Impact-parameter dependence of the electronic energy loss of protons in collisions with atoms

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We calculate the energy transferred by a swift incident particle to a stationary atom as a function of the impact parameter. The calculation is based on a local-density approximation and on the electron-gas model. We apply Thomas-Fermi and Lenz-Jensen atomic models, and we study the general scaling properties of the energy loss as a function of the impact parameter and velocity, in terms of the target atomic number Z_2. With the same description we calculate the stopping cross section as a function of Z_2, and compare it with existing experimental results. Finally, we compare our theory with the experimental results of Eckardt *et al.* for the angular dependence of the energy loss of protons transmitted through thin solid foils.

I. INTRODUCTION

The phenomenon of energy loss of swift ions in solids has been studied thoroughly, and its general properties are reasonably well understood. From such studies a standard stopping-power theory has also been established. However, from a practical point of view several problems still remain, because a simultaneous treatment of atomic excitations, many-body effects and other processes becomes in many cases prohibitively long. In consequence, several models and approximations have been developed.

Recently, some experimental and theoretical work has focused on the analysis of the angular dependence of the energy loss of protons in thin solid foils.[1-5] In particular, a multiple-scattering analysis of the data[3] permits us to study the energy loss in individual collisions, Q, as a function of the scattering angle θ, and thereafter as a function of the impact parameter b. This development opens new ways to obtain clear information on the angular and impact-parameter dependences of the energy loss process; moreover, a better understanding of this dependence may permit a more stringent test of some of the models currently used in the literature.

Previous descriptions of the average energy loss of protons in matter[6,7] (stopping power) made use of a local approximation for the contribution of atomic electrons to the stopping number, in terms of the local plasma frequency $\omega_P(r)$ and Fermi velocity $v_F(r)$. The calculations give accurate results for the stopping power. Even some particular properties in the atomic number dependence (Z_2 oscillations) for the intermediate velocities, can be described by using Hartree-Fock atomic densities.[8] However, there is so far no evidence of whether the same theoretical picture can describe the impact-parameter dependence of Q in a satisfactory manner. Therefore, calculations of $Q(b)$ will be important to illustrate the applicability of those models. Some, evaluations are already contained in previous work,[2,9,10] but the results are not conclusive.

In this paper we provide a description of the impact-parameter dependence of the energy loss, using the general properties of the statistical atomic model. We base our calculation on a local-density approximation and on the electron-gas model. We then introduce the Thomas-Fermi (TF) and Lenz-Jensen (LJ) descriptions, and analyze the general scaling properties of the energy-loss function Q, with atomic number Z_2. The models and approximations are described in Sec. II.

In Sec. III we study the impact-parameter dependence of Q, we calculate the stopping cross section for any element, and finally we obtain the angular dependence of Q and compare theoretical and experimental results for $Q(\theta)$.

We summarize our conclusions in Sec. IV.

II. MODELS AND APPROXIMATIONS

A. Local-density approximation

The approach we will consider is basically an extension of previous treatments of the stopping power of atomic systems using electron-gas concepts.[6,7]

We will consider a local description of the energy loss, in terms of the atomic electron density $\rho(r)$. Therefore, the energy loss of a particle of charge $Z_1 e$ can be expressed as (we use atomic units throughout this paper):

$$-\frac{dE}{dX}(\mathbf{r})=\frac{4\pi Z_1^2}{v^2}\rho(\mathbf{r})L(\rho(\mathbf{r}),v)\ , \tag{1}$$

where $L(\rho,v)$ is the usual stopping logarithm.[11]

Hence, we can write the energy transferred to the atomic electrons $Q(b)$, in a collision with impact parameter b, as the line integral

$$Q(b)=\int dl\left[-\frac{dE}{dx}(\mathbf{r})\right]\Bigg|_{\mathbf{r}=\mathbf{r}(l)}\ , \tag{2}$$

where the integration is taken along the particle trajectory

$\mathbf{r}=\mathbf{r}(l)$. We will make use of the straight-line approximation, and will consider the particle moving in the z direction, $l=z$, with $-\infty<z<\infty$. Thus we get

$$Q(b)=\frac{8\pi Z_1^2}{v^2}\int_0^\infty dz\,\rho(r)L(\rho(r),v) \tag{3}$$

with $r=(z^2+b^2)^{1/2}$, and where the electron distribution is considered as spherically symmetric.

