

Z_1^3 correction to the stopping power of an electron gas for ions

J.M. Pitarke

Materia Kondentsatuaren Fisika Saila, Zientzi Falkultatea, Euskal Herriko Unibertsitatea, 644 Posta kutxatila, 48080 Bilbo, Basque Country, Spain

R.H. Ritchie

Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, Tennessee 37831-6123, and The University of Tennessee, Department of Physics, Knoxville, Tennessee 37996, USA

P.M. Echenique

Materialeen Fisika, Kimika Falkultatea, Euskal Herriko Unibertsitatea, 1072 Posta kutxatila, 20080 Donostia, Basque Country, Spain

A diagrammatic analysis of many-body interactions between a moving ion and an electron gas is made. The Z_1^3 correction to the stopping power of the medium for the penetrating ion is derived using Feynman diagrams, and the contributing terms leading to significant Z_1^3 corrections to the stopping power at low velocities of the ion are evaluated, as a function of the velocity of the ion, in the random-phase approximation.

Since the original papers of Böhr [1] and Bethe [2], the energy loss of a charged particle in matter has been the subject of continuing interest. Classic first-order perturbation theories lead to a stopping power proportional to the square of the projectile charge Z_1 . However, from measurements on positive and negative pions [3] it was known that the stopping power exhibits a dependence on the sign of the charge; recently, measured energy losses of protons and antiprotons in silicon and gold have been reported [4–6] and the Z_1^3 correction to the stopping power has been extracted, assuming that the Born series exist for these collisions and that other terms proportional to odd powers of Z_1 are negligible in the velocity regimes under study.

The so-called Barkas correction to the stopping power was first calculated by Ashley, Ritchie and Brandt [7] for distant collisions only, using a classical perturbation calculation for a harmonic oscillator; they included the polarization of target atoms by the projectile and found a correction term that, in lowest order, is proportional to Z_1^3 , and was later proven by Hill and Mertzbacher [8] to approach the result of the second Born approximation at large impact parameters. Later on, Jackson and McCarthy [9] performed a similar classical but relativistic calculation, and set the minimum impact parameter equal to the radius of the quantum mechanical harmonic oscillator, to find a standard high-velocity limit of the Barkas term.

Subsequently, the contribution to the Z_1^3 term from

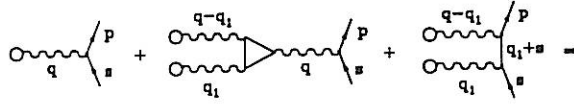
close collisions, which had been argued to be negligible, was estimated by Lindhard [10], studying stopping by a free electron gas at rest, to be comparable to the distant-collisions contribution as calculated by Jackson and McCarthy. Since then, more rigorous quantum-mechanical calculations of the Barkas effect have appeared [11–14], using both the harmonic oscillator [11] and electron gas model of the target [12–14], but a quantitative evaluation of the Barkas correction to the stopping power of an electron gas where a low- or high-velocity assumption does not enter explicitly remained to be done.

In this paper we investigate the Z_1^3 correction to the stopping power of an electron gas for ions, including the zero-point motion of the Fermi gas. In particular, an alternative derivation of the Z_1^3 term is presented, following procedures of many-body perturbation theory, and a quantitative evaluation of the contributing terms leading to significant Z_1^3 corrections to the stopping power at low velocities of the ion is carried out, as a function of the velocity of the ion, in the random-phase approximation (RPA), thereby analysing the range of validity of the previously studied low-velocity limit.

We consider an electron gas of density n through which an ion of charge Z_1 and velocity v passes. Treating the heavy particle as a prescribed source of energy and momentum, the matrix element of the S -matrix for the electron gas-heavy ion system corre-

sponding to the process of carrying the system from an initial state $a_s^+|0\rangle$ to a final state $a_p^+|0\rangle$ can be represented in momentum space up to second order in the ion charge as (we use atomic units throughout, i.e., $e = m = \hbar = 1$)

$$S_{fi} = \langle 0 | a_p S a_s^+ | 0 \rangle =$$



$$\Omega^{-1} \left\{ 2\pi i Z_1 V_q \delta[q^0 - q \cdot v] + i Z_1^2 \int \frac{d^4 q_1}{(2\pi)^2} V_q V_{q_1} V_{q-q_1} M_{q,q_1} \delta[q_1^0 - q_1 \cdot v] \times \delta[q^0 - q_1^0 - (q - q_1) \cdot v] - i Z_1^2 \int \frac{d^4 q_1}{(2\pi)^2} V_{q_1} V_{q-q_1} G_{q_1+s} \delta[q_1^0 - q_1 \cdot v] \times \delta[q^0 - q_1^0 - (q - q_1) \cdot v] \right\}, \quad (1)$$

