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Z^3 corrections to the scattering of electrons and positrons in atoms and to the energy loss of fast particles in solids

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A calculation of the elastic scattering cross section for the screened Coulomb potential of a charge Ze provides second-order terms, of relativistic and nonrelativistic origin, that are proportional to Z^3. Here we study the Z^3 effects in the elastic scattering of electrons and positrons in atoms and in the energy loss of fast charged particles in solids, for a wide range of energies. Owing to the Z^3 effect, the scattering of electrons in atoms becomes always larger than the scattering of positrons. In the relativistic limit this agrees with the result of McKinley and Feshbach for bare nuclei. The screening effect introduces a nonrelativistic enhancement of the Z^3 correction; this increases the asymmetry between electron and positron scattering. Using the same approach we calculate the contribution from close collisions to the Z^3 correction in the energy loss of fast particles in solids. For nonrelativistic velocities the Z^3 correction shows a behavior similar to the result of Ashley, Ritchie, and Brandt, including distant and close collisions; in the relativistic limit we retrieve the result of Jackson and McCarthy. The limitations of this approach in describing distant collisions, and the validity of the partition rule, are considered.

I. INTRODUCTION

The ionization rate of a fast charged particle in matter differs from that of its antiparticle, as shown by Barkas and other workers.[1,2] Ashley, Ritchie, and Brandt[3–5] studied this effect by extending the model of atomic oscillators introduced by Bohr[6] to describe the energy transfer from a fast particle of charge Ze to the target atoms. In addition to the leading Z^2 dependence of the Bethe-Bloch theory, they obtained a nonrelativistic Z^3 correction owing to distant collision events. The contribution from close collisions to the Z^3 term was also studied,[7–9] with the use of the exact Mott cross section[10] for the scattering of relativistic electrons in a Coulomb field and with the use of the expansion of the differential cross section in powers of Z given by McKinley and Feshbach.[11] The result, however, becomes negligible for nonrelativistic velocities. The contribution from close collisions to the nonrelativistic Z^3 effect in the energy loss was stressed by Lindhard,[12] who estimated nearly equal contributions from both close and distant collisions. Calculations of the Z^3 effect using the free-electron-gas model also supports this conclusion.[13] We can parenthetically notice that, in an impact-parameter description, close collisions may not be expected to be free of distant collision effects, inasmuch as the orbits of the scattering particles extend to infinity.

On the other hand, early experiments[14] of elastic scattering of electrons and positrons in atoms indicated an excess of electron over positron scattering, at large angles θ and for relativistic energies, as predicted by theory. The agreement in electron scattering experiments[15–17] was also good for all the elements with Z between 4 and 79. Scattering ratios of ~ 3, between electrons and positrons in platinum (for $\theta = 57.6°$ and kinetic energies $\simeq 1$ MeV), were measured by Lipkin and White,[18] in agreement with theory but also indicating possible screening effects. Calculations for extreme relativistic[19] and intermediate relativistic energies[20] show important differences between electron and positron scattering by point nuclei of charge Ze. For decreasing kinetic energies or for decreasing Z or θ values, these calculations approach Rutherford cross-section values,[20] as expected for the bare Coulomb potential. With decreasing energies, however, calculations for real atoms should incorporate additional screening effects.

The two phenomena previously described belong to two different experimental areas, but they can be theoretically described in similar terms provided that some simplifications are made from the beginning. This is the approach considered in this paper. First we analyze the effects of the atomic screening on the elastic scattering and the asymmetry between electron and positron scattering in atoms for a wide range of energies. The analysis is based on Dalitz calculation[21] of the second-order scattering amplitude for the Yukawa potential and it provides an extension to the relativistic Z^3 correction given by the formula of McKinley and Feshbach. A similar approach is used to study the contribution from close collisions to the Z^3 correction in the energy loss of fast particles in solids. The results are compared with previous relativistic and nonrelativistic descriptions.

