by total cross sections due to the large number of trajectories necessary to obtain reasonable statistical errors. This is probably the reason why very few calculations have appeared in the literature concerning CTMC differential cross sections. To our knowledge, the most exhaustive work is that of Olson[5] where the $H^+ + H$ system has been studied in detail.

More than one-electron systems have generally been studied by solving a three-body system with one active electron and assuming the independent-electron model.[7,8] For the case of helium targets Pfeifer *et al.*[9] have solved a full four-body problem by means of a Heisenberg core which guarantees the stability of classical two-electron atoms.[10] So far, when considering the independent-electron model, the effect of the other electrons has generally been taken into account by means of Coulomb potentials with appropriate effective charges.[11-13] However, these potentials do not have the correct behavior at small and large distances.

Using the CTMC method, McDowell and Janev[14] have computed single-capture, single ionization, and transfer ionization total cross sections in fast $Au^{q+} + He$ collisions. They have considered a variable-charge potential to describe the interaction between the active electron and the projectile. McDowell and co-workers[15] have also employed general central interactions to study $He^+ + He$ and $He^+ + H$ collisions in the intermediate-energy range.

The main difficulty, when considering general interactions, does not rest with the integration of Hamilton equations, but with the generation of initial electronic conditions. The initial position and momentum coordinates of the electron must be obtained from a set of uniformly distributed variables characterizing a microcanonical distribution. In Sec. II the method we have developed to find these variables for the case of general central interactions is described. For Coulomb interactions the method is equivalent to Abrines and Percival's method, but its numerical advantage is that the Kepler orbit of the electron need not be solved.

This method has been applied to study electron-capture and ionization reactions in $H^+ + He$ and $H^+ + Li^+$ collisions. In order to test the sensitivity of the different cross sections to the potentials representing the interactions between the components of the collision system, the cases of Coulomb effective potentials and model potentials have been considered.

For helium targets we have computed total cross sections for single-ionization, free-electron production, single-capture, and double-ionization processes. We have also obtained singly differential cross sections (SDCS) in the energy and the angle of the ejected electrons. These are, to our knowledge, the first SDCS calculations for more than one-electron systems performed with CTMC methods.

For Li^+ targets we present total cross sections for Li^{2+} production, single capture, and single ionization.

Atomic units are used throughout except where otherwise stated.

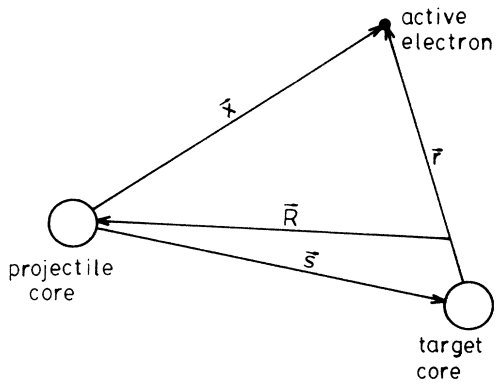

FIG. 1. Collision system.

II. THEORY

A. Dynamics

We consider the three-particle classical collision system of Fig. 1 composed by two frozen cores (projectile and target cores) of masses M_p and M_t and one active electron initially bound to the target core. The Hamiltonian of the system reads

$$H=\frac{p^2}{2\mu}+\frac{P^2}{2M}+V(r)+U(x)+W(s)\ , \tag{1}$$

where $\mu=M_t/(1+M_t)$ and $M=M_p(M_t+1)/(1+M_t+M_p)$. $U(x)$, $V(r)$, and $W(s)$ are, respectively, the electron-projectile, electron—target-core, and core-core interaction potentials. If we note by $\mathbf{R}$ the coordinate relating the projectile to the electron—target-core center of mass, then $\mathbf{p}$ and $\mathbf{P}$ are, respectively, the momenta associated with the coordinates $\mathbf{r}$ and $\mathbf{R}$. We need not consider the kinetic energy of the center of mass of the entire system because it is a constant of motion. For a given set of initial conditions, the dynamics of the system is determined by the classical Hamilton equations:

$$\begin{aligned}&\dot{r}_i=p_i/\mu,\ \ \dot{p}_i=-\frac{\partial H}{\partial r_i},\ \ i=1,2,3\\&\dot{R}_i=P_i/M,\ \ \dot{P}_i=-\frac{\partial H}{\partial R_i},\ \ i=1,2,3\ .\end{aligned} \tag{2}$$

B. Initial conditions

At $t=0$, the initial condition for the projectile is specified by its distance R_0 to the target, its velocity $\mathbf{v}$, and the impact parameter b. Assuming a monoenergetic incident beam, the value of $\mathbf{v}$ is fixed. The initial distance R_0 is taken to be large enough so as to neglect the interaction with the target. The results must be independent of the particular choice of R_0. For the energies commonly considered in this method a practical criterion is to choose R_0 so that the projectile-electron interaction is much smaller than the target-electron interaction. The impact parameter must be chosen so as to reproduce a uniform flux of incident particles. If $b_{\max}$ is the impact parameter above which the ionization and capture processes are negligible, this condition is fulfilled by choosing b^2 uniformly in the interval $[0,b^2_{\max}]$.

