Nonperturbative theory of projectile-electron loss in fast collisions with heavy atomic targets

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The electron loss of He^+ projectiles in heavy targets is studied within the framework of the sudden approximation. The main focus of the present study is in the elastic (screening) contribution to the electron loss. The calculations presented here unitarize the final populations of the projectile and of the target, take into account the nonperturbative character of the collision, and include the possibility of multielectronic transitions in the target atom concomitantly with the loss process. An analytical estimate for the screening contribution is also obtained. [S1050-2947(99)06104-1]

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I. INTRODUCTION

The understanding of collision processes out of the perturbative regime is, as a general rule, limited to single-electron transitions and to collision regimes where only one collision channel contributes significantly. In more complex collisions, where several collision channels are important and many-electron transitions can occur through them, there are few methods that go beyond the usual methodology [1–4] of combining perturbative approaches with the independent electron model (IEM). Indeed, most of the nonperturbative close-coupling calculations, which are the standard alternative to the perturbative approaches, are limited to few-electron systems [5].

Projectile electron loss by heavy atomic targets, in the intermediate-to-high velocity regime, is an example of a collision system that can be quite complex, even for simple projectile ions such as He^+. If the He^+ electron loss occurs through collisions with light atomic targets, first-order perturbation theories give a good theoretical description of the collision dynamics [6,2,3,7]. In this case, the projectile ionization occurs via the interaction with a weak potential, due either to the screened target nucleus (elastic mode) or to the electron-electron interaction (antiscreening mode) with one of the (few) target electrons. In the screening mode the nucleus and the electron cloud of the target act coherently, since the final state of the electron cloud remains unchanged. In the antiscreening mode the target electron cloud changes its state and its effect on the projectile electron cannot be coherently summed with that of the target nucleus. Thus, the screening and antiscreening modes can be alternatively denominated coherent and incoherent modes, respectively.

When the target atomic number increases, the strength of the target field over the projectile electron in close collisions increases substantially and perturbative methods are no longer valid. The projectile ionization probability for the elastic mode can reach values near unity at small impact parameters and, because the antiscreening probability also increases with the number of target electrons, the coupling of the elastic and the antiscreening modes cannot be neglected. Furthermore, due to the large number of target electrons available, target ionization is very likely to happen together with the loss process, which causes the elastic mode to be conditioned to the nonoccurrence of the target ionization. If the projectile is a multiply charged ion, electron capture becomes important in the intermediate-to-low velocity regime and must also be considered in the analysis of the electron loss process.

Some of these difficulties were identified long ago through the use of the free-collision model (FCM) [8,9] in the study of electron-loss probability of H atoms in various gases. As noted by Walters [10], the increase of the static field in heavy targets makes it necessary to go beyond first-order Born approximation to describe the elastic scattering of the projectile electron in this field. More recently, Riesselmann *et al.* [11] used an extension of the FCM to study projectile electron loss of H and H^- on gaseous targets, obtaining a good agreement with experiment.

However, because the FCM is not formulated in terms of the impact parameter of the collision, its use is restricted to cases where the coupling between competitive collision channels either is weak or can be taken into account by further simplifications in the IEM. In general, these conditions do not hold when the projectile charge increases. These restrictions are partially eliminated through the use of nonperturbative, close-coupling calculations. These calculations were introduced in the study of He^+ electron loss in noble gases by Grande *et al.* [12] and, because it is formulated in terms of impact parameters, it allowed these authors to estimate the effect of the joint unitarization of the elastic and antiscreening modes. This last formulation, however, cannot be considered as fully unitarized because the close-coupling method was applied only to the screening mode. As a consequence, the coupling between target ionization and projectile electron loss, for example, is ignored. As we will see in Sec. II B, this coupling plays an important role in the case of heavy targets.

The sudden approximation (SA) is a nonperturbative, unitarized theory (see, e.g., Ref. [13] and the review in Ref. [14]). In this paper the SA is used to study projectile electron loss of He^+ in noble gases. The SA is employed to describe the full colliding system, i.e., to describe the dynamics of both projectile and target electrons. This means that the final populations of both projectile and target states induced by

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the collision are unitarized within this approach. As a consequence, it will be shown that the screening (elastic), antiscreening, and target ionization channels appear naturally from the theory in a unitarized way, without the need of any *ad hoc* assumption. The general theory is presented in Sec. II. The comparison of calculated results with experimental data of He^+ electron loss in noble gases is discussed in Sec. III, where an analytical approximation for the elastic contribution to the electron loss is also introduced. Section IV presents the main conclusions.

Atomic units are used throughout except where otherwise stated.

II. THEORY

A. Sudden perturbation for projectile electron loss

In the impact parameter method the electronic system of colliding partners is described by the time-dependent Schrödinger equation,

$$i\frac{\partial}{\partial t}\Psi(\mathbf{r},\boldsymbol{\tau}_N,t)=(H_i+H_a+V_{\rm int}(t))\Psi(\mathbf{r},\boldsymbol{\tau}_N,t). \tag{1}$$

In Eq. (1), $\Psi(\mathbf{r},\boldsymbol{\tau}_N,t)$ is the electronic wave function of the colliding system, $\mathbf{r}$ is the coordinate of the active electron of the projectile ion with respect to its nucleus, $\boldsymbol{\tau}_N=\{\boldsymbol{\rho}_1,\boldsymbol{\rho}_2,\ldots,\boldsymbol{\rho}_N\}$ is the (3-N)-dimensional vector representing the coordinates of the N atomic target electrons with respect to the target nucleus, H_i and H_a are the electronic Hamiltonian of the projectile ion and of the target atom, respectively, and

$$V_{\rm int}(t)=\frac{Z_1Z_2}{R(t)}-\frac{Z_2}{|\mathbf{R}(t)-\mathbf{r}|}-\sum_{j=1}^{N}\frac{Z_1}{|\mathbf{R}(t)+\boldsymbol{\rho}_j|}+\sum_{j=1}^{N}\frac{1}{|\mathbf{R}(t)+\boldsymbol{\rho}_j-\mathbf{r}|} \tag{2}$$

is the time-dependent interaction between the projectile and the target. In Eq. (2), Z_1 and Z_2 are the nuclear charges of the projectile ion and of the target atom, respectively, and $\mathbf{R}(t)$ is the internuclear distance. The first term on the right-hand side of Eq. (2) is independent of the electron coordinates and can be eliminated by a simple phase transformation of the wave function, a procedure that will be followed below. In this work, $\mathbf{R}(t)$ is assumed to be a straight line, $\mathbf{R}(t)=\mathbf{b}+\mathbf{v}t$, determined by the relative (collision) velocity $\mathbf{v}$ and by the impact parameter $\mathbf{b}$, $(\mathbf{b}\cdot\mathbf{v}=0)$.

