Stopping power for partially stripped ions

Yong-Ki Kim and Kwok-tsang Cheng
Argonne National Laboratory, Argonne, Illinois 60439
(Received 10 December 1979)

The Bethe formula for the stopping power for bare ions is extended to the collisions between partially stripped ions and neutral atoms. The resulting formulas can be presented in the same form as the original Bethe formula by replacing the nuclear charge of the projectile Z and the mean excitation energy I by Z_{eff} and I_{eff}, respectively. Both Z_{eff} and I_{eff} contain contributions from excitations (including ionizations) of the target by the projectile, excitations of the projectile by the target, and mutual excitations. They are defined in terms of projectile and target properties that can be calculated from first principles. Expressions for Z_{eff} and I_{eff} reduce to those in the Bethe formula for bare incident ions. Formulas for atom-atom and ion-ion collisions are also presented. Comparison with experimental data on Ar ions in Ar gas indicates that the new formula is reliable for projectile energies greater than a few MeV/amu.

I. INTRODUCTION

The stopping power for a bare projectile of charge $Z^{(p)}e$ and speed $v^{(p)}$ is given by the Bethe formula[1]

$$-\frac{dE}{dx}=N_0\,\mathcal{R}\,\frac{4\pi a_0^2}{T/\mathcal{R}}\,2N^{(t)}(Z^{(p)})^2\ln\left(\frac{4T}{I^{(t)}}\right), \qquad (1)$$

where N_0 is the density of target atoms, a_0 is the Bohr radius, and $T=\frac{1}{2}m_e(v^{(p)})^2$ with the electron rest mass m_e, $\mathcal{R}$ is the Rydberg energy, $N^{(t)}$ is the number of electrons in the target, and $I^{(t)}$ is the mean excitation energy of the target. Throughout this paper we use superscripts (p) for the incident projectile and (t) for the target. The mean excitation energy I of an atom or ion with N electrons is defined in terms of the dipole oscillator strength distribution $L(0)$ as[1,2]:

$$N\ln\left(\frac{I}{\mathcal{R}}\right)=L(0)=\sum_{n\neq 0}f_n\ln\left(\frac{E_n}{\mathcal{R}}\right), \qquad (2)$$

where f_n is the dipole oscillator strength for the transition from the ground state $|0\rangle$ to the excited state $|n\rangle$, E_n is the transition energy, and the summation includes all discrete and continuum excitations.

The Bethe formula is based on the first Born approximation, and it is valid for fast bare ions. The factor of 2 in front of $(Z^{(p)})^2$ in Eq. (1) emphasizes the fact that glancing collisions and knock-on collisions contribute equally [i.e., $(Z^{(p)})^2$ each] to the stopping power.

When both the projectile and the target carry orbital electrons, energy loss due to collisional excitations occurs through one of the three mechanisms: (a) excitation of the target while the projectile remains in the ground state, (b) excitation of the projectile while the target remains unexcited, and (c) excitation of both the projectile and the target. For a bare projectile, only mechanism (a) applies.

Also, for a bare projectile, any energy loss by the ion results in the slowing down of the ion as well as energy deposition in the target. For a partially stripped ion, however, process (b) above slows down the ion but no energy is deposited in the target. The process simply converts the kinetic energy of the projectile to its internal energy. For instance, in an experiment where the projectile beam passes through a thin foil, different values of dE/dx will be obtained depending on whether the energy deposited in the foil is measured or the loss in kinetic energy of the ion is measured.

The situation becomes more complicated if the projectile is in a metastable state. In such a case, the target can be excited without slowing down the projectile, and it is even possible that the ion is accelerated after a collision (particularly for light projectile on heavy target) by converting its internal energy to kinetic energy.

In the present work, we develop the theory for the loss in kinetic energy of the projectile; i.e., we include process (b) in the derivation of the stopping power. We also assume that all projectiles are in the ground state.

Qualitatively, for glancing collisions with large impact parameters, electrons in the target atom see a fully screened charge of the projectile, whereas the bare nuclear charge of the projectile is responsible for knock-on collisions with small impact parameters. These conclusions are clearly reflected in the results presented below.

In reality, due to electron pick-up and stripping, the charge state of the projectile changes during the passage through a layer of target. The usual procedure to account for the fluctuation of the charge state is to replace $Z^{(p)}$ in Eq. (1) by an effective charge $\gamma^{(p)}$ which is often determined empirically.[3] For comparison with experiment, empirical terms such as the inner-shell correction[2] are also added to Eq. (1).

