Relativistic theory of stopping for heavy ions

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We calculate the electronic stopping power and the corresponding straggling for ions of arbitrary charge number, penetrating matter at any relativistic energy. The stopping powers are calculated by a simple method. Its starting point is the deviation of the precise theory from first-order quantum perturbation. We show that this deviation can be expressed in terms of the transport cross section, $\sigma_{\rm tr}$, for scattering of a free electron by the ion. In the nonrelativistic case the deviation is precisely the Bloch correction to Bethe's formula; we look into the nonrelativistic case in order to clarify both some features of our method and a seeming paradox in Rutherford scattering. The corresponding relativistic correction is obtained from $\sigma_{\rm tr}$ for scattering of a Dirac electron in the ion potential. Here, the major practical advantage of the method shows up; we need not find the scattering distribution, but merely a single quantity, $\sigma_{\rm tr}$, determined by differences of successive phase shifts. For a point nucleus our results improve and extend those of Ahlen. Our final results, however, are based on atomic nuclei with standard radii. Thereby, the stopping is changed substantially already for moderate values of $\gamma=(1-v^2/c^2)^{-1/2}$. An asymptotic saturation in stopping is obtained. Because of finite nuclear size, recoil corrections remain negligible at all energies. The average square fluctuation in energy loss is calculated as a simple fluctuation cross section for a free electron. The fluctuation in the relativistic case is generally larger than that of the perturbation formula, by a factor of ~ 2–3 for heavy ions. But the finite nuclear radius leads to a strong reduction at high energies and the elimination of the factor γ^2 belonging to point nuclei.

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I. INTRODUCTION

When swift ions move through matter, their dissipation of energy is almost exclusively due to interaction with and energy transfer to electrons. In this paper we study the corresponding stopping powers for light and heavy ions when their velocity approaches the velocity of light, i.e., from near-relativistic energies and up to any extreme relativistic energy. The aim is to account for both average energy loss and straggling in energy loss, and to obtain results that are accurate for all values of the projectile charge. In order to do this, we have to perform precise quantum mechanical calculations for Dirac electrons scattered by a Coulomb potential. We make a shortcut as compared with previous calculations and obtain the stopping and straggling in a direct manner.

Our treatment has close connections to the Bethe-Bohr-Bloch description of nonrelativistic slowing down. Bohr's paper from 1913 [1] treats the electronic stopping of a swift charged particle within classical mechanics, with perturbation theory for distant collisions, leading to an adiabatic limit of energy transfer determined by orbital frequencies of electrons, but with a precise description of close collisions. In Bethe's 1930 paper [2], first-order quantum perturbation theory is used for all collisions. The adiabatic limit is determined by transition frequencies and, although this may not be obvious, there is essentially agreement with the classical adiabatic concept (cf. also Sec. III). The discussion by Bloch [3] bridges the gap between the two treatments. This situation is described in Bohr's renowned survey paper from 1948 [4]. It is shown there that, for a collision between an ion of charge number Z_1 and an electron with relative velocity v, the dimensionless parameter

$$\kappa \equiv 2\eta = \frac{2Z_1 e^2}{\hbar v}, \tag{1}$$

allows quantum perturbation theory when small, but permits a classical treatment when large compared to unity. Note that in connection with the Dirac equation it will be convenient to use the symbol η instead of Bohr's κ.

There are two corrections to this picture of slowing down of swift ions, however. First, as shown by Bohr [4], ions for which $\kappa > 1$ will also carry electrons, with processes of capture and loss. This leads to a considerable change of stopping for heavy ions because of the reduction of charge, due to screening by electrons bound to the ion. Second, the Bethe-Bohr-Bloch description contains only terms even in Z_1, or κ. The so-called Barkas correction is of a different kind, being odd in Z_1; its dominating term behaves as Z_1^3 and is important in both classical and quantum descriptions.

When we now return to the relativistic case, the above two nonrelativistic corrections become small and are completely negligible for large values of $\gamma=(1-v^2/c^2)^{-1/2}$. They are therefore not relevant to our central purpose; we shall later indicate the approximate magnitude of these corrections.

The Bethe perturbation formula was extended to relativistic energies, cf. Bethe [5], Fano [6], and Jackson [7]. This leads to accurate results for slowing down of ions with low charge number, such as protons and α particles; but with one reservation for large γ, as we shall see later.

The situation becomes more complicated for relativistic heavy nuclei. This is indicated by Bohr's parameter κ in (1), which remains pertinent in the relativistic case. Since $v<c$, κ can easily become comparable to or larger than unity, which gives one indication that quantum perturbation theory is not accurate in close collisions. Furthermore, it is important to use the relativistic Dirac equation for electrons. In a review paper from 1980, Ahlen has given an expression for the average energy loss for heavy relativistic ions [8,9].

He there relies on early calculations of scattering of Dirac electrons by point nuclei. These results are in parametrized form, and the resulting stopping contains a set of terms with Z_1 up to the power seven. This is not a perturbation expansion, however. We shall find that Ahlen's expression has reasonable accuracy — within a few percent — for moderate values of γ.

In the following, we present a thorough discussion, prior to the calculations. In Sec. II we attempt to account for all terms in the formula for the average energy loss of a swift ion. The central quantity to be calculated is introduced as the deviation ΔL from the value of L for perturbation theory, cf. (2) and (4). This quantity is shown to be given by the change in transport cross section of an electron with relative velocity v scattered by the ion. In Sec. III we consider the nonrelativistic case. Here, the deviation ΔL turns out to be the Bloch correction; it is confined to close collisions and in this connection we resolve some seeming paradoxes in the basic Rutherford scattering. In Secs. II and III we also treat the fluctuation in energy loss. Next, in Sec. IV, as an introduction to the relativistic treatment, the Dirac equation is applied to transport cross sections. In Sec. V we calculate ΔL for a point nucleus, obtaining fair agreement with the results of Ahlen; but this is a preliminary result. The realistic case of a nucleus with standard radius is studied in Sec. VI. We find considerable reductions as compared with a point nucleus, for large γ. In Sec. VII the fluctuation in energy loss is obtained; it is strongly reduced for large γ because of finite nuclear radii. Finally, in Sec. VIII we comment on the results obtained.

II. THE BASIC STOPPING FORMULAE

A. Average energy loss

The electronic stopping power, for a nucleus with charge $Z_1 e$ in a random substance with charge number Z_2, can be written as

$$-\frac{dE}{dx}=\frac{4\pi Z_1^2 e^4}{mv^2}NZ_2 L; \tag{2}$$

$NZ_2=n$ is the average density of electrons, and m the electron mass. We can now introduce a standard function, L_{stand}, which in the main represents a quantum mechanical perturbation formula,

$$L_{\text{stand}}=\ln\left(\frac{2mv^2}{I}\gamma^2\right)-\frac{v^2}{c^2}-\frac{1}{2}\delta, \tag{3}$$

with $\gamma=(1-v^2/c^2)^{-1/2}$. Moreover, I is given by Bethe's result $Z_2 \ln I=\Sigma_n f_{n0}\ln(\hbar|\omega_{n0}|)$, and determined by dipole oscillator strengths f_{n0} and transition frequencies ω_{n0}. The function $-\delta/2$ is the familiar density effect correction of Fermi [10], modifying the adiabatic limit in distant collisions for sufficiently large γ.

The function L_{stand} in (3) depends only on the velocity v of the particle, on the atomic number Z_2 of the medium, and on the average electron density n as contained in the density effect. Thus, it does not depend on the charge number Z_1 of the particle, and in fact L_{stand} represents relativistic first-order quantum perturbation theory, implying that $dE/dx \propto Z_1^2$. The basic relativistic increase of L_{stand} is contained in $\ln\gamma^2-v^2/c^2$ and has equipartition, i.e., exactly equal contributions, $\ln\gamma-v^2/2c^2$, from close and distant collisions. But the increase due to distant collisions will be saturated by the density effect correction, $-\delta/2$, for sufficiently large γ. There remains only $\ln\gamma$ from close collisions in the relativistic increase of L_{stand}. It should be noted that, for simplicity, we have omitted one term belonging to first-order perturbation theory, i.e., the small shell correction due to the finite orbital velocities of the target electrons. The full term belonging to first-order quantum perturbation theory is therefore $L_{\text{pert}}=L_{\text{stand}}+\delta L_{\text{shell}}$. In (3) we have also omitted the so-called Mott term, proportional to $Z_1 v/c^2$, and formally belonging to higher-order scattering theory.

We have mentioned the shell effect, the Barkas effect, and the screening by a captured electron. Introducing these three minor corrections, we can now write for the difference between the true L in (2) and L_{stand} in (3),

$$L-L_{\text{stand}}=\Delta L+\delta L_{\text{shell}}+\delta L_{\text{Barkas}}+\delta L_{\text{scr}}, \tag{4}$$

where ΔL is the quantity we want to derive; it arises from the deviation of scattering from quantum perturbation theory. Note here that the formulas (2), (3), and (4) apply in nonrelativistic theory too. In that case, ΔL represents precisely Bloch's correction to the Bethe stopping formula.

It is appropriate to make a few guiding comments concerning the magnitude of the three correction terms in (4), when we approach the relativistic region. We note that the relative correction in stopping is less than 1% when $|\delta L|<0.1$, since $L\sim 10$. In most cases by far the corrections are below this limit and thus negligible. The standard nonrelativistic shell correction is known fairly accurately, $\delta L_{\text{shell}}\cong -1.5 Z_2^{4/3} v_0^2/v^2$, where the numerator represents the Thomas-Fermi estimate of $\langle v_e^2\rangle$, the average square of electron velocities in the atom. Thus, the standard shell correction is completely negligible when $v\to c$. Next, a cursory estimate of the Barkas correction is $\delta L_{\text{Barkas}}\sim(4Z_1 e^2/mv^2)(\bar{\omega}/v)L$ [11], where $\bar{\omega}$ is a representative frequency of the atom, $\bar{\omega}\sim Z_2$ Rydberg. This correction is completely negligible for $v\to c$, unless both Z_1 and Z_2 are large, in which case it may approach 1%. Finally, δL_{scr} is due to the probability of the ion carrying an electron, from balance between capture and loss, and with a consequent screening of the ion potential. This correction is less easily formulated in a simple way. It is usually negligible, unless both Z_1 and Z_2 are large, where it may attain a magnitude $\sim -1\%$.

