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Partial stopping power and straggling effective charges of heavy ions in condensed matter

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The stopping-power effective charge (SPEC) has been formulated in the Brandt-Kitagawa (BK) model. In the effective-charge theory, the stopping power of heavy ions can be obtained by scaling using the SPEC with a mean charge state. Based on the BK treatment for the statistical ion screening and the dielectric function, a formula for the straggling effective charge (SGEC) has been obtained. The SGEC, which is different from the SPEC, provides the scaling of collisional (without charge exchange) straggling in the effective-charge theory. To properly describe the stopping power and straggling of heavy projectiles in condensed matter, partial effective charges (PEC's) are introduced to describe the charge-state-dependent stopping power and straggling in a charge-state model. The partial stopping power and straggling of projectiles with a fixed charge state can be obtained by scaling to those of the bare nucleus with related PEC's. This allows the calculation of the total stopping power and straggling of heavy projectiles in a charge-state description including the charge-exchange effect.

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I. INTRODUCTION

Stopping power and straggling are the most important parameters of the energy-loss process of energetic ions passing through matter. The energy-loss process of heavy ions is complicated because of the charge-exchange effect which leads to charge-state fluctuations. The stopping power of heavy ions has been studied extensively and described by the effective-charge concept [1]. With the dielectric-function method [2], Brandt and Kitagawa (BK) [3] have derived a well-known formula by describing the electronic density distribution in a statistical manner. Comprehensive data compilations have led to a widely used empirical formula [4] for the stopping power of heavy ions based on the BK theory. By introducing the charge states of a projectile into the transport equation, the contributions from the charge-exchange effect can be derived in addition to the collisional term (for the projectile with a fixed charge state) of stopping power and straggling [5,6]. However, energy straggling has not been studied as extensively as stopping power because of the difficulties associated with charge-exchange effect [7,8]. By applying the stopping-power effective charge (SPEC) to the collisional straggling, an empirical formula for energy straggling [9] has been obtained including the charge exchange contribution. Although the effective-charge model well describes the stopping power, there are ambiguities in describing the screening of ions in condensed matter [10].

Recently, more promising studies have been presented in a charge-state description. Some calculations [3,11–13] and measurements [14–22] have been available for the charge-state-dependent stopping power and straggling. A Monte Carlo simulation [23] with a charge-state model predicted large discrepancies from TRIM [4], which is based on the BK effective-charge theory, for implanted range and range straggling. A general statistical description [6] for stopping power and straggling has been presented including the charge-exchange effect, in which the Bethe-Landau integral [24] for the energy-loss spectrum of a point charge was generalized into a square matrix to include the incoming and outgoing charge states. In a charge-state approach [25], good agreement with available experimental data for the total stopping power of H and He ions in Al has been demonstrated. In the case of heavy ions, however, the charge-state model is very complicated and not practical for a full calculation of the contribution from each charge state.

The stopping power and straggling can be divided into a collisional contribution (without charge exchange) and a charge-exchange contribution (from charge-state fluctuations) [5–9,11,25]. So far, some theoretical and experimental studies have been performed on the charge-exchange contribution to energy straggling [5–9,11]. The straggling effective charge (SGEC) for heavy ions, which could be used for the scaling of collisional straggling, has not been studied. Instead, the effective charge derived from stopping power was used to perform the approximate scaling of collisional straggling [9,26]. However, the SGEC is different from the SPEC because energy straggling corresponds to the second-order momentum of the energy-loss process while stopping power corresponds to the first-order momentum. The SPEC derived from stopping power may be inadequate to describe the collisional straggling. To properly understand the stopping power and straggling of heavy ions, including the charge-exchange effect, it is necessary to clarify the effective-charge concept and combine it with the charge-state model.

In this paper, PEC's are introduced to describe the contribution to the stopping power and straggling from each charge state of heavy ions in condensed matter. The partial SPEC, which has been formulated in the BK treatment [3], is summarized in Sec. II. In Sec. III, a formula for the partial SGEC is derived within the BK approximation. Discussion is presented in Sec. IV with at-

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tention drawn to the nonlinear response effect [32] at low ion velocities, followed by the conclusion in Sec. V. Atomic units (a.u.) $e=\hbar=m=1$ are used below except when stated otherwise.