To describe projectile electron loss at relatively high collision velocities, $v>v_i$ (a stricter condition is $v\gg v_i$, where v_i is the orbital velocity of the electron in the projectile ion), in collisions with heavy atoms, when $Z_2>v$, and, correspondingly, the perturbation theory is invalid, the sudden approximation can be used when the effective collision time τ_{coll} is small compared to the orbiting time τ_i of the electron in the ion. The effective collision time can be estimated as $\tau_{coll}\simeq a_{at}/v$, where $a_{at}\sim a_0=1$ a.u. is the atomic dimension. Estimating the orbiting time as $\tau_i\simeq a_i/v_i$, where $a_i\simeq a_0n^2/Z_1$ is the characteristic dimension of the projectile ion and $v_i\simeq v_0Z_1/n$ (n is the principal quantum number of the electron state in the projectile and $v_0=1$ is the Bohr velocity), we have $\tau_i\simeq\tau_0\ n^3/Z_1^2$, where $\tau_0=1$ is the characteristic atomic time. Thus, the sudden approximation can be applied to treat the electron transitions in the projectile ion when the collision velocity satisfies the condition $v>v_0Z_1^2/n^3=Z_1^2/n^3$ (a stricter condition would be $v\gg Z_1^2/n^3$).

Below, Eq. (1) is solved with the interaction (2) in the zeroth order of the sudden approximation (see Ref. [14]). It should be noted that, for collisions with heavy atoms, the interaction can be sudden for the electron of the ion and for outer electrons of the atom, but may not be sudden for inner, tightly bound, electrons of the atom. Therefore, it is convenient to divide all atomic electrons into two groups. The first group contains inner, tightly bound electrons with orbiting times smaller than the collision time (passive atomic electrons). For these electrons the interaction with the ion (with not a very high charge) is a weak perturbation. Thus, it will be considered that these electrons are only spectators in the collision and that their role is restricted to the partial screening of the target atomic nucleus. The second group contains atomic outer electrons with orbiting times larger than the effective collision time (active atomic electrons).

To go further, it is considered here that the wave function of the Schrödinger equation (1) depends only on the coordinates of the projectile electron and of the target *active* electrons. The interaction term (2) can be approximated as

$$V_{\rm int}(t)=-\frac{f_2(|\mathbf{R}(t)-\mathbf{r}|)}{|\mathbf{R}(t)-\mathbf{r}|}-\sum_{j=1}^{n_a}\frac{Z_1}{|\mathbf{R}(t)+\boldsymbol{\rho}_j|}+\sum_{j=1}^{n_a}\frac{1}{|\mathbf{R}(t)+\boldsymbol{\rho}_j-\mathbf{r}|}, \tag{3}$$

where $-\{[f_2(|\mathbf{R}(t)-\mathbf{r}|)]/|\mathbf{R}(t)-\mathbf{r}|\}$ is the interaction of the electron of the projectile with the target nucleus, partially screened by the passive electrons of the target,

$$-\frac{f_2(|\mathbf{R}(t)-\mathbf{r}|)}{|\mathbf{R}(t)-\mathbf{r}|}=-\frac{Z_2}{|\mathbf{R}(t)-\mathbf{r}|}+\left\langle\sum_{p=1}^{n_p}\frac{1}{|\mathbf{R}(t)+\boldsymbol{\rho}_p-\mathbf{r}|}\right\rangle, \tag{4}$$

where n_a and n_p are the numbers of active and passive atomic electrons, respectively, and the symbol $\langle\cdots\rangle$ represents the averaging over the charge density of the target passive electrons. Note that $\lim_{x\to0}f_2(|\mathbf{x}|)=Z_2$.

In the zeroth order of the sudden approximation the transition amplitude, $A_{0\to n}^{0\to m}$, for the projectile ion being in a final state $\psi_n(\mathbf{r})$ and the target atom being in a final state $\chi_m(\boldsymbol{\tau}_{n_a})$ after the collision, reads (see, e.g., Ref. [14])

$$A_{0\to n}^{0\to m}=\langle\psi_n(\mathbf{r})\chi_m(\boldsymbol{\tau}_{n_a})|\exp\left(-i\int_{-\infty}^{+\infty}V_{\rm int}(t)dt\right)\times|\psi_0(\mathbf{r})\chi_0(\boldsymbol{\tau}_{n_a})\rangle, \tag{5}$$

where $\psi_0(\mathbf{r})$ and $\chi_0(\boldsymbol{\tau}_{n_a})$ are the initial states of the ion and the atom, respectively, and $\boldsymbol{\tau}_{n_a}=\{\boldsymbol{\rho}_1,\boldsymbol{\rho}_2,\ldots,\boldsymbol{\rho}_{n_a}\}$ is the (3-n_a)-dimensional vector representing the coordinates of the $\mathbf{n}_a$ atomic target *active* electrons with respect to the target nucleus.

B. Elastic contribution from the target (screening)

From Eq. (5), it follows that the amplitude for projectile excitation or loss, when the atomic electrons remain in their initial states (i.e., the elastic amplitude), is given by

$$A_{0\to n}^{0\to 0}=\langle \psi_n(\mathbf{r})\chi_0(\boldsymbol{\tau}_{n_a})|\exp\left(-i\int_{-\infty}^{+\infty}V_{\rm int}(t)dt\right)\times|\psi_0(\mathbf{r})\chi_0(\boldsymbol{\tau}_{n_a})\rangle. \quad (6)$$

If one defines

$$V_{\rm scr}(t)=-\frac{f_2(|\mathbf{R}(t)-\mathbf{r}|)}{|\mathbf{R}(t)-\mathbf{r}|}+\langle\chi_0(\boldsymbol{\tau}_{n_a})|\sum_{j=1}^{n_a}\frac{1}{|\mathbf{R}(t)+\boldsymbol{\rho}_j-\mathbf{r}|}|\chi_0(\boldsymbol{\tau}_{n_a})\rangle =-\frac{Z_2}{|\mathbf{R}(t)-\mathbf{r}|}+\langle\chi_0(\boldsymbol{\tau}_N)|\sum_{j=1}^{N}\frac{1}{|\mathbf{R}(t)+\boldsymbol{\rho}_j-\mathbf{r}|}|\chi_0(\boldsymbol{\tau}_N)\rangle \quad (7)$$

as the screened potential of the target atom, which can be very strong at small impact parameters, and

$$\Delta V=-\sum_{j=1}^{n_a}\frac{Z_1}{|\mathbf{R}(t)+\boldsymbol{\rho}_j|}+\sum_{j=1}^{n_a}\frac{1}{|\mathbf{R}(t)+\boldsymbol{\rho}_j-\mathbf{r}|}-\langle\chi_0(\boldsymbol{\tau}_{n_a})|\sum_{j=1}^{n_a}\frac{1}{|\mathbf{R}(t)+\boldsymbol{\rho}_j-\mathbf{r}|}|\chi_0(\boldsymbol{\tau}_{n_a})\rangle, \quad (8)$$

so that $V_{\rm int}=V_{\rm scr}+\Delta V$, Eq. (6) can be written, using the completeness relation for the projectile states, as

$$A_{0\to n}^{0\to 0}=\langle\psi_n|\exp\left(-i\int_{-\infty}^{+\infty}V_{\rm scr}(t)dt\right)G(\mathbf{r})|\psi_0\rangle =\sum_{n'}\langle\psi_n|\exp\left(-i\int_{-\infty}^{+\infty}V_{\rm scr}(t)dt\right)\times|\psi_{n'}\rangle\langle\psi_{n'}|G(\mathbf{r})|\psi_0\rangle, \quad (9)$$

where

$$G(\mathbf{r})=\int\prod_{j=1}^{n_a}d\boldsymbol{\rho}_j|\chi_0(\boldsymbol{\tau}_{n_a})|^2\exp\left(-i\int_{-\infty}^{+\infty}\Delta V\,dt\right). \quad (10)$$

