

## Density Effect in Ionization Energy Loss of Charged Particles

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A more rigorous justification is given for the statement made by Aage Bohr that for an incident particle of relativistic velocity, the electrostatic effect of the surrounding electrons is negligible and the main factor in the screening is due to the electromagnetic interactions which limit the impact parameter to a value  $c/\Omega$ , where  $\Omega = (4\pi ne^2/m)^{1/2}$  and  $n$  is the electron density in the medium.

### I. INTRODUCTION

THE density effect, originally suggested by Swann,<sup>1</sup> accounts for the reduction in the ionization energy loss of charged particles due to the polarization of the medium, and a quantitative theory of this effect has been given by Fermi.<sup>2</sup> The work of Fermi has been further extended and refined and a great many investigations have been devoted to this subject.<sup>3</sup> The density effect has also been studied by Bohr,<sup>4</sup> who emphasized certain intuitional and microscopic aspects whereas previous investigations were based mostly on rigorous solution of Maxwell's equations in a macroscopic medium. Bohr was particularly interested in the adiabatic limit of the impact parameter beyond which no appreciable energy transfer occurs, and showed by means of ingenious microscopic considerations how the electromagnetic field of the perturbed electrons is effective in setting this adiabatic limit.

The arguments presented by Bohr are based to a large extent on rather cursory calculations. It seemed, therefore, desirable to undertake more exact calculations to show whether and to what extent the Bohr theory is valid. The results obtained in this investigation show a satisfactory agreement with the results obtained by Bohr.

### II. ARGUMENTS OF BOHR

Bohr's considerations are based on the existence of a maximum impact parameter defining the adiabatic limit beyond which the effect of the moving particle is negligible. For relativistic velocities of the particle, i.e., for  $V \rightarrow c$ , for a medium of low density, the adiabatic limit  $d_1$  increases indefinitely with  $V$ , i.e.,

$$d_1 = V\gamma/\omega_1, \quad (1)$$

where  $\gamma = 1/(1-\beta^2)^{1/2}$ . We assume that the medium is composed of atoms characterized by a binding frequency  $\omega_1$ .

In case of a dense medium the situation changes entirely. According to Bohr, electromagnetic forces enter into the effect caused by the electrons in the

medium that are perturbed by the moving particle. As shown by Bohr, these forces limit the impact parameter, which for increasing  $V$  tends to a value

$$d_2 = c/\Omega, \quad (2)$$

where  $\Omega = (4\pi ne^2/m)^{1/2}$  and  $n$  is the electron density in the medium.

The expression (2) has been derived by considering an electron at a distance  $\rho$  from the particle track. Bohr<sup>5</sup> calculated that the field due to the retarded action of all electrons in the medium perturbed by the particles and acting on the electron at a distance  $\rho$  is:

$$E_{\text{ret}}^m \sim (e^2 n \rho^2 / c^2) \ddot{\eta}, \quad (3)$$

where  $\ddot{\eta}$  is the acceleration of the electron due to the field of the particle. The field

$$E^p = m\ddot{\eta}/e, \quad (4)$$

and is directed against  $E_{\text{ret}}^m$ . Therefore, as observed by Bohr, we obtain from (3) and (4) that

$$E_{\text{ret}}^m \ll E^p, \quad (5)$$

for  $\rho \ll c/\Omega$ .

From this observation Bohr concluded that  $\rho = c/\Omega$  represents the adiabatic limit beyond which the interaction of the incident particle with the surrounding medium is negligible.<sup>5</sup>

The above argument presented by Bohr is rather cursory. No consideration has been given to the impact parameter  $\rho > c/\Omega$ . In order to support Bohr's result, it would be necessary to show that for  $\rho > c/\Omega$  the field produced by the retarded action of the perturbed electrons is equal and opposite to the field due to the direct action of the incident particle and, therefore, the medium remains unperturbed. This has not been done by Bohr.

It should be noted that the expression (3) is not rigorous and cannot be applied for  $\rho > c/\Omega$ . This can be shown by taking<sup>6</sup>

$$\ddot{\eta} \sim Z_1 e^2 \gamma / \rho^2, \quad (6)$$

(where  $Z_1 e$  is the charge of the incident particle) and substituting the expression (6) in (3) we obtain that for any substantially large impact parameter  $\rho$  the field  $E_{\text{ret}}^m$  is constant, i.e.,

$$E_{\text{ret}}^m \sim Z_1 e^4 n \gamma / c^2, \quad (7)$$

<sup>5</sup> See reference 4, p. 23.