As in the method of Abrines and Percival,[1] the initial electronic state is obtained from the microcanonical distribution,

$$f(\mathbf{r},\mathbf{p})=k\delta(E_i-p^2/2\mu-V(r))\ , \tag{3}$$

where k is a normalization constant and E_i is the ionization potential of the active electron. The electronic coordinate is confined to the intervals where the relation

$$p^2/2\mu=E_i-V(r)>0 \tag{4}$$

is verified. For the sake of simplicity we shall assume that the equation

$$E_i-V(r)=0 \tag{5}$$

has only one root. The values of r are then confined to the single interval $0<r<r_0$, r_0 being that root. Potentials satisfying this condition represent the electron-core interaction for a wide variety of physical cases. However, the method can be straightforwardly generalized to more general interactions.

In order to generate an initial condition for the active electron, we must perform a transformation from the variables $(\mathbf{r},\mathbf{p})$ to a set of uniformly distributed variables completely specifying the initial state of the system [given by (3)]. This transformation is a combination of two successive changes of coordinates, described as follows. First, we perform a transformation

$$(\mathbf{r},\mathbf{p})\rightarrow(E,r,\nu_r,\nu_p,\varphi_r,\varphi_p) \tag{6}$$

defined by the relations

$$\begin{aligned}&x=r(1-\nu_r^2)^{1/2}\cos\varphi_r\ ,\\&y=r(1-\nu_r^2)^{1/2}\sin\varphi_r\ ,\\&z=r\nu_r\ ,\\&p_x=\{2\mu[E-V(r)]\}^{1/2}(1-\nu_p^2)^{1/2}\cos\varphi_p\ ,\\&p_y=\{2\mu[E-V(r)]\}^{1/2}(1-\nu_p^2)^{1/2}\sin\varphi_p\ ,\\&p_z=\{2\mu[E-V(r)]\}^{1/2}\ .\end{aligned} \tag{7}$$

The new variables are confined to the intervals

$$\begin{aligned}&E\in(-\infty,0),\ \ r\in[0,r_0]\ ,\\&\nu_r,\nu_p\in[-1,1],\ \ \varphi_r,\varphi_p\in[0,2\pi]\ .\end{aligned} \tag{8}$$

The Jacobian of this transformation is

$$J_1=\mu r^2\{2\mu[E-V(r)]\}^{1/2}\ . \tag{9}$$

The initial distribution for the new variables is then

$$k\mu r^2\{2\mu[E_i-V(r)]\}^{1/2}\delta(E-E_i)\ . \tag{10}$$

Now, we perform a second transformation from the variable r to the variable w given by

$$w(r)=\int_0^r dr'\mu r'^2\{2\mu[E_i-V(r')]\}^{1/2}\ . \tag{11}$$

For $r<r_0$ w is always within the interval

$$0<w<w(r_0)\ . \tag{12}$$

The Jacobian of this transformation is

$$J_2 = dr/dw = \mu^{-1} r^{-2} \{2\mu[E_i - V(r)]\}^{-1/2} . \quad (13)$$

This leads to the required distribution,

$$f(E,w,\nu_r,\nu_p,\varphi_r,\varphi_p) = k\delta(E - E_i) , \quad (14)$$

which is, as desired, independent of the variables $(w,\nu_r,\nu_p,\varphi_r,\varphi_p)$. Now, an initial condition for the active electron can be easily generated. It suffices to select at random those variables in the intervals

$$w \in [0, w(r_0)], \quad \varphi_r \in [0,2\pi], \quad \varphi_p \in [0,2\pi] ,$$
$$\nu_r \in [-1,1], \quad \nu_p \in [-1,1] . \quad (15)$$

The corresponding initial conditions for $\mathbf{r}$ and $\mathbf{p}$ are then obtained from relations (7) and (11). For practical reasons the value of r corresponding to a particular choice of w may be interpolated from a table of r versus w numerically computed from (11) at the beginning of the calculations.

III. RESULTS

A computer program has been written to calculate classical electron-capture and ionization cross sections using the Monte Carlo method. The program allows the use of general potentials to describe the core-core and electron-core interactions. The initial electronic state is calculated following the method described in Sec. II. In order to test the program, initial runs have been made for the $H^+ + H(1s)$ system. The results obtained reproduce the ionization and charge-transfer total cross sections as well as the differential cross sections here considered for the electron ejection calculated by Olson.[5]

The program has been then employed to study the collisions of protons with helium and singly ionized lithium targets. Following the independent-electron model, the cross sections here studied have been obtained from the results of the one-electron reactions

$$H^+ + X(1s,1s) \rightarrow H^+ + X(1s) + e^- , \quad (16)$$

$$H^+ + X(1s,1s) \rightarrow H + X(1s) , \quad (17)$$

$$H^+ + X(1s,1s) \rightarrow H^+ + X(1s,*) , \quad (18)$$

where X stands either for He or Li^+ and $*$ means any bound state.