Considering the $\mathbf{r}$-dependent part of the interaction $\Delta V(\mathbf{r},\boldsymbol{\tau}_{n_a},t)$ as a weak perturbation acting on the active electron of the projectile, Eq. (9) can be rewritten approximately as

$$A_{0\to n}^{0\to 0}\simeq\langle\psi_n|\exp\left(-i\int_{-\infty}^{+\infty}V_{\rm scr}(t)dt\right)|\psi_0\rangle\langle\psi_0|G(\mathbf{r})|\psi_0\rangle, \quad (11)$$

where the only term kept in the sum over n' is the one which gives a nonvanishing value in the limit

$$\sum_{j=1}^{n_a}\frac{1}{|\mathbf{R}(t)+\boldsymbol{\rho}_j-\mathbf{r}|}-\langle\chi_0|\sum_{j=1}^{n_a}\frac{1}{|\mathbf{R}(t)+\boldsymbol{\rho}_j-\mathbf{r}|}|\chi_0\rangle\to 0.$$

Assuming a small ion charge ($Z_1<v$) and keeping only the first three terms of the expansion of the exponent containing the term ΔV in Eq. (11), the elastic probability, $P_{0\to n}^{\rm el}(b)=|A_{0\to n}^{0\to 0}|^2$, can be written, after some elementary but rather cumbersome algebra, as

$$P_{0\to n}^{\rm el}(b)=\left|\langle\psi_n|\exp\left(-i\int_{-\infty}^{+\infty}V_{\rm scr}(t)dt\right)|\psi_0\rangle\right|^2\times\left(1-\sum_{m\neq 0}\left|\langle\chi_m|\int_{-\infty}^{+\infty}V_0(t)dt|\chi_0\rangle\right|^2\right), \quad (12)$$

where

$$V_0(t)=\sum_{j=1}^{n_a}\left(-\frac{Z_1}{|\mathbf{R}(t)+\boldsymbol{\rho}_j|}+\langle\psi_0|\frac{1}{|\mathbf{R}(t)+\boldsymbol{\rho}_j-\mathbf{r}|}|\psi_0\rangle\right) \quad (13)$$

is the net potential of the projectile acting on the target electrons, assuming the projectile electron to be ''frozen'' in its ground state.

Noticing that

$$p_{0\to n}^{\rm scr}(b)=\left|\langle\psi_n|\exp\left(-i\int_{-\infty}^{+\infty}V_{\rm scr}(t)dt\right)|\psi_0\rangle\right|^2 \quad (14)$$

is the probability of the projectile electron to make a transition in the field of the screened target atom in the ground state, one can write Eq. (12) as

$$P_{0\to n}^{\rm el}(b)=p_{0\to n}^{\rm scr}(b)\left(1-\sum_{m\neq 0}\left|\langle\chi_m|\int_{-\infty}^{+\infty}V_0(t)dt|\chi_0\rangle\right|^2\right). \quad (15)$$

Equation (15) is the first main result of this paper. Since the zeroth-order sudden approximation assumes the electrons (with respect to their nuclei) to be frozen during the collision time, Eq. (15) is in agreement with this assumption. This equation has a simple physical meaning: the elastic probability is equal to the screening probability of the projectile electron to make a transition in the field of the target atom in the ground state, multiplied by the probability of the target atom to remain in this state during the collision. This last term can, then, be rewritten as

$$1-\sum_{m\neq 0}\left|\langle\chi_m|\int_{-\infty}^{+\infty}V_0(t)dt|\chi_0\rangle\right|^2=1-P_{\rm exc}^a(b)-P_{\rm ion}^a(b), \quad (16)$$

where $P_{\rm ion}^a(b)$ and $P_{\rm exc}^a(b)$ are the probabilities of ionization and excitation of the target by the projectile, respectively.

For multielectron atoms the ionization channel dominates over the excitation to discrete states and one can set approximately

$$1-\sum_{m\neq 0}\left|\langle\chi_m|\int_{-\infty}^{+\infty}V_0(t)dt|\chi_0\rangle\right|^2\simeq 1-P_{\rm ion}^a(b), \quad (17)$$

From Eqs. (15) and (17) it follows that

$$P^{\rm el}_{0\to n}(b)=p^{\rm scr}_{0\to n}(b)[1-P^{a}_{\rm ion}(b)]. \tag{18}$$

It is worth noting that Eq. (18) appears naturally in the approach used in this work. In perturbative approaches, on the other hand, the product of probabilities like that of Eq. (18) appears in an *ad hoc* way, in connection with the independent electron model (see Ref. [1]).

The probability $p^{\rm scr}_{0\to n}(b)$ describes electron transitions in the projectile induced by the interaction $V_{\rm scr}(t)$ between the projectile electron and the target atomic field, which strongly depends on the impact parameter and varies rapidly from very large magnitudes, at $b\to 0$, to negligible ones, at $b \sim a_{at}\sim 1$. Therefore, one can assume that the probability $P^{a}_{\rm ion}(b)$ is a rather smooth function of the impact parameter b as compared to the probability $p^{\rm scr}_{0\to n}(b)$ for electron transitions in the ion and can be approximated by its value at $b=0$ in the calculation of $P^{\rm el}_{0\to n}(b)$ in Eq. (18). Then, the elastic cross section can be obtained from Eqs. (15) and (18) as

$$\begin{aligned}\sigma^{\rm el}_{n}&=2\pi\int_0^\infty db\, b P^{\rm el}_{0\to n}(b)\\ &\simeq 2\pi[1-P^{a}_{\rm ion}(b=0)]\\ &\quad\times\int_0^\infty db\, b\left|\langle\psi_n|\exp\left(-i\int_{-\infty}^{+\infty}V_{\rm scr}(t)dt\right)|\psi_0\rangle\right|^2.\end{aligned} \tag{19}$$

This expression is the second main result of this paper and it will be used in Sec. III to describe collisions of He^{+} ions with noble gases.

