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Nonlinear quantum hydrodynamical model of the electron gas

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Abstract

It is well known that the hydrodynamical model of the electron gas is suitable when the electron density can be considered as the fundamental quantity, small wavelength effects being less important. This is the case when the electron gas is excited by the passage of swift charged particles. In this paper we make use of the quantum hydrodynamical model of the electron gas to derive, within this model, the nonlinear wake potential of fast charged particles passing through matter, the Barkas effect, and double-plasmon excitation probabilities. This is compared with results obtained by following many-body schemes within the random-phase-approximation.

1. Introduction

The study of the dynamical properties of an inhomogeneous medium dates from the earliest days of modern physics. The first hydrodynamical treatment of a degenerate electron gas was developed by Bloch [1]. He derived the equations of motion of the statistical atom, and demonstrated not only the steady state solutions found in the works of Thomas [2] and Fermi [3], but also oscillations about this state. Utilizing the approximate correspondence between the frequencies of these hydrodynamical disturbances and the actual excitation frequencies of the atomic electrons, Bloch found a formula for the electronic stopping of a swift charged particle in matter. Later, Ritchie [4] predicted the existence of surface plasma oscillations using the hydrodynamical model for the conduction electrons in a plasma slab. Also, several approaches have been made to construct approximate dynamical response functions for conduction electrons in an infinite plasma by considering the medium as a uniform electron gas with small density gradients.

In this paper we consider the interaction between an external particle of charge Z_1e and velocity v_0 with an electron gas immersed in a uniform background of positive charge, and will focus on the study of the electronic density wake induced by the passage of the projectile. For high enough velocities of the traveling charged particle, i.e., $v_0 > 1.5v_F$, v_F being the Fermi velocity of the target, the traveling charged particle can excite collective modes in the electron gas. These long wavelength excitations,

called plasmons, which appear as a consequence of the long range Coulomb interaction, are suitable to be studied within a hydrodynamical treatment of the electron gas. Also, in these conditions electron–hole excitations of energy below the plasmon energy are less important, and higher energy electron–hole excitations can be included through gradient density corrections in the hydrodynamical Hamiltonian.

Since the hydrodynamical equations are themselves nonlinear, nonlinear effects may be studied in a straightforward manner, and we describe the system in the framework of the quantum hydrodynamical model [5], which enables us to employ field theoretic perturbation techniques. Then, after applying many-body perturbation theory we derive the nonlinear wake potential of fast charged particles passing through matter, the Z_1^3 effect in the electronic stopping power, and double plasmon excitation probabilities. Finally, we compare these results with previous results obtained in the random-phase-approximation (RPA) [6–9].

2. Theory

Within a hydrodynamical model, we consider that the collective motion of the electron gas may be described in terms of the displacement of electrons from their original uniform state, and assume that all relevant physical quantities can be expressed in terms of the electron density, $n(r, t)$. We approximate the internal energy as a sum of the classical Coulomb energy and the Thomas–Fermi–Weizsäcker functional [10], and the exchange–correlation energy is neglected, therefore, at this point. Finally, the

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electron gas is treated as a fluid having an irrotational flow, and a velocity potential, $\psi(\mathbf{r}, t)$, can be introduced according to the definition $\mathbf{v}(\mathbf{r}, t) = -\nabla\psi(\mathbf{r}, t)$.

Hence, the Hamiltonian, $H(t)$, of the system is found to be

$$H(t) = \int d^3r \mathcal{H}(\mathbf{r}, t), \quad (1)$$

where $\mathcal{H}(\mathbf{r}, t)$ represents the density Hamiltonian:

$$\begin{aligned} \mathcal{H} = & \frac{1}{2}m_e n(\nabla\psi)^2 + \frac{3}{10}(3\pi^2)^{2/3} \frac{\hbar^2}{m_e} n^{5/3} \\ & + \frac{\hbar^2}{8m_e} \frac{(\nabla n)^2}{n} - \frac{1}{2}e(n - n_0)U_{\text{ind}} - e(n - n_0)U_{\text{ext}}. \end{aligned} \quad (2)$$

The first term here is the hydrodynamical kinetic energy. The second term represents the internal kinetic energy of a uniform system, enclosing the description of the fluid as a quantum electron gas, and the term proportional to $(\nabla n)^2$ is the von-Weizsäcker term, coming from the second order gradient expansion for noninteracting electrons. U_{ind} is the induced electronic potential and U_{ext} represents the potential energy of the interaction with the external field. U_{ind} and U_{ext} can be obtained from the Poisson equation:

$$\nabla^2 U_{\text{ind}} = 4\pi e(n - n_0), \quad (3)$$

and

$$\nabla^2 U_{\text{ext}} = -4\pi eZ_1\delta(\mathbf{r} - \mathbf{v}_0 t), \quad (4)$$

assuming that the moving charged particle is at the origin when $t = 0$. The constant electronic density deep in the interior of the electron gas and far from the position of the projectile, n_0 , is subtracted from the actual electron density, $n(\mathbf{r}, t)$, in order to account, within the jellium model, for the background positive charge.

