Screening and antiscreening by projectile electrons in high-velocity atomic collisions

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The scattering amplitude for a projectile of nuclear charge Z_1 carrying N electrons colliding with an atomic target with charge Z_2, evaluated in the first Born approximation using hydrogenic wave functions, is compared with recent experimental results. In the present approximation where the minimum momentum transfer $t_{\min}$ is considered to be approximately independent of the final state of the projectile, the differential cross sections separate into a product of one term that depends only on the target times the square $Z_1^2(t)$ of an effective projectile charge. Here an analytic expression for $Z_1^2(t)$ is given for 2, 1, and 0 electrons. Some total ionization cross-section ratios are also given.

I. INTRODUCTION

While there have been numerous theoretical studies[1-8] of the projectile charge dependence of cross sections for inner shell vacancy production at intermediate and high velocities by a fully stripped ion, less theoretical attention has been given to cases where the incident ions (or atoms) carry electrons into the collision. For vacancy production by direct Coulomb ionization, cross sections for projectiles of charge Z_1 carrying N electrons may be evaluated in the plane-wave Born approximation (PWBA). Cross sections for scattering of atomic hydrogen by atomic hydrogen were first evaluated by Bates and Griffing[9] in 1953 where a closure relation was used to sum over the final states of the projectile. Subsequently, these results were generalized[10-18] to simple systems with a few projectile electrons. Recently, Gillespie[15] published a comprehensive study for various many-electron systems at high velocities.

In 1978, Stolterfoht[19] analyzed experimental double differential ionization cross sections for projectiles of various charge. In taking the ratio of these cross sections for various charge states it was expected that the target dependence would cancel. In this way an effective charge of the projectile was derived. This effective projectile charge was plotted as a function of the electron energy and related to the adiabatic radius using the Massey criterion. In this paper it is shown that in the PWBA approximation this effective projectile charge is entirely independent of the target if differences in energy of the final projectile state are negligible (e.g., in comparison to the excitation energy of the target). Thus the earlier analysis is confirmed.

Expressions for projectiles carrying an arbitrary number of electrons have been derived by Briggs and Taulbjerg[17] in the PWBA approximation, by Gillespie[16] using an expansion in $(v_0/v)^2$, where v_0 is the Bohr velocity, and by Inokuti[18] using the Bethe approximation. Extensive tables for various systems with nonhydrogenic electrons are given by Gillespie[16] for the evaluation of many cross sections including the relative elastic and inelastic contributions of the projectile. However, no simple analytic expressions for projectile charge dependence of excitation cross sections has been given. In this paper, a simple analytic expression is given for the effective charge of a projectile carrying 0, 1, or 2 hydrogenic electrons, assuming that the minimum momentum transfer in the collision is approximately independent of the energy of the final state of the projectile, and that the target is always ionized. Comparisons are made to recent experimental[20-23] determinations of the effective projectile charge for He^+ on Ar and H_2O, illustrating how the effective projectile charge varies. Also predictions are made corresponding to experiments[24] now in progress using He^0. Furthermore, comparisons are made to a simple screening model recently[25] proposed.

For bare projectiles of charge Z_1 the PWBA cross section is given by $Z_1^2|\tilde{f}(t)|^2$, where t is the momentum transfer. For projectiles carrying N electrons, the PWBA cross section may be expressed[16-18] as $Z_1^2(t)\ |\tilde{f}(t)|^2$, where $Z_1^2(t)$ represents an effective projectile charge squared which is independent of the target and $\tilde{f}(t)$ depends on the target independent of the projectile. Hence there is a separation of projectile and target contributions in the PWBA cross section. Furthermore, the projectile electron contribution $Z_1^2(t)$ may increase or decrease the cross sections relative to a bare projectile. Specifically, for small t (corresponding to large impact parameters), $Z_1^2(t)$ goes to $(Z_1-N)^2$ corresponding to screening of the projectile charge Z_1 by electrons. At large t (corresponding to small impact parameters), $Z_1^2(t)$ goes to Z_1^2+N corresponding to scattering incoherently by the projectile nucleus and N electrons. In this paper $Z_1(t)$ is evaluated in a simple closed form for $N=0$, 1, and 2, for hydrogenic systems.