II. PARTIAL STOPPING-POWER EFFECTIVE CHARGE (PSPEC)

The probability of energy transfer from an energetic projectile to a free-electron gas is described by the random-phase dielectric function $\epsilon(k,\omega)$ approximation [2]. Brandt and Kitagawa [3] have derived a formula for the PSPEC in a variational statistical approximation. The results are summarized briefly below.

The stopping power of a singly charged projectile can be expressed by

$$S\equiv\frac{dE}{dx}=\frac{2}{\pi v^2}\int_0^\infty\frac{dk}{k}|\rho(k)|^2\int_0^{kv}d\omega\,\omega\,\mathrm{Im}\left[\frac{-1}{\epsilon(k,\omega)}\right], \tag{1}$$

where v is the projectile velocity and $\rho(k)$ is the Fourier transform of the spatial charge density $\rho(\mathbf{r})$ (total of nuclear and electronic charge densities) in the rest frame of the projectile. A spherically symmetric charge distribution was assumed in a statistical approximation,

$$\rho(R)=Z_1\delta(R)-\frac{N_e}{4\pi\Lambda_0^3}\frac{\Lambda_0}{R}e^{-R/\Lambda_0}, \tag{2}$$

where Z_1 is the atomic number of the projectile and N_e is the number of electrons still bound to the projectile nucleus. By finding the minimum internal energy of the projectile (nucleus and bound electrons), the screening length Λ_0 was determined by

$$\Lambda_0=\frac{2a(1-q)^{2/3}}{Z_1^{1/3}[1-(1-q)/7]}a_0, \tag{3}$$

with $a=0.240$ and $a_0=1$ a.u. = 0.529 Å is the Bohr radius. For the K-shell electrons, BK suggested $\Lambda_0=a_0/Z_{1K}$ with $Z_{1K}=Z_1$ for $N_e=1$ and $Z_{1K}=Z_1-0.3$ for $N_e=2$.

By taking into account the static screening effect of conduction electrons in the medium, the projectile screening length in condensed matter was improved to be [27]

$$\Lambda=\Lambda_0/(1-\tfrac{2}{3}k_{\mathrm{TF}}^2\Lambda_0^2), \tag{4}$$

where $k_{\mathrm{TF}}=(4k_F/\pi)^{1/2}$ is the Thomas-Fermi (TF) screening wave number and $k_F=(3\pi^2n)^{1/3}$ is the Fermi wave number with the conduction-electron density $n=3/4\pi r_s^3$. The one-electron radius r_s is the radius of the average volume occupied by each conduction electron of the medium. The screening lengths Λ_0 and Λ are shown in Fig. 1 for different ionizations $q=1-Ne/Z_1$. More screening was expected for lower charge states. Additional contributions to the stopping power and straggling of slow heavy atoms from the static screening have been studied, showing an improved agreement with experimental data [27].

The Fourier transform of $\rho(\mathbf{r})$ with spherical symmetry, Eq. (2), yields

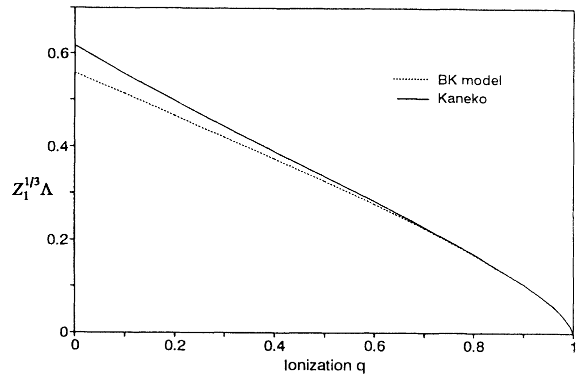

FIG. 1. Comparison of the modified ion screening radius, Eq. (4), with the BK result, Eq. (3), as a function of ionization fraction q.

$$\rho(k)=Z_1\frac{q+(k\Lambda)^2}{1+(k\Lambda)^2}. \tag{5}$$

From Eqs. (1) and (5) with suitable approximations for the dielectric function, one can obtain the partial stopping power. The PSPEC fraction is expressed by

$$\zeta(q)\equiv[S(q)/S(q=1)]^{1/2}, \tag{6}$$

where $S(q=1)$ is the stopping power for the bare nucleus of the projectile.