<sup>6</sup> See reference 4, p. 8, Formula (3.1).

<sup>1</sup> W. F. G. Swann, *J. Franklin Inst.* **226**, 598 (1938).

<sup>2</sup> E. Fermi, *Phys. Rev.* **57**, 485 (1940).

<sup>3</sup> For a review of the literature, see, for instance, F. Sauter, in *Kosmische Strahlung*, edited by W. Heisenberg (Springer Verlag, Berlin, 1953), pp. 456-481.

<sup>4</sup> Aage Bohr, *Kgl. Danske Videnskab. Selskab, Mat.-fys. Medd.* **24**, No. 19 (1949).

which obviously is not in agreement with the physical reality.

### III. EXACT CALCULATIONS

As pointed out by Bohr, the screening effect of the medium on the incident charged particle depends on the velocity of the particle. For a low velocity, one has to consider only the electrostatic forces between the electrons of the medium and these forces are only of secondary importance in the stopping power. For a relativistic velocity, the electrostatic effects are negligible and the stopping power is determined mainly by electromagnetic interactions between the electrons in the medium.

In order to determine separately the electrostatic and electromagnetic effects, we shall examine the longitudinal and transverse components of the field. Since the longitudinal component is irrotational, it will be associated with electrostatic effects and since the transverse component is divergence-free, it will be associated with electromagnetic interactions. It should be noted in that connection that the retarded field of the perturbed electrons which has been calculated by Bohr is not identical to the transverse component of the electromagnetic field.

To calculate in a precise manner the effect of the transverse and longitudinal fields in the dielectric medium we begin with Maxwell's equations:

$$\begin{aligned} -\nabla \times \mathbf{E} &= -\frac{1}{c} \frac{\partial \mathbf{H}}{\partial t}; & \nabla \cdot \mathbf{H} &= 0; \\ \nabla \times \mathbf{H} &= -\frac{\epsilon}{c} \frac{\partial \mathbf{E}}{\partial t} + \frac{4\pi}{c} Z_1 e \mathbf{V} \delta(\mathbf{r} - \mathbf{V}t), \\ \epsilon \nabla \cdot \mathbf{E} &= 4\pi Z_1 e \delta(\mathbf{r} - \mathbf{V}t), \end{aligned} \quad (8)$$

and

$$\mathbf{E}_i(z, \rho, \varphi) = \frac{-iZ_1 e}{2\pi^2 V} \int_0^{2\pi} d\varphi' \int_0^\infty \kappa d\kappa \int_{-\infty}^\infty \frac{d\omega \mathbf{k} \exp[ik\rho \cos(\varphi - \varphi') + i\omega(z - Vt)/V]}{(\kappa^2 + \omega^2/V^2)\epsilon(\omega)}, \quad (14)$$

where  $(z, \rho, \varphi)$  are the coordinates of the field point in a cylindrical system of coordinates whose axis is coincident with the particle track. The location of the incident particle at time  $t$  is given by  $z - Vt = 0$ .

An electron in the medium located at a distance  $\rho$  from the particle track is in the process of undergoing collision with the particle and simultaneously is acted upon by other electrons in the medium. We determine the net fields acting on an electron at  $\rho$  and at  $z = Vt$  and, then, by carrying out the integrals given in Eqs. (14) and (15), we find that only the components of the longitudinal and transverse fields which are perpendicular to

in which we assume the medium to be infinite homogeneous, nonmagnetic, and characterized by a dielectric constant  $\epsilon(\omega)$ .

We now analyze  $\mathbf{E}$ ,  $\mathbf{H}$ , and the incident charge into Fourier components,

$$\left\{ \begin{array}{l} \mathbf{E}(\mathbf{r}, t) \\ \mathbf{H}(\mathbf{r}, t) \\ \delta(\mathbf{r} - \mathbf{V}t) \end{array} \right\} = \int d\mathbf{k} \exp[i\mathbf{k}(\mathbf{r} - \mathbf{V}t)] \left\{ \begin{array}{l} \mathbf{E} \\ \mathbf{H} \\ (2\pi)^{-3} \end{array} \right\}, \quad (9)$$

so that Maxwell's equations become

$$\begin{aligned} i\mathbf{k} \times \mathbf{E} &= i\omega \mathbf{H}/c, & \mathbf{k} \cdot \mathbf{H} &= 0, \\ i\mathbf{k} \times \mathbf{H} &= -i\omega \epsilon(\omega) \mathbf{E}/c + Z_1 e \mathbf{V}/2\pi^2 c, \\ \epsilon i\mathbf{k} \cdot \mathbf{E} &= Z_1 e/2\pi^2. \end{aligned} \quad (10)$$

