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Nonlinear wake in the random-phase-approximation

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Abstract

We have formulated a diagrammatic analysis to study the many-body interactions between a moving ion passing through a solid, modeling the solid by an electron gas embedded in a uniformly distributed positive background. Using Feynman diagrams, a derivation of the first nonlinear correction (proportional to Z_1^2 , Z_1 being the ion charge) to the induced potential and electron density is presented. These magnitudes are evaluated numerically using the full random-phase-approximation to describe the shielded interaction.

1. Introduction

Since the pioneering work of Bohr [1], much research has been oriented to the evaluation of the electron density induced by the passage of swift ions through a solid [2]. The evaluation of this so-called wake was first presented by Neufeld and Ritchie [3] by using a local dielectric function as the linear response of the medium. Then, Echenique, Ritchie and Brandt [4] used the plasmon-pole approximation to the dielectric function, and, finally, Mazarro, Echenique and Ritchie [5] evaluated the wake potential in the full random-phase-approximation (RPA), also on the basis of a linear response of the medium. However, there exists a variety of experimental conditions where there is a need for a nonlinear theory of the electronic polarization and the wake potential.

An approximate theory of the nonlinear wake had been developed by Faibis et al. [6] by using Coulomb scattering, but the first nonlinear theory that accounted for collective phenomena was presented by Esbensen and Sigmund [7] in the static electron gas approximation. Then, nonlinear hydrodynamical descriptions of the wake potential have been formulated very recently, accounting for the low [8] and high [9] velocity regimes, but an evaluation of the second-order electronic wake that is valid for nonrelativistic arbitrary velocities had not been published yet [10].

As far as the electronic stopping power is concerned, the so-called Z_1^3 or Barkas [11] correction had been first evaluated by Ashley, Ritchie and Brandt [12] by using classical perturbation theory for a harmonic oscillator, and it has only very recently been evaluated by Pitarke et al. [13,14] for an electron gas in the full RPA. The key feature of this calculation was the evaluation, within the RPA, of

both the real and the imaginary part of the quadratic density response function of the medium, and this evaluation enables us, therefore, to go further and present a calculation of the second-order electronic wake.

2. Quantum theory of the wake potential

We consider a point charge, $Z_1 e$, moving with constant velocity v through an isotropic homogeneous electron gas embedded in a uniformly distributed positive background. The electric potential operator, at point r , induced by the electron gas and the positive background is (we use atomic units throughout, i.e., $e^2 = \hbar = m_e = 1$):

$$V(r) = - \sum_{r_e} \frac{1}{|r - r_e|} + V_{BG}, \quad (1)$$

where r_e represents the electron position operator, and V_{BG} , the interaction between a test positive unit charge at r and the positive background. In the representation of second quantization [15] one finds:

$$V(r) = -V^{-1} \sum_{k,q;q \neq 0,\lambda} v_q e^{iq \cdot r} a_{\lambda}^{\dagger}(k) a_{\lambda}(k+q), \quad (2)$$

where $a_{\lambda}^{\dagger}(k)$ and $a_{\lambda}(k)$ represent creation and destruction operators, respectively, of well-defined free electron k momentum and λ spin states, and $v_q = 4\pi/q^2$. In the following equations the sum over electron spin states will be implicitly assumed.

Then, the wake potential is found as the mean value of the interaction potential operator:

$$\phi(r, t) = \frac{\langle \Omega_0 | (V')^H(r, t) | \Omega_0 \rangle}{\langle \Omega_0 | \Omega_0 \rangle}, \quad (3)$$

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where $(V')^H(\mathbf{r}, t)$ and $|\Omega_0\rangle$ are the induced potential of Eq. (2) and the ground state, respectively, in the Heisenberg representation.

Treating the moving charged particle as an external source of momentum and energy, the Hamiltonian of the system, which depends explicitly on the time, can be expressed in the representation of second quantization as

$$H = H'_0 + H_{\text{int}}, \quad (4)$$

where

$$H'_0 = \sum_k E_k a^\dagger(\mathbf{k}) a(\mathbf{k}), \quad (5)$$

$$E_k = k^2/2,$$

$$H_{\text{int}} = H_{e-e} + H_{i-e}, \quad (6)$$

$$H_{e-e} = \frac{V^{-1}}{2} \sum_{\mathbf{p}, \mathbf{p}_1, \mathbf{q}; \mathbf{q} \neq 0} \frac{4\pi}{q^2} \times a^\dagger(\mathbf{p} - \mathbf{q}) a(\mathbf{p}) a^\dagger(\mathbf{p}_1 + \mathbf{q}) a(\mathbf{p}_1), \quad (7)$$

and

$$H_{i-e} = -V^{-1} Z_1 \sum_{\mathbf{k}, \mathbf{q}; \mathbf{q} \neq 0} \frac{4\pi}{q^2} e^{i\mathbf{q} \cdot \mathbf{r}} a^\dagger(\mathbf{k}) a(\mathbf{k} + \mathbf{q}). \quad (8)$$