II. ELASTIC SCATTERING OF ELECTRONS AND POSITRONS

The relativistic calculation of Rutherford scattering using classical mechanics shows a singular behavior at small distances, as the particle can be captured by the scattering center[22]; but for impact parameters much larger than the capture radius, the result may be approximated by simply including the relativistic mass correction in the differential scattering cross section, namely,

$$\frac{d\sigma_{\mathrm{Ruth}}}{d\Omega}=\frac{Z^2e^4}{m^2v^4}\frac{(1-\beta^2)}{4\sin^4\theta/2}\,, \tag{1}$$

which applies to the scattering of a particle of rest mass m (in our case the electron mass) and velocity $v=\beta c$ by a fixed point charge Ze; θ is the scattering angle and $d\Omega=\sin\theta\, d\theta\, d\phi$.

The first-order Born approximation for relativistic energies gives the following result, both for electron and positron scattering:

$$\frac{d\sigma^{(1)}}{d\Omega}=\frac{d\sigma_{\mathrm{Ruth}}}{d\Omega}\left[1-\beta^2\sin^2\frac{\theta}{2}\right]. \tag{2}$$

The factor $(1-\beta^2\sin^2\theta/2)$ is associated with the electron spin (it would be one for the scattering of a zero-spin particle); Eq. (2) includes both helicity flip and helicity nonflip processes. The Z dependence, however, remains unchanged.

The exact solution to the Coulomb scattering of a Dirac particle, as given by Mott,[10,23] is a partial-wave summation that must be calculated numerically.[19,20] The correct expansion in powers of Z, as given by McKinley and Feshbach[11] for the first two terms,

$$\frac{d\sigma^{(2)}}{d\Omega}=\frac{d\sigma_{\mathrm{Ruth}}}{d\Omega}\left[1-\beta^2\sin^2\frac{\theta}{2}\right.\\ \left.\pm\pi\frac{Z}{137}\beta\sin\frac{\theta}{2}\left[1-\sin\frac{\theta}{2}\right]\right], \tag{3}$$

introduces a Z^3 dependence in the cross section of relativistic electrons (+ sign) and positrons (− sign).

Let us consider now the effects related to the screening of the nucleus by the atomic electrons. The atomic potential will be approximated by

$$V(r)=\frac{Ze^2}{r}\exp\left[\frac{-r}{\lambda}\right], \tag{4}$$

where $\lambda\equiv q_s^{-1}$ represents the atomic screening distance; it could also be written as $\lambda=aZ^{-1/3}$, where $a=0.885\mu a_0$ and a_0 is the Bohr radius. Values of μ for some elements can be obtained from experiments[24]; the values $\mu=1$ and 3 will be used here only for illustrative purposes. The approximation of scattering by a static potential applies from electron (positron) energies of ~ 1 keV, where polarization and exchange corrections are important,[23] up to extreme relativistic energies ~ 10 MeV, where the finite size of the nucleus must be considered.[25,26] At these high energies radiative corrections become also important, especially for large scattering angles.[24] In addition we restrict our discussion to a range of v and Z values consistent with the applicability of the Born approximation.

The scattering amplitude obtained by Dalitz[21] provides the first two terms in the expansion of the cross section in powers of Z, which in ordinary units becomes

$$\frac{d\sigma}{d\Omega}=\frac{4Z^2e^4m^2\gamma^2}{\hbar^4(q^2+q_s^2)^2}\left[\left[1-\beta^2\sin^2\frac{\theta}{2}\right]\left[1-\frac{Z\alpha E}{\pi^2\hbar c}(q^2+q_s^2)\mathrm{Re}(I+J)\right]-\frac{Z\alpha m^2c^3}{\pi^2\hbar E}(q^2+q_s^2)\mathrm{Re}(I-J)\right], \tag{5}$$

where $\beta=v/c$, $\hbar q=2p\sin\theta/2$, $\gamma=(1-\beta^2)^{-1/2}$, $\alpha=e^2/\hbar c$; $p\equiv\hbar k=Ev/c^2$ is the momentum of the electron and E is its energy. The real parts of I and J, calculated from the integrals obtained by Dalitz, become

$$\mathrm{Re}(I)=-\frac{2\pi^2}{q\kappa^2}\tan^{-1}\left[\frac{qq_s}{2\kappa^2}\right], \tag{6}$$