II. THEORY

As a brief illustration of the theory, consider a projectile with two electrons and a target with one electron corresponding to our calculations in the next section. Generalization to systems with more electrons has been given by Gillespie,[16] Inokuti,[18] and Briggs and Taulbjerg.[17]

The Hamiltonian for a system with two projectile electrons with coordinates $\vec{r}_1', \vec{r}_1''$ and one target electron with coordinate $\vec{r}_2$ is

$$H=-\frac{\nabla_M^2}{2M}-\frac{\nabla_1'^2}{2}-\frac{Z_1}{r_1'}-\frac{\nabla_1''^2}{2}-\frac{Z_1}{r_1''}+\frac{1}{|\vec{r}_1'-\vec{r}_1''|}-\frac{\nabla_2^2}{2}-\frac{Z_2}{r_2}+V\,, \tag{1}$$

where

$$V=\frac{Z_1Z_2}{R}-\frac{Z_2}{|\vec{R}+\vec{r}_1'|}-\frac{Z_2}{|\vec{R}+\vec{r}_1''|}-\frac{Z_1}{|\vec{R}-\vec{r}_2|}+\frac{1}{|\vec{R}-\vec{r}_2+\vec{r}_1'|}+\frac{1}{|\vec{R}-\vec{r}_2+\vec{r}_1''|}\,. \tag{2}$$

The cross section for ionizing electron two is given[10] by

$$\frac{d\sigma}{d\vec{k}\,dt}(1s\text{-}\epsilon;1s\text{-}n'l';1s\text{-}n''l'')=\frac{1}{2\pi v^2}t|f(t)|^2\,, \tag{3}$$

where t is the momentum transfer energy for the system and $n'l'$ ($n''l''$) denotes the final state of projectile electron $1'$ ($1''$). The speed of the projectile relative to the target is v.

The PWBA expression[26,27] for the scattering amplitude $f(t)$ is, ignoring antisymmetry of target and projectile electron wave functions,

$$f(t)=\int d\vec{R}\,d\vec{r}_1'd\vec{r}_1''d\vec{r}_2 e^{i\vec{R}\cdot\vec{t}}\phi^*_{n'l'n''l''}(\vec{r}_1',\vec{r}_1'')\phi^*_C(\vec{r}_2)\times\left(\frac{Z_1Z_2}{R}-\frac{Z_2}{|\vec{R}+\vec{r}_1'|}-\frac{Z_2}{|\vec{R}+\vec{r}_1''|}-\frac{Z_1}{|\vec{R}-\vec{r}_2|}+\frac{1}{|\vec{R}-\vec{r}_2+\vec{r}_1'|}+\frac{1}{|\vec{R}-\vec{r}_2+\vec{r}_1''|}\right)\times\phi_{1s1s}(\vec{r}_1',\vec{r}_1'')\phi_{1s}(\vec{r}_2)\,. \tag{4}$$

Since the atomic wave functions are orthogonal, the first three terms in Eq. (4) do not contribute and the fourth term contributes only when neither projectile electron is excited. Separating out the Coulomb scattering amplitude in the usual fashion[26] using

$$\int\frac{1}{|\vec{R}-\vec{r}|}e^{i\vec{R}\cdot\vec{t}}d\vec{R}=e^{i\vec{r}\cdot\vec{t}}\int\frac{e^{i\vec{R}'\cdot\vec{t}}}{R'}d\vec{R}'=\frac{4\pi}{t^2}e^{i\vec{r}\cdot\vec{t}}\,, \tag{5}$$

$$f(t)=\frac{4\pi}{t^2}\tilde{\Phi}_1(1s\text{-}n'l';1s\text{-}n''l'';t)\Phi_2(1s\text{-}nl;t)\,. \tag{6}$$

Here is evident the basic separation of $f(t)$ into a product of one term depending only on the target, Φ_2, multiplied by another term depending only on the projectile, Φ_1, where

$$\Phi_2(1s\text{-}nl;t)=-\int d\vec{r}_2\phi^*_{nl}(\vec{r}_2)\phi_{1s}(\vec{r}_2)e^{i\vec{r}_2\cdot\vec{t}}\,(nl\neq 1s) \tag{7}$$

and

$$\tilde{\Phi}_1(1s\text{-}n'l',1s\text{-}n''l'';t)=-\int d\vec{r}_1'd\vec{r}_1''\phi^*_{n'l'n''l''}(\vec{r}_1',\vec{r}_1'')\phi_{1s1s}(\vec{r}_1',\vec{r}_1'')(Z_1-e^{i\vec{r}_1'\cdot\vec{t}}-e^{i\vec{r}_1''\cdot\vec{t}})\,. \tag{8}$$

Note that the PWBA amplitude is a product of a target amplitude, Φ_2, times a projectile amplitude, $\tilde{\Phi}_1$, where $\tilde{\Phi}_1$ is a sum of contributions from the nucleus and each electron.