According to the variational principle one writes

$$\delta \int_{t_1}^{t_2} L dt = 0, \quad (5)$$

where the Lagrangian function, L , is obtained in the usual way in terms of the Hamiltonian of the system, and both the continuity equation and the Bernoulli equation can be derived:

$$\frac{\partial n}{\partial t} - \nabla(n\nabla\psi) = 0 \quad (6)$$

and

$$\begin{aligned} \frac{\partial \psi}{\partial t} = & \frac{1}{2}(\nabla\psi)^2 + \frac{\hbar^2}{2m_e^2}(3\pi^2)^{3/2}n^{2/3} - \frac{\hbar^2}{8m_e^2} \frac{(\nabla n)^2}{n^2} \\ & - \frac{\hbar^2}{4m_e^2} \frac{\nabla^2 n}{n} - \frac{e}{m_e}(U_{\text{ind}} + U_{\text{ext}}), \end{aligned} \quad (7)$$

respectively.

These are nonlinear equations, difficult to solve. Recently, these equations have been solved perturbatively with respect to the strength of the external potential, and first order corrections to the stopping power and the wake potential, valid for high velocities of the penetrating charged particle, have been obtained [11].

In order to develop a nonlinear quantum hydrodynamical model of the electron gas, which employs many body theoretic perturbation techniques, we first expand the electronic density and the velocity potential as

$$n(\mathbf{r}, t) = n_0 + n_1(\mathbf{r}, t) + \dots \quad (8)$$

and

$$\psi(\mathbf{r}, t) = 0 + \psi_1(\mathbf{r}, t) + \dots, \quad (9)$$

respectively, where it is assumed, e.g., that $n_0 \gg n_1 \gg \dots$. Then, inserting these expansions into the Euler–Lagrange equations, i.e., Eqs. (6) and (7), and collecting quantities of the same order we find zeroth and first order continuity and Bernoulli equations, and after insertion into Eq. (2) we obtain:

$$\mathcal{H} = \mathcal{H}_G + \mathcal{H}_0 + \mathcal{H}_1 + \mathcal{H}_{\text{ext}}, \quad (10)$$

where

$$\mathcal{H}_G = \frac{3}{10}(3\pi^2)^{2/3} \frac{\hbar^2}{m_e} n_0^{5/3}, \quad (11)$$

$$\begin{aligned} \mathcal{H}_0 = & \frac{1}{2}m_e n_0(\nabla\psi_1)^2 + \frac{1}{2}(3\pi^2)^{2/3} \frac{\hbar^2}{m_e} n_0^{2/3} n_1 \\ & + \frac{\hbar^2}{8m_e} \frac{(\nabla n_1)^2}{n_0} - \frac{1}{2}eU_{\text{ind}}^{(1)} n_1, \end{aligned} \quad (12)$$

$$\mathcal{H}_1 = \frac{1}{2}m_e n_1(\nabla\psi_1)^2 - \frac{\hbar^2}{8m_e} \frac{(\nabla n_1)^2 n_1}{n_0^2}, \quad (13)$$

and

$$\mathcal{H}_{\text{ext}} = -en_1 U_{\text{ext}}. \quad (14)$$

$\mathcal{H}_G$ is the ground state energy of the electron gas in the frame of the Thomas–Fermi model, and $U_{\text{ind}}^{(1)}$ represents the solution of Eq. (3) when n is replaced by $n_0 + n_1$. The linear deviation from the ground state is obtained through $\mathcal{H}_0$, and $\mathcal{H}_1$, which goes to a higher order in the perturbed electronic density, appears as a consequence of the nonlinearity of the system.