B. Interaction potentials

The potential $V(r)$ between the active electron and the frozen Li^{2+} or He^+ cores in Eq. (1) has been represented either by an effective Coulomb potential or by a model potential. These interactions read

$$V_{\text{eff}}(r) = -Z_{\text{eff}}/r , \quad (19)$$

$$V_{\text{mod}}(r) = \left\langle \psi_{SZ(1s^2)}(\mathbf{r}') \left| \frac{1}{|\mathbf{r}-\mathbf{r}'|} \right| \psi_{SZ(1s^2)}(\mathbf{r}') \right\rangle - Z_T/r$$
$$= -[Z_T - 1 + (1 + Z_{\text{eff}} r) e^{-2Z_{\text{eff}} r}]/r , \quad (20)$$

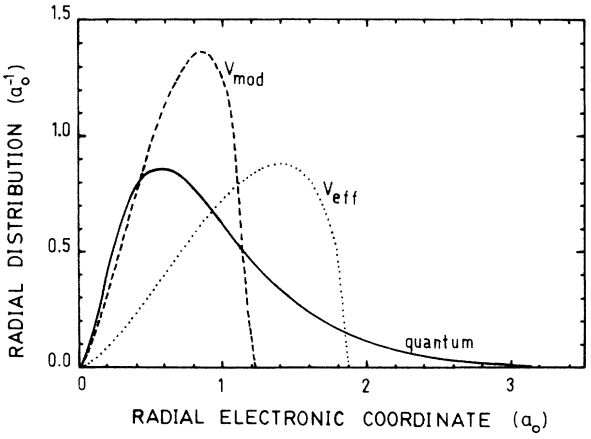

FIG. 2. Radial distributions for He. Theory: V_{mod} (— — —), V_{eff} (· · · ·), quantum (——) (Ref. 16).

where Z_T is the nuclear charge of the target, $Z_{\text{eff}} = Z_T - \frac{5}{16}$, and $\psi_{SZ(1s^2)}(r)$ is the corresponding single-zeta (SZ) function of the target. It must be noted that only V_{mod} has the correct behavior at large and small distances, i.e.,

$$V_{\text{mod}}(r) \rightarrow -(Z_T - 1)/r \quad \text{as } r \rightarrow \infty$$
$$V_{\text{mod}}(r) \rightarrow -Z_T/r \quad \text{as } r \rightarrow 0 . \quad (21)$$

Initial electronic position and momentum distributions are obtained from the microcanonical distribution [Eq. (3)] as

$$P(r) = 4\pi r^2 \int d\mathbf{p} f(\mathbf{r},\mathbf{p}) ,$$
$$P(p) = 4\pi p^2 \int d\mathbf{r} f(\mathbf{r},\mathbf{p}) \quad (22)$$

which depend on the interaction potential $V(r)$ through $f(\mathbf{r},\mathbf{p})$. Distributions resulting from the use of potentials (19) and (20) are compared in Figs. 2 and 3—for the He case—with the corresponding quantum distributions obtained from the multiple-zeta function of Clementi and Roetti.[16] The model-potential momentum distribution

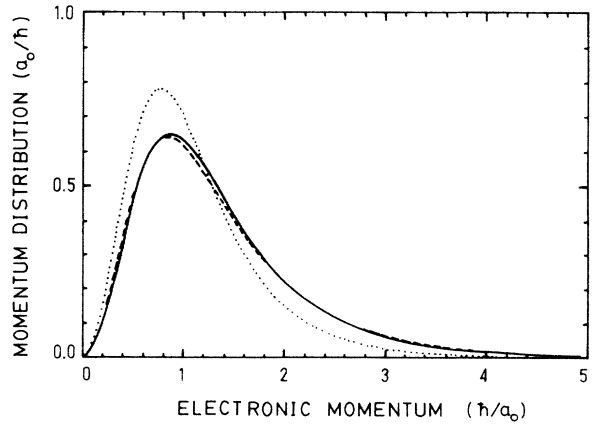

FIG. 3. Momentum distributions for He. Theory: V_{mod} (— — —), V_{eff} (· · · ·), quantum (——) (Ref. 16).

reproduces almost exactly the quantum-mechanical one. We recall that for hydrogenic systems quantum and classical momentum distributions are identical.[1] As pointed out by Percival and Richards,[17] this coincidence is essential for the success of the CTMC approximation. On the other hand, the momentum distribution obtained with V_{eff} does not coincide with the quantum-mechanical one. This is so, independently of the kind of wave function used. In fact, the single-zeta function and multiple-zeta function lead to very similar distributions. However, if the binding energy of the active electron is taken to be $E_i=-Z_{\text{eff}}^2/2$, the classical momentum distribution becomes identical to the single-zeta distribution. With this choice of E_i, the radial distribution obtained with V_{eff} is almost coincident with that obtained with V_{mod} and the correct ionization potential. However, the electron-capture and ionization cross sections that result in this case are too small due to the fact that the electron is excessively bound.