Cross sections for target ionization may be evaluated from Eqs. (6)–(8) for any final state of the projectile. Note that a given value of t corresponds to different scattering angles of the projectile for different projectile states since t depends on ΔE, v, and the scattering angle. In this paper we consider cross sections for the ionization of the target summed over all final states of the projectile, namely,

$$\frac{d\sigma}{d\vec{k}\,dt}(1s-\epsilon;1s-\Sigma';1s-\Sigma'')=\frac{8\pi}{v^2}\sum_{n'l'}\sum_{n''l''}\frac{1}{t^2}\left|\tilde{\Phi}_1(1s\text{-}n'l';1s\text{-}n''l'',t)\Phi_2(1s\text{-}\vec{k};t)\right|^2, \tag{9}$$

where $\vec{k}$ is the momentum of the ejected electron. At fixed t, closure may be expressed[28] by

$$\sum_{NL}|\Phi(1s\text{-}NL;t)|^2=\sum_{NL}\langle 1s|NL\rangle\langle NL|1s\rangle=1$$

or (10)

$$\sum_{NL\neq 1s}|\Phi(1s\text{-}NL;t)|^2=1-|\Phi(1s-1s;t)|^2 .$$

For $t\simeq t_{\min}$ closure does not apply unless a common value of $t_{\min}$ is chosen for all final states NL. In general $t_{\min}=\Delta E/v$ will vary depending on how the projectile electrons are excited. However, when the projectile is neutral, $t|f(t)|^2$ goes to zero[16,26] for small t, so that at large v it is possible to set $t_{\min}$ to zero. In other cases the variation in ΔE is small, e.g., if $Z_1^2\ll Z_2^2$ then for K shell excitation ΔE is dominated by the target ionization energy. In some cases the variation in $t_{\min}$ is not negligible.[16] We choose $t_{\min}$ as the smallest value of $t_{\min}$, namely, the ionization energy for the target electron in our calculations.

Then, using orthonormality in Eq. (8), and closure,

$$\begin{aligned}\sum_{n'l'}\sum_{n''l''}|\tilde{\Phi}_1(1s\text{-}n'l';1s\text{-}n''l'';t)|^2&=[|Z_1-\Phi_1(1s\text{-}1s;1s\text{-}1s,t)-\Phi_1(1s\text{-}1s;1s\text{-}1s,t)|^2]\\&\quad+[1-|\Phi_1(1s\text{-}1s;1s\text{-}1s;t)|^2]+[1-|\Phi_1(1s\text{-}1s;1s\text{-}1s;t)|^2]\\&\equiv|Z_1(t)|^2,\end{aligned} \tag{11}$$

with

$$\Phi_1(1s\text{-}1s;1s\text{-}1s;t)=\int d\vec{r}_1'd\vec{r}_1''\phi_{1s1s}(\vec{r}_1',\vec{r}_1'')e^{i\vec{r}_1'\cdot\vec{t}}\phi_{1s1s}(\vec{r}_1',\vec{r}_1'')$$

so that

$$\frac{d\sigma}{d\vec{k}\,dt}(1s\text{-}\epsilon;1s\text{-}\epsilon';1s\text{-}\epsilon'')=\frac{8\pi}{v^2}t^{-3}|Z_1(t)|^2|\Phi_2(1s\text{-}\vec{k})|^2 . \tag{12}$$

The expression, $|Z_1(t)|^2$, behaves as the square of an effective projectile charge. This quantity is independent of the target, and the target amplitude is independent of the projectile contribution. The first, second, and third terms in square brackets in Eq. (11) represent elastic scattering for the projectile, a sum over excited states of electron $1'$ and a sum over excited states of $1''$, respectively. At large t, $\Phi_1(1s\text{-}1s;1s\text{-}1s;t)$ goes to zero, and $|Z_1(t)|^2$ goes to Z_1^2+2 corresponding to independent scattering by the nucleus and each of the two projectile electrons. The last two terms in square brackets of Eq. (11), giving rise to $|Z_1(t)|^2>Z_1^2$ at small t, are referred to in the literature[15-18] as the projectile (or sometimes x-ray) incoherent scattering function or as the Compton scattering factor.