where $q = (p - s, \omega_p - \omega_s)$, $\omega_p = p^2/2$ being the energy of an electron with momentum p , and it is understood that (p, s) lies in the (unoccupied, occupied) part of momentum space. Ω is the normalization volume, V_q , represented by wavy lines, gives account of the effective interaction [15], i.e.,

$$V_q = \frac{4\pi}{q^2} \epsilon_q^{-1}, \quad (2)$$

and G_k^0 , represented by solid lines, is the zero-order propagator for an electron gas,

$$G_k^0 = \frac{1 - n_k}{k_0 - \omega_k + i\delta} + \frac{n_k}{k_0 - \omega_k - i\delta}, \quad (3)$$

where $k = (k, k^0)$ is the four-vector representing the momentum-energy of the electron, and n_k is the occupation number,

$$n_k = \theta(k_F - |k|), \quad (4)$$

k_F being the Fermi momentum, and $\theta(x)$ the Heaviside function.

The first diagram in eq. (1), which is represented by a wavy line leading from an external point to a fermion-scattering vertex, describes a process in which an electron is scattered once from the linearly screened ion potential, while the second and third diagrams describe processes in which an electron is scattered once from the quadratically screened ion potential and twice from the linearly screened ion potential, respec-

tively, ϵ_q is the linear response function of the medium, that is,

$$\epsilon_q = 1 - \frac{4\pi}{q^2} \Lambda_q, \quad (5)$$

where Λ_q is a sum over all proper polarization subdiagrams:

$$i\Lambda_q = \text{shaded bubble} - \text{empty bubble} + \text{bubble with fermion line} + \text{bubble with fermion line and wavy line} + \dots \quad (6)$$

and M_{q,q_1} is the quadratic response function of the medium, represented by the triple vertex diagram:

$$M_{q,q_1} = \text{triangle with wavy line} - \text{triangle with wavy line and fermion line} + \text{triangle with wavy line and fermion line and wavy line} + \dots \quad (7)$$

Therefore, the transition rate, γ , for a process leading to any possible momentum transfer to the electron gas, is given, in the limit as the interaction time $T \rightarrow \infty$, up to third order in the ion charge by

$$\gamma = 2\Omega^2 \int \frac{d^3 p}{(2\pi)^3} \int \frac{d^3 s}{(2\pi)^3} \frac{|S_{fi}|^2}{T} = \gamma^{(2)} + \gamma_1^{(3)} + \gamma_2^{(3)}, \quad (8)$$

where

$$\gamma^{(2)} = 8(2\pi)^3 Z_1^2 \int \frac{d^3 p}{(2\pi)^3} \int \frac{d^3 s}{(2\pi)^3} \frac{\delta(q^0 - q \cdot v)}{q^4 |\epsilon_q|^2}, \quad (9)$$

$$\gamma_1^{(3)} = 2^6 (2\pi)^5 Z_1^3 \int \frac{d^3 p}{(2\pi)^3} \int \frac{d^3 s}{(2\pi)^3} \int \frac{d^3 q_1}{(2\pi)^3} \times \frac{\text{Re}[\epsilon_{q_1}^{-1} \epsilon_{q-q_1}^{-1} M_{q,q_1}] \delta(q^0 - q \cdot v)}{q^4 q_1^2 |q - q_1|^2 |\epsilon_q|^2} \quad (10)$$

and

$$\gamma_2^{(3)} = -2^5 (2\pi)^4 Z_1^3 \int \frac{d^3 p}{(2\pi)^3} \int \frac{d^3 s}{(2\pi)^3} \int \frac{d^3 q_1}{(2\pi)^3} \times \frac{\text{Re}[(\epsilon_q^{-1})^* \epsilon_{q_1}^{-1} \epsilon_{q-q_1}^{-1} G_{q_1+s}^0] \delta(q^0 - q \cdot v)}{q^2 q_1^2 |q - q_1|^2}, \quad (11)$$

with $q_1^0 = q_1 \cdot v$. The stopping power of the medium for the penetrating ion, i.e., the average energy loss of the ion per path length, is then obtained after multiplying each contribution to the transition rate by the energy transferred in the corresponding process, q^0 , and dividing by the velocity of the ion.