In this paper we generalize the Bethe formula, Eq. (1), to ion-ion, ion-atom, and atom-atom collisions, utilizing sum rules on the Born cross section for such collisions.[4] Further refinement of the Bethe formula (e.g., charge pick-up, inner-shell, and Z^3 corrections) is beyond the scope of the present work. The generalization of the Bethe formula does not involve any empirical adjustments. Atomic constants that appear in the final results can be determined either from first principles or from experimental data such as the dipole oscillator strength distribution and x-ray form factors. As an illustration, the stopping power for Ar ions colliding with Ar gas is calculated according to the generalized formula and compared with experiment.

II. THEORY

A. Preliminary

It is convenient to define the mean energy-loss cross section, σ_E, by

$$-dE/dx = N_0 \mathcal{R} \sigma_E \,, \tag{3}$$

where σ_E is the sum of all excitation energies weighted by corresponding inelastic cross sections:

$$\sigma_E = \sum_{n\neq 0} \sigma_{0n} \frac{E_n^{(t)}}{\mathcal{R}} + \sum_{m\neq 0} \sigma_{m0} \frac{E_m^{(p)}}{\mathcal{R}} + \sum_{m\neq 0} \sum_{n\neq 0} \sigma_{mn} \frac{(E_m^{(p)} + E_n^{(t)})}{\mathcal{R}} \,. \tag{4}$$

In Eq. (4) σ denotes collision cross sections. The first subscript of σ refers to the excitation of the projectile and the second one of the target (0 for elastic scattering). The first, second, and third sums on the right-hand side (RHS) of Eq. (4) correspond to energy-loss mechanisms (a), (b), and (c) of Sec. I, respectively.

In the Born approximation, the collision cross section σ_{mn} for the excitation of the projectile to state $|m\rangle$ and the target to state $|n\rangle$ ($m=0$ and $n=0$ included) is given by[4]

$$\sigma_{mn} = \frac{4\pi a_0^2}{T/\mathcal{R}} \int_{Q_{\min}(m,n,T)}^{Q_{\max}(m,n,T)} |F_m^{(p)}(Q)|^2 \, |F_n^{(t)}(Q)|^2 \frac{dQ}{Q^2} \,, \tag{5}$$

where $Q \equiv (Ka_0)^2$ is defined in terms of momentum transfer $\vec{K}\hbar$. For fast collisions[4]

$$Q_{\min} \cong (E_m^{(p)} + E_n^{(t)})^2 / 4T\mathcal{R} \,. \tag{6a}$$

The maximum momentum transfer is limited to

$$Q_{\max} \cong 4T/\mathcal{R} \tag{6b}$$

for heavy projectiles.[5]

For a particle with nuclear charge Ze and N electrons, the Born form factors in Eq. (5) are defined as

$$F_n(Q) = \left\langle n \left| Z - \sum_j e^{i\vec{K}\cdot\vec{r}_j} \right| 0 \right\rangle , \tag{7}$$

where $\vec{r}_j$ is the position vector of the jth electron. For elastic scattering, $F_0(Q)$ can be expressed in terms of the x-ray form factor $F(Q)$ as

$$F_0(Q) = Z - F(Q) = Z - \left\langle 0 \left| \sum_j e^{i\vec{K}\cdot\vec{r}_j} \right| 0 \right\rangle , \tag{8}$$

while for inelastic scattering, $F_n(Q)$ ($n \neq 0$) is related to the generalized oscillator strength[1] (GOS) $f_n(Q)$ as

$$|F_n(Q)|^2 = Q(\mathcal{R}/E_n) f_n(Q) = \left| \left\langle n \left| \sum_j e^{i\vec{K}\cdot\vec{r}_j} \right| 0 \right\rangle \right|^2 . \tag{9}$$

For small Q, the elastic form factor $F_0(Q)$ and the GOS $f_n(Q)$ can be expanded into power series of Q:

$$F_0(Q) = \zeta + a_1 Q + a_2 Q^2 + \cdots \,, \tag{10}$$

$$f_n(Q) = f_n + b_1 Q + b_2 Q^2 + \cdots \,, \tag{11}$$

where $\zeta = Z - N$ is the net charge, f_n is the dipole oscillator strength used in Eq. (2), and $a_1, a_2, \ldots, b_1, b_2, \ldots$ are atomic constants related to the expectation values of powers of r. For large Q, asymptotic behavior of $F_0(Q)$ and $f_n(Q)$ is also known[6,7]:

$$F_0(Q) = Z - (a_1' Q^{-2} + a_2' Q^{-3} + \cdots) \,, \tag{12}$$

$$f_n(Q) = b_1' Q^{-3} + b_2' Q^{-4} + \cdots \,, \tag{13}$$

where $a_1', a_2', \ldots, b_1', b_2', \ldots$ are again atomic constants that can be calculated from the wave functions.