Note that the overshoot, i.e., $|Z_1(t)|^2>Z_1^2$, appears only after the sum over final states of the projectile has been performed. If the projectile is elastically scattered, then $(Z_1-N)^2\le|Z_1(t)|^2\le Z_1^2$, i.e., the effective nuclear charge never exceeds the bare nuclear charge. This is evident from Eq. (4), keeping in mind that the first three potentials therein do not contribute. Excitation of the projectile is caused only by the electron-electron interactions in first order perturbation theory. Consequently, for any individual excited state of the projectile, $|Z_1(t)|^2\le N$. For two projectile electrons considered here $N=2$.

For hydrogenic wave functions $|Z_1(t)|^2$ may be evaluated in closed form, namely,

$$\begin{aligned}|Z_1(t)|^2=Z_1^2+2-4Z_1|1+(t/2Z_1)^2|^{-2}\\+2|1+(t/2Z_1)^2|^{-4}.\end{aligned} \tag{13}$$

For a projectile with one electron, there are similar expressions, namely,

$$\begin{aligned}|Z_1(t)|^2=|Z_1-\phi_1(1s\text{-}1s;t)|^2\\+1-|\phi_1(1s\text{-}1s;t)|^2\end{aligned} \tag{14}$$

and for hydrogenic wave functions,

$$|Z_1(t)|^2 = Z_1^2 + 1 - 2Z_1|1 + (t/2Z_1)^2|^{-2} . \quad (15)$$

Here, as t goes to zero $|Z_1(t)|^2$ goes to $(Z_1 - 1)^2$ and as t goes to infinity $|Z_1(t)|^2$ goes to $Z_1^2 + 1$. For a bare nucleus

$$|Z_1(t)|^2 = Z_1^2 , \quad (16)$$

which is independent of t. For a projectile with more than two electrons, $\Phi_1(1s\text{-}1s\ 1s\text{-}1s;t)$ is replaced[29] by the corresponding elastic scattering amplitude $\Phi_1(1s\text{-}1s;1s\text{-}1s;2s\text{-}2s;\ldots;nl\text{-}nl;t)$. Thus, for a projectile with N electrons $|Z_1(t)|^2$ will behave qualitatively as illustrated in Fig. 1.

III. EXPERIMENTAL COMPARISON AND DISCUSSION

In Figs. 2 and 3, Eq. (14) is compared with observed determinations[20-23] of $Z_1(t)$ for He^+ on Ar and H_2O. In these figures $Z_1(t)$ is plotted as a function of t^{-1} which may be regarded as an effective collision distance, b_{eff}.

The peak evident in the data at 1.2 MeV in Fig. 3 is thought to be due to electrons coming from the projectile. For comparison to the present theory, which differentiates between projectile and target electrons, this peak should be ignored. It should also be stressed that the data shown here do not correspond to a particular momentum transfer, but rather is averaged over all momentum transfers greater than the minimum momentum transfer of the collision, t_{min}. That is, the data come from differential observations corresponding to

$$\frac{d\sigma}{d\vec{k}} = \int_{t_{min}}^{t_{max}} \frac{d\sigma}{d\vec{k}\,dt}\,dt ,$$

with $t_{max} \cong \infty$.

Now, from Eq. (12) this corresponds to

$$\frac{d\sigma}{d\vec{k}} = \frac{8\pi}{v^2}\int_{t_{min}}^{t_{max}} dt\, t^{-3}|Z_1(t)|^2|\Phi_2(1s\text{-}\vec{k})|^2 .$$

In the analysis of the data it is argued that $t^{-3}|\Phi_2(1s\text{-}\vec{k})|^2$ is peaked about $t = t_{min}$. As a consequence, the ratio of double differential cross sections is independent of the target. Hence, for He^+ and He^{2+}

$$\left.\frac{d\sigma}{d\vec{k}}\right|_{He^+} \Big/ \left.\frac{d\sigma}{d\vec{k}}\right|_{He^{2+}} = \frac{|Z_1(t_{min})|^2}{Z_1^2}$$

or

$$Z_1(t_{min}) = Z_1\left(\left.\frac{d\sigma}{d\vec{k}}\right|_{He^+} \Big/ \left.\frac{d\sigma}{d\vec{k}}\right|_{He^{2+}}\right)^{1/2}$$

corresponding to reported[19,20] results, where

$$t_{min} = \frac{k^2 + I}{v} = \frac{E_R + I}{v} \cong t ,$$

with I equal to the ionization energy of the target, i.e., the target excitation energy is ignored and