In the lowest order approximation to Λ_q and M_{q,q_1} (random-phase-approximation), they are described by the empty bubble and the empty triangle diagram, respectively. The empty bubble was first evaluated by

Hubbard [16] and it coincides for positive values of the energy component of q with Lindhard's function [17]. On the other hand, the real part of the empty triangle diagram has recently been evaluated analytically by Cenni and Saracco [18] for arbitrary momentum and energy, and the imaginary part by Hu and Zaremba [14]; however, it is an alternative derivation of the imaginary part of the triple vertex function, which we give as [19]

$$\text{Im } M_{q,q_1} = -[H_{q,q_1} + H_{q_1,q} + H_{(q-q_1),-q_1}], \quad (12)$$

that enables us to express the Z_1^3 correction to the stopping power in terms of both the real and the imaginary part of the triple vertex function.

In particular, if one considers only contributions that are not negligible at low velocities of the ion, the Z_1^3 correction to the stopping power can be written in the following way:

$$\begin{aligned} S^{(3)} = & \frac{4Z_1^3}{\pi^3 v} \int dq \frac{q^0}{q^2} \\ & \times \int dq_1 \{ \text{Im}(-\epsilon_q^{-1}) \text{Re } \epsilon_{q_1}^{-1} \text{Re } \epsilon_{q-q_1}^{-1} \text{Re } M_{q,q_1} \\ & + H_{q,q_1} \text{Re } \epsilon_q^{-1} \text{Re } \epsilon_{q_1}^{-1} \text{Re } \epsilon_{q-q_1}^{-1} \} \\ & \times \{ q_1^2 |q - q_1|^2 \}^{-1} \\ & (q^0 > 0), \end{aligned} \quad (13)$$

with $q^0 = q \cdot v$ and $q_1^0 = q_1 \cdot v$; then, in the low-velocity limit, i.e., when the low-frequency limit of ϵ_q and M_{q,q_1} are substituted into eq. (13), one finds an expression for the Z_1^3 correction to the stopping power that is linear in the velocity of the ion and is exactly equivalent to eq. (2.18) of Hu and Zaremba. The remaining contributions to the stopping power not included in eq. (13) are, in the low-velocity limit, of higher order in the velocity of the ion, and become of importance only for velocities higher than approximately half the Fermi velocity of the medium [19].

We have also calculated the Z_1^3 contribution to the stopping power of an electron gas, after substitution of the full RPA ϵ_q and M_{q,q_1} functions into eq. (13), and we have obtained the result plotted in fig. 1 by a solid line, as a function of the velocity of the projectile, for the electron density parameter $r_s = 2.07$ ($n^{-1} = (4\pi/3)r_s^3$) corresponding to an electron gas of a density equal to that of aluminum; the contributions coming from the imaginary part of the linear response function, which can be interpreted as arising from excitations generated by the quadratically screened ion potential, and coming from H_{q,q_1} , which arises from multiple scattering of the electrons by the linearly screened ion potential, are plotted separately (dashed and dashed-dotted line, respectively); the dotted line represents the low-velocity limit already computed in

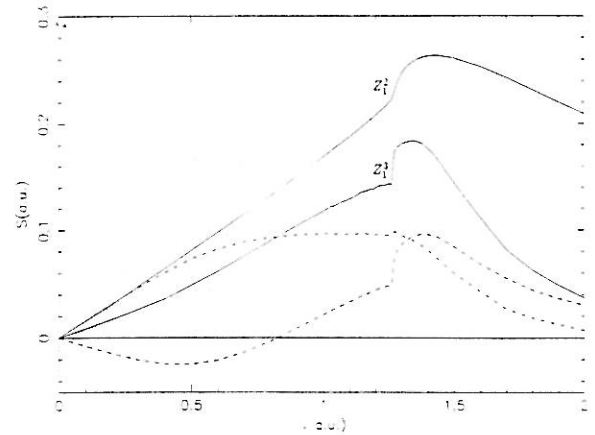


Fig. 1. Contributions to the stopping power that are proportional to Z_1^2 and Z_1^3 , in the RPA, as a function of the velocity of the ion, for $r_s = 2.07$ and $Z_1 = 1$. The solid lines correspond to the total Z_1^2 contribution and the Z_1^3 contribution of eq. (13), and the dotted lines represent the corresponding low-velocity limits. Contributions to eq. (13) coming from the imaginary part of ϵ_q and from H_{q,q_1} are represented by dashed and dashed-dotted lines, respectively.

ref. [14], thereby showing that the range of validity of the linear velocity dependence of the Z_1^3 correction to the stopping power persists up to velocities approaching half the Fermi velocity of the electron gas. For comparison, the total contribution to the stopping power that is proportional to Z_1^2 obtained in the RPA approximation is also plotted, together with the corresponding low-velocity limit obtained when the low-frequency limit of the linear response function is substituted.