In calculating the stopping power, it is convenient to introduce the incoherent scattering function $S(Q)$ which appears in the sum rules for the Born cross sections[6,8-10]

$$NS(Q) = Q \sum_{n\neq 0} \left(\frac{\mathcal{R}}{E_n} \right) f_n(Q) \,. \tag{14}$$

For small Q,

$$S(Q) = c_1 Q + c_2 Q^2 + \cdots \,, \tag{15}$$

while for large Q,

$$S(Q) = 1 + c_1' Q^{-2} + c_2' Q^{-3} + \cdots \,, \tag{16}$$

where $c_1, c_2, \ldots, c_1', c_2', \ldots$ are atomic constants.

To derive the Bethe formula, Eq. (1), the projectile is taken as a bare charge ($N^{(p)}=0$), and the first sum on the RHS of Eq. (4) is carried out, keeping only two leading terms ($\ln T/T$ and T^{-1}) in the expansion of the cross section σ_{0n} in inverse powers of T.[11] Higher-order terms of the Born approximation compete with other mechanisms that were excluded from the Born approximation such as the electron exchange, distortion of the charge distribution of the projectile as well as that of the target. To extend the Bethe formula to partially stripped ions, we also retain the same leading terms only.

B. Ion-ion collision

As we have mentioned before, there are three mechanisms leading to energy losses. We discuss their respective contributions.

1. Projectile elastic, target inelastic

From Eqs. (5)–(9), the first term on the RHS of Eq. (4) becomes

$$I_{\mathrm{el,inel}}=\sum_{n\neq 0}\sigma_{0n}E_n^{(t)}/\mathcal{R}$$

$$=\frac{4\pi a_0^2}{T/\mathcal{R}}\sum_{n\neq 0}\int_{Q_{\min}}^{Q_{\max}}|F_0^{(p)}(Q)|^2 f_n^{(t)}(Q)\,\frac{dQ}{Q}\,. \tag{17}$$

From the series expansion of $F_0(Q)$ and $f_n(Q)$ near $Q=0$ [Eqs. (10), (11)] and the definition of $Q_{\min}$ [Eq. (6a)], we have

$$\int_0^{Q_{\min}}[|F_0^{(p)}(Q)|^2 f_n^{(t)}(Q)-(\zeta^{(p)})^2 f_n^{(t)}]\,\frac{dQ}{Q}=O(Q_{\min})$$

$$\cong O(T^{-1})\,. \tag{18}$$

We can thus extend the lower limit of integration to zero in Eq. (17) and replace $Q_{\max}$ by $4T/\mathcal{R}$ [Eq. 6(b)]:

$$I_{\mathrm{el,inel}}=\frac{4\pi a_0^2}{T/\mathcal{R}}\sum_{n\neq 0}\left[\int_0^{4T/\mathcal{R}}[|F_0^{(p)}(Q)|^2 f_n^{(t)}(Q)-(\zeta^{(p)})^2 f_n^{(t)}]\,\frac{dQ}{Q}+2(\zeta^{(p)})^2 f_n^{(t)}\ln\left(\frac{4T}{E_n^{(t)}}\right)\right]+O(T^{-2})\,. \tag{19}$$

Since the limits of integration are constants now, we can interchange the summation and the integration. Utilizing the Kuhn-Reich sum rule $\sum_{n\neq 0}f_n=N$ and the Bethe sum rule $\sum_{n\neq 0}f_n(Q)=N$, we get

$$I_{\mathrm{el,inel}}=\frac{4\pi a_0^2}{T/\mathcal{R}}\left[N^{(t)}\int_0^{4T/\mathcal{R}}[|F_0^{(p)}(Q)|^2-(\zeta^{(p)})^2]\,\frac{dQ}{Q}+2N^{(t)}(\zeta^{(p)})^2\ln\left(\frac{4T}{\mathcal{R}}\right)-2(\zeta^{(p)})^2 N^{(t)}\ln\left(\frac{I^{(t)}}{\mathcal{R}}\right)\right]+O(T^{-2})\,, \tag{20}$$

where $I^{(t)}$ is the mean excitation energy of the target defined in Eq. (2). To factor out the leading T^{-1} dependence in the above expression, we rewrite the integral on the RHS as

$$I_F=\int_0^{4T/\mathcal{R}}[|F_0(Q)|^2-\zeta^2]\frac{dQ}{Q}$$

$$=\int_0^{Q_1}[|F_0(Q)|^2-\zeta^2]\,\frac{dQ}{Q}-\int_{Q_1}^{\infty}[Z^2-|F_0(Q)|^2]\frac{dQ}{Q}$$

$$+\int_{Q_1}^{4T/\mathcal{R}}(Z^2-\zeta^2)\,\frac{dQ}{Q}+\int_{4T/\mathcal{R}}^{\infty}[Z^2-|F_0(Q)|^2]\,\frac{dQ}{Q} \tag{21}$$