Concerning the position distribution, the model potential is better than the effective charge to predict the most probable value of the quantum distribution.

In the Appendix the classical mean value of the total energy of the helium atom is calculated. It is observed that only V_{mod} gives a correct value of this magnitude.

In view of the discussion above, it becomes clear that model interactions like V_{mod} provide a more realistic description of the atom than V_{eff}. Although only the analysis of the He case has been presented, similar conclusions are reached for Li^+ ions.

As the projectile (H^+) is a structureless particle of charge equal to one, the core-core interaction has been taken to be, in each case, as given by (19) and (20), but with opposite sign.

B. Total cross sections

The possible reaction channels for the systems studied here are

$$\begin{aligned}
&H^+ + X \rightarrow H^+ + X^+ + e^- \quad \text{(single ionization)}, \\
&H^+ + X \rightarrow H^+ + X^{2+} + 2e^- \quad \text{(double ionization)}, \\
&H^+ + X \rightarrow H + X^{2+} + e^- \quad \text{(transfer ionization)}, \\
&H^+ + X \rightarrow H + X^+ \quad \text{(single capture)}, \\
&H^+ + X \rightarrow H^- + X^{2+} \quad \text{(double capture)}, \\
&H^+ + X \rightarrow H^+ + X \quad \text{(elastic and excitation)}.
\end{aligned} \tag{23}$$

Suppose P_c, P_i, and P_e are, respectively, the electron-capture, ionization, and excitation probabilities of reactions (16), (17), and (18) for a given impact parameter and collision velocity. Following the independent-electron model the probabilities for reactions (23) are, respectively, given by

$$\begin{aligned}
P_{\text{si}} &= 2P_iP_e \ , \\
P_{\text{di}} &= P_iP_i \ , \\
P_{\text{ci}} &= 2P_cP_i \ , \\
P_{\text{sc}} &= 2P_cP_e \ , \\
P_{\text{dc}} &= P_cP_c \ , \\
P_{\text{ee}} &= P_eP_e \ .
\end{aligned} \tag{24}$$

Since $P_c+P_i+P_e=1$, relations (24) preserve unitarity. The probability for free-electron production is obtained by addition of P_{si}, P_{di}, and P_{ci}, giving

$$P_{e^-}=2P_i-P_i^2 \ . \tag{25}$$

The total cross section for a particular process is calculated by integration of the corresponding probability over the impact parameter. For example, the total cross section for single ionization is

$$\sigma_{\text{si}}=\int_0^{b_{\max}} db\, 2\pi b P_{\text{si}}(b) \ , \tag{26}$$

where we have explicitly written the dependence of P_{si} on the impact parameter b.

We shall first present out theoretical results for H^+ + He collisions in the energy range 60—1000 keV. In Fig. 4 the total cross sections σ_{si}, σ_{e^-} σ_{sc}, and σ_{di} are, respectively, shown for single ionization, free-electron production, single capture, and double ionization. In all