The description of the energy loss along the trajectory, in terms of the local density $\rho(r)$, will be referred to as the local-density approximation (LDA) for the energy loss.

In order to calculate $Q(b)$ in Eq. (3) we will apply some well-known results for the energy loss of charged particles in an electron gas. The stopping number $L(\rho,v)$ becomes in this case a function of the ion velocity v, and of the Fermi velocity v_F and plasma frequency ω_P of the gas. In particular, the following analytical approximations are obtained:[11]

(i) for $v<v_F$,

$$L\cong C(\chi)\left[\frac{v}{v_F}\right]^3, \tag{4}$$

where

$$C(\chi)=\frac{1}{2(1-\chi^2/3)^2}\left[\ln\left[\frac{1+\frac{2}{3}\chi^2}{\chi^2}\right]-\frac{1-\chi^2/3}{1+\frac{2}{3}\chi^2}\right] \tag{5}$$

and $\chi^2=1/(\pi v_F)$ is a density-dependent parameter;

(ii) for $v>v_F$,

$$L\cong\ln\left[\frac{2v^2}{\omega_P}\right]-\frac{3}{5}\left[\frac{v_F}{v}\right]^2. \tag{6}$$

Since in this description of the atom the Fermi velocity v_F is a function of r, we can differentiate between two regions: (a) an inner region, $r<r_0$, where $v<v_0$ and the value of L can be approximated by Eq. (4); (b) an outer region, $r>r_0$, where $v>v_0$ and Eq. (6) can be used. The velocity v_0 is close to the Fermi velocity v_F: $v_0=\alpha v_F$ with $\alpha\cong 1$. Since it is convenient to use a continuous energy loss function, the value of v_0 will be taken as the point of intersection of the low-velocity and high-velocity approximations, Eq. (4) and Eq. (6). Numerical calculations for the electron gas[11] show that this criterion yields accurate analytical approximations as compared with the exact values.

B. Thomas-Fermi and Lenz-Jensen models

The description we have outlined can be cast in a convenient form by the use of the scaling properties contained in the TF and LJ models.

In the TF model, the density $\rho(r)$ is of the form $\rho(r)=Z_2^2 f(x)$, where $x=rZ_2^{1/3}/a$, Z_2 is the target atomic number and $a\cong 0.885$. The function $f(x)$ is given by

$$f(x)=\frac{32}{9\pi^3}\left[\frac{\phi(x)}{x}\right]^{3/2}, \tag{7}$$

where $\phi(x)$ is the TF function. Hence, the energy loss can be written as

$$Q=8\pi a\frac{Z_1^2 Z_2^{5/3}}{v^2}\int_0^\infty dz' f(x)L(Z_2^2 f(x),v) \tag{8}$$

in terms of the reduced variables $z'=zZ_2^{1/3}/a$, $b'=bZ_2^{1/3}/a$, and $x=rZ_2^{1/3}/a=[(z')^2+(b')^2]^{1/2}$. The values of L are now given by

$$L\cong\begin{cases} C(\chi)\left[\dfrac{v}{v_F}\right]^3=\dfrac{v^3}{3\pi^2 Z_2^2}\dfrac{C(\chi)}{f(x)}, & x<x_0 \quad (9)\\ \ln\left[\dfrac{v^2}{Z_2[\pi f(x)]^{1/2}}\right]-\dfrac{3}{5}\left[\dfrac{v_F}{v}\right]^2, & x>x_0 \quad (9')\end{cases}$$

where we used the relations $v_F^3=3\pi^2\rho=3\pi^2 Z_2^2 f(x)$, $\omega_P=(4\pi\rho)^{1/2}=Z_2[4\pi f(x)]^{1/2}$. The value of $x_0=r_0 Z_2^{1/3}/a$ is the solution of the intersecting condition $v=v_0(r_0)=\alpha v_F(r_0)$, which can also be put in the form $v^3/Z_2^2=3\pi^2\alpha^3 f(x_0)$.