C. Total contribution from the target

1. General expressions

In cases where the final state of the target atom is not observed, the probability of projectile excitation or loss is given by

$$\begin{aligned}P_{0\to n}(b)&=\sum_m |A^{0\to m}_{0\to n}|^2=\int d\mathbf{r}\int d\mathbf{r}'\,\psi_n^*(\mathbf{r})\psi_0(\mathbf{r})\\ &\quad\times\psi_n(\mathbf{r}')\psi_0^*(\mathbf{r}')\int\prod_{j=1}^{n_a}d\boldsymbol{\rho}_j|\chi_0(\boldsymbol{\tau}_{n_a})|^2\\ &\quad\times\exp\left(-i\int_{-\infty}^{+\infty}[V_{\rm int}(\mathbf{r},t)-V_{\rm int}(\mathbf{r}',t)]dt\right).\end{aligned} \tag{20}$$

When deriving Eq. (20), the completeness relation for the atomic states χ_m was used. It should be noted that the use of

$$\sum_m |\chi_m(\boldsymbol{\tau}_{n_a})\rangle\langle\chi_m(\boldsymbol{\tau}_{n_a})|=I,$$

is, in fact, an approximation whose accuracy is not easy to estimate, because the functions $\chi_m(\boldsymbol{\tau}_{n_a})$ describe only the active electrons of the total target atomic system. The states that form a complete basis set are the states $\chi_m(\boldsymbol{\tau}_N)$.

In the sudden approximation used here, unlike perturbative approaches, the sum over the population probabilities of all states (including both projectile and target states) is exactly equal to 1,

$$\sum_n P_{0\to n}(b)=\sum_n\sum_m |A^{0\to m}_{0\to n}|^2=1. \tag{21}$$

Equation (21) follows straightforwardly from Eq. (20) and the completeness relation for the projectile states ψ_n.

Equation (20) can be rewritten as

$$\begin{aligned}P_{0\to n}(b)&=\int d\mathbf{r}\int d\mathbf{r}'\,\psi_n^*(\mathbf{r})\psi_0(\mathbf{r})\psi_n(\mathbf{r}')\psi_0^*(\mathbf{r}')\\ &\quad\times\exp\left(-i\int_{-\infty}^{+\infty}[V_{\rm scr}(\mathbf{r},t)-V_{\rm scr}(\mathbf{r}',t)]dt\right)\\ &\quad\times\int\prod_{j=1}^{n_a}d\boldsymbol{\rho}_j|\chi_0(\boldsymbol{\tau}_{n_a})|^2\exp\left(-i\int_{-\infty}^{+\infty}[\Delta V(\mathbf{r},\boldsymbol{\tau}_{n_a},t)\right.\\ &\quad\left.-\Delta V(\mathbf{r}',\boldsymbol{\tau}_{n_a},t)]dt\right).\end{aligned} \tag{22}$$

It should be noted that, in contrast to the screening electron transition probability (15), Eqs. (20) and (22) do not contain the interaction term $\Sigma_{j=1}^{n_a}[Z_1/|\mathbf{R}(t)+\boldsymbol{\rho}_j|]$. The reasons for this are the following: (i) no interaction can change the total probability to find the atomic target in some of its states — a sum over all atomic states for atomic population probabilities is equal to unity; (ii) the interaction term in question is independent of the coordinates of the electron in the ion; and (iii) the summation over all atomic states of the target has already been done in Eqs. (20) and (22).

Expanding the exponential term in Eq. (22), which contains the weak perturbation $[\Delta V(\mathbf{r},\boldsymbol{\tau}_{n_a},t)-\Delta V(\mathbf{r}',\boldsymbol{\tau}_{n_a},t)]$, into series and keeping the first three terms one obtains, after some straightforward but cumbersome calculations,

$$\begin{aligned}P_{0\to n}(b)&=\int d\mathbf{r}\int d\mathbf{r}'\,\psi_n^*(\mathbf{r})\psi_0(\mathbf{r})\psi_n(\mathbf{r}')\psi_0^*(\mathbf{r}')\\ &\quad\times\exp\left(-i\int_{-\infty}^{+\infty}[V_{\rm scr}(\mathbf{r},t)-V_{\rm scr}(\mathbf{r}',t)]dt\right)\\ &\quad\times\left(1-\frac{1}{2}\sum_{m\neq 0}|f_m(\mathbf{r},b)|^2-\frac{1}{2}\sum_{m\neq 0}|f_m(\mathbf{r}',b)|^2\right.\\ &\quad\left.+\sum_{m\neq 0}f_m(\mathbf{r},t)f_m^*(\mathbf{r}',b)\right),\end{aligned} \tag{23}$$

where

$$f_m(\mathbf{r},b)=\langle\chi_0|\int_{-\infty}^{+\infty}dt\sum_{j=1}^{n_a}\frac{1}{|\mathbf{R}(t)+\boldsymbol{\rho}_j-r|}|\chi_m\rangle. \tag{24}$$

It is interesting to note that the unitarity is still kept in Eq. (23): $\Sigma_n P_{0\to n}(b)\equiv 1$ for any b.

2. Close and distant collision limits

Equation (23) can be further simplified for two limiting cases: close collisions, where $b < a_{at} \sim 1$, and distant collisions, where $b \gg 1$.

For collisions with heavy atomic targets at $b < 1$, where the interaction V_{scr} is very strong, one can neglect in Eq. (23) the terms containing the antiscreening part of electron-electron interactions, which results in

$$P_{0\to n}(b) = \left| \int d\mathbf{r}\, \psi_n^*(\mathbf{r}) \psi_0(\mathbf{r}) \exp\left(-i \int_{-\infty}^{+\infty} V_{scr}(\mathbf{r},t) dt \right) \right|^2. \tag{25}$$

This equation describes the transitions of the projectile electron due to the interaction with the atomic target, the electrons of which are ''frozen'' during the collision time. It should be noted that, since the summation over all states of the target was carried out, the target is allowed to be in any of its possible states after the collision, in contrast to the elastic mode.

For distant collisions, the short-range interaction V_{scr} vanishes, and it follows straightforwardly from Eq. (23) that

$$P_{0\to n}(b) = \sum_{m\neq 0} \left| \langle \psi_n \chi_m | \int_{-\infty}^{+\infty} dt \sum_{j=1}^{n_a} \frac{1}{|\mathbf{R}(t) + \boldsymbol{\rho}_j - \mathbf{r}|} | \psi_0 \chi_0 \rangle \right|^2. \tag{26}$$

In this case, the total transition probabilities of the projectile electron are reduced to the antiscreening mode, which is known to dominate over the screening mode in distant collisions [6].

3. Perturbative limit

In cases where all interactions are weak, the exponential term in Eq. (23) can be expanded in series. Keeping the first three terms of this expansion one obtains

$$\begin{aligned} P_{0\to n}(b) = & \left| \langle \psi_n | \int_{-\infty}^{+\infty} V_{scr}(\mathbf{r},t) dt | \psi_0 \rangle \right|^2 \\ & + \sum_{m\neq 0} \left| \langle \psi_n \chi_m | \int_{-\infty}^{+\infty} dt \sum_{j=1}^{n_a} \frac{1}{|\mathbf{R}(t) + \boldsymbol{\rho}_j - \mathbf{r}|} \right. \\ & \left. \times | \psi_0 \chi_0 \rangle \right|^2. \end{aligned} \tag{27}$$

This equation describes the total probability of the projectile electron transitions as a sum of the screening and antiscreening electron transition probabilities. It coincides with the result for the total probability, obtained in the first order of the perturbation theory [6], if one disregards the factors $\exp(-i\omega_{if}t)$ [15], where ω_{if} are the transition frequencies, which are neglected in the sudden approximation [14]. It should be noted that, in contrast to Eq. (27), obtained in the perturbative regime, Eq. (23), in general, does not allow such a simple separation for the total transition probability.