Solving for  $\mathbf{E}$  and dividing it into two components,  $\mathbf{E}_l$  and  $\mathbf{E}_t$ , parallel and perpendicular, respectively, to the propagation vector we find

$$\mathbf{E}_l = -\frac{iZ_1 e \mathbf{k}}{2\pi^2 k^2 \epsilon(\omega)}, \quad (11)$$

$$\mathbf{E}_t = \frac{iZ_1 e \omega}{2\pi^2 c^2} \frac{\mathbf{V} - (\mathbf{k} \cdot \mathbf{V})\mathbf{k}/k^2}{(k^2 - \omega^2 \epsilon(\omega)/c^2)}. \quad (12)$$

Going back into configuration space, we first divide the vector  $\mathbf{k}$  into components  $\omega/V$  and  $\kappa$ , parallel and perpendicular, respectively, to the particle track,

$$k^2 = \kappa^2 + \omega^2/V^2; \quad d\mathbf{k} = \kappa d\kappa d\varphi' d\omega/V. \quad (13)$$

We find

the track are not zero at the field point in question. We designate these by  $E_l(\rho)$  and  $E_t(\rho)$ , respectively. Also let

$$\mathbf{E}(\rho) = \mathbf{E}_l(\rho) + \mathbf{E}_t(\rho). \quad (16)$$

The symbols  $E_l$  and  $E_t$  shall be provided with superscripts  $p$  and  $m$  designating field generated by the "particle" and the "medium", respectively. By the straightforward application of Maxwell's equations to our dispersive medium, we obtain the following results that are valid for relativistic velocities and for a dielectric constant obtained from harmonic oscillator model.

The electric field due to the particle alone is

$$E_{t^p}(\rho) = Z_1 e (1 - \gamma) \frac{d}{d\rho} \left( \frac{1}{\rho} \right), \quad (17)$$

$$E_{l^p}(\rho) = -Z_1 e \frac{d}{d\rho} \left( \frac{1}{\rho} \right), \quad (18)$$

$$E^p(\rho) = -\gamma Z_1 e \frac{d}{d\rho} \left( \frac{1}{\rho} \right). \quad (19)$$

The electric field due to the action of the medium is

$$E_t^m(\rho) = \frac{d}{d\rho} \left[ \Phi(\rho) - \frac{Z_1 e}{\rho} \right] + \gamma Z_1 e \frac{d}{d\rho} \frac{1 - \exp(-\Omega\rho/V)}{\rho}, \quad (20)$$

$$E_l^m(\rho) = \frac{d}{d\rho} \left[ \frac{Z_1 e}{\rho} - \Phi(\rho) \right], \quad (21)$$

$$E^m(\rho) = \gamma Z_1 e \frac{d}{d\rho} \frac{1 - \exp(-\Omega\rho/V)}{\rho}, \quad (22)$$

where  $\Phi(\rho)$  is the scalar potential in the medium.  $\Phi(\rho)$  represents the Coulomb potential of the particle for points close to the particle. The value of  $\Phi(\rho)$  for points distant from the particle is given in the Appendix, Eqs. (A-3) to (A-6).

We obtain from (22) that for small values of  $\rho$  the electric field exerted by the medium is

$$E^m \sim \gamma Z_1 e \left( -\frac{\Omega^2}{2V^2} + \frac{\Omega^3 \rho}{3V^3} - \frac{\Omega^4 \rho^2}{8V^4} + \dots \right). \quad (23)$$

We shall retain the first term in this expansion and compare it with the electric field due to the particle alone as given by (19). The field due to the medium acts in the direction opposite to the field of the particle. We obtain, however, that for  $p \ll V/\Omega$ ,

$$E^m \ll E^p. \quad (24)$$

Consequently, for small impact parameters the shielding effect of the medium is negligible and the inequality (24) derived on rigorous grounds is in agreement with Bohr's inequality.