For small impact parameters, such that $b'<x_0$, the integration in Eq. (8) splits into two separate integrals according to Eqs. (9) and (9'). For larger impact parameters, $b'>x_0$, the expression (9') applies over the whole range of integration.

Equation (8) leads now to interesting scaling properties First, it is convenient to define a reduced energy loss

$$Q'=Q\frac{v^2}{Z_1^2 Z_2^{5/3}} \tag{10}$$

which is a function of the impact parameter b, the velocity v, and the atomic number Z_2. The impact-parameter dependence appears only through the variable $b'=bZ_2^{1/3}/a$, as expected in the TF scaling. On the other hand, the velocity dependence, by Eqs. (9) and (9'), appears in terms of two characteristic velocities, namely,

$$v'=v/Z_2^{1/2},\quad v''=v/Z_2^{2/3}. \tag{11}$$

Therefore, the velocity dependence cannot be reduced to a single parameter. The reason for this is that the stopping logarithm $L(\rho,v)$ is a function of v/v_F at low velocities and a function of v/ω_P at high velocities [leading term in Eq. (9')]. The existence of two velocity scales is not very upsetting since the ratio $v'/v''=Z_2^{1/6}$ has a very weak dependence on Z_2. Moreover, Eq. (9) has an additional Z_2 dependence through the function $C(\chi)$, but as shown by Lindhard and Winther,[11] $C(\chi)$ also changes weakly with density.

In conclusion, a universal scaling of the reduced energy loss Q' in terms of impact parameter and of a single velocity parameter cannot be achieved, but nevertheless an approximate scaling can be used.

The previous analysis can also be done using the Lenz-Jensen model for $\rho(r)$. In this case the density of electrons takes the form

$$\rho(r)=Z_2^2 g(y), \tag{12}$$

where $y=(\gamma r Z_2^{1/3})^{1/2}$, $\gamma=10.91$, and the function $g(y)$

has a simple analytical form.[12,13]

To compare with the TF model we notice that $y^2=\gamma a x$, where $x=rZ_2^{1/3}/a$ is the TF variable. Therefore, we can use the same formulation of Eqs. (8)—(9'), with the replacement of $f(x)$ by the appropriate LJ function, namely,

$$f_{\mathrm{LJ}}(x)\equiv g((\gamma a x)^{1/2}) .$$

III. CALCULATIONS

A. Impact-parameter dependence

Following the approach described before, we performed calculations using both the TF and LJ models.

In Fig. 1, parts (a) and (b), we show the results for the reduced energy loss $Q'=Q(b,v,Z_2)v^2/(Z_1^2Z_2^{5/3})$ (in atomic units) as a function of the reduced impact-parameter $b'=bZ_2^{1/3}/a$, for reduced velocities $v/Z_2^{1/2}=0.4$ in part (a) and $v/Z_2^{1/2}=0.90$ in part (b). The difference between the TF and LJ models becomes larger at low velocities, and it is more important for large impact parameters. The origin of this difference can be assigned to the asymptotic behavior of the TF density, which decays too slowly for large distances. Since the TF and LJ densities agree at intermediate and small distances, the difference becomes less important for smaller impact parameters. For large velocities, $v/Z_2^{1/2}\gg 1$, the TF and LJ models agree very well.

In Fig. 2 we show results corresponding to a reduced velocity $v'=v/Z_2^{1/2}=1.5$, and for various values of Z_2 and v ($Z_2=10$, 60, and 100). For large impact parameters, $b'>1$, we find a good scaling of velocities according to $v/Z_2^{1/2}$ [see the leading term in Eq. (9')], and therefore the curves coincide. For smaller impact parameters the particle penetrates the inner atomic region, hence both Eqs. (9) and (9') must be used in the integration, and in consequence, the scaling is lost.