B. Fluctuation in energy loss

We shall also calculate the average square fluctuation in energy loss, $\Omega^2=\langle(\delta E-\langle\delta E\rangle)^2\rangle$, where δE is the energy loss. We consider high velocities where we can disregard the minor quantum corrections in distant collisions. The average square fluctuation is then entirely dependent on the close collisions, and we formulate its increase as

$$\frac{d\Omega^2}{dx}=4\pi Z_1^2 e^4 NZ_2\gamma^2 X, \tag{5}$$

which represents Rutherford scattering when the function X is unity. With first-order quantum perturbation theory the Dirac equation leads to

$$X=1-\frac{v^2}{2c^2}, \tag{6}$$

so that this value of X corresponds to L_{stand} in (3). We shall obtain X by a direct calculation analogous to that for ΔL.

When we turn to the possibilities of measuring the average energy loss and its average square fluctuation, we find that this depends on the thickness of the target. In point of fact, for sufficiently thick targets, the energy-loss distribution will be Gaussian around the average energy loss, and with width Ω. For thin targets, one finds a Landau-type distribution of smaller peak width, with a long tail towards large energy losses; it may then be difficult to assess the average energy loss, as discussed in Sec. VII.

C. The method of transport cross section

In this subsection we give a brief survey of a method based on transport cross sections, which method accounts for high-velocity stopping in a precise manner, thereby elucidating the connection between classical and quantal treatments. This method has been used of old in unpublished lecture notes by one of us [12], and it has later been applied by other authors as well; cf. [13,14]. We use the method here because it vastly simplifies the relativistic calculations with Dirac electrons.

The essence is to calculate the scattering of electrons at rest, more precisely the transport cross section σ_{tr} for free electrons with relative velocity v scattered by the Coulomb potential of the ion. We may first indicate why ΔL in (4) is given by the difference, $\sigma_{\text{tr}}-\sigma_{\text{tr}}^{\text{pert}}$, between the transport cross sections for exact scattering and quantal perturbation. In point of fact, ΔL in (4) represents the difference $L-L_{\text{stand}}$ between exact calculation and first-order quantum treatment. The difference does not occur in distant collisions, near the adiabatic limit, where we have perturbation anyway. Moreover, we have in (4) eliminated, first, the shell effect correction δL_{shell} due to electrons not being at rest before the collision; second, the effect δL_{scr} of electrons bound by the ion and thus screening the potential and being captured or lost; third, the Barkas correction, δL_{Barkas}, in which the force from the atom initially counteracts the force from the ion and thereby modifies the free scattering. When, therefore, we have eliminated all atomic corrections, including capture and loss, we are left with the estimate of scattering of free electrons at rest by the pure ion potential, comparing an exact result with the first Born approximation. We have thus arrived at an estimate similar to that made by Bloch, but on a surer footing, not least because we have taken the Barkas effect into account.

Let us therefore consider the energy loss by a heavy ion of velocity v colliding with electrons at rest. The energy transfer T is given by

$$T=T_0\sin^2\frac{\theta}{2}, \tag{7}$$

where θ is the deflection in the center-of-mass frame. Moreover, T_0 is the maximum energy transfer. The contribution to average energy loss will be

$$-\frac{dE}{dx}=NZ_2\int T\,d\sigma=NZ_2\frac{T_0}{2}\sigma_{\text{tr}},$$

$$\sigma_{\text{tr}}=\int d\sigma(1-\cos\theta), \tag{8}$$

where $d\sigma$ is the differential cross section for deflection θ. We shall here assume that $T_0=2mv^2\gamma^2$. Note that it then follows from (8) and (2) that the contribution to L from σ_{tr} is

$$L_{\text{tr}}=\sigma_{\text{tr}}/(\pi\kappa^2\lambda\!\!\!^{-2}). \tag{9}$$

Since the ions with which we are concerned have mass ratio $M/m\approx A\times 1836$ the formula for T_0 is accurate in the center-of-mass frame both in the nonrelativistic case and for large γ, e.g., for $\gamma=1000$ when A is large. In such cases the formulas also hold in the initial rest frame of the ion, where then θ represents the deflection in this frame. For exceedingly high values of γ we can still apply the above formulas in the ion rest frame, if wide angle scattering is suppressed, cf. the introductory discussion in Sec. VI.

III. NONRELATIVISTIC CASE AND BLOCH CORRECTION

In the basic nonrelativistic case we meet with a seeming paradox concerning ΔL. In point of fact, for a Coulomb potential, $-Z_1e^2/r$, Rutherford scattering is valid not only classically and in exact quantum theory, but also in first-order quantum perturbation, i.e., $d\sigma/d\theta$ or $d\sigma/dT$ are the same in the three cases. And yet differences like $\sigma_{\text{tr}}-\sigma_{\text{tr}}^{\text{pert}}$, which describe the Bloch correction, are not zero. In order to clarify this situation we shall treat the transport cross section in some detail.

Consider then scattering in any spherically symmetric potential. As to the quantum mechanical transport cross section we have to integrate the product of $(1-\cos\theta)$ and two scattering wave functions containing Legendre polynomials $P_l(\cos\theta)$, where l is the angular momentum. It follows that, $\lambda=2\pi\lambda\!\!\!^{-}$ being the wavelength of the relative motion,

$$\sigma_{\text{tr}}^{\text{qu}}=4\pi\lambda\!\!\!^{-2}\sum_{l=0}(l+1)\sin^2(\delta_l-\delta_{l+1}), \tag{10}$$

so that the transport cross section is determined by the differences of phase shifts for successive angular momenta.

In the classical description we can write $d\sigma=2\pi q\,dq$, where q is the impact parameter, and $\vartheta=\vartheta(q)$ is the classical angle of deflection:

$$\sigma_{\text{tr}}^{\text{cl}}=4\pi\int q\,dq\sin^2[\vartheta(q)/2]. \tag{11}$$

Now, a well-defined impact parameter q is not in accord with quantum concepts. Instead, we can use angular momentum which classically is $L=pq$, and we may put it equal to $l'\hbar$, so that (11) becomes

$$\sigma_{\rm tr}^{\rm cl}=4\pi\lambda\!\!\!^{-2}\int l'dl'\sin^2[\vartheta(l'\lambda\!\!\!^{-})/2]. \tag{12}$$

There is a close correspondence between (10) and (12). Thus, the summation over $l=0,1,2,\ldots$ is replaced by an integration over l'. We therefore have a simple connection between classical and quantum angular momenta, and either of them are constants of the motion. Furthermore, the correspondence implies that the classical deflection connects to phase shift differences, $\vartheta(\lambda\!\!\!^{-}l')/2\leftrightarrow\delta_l-\delta_{l+1}$, where it is plausible to conclude that $l'\leftrightarrow l+1/2$. This result for deflections is in accord with findings of Landau and Lifshitz [15], derived by a different argument.

After these general considerations we return to the actual case of Rutherford scattering. The quantum phase shifts are familiar,

$$\delta_l=-\arg\Gamma\left(l+1+\frac{i\kappa}{2}\right)+\frac{\kappa}{2}\ln 2kr, \tag{13}$$

where the last term is the common divergent phase shift. From (13) we get an extremely simple formula for the phase shift differences:

$$\delta_l-\delta_{l+1}=\arg\left(l+1+\frac{i\kappa}{2}\right) \tag{14a}$$

or

$$\sin^2(\delta_l-\delta_{l+1})=\frac{\kappa^2/4}{(l+1)^2+\kappa^2/4}. \tag{14b}$$

It is preferable to express the transport cross section $\sigma_{\rm tr}$ in terms of the L factor in stopping. We therefore apply Eq. (9), so that Eqs. (10) and (14) lead to the simple result

$$L_{\rm tr}^{\rm qu}=\sum_{l=0}\frac{l+1}{(l+1)^2+\kappa^2/4}. \tag{15}$$

In first-order perturbation we can disregard κ^2, and find

$$L_{\rm tr}^{\rm pert}=\sum_{l=0}\frac{1}{l+1}. \tag{16}$$

Since classical Rutherford scattering connects impact parameter and scattering angle by the formula

$$\tan(\vartheta/2)=Z_1e^2/(mv^2q)=(\kappa/2)(1/l'), \tag{17}$$

the classical formula (12) becomes

$$L_{\rm tr}^{\rm cl}=\int dl'\frac{l'}{l'^2+\kappa^2/4}. \tag{18}$$

As is characteristic for the L factor, the above three formulas would diverge logarithmically if there were no upper limit, i.e., the adiabatic limit $l_{\rm ad}$. Since the classical adiabatic impact parameter is $q_{\rm ad}=2v/\omega C$ for a frequency ω ($C=1.781$, and $\ln C=0.5771$ is Euler's constant), we should in (18) integrate up to $l_{\rm ad}=2mv^2/(\hbar\omega C)$, leading to Bohr's formula $L_{\rm tr}^{\rm cl}=\ln(2mv^2/|Z_1e^2|\omega C)$. With the same upper limit we find from (16) Bethe's formula for high velocities, $L_{\rm tr}^{\rm pert}=\ln(2mv^2/\hbar\omega)$. This upper limit applies of course also in the general formula (15), which contains (16) and (18) as limits for $\kappa\ll 1$ and $\kappa\gg 1$, respectively. It is to be noted that in assessing $l_{\rm ad}$ in the above manner we have verified that the adiabatic limit is common to the nonrelativistic Bohr and Bethe treatments, as indicated in the Introduction.