Consider now the region of large impact parameters corresponding to  $\rho \gg V/\Omega$ . Referring to (19) and (22), it is seen that for this region we have

$$E^m = -E^p, \quad (25)$$

and, consequently, the shielding effect is complete—i.e., it cancels entirely any effect due to the charged incident particle. The inequality (25) expresses the effect of the total electric field. However, it is apparent from (20) and (22) that for  $V \rightarrow c$  (or for  $\gamma$  increasing indefinitely),  $E_t^m \rightarrow E^m$  and, consequently, we may conclude that the shielding is caused primarily by the electromagnetic interaction of the electrons in the medium.

The authors wish to express their gratitude to Dr. Aage Bohr for an interesting conversation on the above subject and comments.

#### APPENDIX

For the sake of completeness, we shall give the expressions for longitudinal and transverse components of the electric field at all positions relative to the incident relativistic charged particle. The assumptions are, as stated before, (1) that the dielectric constant may be adequately represented by the usual expression

$$\epsilon(\omega) = 1 + \frac{4\pi N e^2}{m} \sum_i \frac{f_i}{\omega_i^2 - i g_i \omega - \omega_i^2},$$

where  $N$  is the number of atoms per  $\text{cm}^3$  in the medium,  $f_i$ ,  $\omega_i$ , and  $g_i$  are the oscillator strength, resonant frequency, and damping constant belonging to the  $i$ th atomic transition, and (2) that the particle is in the relativistic region, i.e., that  $\gamma = 1/(1 - \beta^2)^{1/2} \gg 1$ . The fields given here, in fact, comprise the first two terms of expansions in inverse powers of  $\gamma$ , e.g.,

$$E_t = \gamma E_t^{(1)} + E_t^{(2)} + O(\gamma^{-1}).$$

Using the formulation given in Eqs. (14) and (15), one finds for the components of the fields in the  $\rho$  direction (perpendicular to the particle track):

$$E_{t\rho} = \frac{\partial}{\partial\rho} \left\{ \Phi(r) - \frac{\gamma Z_1 e \exp[\Omega(\rho^2 + \gamma^2 z^2)^{1/2}/V]}{(\rho^2 + \gamma^2 t^2)^{1/2}} \right\} + (E_{t\rho})_{\text{Čerenkov}} \quad (A-1)$$

$$E_{l\rho} = -\frac{\partial}{\partial\rho} \Phi(r), \quad (A-2)$$

where the scalar potential  $\Phi(r)$  has the following forms:

(a) For field points close to the incident particle,

$$\Phi(r) = z_1 e / r, \quad \text{where } r = (z^2 + \rho^2)^{1/2}. \quad (A-3)$$

(b) If the field point is far from the particle and if none of the  $\omega_i$  are zero (the dielectric is an insulator),

$$\Phi(r) = \frac{1}{1 + \Omega^2 \sum_i (f_i / \omega_i^2)} \frac{Z_1 e}{r}. \quad (A-4)$$

(c) If the field point is far from the particle and if one of the  $\omega_i$ , say  $\omega_1$ , is identically zero, then

$$\Phi(r) = -\frac{Z_1 e g_1 V}{f_1 \Omega^2} \frac{d}{dz} \left( \frac{1}{r} \right). \quad (A-5)$$

(d) If the field point is far from the particle,  $\omega_1 = 0$  and  $g_1 = 0$

$$\Phi(r) = \frac{Z_1 e V^2}{f_1 \Omega^2} \frac{d^2}{dz^2} \left( \frac{1}{r} \right). \quad (A-6)$$

The  $z$  components (parallel with the particle track) are

$$E_{tz} = \frac{\partial}{\partial z} \left\{ +\Phi(r) - \frac{Z_1 e \exp[-\Omega(\rho^2 + \gamma^2 z^2)^{1/2}/V]}{\gamma (\rho^2 + \gamma^2 z^2)} \right\} - Z_1 e \frac{\Omega^2 z}{V^2 |z|} \int_{\gamma|z|}^{\infty} dx \frac{\exp[-\Omega(\rho^2 + x^2)^{1/2}/V]}{(\rho^2 + x^2)^{3/2}}, \quad (\text{A-7})$$

$$E_{tz} = -\frac{\partial}{\partial z} \Phi(r). \quad (\text{A-8})$$

The additional term in the expression for  $E_t$  corresponds to the existence of the Čerenkov wake behind the particle ( $z < 0$ ). Assuming for simplicity that only one of the resonances at  $\omega = \omega_1$  is important in the expression for dielectric constant, we find that

$$(\mathbf{E}_t)_{\text{Čerenkov}} = \frac{2Z_1 e \omega_1^3}{\Omega(\Omega^2 + \omega_1^2)} \nabla (\omega_1 z^2 / \Omega^2 - \rho^2)^{-1/2} \quad \text{if } \omega_1 z / \Omega < -\rho, \quad (\text{A-9})$$

and

$$(\mathbf{E}_t)_{\text{Čerenkov}} = 0 \quad \text{if } \omega_1 z / \Omega > -\rho. \quad (\text{A-10})$$