Here, Q_1 is an arbitrary constant. For convenience, we choose $Q_1=1$. From the asymptotic behavior of $F_0(Q)$ [Eq. (12)], we find that the last integral on the RHS of Eq. (21) is of the order of T^{-2}. Thus,

$$I_F=\int_0^1[|F_0(Q)|^2-\zeta^2]\,\frac{dQ}{Q}-\int_1^{\infty}[Z^2-|F_0(Q)|^2]\,\frac{dQ}{Q}$$

$$+(Z^2-\zeta^2)\ln(4T/\mathcal{R})+O(T^{-2})\,. \tag{22}$$

If we define G_F as

$$(Z^2+\zeta^2)\ln\left(\frac{G_F}{\mathcal{R}}\right)=\int_1^{\infty}[Z^2-|F_0(Q)|^2]\,\frac{dQ}{Q}$$

$$-\int_0^1[|F_0(Q)|^2-\zeta^2]\frac{dQ}{Q}\,, \tag{23}$$

then, from Eqs. (20)–(23),

$$I_{\mathrm{el,inel}}=\frac{4\pi a_0^2}{T/\mathcal{R}}\left[N^{(t)}[(Z^{(p)})^2+(\zeta^{(p)})^2]\ln\left(\frac{4T}{G_F^{(p)}}\right)\right.$$

$$\left.-2(\zeta^{(p)})^2N^{(t)}\ln\left(\frac{I^{(t)}}{\mathcal{R}}\right)\right]+O(T^{-2})\,. \tag{24}$$

2. Projectile inelastic, target elastic

In this case, the result is the same as Eq. (24) with superscripts p and t interchanged:

$$I_{\text{inel,el}} = \frac{4\pi a_0^2}{T/\mathcal{R}}\left[N^{(p)}[(Z^{(t)})^2 + (\zeta^{(t)})^2]\ln\left(\frac{4T}{G_F^{(t)}}\right) - 2(\zeta^{(t)})^2 N^{(p)}\ln\left(\frac{I^{(p)}}{\mathcal{R}}\right)\right] + O(T^{-2}). \tag{25}$$

3. Projectile inelastic, target inelastic

For the third sum on the RHS of Eq. (4), we have, from Eq. (9),

$$I_{\text{inel,inel}} = \sum_{m\neq 0, n\neq 0} \sigma_{mn}\frac{(E_m^{(p)}+E_n^{(t)})}{\mathcal{R}} = \frac{4\pi a_0^2}{T/\mathcal{R}}\sum_{m\neq 0, n\neq 0}\int_{Q_{\min}}^{Q_{\max}}\left(f_m^{(p)}(Q)\frac{f_n^{(t)}(Q)}{E_n^{(t)}/\mathcal{R}} + \frac{f_m^{(p)}(Q)}{E_m^{(p)}/\mathcal{R}}f_n^{(t)}(Q)\right)dQ. \tag{26}$$

From the series expansion of $f_n(Q)$ [Eq. (11)], we can extend the lower limit of integration from $Q_{\min}$ to zero in Eq. (26) by neglecting terms of order T^{-2}. Utilizing the Kuhn-Reich and the Bethe sum rules, and from the definition of the incoherent scattering function $S(Q)$ given by Eq. (14), we have

$$I_{\text{inel,inel}} = \frac{4\pi a_0^2}{T/\mathcal{R}} N^{(p)}N^{(t)}\left(\int_0^{4T/\mathcal{R}} S^{(p)}(Q)\frac{dQ}{Q} + \int_0^{4T/\mathcal{R}} S^{(t)}(Q)\frac{dQ}{Q}\right) + O(T^{-2}). \tag{27}$$

To extract the leading T^{-1} terms on the RHS of the above relation, we set

$$\int_0^{4T/\mathcal{R}} S(Q)\,\frac{dQ}{Q} = \int_0^1 S(Q)\,\frac{dQ}{Q} - \int_1^\infty [1-S(Q)]\,\frac{dQ}{Q} + \ln(4T/\mathcal{R}) + O(T^{-2}), \tag{28}$$

where we have made use of the asymptotic behavior of $S(Q)$ given in Eq. (16). If we define G_S such that

$$\ln\left(\frac{G_S}{\mathcal{R}}\right) = \int_1^\infty [1-S(Q)]\,\frac{dQ}{Q} - \int_0^1 S(Q)\,\frac{dQ}{Q}, \tag{29}$$

we then have

$$I_{\text{inel,inel}} = \frac{4\pi a_0^2}{T/\mathcal{R}}\, 2N^{(p)}N^{(t)}\ln\left(\frac{4T}{(G_S^{(p)}G_S^{(t)})^{1/2}}\right) + O(T^{-2}). \tag{30}$$