We shall now attempt to elucidate the three formulas (15), (16), and (18) by combining them into one, albeit only in an approximate manner. We know that the Bohr formula for stopping is obtained from (18) when the integration is from 0 to $l_{\rm ad}$, as it must be in classical physics. But we can modify this by considering the correspondence between the classical angle of deflection $\vartheta=\vartheta(\lambda\!\!\!^{-}l')$, and the quantum phase shifts $2(\delta_l-\delta_{l+1})$, as alluded to after (12). There, it was indicated that $l'=l+1/2$ gives a suitable correspondence to quantum theory, so that the integration in (18) might start from 1/2. In point of fact, the association to (15) becomes closest if 1/2 is replaced by $C^{-1}\approx 0.56$. This gives the following approximation to (15):

$$L_{\rm tr}=\int_0^{l_{\rm ad}}dl\,\frac{l+C^{-1}}{(l+C^{-1})^2+\kappa^2/4}=\ln\frac{l_{\rm ad}}{\sqrt{C^{-2}+\kappa^2/4}}. \tag{19}$$

It is seen that this formula represents the Bethe and Bohr formulas, respectively, for small and large values of κ. In between, it gives a fair approximation to (15), deviating nowhere more than 0.05.

The numerator and denominator in the logarithm in (19) are measured in units of angular momentum, or — if multiplied by $\lambda\!\!\!^{-}$ — in units of impact parameter. Since the denominator gives the impact parameter at which wide angle scattering commences, we find that for classical scattering it is at $\lambda\!\!\!^{-}\kappa/2$, for perturbation theory at $\lambda\!\!\!^{-}C^{-1}$, and for the precise quantum calculation at $\sim\lambda\!\!\!^{-}(C^{-2}+\kappa^2/4)^{1/2}$. The difference in the values of (15), (16), and (18) is therefore due to the close collisions.

We now return to our original aim of finding ΔL in the nonrelativistic limit. From (15) and (16),

$$\Delta L=\sum_{l=0}\left[\frac{l+1}{(l+1)^2+\kappa^2/4}-\frac{1}{l+1}\right], \tag{20}$$

and, in contrast to (15) and (16), this formula converges for unrestricted summation. In fact, let us stipulate that the sum in (20) goes to infinity; we make a negligible error, approximately $-\kappa^2/(8l_{\rm ad}^2)$.

The result (20) is Bloch's correction to the Bethe formula. It can be expressed in terms of the logarithmic derivative of the gamma function, $\Delta L=-\mathrm{Re}\psi(1+i\kappa/2)-\ln C$. Within the non-relativistic description of electrons without spin we therefore have a complete formula for L, i.e., (4), including all corrections.

For small values of κ in (20), we can expand and find $\Delta L\approx-1.202(\kappa/2)^2$; for moderate values of κ the correction ΔL is nearly linear in κ. But (20) is not applicable when $\kappa\gg 1$, because the scattering is changed by screening of the charge Z_1e, due to electrons residing on the ion. It may be added that, if we could use antinuclei with high negative charge numbers Z_1, there would be no capture of electrons and (20) should be relevant also for $|\kappa|\gg 1$.

We now turn to the increase in energy fluctuation, as described by (5). It is dominated by the close collisions. We

disregard the quantum corrections belonging to distant collisions, because they are negligible at high velocities. We are therefore concerned with scattering of electrons at rest, i.e., precisely the physical situation described by the transport cross section in the calculation of ΔL. Our purpose here is again to prepare the ground for the relativistic Dirac treatment by considering the nonrelativistic description, as well as to resolve a seeming paradox in the latter case.

Consider then the transport fluctuation cross section,

$$Q=\int d\sigma(1-\cos\theta)^2, \tag{21}$$

which is connected to the specific increase in energy loss fluctuation by

$$\frac{d\Omega^2}{dx}=NZ_2\frac{T_0^2}{4}Q. \tag{22}$$

The nonrelativistic expression for Q, for a spherically symmetric potential, and derived analogously to (10), is

$$Q^{\mathrm{qu}}=4\pi\lambda\!\!\!^{-2}\sum_{l=0}(l+1)\left\{2\sin^2(\delta_{l+1}-\delta_l)-\frac{l+2}{2l+3}\sin^2(\delta_{l+2}-\delta_l)\right\}. \tag{23}$$

The corresponding classical expression is found directly from (21). We write the impact parameter as $q=\lambda\!\!\!^{-}l'$, and find in analogy to (12)

$$Q^{\mathrm{cl}}=8\pi\lambda\!\!\!^{-2}\int_0 l'dl'\sin^4\frac{\vartheta}{2}. \tag{24}$$

In the quantum expression (23) it only remains to apply the phase shifts from (13) and (14). When these are introduced in (23), with $T_0=2mv^2$, we get directly

$$\frac{d\Omega^2}{dx}=4\pi Z_1^2e^4NZ_2\sum_{l=0}\frac{l+1}{(l+1)^2+\kappa^2/4}\frac{l+2+\kappa^2/2}{(l+2)^2+\kappa^2/4}=4\pi Z_1^2e^4NZ_2. \tag{25}$$

In order to obtain the last result, we have here rewritten the sum as

$$\sum=\sum_{l=0}\left(\frac{l+1+\kappa^2/4}{(l+1)^2+\kappa^2/4}-\frac{l+2+\kappa^2/4}{(l+2)^2+\kappa^2/4}\right)=\frac{1+\kappa^2/4}{1+\kappa^2/4}=1.$$

This result shows that Rutherford scattering — whether in the Born approximation, classically, or in precise quantum formulation — always gives the simple result (25). In fact, in all cases where the location in space of the scattering process is immaterial, we can use the simple Rutherford formula. This is because the scattering amplitude, when summed freely over angular momenta, gives the Rutherford amplitude. In the case of stopping, however, the cutoff at the adiabatic distance is essential, and the spatial distribution becomes important.

It only remains to see whether our classical interpretation of the Bloch correction can hold in the present case. In fact, (19) contains a generalized expression for $\sin^2\vartheta/2$, which is seen to be proportional to $1/\{(l+C^{-1})^2+\kappa^2/4\}$. Since $\sin^2\vartheta/2$ is to be generally applicable it must have a maximum value equal to unity, and it follows that $\sin^2\vartheta/2\rightarrow(C^{-2}+\kappa^2/4)/\{(l+C^{-1})^2+\kappa^2/4\}$, and a factor $(\kappa^2/4)/(C^{-2}+\kappa^2/4)$ comes outside the integral. Corresponding to this, we find for the reformulation of (24)

$$Q=\frac{\kappa^2/4}{C^{-2}+\kappa^2/4}8\pi\lambda\!\!\!^{-2}\int_0^\infty dl(l+C^{-1})\frac{(C^{-2}+\kappa^2/4)^2}{\{(l+C^{-1})^2+\kappa^2/4\}^2}, \tag{26}$$

and with (22), we obtain exactly the result (25).

We have hereby a simple description of the quantum Rutherford scattering in close collisions, as seen in a classical interpretation. The scattering is scaled essentially to larger impact parameters q. At the same time the differential cross section $2\pi qdq$ is to be reduced by a *probability* of scattering, $(\kappa^2/4)/\{C^{-2}+\kappa^2/4\}$. When κ is small, the reduction is proportional to Z_1^2, as expected in first-order quantum perturbation. This should give a simple understanding of the interpretation problems encountered in Bloch's correction, i.e., σ_{tr}, as well as in Q.

IV. TRANSPORT CROSS SECTION FOR DIRAC ELECTRONS

In the previous sections we have made it clear that the central correction ΔL to a perturbation formula for the stopping logarithm is simply determined by the difference between the transport cross sections σ_{tr} and $\sigma_{\mathrm{tr}}^{\mathrm{pert}}$ for scattering of electrons of relative velocity v by the nucleus. We shall now apply the Dirac equation, and need at first the scattering theory for electrons with velocity v in a spherically symmetric potential.

For a spin-1/2 particle, the scattering amplitude may be expressed as [15,16]

$$f(\theta)=A(\cos\theta)+B(\cos\theta)\mathbf{n}\cdot\boldsymbol{\sigma}, \tag{27}$$

where the components of $\boldsymbol{\sigma}$ are the usual Pauli matrices and $\mathbf{n}$ is a unit vector perpendicular to the incident and exit directions. The scattering cross section summed over final spin values yields for an unpolarized initial state simply [15]

$$\frac{d\sigma}{d\Omega}=|A|^2+|B|^2. \tag{28}$$

Explicit expressions for the quantities A and B appearing in (27) and (28) are given for the nonrelativistic case in Ref. [15]. These expressions may be adapted to the relativistic case simply by replacing the nonrelativistic phase shifts by the proper relativistic ones. The result is [16]

$$A=\frac{\lambda\!\!\!^{-}}{2i}\sum_{l=0}^{\infty}[(l+1)(e^{2i\delta_{-l-1}}-1)+l(e^{2i\delta_l}-1)]P_l(\cos\theta),$$

$$B=\frac{\lambda\!\!\!^{-}}{2}\sum_{l=1}^{\infty}(e^{2i\delta_{-l-1}}-e^{2i\delta_l})P_l^1(\cos\theta), \tag{29}$$

where $\lambda\!\!\!^{-}$ relates to the electron momentum $p=\gamma mv$ as $\lambda\!\!\!^{-}=\hbar/p$, P_l is a Legendre polynomial and P_l^1 is an associated Legendre function, cf. [17]. Indices l and $-l-1$ refer to states where the upper (''large'') component of the electron spinor has orbital angular momentum l while the total angular momentum j assumes the values $j=l-1/2$ and $j=l+1/2$. The expressions (29) may be inserted in (28) which, in turn, may be applied in (8). Upon integration over angles, and after some algebra, the following expression for the transport cross section results:

$$\sigma_{\rm tr}=4\pi\lambda\!\!\!^{-2}\sum_{l=0}\,(l+1)\left[\frac{l+2}{2l+3}\sin^2(\delta_{-l-1}-\delta_{-l-2})+\frac{l}{2l+1}\sin^2(\delta_{l+1}-\delta_l)+\frac{1}{(2l+1)(2l+3)}\times\sin^2(\delta_{l+1}-\delta_{-l-1})\right]. \tag{30}$$

The result (10), valid for spinless particles, is obtained by putting $\delta_l=\delta_{-l-1}$. By the same substitution, the expressions (29) reduce (27) to the usual expression for the nonrelativistic scattering amplitude.