The adiabatic theorem, necessary for the application of standard many-body techniques, implies the following reversibility requirement:

$$S |\Phi_0\rangle = e^{i\alpha} |\Phi_0\rangle, \quad (9)$$

where S is the scattering matrix

$$S = U'(+\infty, -\infty), \quad (10)$$

U' is the evolution operator

$$U'(t_1, t_0) = T \left[\exp - i \int_{t_0}^{t_1} H_{\text{int}}^1(t) dt \right], \quad (11)$$

T is the time ordering operator, $|\Phi_0\rangle$ is the ground state in the interaction representation, and $H_{\text{int}}(t)$ represents the perturbing Hamiltonian in the interaction representation. Nevertheless, the former adiabatic condition is not verified in the presence of time dependent Hamiltonians, so that the system is not returned to the ground state as the time goes to infinity [16]. As a result, standard Feynman diagrams cannot be applied, but we have found the retarded prescription necessary for the fulfillment of the causality and the computing of the actual response functions involved.

Treating the interaction between the external source of momentum and energy and the electron gas separately from the interactions inside the electron gas, Eq. (3) can be displayed in a new interaction representation; in this representation we consider the free Hamiltonian as follows

$$H_0 = H'_0 + H_{e-e}, \quad (12)$$

while the perturbative Hamiltonian involves the interaction between the incoming charged particle and the electron gas. This representation is equivalent to the Heisenberg representation when the interaction between the moving particle and the electron gas is not taken into account. Therefore, this picture will be identified with an H superscript but without any comma to be distinguished from the former full Heisenberg representation.

In this representation Eq. (3) can be rewritten as follows

$$\phi(\mathbf{r}, t) = \frac{\langle \Psi_0 | U^+(t, -\infty) V^H(\mathbf{r}, t) U(t, -\infty) | \Psi_0 \rangle}{\langle \Psi_0 | U^+(t, -\infty) U(t, -\infty) | \Psi_0 \rangle}, \quad (13)$$

where $|\Psi_0\rangle$ represents the ground state of the Hamiltonian of Eq. (12), and U is the evolution operator

$$U(t_1, t_0) = T \left[\exp - i \int_{t_0}^{t_1} H_{i-e}^H(t) dt \right]. \quad (14)$$

For the evaluation of this magnitude, the electron–electron interaction and the interaction between the moving particle and the electron gas can be studied separately, when this representation is considered. For this reason, the screening due to the induced electronic density may be computed up to infinite order in the electron interaction, on the ground of quantum field theory.

Finally, by expanding the evolution operator, U , nonlinear corrections to the wake potential can be systematically obtained.

2.1. The linear wake potential

An expansion of Eq. (13) gives, up to first order in the ion charge:

$$\begin{aligned} \phi(\mathbf{r}, t)^{Z_1} &= \frac{Z_1 i}{V^2} \int_{-\infty}^{\infty} dt_1 \sum_{\mathbf{q}, \mathbf{q}_1} \left\{ \nu_{\mathbf{q}} \nu_{\mathbf{q}_1} e^{i\mathbf{q} \cdot \mathbf{r}} e^{i\mathbf{q}_1 \cdot \mathbf{r}} \Theta(t - t_1) \right. \\ &\quad \times \frac{\langle \Psi_0 | [n^H(\mathbf{q}_1, t_1), n^H(\mathbf{q}, t)] | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} \left. \right\}, \end{aligned} \quad (15)$$

where $n(\mathbf{q}, t)$ is the electronic density operator

$$n(\mathbf{q}, t) = V^{-1} \sum_{\mathbf{k}} a^\dagger(\mathbf{k}, t) a(\mathbf{k} + \mathbf{q}, t), \quad (16)$$

and the retarded density correlation function is defined as

$$\begin{aligned} iD^R(\mathbf{q}, t; \mathbf{q}_1, t_1) &= \Theta(t - t_1) \frac{\langle \Psi_0 | [n^H(\mathbf{q}, t), n^H(\mathbf{q}_1, t_1)] | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle}, \end{aligned} \quad (17)$$

which preserves the causality of the system.