At high velocities where the projectile can excite plasmons in the medium, BK used the plasmonpole approximation [28] of the dielectric function and obtained the PSPEC of projectiles with ionization q,

$$\zeta^2(q)=q^2+(1-q)\times\left[(1-q)\left[\frac{1}{1+(k_+\Lambda)^2}-\frac{1}{1+(k_-\Lambda)^2}\right]+(1+q)\ln\frac{1+(k_+\Lambda)^2}{1+(k_-\Lambda)^2}\right]\Big/\ln(k_+^2/k_-^2), \tag{7}$$

where

$$k_\pm=\{2(v^2-\beta^2)\pm2[(v^2-\beta^2)^2-\Omega_p^2]\}^{1/2}, \tag{8}$$

with $\beta=3k_F^2/5$ and the collective frequency $\Omega_p=(\omega_p^2+\omega_g^2)^{1/2}$, where the plasmon frequency $\omega_p=(4\pi n)^{1/2}=(3/r_s^3)^{1/2}$ and ω_g is the effective band-gap energy of semiconductors or insulators [3]. From Eq. (8), a threshold velocity for the projectile to excite plasmons in the medium is determined by

$$v_{\mathrm{thr}}=(\beta^2+\Omega_p)^{1/2}. \tag{9}$$

At low velocities $v<v_F$ (Fermi velocity), the PSPEC fraction was approximated by

$$\zeta(q)=q+C(k_F)(1-q)\ln[1+(2k_F\Lambda)^2], \tag{10}$$

where

$$C(k_F)=\frac{\pi k_F}{(1+\pi k_F)I(\pi k_F)}-\frac{2}{\pi k_F},$$
$$I(z)=\ln(1+z)-\frac{z}{1+z}. \tag{11}$$

The first and second terms in Eq. (10) represent the contributions from the distant collision and the close collision respectively in the BK effective-charge theory [3,4].

III. PARTIAL STRAGGLING EFFECTIVE CHARGE (PSGEC)

With the dielectric function method, the energy-straggling cross section of a singly charged projectile with velocity v can be expressed by

$$\frac{\Omega^2}{Ndx}=\frac{2}{N\pi v^2}\int_0^\infty \frac{dk}{k}|\rho(k)|^2\int_0^{kv}d\omega\,\omega^2\mathrm{Im}\left[\frac{-1}{\epsilon(k,\omega)}\right], \tag{12}$$

where N is the atomic density of the medium. The PSGEC fraction of energy straggling is defined by

$$\eta(q)\equiv[\Omega(q)/\Omega(q=1)]^{1/2}, \tag{13}$$

where $\Omega(q=1)$ is the energy straggling for the bare nucleus of the projectile. Following the treatment as for stopping power, an analytical formula for η can be obtained.

At high velocities $v>v_{\mathrm{thr}}$, one can use the plasmonpole approximation [28] for the dielectric function in the limit of no damping process [3]

$$\mathrm{Im}\left[\frac{-1}{\epsilon(k,\omega)}\right]=\frac{\pi\omega_p^2}{2A}\delta(\omega-A), \tag{14}$$

with $A^2=\Omega_p^2+\beta^2k^2+k^4/4$. From Eqs. (5), (12), and (14), one obtains

$$\frac{\Omega^2}{Ndx}=\frac{\omega_p^2}{Nv^2}\int_{k_-}^{k_+}\frac{dk}{k}\rho^2(k)(\Omega_p^2+\beta^2k^2+k^4/4)^{1/2}$$
$$=\frac{\omega_p^2\Omega_pZ_1^2}{2Nv^2}\eta^2(q)f(1), \tag{15}$$