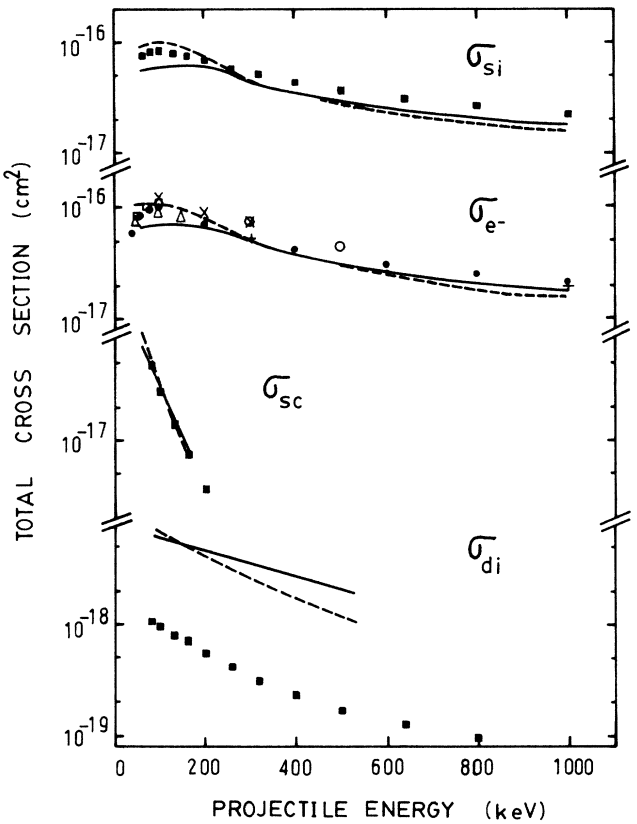

FIG. 4. H^+ + He total cross section for single ionization (σ_{si}), free-electron production (σ_{e^-}), single capture (σ_{sc}), and double ionization (σ_{di}) as a function of the projectile energy. Experiments: ■, Shah and Gilbody (Ref. 18); □, Rudd and Madison (from Ref. 19); △, Rudd and Jorgensen (from Ref 19); ×, Rudd, Sautter and Bailey (from Ref. 19); +, Toburen (from Ref. 19); ○, Stolterfoht *et al.* (Ref. 19); ●, Barnett *et al.* (Ref. 20). Theory: V_{mod} (——), V_{eff} (— — —).

cases, the results obtained with V_{eff} or V_{mod} are compared with experimental data. In order to ensure error bars of 10% in σ_{e^-}, σ_{si}, and σ_{sc} the integration of 3000–4000 trajectories is required. For double ionization the number of trajectories is to be multiplied by ten. We have considered the value $E=-0.904$ in formula (3) for both potentials. As the collision energy increases from 60 keV to 1 MeV, the maximum impact parameter ($b_{\max}$) contributing to the ionization cross section decreases, in the case of V_{eff} interactions, from $3.3a_0$ to $1.8a_0$ and from $2.4a_0$ to $1.3a_0$ when V_{mod} interactions are considered. For capture processes, $b_{\max}$ is less then or equal to the one used for ionization and decreases more rapidly for increasing energies.

Good agreement is observed between theoretical and experimental results for σ_{si} and σ_{e^-}. As electron-capture and ionization probabilities (respectively, P_c and P_i) are very small, almost all the contribution to σ_{e^-} comes from σ_{si}. No important differences are observed between the results obtained with V_{eff} or V_{mod} except for the lower energies where those calculated with V_{eff} are approximately 1.7 times those with V_{mod}. In the high-energy range it seems that both calculations lead, within present statistical errors, to the same result. The results obtained with V_{eff} are coincident with those calculated by Olson.[12]

The results obtained for σ_{sc} are in very good agreement with the experimental measurements by Shah and Gilbody.[18] Those calculated with V_{eff} reproduce classical calculations by Olson[12] for the present system. The energy range where this reaction has been studied is smaller than the one used for ionization since above 200 keV larger statistics should be considered in order to obtain 10% error bars.

CTMC calculations by Olson (mentioned in Ref. 12) using an effective charge interaction lead to results for double-ionization cross sections that are 1 order of magnitude below those for single ionization. Our calculations using the same interaction confirm these results. However, the experimental measurements by Shah and Gilbody[18] are still another order of magnitude smaller. We have found no improvement when the model potential is used in the calculations. As V_{mod} is supposed to give a good representation of the target core, the reason for the mismatch between theoretical and experimental results does not seem to be the use of a particular kind of interaction, but rather the assumption of the independent-electron model. Finally, we have calculated total cross sections for the transfer-ionization reaction (not presented) and compared it with the data of Shah and Gilbody,[18] but the same conclusions as for σ_{di} are obtained.

Concerning the $H^+ + Li^+$ system, we have performed classical calculations to compute electron-capture and ionization reactions in the center-of-mass energy range 85–350 keV. Experimental cross sections by Sewell *et al.*[21] for Li^{2+} production ($\sigma_{Li^{2+}}$) and single-electron capture (σ_{sc}) are available in this energy range for the present collisional system. In Fig. 5 we, respectively, show the total cross sections $\sigma_{Li^{2+}}$, σ_{si}, and σ_{sc} for Li^{2+} production single ionization and single-electron capture. Total cross section $\sigma_{Li^{2+}}$ may be obtained by addition of