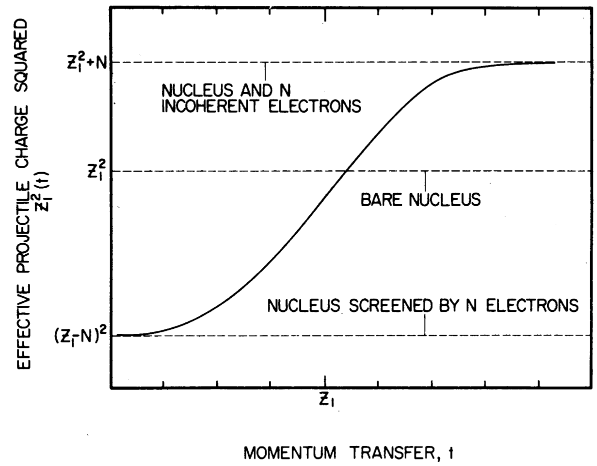

FIG. 1. Sketch of effective projectile charge squared, $|Z_1(t)|^2$, as a function of the momentum transfer t for a projectile with nuclear charge Z_1 carrying N electrons.

E_R equal to the energy of the ejected electron. Furthermore, it is assumed that $b_{eff} = t^{-1}$. Consequently, there are contributions in the data from $t > t_{min}$ corresponding to smaller b_{eff}. Correcting for this effect would shift the data to the left, toward a higher mean value of t, and into better agreement with theory.

A point to be stressed here is the fact that theory predicts that $Z_1(t)$ is independent of the target. Indeed is it clear that for two rather different targets, Ar and H_2O, there is evidence that $Z_1(t)$ does not depend very much, if at all, on the target.

Also shown in Figs. 2 and 3 are results of calculations[25] using an effective screening for the

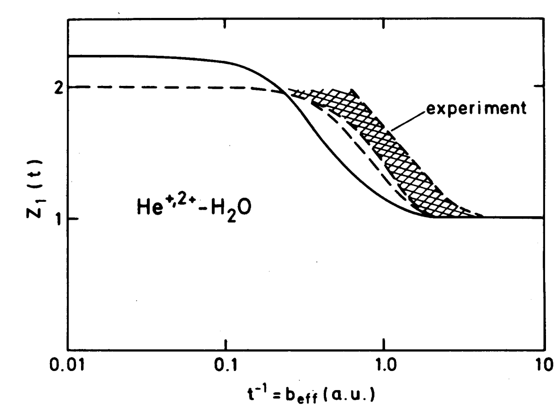

FIG. 2. Plot of $Z_1(t)$ vs $t^{-1} = b_{eff}$ for $He^+ + H_2O$. Data analysis of Toburen *et al.* (Ref. 23) assumes that $t = t_{min}$. The solid curve represents the present Born calculation, and the dashed curve corresponds to calculations (Ref. 25) with variable screened projectile charges.

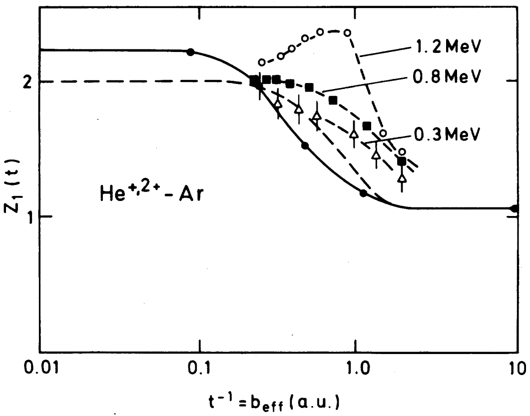

FIG. 3. Plot of $Z_1(t)$ vs $t^{-1}=b_{\text{eff}}$ for $He^{+}+Ar$. Data analysis of Toburen *et al.* (Ref. 22) assumes that $t=t_{\min}$. The solid curve represents the present Born calculation, and the dashed curve corresponds to calculations based on variable screened projectile charges.