where

$$\eta^2(q)=f(q)/f(1), \tag{16}$$
$$f(q)=q^2\ln\frac{k_+^2}{k_-^2}+(1-q)^2\left[\frac{f_1(k_+\Lambda)}{1+(k_+\Lambda)^2}-\frac{f_1(k_-\Lambda)}{1+(k_-\Lambda)^2}\right]+[f_1(k_+\Lambda)-f_1(k_-\Lambda)]$$
$$+(1-q)\frac{(1+q)(2-b)+4c-2b}{2\sqrt{1-b+c}}\left[\ln\frac{1+(k_+\Lambda)^2}{1+(k_-\Lambda)^2}-\ln\frac{f_2(k_+\Lambda)}{f_2(k_-\Lambda)}\right]-q^2\ln\frac{f_3(k_+\Lambda)}{f_3(k_-\Lambda)}+\frac{b-4c(1-q)}{2\sqrt{c}}\ln\frac{f_4(k_+\Lambda)}{f_4(k_-\Lambda)},$$

with

$$f_1(z)=\sqrt{1+bz^2+cz^4},$$
$$f_2(z)=2-b+bz^2-2cz^2+2\sqrt{1-b+c}\,f_1(z),$$
$$f_3(z)=2+bz^2+2f_1(z),$$
$$f_4(z)=b+2cz^2+2\sqrt{c}\,f_1(z), \tag{17}$$
$$b=(\beta/\Omega_p\Lambda)^2,$$
$$c=1/(2\Omega_p\Lambda^2)^2.$$

At high velocities ($v\to\infty$), Eq. (8) gives $k_+\simeq 2v\to\infty$ and $k_-\simeq\Omega_p/v\to 0$, then $\eta^2(q)\to 1$ and $f(1)\simeq 2v^2/\Omega_p$. The conduction-electron density is $n=Z_2N$ because all the target electrons can be treated as free electrons at such high projectile velocities. Therefore, $\omega_p^2=4\pi n=4\pi Z_2N$ and Eq. (15) becomes the well-known Bohr formula [29]

$$\Omega_B^2=4\pi Z_1^2Z_2Ndx. \tag{18}$$

It should be noted that, at high velocities, Eq. (15) turns into the Bohr straggling for projectiles with any charge state other than that which is only for fully stripped ions (bare nucleus).

At low velocities $v<v_F$, the dielectric function is described as [3]

$$\mathrm{Im}\left[\frac{-1}{\epsilon(k,\omega)}\right]\simeq\begin{cases}\dfrac{2k\omega}{(k^2+k_D^2)^2} & \text{for } k\le 2k_F\\ 0 \text{ for } k>2k_F,\end{cases} \tag{19}$$

with a screening constant $k_D=(4k_F/\pi)^{1/2}$. Inserting Eqs. (5) and (19) into Eq. (12), the energy-straggling cross section is obtained as

$$\frac{\Omega^2}{Ndx}=\frac{v^2}{\pi N}\int_0^{2k_F}dk\frac{k^4}{(k^2+k_D^2)^2}\rho^2(k)$$
$$=\frac{k_FZ_1^2}{\pi N}\eta^2v^2[J(\pi k_F)+2], \tag{20}$$

where the PSGEC fraction is expressed by

$$\eta^2(q)=\left\{\left[1-\frac{1-q}{1-(k_D\Lambda)^2}\right]^2+\frac{2}{J(\pi k_F)}+\left[\frac{1-q}{1-(k_D\Lambda)^2}\right]^2\frac{J(4k_F^2\Lambda^2)}{J(\pi k_F)}\right.$$
$$\left.+4\frac{1-q}{1-(k_D\Lambda)^2}\left[1-\frac{1-q}{1-(k_D\Lambda)^2}\right]\frac{M(k_F,\Lambda)}{J(\pi k_F)}\right\}\Bigg/\left[1+\frac{2}{J(\pi k_F)}\right], \tag{21}$$

with

$$J(z)=\frac{1}{1+z}-3\frac{\tan^{-1}(\sqrt{z}\,)}{\sqrt{z}},$$
$$M(k_F,\Lambda)=\frac{1}{1-(k_D\Lambda)^2}\left[4k_F^2\Lambda^2\frac{\tan^{-1}(\sqrt{\pi k_F})}{(\pi k_F)^{3/2}}-\frac{\tan^{-1}(2k_F\Lambda)}{2k_F\Lambda}\right]. \tag{22}$$