$$\mathrm{Re}(J)=\frac{q_s^2+2k^2}{2k^2\cos^2\theta/2}\mathrm{Re}(I)+\frac{\pi^2}{2k^3\cos^2\theta/2}\tan^{-1}\left[\frac{2k}{q_s}\right]-\frac{\pi^2\tan^{-1}(q/2q_s)}{2k^3\sin\theta/2\cos^2\theta/2}, \tag{7}$$

where

$$\kappa=(q_s^4+4q_s^2k^2+q^2k^2)^{1/4}. \tag{8}$$

Relative to the Rutherford cross section, Eq. (1), the result for finite λ, Eq. (5), can be written for electrons ($d\sigma_-$) and positrons ($d\sigma_+$) in the convenient form

$$\frac{d\sigma_\mp}{d\sigma_{\mathrm{Ruth}}}=\frac{y^4}{(y^2+y_0^2)^2}\left[a_0(y)\pm\left[\frac{Zv_0}{v}\right]a_1(y)\pm\left[\frac{Zv_0v}{c^2}\right]a_2(y)\right], \tag{9}$$

where $v_0=e^2/\hbar$ is the Bohr velocity, and

$$a_0(y)=1-\beta^2y^2=1-\beta^2\sin^2\frac{\theta}{2}, \tag{10a}$$

$$a_1(y)=\left[\frac{4}{ys}\right](y^2+y_0^2)(1+\beta^2y_0^2-\tfrac{1}{2}\beta^2y^2)\times\tan^{-1}\left[\frac{yy_0}{s}\right], \tag{10b}$$

$$a_2(y)=\left[\frac{2}{y}\right](y^2+y_0^2)\left[\tan^{-1}\left[\frac{y}{2y_0}\right]-y\tan^{-1}\left[\frac{1}{y_0}\right]\right], \tag{10c}$$

$$s=(y^2+4y_0^2+4y_0^4)^{1/2}.$$

In these equations we have introduced the notation

$$y=\sin\frac{\theta}{2},\quad y_0=\frac{\hbar}{2p\lambda}=\frac{\hbar q_s}{2\gamma mv}. \tag{11}$$

The dependence on β and y_0 of the functions $a_i(y)$ is implicitly assumed.

For $\lambda\rightarrow\infty$ (Coulomb potential), this result contains the previous approximations, Eqs. (1)–(3), in the limiting cases where each of them applies. The term $a_0(y)$ in Eq. (9) represents the contribution of the first-order Born approximation to the differential scattering cross section. The second-order terms $a_1(y)$ and $a_2(y)$ introduce a Z^3 correction in the differential cross section. The function $a_1(y)$ is important for the nonrelativistic behavior of Eq. (9); it is clearly related to the screening and it vanishes for $\lambda\rightarrow\infty$. The function $a_2(y)$ provides an extension to the relativistic McKinley and Feshbach correction, Eq. (3), for a screened field.

The difference between electron and positron scattering can be analyzed in terms of the ratio

$$\Delta\equiv\frac{1}{Z\alpha}\frac{d\sigma_--d\sigma_+}{d\sigma_-+d\sigma_+}=\frac{a_1(y)+\beta^2a_2(y)}{\beta a_0(y)}, \tag{12}$$

as obtained from Eq. (9), with $\alpha=e^2/\hbar c\cong 1/137$. This is shown in Fig. 1 for $y=\sin\theta/2=0.5$ (i.e., $\theta=60°$); the dash-dot line represents the result for the case $\lambda=\infty$ (Coulomb potential), i.e.,

$$\Delta=\pi\beta y\frac{1-y}{1-\beta^2y^2},$$

obtained from Eq. (3), which corresponds to $a_1(y)=0$ and $a_2(y)=\pi y(1-y)$. Screening effects are responsible for the differences between the results for $\lambda=\infty$ (dashed-dot line) and for finite λ (solid lines for $Z\alpha=0.2$, dashed lines for $Z\alpha=0.1$). These effects are negligible for $v\gtrsim 100v_0$ ($\beta\gtrsim 0.7$), but they dominate for nonrelativistic velocities where Δ reaches its highest values.