A Fourier expansion of the electronic density finds the well-known normal modes of oscillation of the linearized Euler–Lagrange equations, which we shall refer after quantization as plasmons, and the linearized Hamiltonian, $\mathcal{H}_0$, can be quantized to become:

$$\mathcal{H}_0 = \frac{1}{V} \sum_{\mathbf{q}} \hbar \omega_{\mathbf{q}} \hat{b}^+(\mathbf{q}, t) \hat{b}(\mathbf{q}, t), \quad (15)$$

where V represents the normalization volume, $\hat{b}^+(\mathbf{q}, t)$

and $\hat{b}(q, t)$ are creation and annihilation Bose–Einstein operators, and

$$\omega_q^2 = \omega_p^2 + \beta^2 q^2 + \frac{\hbar^2 q^4}{4m_e^2}, \quad (16)$$

β representing the speed of propagation of hydrodynamic disturbances in the electron gas, and ω_p , the so-called plasma frequency. β can be chosen to be $\sqrt{3/5} v_F$, as obtained in the collective description of the electron gas of Pines and Bohm [12].

The Hamiltonian $\mathcal{H}_1$ of Eq. (13), which describes the triple-vertex interaction between three excitations due to the nonlinear properties of the system, can also be quantized and be expressed, in the limit as $V \rightarrow \infty$, as follows:

$$\begin{aligned} \mathcal{H}_1 = & \frac{1}{2} \left(\frac{\hbar^3}{n_0 m_e} \right)^{1/2} \int \frac{d\omega_1}{2\pi} \frac{d\omega_2}{2\pi} \frac{d\omega_3}{2\pi} \frac{d^3 q_1}{(2\pi)^3} \frac{d^3 q_2}{(2\pi)^3} \\ & \times \left\{ \frac{q_2 \cdot (q_1 - q_2)}{|q_2| |q_1 - q_2|} |q_1| \omega_2 \omega_3 \right. \\ & \left. - \frac{\hbar^2}{4m_e^2} (q_1 \cdot q_2 |q_1| |q_2| |q_1 - q_2|) \right\} \\ & \times \frac{\hat{\phi}(q_1, \omega_1) \hat{\phi}(q_2, \omega_2) \phi(q_1 - q_2, \omega_3)}{(\omega_{q_1} \omega_{q_2} \omega_{q_1 - q_2})^{1/2}} \\ & \times e^{-i(\omega_1 + \omega_2 + \omega_3)t}, \end{aligned} \quad (17)$$

where

$$\hat{\phi}(q, \omega) = \frac{\hat{b}_{q,\omega} + \hat{b}_{-q,\omega}^\dagger}{2}. \quad (18)$$

This Hamiltonian exactly agrees with the result obtained by Ashley and Ritchie [13] employing a simplified version of the RPA as originated by Pines and Bohm for treatment of collective phenomena, if one neglects plasmon dispersion throughout. For the Hamiltonian of Eq. (14), describing the interaction of the electron gas with the external moving charge, we find:

$$\mathcal{H}_{\text{ext}} = -Z_1 \int \frac{d^3 q}{(2\pi)^3} \frac{4\pi e^2}{q} \left(\frac{\hbar n_0}{m_e \omega_q} \right)^{1/2} e^{iq \cdot v_0 t} \hat{\phi}(q, t). \quad (19)$$

Thus, the perturbing Hamiltonian of the system is the sum of two different contributions:

$$\mathcal{H}_{\text{int}} = \mathcal{H}_1 + \mathcal{H}_{\text{ext}}, \quad (20)$$

where $\mathcal{H}_1$, given by Eq. (17), describes the interaction originated in the electron gas between three excitations, and $\mathcal{H}_{\text{ext}}$, given by Eq. (19), encloses the interaction between the external charge and the electron gas.

3. Applications

In the following we shall apply this nonlinear quantum hydrodynamical model of the electron gas to study nonlinear effects involved in different quantities related with the disturbance created by the incoming charged particle on the electron gas.

3.1. The wake potential

The scalar potential of the interaction between a test unit positive charge at an arbitrary point r and the electron gas, which appears as a consequence of the deviation of electrons from their equilibrium positions originated by the incoming charged particle, is, in the representation of second quantization:

$$\hat{V}_w(r, t) = - \int \frac{d^3 q}{(2\pi)^3} \frac{4\pi e}{q} \left(\frac{\hbar n_0}{m_e \omega_q} \right)^{1/2} e^{iq \cdot r} \hat{\phi}(q, t), \quad (21)$$

where ω_q and $\hat{\phi}(q, t)$ are given by Eqs. (16) and (18), respectively.