In order to get an analogy with the perturbative limit, Eq. (27), the probability $P_{0\to n}(b)$ can be rewritten as

$$P_{0\to n}(b) = \sum_m |A_{0\to n}^{0\to m}|^2 = |A_{0\to n}^{0\to 0}|^2 + \sum_{m\neq 0} |A_{0\to n}^{0\to m}|^2. \tag{28}$$

The first term in the right-hand side of Eq. (28) is the elastic probability, $P_{0\to n}^{el}$, determined by Eq. (15). The second term is the inelastic contribution to the total probability and can be split into two parts. One corresponds to the antiscreening mode, $P_{0\to n}^{anti}$, calculated in the first order of the perturbation theory. The other, $\Delta P(b)$, accounts for electron-nucleus interactions occurring together with the antiscreening part of the electron-electron interaction. $\Delta P(b)$ can be either positive or negative, and goes to zero in the perturbative limit.

Thus, Eq. (28) takes the form

$$P_{0\to n}(b) = P_{0\to n}^{el}(b) + P_{0\to n}^{anti}(b) + \Delta P(b). \tag{29}$$

III. RESULTS AND DISCUSSION

In the case of ionization, the final state of the projectile electron is in the continuum, with momentum $\mathbf{k}$ and a corresponding Coulomb wave function $\psi_{\mathbf{k}}$. Thus, the elastic part, σ_{loss}^{el}, of the total cross section for the electron loss can be written as

$$\sigma_{loss}^{el} = 2\pi \int_0^{\infty} db\, b P_{loss}^{el}(b), \tag{30}$$

where

$$P_{loss}^{el}(b) = \int d\mathbf{k}\, P_{0\to\mathbf{k}}^{el}(b). \tag{31}$$

Following Eq. (19) one can, then, write

$$\begin{aligned} P_{loss}^{el}(b) \simeq & [1 - P_{ion}^{a}(0)] \int d\mathbf{k}\, p_{0\to\mathbf{k}}^{scr}(b) \\ = & [1 - P_{ion}^{a}(0)] \\ & \times \int d\mathbf{k} \left| \langle \psi_{\mathbf{k}} | \exp\left(-i \int_{-\infty}^{+\infty} V_{scr}(t) dt \right) | \psi_0 \rangle \right|^2. \end{aligned} \tag{32}$$

Using the analytical screening function from Ref. [16],

$$V_{scr}(t) = -\frac{Z_2}{|\mathbf{R}(t) - \mathbf{r}|} \sum_{i=1}^{3} A_i \exp[-\alpha_i |\mathbf{R}(t) - \mathbf{r}|], \tag{33}$$

where A_i and α_i are tabulated parameters from the above reference, the integration over t in expression (32) can be done analytically, giving

$$\sigma_{\rm loss}^{\rm el}=[1-P_{\rm ion}^{a}(0)]2\pi\int_0^\infty db\, b \times\int d\mathbf{k}\left|\langle\psi_{\mathbf{k}}|\exp\left(-i\frac{2Z_2}{v}\sum_i A_i K_0(\alpha_i|\mathbf{b}-\mathbf{r}_\perp|)\right)\times|\psi_0\rangle\right|^2 =[1-P_{\rm ion}^{a}(0)]\,S_{\rm loss}^{\rm scr}, \quad (34)$$

where $S_{\rm loss}^{\rm scr}$ is the screening contribution to the loss cross section, K_0 is the modified Bessel function of the second kind, and $\mathbf{r}_\perp$ is the transverse part of the vector $\mathbf{r}$, which is perpendicular to the collision velocity $\mathbf{v}$.

Numerical calculations for $S_{\rm loss}^{\rm scr}$ show that, for collisions of He^+ with Ne, Ar, Kr, Xe at not very high collision velocities, this magnitude is much larger than the geometric cross section of He^+, $\sigma_{\rm geom}^{\rm He+}\simeq\pi/4\simeq0.8$ a.u. Thus, large impact parameters (as compared to the characteristic dimension of He^+) contribute most to $S_{\rm loss}^{\rm scr}$. Expanding $K_0(\alpha_i|\mathbf{b}-\mathbf{r}_\perp|)$ in series with respect to $r_\perp/b$ and keeping only the ''monopole'' and ''dipole'' terms one obtains

$$\sigma_{\rm loss}^{\rm el}\approx[1-P_{\rm ion}^{a}(0)]2\pi\int_0^\infty db\, b\int d\mathbf{k}\left|\langle\psi_{\mathbf{k}}|\exp\left(-i\frac{2Z_2}{v}\sum_i A_i\alpha_i K_1(\alpha_i b)\frac{\mathbf{b}\cdot\mathbf{r}_\perp}{b}\right)|\psi_0\rangle\right|^2 =[1-P_{\rm ion}^{a}(0)]2\pi\int_0^\infty db\, b\int d\mathbf{k}|\langle\psi_{\mathbf{k}}|\exp(-i\mathbf{q}\cdot\mathbf{r})|\psi_0\rangle|^2, \quad (35)$$

where K_1 is the modified Bessel function of the second kind and

$$\mathbf{q}=\frac{2Z_2\mathbf{b}}{vb}\sum_i A_i\alpha_i K_1(\alpha_i b) \quad (36)$$

can be interpreted as the mean momentum transferred to the projectile electron by the screened field of the atomic target. In the above approximation the projectile electron is considered, during the collision, as a free classical particle. This approximation is justified if (i) the effective collision time is small compared to the orbiting time of the electron in the projectile; and (ii) the ''strength'' of the atomic field, acting on the electron of the ion, is almost homogeneous within distances of the order of the size of the electron wave packet $\sim a_i$. Condition (i) corresponds to the validity of the sudden approximation. However, it is unlikely that the second condition can be well justified for a short-range screened atomic potential. Therefore, one should expect that, in principle, the function

$$p(b)=\int d\mathbf{k}|\langle\psi_{\mathbf{k}}|\exp(-i\mathbf{q}\cdot\mathbf{r})|\psi_0\rangle|^2 \quad (37)$$

could be regarded only as a rough approximation for the probability

$$p_{\rm loss}^{\rm scr}(b) =\int d\mathbf{k}\left|\langle\psi_{\mathbf{k}}|\exp\left(-i\frac{2Z_2}{v}\sum_i A_i K_0(\alpha_i|\mathbf{b}-\mathbf{r}_\perp|)\right)\times|\psi_0\rangle\right|^2. \quad (38)$$

Figure 1 presents an example of calculations for the probability $p_{\rm loss}^{\rm scr}(b)$ using Eq. (38), together with simplified versions of this equation given by Eq. (37) and Eq. (A4) (see below).