Combining results of Eqs. (24), (25), and (30), σ_E for ion-ion collision becomes

$$\sigma_E(\text{ion-ion}) = \frac{4\pi a_0^2}{T/\mathcal{R}}\, 2N^{(t)}Z_{\text{eff}}^2\ln\left(\frac{4T}{I_{\text{eff}}}\right), \tag{31}$$

where Z_{eff} and I_{eff} are defined as

$$2N^{(t)}Z_{\text{eff}}^2 = N^{(t)}[(Z^{(p)})^2 + (\zeta^{(p)})^2] + N^{(p)}[(Z^{(t)})^2 + (\zeta^{(t)})^2] + 2N^{(p)}N^{(t)} \tag{32}$$

and

$$\begin{aligned} 2N^{(t)}Z_{\text{eff}}^2\ln(I_{\text{eff}}/\mathcal{R}) = {}& N^{(t)}[(Z^{(p)})^2 + (\zeta^{(p)})^2]\ln(G_F^{(p)}/\mathcal{R}) \\ &+ N^{(p)}[(Z^{(t)})^2 + (\zeta^{(t)})^2]\ln(G_F^{(t)}/\mathcal{R}) + 2(\zeta^{(p)})^2N^{(t)}\ln(I^{(t)}/\mathcal{R}) \\ &+ 2(\zeta^{(t)})^2N^{(p)}\ln(I^{(p)}/\mathcal{R}) + N^{(p)}N^{(t)}\ln(G_S^{(p)}G_S^{(t)}/\mathcal{R}^2). \end{aligned} \tag{33}$$

It is obvious that Eq. (31) is a generalization of the Bethe formula given in Eq. (1) by replacing $Z^{(p)}$ and $I^{(t)}$ by Z_{eff} and I_{eff}, respectively. We can understand the role and origin of each term in Eq. (32) easily. The first term on the RHS of Eq. (32), $N^{(t)}(Z^{(p)})^2$, comes from the excitation of the target electrons ($N^{(t)}$) by the bare charge of the projectile as a result of close collisions with large momentum transfers. The second term, $N^{(t)}(\zeta^{(p)})^2$, arises from distant collisions (small momentum transfers) where the target "sees" a fully screened projectile. The third and fourth terms are the same as the first two with the roles of the projectile and the target interchanged. The last term of Eq. (32), of course, comes from the mutual excitation of the projectile electrons ($N^{(p)}$) and those of the target ($N^{(t)}$) by close collisions.

The terms contributing to I_{eff} [Eq. (33)] come both from close and distant collisions; they are well defined in terms of the projectile and target properties, but their evaluation requires the knowledge of the x-ray form factors [Eqs. (8) and (23)], incoherent scattering functions [Eqs. (14) and (29)], and the dipole oscillator strength distribution [Eqs. (2), (24), and (25)]. These properties can be measured from x-ray scattering, electron scattering, and photoabsorption experiments, unrelated to the ion-atom collision we are focusing upon here. They can also be calculated from wave functions if they are known. The term that is most difficult to calculate theoretically is $\ln(I/\mathcal{R})$ defined in Eq. (2), because the summation covers all dipole-allowed states including the continuum. One can deduce $\ln(I/\mathcal{R})$, however, if any of the stopping powers for fast bare particles (protons, electrons, α particles, etc.) are known for the same target.

Since I_{eff} appears in a denominator in Eq. (31), a larger value of I_{eff} leads to a smaller stopping power. The contributions from mechanisms (a), (b), and (c) are divided into Z_{eff} and I_{eff} [Eqs. (32) and (33)] in such a way that all binding effects of the electrons in the projectile and the target are put in I_{eff}. As a result, the RHS of Eq. (32) amounts to treating the electrons on the projectile and the target as free electrons. The first term on the RHS of Eq. (33) represents the screening of the projectile nucleus by the electrons on it during the excitation of the target electrons. The second term accounts for the screening of the target nucleus during the excitation of the projectile electrons. The third and fourth terms similarly adjust for the binding effects in the contribution of glancing collisions [ζ^2 terms in Eq. (32)]. The last term of Eq. (33) stems from the binding effects in mechanism (c), and this term is the smallest in magnitude.

C. Ion-atom collisions

Since there is no net charge on the target ($\zeta^{(t)}=0$), we have, from Eqs. (31)–(33)

$$\sigma_E(\text{ion-atom}) = \frac{4\pi a_0^2}{T/\mathcal{R}}\, 2N^{(t)}Z_{\text{eff}}^2 \ln\left(\frac{4T}{I_{\text{eff}}}\right), \tag{34}$$

where

$$2N^{(t)}Z_{\text{eff}}^2 = N^{(t)}[(Z^{(p)})^2 + (\zeta^{(p)})^2] + N^{(p)}(Z^{(t)})^2 + 2N^{(p)}N^{(t)} \tag{35}$$

and

$$2N^{(t)}Z_{\text{eff}}^2 \ln(I_{\text{eff}}/\mathcal{R}) = N^{(t)}[(Z^{(p)})^2 + (\zeta^{(p)})^2]\ln(G_F^{(p)}/\mathcal{R}) + N^{(p)}(Z^{(t)})^2\ln(G_F^{(t)}/\mathcal{R}) + 2(\zeta^{(p)})^2 N^{(t)}\ln(I^{(t)}/\mathcal{R}) + N^{(p)}N^{(t)}\ln(G_S^{(p)}G_S^{(t)}/\mathcal{R}^2)\,. \tag{36}$$