We note, however, that even when Z_2 changes by a factor 10 the reduced energy loss $Q'=Qv^2/(Z_1^2Z_2^{5/3})$ changes less than 60% (larger difference for $b=0$). This means that the approximate scaling still becomes useful.

B. Stopping cross section

The calculations of the atomic stopping cross section S_a can be formulated using the same approach considered before for $Q(b)$. The relation between both quantities is

$$S_a=-\frac{1}{N}\left\langle\frac{dE}{dx}\right\rangle=2\pi\int_0^\infty Q(b)b\,db \tag{13}$$

which yields

$$S_a=\frac{(4\pi)^2Z_1^2}{v^2}\int_0^\infty \rho(r)L(\rho(r),v)r^2\,dr . \tag{14}$$

This integral was calculated using the approximations of Eqs. (9) and (9'), and using also the TF and LJ models. In Fig. 3, parts (a) and (b), we show the results for α particles with energies of 0.8 MeV and 4 MeV, as a function of atomic number Z_2, together with experimental results from various authors[14] collected by Chu *et al.*[8] The experimental data show the characteristic Z_2 oscillations due to atomic shell effects.

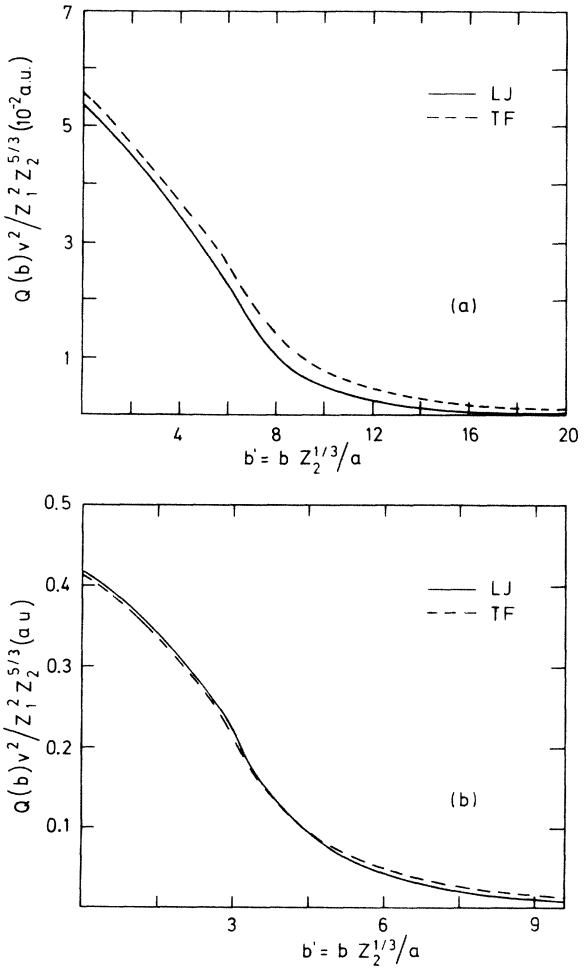

FIG. 1. Reduced energy loss $Q'=Qv^2/Z_1^2Z_2^{5/3}$ as a function of $b'=bZ_2^{1/3}/a$ (in a.u.), for reduced velocities $v'=v/Z_2^{1/2}=0.4$ in part (a) and $v'=0.9$ in part (b). The solid curve corresponds to the LJ model and the dashed curve to the TF model.

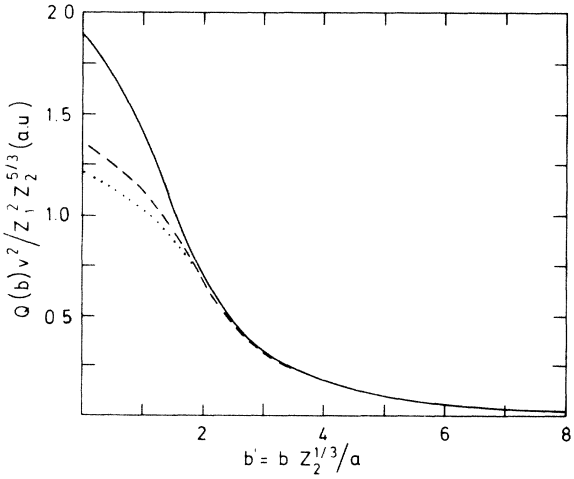

FIG. 2. Impact-parameter dependence of the reduced energy loss $Q'=Qv^2/Z_1^2Z_2^{5/3}$, for $v'=v/Z_2^{1/2}=1.5$ and for $Z_2=10$ (solid line), 60 (dashed line), and 100 (dotted line), as calculated using the LJ model.