The ratio between positron and electron differential scattering cross sections,

$$R(y)\equiv\frac{d\sigma_+}{d\sigma_-}=\frac{1-Z\alpha\Delta}{1+Z\alpha\Delta}, \tag{13}$$

is shown as a function of the scattering angle θ in Fig. 2(a) for $\lambda=\infty$ and in Fig. 2(b) for $\lambda=aZ^{-1/3}$, according to Eqs. (3) and (9), respectively. The Z^3 effect shown in Fig. 2(a) disappears for nonrela-

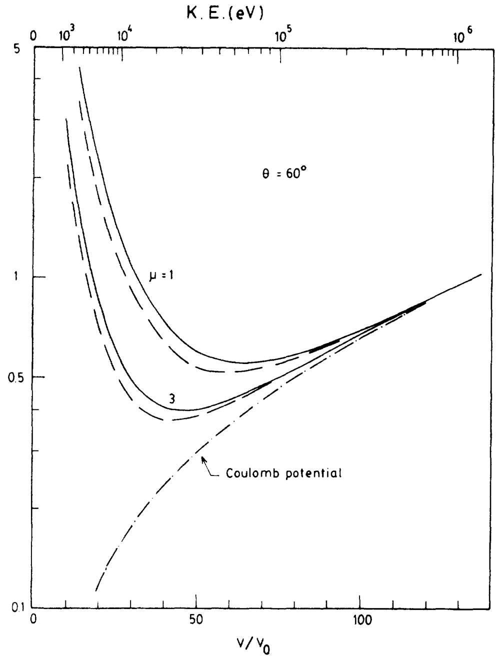

FIG. 1. Z^3 correction to the differential scattering cross section, as given by the ratio $\Delta = (Z\alpha)^{-1} \times (d\sigma_- - d\sigma_+)/(d\sigma_- + d\sigma_+)$, according to Eqs. (10) and (12), as a function of the velocity v and for scattering angle $\theta = 60°$. The upper scale gives the kinetic energy of the electrons or positrons. Calculations for screened potentials, with parameters $\mu = 1$ and $\mu = 3$, are illustrated with solid lines for $Z\alpha = 0.2$ and with dashed lines for $Z\alpha = 0.1$. The dashed-dot line gives the Z^3 correction to the scattering by bare nuclei.

tivistic velocities where $R(y) \to 1$, when approaching Rutherford scattering.[20] When screening is taken into account, as in Fig. 2(b), a stronger nonrelativistic effect develops, which further reduces the relative scattering of positrons (and increases the scattering of electrons).

III. ENERGY LOSS OF FAST PARTICLES IN SOLIDS

We consider now the Z^3 effect in the energy loss of fast particles in solids, with the use of an approximation that permits one to outline the relation with the scattering problem. Here we use the second-order Born approximation for the scattering by a screened potential, Eq. (4), where the screening distance shall be regarded as conveying information on the dynamical response of the medium; the appropriate scale of distances is set if we take[27,28] $\lambda = \gamma v / g\omega$, where $v = \beta c$ is the particle velocity, $\gamma = (1-\beta^2)^{-1/2}$, g is a number of order unity, and ω is an oscillator frequency. An average over the appropriate oscillator strength distribution could eventually be performed at a later stage, following the usual approach of considering the medium in a statistical sense.[4,29] This is a standard approach that will not be discussed here. The energy loss per unit distance can be calculated from the integral

$$S \equiv \frac{dE}{dx} = n \int Q\, d\sigma \,, \tag{14}$$

where n is the density of electrons in the medium and Q is the energy transfer in the laboratory frame. The integral can be written in terms of the center-of-mass variable $y = \sin\theta/2$, with the use of Eq. (9) for the differential cross section, where the