Here G_F and G_S are defined in Eqs. (23) and (29), respectively, with $\zeta^{(t)}=0$. The origin of Z_{eff} is the same as in the case of ion-ion collision, except for the lack of the distant collision term [$N^{(p)}(\zeta^{(t)})^2$ in Eq. (32)], because there is no net charge on the target as seen by the projectile at a distance.

If the incident projectile is a bare ion, we have $N^{(p)}=0$ and $F_0^{(p)}(Q)=Z^{(p)}=\zeta^{(p)}$. As a result, $G_F^{(p)}=\mathcal{R}$, $Z_{\text{eff}}=Z^{(p)}$, $I_{\text{eff}}=I^{(t)}$, and Eq. (34) simply reduces to the Bethe formula of Eq. (1).

D. Atom-atom collisions

Since there is no net charge on either the projectile or the target, we have $\zeta^{(p)}=\zeta^{(t)}=0$. From Eqs. (31)–(33),

$$\sigma_E(\text{atom-atom}) = \frac{4\pi a_0^2}{T/\mathcal{R}}\, 2N^{(t)}Z_{\text{eff}}^2 \ln\left(\frac{4T}{I_{\text{eff}}}\right) + O(T^{-2})\,, \tag{37}$$

where

$$2N^{(t)}Z_{\text{eff}}^2 = N^{(t)}(Z^{(p)})^2 + N^{(p)}(Z^{(t)})^2 + 2N^{(p)}N^{(t)} \tag{38}$$

and

$$2N^{(t)}Z_{\text{eff}}^2 \ln(I_{\text{eff}}/\mathcal{R}) = N^{(t)}(Z^{(p)})^2 \ln(G_F^{(p)}/\mathcal{R}) + N^{(p)}(Z^{(t)})^2 \ln(G_F^{(t)}/\mathcal{R}) + N^{(p)}N^{(t)}\ln(G_S^{(p)}G_S^{(t)}/\mathcal{R}^2)\,. \tag{39}$$

The origin of the terms in Z_{eff} is the same as that in the case of the ion-ion collision, except for the lack of any distant collision terms [$N^{(t)}(\zeta^{(p)})^2$ and $N^{(p)}(\zeta^{(t)})^2$ in Eq. (32)].

III. DISCUSSION

As is clear from the original work by Bethe and the derivations in Sec. II, the stopping power formulas (31)–(39) should be used at high energies. In principle the projectile speed should be much faster than any of the orbital speeds of the electrons attached to the projectile or the target. With the ion accelerators currently available, only light ions can be accelerated to sufficiently high speed to satisfy the validity of the underlying Born approximation. At such high speeds, however, the light ions are likely to be stripped fully by the target. Furthermore, each term in the stopping power formulas (31)–(39) was calculated with the assumption that the net charge of the projectile remains constant, which is somewhat unrealistic. The actual charge state of the projectile will be determined by the competition between stripping and charge pick-up, as was mentioned earlier. Experimental evidences[12] are such that the electrons on the projectile will be stripped if their orbital velocities are of the same order or slower than the projectile speed.

The preceding derivations are based on particle-particle collision cross section, and the formulas presented here are appropriate for collisions in the gas phase. If the gas pressure is sufficient to establish an equilibrium charge distribution of the projectile, one can use the most probable charge state as $\zeta^{(p)}$ in Eqs. (31)–(39). Our results on Ar ions presented below show that the stopping powers are not very sensitive to a small change in $\zeta^{(p)}$ as long as $\zeta^{(p)}$ is sufficiently different from zero or from $Z^{(p)}$.

If the charge-state distribution of the incident ion is known, one could accordingly used the weighted sum of the stopping power for each charge state. For a projectile in metastable state we must distinguish the loss of the kinetic energy and that of the internal energy of the ion as we mentioned in the Introduction. Furthermore, we must understand the partition of the released internal energy among competing processes—excitation and ionization of the target, acceleration of the target, and acceleration of the projectile, which depend on details such as energy levels, ionization potentials, and masses of the projectile and the target.

Although extended formulas for the stopping power have room for further improvement, it can nevertheless provide, in its present form, useful estimates of the $-dE/dx$ in high-energy ion-atom collisions where there are no proven methods.