In conclusion, the contributing terms leading to significant Z_1^3 corrections to the stopping power at low velocities of the ion have been derived following procedures of many-body perturbation theory, they have been evaluated numerically, as a function of the velocity of the ion, using the random-phase approximation to the linear and quadratic response functions, and it has been found that the Z_1^3 contribution to the stopping power is almost linear in the velocity of the ion up to velocities approaching half the Fermi velocity of the electron gas. A more detailed presentation of the derivation of the Z_1^3 correction to the stopping power and quantitative calculations of the full Z_1^3 correction in the RPA, as a function of the velocity of the ion, will be published elsewhere [19].

Acknowledgements

This work has been supported by the University of the Basque Country and the Spanish Comisión Asesora

Científica y Técnica (CAICYT). One of the authors (J.M.P.) gratefully acknowledges support by Eusko Ikaskuntza.

References

- [1] N. Böhr, *Philos. Mag.* 25 (1913) 10.
- [2] H.A. Bethe, *Ann. Phys. (Leipzig)* 5 (1930) 325.
- [3] W.H. Barkas, N.J. Dyer and H.H. Heckman, *Phys. Rev. Lett.* 11 (1963) 26; 11 (1963) 138 (E).
- [4] L.H. Andersen, P. Hvelplund, H. Knudsen, S.P. Møller, J.O.P. Pedersen, E. Uggerhøj, K. Elsener and E. Morenzoni, *Phys. Rev. Lett.* 62 (1989) 1731.
- [5] R. Medenwald, S.P. Møller, E. Uggerhøj, T. Worm, P. Hvelplund, H. Knudsen, K. Elsener and E. Morenzoni, *Nucl. Instr. and Meth.* 58 (1991) 1.
- [6] R. Medenwald, S.P. Møller, E. Uggerhøj, T. Worm, P. Hvelplund, H. Knudsen, K. Elsener and E. Morenzoni, *Phys. Lett. A* 155 (1991) 155.
- [7] J.C. Ashley, R.H. Ritchie and W. Brandt, *Phys. Rev. B* 5 (1972) 2393; 8 (1973) 2402; 10 (1974) 737.
- [8] K.W. Hill and E. Merzbacher, *Phys. Rev. A* 9 (1974) 156.
- [9] J.D. Jackson and R.L. McCarthy, *Phys. Rev. B* 6 (1972) 4131.
- [10] J. Lindhard, *Nucl. Instr. and Meth.* 132 (1976) 1.
- [11] H. Mikkelsen and P. Sigmund, *Phys. Rev. A* 40 (1989) 101.
- [12] H. Esbensen, Ph.D. thesis, University of Aarhus, 1977, unpublished;
H. Esbensen and P. Sigmund, *Ann. Phys.* 201 (1990) 152.
- [13] C.C. Sung and R.H. Ritchie, *Phys. Rev. A* 28 (1983) 674.
- [14] C.D. Hu and E. Zaremba, *Phys. Rev. B* 37 (1988) 9268.
- [15] T.D. Schultz, *Quantum Field Theory and the Many Body Problem* (Gordon and Breach, New York, 1964);
A.L. Fetter and J.D. Walecka, *Quantum Theory of Many-Particle Systems* (McGraw-Hill, New York, 1971).
- [16] J. Hubbard, *Proc. Phys. Soc. (London)* A68 (1955) 978.
- [17] J. Lindhard, *K. Dan. Vidensk. Selsk. Mat. Fys. Medd.* 28 (1954) 28.
- [18] R. Cenni and P. Saracco, *Nucl. Phys. A* 487 (1988) 279.
- [19] J.M. Pitarke, R.H. Ritchie, P.M. Echenique and E. Zaremba, *Phys. Rev. B*, to be published.