Fig. 1. Feynman diagram representing the linear wake potential generated by a moving ion. The dashed line, representing a Coulomb bare interaction, leads from an external point, corresponding to the external source of energy and momentum, to an internal vertex. Another dashed line leads from an internal vertex to a cross representing a test unit charge.

It is of interest, at this point, to define the time-ordered counterpart of Eq. (17):

$$iD^{T.O.}(q, t; q_1, t_1) = \frac{\langle \Psi_0 | T[n^H(q, t)n^H(q_1, t_1)] | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle}, \quad (18)$$

since Eq. (17) can be obtained from Eq. (18) by turning all the imaginary parts of the frequencies to be positive. This allows us, therefore, to derive Eq. (15) after an evaluation of the time-ordered linear wake represented diagrammatically in Fig. 1 [10]. The double internal vertex of this figure represents the exact linear density response function of the medium, χ_q , which is approximated, in the RPA, by summing over the infinite set of diagrams containing a string of empty bubbles (see Fig. 2):

$$\chi_q = \chi_q^0 + \chi_q^0 \nu_q \chi_q, \quad (19)$$

where χ_q^0 represents the so-called linear density response function of the noninteracting electron gas:

$$\chi_q^0 = -2i \int d^4k G_k^0 G_{k+q}^0. \quad (20)$$

Consequently, Eq. (15) gives, in the RPA, the following result:

$$\phi(r, t)^{Z_1} = Z_1 \int \frac{d^3q}{(2\pi)^3} e^{iq \cdot (r - vt)} \nu_q [(\epsilon^R(q, q \cdot v)^{-1} - 1)], \quad (21)$$

where

$$(\epsilon_q^R)^{-1} = 1 + \nu_q \chi_q^R. \quad (22)$$

Eq. (21) exactly coincides with the standard expression for the linear induced electric potential [2].



Fig. 2. Diagrammatic representation of the linear density response function, χ_q , approximated in the RPA by summing over the infinite set of diagrams containing a string of empty bubbles.

2.2. The second-order wake potential

An expansion of Eq. (17) gives for the contribution to the wake potential that is proportional to the second power of the ion charge:

$$\begin{aligned} \phi(r, t)^{Z_1^2} &= \frac{Z_1^2}{V^3} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dt_1 dt_2 \sum_{q, q_1, q_2} \nu_q \nu_{q_1} \nu_{q_2} \\ &\times e^{iq \cdot r} e^{iq_1 \cdot vt_1} e^{iq_2 \cdot vt_2} \Theta(t - t_1) \Theta(t_1 - t_2) \\ &\times \frac{\langle \Psi_0 | [[n^H(q, t), n^H(q_1, t_1)], n^H(q_2, t_2)] | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle}, \end{aligned} \quad (23)$$

or

$$\begin{aligned} \phi(r, t)^{Z_1^2} &= \frac{Z_1^2}{V^3} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dt_1 dt_2 \sum_{q, q_1, q_2} \nu_q \nu_{q_1} \nu_{q_2} \\ &\times e^{iq \cdot r} e^{iq_1 \cdot vt_1} e^{iq_2 \cdot vt_2} Y^R(q, t; q_1, t_1; q_2, t_2), \end{aligned} \quad (24)$$

where the retarded quadratic response function, Y^R , is defined as

$$\begin{aligned} Y^R(q, t; q_1, t_1; q_2, t_2) &= \{\Theta(t - t_1) \Theta(t_1 - t_2) \\ &\times \langle \Psi_0 | [[n^H(q, t), n^H(q_1, t_1)], n^H(q_2, t_2)] | \Psi_0 \rangle\} \\ &\times \{\langle \Psi_0 | \Psi_0 \rangle\}^{-1}. \end{aligned} \quad (25)$$

A similar method as the one considered in the evaluation of the linear term may be developed to study the relationship between this retarded quadratic response function and the following time ordered one:

$$\begin{aligned} Y^{T.O.}(q, t; q_1, t_1; q_2, t_2) &= \frac{1}{2} \frac{\langle \Psi_0 | T[n^H(q, t)n^H(q_1, t_1)n^H(q_2, t_2)] | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle}. \end{aligned} \quad (26)$$

We define the frequencies w , w_1 and w_2 as the Fourier transform variables of t , t_1 and t_2 , respectively, and turning them, in $Y^{T.O.}$, into $w + i\eta$, $w_1 - i\eta$ and $w_2 - i\eta$

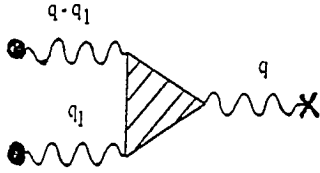


Fig. 3. Feynman diagram representing the second order nonlinear wake potential generated by a moving ion. Wavy lines represent effective interactions.