It is convenient to characterize the partial waves corresponding to a total angular momentum quantum number j by the quantum number $\kappa=\pm(j+1/2)$, which may take on any nonzero integer value. The quantum number j may be recovered from κ as $j=|\kappa|-1/2$, while the orbital angular momentum quantum number l assumes the value

$$l=\begin{cases}\kappa=j+1/2 & \text{for } \kappa>0\\ -\kappa-1=j-1/2 & \text{for } \kappa<0\end{cases}. \tag{31}$$

In terms of the quantum number κ and after renumbering for positive κ values, Eq. (30) may be formulated as

$$\sigma_{\rm tr}=4\pi\lambda\!\!\!^{-2}\sum_{\kappa}\,|\kappa|\left[\frac{\kappa-1}{2\kappa-1}\sin^2(\delta_\kappa-\delta_{\kappa-1})+\frac{1/2}{4\kappa^2-1}\sin^2(\delta_\kappa-\delta_{-\kappa})\right]. \tag{32}$$

Both terms in brackets in (32) correspond to a difference of $\Delta l=1$ (for the upper, so-called large, component of the electron spinor), but while in the first term also $\Delta j=1$, the second term corresponds to $\Delta j=0$. Accordingly, the second term will be called the spin-flip contribution. In the ultrarelativistic limit $\delta_{-\kappa}\to\delta_\kappa$ [16] whereby Eq. (32) reduces to a form rather similar to, though not identical to, the nonrelativistic result (10).

It should be emphasized that (30) and (32) hold for any spherically symmetric potential. For potentials that at large distances vary as the Coulomb potential, the situation is completely analogous to the nonrelativistic case. Thus, the sums in (30) and (32) formally have a logarithmic divergence. But in ΔL we are always concerned with the difference $\sigma_{\rm tr}-\sigma_{\rm tr}^{\rm pert}$, which difference is absolutely convergent, and has contributions only from close collisions just like its non-relativistic counterpart, the Bloch correction.

V. PRELIMINARY RESULTS FOR STOPPING POWER: POINTLIKE NUCLEI

We shall now apply the general results obtained in the previous section to the case of the Coulomb potential of a point charge Z_1e. We thereby obtain the stopping of a point nucleus, and our results can be compared directly with those of Ahlen [8,9]. The results in this section are only preliminary; in the following section we treat the proper case of nuclei with finite radii, and then quite considerable modifications are obtained when the Lorentz factor γ is large (for heavy ions, typically $\gamma>10$).

In the relativistic case, the Coulomb phase shifts assume the form [16]

$$\delta_\kappa=\xi_\kappa-\arg\Gamma(s_\kappa+1+i\eta)-\frac{1}{2}\pi s_\kappa+\frac{1}{2}\pi l, \tag{33}$$

where η is defined in (1), that is, $\eta\equiv\alpha Z_1c/v$ with α denoting the fine-structure constant. The sign of η is positive for attractive interaction but negative in the case of repulsion (negative Z_1 *or* negative-energy electron states). Note that for relativistic scattering, which is the subject of the rest of this paper, Bohr's κ is replaced by 2η while the symbol κ is reserved for the quantum number introduced in the previous section. The quantities s_κ and ξ_κ are defined as

$$s_\kappa=\sqrt{\kappa^2-(\alpha Z_1)^2},\quad e^{2i\xi_\kappa}=\frac{\kappa-i\eta/\gamma}{s_\kappa-i\eta}. \tag{34}$$

The quantity γ is the total particle energy measured in units of the rest energy, $\gamma=E/mc^2$. Since we consider solutions to the Dirac equation of positive energy only, this energy measure is of course identical to the usual Lorentz factor defined previously. Let us first consider the last term in (32) where we replace 1/2 in the numerator by 1 and sum over positive values of κ only. With

$$\tan(\delta_\kappa-\delta_{-\kappa})=-\frac{\eta}{\gamma\kappa}, \tag{35}$$

the spin-flip ($\Delta j=0$) contribution to the stopping logarithm may be written in closed form as

$$L_{\rm tr}^{\rm spin\ flip}=\frac{1}{\gamma^2}\sum_{\kappa\geqslant 1}\frac{\kappa}{4\kappa^2-1}\frac{1}{\kappa^2+(\eta/\gamma)^2}, \tag{36}$$

where $L_{\rm tr}$ as usual connects to the transport cross section as $L_{\rm tr}=(4\pi\eta^2\lambda\!\!\!^{-2})^{-1}\sigma_{\rm tr}$. The sum is convergent and easy to evaluate numerically. An equally simple expression has not been found for the first sum in (32); as compared to the nonrelativistic case the situation is now complicated by the fact that s_κ is not an integer. For the phase-shift differences entering this part of (32), the following expression holds:

$$\delta_\kappa-\delta_{\kappa-1}=\frac{1}{2}\arctan\frac{\eta(s_{\kappa-1}-s_\kappa)}{s_\kappa s_{\kappa-1}+\eta^2}+\frac{1}{2}\arctan\frac{\eta/\gamma}{\kappa(\kappa-1)+(\eta/\gamma)^2}-\arg\Gamma(s_\kappa+1+i\eta)+\arg\Gamma(s_{\kappa-1}+1+i\eta)-\frac{\pi}{2}\left(s_\kappa-s_{\kappa-1}-\frac{\kappa}{|\kappa|}\right). \tag{37}$$

As opposed to the spin-flip term, the first sum in (32) has the familiar logarithmic divergence. However, in the limit of large $|\kappa|$, $\sin^2(\delta_\kappa-\delta_{\kappa-1})$ tends to the value $(\eta/\kappa)^2$ whereby the contribution to $L_{\rm tr}$ tends to $1/|\kappa|$ and thus becomes independent of both η and γ.

Let us consider the perturbation limit, that is, $\eta\to 0$ and, of course, $\alpha Z_1(=\eta v/c)\to 0$. Here $\sin^2(\delta_\kappa-\delta_{\kappa-1})$ in (32) assumes the form

$$\sin^2(\delta_\kappa-\delta_{\kappa-1})=\left(\frac{\eta}{\kappa}\right)^2\left(1+\frac{1-1/\gamma}{2(\kappa-1)}\right)^2, \quad |\eta|\ll 1 . \tag{38}$$

In the nonrelativistic limit, i.e., $\gamma\to 1$, the second factor on the right-hand side of (38) approaches 1, and upon insertion into (32) and application of the expression (36) for the spin-flip contribution (in the limit $\eta\to 0$), the result (16) is obtained. It may be noted that the spin-flip term contributes 1/3 for $l=0$ (and that its relative contribution decreases rapidly with increasing l; the total value of the sum is $2\ln 2-1$). By insertion of (38) in (32) and application of (36) we obtain

$$L_{\rm tr}^{\rm pert}=\sum_{\kappa\geqslant 1}\frac{1}{\kappa}-\frac{5}{8}+\frac{1}{4\gamma}+\frac{3}{8\gamma^2}+\frac{1}{2}\left(1-\frac{1}{\gamma}\right)^2\sum_{\kappa\geqslant 2}\frac{1}{\kappa(\kappa^2-1)}. \tag{39}$$

Here the last sum converges rapidly. If it is extended to infinity (39) reduces to the simple result

$$L_{\rm tr}^{\rm pert}=\sum_{\kappa\geqslant 1}\frac{1}{\kappa}-\frac{v^2}{2c^2}, \quad |\eta|\ll 1 . \tag{40}$$

The last term, which has the remarkable feature of being independent of Z_1, is due to the spin of the electron: In a first Born approximation the differential scattering cross section equals the nonrelativistic Rutherford cross section times a factor $1-(v/c)^2\sin^2\theta/2$, where the second term is due to spin, cf. [16,18]. Our perturbation value for the transport cross section (40) leads to a stopping logarithm for close collisions of $\ln(Cq'\gamma mv/\hbar)-v^2/2c^2+1/2\kappa_{\max}+\cdots$ for $\kappa_{\max}\equiv q'\gamma mv/\hbar$ where q' is a fixed, γ-independent impact parameter which separates close and distant collisions. By addition of the contribution from distant collisions as obtained in a semiclassical perturbation treatment, i.e., by addition of $\ln(2\gamma\hbar v/ICq')-v^2/2c^2-\delta/2$ to the logarithmic factor, our result reproduces that of standard perturbation calculations, i.e., $L_{\rm stand}$ in (3). Note that the correction $-v^2/c^2$ receives equal contributions from close and distant collisions; see also [6,7].

In the ultrarelativistic limit, $\gamma\to\infty$, the result for ΔL, defined as the difference $L_{\rm tr}-L_{\rm tr}^{\rm pert}$, becomes independent of energy. From the expression (36) it is obvious that the spin-flip contribution vanishes in the high-energy limit. As far as the remaining terms are concerned, we note that $\eta\to\alpha Z_1$ when $\gamma\to\infty$, whereby the entire energy dependence of the phase-shift difference (37) is in the second arctan. Obviously, this term vanishes in the limit of high energies.