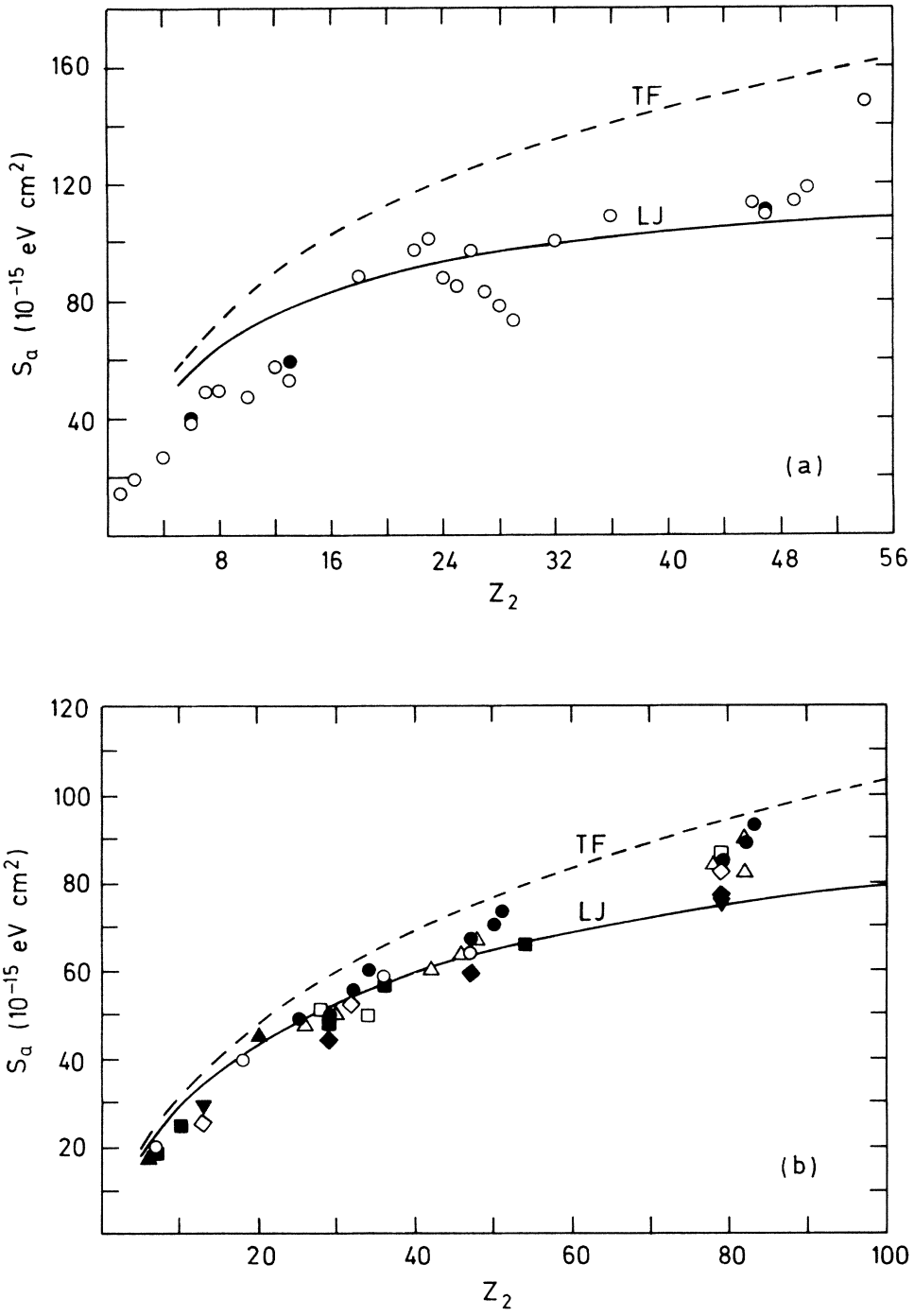

FIG. 3. Atomic stopping cross section S_a as a function of atomic number Z_2, for α particles with energies of 0.8 MeV [part (a)] and 4 MeV [part (b)]. The solid and dashed curves correspond to the present calculations using the LJ and TF models.