The term $[J(\pi k_F)+2]$ in Eq. (20) accounts for the screening of the medium on energy straggling, which is different from $I(\pi k_F)$ accounting for the screening on stopping power. Following the BK description, the parameter $2k_F\Lambda \sim 4\Lambda r_s^{-1}$, which is a measure of the ion screening radius Λ relative to the electron spacing r_s of the medium, can be treated as small. Introducing a variable $\Delta \equiv 1-\tan^{-1}(2k_F\Lambda)/2k_F\Lambda$, Eq. (21) can be expanded in the limit of small $2k_F\Lambda$ or $\Delta \to 0$,

$$\eta=\eta_{\Delta=0}+\Delta\left.\frac{d\eta}{d\Delta}\right|_{\Delta=0}. \tag{23}$$

With $J(0)=-2$, $M(k_F,0)=-1$, and $\eta(q)|_{\Delta=0}=q$ according to Eq. (21), differentiation of Eq. (21) at $\Lambda=0$ leads to

$$\eta(q)\simeq q+D(k_F)(1-q)\left[1-\frac{\tan^{-1}(2k_F\Lambda)}{2k_F\Lambda}\right], \tag{24}$$

where

$$D(k_F)=\frac{2\pi k_F}{(1+\pi k_F)[2+J(\pi k_F)]}-\frac{5}{\pi k_F} \tag{25}$$

is a coefficient weakly depending on k_F (or r_s); e.g., $D(k_F)=1.71$, 1.74, 1.78, and 1.95 for $r_s=1.49$, 1.66, 2.12, and 5.88, respectively. The validity and universal behavior of Eq. (23) are demonstrated in Fig. 2, together with that of Eq. (10) for comparison.

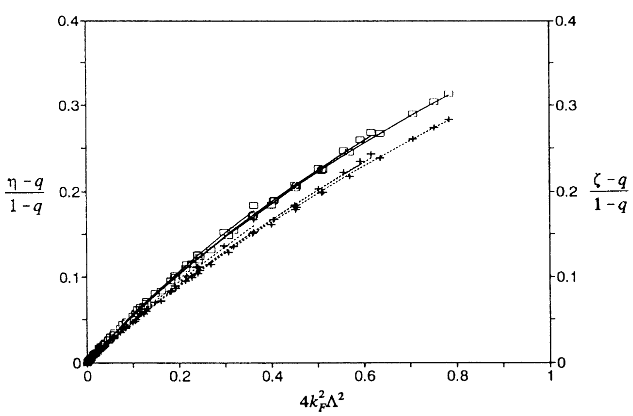

FIG. 2. Demonstration for the equivalence of the approximation expression, Eq. (24), to the exact formula, Eq. (21), of energy straggling (——, □) in the form of $(\eta-q)/(1-q)$ vs $(2k_F\Lambda)^2$, together with $(\zeta-q)/(1-q)$ of stopping power [3] (— — —, +) for comparison. The lines represent the results from Eqs. (10) and (24) for $Z_1 \geq 5$ at all degrees of ionization, while the data symbols are calculated from the exact expressions for $Z_1=6,7,18,53,92$ each at ionizations $q=0.197$, 0.447, and 0.852, in targets with $r_s=1.49$ (Au), 1.66 (C), 2.12 (Al), and 5.88 (Cs). The screening length, Eq. (4), is used.

IV. DISCUSSION

The PSPEC (ζ) and PSGEC (η) are expressed by Eqs. (7), (10), (16), and (24), respectively, in the frame of the linear response theory [2,3] for slow and swift projectiles with a fixed charge state (or ionization fraction q). The energy dependence of the PEC's for C neutral atoms and C^{5+} ions in carbon ($r_s=1.66$) is shown in Fig. 3. A similar feature as discussed for He^+ ions in solids based on numerical calculations [11,12] is observed. The fractions ζ and η are constants at low energies and increase gradually with increasing energy until $\zeta^2 \to (1+q^2)/2$ and $\eta^2 \to 1$ at the high-energy limit. There is a mismatch at velocities around v and $v_{\rm thr}$ between the low- and high-velocity approximations, which is due to the limitation of Eqs. (14) and (19) for the dielectric function at such ve-