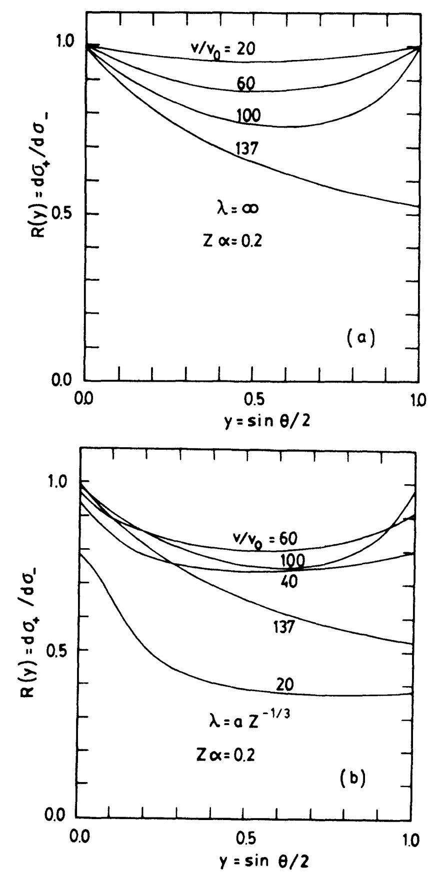

FIG. 2. Ratio between positron ($d\sigma_+$) and electron ($d\sigma_-$) differential scattering cross sections as a function of the scattering angle variable $y = \sin\theta/2$ for $Z\alpha = 0.2$ and for several values of the velocity v. (a) corresponds to the scattering by bare nuclei as predicted by the formula of McKinley and Feshbach, Eq. (3). (b) applies to the screened Coulomb potential, Eq. (4), with $\mu = 1$; here the asymmetry between electron and positron scattering becomes important at large angles (close collisions), both for relativistic and nonrelativistic velocities.

positive and negative signs in the right-hand side correspond here to positive and negative values of the charge of the scattering center. The value of Q in the laboratory frame, in terms of the spatial component of the four-momentum transfer $q^\mu=(\vec{q},0)$ in the center-of-mass frame ($\hbar|\vec{q}|=2p\sin\theta/2=2py$, $p=\gamma mv$), is

$$Q=\frac{\hbar^2|\vec{q}|^2}{2m}=\frac{2p^2}{m}y^2\,, \tag{15}$$

like in the nonrelativistic case. From Eqs. (9), (14), and (15) we get

$$S=\frac{4\pi nZ^2e^4}{mv^2}\int_0^1\frac{y^3dy}{(y^2+y_0^2)^2}\times\left[1-\beta^2y^2\pm\frac{Zv_0}{v}a_1(y)\pm\frac{Zv_0v}{c^2}a_2(y)\right], \tag{16}$$

where

$$y_0=\frac{\hbar}{2p\lambda}=\frac{g\hbar\omega}{2mv^2}(1-\beta^2)\,. \tag{17}$$

The leading term in the energy loss, of order Z^2, can be calculated immediately and for $y_0 \ll 1$ it becomes

$$S_0=\frac{4\pi nZ^2e^4}{mv^2}\left[\ln\left[\frac{1}{y_0}\right]-\frac{1}{2}-\frac{1}{2}\beta^2\right]. \tag{18}$$

With the use of Eq. (17) for y_0 we can check the agreement with the relativistic Bethe formula,

$$S_{\text{Bethe}}=\frac{4\pi nZ^2e^4}{mv^2}\left[\ln\left[\frac{2mv^2}{\hbar\omega}\right]-\ln(1-\beta^2)-\beta^2\right]. \tag{19}$$