Surprisingly, numerical calculations for cross sections using Eq. (35) give a good agreement with calculations using Eq. (34) for a wide range of the collision parameters Z_2 and v where $S_{\rm loss}^{\rm scr}$ is much larger than the geometric cross section $\sigma_{\rm geom}^{\rm He+}$ of the projectile. This agreement improves for increasing values of $S_{\rm loss}^{\rm scr}$, i.e., when the collision energy decreases and/or when the atomic number Z_2 increases. This good agreement with the full calculations, given by Eq. (34) (see below), encourages one to make further simplifications in order to obtain a simple analytical expression for the screening cross section for electron loss.

For the atomic targets studied, Ne, Ar, Kr, and Xe, the values of the parameters α_i and A_i are such that the term

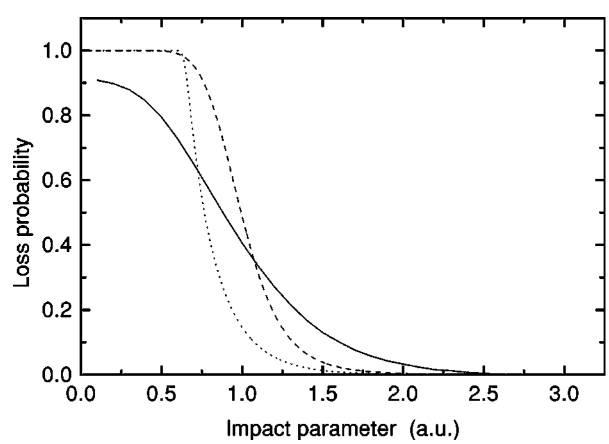

FIG. 1. Probability $p_{\rm loss}^{\rm scr}(b)$ for He^+ collisions with Kr at the projectile energy 4 MeV: the solid, dashed, and dotted lines represent results of calculations using Eqs. (38), (37), and (A4), respectively.

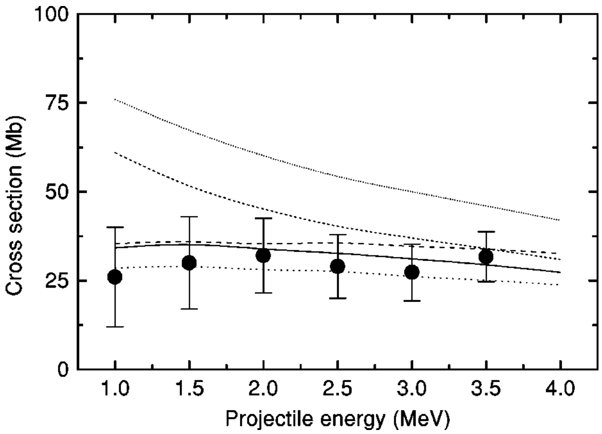

FIG. 2. Elastic cross section for He^+ electron loss in collisions with Ne as a function of the projectile energy. Theory: thick solid line, Eq. (34); dashed line, Eq. (35); dotted line, Eq. (39); thin-solid line, calculations using Eq. (34), when the ionization of the target is not taken into account ($P^a_{ion}=0$); dash-dotted line, coupled-channel results of Ref. [12] for the screening cross section. Experiment: solid circles (Refs. [17,18]).

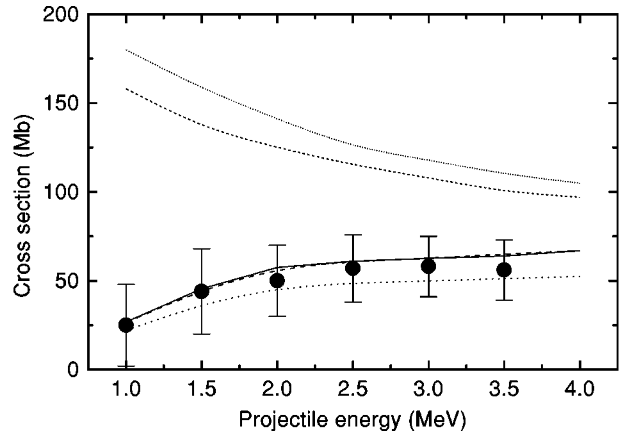

FIG. 3. Same as in Fig. 2, but for the Kr target.

with the lowest value of α_i in the sum in Eq. (33) [and of corresponding sums in Eqs. (34) and (35)] gives the main contribution to cross sections, given by Eqs. (34) and (35). Keeping only this term, the following simple analytical estimate can be obtained for the screening contribution in cases where the collision velocity is not very high, i.e., $Z_2^2A_{\min}^2\alpha_{\min}^2/(Z_1^2v^2)\gg 1$ (see Appendix),

$$\sigma_{\rm loss}^{\rm el}\approx[1-P_{\rm ion}^a(0)]\times\Bigg[\frac{\pi}{4\alpha_{\min}^2}\ln^2\Bigg(\frac{1.13\pi Z_2^2A_{\min}^2\alpha_{\min}^2}{Z_1^2v^2\ln\Big(\frac{1.13\pi Z_2^2A_{\min}^2\alpha_{\min}^2}{Z_1^2v^2}\Big)}\Bigg)+\frac{\pi}{2\alpha_{\min}^2}\ln\Bigg(\frac{1.13\pi Z_2^2A_{\min}^2\alpha_{\min}^2}{Z_1^2v^2}\Bigg)\Bigg], \tag{39}$$

where $\alpha_{\min}$ is the smallest value from the set of parameters α_i, and $A_{\min}$ is the corresponding value from the set of parameters A_i.

In order to estimate the ionization probability $P^a_{\rm ion}(b=0)$ of the target atom the following procedure was used. The ionization probability in close collisions with He^+ was assumed to be approximately equal to the ionization probability in close collisions with protons multiplied by some factor, i.e.,

$$P^a_{\rm ion}(0,{\rm He}^+)=z_{\rm eff}^2P^a_{\rm ion}(0,p^+),$$

where $z_{\rm eff}$ can be interpreted as an effective charge of He^+ ''seen'' by atomic electrons in close collisions, and which is taken here as a free parameter. In general, the magnitude of $z_{\rm eff}$ is within the limits $1\le z_{\rm eff}\le 2$. Choosing $z_{\rm eff}^2=1.8$, a good agreement with the experimental data for collisions with Ne, Ar, and Kr was obtained. Ionization probabilities for Ne and Ar in collisions with protons were evaluated from the semiclassical calculations of Hansteen, Johnsen, and Kocbach [20]. Ionization probabilities for Kr in collisions with protons were estimated as follows. Since, for the range of collision velocities studied in Refs. [17,18], single ionization cross sections for Ar and Kr in collisions with protons are roughly the same [19], the total probability for ionization of the $4s$ and $4p$ shells of Kr was assumed to be the same as the total probability for ionization of the $3s$ and the $3p$ shells of Ar. The ionization probability of the $3d$ shell of Kr was also obtained from Ref. [20].