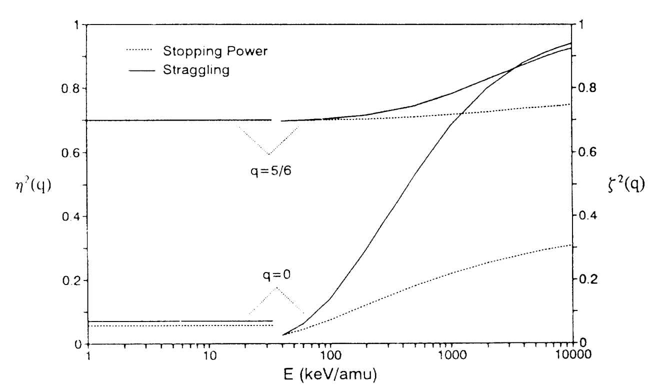

FIG. 3. The energy dependence of the PSPEC and PSGEC fractions for C atoms ($q=0$) and C^{5+} ions in carbon ($r_s=1.66$). Equations (10) and (24) are used for low energies, with Eqs. (7) and (16) for high energies.

locities. Such an energy dependence is more significant for lower charge state for both ζ and η, while η increases more rapidly than ζ. Figure 4 illustrates ζ and η versus the ionization fraction q for low energy and 3 MeV/amu C projectiles in carbon ($r_s = 1.66$). At high energies, there is a stronger dependence on q for ζ than for η, while there is no significant difference at low energies. It is noticed that, at high energies, the singly charted projectile with minimum η^2 is not a neutral atom but a partially stripped ion ($0<q<1$), as shown in Figs. 3 and 4. This may be explained as follows. In the case of electronic straggling, the most important contribution comes from large energy transfers (i.e., close collision) [30]. At high velocities, the collisions between the target electrons and the projectile occur close to the inner atomic shells of the projectile. Therefore, the outer-shell bound electrons have no significant screening effect on the electronic straggling except a small contribution due to collisions with the target electrons (small energy transfers).

In the BK effective-charge theory, only the low-velocity formula, Eq. (10), has been used by BK to describe the stopping power of heavy ions [3,4]. On the other hand, little attention has been paid to the high-velocity formula, Eq. (7). In the effective-charge model, the mean projectile ionization is expressed as $\bar{q} = 1 - \exp(-v_r/v_0 Z_1^{2/3})$ where v_0 is the Bohr velocity and v_r is the mean relative velocity between the projectile and the conduction electrons in the medium [3,4]. The SPEC and SGEC versus $y_r = v_r/v_0 Z_1^{2/3}$ for C ions with the mean ionization $\bar{q}$ have been calculated with both the low- and high-velocity approximations as shown in Fig. 5. Only a slight difference between Eqs. (7) and (10) is observed at medium energies (y_r from 1 to 3), which implies that Eq. (10) with its simplicity may provide reasonable estimates for ζ even at medium and high velocities, as illustrated in Fig. 5.

For energy straggling, there are significant differences not only between Eqs. (16) and (24), but also between ζ and η at medium energies. In the case of heavy ions, however, the effective charge derived from stopping power may still provide reasonable approximations for

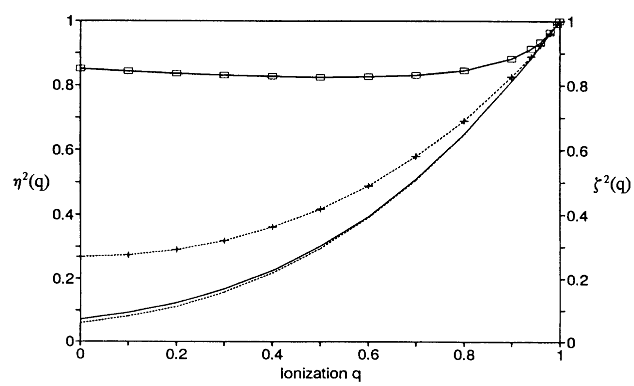

FIG. 4. The PSPEC and PSGEC fractions for C projectiles in carbon ($r_s = 1.66$) vs projectile ionization fraction q. ——, η, Eq. (24); — — — —, ζ, Eq. (10); —□—, η, Eq. (16) at 3 MeV/amu; — — — + — — —, ζ, Eq. (7) at 3 MeV/amu.