In the general nonperturbative case a numerical computation is required for the determination of $L_{\rm tr}$. In view of the results (32), (36), and (40) we have

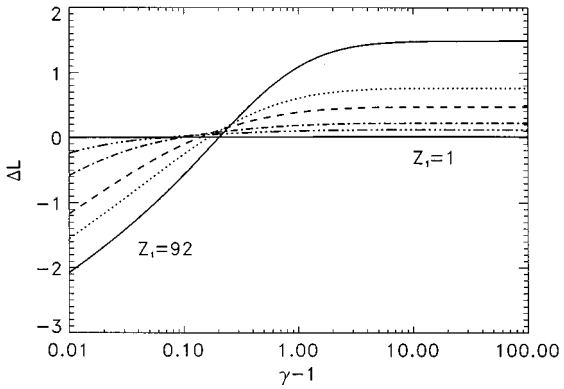

FIG. 1. Close-collision contribution ΔL as a function of $\gamma-1$ (projectile kinetic energy in units of the rest energy) for projectile charges $Z_1=1$, 10, 18, 36, 54, and 92. The quantity ΔL gives the correction to the perturbation value of the stopping logarithm (3) and is computed for the Coulomb potential of point nuclei; cf. (41) and (37). Finite nuclear size will affect the results substantially at high γ values; cf. Figs. 5–7.

$$\Delta L=\sum_{\substack{\kappa=-\infty\\(\kappa\neq 0)}}^{\infty}\left[\frac{|\kappa|}{\eta^2}\frac{\kappa-1}{2\kappa-1}\sin^2(\delta_\kappa-\delta_{\kappa-1})-\frac{1}{2|\kappa|}\right]+\frac{1}{\gamma^2}\sum_{\kappa=1}^{\infty}\frac{\kappa}{4\kappa^2-1}\frac{1}{\kappa^2+(\eta/\gamma)^2}+\frac{v^2}{2c^2}, \tag{41}$$

where summations have been extended to infinity since the exact choice of $\kappa_{\max}$ is immaterial due to the rapid convergence of the series. The phase-shift differences appearing in the first term are given by (37). Their determination requires computation of the argument of the complex gamma function. This, however, is very simple by application of the very precise "magic" formula for $\Gamma(z)$ given in [19]. As a check of the numerical calculations, we have produced a ΔL of zero (up to 1 part in 10^6) for $Z_1\to 0$. The formula (41) represents the relativistic generalization of the nonrelativistic result (20), i.e., of the Bloch correction.

Figure 1 presents the calculated ΔL for a wide range of energies and charges. For $Z_1=1$, our result is hardly distinguishable from first-order perturbation theory. At nonrelativistic energies, the stopping approaches the Bohr value for high charges. This shows up through negative values of ΔL. As noted in Secs. I–III, the ions will carry electrons at low energies, however, and the curves cannot be applied with any accuracy here. For high charges and relativistic energies, ΔL becomes positive. In the ultrarelativistic limit, the result for ΔL is independent of energy as discussed above.

Figure 2 demonstrates explicitly the agreement between the general nonperturbative result for ΔL and the nonrelativistic formula (20), $\Delta L_{\rm NR}\equiv-\eta^2\Sigma_{l=0}(l+1)^{-1}[(l+1)^2+\eta^2]^{-1}$, at low energies. The figure displays $\Delta L-\Delta L_{\rm NR}$ for the same projectile charges and collision energies as shown in Fig. 1. For $\gamma\to 1$ curves approach 0 for all charge numbers and for $Z_1\to 0$ the results approach 0 for any energy. For moderate charge numbers, the curves display essentially the linear Mott correction $Z_1\alpha\pi v/2c$, for the latter see, e.g. [20], (in the limit $v\to c$, the correction $Z_1\alpha\pi v/2c$

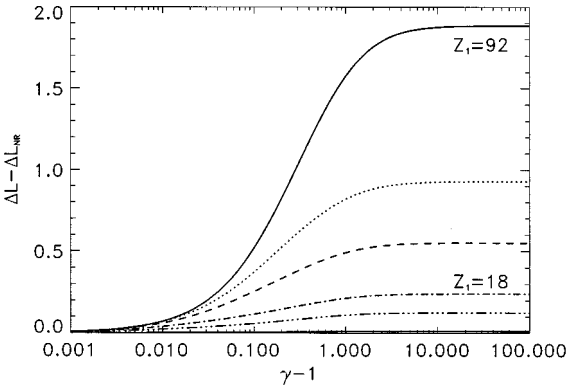

FIG. 2. As Fig. 1 but subtracting ΔL_{NR} from the ordinate. The quantity ΔL_{NR} is the nonrelativistic Bloch correction given by the expression (20).

assumes the values of 0.115, 0.206, and 0.413 for $Z_1=10$, 18, and 36, whereas the numerical calculation in these three cases gives 0.119, 0.220, and 0.473). Hence, for moderate charge numbers, the stopping is approximately obtained by adding the nonrelativistic ΔL_{NR} and the linear Mott correction to the relativistic L_{stand} of (3).

Figure 3 illustrates the distribution of $\Delta L-v^2/2c^2$ over angular momenta for some typical cases. A few angular momenta give sizable contributions. For the case of $Z_1=36$ and $\gamma=2$, values of $|\kappa|$ larger than 8 contribute 0.043 to ΔL; for $Z_1=92$ values of $|\kappa|$ larger than 8 contribute 0.133 at $\gamma=100$ and 0.112 at $\gamma=2$. It may be noted that those angular momenta that give sizable contributions to the sum (41) correspond to impact parameters much smaller than atomic radii.

It is of interest to compare our results to those quoted by Ahlen [8,9]. In making the comparison we can disregard the small Barkas term. Then his stopping-power formula splits into four parts: one term corresponding to the perturbation result, another to the nonrelativistic Bloch correction, a term contributing a correction $G/2$ to the logarithm L, and finally the density-effect correction. In the determination of the correction $G/2$, which Ahlen calls the Mott correction, he relies on early calculations of scattering of Dirac electrons by point nuclei. These results are in parametrized form, and $G/2$ is

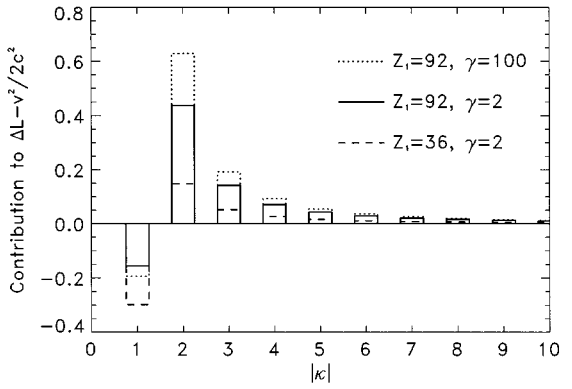

FIG. 3. Distribution over $|\kappa|$ of the contribution to $\Delta L-v^2/2c^2$; cf. Eq. (41). Each box represents two quantum numbers $\pm|\kappa|$.

composed of a set of terms with Z_1 up to the seventh power. If we subtract ΔL_{NR} from our computed value of ΔL as in Fig. 2, we may compare to Ahlen's correction $G/2$. For $Z_1=1$ good agreement is obtained at all energies tested ($0.01\leqslant\gamma-1\leqslant 100$) but the correction itself is small, not exceeding 0.012. For high charges good values are obtained with Ahlen's estimate at high energies, whereas poor values are obtained at low energies. We may quote some examples. Our result for $\Delta L-\Delta L_{\mathrm{NR}}$ increases with energy for positive charges; cf. Fig. 2. For $Z_1=84$ and 92, the value at $\gamma=100$ is 1.67 and 1.88, respectively. For $Z_1=84$, Ahlen's $G/2$ agrees with our number to the two decimals displayed here (with his parameter $\cos\chi$ set to 0.440). For $Z_1=92$, the estimate is higher than our value by 0.09 (with $\cos\chi=0.405$). At $\gamma=1.5$ our values for the same two charge numbers are 1.18 and 1.29, whereas Ahlen's are higher by 0.07 and 0.15. At $\gamma=1.2$ our values are 0.78 and 0.82, whereas Ahlen's are lower by 0.10 and 0.19. At still lower energies Ahlen's $G/2$ becomes virtually useless. These results correspond well with the author's claim that his estimate of $G/2$ contributes an uncertainty of no more than a few percent to the average energy loss provided $v/c>|Z_1|/100$. It should be remembered, however, that at high energies, beginning at $\gamma\simeq 10$, the results are modified substantially due to finite nuclear size.

In [14] the quantity $\Delta L-\Delta L_{\mathrm{NR}}$ was calculated for point-like nuclei essentially by the present method. There is fair agreement between our results and those presented in [14]. For $Z_1=92$ the deviation is nowhere larger than 0.05.

In a recent publication by Scheidenberger *et al.* [21], measurements of the average energy loss are reported for projectiles with γ values close to 2 and atomic numbers of 8, 18, 36, and 54. The authors compare to theoretical values that correspond to the sum of L_{stand} of (3), the nonrelativistic Bloch correction, and their own estimate of what is called the Mott correction (cf. Ahlen's $G/2$). In general, good agreement is obtained between theoretical and experimental results. The difference between the theoretical values for the full stopping power and the perturbation value corresponding to L_{stand} of (3) as read off the table in [21] are in good agreement with our results for ΔL. For the considered collision systems, the largest ΔL value encountered is 0.571 according to our calculations.