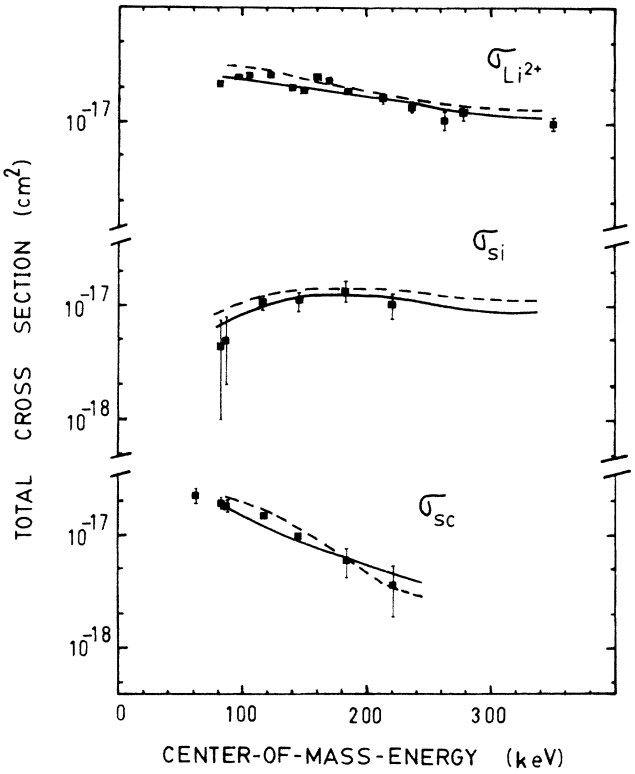

FIG. 5. $H+Li^+$ total cross sections for Li^{2+} production ($\sigma_{Li^{2+}}$), single ionization (σ_{si}), and single capture (σ_{sc}) as a function of the center-of-mass energy. Experiments: ■, Sewell *et al.* (Ref. 21). Theory: V_{mod} (——), V_{eff} (— — —).

σ_{si} and σ_{sc}. Depending on the interaction V_{eff} and V_{mod} considered, the maximum impact parameters contributing to the ionization process are, respectively, $1.5a_0$ and $1a_0$ for all the energy range here studied. For capture reactions the maximum impact parameter decreases with increasing energies from $1.8a_0$ and $1.4a_0$ to $1a_0$ and $0.8a_0$ for V_{eff} and V_{mod}, respectively. For both interactions, the value $E_i=-2.78$ has been used. Approximately 3000–4000 trajectories are sufficient to obtain the results with reasonable error limits (10%). It may be seen that both the results corresponding to the interactions V_{eff} and V_{mod} are in fair agreement with the experimental results by Sewell. As is also the case for He targets, total cross sections are not too sensitive to the change from V_{eff} to V_{mod}. We note that unpublished CTMC calculations by Olson are presented in the paper of Sewell *et al.* As details of those calculations are not available to us, we cannot explain the difference between Olson's results and ours. For other systems such as $H^+ + H$ and $H^+ + He$ we have found almost exact agreement with results by this author.

C. Differential cross sections

A review of experimental differential cross sections for electron ejection in $H^+ + He$ collisions has been published by Rudd, Toburen, and Stolterfoht[19] in the impact energy range 5 keV–5 MeV.

The way to calculate SDCS for reactions (16) and (17) is as follows. Let N_Ω denote the number of ejected electrons that are detected in the solid-angle interval $(\Omega-\Delta\Omega/2,\Omega+\Delta\Omega/2)$ and N_E the number of those in the final energy interval $(E-\Delta E/2,E+\Delta E/2)$. The corresponding SDCS are obtained by means of relations

$$\frac{d\sigma}{d\Omega}=\frac{N_\Omega}{N\Delta\Omega}\pi b_{\max}^2 ,$$
$$\frac{d\sigma}{dE}=\frac{N_E}{N\Delta E}\pi b_{\max}^2 , \tag{27}$$

where N is the total number of trajectories that have been integrated. Intervals in angle and energy must always be chosen so as to provide a smooth variation of the SDCS and to guarantee an error of the order of 10%. In order to compute a SDCS for two electrons we have multiplied by the two expressions (27). This is consistent with the fact that in (25) the term P_i^2 may be neglected in comparison with $2P_i$.

In Fig. 6 we show the SDCS as a function of the energy of the ejected electron for impact energies of 100 and 500 keV. A total of 30000 and 50000 trajectories were, respectively, integrated at 100 and 500 keV. At 100 keV the results obtained with V_{eff} are in very good agreement with the experimental results by Rudd, Sautter, and Bailey (from Ref. 19). The agreement is also good with the measurements by Rudd and Madison (from Ref. 19) except at very low energies where the experimental results decrease. On the other hand, the theoretical calculations with V_{mod} interactions reproduce correctly the results by Rudd and Jorgenson (from Ref. 19) except for low energies of the ejected electron. For 500-keV projectiles, both interactions lead to the same differential cross section for all the electronic energy range under consideration. However, the theoretical results underestimate the experimental measurements by Stolterfoht *et al.* (from Ref. 19). It is to be noted that also the the total cross section measured by this author is greater than the corresponding theoretical values and the general trend of the experimental results by Barnett *et al.*[20]

In Fig. 7 we show the SDCS as a function of the angle of the ejected electron for impact energies of 100 and 500 keV. At 100 keV the results show good agreement with the experimental data. At 500 keV, as for the energy distribution, the angular cross section is less sensitive to the choice of the interactions than at 100 keV, except for the small-angle region where V_{mod} gives greater results than V_{eff}.