Formulas (31), (34), and (37) can be extended to projectiles with relativistic speed as in the case of the bare projectile[13] by replacing

(a) $4\pi a_0^2 \mathcal{R}/T$ by $4\pi a_0^2 \alpha^2/\beta^2$,

and

(b) $\ln\left(\frac{4T}{I_{eff}}\right)$ by $\ln\left(\frac{4\beta^2\mathcal{R}}{(1-\beta^2)\alpha^2 I_{eff}}\right)-\beta^2$,

where α is the fine-structure constant and $\beta = v^{(p)}/c$, c being the speed of light. Thus, the relativistic form of Eqs. (31), (34), and (37) becomes

$$\sigma_E = \frac{4\pi a_0^2 \alpha^2}{\beta^2} 2N^{(t)} Z_{eff}^2 \left[\ln\left(\frac{4\beta^2\mathcal{R}}{(1-\beta^2)\alpha^2 I_{eff}}\right) - \beta^2\right]. \quad (40)$$

TABLE I. Constants for the stopping powers for $Ar^{\zeta+}$ in Ar. [$N^{(t)}=18$, $\ln(G_F^{(t)}/\mathcal{R})=3.418$, $\ln(G_S^{(t)}/\mathcal{R})=2.034$, $I^{(t)}=179$ eV.]

Ion	$N^{(p)}$	$\ln(G_F^{(p)}/\mathcal{R})$	$\ln(G_S^{(p)}/\mathcal{R})$	Z_{eff}	I_{eff} (eV)
Ar^{18+}	0	0	0	18	179.0
Ar^{17+}	1	0.3534	5.334	17.79	224.7
Ar^{16+}	2	0.7242	5.292	17.61	280.9
Ar^{15+}	3	0.9435	4.368	17.45	298.8
Ar^{14+}	4	1.171	3.887	17.32	317.0
Ar^{13+}	5	1.422	3.817	17.22	340.3
Ar^{12+}	6	1.678	3.751	17.15	363.3
Ar^{11+}	7	1.937	3.686	17.10	385.4
Ar^{10+}	8	2.195	3.622	17.09	406.3
Ar^{9+}	9	2.450	3.557	17.10	425.3
Ar^{8+}	10	2.698	3.491	17.15	442.3
Ar^{7+}	11	2.840	3.193	17.22	428.8
Ar^{6+}	12	2.972	2.933	17.32	416.9
Ar^{5+}	13	3.090	2.771	17.45	407.0
Ar^{4+}	14	3.192	2.618	17.61	398.7
Ar^{3+}	15	3.276	2.471	17.79	392.3
Ar^{2+}	16	3.341	2.327	18.00	387.7
Ar^{+}	17	3.385	2.181	18.23	385.0
Ar	18	3.418	2.034	18.49	385.9

IV. COMPARISON WITH EXPERIMENT: $Ar^{\zeta+}$ IN Ar

As an example, we compare our theoretical result for Ar ions in Ar gas with the experiment by Martin and Northcliffe.[14] The constants presented in Table I were calculated from Hartree-Fock wave functions corresponding to average configuration of each ion. The mean excitation energy of Ar, $I=179$ eV, was deduced from semiempirical oscillator strength distributions by Eggarter.[15] The data in Table I show that there is a broad

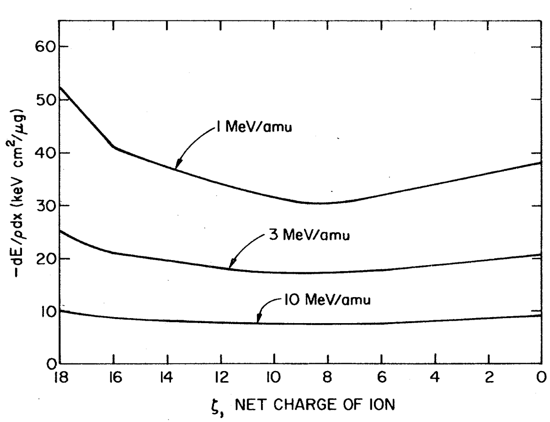

FIG. 1. Stopping powers for $Ar^{\zeta+}$ in Ar gas at different incident energies as functions of the charge state ζ. The value of $\rho=1783.7$ μg/cm^3 is used for the density of argon gas. The curves are calculated from Eqs. (34)–(36) and the data in Table I.