These expressions are approximately valid as long as the field point is located sufficiently far from the surface of the cone  $z = -\Omega\rho/\omega_1$ . The apparent singularity on this cone does not exist but arises from the approximation to the more exact expression for  $(\mathbf{E}_t)_{\text{Čerenkov}}$ . It is to be noted that the angle of opening of the cone in the expression for  $E_t$  is

$$\vartheta = \tan^{-1}(\omega_1/\Omega). \quad (\text{A-11})$$

The third term in (A-7) for  $E_{tz}$ , i.e.,

$$(E_{tz})_3 = Z_1 e \frac{\Omega^2 z}{V^2 |z|} \int_{\gamma|z|}^{\infty} dx \frac{\exp[-\Omega(\rho^2 + x^2)^{1/2}/V]}{(\rho^2 + x^2)^{3/2}} \quad (\text{A-12})$$

is of some interest and does not appear to have been noted before. This portion of the field is independent of the resonant frequency  $\omega_1$ , but goes to zero for very low medium density. Exactly the same term arises in the transverse field expressions for a particle passing through a plasma.<sup>7</sup> This term is antisymmetric in the  $z$  coordinate and possesses a discontinuity at  $z=0$ . It arises from the Lorentz-contracted field of the line polarization charge which exists behind the incident particle.

<sup>7</sup> J. Neufeld and R. H. Ritchie, Phys. Rev. **98**, 1632 (1955).

## Dipolar Sums in the Primitive Cubic Lattices

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Dipole-wave sums, important in many magnetic and electric problems involving dipole-dipole interactions, are defined, and numerical values are given at sets of independent points in  $\mathbf{k}$ -space equivalent to a 512-fold sampling of the first Brillouin zone of each of the three primitive cubic lattices. Strong size, shape, and position dependence of these sums is shown to occur in a pathological region about the origin in  $\mathbf{k}$ -space. The dipole-wave sums are shown to be related to dipole-field factors at points within the unit cell. The dipolar anisotropy energy in the antiferromagnet MnO is discussed as an illustration of the use of dipole-wave sums.

### I. INTRODUCTION

WE introduce the lattice sums

$$S_n(\mathbf{k}) = \rho^{-1} \sum_i' |\mathbf{r}_i|^{-n} \exp(i\mathbf{k} \cdot \mathbf{r}_i); \quad (\text{1a})$$

$$S_n^{ij}(\mathbf{k}) = \rho^{-1} \sum_i' r_i^i r_i^j |\mathbf{r}_i|^{-n} \exp(i\mathbf{k} \cdot \mathbf{r}_i). \quad (\text{1b})$$

Here  $i, j = x, y, z$ ; the primed sum is to be taken over all lattice vectors  $\mathbf{r}_i$  except  $\mathbf{r}_i = 0$ ; and  $\rho$  is the number of lattice points per unit volume.

Specifically, we shall be interested in  $S_3(\mathbf{k})$  and  $S_5^{ij}(\mathbf{k})$ , which we shall call *dipole-wave sums*. Our interest in these sums arises from their importance in

many magnetic problems involving dipole-dipole interactions. In particular, we have made extensive use of dipole-wave sums in the quantum-mechanical problem of dipolar ferromagnetism.<sup>1</sup> Furthermore, these sums find use in the calculation of dipole-field factors (see Secs. VI, VII, and VIII) and of exciton energies.<sup>2</sup> They are important in the considerations of lattice stability of polar crystals that arise, for example, in connection with ferroelectrics and antiferroelectrics.

<sup>1</sup> M. H. Cohen and F. Keffer, Phys. Rev. **94**, 1412 (1954), and following paper [Phys. Rev. **99**, 1135 (1955)].

<sup>2</sup> W. R. Heller and A. Marcus, Phys. Rev. **84**, 809 (1951).