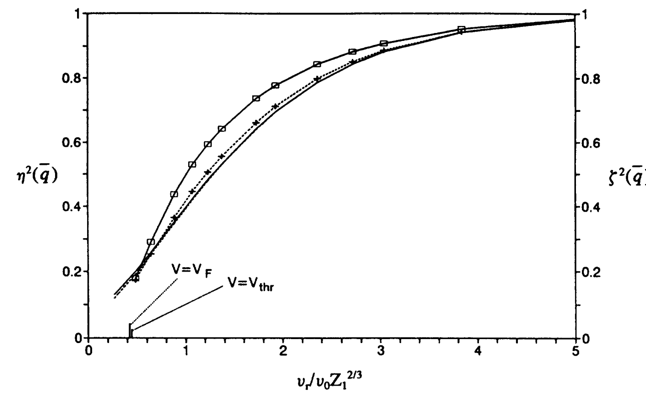

FIG. 5. The SPEC and SGEC fractions for C ions with mean ionization fraction $\bar{q} = 1 - \exp(-v_r/v_0 Z_1^{2/3})$ in carbon ($r_s = 1.66$) vs $y_r = v_r/v_0 Z_1^{2/3}$ in the BK effective-charge theory. ——, η, Eq. (24); — — — —, ζ, Eq. (10); —□—, η, Eq. (16); and — — — + — — —, ζ, Eq. (7).

the scaling of collisional straggling because the difference between ζ and η is relatively small compared with the charge-exchange straggling of heavy ions [9].

The PEC's Eqs. (7), (10), (16), and (24), are derived for projectiles with a fixed charge state (or ionization fraction q). Experimental data [14–22] for the partial stopping power of heavy ions with "frozen" charge states have become available recently. Figure 6 illustrates the ratio of the measured PSPEC to the BK results with low- and high-velocity approximations for different projectile ionizations, while most of the data were measured at the projectile energy of 3 MeV/amu. There is a better agreement for higher charge states than for lower ones. For heavy projectiles with low charge states (more bound electrons), the projectile excitations [13] and many-body interactions may become important. The BK results from Eqs. (7) and (10) agree with the experiments to within 10% of most of the data points, while there is a better agreement for the high-energy expression, Eq. (7), as expected. Unfortunately, no experiments are available for the measurements of the partial energy straggling, which could be used to verify the PSGEC.

It should be pointed out that Eqs. (7), (10), (16) and (24) are derived based on the dielectric-function method and BK model, which is essentially the linear-response theory. The high-velocity expressions, Eqs. (7) and (16), are appropriate because there is no significant nonlinear effect at high ion velocities. At low velocities ($v < v_F$), the BK model does not show any of the well-known Z_1 oscillation of the stopping power [37] and energy straggling [38,39]. Instead, it gives a reasonable average description of the effective charge as a function of Z_1 for different r_s values [32,37]. Taking into account the nonlinear response, the stopping power and energy straggling of slow ions moving in an electron gas can be calculated using the phase-shift method with the density-function theory [31,32,37–40]. At low ion velocities, a more appropriate PSPEC and PSGEC should be obtained according to Eqs. (6) and (13) while the partial stopping power and straggling of a singly charged ion can be calculated

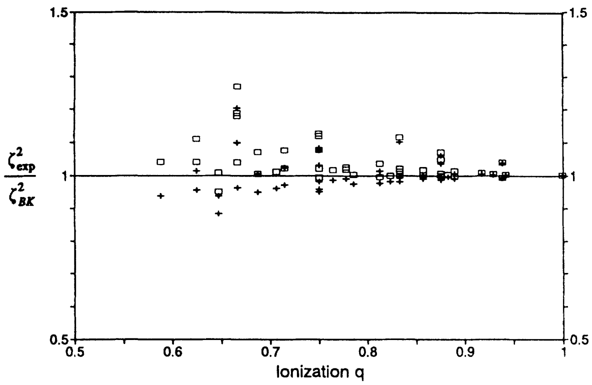

FIG. 6. Ratios of the measured PSPEC to that of BK results with low- (□) and high- (+) velocity approximations for various ionization fractions q. Experimental results are taken from Refs. [15–22] with different combinations of targets and heavy ions at different energies.

from the nonlinear density-function theory dealing with many-body problem.