The agreement with the LJ model becomes better at both energies. As already observed in the calculations of $Q(b)$, the results for the TF model are larger due to the slower decay of the density $\rho(r)$ for large values of r.

With increasing energies the difference between the TF and LJ models fades away, and also the agreement with the experiments improves significantly.

Previous calculations of stopping cross sections using more accurate Hartree-Fock densities[8] follow the experimental results quite closely. Moreover, a simultaneous convergence of theoretical and experimental results, and a damping of the Z_2 oscillations, occur with increasing energies.

C. Angular dependence

In order to compare our calculations with available experimental results for the angular dependence of the ener-

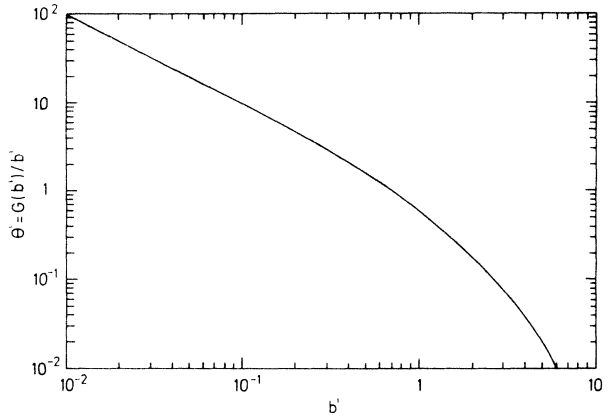

FIG. 4. Reduced scattering angle $\theta'=G(b')/b'$, from Eqs. (15) and (16), as a function of $b'=bZ_2^{1/3}/a$. The limit $\theta'\cong 1/b'$ (Coulomb potential) is obtained for $b'<1$.

gy loss of protons in solid targets, we now consider the energy loss Q as a function of the scattering angle θ in a single collision with impact parameter b. The transformation from $Q(\theta)$ to the measured energy loss $\Delta E(\theta_e)$ in terms of the emergence angle θ_e can be carried out through a multiple-scattering formulation as discussed by Jakas *et al.*[3]

Using the results of Lindhard, Nielsen, and Scharff[15] for the Lenz-Jensen (LJ) potential we can write the relation between θ and b, for small angles of scattering, in the form

$$\theta=\frac{2Z_1Z_2^{4/3}}{aM_1v^2}\frac{G(b')}{b'}\ , \tag{15}$$

where $b'=bZ_2^{1/3}/a$ and M_1 is the mass of the incident particle. The function $G(u)$ is given by

$$G(u)=\int_0^{\pi/2}[\cos\alpha\phi_{\rm LJ}(u/\cos\alpha)-u\phi'_{\rm LJ}(u/\cos\alpha)]d\alpha\ , \tag{16}$$

where $\phi_{\rm LJ}$ is the screening function of the LJ potential.[12,13]

It is convenient to define a reduced angle $\theta'=\theta aM_1v^2/(2Z_1Z_2^{4/3})$, which according to Eq. (15) is a universal function of the reduced impact parameter b'. This function is shown in Fig. 4. Results for the electronic energy loss $Q(\theta)$ in the collision of the 200-KeV protons with atoms of Al and C are shown in Figs. 5(a) and 5(b). The circles are data for $Q(\theta)$ obtained by Jakas *et al.*[3,4] from the analysis of their experimental results.

The figures show a qualitative agreement between theory and experiments. The fact that the calculations give in both cases larger results can be related to the similar behavior of the stopping cross section at this energy [see Fig. 3(a)]. We think that the use of more accurate atomic density distributions will improve this agreement in quantitative terms.