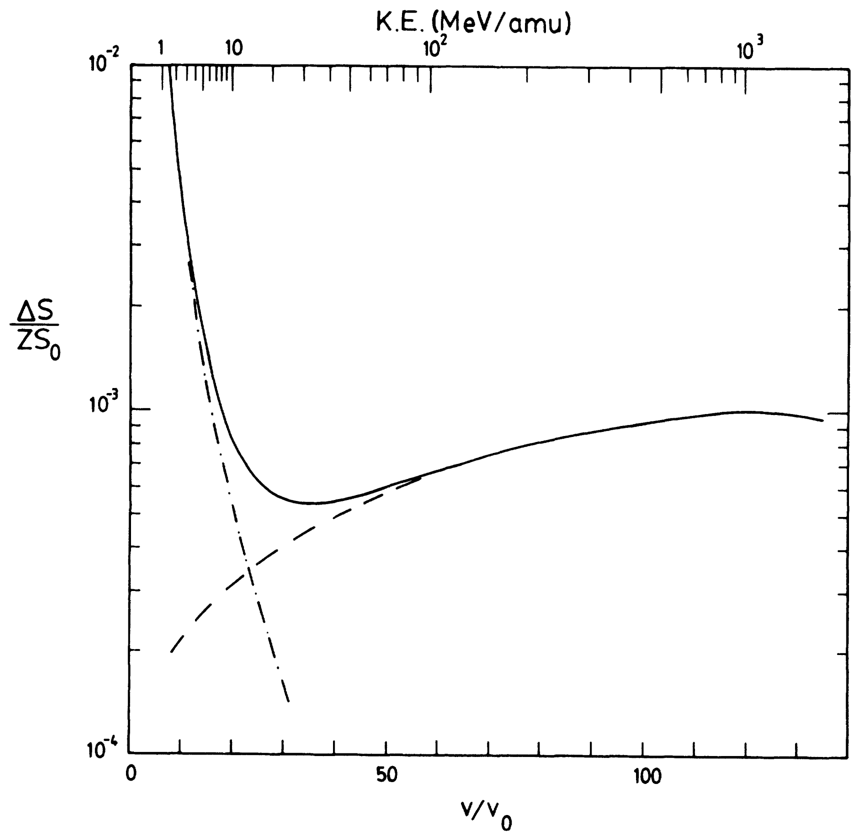

FIG. 3. Z^3 correction to the energy loss ΔS divided by ZS_0 from Eqs. (18) and (20). The relativistic limit of Eq. (21) is indicated with a dashed line and it agrees with the calculation of the close-collision effect (Fermi correction) by McKinley and Feshbach. The nonrelativistic approximation of Eq. (22), dash-dot line, includes similar contributions from both close and distant collisions.

The term $\ln(1-\beta^2)$ is correctly obtained with equal contributions from close ($y \sim 1$) and distant ($y \sim 0$) collisions. The term $-\frac{1}{2}\beta^2$ in Eq. (18) comes from close collisions and is only half of the term $-\beta^2$ in Eq. (19); the other half should come from distant collisions, but it is not obtained with this model.

The Z^3 correction to the stopping power is given by

$$\Delta S = \frac{4\pi n Z^3 e^4}{mv^2} \int_0^1 \frac{y^3 dy}{(y^2+y_0^2)^2} \left[\frac{v_0}{v} a_1(y) + \frac{v_0 v}{c^2} a_2(y) \right] ; \tag{20}$$

this reduces to the relativistic and nonrelativistic results, in the appropriate limits, as illustrated in Fig. 3. For $\beta \rightarrow 1$ we retrieve the "Fermi correction" as calculated by Jackson and McCarthy,[9] namely,

$$\Delta S_{\beta \simeq 1} \cong \left[\frac{4\pi n Z^3 e^4}{mv^2} \right] \frac{\pi}{2} \frac{v_0 v}{c^2} , \tag{21}$$

which is entirely due to close collisions with a bare Coulomb potential. For $\beta << 1$ we obtain a characteristic v^{-3} dependence in $\Delta S / Z S_0$ similar to the result of Ashley, Ritchie, and Brandt,[4] but including now close collisions, as given by

$$\Delta S_{\beta << 1} \cong \left[\frac{4\pi n Z^3 e^4}{mv^2} \right] \frac{2ge^2\omega}{mv^3} \ln \left[\frac{mv^2}{2^{1/3} g \hbar \omega} \right] . \tag{22}$$

These two limits are indicated in Fig. 3 with a dashed line, Eq. (21), and with a dash-dot line, Eq. (22).