(η is an arbitrary infinitesimal positive quantity) gives the retarded function, Y^R . Now, a change in the q_1 wave vector sign in Eq. (24) integral makes all the frequency imaginary parts positive, resulting, therefore, to the usual retarded prescription.

Thus, following this prescription, the second-order wake potential can be derived after an evaluation of the corresponding time-ordered second-order wake potential, represented diagrammatically in Fig. 3 [10]. The triple vertex of this figure represents the exact quadratic density response function of the medium, M_{q,q_1} , which is approximated, in the RPA, by the corresponding empty triangle diagram:

$$M_{q,q_1} = 2i \int d^4k G_k^0 G_{k+q}^0 G_{k+q_1}^0. \quad (27)$$

Consequently, we finally find, within the RPA, the following expression for the second-order wake potential:

$$\begin{aligned} \phi^{Z_1}(\mathbf{r}, t) &= Z_1^2 \int \frac{d^3q}{(2\pi)^3} e^{i\mathbf{q} \cdot (\mathbf{r} - \mathbf{v}t)} \nu_q \int \frac{d^3q_1}{(2\pi)^3} \nu_{q_1} \nu_{q-q_1} \\ &\times (\epsilon_{q,q,v}^R)^{-1} (\epsilon_{q_1,q_1,v}^R)^{-1} (\epsilon_{q-q_1,(q-q_1),v}^R)^{-1} \\ &\times M_{q,q,v;q_1,q_1,v}^R, \end{aligned} \quad (28)$$

where M_{q,q_1}^R represents the retarded counterpart of M_{q,q_1} of Eq. (27).

The gradient of this nonlinear contribution to the induced potential at the position of the ion, multiplied by the ion charge, gives a result for the corresponding contribution to the stopping power that is equivalent to the one obtained in Refs. [13,14] after an open diagrammatic analysis of the many-body interactions between the moving charged particle and the electron gas [10].

Finally, the evaluation of the polarization charge distribution is obtained through the Poisson relation:

$$\delta n(\mathbf{q}, \omega) = -\frac{q^2}{4\pi} \phi(\mathbf{q}, \omega). \quad (29)$$

3. Results

In this section numerical computations of the nonlinear wake and polarization density are presented, as obtained in the full RPA.

The first-order induced electron density at the position of the ion can be approximated, in the high velocity regime, by [2]:

$$\delta n/n_0 = \pi/\nu. \quad (30)$$

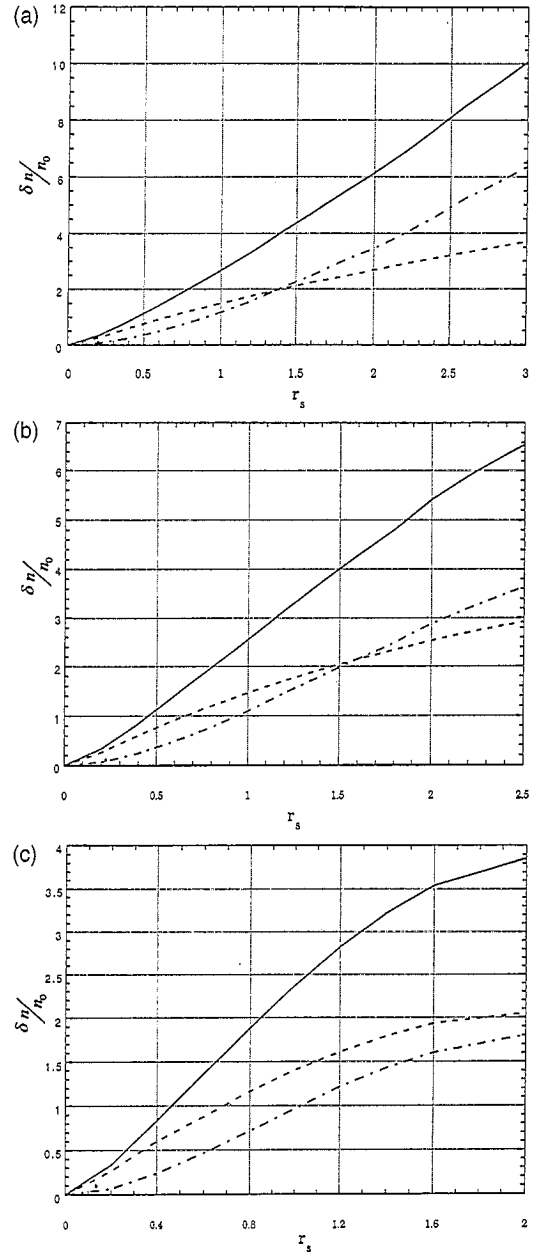


Fig. 4. First (dashed line) and second (dashed-dotted line) order induced density at the position of an ion of charge unity ($Z_1 = 1$) moving with velocities $\nu = 0.5$ (a), $\nu = 1$ (b) and $\nu = 1.5$ (c), as a function of r_s . The total induced density, up to second order in the ion charge, is represented by a solid line.