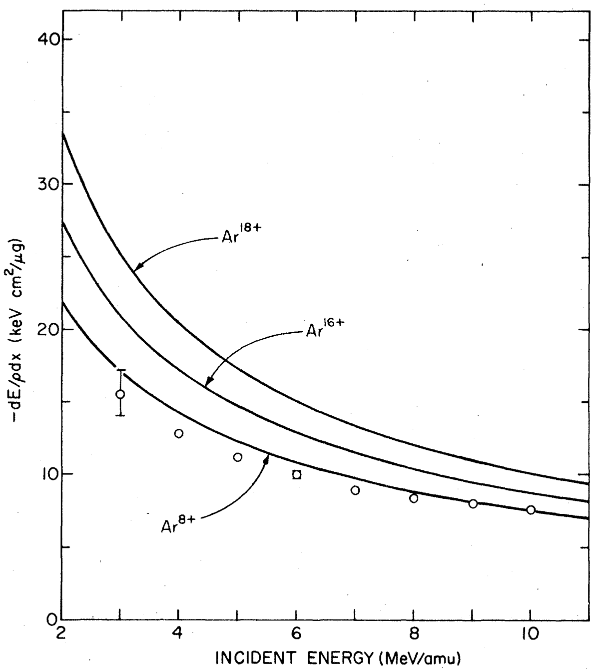

FIG. 2. Stopping powers for $Ar^{\zeta+}$ in Ar gas at different ζ as functions of incident energy. Solid curves are based on the present theory, and the circles represent the experimental data by Martin and Northcliffe (Ref. 14).

minimum in Z_{eff} near Ar^{10+} and a less broad maximum in I_{eff} at Ar^{8+}. The stopping power at a given projectile energy shows a minimum (as a function of charge state) near Ar^{8+}.

The effective charges for Ar^{+} and neutral Ar (as projectile) exceed 18 because of the contributions from mechanisms (b) and (c) mentioned in the Introduction. For ions of low-charge states, the terms with $\ln(G_F/\mathcal{R})$ in Eq. (36) dominate the value of I_{eff}. For ions of high-charge states, the major contribution to I_{eff} comes from the $\ln(I^{(t)}/\mathcal{R})$ term.

In Fig. 1, we present stopping powers for Ar ions in Ar gas at three projectile energies. We note that the stopping power for Ar^{8+} is the smallest at all projectile energies ($\leq$10 MeV/amu) as expected from the largest value of I_{eff} of the ion, although the stopping powers for ions with $\zeta = 5-10$ are all within 10% of each other. The minimum at Ar^{8+} and a sharp bend at Ar^{16+} reflect the closed-shell structures of the ions; Ar^{8+} lost all M electrons, and Ar^{16+} has only K electrons.

Also, Fig. 1 clearly shows that the $-dE/dx$ for bare projectiles is the largest. Since a bare projectile is likely to pick up electrons as it goes through target gas, actual $-dE/dx$ will be less than that for a bare ion.

In Fig. 2, we compare our results with the experiment by Martin and Northcliffe.[14] In their experiment, the charge state of the incident ion was Ar^{3+}, but the charge states of the ion after the collision were not determined. The collision cell was sealed by Ni foils at both ends and the ions must have had various charge states (>3+) in the collision cell. Among the values for various charge states, $-dE/dx$ for Ar^{8+}, the lowest one, agrees best with the experiment. At high incident energies, however, the experimental data seem to be headed toward theoretical values with higher-charge states. Since a projectile of 10 MeV/amu in the target gas is likely to carry only K electrons with it at the most, Fig. 2 suggests that the extended Bethe formula slightly overestimates the stopping power.

ACKNOWLEDGMENTS

The authors are indebted to Dr. G. H. Gillespie and Dr. M. Inokuti for valuable discussions. This work was performed under the auspices of the U. S. Department of Energy.

[1]H. A. Bethe, Ann. Phys. 5, 325 (1930).
[2]U. Fano, Annu. Rev. Nucl. Sci. 13, 1 (1963).
[3]See, for instance, J. F. Ziegler, *Helium Stopping Powers and Ranges in All Elements* (Pergamon, New York, 1977).
[4]G. H. Gillespie, Phys. Rev. A 15, 563 (1977).
[5]See, for instance, L. D. Landau and E. M. Lifshitz, *Quantum Mechanics, Non-Relativistic Theory* (Pergamon, Oxford, 1965), 2nd ed., p. 587.
[6]O. Goscinski and P. Lindner, J. Chem. Phys. 52, 2539 (1970).
[7]E. N. Lassettre, J. Chem. Phys. 43, 4479 (1965).
[8]V. H. Smith, Jr., Chem. Phys. Lett. 7, 226 (1970).
[9]M. Inokuti, Y.-K. Kim, and R. L. Platzman, Phys. Rev. 164, 55 (1967).
[10]Y.-K. Kim and M. Inokuti, Phys. Rev. 165, 39 (1968).
[11]M. Inokuti, Rev. Mod. Phys. 43, 297 (1971).
[12]H. D. Betz, Rev. Mod. Phys. 44, 465 (1972).
[13]H. A. Bethe, Z. Phys. 76, 293 (1938).
[14]F. W. Martin and L. C. Northcliffe, Phys. Rev. 128, 1166 (1962).
[15]E. Eggarter, J. Chem. Phys. 62, 833 (1975).