It may be of interest to display the effect of the electron spin. For scalar electrons, the formula (10) holds at any energy and we therefore merely need their relativistic phase shifts. For the Coulomb potential, the radial Klein-Gordon equation takes the same form as the nonrelativistic Schrödinger equation except for a replacement of $l(l+1)$ by $l(l+1)-(\alpha Z_1)^2$ in the angular-momentum barrier. The analysis of the Klein-Gordon equation is then similar to the analysis of the Schrödinger equation if the angular momentum l in the Schrödinger equation is replaced by an effective angular momentum $l^*=-1/2+\sqrt{(l+1/2)^2-(\alpha Z_1)^2}$; cf. [22]. As a result, the Klein-Gordon phase shifts take the form $\delta_l^{\mathrm{KG}}=-\arg\Gamma(l^*+1+i\eta)-(\pi/2)(l^*-l)+\eta\ln(2kr)$. In the determination of L, an approach based on the Klein-Gordon equation does not contain the term $-v^2/2c^2$; cf. [16], but yields twice the Mott correction $Z_1\alpha\pi v/2c$ for low charge numbers; cf. [20]. Accordingly, we show in Fig. 4 the differ-

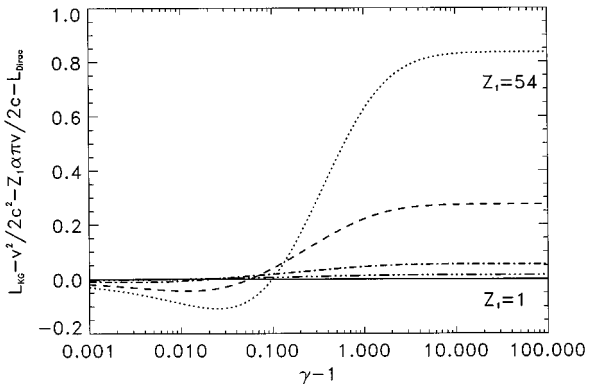

FIG. 4. Spin effects. The figure shows the difference between $L_{\mathrm{KG}}-v^2/2c^2-Z_1\alpha\pi v/2c$ and L_{Dirac} for the same γ values and charges (except $Z_1=92$) as in Fig. 1. See text for details.

ence between $L_{\mathrm{KG}}-v^2/2c^2-Z_1\alpha\pi v/2c$ and L_{Dirac}. For point charges, the solution of the Klein-Gordon equation requires $\alpha Z_1<1/2$, for which reason we have excluded $Z_1=92$ from our usual set of projectile charges; cf. Figs. 1 and 2. For moderate charge numbers $Z_1\leqslant 20$, additional spin-effects amount to less than 0.1 (which correspond to typically 1% of the total L value). On the other hand, as the charge number increases beyond 20, the curves of Fig. 4 start to deviate substantially from 0.

VI. FINAL RESULTS FOR STOPPING POWER: FINITE NUCLEAR SIZE

At high relativistic energies the finite size of the projectile nucleus must become important for electron scattering. Thus, an electron with rectilinear classical motion will encounter the nucleus when its angular momentum is $pR\simeq\gamma mcR$, where R is the nuclear radius. If this angular momentum is of order of $\hbar/2$, we may expect modification of the first few quantum phase shifts as compared to those for a point nucleus. With a standard value for the nuclear radius this criterion demands $1=\gamma mcR2/\hbar\simeq\gamma A^{1/3}/160$, where A is the projectile mass number. Reduction of stopping may therefore occur already for moderate values of γ. The corresponding reduction of straggling should be even larger, since straggling depends entirely on close collisions.

We note, moreover, that, because of the finite nuclear radius, the potential has a maximum depth of order of $4Z_1A^{-1/3}mc^2$. We can therefore expect that for sufficiently high relative energy γmc^2 of the electron, the stopping can again be calculated by means of first-order perturbation theory, i.e., it is proportional to Z_1^2. In first-order quantum perturbation theory, the scattering has an effective maximum momentum transfer of $\hbar k_{\max}\simeq\hbar/R$. This maximum momentum transfer has a decisive influence on the calculations. It follows that the recoil velocity u of the nucleus, originally at rest, is at most $u/c\simeq(6A^{4/3})^{-1}$ for standard nuclear radius. The maximum recoil velocity is thus exceedingly small, except perhaps in the case of the proton. Independently of the value of γ, we therefore use the *initial rest frame* of the ion for our formulation of scattering.

The above allows us to make a simple conclusion about asymptotic stopping. Since classical scattering has an effective minimum impact parameter $q_{\min}\approx R$, and similarly quantum perturbation has $k_{\max}\approx 1/R$, we have essentially the same cutoff in both cases. Accordingly, we expect that for all charge numbers the L functions converge to the value $L\rightarrow\ln(q_{\mathrm{ad}}/R)$, where q_{ad} is the effective adiabatic cutoff. In the following, we shall see how far these simple predictions are substantiated by the precise calculations.

The basis for our calculation is the results of Sec. IV, which hold in general for any spherically symmetric potential. In order to find the effect of finite nuclear size, we have to compute the corresponding phase shifts or, rather, differences in successive phase shifts. To this end, we shall assume the nuclear charge to be distributed homogeneously over a sphere of radius R, which we choose as $1.18\,A^{1/3}\times 10^{-13}$ cm, cf. [23], with the value of A taken according to the atomic weight. We proceed as described by Bhalla and Rose [24]; see also [25]. For any given value of κ, the radial wave functions of the electron outside the nucleus may now be expressed as a linear combination of the regular and the irregular (or singular) solutions of the Dirac equation obtained for the pure Coulomb potential for the same κ. Inside R, the radial wave functions are expressed as a series in the radial distance r. The full solution to the Dirac equation, and thereby the phase shift, is obtained by joining the two sets of solutions at R.

Let g and f denote the upper (or "large") and lower (or "small") components. For $\kappa<0$ the expansions for $r<R$ may be written as

$$G_{\mathrm{int}}\equiv rg_{\mathrm{int}}=\rho^k\sum_{n=0}^{\infty}a_n\rho^{2n},\quad F_{\mathrm{int}}\equiv rf_{\mathrm{int}}=\rho^{k+1}\sum_{n=0}^{\infty}b_n\rho^{2n},\tag{42}$$

where $k\equiv|\kappa|$, $\rho\equiv r/R$, and the subscript "int" stands for interior. For $\kappa>0$ the powers outside the summations are interchanged between the two components. Insertion of the expansions (42) in the Dirac equation leads to the following recurrence relations for the coefficients for $\kappa<0$:

$$a_0=-\frac{(2k+1)}{R(\gamma-1)+3\alpha Z_1/2}b_0,$$

$$2a_1=[R(\gamma+1)+3\alpha Z_1/2]b_0,$$

$$(2k+2n+1)b_n=-[R(\gamma-1)+3\alpha Z_1/2]a_n+(\alpha Z_1/2)a_{n-1},$$

$$2(n+1)a_{n+1}=[R(\gamma+1)+3\alpha Z_1/2]b_n-(\alpha Z_1/2)b_{n-1}.\tag{43}$$

The recurrence relations for $\kappa>0$ are obtained by interchanging the a and b coefficients in (43) and simultaneously changing the signs of γ and Z_1. For $r>R$, we write the G and F functions as $G_{\mathrm{ext}}=c_1G^{(r)}+c_2G^{(s)}$ and $F_{\mathrm{ext}}=c_1F^{(r)}+c_2F^{(s)}$ where the superscripts identify the regular and singular Coulomb solutions. Matching at the nuclear surface then yields

$$H\equiv c_2/c_1=\frac{F^{(r)}/G^{(r)}-F_{\mathrm{int}}/G_{\mathrm{int}}}{F_{\mathrm{int}}/G_{\mathrm{int}}-F^{(s)}/G^{(s)}}\frac{G^{(r)}}{G^{(s)}},\tag{44}$$

where all ratios are taken at $r=R$. The requested phase shift assumes the form

$$\delta_\kappa = \arg[\exp(i\delta_\kappa^{(r)}) + H\exp(i\delta_\kappa^{(s)})], \tag{45}$$

where the phase shift $\delta_\kappa^{(r)}$ for the regular Coulomb component is given by (33) whereas that for the singular component $\delta_\kappa^{(s)}$ is obtained from the same equation by the substitution $s_\kappa \to -s_\kappa$. The ratio between the two regular Coulomb components at $r=R$ may be written as

$$\frac{F^{(r)}}{G^{(r)}} = \sqrt{\frac{\gamma-1}{\gamma+1}}\frac{\mathrm{Re}\Lambda^{(r)}}{\mathrm{Im}\Lambda^{(r)}} \tag{46}$$

(include a minus sign in front of the square root for states of negative energy) where $\mathrm{Re}\Lambda^{(r)}$ and $\mathrm{Im}\Lambda^{(r)}$ denote the real and imaginary parts of $\Lambda^{(r)}$, respectively,

$$\Lambda^{(r)} \equiv e^{i(\xi_\kappa - pR/\hbar)}{}_1F_1(s_\kappa+1+i\eta, 2s_\kappa+1, 2ipR/\hbar) \tag{47}$$

and ${}_1F_1$ is the confluent hypergeometric function. For the ratio of the singular components an identical set of equations holds except for the substitution $s_\kappa \to -s_\kappa$ everywhere in Λ. For the ratio between the two G components we have

$$\frac{G^{(r)}}{G^{(s)}} = \frac{|\Gamma(s_\kappa+1+i\eta)|}{|\Gamma(-s_\kappa+1+i\eta)|}\frac{\Gamma(-2s_\kappa+1)}{\Gamma(2s_\kappa+1)}(2pR/\hbar)^{2s_\kappa}\frac{\mathrm{Im}\Lambda^{(r)}}{\mathrm{Im}\Lambda^{(s)}}. \tag{48}$$

Finally, the ratio $F_{\mathrm{int}}/G_{\mathrm{int}}$ is given by the ratio of the sum of the corresponding coefficients where we arbitrarily choose $a_0=1$ for $\kappa>0$ and $b_0=1$ for $\kappa<0$.

We have computed the modifications of the phase shifts relative to the Coulomb case for gold and $\gamma=225$ $[pR/\hbar=4.0]$ and compared to the modifications reported by Yennie, Ravenhall, and Wilson [26]; see also [18]. These authors compute in a special high-energy approximation where $\delta_\kappa=\delta_{-\kappa}$. For any given value of $|\kappa|$ our two results closely bracket that of [26]. For all values of $|\kappa|$ the deviations are comparable to the actual difference computed between modifications for $\pm|\kappa|$. This difference decreases with increasing values of $|\kappa|$. It attains its maximum of 0.0024 at $|\kappa|=1$. This number is small compared to the modification of -0.8582 reported in [26] for $j=1/2$.