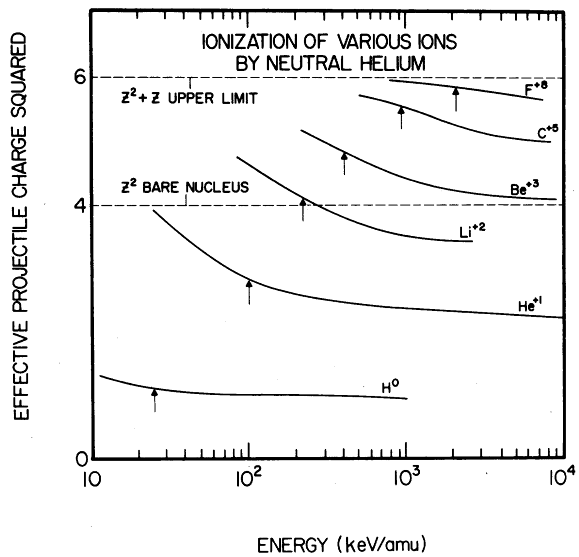

FIG. 4. PWBA calculations of $Z_1^2\,\sigma_{He^0}/\sigma_{He^{2+}}$ versus collision velocity in keV/amu for ionization of various one electron targets from H to F^{8+} by He^0 and He^{2+}. All final states of He^0 have been summed. The arrows indicate the velocity matching of the He projectile with target electrons, $v=Z_2$. The ratio shown represents an average of $|Z_1(t)|^2$ over momentum transfers.

nucleus. Note that the screening calculations do not predict $Z_{\text{eff}}>Z_1$ at large momentum transfer. However, as discussed below, use of the Born approximation is questionable in the large t limit, corresponding to close collisions where the field strengths may be large.

Results for relative total cross sections for ionization of single electron targets by He^{2+} and He^0 are given in Fig. 4, where we plot $Z_1^2\sigma_{He^0}/\sigma_{He^{2+}}$ versus velocity for a number of one electron targets. This figure corresponds to an averaging $Z_1^2(t)$ over t. Namely,

$$\sigma_{\text{tot}}=\int d\vec{k}\,dt\frac{d\sigma}{d\vec{k}\,dt}$$
$$=\int_0^\infty k^2dk\int d\Omega_k\int_{(k^2+I)/2v}^\infty dt\,t^{-3}|Z_1(t)|^2\times|\Phi_1(1s-\vec{k})|^2\,.$$

The integral over $d\Omega_k$ was done analytically, and integrals over t and k have been evaluated numerically. At low velocities the average charge squared tends towards the Z_1^2+N limit while at high velocities it tends toward the $(Z_1-N)^2$ limit. Roughly speaking at the lower velocities the interaction tends to be a close encounter and the projectile target and nucleus scatter incoherently. At high velocities the interaction region tends to move to larger distances and screening of the projectile nucleus by the projectile electrons becomes important. We also note that the screening, i.e., $Z_1^2\sigma_{He^0}/\sigma_{He^{2+}}$, does not scale to v/Z_2. Hence PWBA cross sections do not follow a universal curve[1,30] when the projectile carries electrons into the collision.

Now consider briefly the validity of these PWBA results. The general criterion[31,32] usually required at high energies is that $v_0a\ll 1$, where V_0 and a are the strength and range of the interaction potential. More specific criteria required by Madison and Merzbacher[1] for direct Coulomb ionization by bare projectiles are $Z_1/Z_2\ll 1$ and $Z_1/Z_2\ll v$. These criteria correspond to a weak disturbance of the target by the interaction. However, since here the Born approximation has been applied to both target and projectile electron states, it is necessary that both the target and projectile electrons be weakly disturbed. Now if $Z_2\lesssim Z_1$ then at sufficiently high velocities one may expect the usual criteria to apply where the projectile nucleus is effectively screened by the projectile electrons. However, if $Z_2>Z_1$, whenever Z_1 is close enough to ionize the electron on Z_2 then Z_2 may strongly influence the relatively weakly bound electrons on Z_1. This may occur even at high velocities for neutral projectiles since the screening damps out the cross sections at small t, i.e., $Z_1^2(t)\to(Z_1-Z_1)=0$ as t goes to zero. This screening forces the cross section to larger momentum transfers where the interaction is not so gentle, and the projectile electrons are strongly perturbed.

There are, in addition, restrictions on PWBA calculations for projectiles carrying electrons imposed by ignoring variation of $t_{\min}=\Delta E/v$ with final projectile states.[16] These effects may be large when v is small or when $Z_1 \gtrsim Z_2$ where ΔE changes appreciably. Also antisymmetrization[6] of projectile and target electrons, which we have ignored, may be important at the lower velocities.

In conclusion, simple analytic expressions for the effective projectile charge, $Z_1(t)$ based on the first Born approximation are given, and compared to recently observed results. There is evidence that the effective projectile charge is independent of the target in the cases considered here.

Note added in proof. Our theory is equivalent to that in the very recent paper by Manson and Toburen,[33] except that they also include cross sections for elastic and inelastic scattering of the target.

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