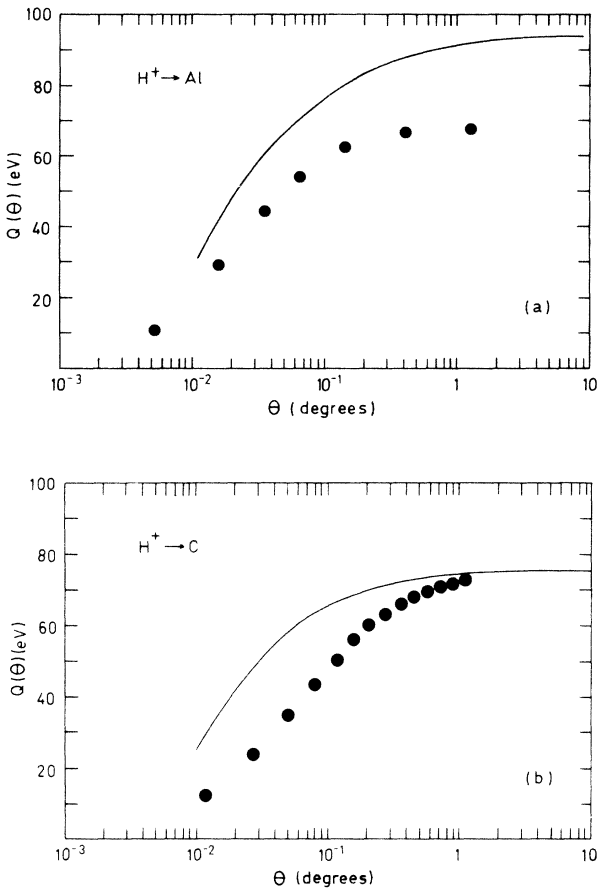

FIG. 5. Electronic energy loss function $Q(\theta)$ vs scattering angle θ, for 200-KeV protons on (a) Al and (b) C targets. The data were obtained by Jakas *et al.* (Refs. 3 and 4) from beam-foil experiments. The curves show the calculations described in the text.

IV. DISCUSSION AND CONCLUSIONS

Our study of the impact-parameter dependence of the energy loss is based on several approximations. First we introduce a local approximation which permits us to integrate the energy loss, for a given impact parameter, along the trajectory of the particle. We make use of analytical results for the electron-gas model and consider the Thomas-Fermi and Lenz-Jensen models for the atomic electron density.

A few general properties can be obtained from this analysis. The energy loss Q and the impact parameter b scale according to $Z_1^2Z_2^{5/3}/v^2$ and $Z_2^{-1/3}$, respectively. The velocity scaling is not unique since two variables related to low-velocity and high-velocity approximations ($v/Z_2^{2/3}$ and $v/Z_2^{1/2}$, respectively) appear in the description.

By integrating $Q(b)$ over impact parameters we make contact with an independent measurable quantity, namely, the stopping cross section. This permits another check of the model, since experimental and theoretical results are available for a wide range of Z_2 values. The Lenz-Jensen model provides a good first approximation to such results. At low velocities the Z_2 oscillations due to outer atomic shells produce individual discrepancies, but the agreement improves significantly with increasing energies. Apart

from individual deviations due to shell efects, we conclude that the model contains all dominant terms depending on Z_2.

Experimental access to the impact-parameter dependence of Q is possible from the analysis of the angular dependence of energy loss data. The comparison with theory is made in terms of the quantity $Q(\theta)$. The agreement with experimental results for 200-KeV protons in C and Al can be considered satisfactory. One should notice that in this range of energies the contribution of the outer atomic shells is important, while the statistical model is more appropriate to describe the behavior of the intermediate shells.

For a careful analysis of these differences a more extensive test of the energy loss model would be desirable. This could be achieved only by a systematic study of the angular dependence of the energy loss at various energies and for a wide range of atomic numbers Z_2. Therefore, a considerable experimental effort in this direction is also required.

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