In Figs. 5 and 6 we display our result for ΔL for finite radius R of the projectile nucleus. As opposed to the case of pointlike nuclei, where ΔL tends to a constant at high energies, Fig. 1, the finite value of R now causes ΔL to decrease below this asymptote and eventually become negative. The effect of finite nuclear size obviously sets in earlier for high than for low charge numbers, for uranium a 1% effect on the stopping occurs already at $\gamma\simeq 10$. Surprisingly, however, all curves very nearly pass through a common point close to $\gamma=85$ and $\Delta L=0$. A similar "fix point" appeared at low energies; cf. Figs. 1 and 5. For sufficiently large energies the dependence of ΔL on γ is logarithmic, so that the contribution to L from close collisions saturates, as predicted in the initial comments in the present section. This implies that at ultra-relativistic energies the average energy loss becomes independent of energy, since the density effect saturates the contribution from distant collisions at an impact parameter

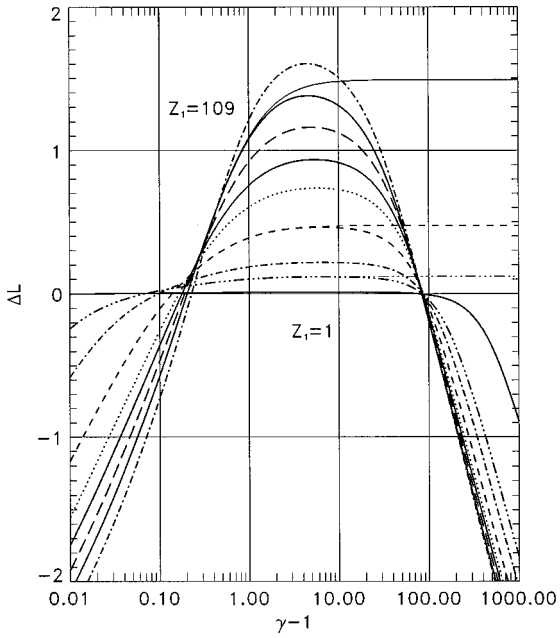

FIG. 5. Stopping for finite nuclear size. The curves display the values of ΔL for atomic numbers $Z_1=1$, 10, 18, 36, 54, 66, 79, 92, and 109 as computed for spherical nuclei of radius $1.18A^{1/3}\times 10^{-13}$ cm and homogeneous charge distribution. The value of A is chosen according to the atomic weight. The thin lines tending to constant values at high γ show ΔL for point nuclei of charge numbers 10, 36, and 92; cf. Fig. 1.

$q_{\mathrm{ad}}=v/\omega_{\mathrm{pl}}$, the quantity $\omega_{\mathrm{pl}}=\sqrt{4\pi ne^2/m}$ denoting the plasma frequency corresponding to the average density $n=NZ_2$ of target electrons. The high-energy ends of the curves displayed in Fig. 5 are all nearly equal to $-\ln(\gamma Rmc/\hbar)+v^2/2c^2$. This is seen more clearly in Fig. 7. If we add the high-energy asymptote to L_{stand} of (3) with the

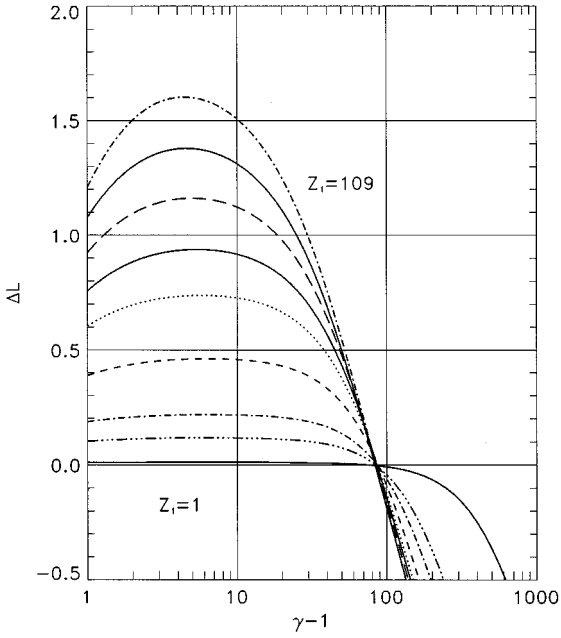

FIG. 6. Same as Fig. 5 but enhancing the region of intermediate γ values.

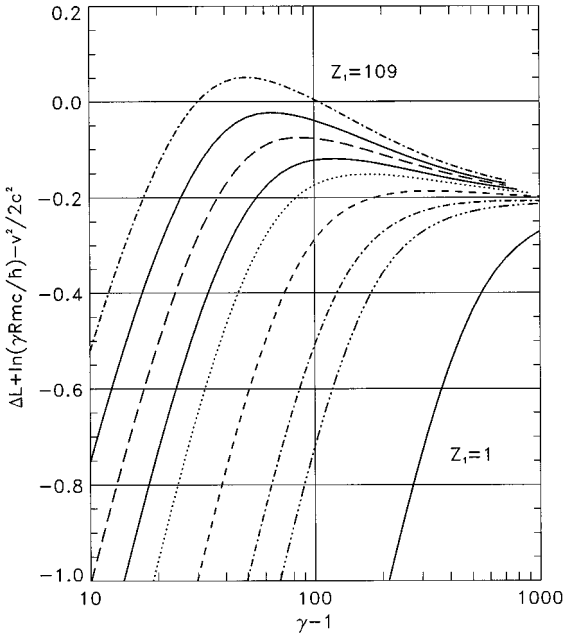

FIG. 7. Difference between ΔL and $-\ln(\gamma Rmc/\hbar)+v^2/2c^2$ for the high-energy part of the data displayed in Fig. 5. The curves indicate that the close-collision contribution to the stopping asymptotically tends to a constant.

density effect correction having the asymptotic value quoted in [8], we arrive at the simple result

$$L\rightarrow\ln(2c/R\omega_{\rm pl})-0.2=\ln(1.64c/R\omega_{\rm pl}) \tag{49}$$

for the total stopping logarithm in the ultrarelativistic limit. In this limit L depends very weakly on target and projectile parameters, having values $L\approx 14$ in condensed matter.

In the relativistic case, in contrast to the nonrelativistic case, the correction ΔL depends on the sign of the interaction as well as on its magnitude. In order to illustrate this, we display in Fig. 8 the difference in ΔL values for positive and negative charge numbers. This hypothetical case may also be conceived as the difference between electron and positron transport cross sections in scattering by ordinary nuclei. The curves in Fig. 8 are computed for finite nuclear size; for any charge number, the curve for pointlike nuclei is obtained

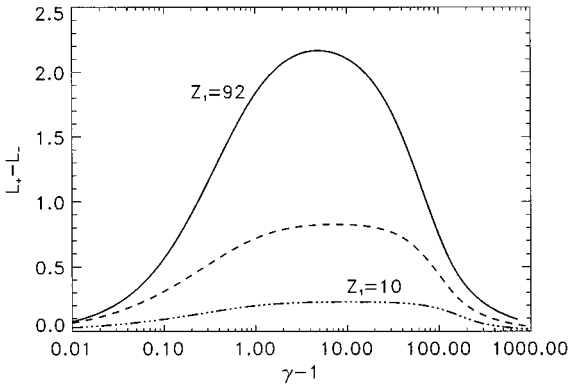

FIG. 8. Difference $L_+-L_-=\Delta L_+-\Delta L_-$ in stopping logarithm for nuclei and antinuclei of finite size for charge numbers 10, 36, and 92.

essentially by continuing from the maximum of the present curve at constant value. As soon as the energy is relativistic, that is, $\gamma-1>1$, the difference is surprisingly close to being linear in $|Z_1|$ until the effect of the finite nuclear size sets in. Although the difference between particle and antiparticle stopping is very nearly equal to twice the linear Mott correction, subtraction of this correction from $\Delta L-\Delta L_{\rm NR}$ still leaves a variation of about one unit for the range of charge and energy shown in Figs. 1 and 2 for both signs of the interaction; see also the discussion of Fig. 2.

It may be noted that the influence of the finite nuclear size on the stopping is not independent of the sign of the projectile charge. This result shows up through a later onset of nuclear-size effects for the case of repulsion than for the case of attraction displayed in Fig. 5. As to the difference between the values of ΔL encountered in the two cases we note from Fig. 8 that this falls back towards zero at high energies.

VII. FLUCTUATION IN ENERGY LOSS

Let us now turn to the question of fluctuation in energy loss. As discussed in Sec. II, a determination of the mean square fluctuation requires determination of the cross section Q, Eq. (21). For a spin-1/2 particle, the evaluation of this cross section follows the same steps as the evaluation of the transport cross section in Sec. IV. In analogy to (30), we obtain the following result:

$$Q=2\sigma_{\rm tr}-4\pi\lambda\!\!\!^{-2}\sum_{l=0}^{\infty}(l+1)(l+2)\left[\frac{l}{(2l+1)(2l+3)}\sin^2(\delta_{l+2}-\delta_l)+\frac{l+3}{(2l+3)(2l+5)}\sin^2(\delta_{-l-1}-\delta_{-l-3})\right.$$
$$\left.+\frac{2}{(2l+1)(2l+3)(2l+5)}\sin^2(\delta_{-l-1}-\delta_{l+2})+\frac{l}{(l+2)(2l+1)}\left(\frac{1}{4(l+1)^2-1}+\frac{1}{4l^2-1}\right)\sin^2(\delta_l-\delta_{-l-1})\right]. \tag{50}$$

This expression is valid quite generally and without reference to any specific (though centrally symmetric) scattering potential. In the spinless limit, which is obtained by taking $\delta_l=\delta_{-l-1}$, the formula reduces to the considerably simpler result (23).