It is also illustrative to divide the range of integration in Eq. (20) between distant collisions for $0 \le y \le y_c$ and close collisions, $y_c \le y \le 1$, where $y_c = \hbar / 2mv\gamma r_c$, and we take[9] $r_c = (\hbar / 2m\omega)^{1/2}$, which is the amplitude of the quantum-mechanical harmonic oscillator. This separates nearly equal contributions to the leading term S_0, as required by the partition rule of Bohr.[30] As for the Z^3 term, this calculation yields a contribution from close collisions that may be larger than 50% at nonrelativistic energies and increases up to 100% for relativistic particles. This prevents application of the partition rule to the Z^3 term in the energy loss, with close collisions predominating at high energies.

The role of close collisions is further emphasized if one considers the Z^3 effect on the *straggling* of the energy-loss distribution, which is obtained from[30]

$$\begin{aligned} \Omega^2 &= n \int Q^2 d\sigma \\ &= 2\gamma^2 \Omega_B^2 \int_0^1 \frac{y^5 dy}{(y^2+y_0^2)^2} \\ &\quad \times \left[1 - \beta^2 y^2 \pm \frac{Zv_0}{v} a_1(y) \pm \frac{Zv_0 v}{c^2} a_2(y) \right] , \end{aligned} \tag{23}$$

where $\Omega_B^2 = 4\pi n Z^2 e^4$ is the value of the straggling calculated by Bohr. This integral is easily evaluated when $y_0 << 1$, both for the relativistic and nonrelativistic cases, with the results

$$\Omega_{\beta \simeq 1}^2 \cong \gamma^2 \Omega_B^2 \left[1 \pm \frac{\pi}{12} Z \frac{v_0 v}{c^2} \right] , \tag{24a}$$

$$\Omega_{\beta << 1}^2 \cong \Omega_B^2 \left[1 \pm \frac{2Ze^2 g\omega}{mv^3} \right] . \tag{24b}$$

Thus, the Z^3 correction for the straggling has a velocity dependence similar to that of the stopping power illustrated in Fig. 3, but it is due to close collisions over the whole velocity range. This behavior can ultimately be traced back to the velocity dependence of the differential scattering cross section in Fig. 1.

Because of the restrictive assumptions made in this calculation of the energy loss, we will not push these results much further. We can just recall that consistent analyses of energy-loss experiments can be carried on by including both distant- and close-collision contributions to the Z^3 term and an additional higher-order Z^4 correction.[12,31,32]

IV. CONCLUSIONS

The asymmetries in the scattering of fast electrons and positrons in atoms and in the energy-loss rates for fast particles and antiparticles in solids, can be studied in analogous ways using a second-order analysis of the scattering cross section for the screened Coulomb potential. This introduces correction terms of order Z^3, which distinguish the scattering of each particle according to its sign.

The Z^3 correction for the elastic scattering of electrons and positrons in atoms always increases the scattering of electrons relative to that of positrons. The effect is especially pronounced for large angles of scattering ("close collisions") and it may be of interest for single- and multiple-scattering experiments. In particular, measurements of particle-beam attenuations in thick solid foils give larger transmissions for positrons than for electrons[33,34] in the relativistic energy range where theories have been advanced.[35,36] The analysis of this paper indicates a nonrelativistic enhancement of the asymmetry in the scattering of such particles. A thorough study of the final effects on the penetration of each particle beam should also include the differences in the energy-loss distributions for electrons and positrons[35]; this study has not yet been made for the nonrelativistic case.

The scattering cross section was here applied to the calculation of the energy loss of fast charged particles in solids. The treatment connects previous results dealing with separate relativistic and nonrelativistic Z^3 effects and it indicates a significant contribution from close-collision events. This model is, however, less appropriate to describe excitations produced in distant collisions; in particular, it introduces an effective cutoff for distant excitations through the adiabatic parameter $\lambda=\gamma v/g\omega$, where the value of g can not be calculated by this approach. On the other hand, this resembles the situation of previous distant-collision treatments,[4,9,37] where an inner cutoff distance must be introduced. Although these two approaches seem to complement each other, a proper matching of them cannot be obtained here. This remaining problem could only be solved by a more comprehensive description of close and distant collisions.

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