Results of the numerical calculations for $\sigma_{\rm loss}^{\rm el}$ for He^+ electron loss in collisions with Ne and Kr as a function of the projectile energy are presented in Figs. 2 and 3 together with the difference $\sigma_{\rm loss}^{\rm tot}-\Sigma_{q\neq 0}\sigma_{\rm loss}^q$. In calculating this difference, $\sigma_{\rm loss}^{\rm tot}$ was taken from the total electron loss measurements of Ref. [17] and $\sigma_{\rm loss}^q$ from the coincidence measurements of Ref. [18]. The above sum was carried out for all the measured charge states, q, of the recoiling target ion. In Fig. 4 the results for Ne, Ar, and Kr targets at a fixed projectile energy are presented.

It can be seen from these figures that a good general agreement between theory and experiment is obtained for the full calculation, Eq. (34), as well as for the simplified versions given by Eqs. (35) and (39). Figures 2 and 3 also show

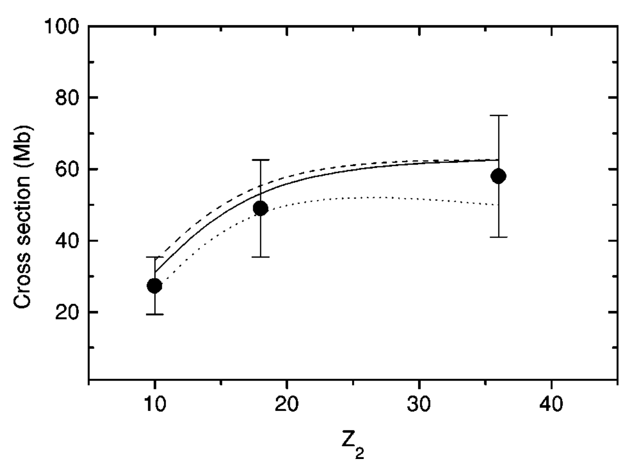

FIG. 4. Elastic cross section for the He^+ electron loss in collisions with Ne, Ar, and Kr at the projectile energy 3 MeV. Theory: solid line, Eq. (34); dashed line, Eq. (35); dotted line, Eq. (39). Experiment: solid circles (Refs. [17,18]).

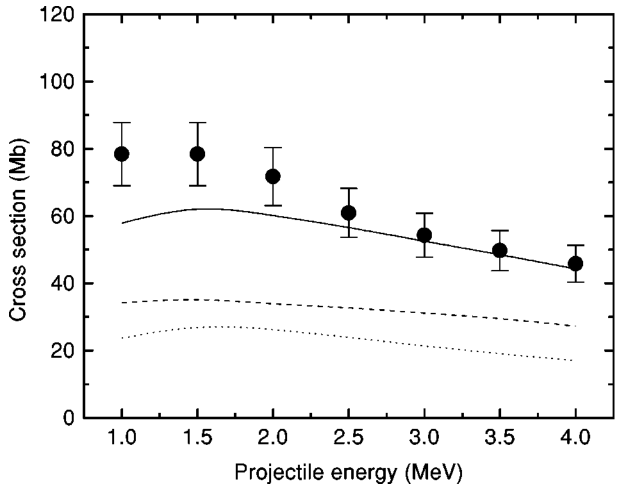

FIG. 5. Total electron loss cross section for collisions of He^+ with Ne as a function of the projectile energy. Theory: dashed line, elastic cross section, Eq. (34); dotted line, perturbative antiscreening cross section (Ref. [21]); solid line, sum of both contributions. Experiment: solid circles (from Ref. [17]).

the importance of the term $[1-P_{\rm ion}^{a}(0)]$ in reducing the screening cross section $S_{\rm loss}^{\rm scr}$, mainly when the projectile energy decreases and the target atomic number increases, as mentioned before. The dependence of $S_{\rm loss}^{\rm scr}$ on the projectile velocity, given by calculations presented here, are very similar to that given by the coupled-channel calculations of Grande *et al.* [12]. However, the coupled-channel calculations give values which are, in general, larger than those obtained from the sudden approximation.

Using Eq. (29) and neglecting the term $\Delta P(b)$ the total electron loss cross section was also estimated. The elastic contribution was calculated using Eq. (34), and the antiscreening contribution was calculated following the extended sum-rule method of Montenegro and Meyerhof [21]. In Figs. 5 and 6 the present calculations are compared with the experimental data of Sant'Anna *et al.* [17] for the total electron loss cross section for Ne and Kr targets, respectively. The rather good agreement obtained between the present calculations and experiment shows that the term $\Delta P(b)$ can be neglected. This means that, in contrast to the elastic contribution, the electron-nucleus interaction is not very important for the inelastic mode. In this intermediate-to-high velocity regime, the elastic and the antiscreening processes contribute at the same foot to the total electron loss cross section. This last conclusion, which was also obtained earlier for light targets [6], could hardly be extrapolated for heavier targets on simple qualitative grounds.

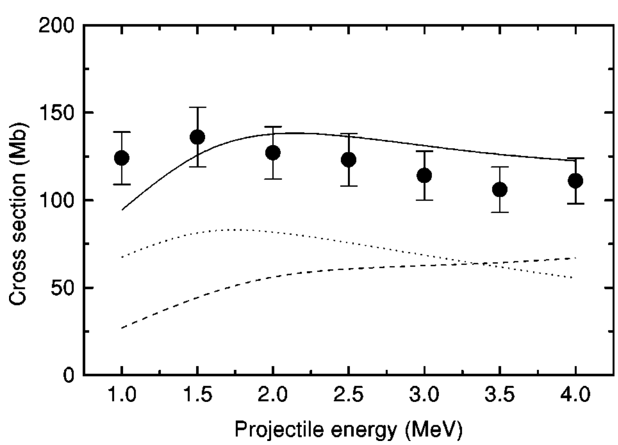

FIG. 6. Same as in Fig. 5, but for the Kr target.

TABLE I. Values of A_{min} and α_{min} for some elements.

Element	A_{min}	α_{min}
He	1.23	2.40
Ne	0.98	2.57
Ar	1.09	2.04
Kr	0.58	1.88
Xe	1.80	0.55

IV. CONCLUSIONS

In this paper a fully unitarized theory, based on the sudden approximation, is used to describe the simultaneous ionizations of the projectile and of the target, including those induced by electron-electron correlation. Within this formalism, the multiparticle aspects of the collision dynamics emerge quite naturally, in contrast to perturbative, or even nonperturbative but partially unitarized, approaches like the free-collision model or coupled-channel calculations, although one loses information about the time evolution of the collision.