It is convenient to formulate (50) in terms of the quantum number κ. The result is

$$Q=2\sigma_{\rm tr}-4\pi\lambda\!\!\!^{-2}\sum_{\kappa=-\infty}^{\infty}|\kappa|\left[\frac{(\kappa-1)(\kappa-2)}{(2\kappa-1)(2\kappa-3)}\sin^2(\delta_\kappa-\delta_{\kappa-2})+\frac{\kappa-1}{(2\kappa-3)(4\kappa^2-1)}\sin^2(\delta_\kappa-\delta_{-\kappa+1})\right.$$
$$\left.+\frac{1}{2}\,\frac{\kappa+1}{2\kappa+1}\left(\frac{1}{4\kappa^2-1}+\frac{1}{4(\kappa+1)^2-1}\right)\sin^2(\delta_\kappa-\delta_{-\kappa-1})\right], \tag{51}$$

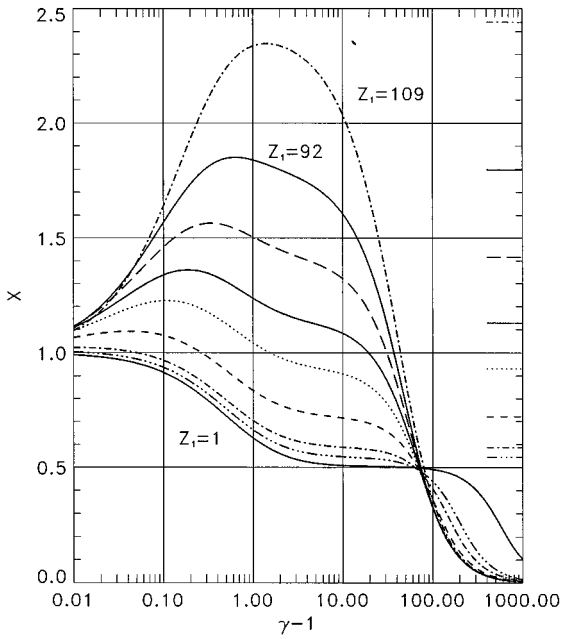

FIG. 9. Straggling for atomic numbers $Z_1=1$, 10, 18, 36, 54, 66, 79, 92, and 109. The curves show the quantity X, defined by Eq. (5), as a function of energy for spherical nuclei of radius $1.18A^{1/3}\times10^{-13}$ cm and homogeneous charge distribution. The horizontal lines to the far right indicate the high-energy values belonging to point nuclei.

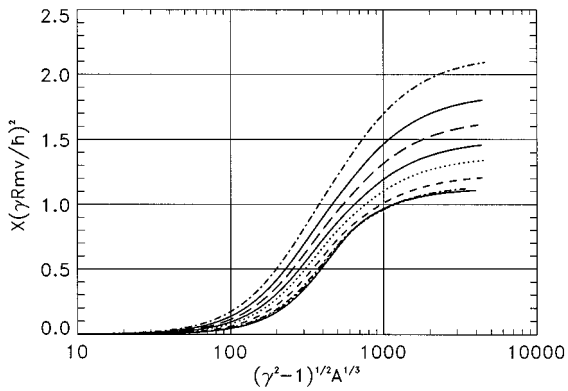

FIG. 10. Ratio of X and $(\lambda\!\!\!^{-}/R)^2$ as a function of $(\gamma^2-1)^{1/2}A^{1/3}$ for the high-energy part of the data displayed in Fig. 9. The curves for charge numbers 1, 10, and 18 are hardly distinguishable.

where $\sigma_{\rm tr}$ is given by (32). The summations of the last two terms in (51) may alternatively be performed solely for positive values of κ if coefficients are doubled.

We have previously, in (5), introduced straggling as a correction factor X times the straggling belonging to Rutherford scattering. According to (22), this factor is connected to Q by $X=Q/(4\pi\lambda\!\!\!^{-2}\eta^2)$. We present the numerical computations for finite nuclear radius only. In Fig. 9 is shown X as a function of $\gamma-1$ in a very wide interval, and for the same atomic numbers as in the case of stopping. At low values of $\gamma-1$, all curves are seen to approach the limit 1. Up to quite high values of $\gamma-1$, the proton represents accurately the perturbation formula $X=1-v^2/2c^2$, belonging to point nuclei. For moderate values of $\gamma-1$, before the effect of nuclear size sets in, the curves for heavier elements rise to values of order of 2, much above the proton curve. We have indicated the high-energy plateaus of X for point nuclei as horizontal lines on the right-hand side of the figure. For large values of $\gamma-1$, the X values decrease, starting with $Z_1=109$, and successively for lower atomic numbers. In the upper end, all curves decrease approximately as γ^{-2}, corresponding to constant values for the straggling Ω^2.

This upper region is shown in a simpler way in Fig. 10, using scaling properties that may be explained briefly as follows. In the wave equation describing scattering, the potential leads to a scaling in terms of a reduced length r/R, and therefore a reduced momentum pR. At very large γ, where the electron mass can be disregarded, and where we can write $(E/c)R=pR$, the full wave equation scales with pR. The result of calculations should therefore be a function of only $pA^{1/3}$ and $\eta=Z_1\alpha$. In Fig. 10, we have used a reduced momentum $(\gamma^2-1)^{1/2}A^{1/3}$ as the abscissa. Let us turn to the magnitude of the straggling, as represented by (5). It is proportional to the maximum energy transfer, which is $T_{\rm max}=p_{\rm max}^2/2m=2mv^2\gamma^2$ in the Rutherford case when M is sufficiently large. We have now instead a maximum momentum transfer $\hbar/R$ in first-order perturbation theory for large γ, and therefore the effective maximum energy transfer is $\approx T_{\rm max}^{\rm eff}\equiv\hbar^2/(2mR^2)$. Accordingly, we measure γ^2X in units of $2T_{\rm max}^{\rm eff}/mc^2$, and this is the scaling unit used as ordinate in Fig. 10. If perturbation theory is valid, the curves from Fig. 9 should merge into one on Fig. 10. This is very nearly so for $Z_1=1$, 10, and 18. The other curves should deviate from this when $Z_1\alpha$ increases. Actually, the curves in Fig. 10 behave approximately as $[1+(\alpha Z_1C)^2]^{1/2}$. The approximate saturation of Ω^2 is also evident.

As mentioned in Sec. II, for sufficiently thick targets the energy-loss distribution will be Gaussian around the average energy loss, and with width Ω. For thin targets, however, one finds a Landau-type distribution of smaller peak width, with a long tail towards large energy losses. The two cases are contained in the Landau-Vavilov distributions [27–29]. The familiar parameter ξ distinguishing between thin and thick targets becomes

$$\xi=\frac{2\pi Z_1^2e^4Z_2Nx}{mv^2T_0X}, \tag{52}$$

where $T_0X=2mv^2\gamma^2X$ is the effective maximum energy transfer. Moreover, the fluctuation parameter X is defined in (5), and its magnitude exhibited in Fig. 9. For $\xi<0.5$ the Landau distribution is obtained [30], and for $\xi\geqslant10$ the distribution is Gaussian. If we introduce the average energy loss $\langle\delta E\rangle$ in (52), we find

$$\xi=\frac{\langle\delta E\rangle}{2LT_0X}=\frac{\langle\delta E\rangle}{E}\frac{A\times1836}{4L(\gamma+1)X}, \tag{53}$$

the formula containing the relative loss of kinetic energy $\langle\delta E\rangle/E$, the mass number A of the ion (with the approxima-

tion $M/M_p \approx A$), and L from (2), $L \sim 10$. It is seen that for increasing values of γ, and even though A is large, it becomes more difficult to obtain a thick target with Gaussian distribution, as long as X remains of order unity. For very large γ, however, the parameter X decreases as γ^{-2}, and we rewrite (53) as

$$\xi = \frac{\langle \delta E \rangle}{E} \frac{A^{5/3}\gamma}{230\, y L}, \tag{54}$$

where $y = X/(\lambda\!\!\!^{-}/R)^2$ is the ordinate in Fig. 10, having asymptotic values $\sim 1-2$. For heavy ions with large energies, the Gaussian limit can then be obtained at quite small values of $\langle \delta E \rangle / E$.

VIII. CONCLUDING REMARKS

The essential points in this paper are, first, that we have been able to calculate relativistic stopping for heavy ions in a simple manner, because its deviation from first-order quantum perturbation can be formulated in terms of a transport cross section. Similarly, the straggling is obtained from a fluctuation cross section.

Second, the finite nuclear radii are important; they lead to a cutoff of momentum transfers at $\sim \hbar/R$. This gives a considerable reduction in stopping, and a large reduction in fluctuation. Because of the cutoff in momentum transfer, scattering can be accounted for in the initial rest frame of the ion for all values of γ, i.e., recoil corrections are negligible.

Third, as a background for the relativistic treatment, we have discussed in detail the nonrelativistic Bloch correction, thereby also illuminating a seeming paradox in Rutherford scattering.

It may be added that in a recent preliminary experiment at CERN, Datz *et al.* [31] have measured stopping of Pb ions with $\gamma = 170$ in carbon. The experimental result for L is 14.5 with an estimated uncertainty of $\pm 10\%$. This is in fair agreement with our theoretical value of $\Delta L = -0.716$, which leads to $L = 14.3$; cf. Fig. 5 and Eq. (3). The asymptotic expression (49) yields 14.2. Note that in the hypothetical case of point nuclei the L value would be 16.3.

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$$\arg\Gamma(s+1+i\eta) = \frac{\eta}{2}\ln\left[\left(s+c+\frac{1}{2}\right)^2+\eta^2\right] + \left(s+\frac{1}{2}\right)\arctan\frac{\eta}{s+c+1/2} - \eta + \arg\left(1+\sum_{n=1}^{6}\frac{C_n}{s+n+i\eta}\right).$$

The value of the c parameter is chosen to 5 while the coefficients C_n assume the values 76.180 091 73, $-86.505\,320\,33$, 24.014 098 22, $-1.231\,739\,516$, $0.120\,858\,003\times10^{-2}$, $-0.536\,382\times10^{-5}$ with increasing order of the index.
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