With the PSPEC and PSGEC, including nonlinear response wherever necessary at low ion velocities, one can describe the total stopping power and straggling at charge-state equilibrium in a charge-state model,

$$S=\sum_q f(q)\left[\zeta^2(q)S_{q=1}+\sum_{q'(\neq q)}\sigma_{q\to q'}U_{q\to q'}\right],$$
$$\Omega^2=\sum_q f(q)\eta^2(q)\Omega^2_{q=1}+\Delta\Omega^2_{\text{chex}}, \tag{26}$$

where $f(q)$ is the equilibrium charge-state fraction of charge state q, $\sigma_{q\to q'}$ is the charge-exchange cross section for charge state q to q', and $U_{q\to q'}$ is the energy transfer in the related charge-exchange process [14,18]. The charge-exchange straggling $\Delta\Omega_{\text{chex}}$ can be expressed analytically for a three-state system if $U_{q\to q'}$ is ignored [6,11],

$$\frac{\Delta\Omega^2_{\text{chex}}}{Ndx}=\frac{2}{D}\{\alpha[(\varepsilon_2-\varepsilon_0)^2 f_0 f_2+(\varepsilon_2-\varepsilon_1)^2 f_1 f_2+(\varepsilon_1-\varepsilon_0)^2 f_0 f_1]-(\varepsilon_2-\varepsilon_1)^2 f_2\sigma_{21}-(\varepsilon_1-\varepsilon_0)^2 f_1\sigma_{10}\}, \tag{27}$$

with

$$\alpha=\sigma_{01}+\sigma_{10}+\sigma_{12}+\sigma_{21},$$
$$D=\sigma_{01}\sigma_{12}+\sigma_{21}\sigma_{01}+\sigma_{21}\sigma_{10}, \tag{28}$$
$$f_0=\sigma_{21}\sigma_{10}/D,\quad f_1=\sigma_{01}\sigma_{21}/D,\quad f_2=\sigma_{01}\sigma_{12}/D,$$

where $\varepsilon_i=S_i/N$ is the stopping cross section and S_i is the stopping power of ions with charge-state i. With $\sigma_{12}=0$ and $\sigma_{21}\neq 0$, Eq. (26) reduces to the well-known two-state expression [7].

The stopping power and straggling of the bare nucleus, $S_{q=1}$ and $\Omega_{q=1}$, can be calculated with the linear-response theory [2,32] or the harmonic-oscillation model [33] at high ion velocities, and with the density-function theory [31,32,37–40] at low ion velocities. Empirically, it may be practical to use the Ziegler-Biersack-Littmark stopping power [4] of protons to obtain the stopping power of fully stripped heavy ions. Chu's numerical results [34] for the energy straggling of protons in matter has been fitted [9] to provide a base set for the straggling of the bare nucleus. The charge-exchange cross section is the most important parameter to describe the charge-exchange process. The dynamic screening and charge-exchange process have been studied and reviewed in more detail recently [32].

V. CONCLUSION

A formula for the partial straggling effective charge (PSGEC), which is different from the partial stopping-power effective charge (PSPEC), has been obtained based on the BK model with the dielectric-function method and a modified screening length of the projectile. This formula provides the effective charge for the scaling of the collisional straggling within the BK effective-charge model. A more general feature is to introduce the PEC's, including nonlinear response [32] at low velocities, into a charge-state description to describe the stopping power and straggling of heavy ions in matter. With the appropriate PEC's, the stopping power and straggling of protons, and knowledge of charge-exchange cross sections, the stopping power and energy straggling of heavy ions can be obtained. Comparison between the charge-state model and recent experiments [35] for the stopping power and straggling of fast C ions in carbon will appear in a further report [36].

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