In Fig. 8 we have represented the ionization probability $P_i(b)$ times the impact parameter b as a function of b for projectile energies of 100 and 500 keV. It may be seen that depending on the potential—V_{eff} or V_{mod}—considered, a very different curve is obtained for the

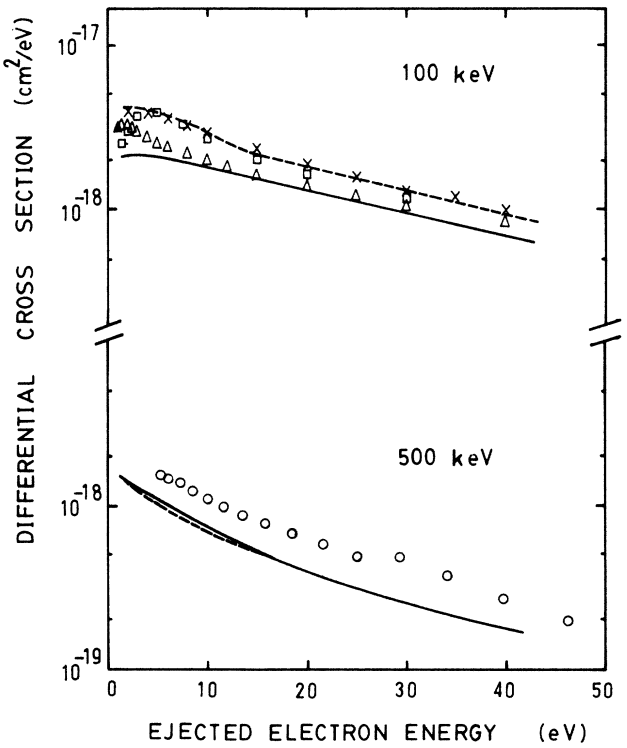

FIG. 6. Differential cross section in the energy of the ejected electron for H^++He collision. Projectile energies are 100 and 500 keV and the values are presented in laboratory coordinates. Experiments: □, Rudd and Madison (from Ref. 19); △, Rudd and Jorgensen (from Ref. 19); ×, Rudd, Sautter, and Bailey (from Ref. 19); ○, Stolterfoht *et al.* (from Ref. 19). Theory: V_{mod} (——), V_{eff} (— — —).

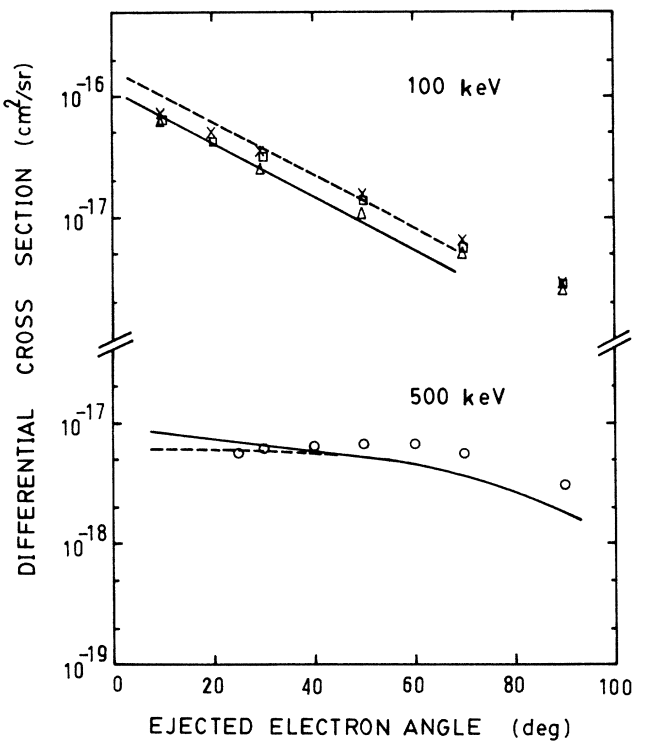

FIG. 7. Differential cross section in the angle of the ejected electron for H^++He collision. The projectile energies are 100 and 500 keV and the values are presented in laboratory coordinates. Experiments: □, Rudd and Madison (from Ref. 19); △, Rudd and Jorgensen (from Ref. 19); ×, Rudd, Sautter and Bailey (from Ref. 19); ○, Stolterfoht *et al.* (from Ref. 19). Theory: V_{mod} (——), V_{eff} (— — —).

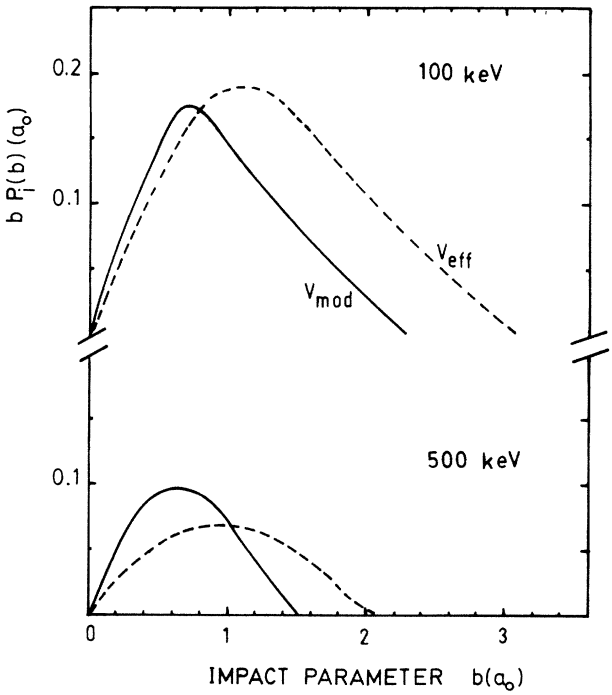

FIG. 8. Electron ionization probability P_i times impact parameter b as a function of b. Theory: V_{mod} (——), V_{eff} (— — —).