The analysis presented here focused mainly on the elastic contribution for electron loss in collisions with heavy targets, in the intermediate-to-high velocity regime. Under these conditions several collision channels contribute at the same time, inducing (multiple) electron transitions in the colliding system, the effects of which over a particular collision channel cannot be ignored. The nonperturbative, fully unitarized, impact-parameter analysis of the collision dynamics showed that, for close collisions, the strong field produced by the partially screened target nucleus on the projectile electron results in a loss probability close to unity. However, because close collisions can, very likely, also ionize the multielectron target, the constraint, imposed by the elastic channel, of keeping the target atom in its ground state can strongly decrease the total elastic contribution to electron loss. In close collisions the antiscreening contribution plays a minor role.

As the impact parameter increases, the screening probability decreases steeply for impact parameters $b \simeq a_{at}+a_i$ due to the decrease of the atomic field of the neutral target. In this range of impact parameters, which can contribute considerably to the total electron loss cross section, complicated inelastic processes appear, which result from the combination of the electron-electron and the nucleus-electron contributions. For distant collisions, the net field produced by the target on the projectile ion is small, and the antiscreening contribution dominates.

The theory presented here not only makes it possible to clarify some important features of the physical processes occurring in such complex collisions, which were hidden in previous approaches, but also showed a good and consistent agreement with experiment for both the elastic contribution and the total electron-loss cross section. It also allowed to obtain an useful, analytical expression to estimate the elastic cross section.

ACKNOWLEDGMENTS

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APPENDIX

Keeping in Eq. (35) only the term with the smallest value of the screening parameters α_i, one obtains

$$\sigma_{\text{loss}}^{\text{el}} \approx [1-P_{\text{ion}}^{a}(0)]2\pi\int_0^\infty db\, b\int d\mathbf{k}\left|\langle\psi_{\mathbf{k}}|\exp\left(-i\frac{2Z_2}{v}A_{\min}\alpha_{\min}K_1(\alpha_{\min}b)\frac{\mathbf{b}\cdot\mathbf{r}_\perp}{b}\right)|\psi_0\rangle\right|^2$$
$$=[1-P_{\text{ion}}^{a}(0)]2\pi\int_0^\infty db\, b\int d\mathbf{k}|\langle\psi_{\mathbf{k}}|\exp(-i\mathbf{q}_1\cdot\mathbf{r})|\psi_0\rangle|^2, \quad \text{(A1)}$$

where

$$\mathbf{q}_1=\frac{2Z_2}{v}A_{\min}\alpha_{\min}K_1(\alpha_{\min}b)\frac{\mathbf{b}}{b}. \quad \text{(A2)}$$

In a range of impact parameters, where $q_1 r \sim q_1 a_i \ll 1$, $P_{\text{loss}}^{\text{el}}(b)$ can be approximated as

$$P_{\text{loss}}^{\text{el}}(b)\simeq[1-P_{\text{ion}}^{a}(0)]\int d\mathbf{k}|\langle\psi_{\mathbf{k}}|\exp(-i\mathbf{q}_1\cdot\mathbf{r})|\psi_0\rangle|^2$$
$$\simeq[1-P_{\text{ion}}^{a}(0)]q_1(b)^2\int d\mathbf{k}|\langle\psi_{\mathbf{k}}|z|\psi_0\rangle|^2$$
$$=[1-P_{\text{ion}}^{a}(0)](0.2834/Z_1)^2q_1(b)^2. \quad \text{(A3)}$$

For small impact parameters, where $q_1 r \sim q_1 a_i > 1$, the magnitude of the integral $\int d\mathbf{k}|\langle\psi_{\mathbf{k}}|\exp(-i\mathbf{q}_1\cdot\mathbf{r})|\psi_0\rangle|^2$ is close to unity. Since the Bessel function $K_1(x)$ decreases rapidly for $x>1$, the electron loss probability can be estimated as

$$P_{\text{loss}}^{\text{el}}(b)\simeq\begin{cases}[1-P_{\text{ion}}^{a}(0)], & b<b_0,\\ [1-P_{\text{ion}}^{a}(0)](0.2834/Z_1)^2q_1(b)^2, & b>b_0,\end{cases} \quad \text{(A4)}$$

where b_0 is the impact parameter satisfying the condition

$$(0.2834/Z_1)^2q_1(b_0)^2=1. \quad \text{(A5)}$$

When the ratio $\eta=(0.2834/Z_1)^2\ (2Z_2A_{\min}\alpha_{\min}/v)^2$ is large, $\eta\gg 1$, (which occurs for collisions of He^+ with Ne, Ar, Kr, and Xe at the collision energies of the measurements of Refs. [17,18]) the point b_0 lies in a region of impact parameters where the asymptotic expansion for $K_1(\alpha_{\min}b)$, $K_1(x)\simeq(\sqrt{\pi/2x})\exp(-x)$, is already valid. In this case, using the asymptotic representation of $K_1(\alpha_{\min}b_0)$, an approximate solution for Eq. (A5) can be written as

$$b_0\simeq\frac{1}{2\alpha_{\min}}\ln\left[\frac{1.13\pi Z_2^2A_{\min}^2\alpha_{\min}^2/(Z_1^2v^2)}{\ln[1.13\pi Z_2^2A_{\min}^2\alpha_{\min}^2/(Z_1^2v^2)]}\right]. \quad \text{(A6)}$$

Using Eqs. (A4) and (A6) to calculate the electron loss cross section, one finally obtains

$$\sigma_{\text{loss}}^{\text{el}}\approx[1-P_{\text{ion}}^{a}(0)]\left(2\pi\int_0^{b_0}db\, b+2\pi\int_{b_0}^\infty db\, b(0.2834/Z_1)^2q_1(b)^2\right)=[1-P_{\text{ion}}^{a}(0)]$$
$$\times\left[\frac{\pi}{4\alpha_{\min}^2}\ln^2\left(\frac{1.13\pi Z_2^2A_{\min}^2\alpha_{\min}^2}{Z_1^2v^2\ln\left(\frac{1.13\pi Z_2^2A_{\min}^2\alpha_{\min}^2}{Z_1^2v^2}\right)}\right)+\frac{\pi}{2\alpha_{\min}^2}\ln\left(\frac{1.13\pi Z_2^2A_{\min}^2\alpha_{\min}^2}{Z_1^2v^2}\right)\right]. \quad \text{(A7)}$$

When evaluating the second integral in the above expression, the asymptotic relation $K_1(x)\simeq(\sqrt{\pi/2x})\exp(-x)$ was used. Equation (A7) gives an analytical approximation for the seven-fold integral

$$\sigma_{\text{loss}}^{\text{el}}=[1-P_{\text{ion}}^{a}(0)]\,2\pi\int_0^\infty db\, b\times\int d\mathbf{k}\left|\langle\psi_{\mathbf{k}}|\exp\left(-i\frac{2Z_2}{v}\sum_i A_iK_0(\alpha_i|\mathbf{b}-\mathbf{r}_\perp|)\right)\times|\psi_0\rangle\right|^2.$$

In order to help the reader, the values of $A_{\min}$ and $\alpha_{\min}$, taken from Ref. [16], for the noble gases are reproduced in Table I.

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