This magnitude increases as the velocity of the ion decreases. Obviously, only at $v > \pi$ the electronic density fluctuation verifies $\delta n < n_0$, where a first-order analysis is useful and applicable. On the other hand, the first-order induced electron density diminishes very rapidly as one separates very little from the position of the ion, and, consequently, the electron density induced at the position of the ion is a very hard test to show the validity of the linear approach.

The analysis of nonlinear terms has to be made with regard to the magnitudes characterizing our interacting system: v , the velocity of the incoming charged particle, and the electron density parameter, $r_s (n_0^{-1} = 4\pi r_s^3/3)$. Also, the perturbation becomes larger as the ion charge is increased; nevertheless, in the following discussion the attention will be paid to the above defined magnitudes, and a projectile of unit charge will be considered.

In Figs. 4a–4c first and second order contributions to the induced electron density at the position of the ion are presented, as a function of the electron density parameter, for projectile velocities of 0.5, 1.0 and 1.5 times Bohr velocity. It is obvious from these figures that nonlinear corrections are relatively smaller at higher densities, which is due to the well known fact that at higher densities the kinetic energy of the electron gas increases and the ion potential becomes, therefore, a relatively smaller perturbation. This can be seen in Figs. 4a and 4b, where the second order contribution gains the linear one at a certain r_s value. On the other hand, as remarked before, nonlinear effects are less important as the ion velocity increases, so that their contribution is, for metallic densities, lower than the linear one for a projectile velocity of 1.5 times Bohr velocity, as shown in Fig. 4c.

First and second order contributions to the wake potential along the axis of motion of the projectile are plotted in

Fig. 5, for a projectile moving with Bohr velocity in an electron gas of a density equal to that of aluminum. The wake potential decreases at the position of the projectile, as a consequence of the nonlinearity of the response, which makes the first minimum deeper, and, on the other hand, the position of this minimum is moved towards the position of the ion. It is interesting to notice, also, that the second order contribution to the wake potential becomes negligible far from the projectile, and as a consequence, the nonlinear wake suffers measurable changes nearby the ion, giving rise, therefore, to a non-negligible nonlinear contribution to the stopping power.

In conclusion, we have presented a many-body-perturbation-theoretic derivation of the wake potential, which enables us to analyze and evaluate, within the full RPA, nonlinear corrections to the electronic potential induced by the passage of charged particles through matter. Calculations of second order contributions to the distribution of both the induced potential and the electronic polarization around the moving charged particle are now in progress, for different values of the velocity of the projectile and the electron density parameter.

Acknowledgements

The authors gratefully acknowledge stimulating discussions with professors P.M. Echenique and R.H. Ritchie. The authors also acknowledge partial financial support by the University of the Basque Country, and one of us, A. Bergara, thanks the “Hezkuntza, Unibertsitate eta Ikerketa Saila” of the Government of the Basque Country for financial support.

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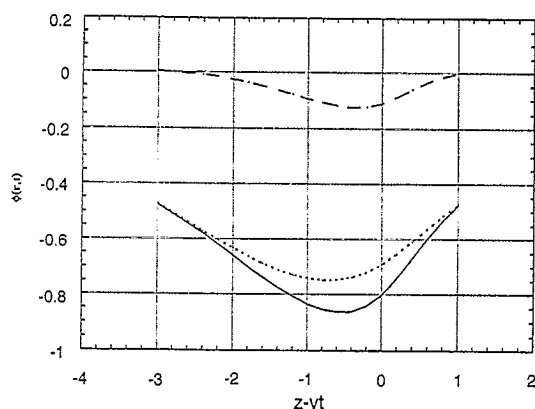


Fig. 5. First (dashed line) and second (dashed-dotted line) order wake potential along the axis of motion for a particle of charge unity ($Z_1 = 1$) moving with a velocity $v = 1$, and $r_s = 2.07$. The total wake potential, up to second order in the ion charge, is represented by a solid line.

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