quantity $bP_i(b)$. However, at 500 keV, this difference is not carried to differential cross sections. As the collision energy increases from 100 to 500 keV, the maximum impact parameter contributing to the ionization cross section decreases. At 1000 keV (not represented) the values of b_{max} obtained with V_{eff} or V_{mod} are exactly coincident with the cutoff of the corresponding position distributions (see Fig. 2). This coincidence comes from the fact that, at high energies, only head-on collisions between the projectile and the electron contribute significantly to ionization.

IV. CONCLUSIONS

We have developed a method that allows the use of general central interactions in the classical treatment of atomic collisions. The classical representation of the He atom has been studied within the independent-electron approximation. It has been shown that, when a model potential is used to represent the interaction of the active electron with the He^+ core, the classical momentum distribution is practically coincident with the quantum one. A similar result is obtained for the total binding energy of the atom. In addition, the interaction's behavior at small and large distances is properly taken into account in the collision dynamics.

For the collision systems studied here, the single-capture and single-ionization total cross sections are not very sensitive to the interaction used. A similar result has been mentioned for the $He^+ + He$ system in the article by McDowell and Janev.[14] However, for the lower energies studied in $H^+ + He$ collisions, the single-ionization total cross section becomes dependent on the particular interaction considered.

The same conclusions are reached for the differential cross sections here studied in spite of the differences in the ionization probabilities $P_i(b)$ when the interactions are changed from V_{eff} to V_{mod}.

Concerning the double-ionization and transfer-ionization cross sections, no agreement was found between theoretical and experimental results. This disagreement, already observed when effective charge interactions are considered, is not solved by the introduction of more realistic interactions as the model potential here employed. We would suggest that a four-body treatment including electronic correlation effects is necessary for the present case or similar ones. Pfeifer and Olson[9] have studied the double-ionization cross sections for $A^{q+} + He$ collisions with a four-body approximation. Although these authors have considered a higher energy range (1—5 MeV/amu) and values of q ranging from 2 to 10, their conclusions about the importance of electronic correlation effects seem to be equally valid for the case here considered.

APPENDIX: CLASSICAL TOTAL ELECTRONIC ENERGY OF HELIUM

The mean value of the total electronic energy of the He atom may be computed within the frame of the independent-electron model. Its value is

$$E_{el}=k^2\int d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{p}_1 d\mathbf{p}_2 H_{el} f(\mathbf{r}_1,\mathbf{p}_1) f(\mathbf{r}_2,\mathbf{p}_2)\ , \tag{A1}$$

where

$$H_{el}=\frac{p_1^2}{2}+\frac{p_2^2}{2}+\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|}-\frac{2}{r_1}-\frac{2}{r_2}\ . \tag{A2}$$

If we make use of the expansion

$$\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|}=4\pi\sum_{l\geq 0}\sum_{m=-l}^{l}(2l+1)^{-1}\frac{r_<^l}{r_>^{l+1}} \times Y_{lm}^*(\theta_1,\varphi_1)Y_{lm}(\theta_2,\varphi_2) \tag{A3}$$

and of the relation

$$\int_{-\infty}^{\infty} dx\, g(x)\delta(f(x))=\sum_i \frac{g_i(x_i)}{|f'(x_i)|}\ , \tag{A4}$$

where the values x_i are the roots of $f(x)$, the integral (A1) may be split in three integrals,

$$E_{el}=32(2)^{1/2}\pi^2 k\left[\int_0^{r_0} dr\, r^2[E_i-V(r)]^{3/2}+2\int_0^{r_0} dr\, r[E_i-V(r)]^{1/2}\right] +512\pi^4 k^2\int_0^{r_0} dr_2\, r_2^2[E_i-V(r_2)]^{1/2}\left[\frac{1}{r_2}\int_0^{r_2} dr_1\, r_1^2[E_i-V(r_1)]^{1/2}+\int_{r_2}^{r_0} dr_1\, r_1[E_i-V(r_1)]^{1/2}\right]\ . \tag{A5}$$

For Coulomb potentials, the first two integrals have a simple analytical result. For V_{mod}, all the integrals must be computed numerically. The values that result for the total electronic energy in the cases of V_{eff} or V_{mod} are, respectively, $E_{\text{el}} = -1.71$ and -2.84. This last value is in fair agreement with the experimental value $E_{\text{el}} = -2.94$.

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