Now, the so-called wake potential is defined as the mean value of this interaction potential:

$$V_w(r, t) = \frac{\langle \Psi_0 | \hat{V}_w^H(r, t) | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle}, \quad (22)$$

where $|\Psi_0\rangle$ is the Heisenberg ground state of the interacting system and $\hat{V}_w^H(r, t)$ represents the interaction potential of Eq. (21) in the Heisenberg picture. In the case of time independent interacting Hamiltonians Gell-Mann and Low's theorem could be applied and the wake potential would be found to be given in terms of interacting operators:

$$V_w(r, t) = \frac{\langle 0 | T [\hat{V}_w^H(r, t) S] | 0 \rangle}{\langle 0 | 0 \rangle}, \quad (23)$$

where $|0\rangle$ represents the ground state of the noninteracting system, and S is the scattering matrix:

$$S = T \left\{ \exp \left[-i\hbar^{-1} \int H_{\text{int}}^H(t) dt \right] \right\}, \quad (24)$$

T being the time-ordering operator. The contribution to the interacting Hamiltonian coming from the interaction with the moving external particle is not time independent; nevertheless, Gell-Mann and Low's theorem can, also, be used in this case if the retarded character of the response functions involved is recovered after applying Wick's theorem to Eq. (23) [6].

The time ordered free propagator of excitations in our quantum hydrodynamical system,

$$D_0(q, t) = -i \frac{\langle 0 | T (\hat{\phi}(q, t) \hat{\phi}^\dagger(q, 0)) | 0 \rangle}{\langle 0 | 0 \rangle}, \quad (25)$$

is obtained after introduction of Eq. (18) into Eq. (25), and we find:

$$D_0(\mathbf{q}, t) = \int \frac{d\omega}{2\pi} \frac{\omega_q}{\omega^2 - (\omega_q - i\delta)^2} e^{-i\omega t}, \quad (26)$$

δ being a positive infinitesimal.

Then, one can apply Wick's theorem to Eq. (23), and we find, up to second order in the ion charge:

$$\begin{aligned} V_W(\mathbf{r}, t) &= Z_1 e^{-1} \int \frac{d^3 q}{(2\pi)^3} v_q \frac{\omega_p^2}{\omega(\omega + i\delta^+) - \omega_q^2} e^{i(\mathbf{q} \cdot \mathbf{r} - \omega t)} \\ &+ Z_1^2 e^2 \hbar^{-3} \int \frac{d^3 q}{(2\pi)^3} \int \frac{d^3 q_1}{(2\pi)^3} e^{i(\mathbf{q} \cdot \mathbf{r} - \omega t)} v_q v_{q_1} v_{q-q_1} \\ &\times D_0^R(\mathbf{q}, \omega) D_0^R(\mathbf{q}_1, \omega_1) \\ &\times D_0^R(\mathbf{q} - \mathbf{q}_1, \omega - \omega_1) \Gamma_{(\mathbf{q}, \omega; \mathbf{q}_1, \omega_1)}, \end{aligned} \quad (27)$$

where

$$\begin{aligned} \Gamma_{(\mathbf{q}, \omega; \mathbf{q}_1, \omega_1)} &= \left(\frac{m_e^3}{\hbar n_0} \right)^{1/2} \frac{1}{|\mathbf{q}| |\mathbf{q}_1| |\mathbf{q} - \mathbf{q}_1|} \frac{1}{(\omega_q \omega_{q_1} \omega_{q-q_1})^{1/2}} \\ &\times Q_{(\mathbf{q}, \omega; \mathbf{q}_1, \omega_1)}, \end{aligned} \quad (28)$$

with

$$\begin{aligned} Q_{(\mathbf{q}, \omega; \mathbf{q}_1, \omega_1)} &= \left(\frac{\hbar}{2m_e} \right)^2 \left\{ \omega \omega_1 |\mathbf{q} - \mathbf{q}_1|^4 + \omega(\omega - \omega_1) q_1^4 \right. \\ &- \omega_1(\omega - \omega_1) q^4 + (\omega - \omega_1)^2 q^2 q_1^2 \\ &- \omega_1^2 q^2 |\mathbf{q} - \mathbf{q}_1|^2 - \omega^2 q_1^2 |\mathbf{q} - \mathbf{q}_1|^2 \\ &\left. + \left(\frac{\hbar}{2m_e} \right)^2 q^2 q_1^2 |\mathbf{q} - \mathbf{q}_1|^2 (q^2 + q_1^2 + |\mathbf{q} - \mathbf{q}_1|^2) \right\}. \end{aligned} \quad (29)$$

v_q represents the Fourier transform of the bare Coulombic interaction,

$$v_q = \frac{4\pi e^2}{q^2}, \quad (30)$$

$\omega = \mathbf{q} \cdot \mathbf{v}_0$, and $\omega_1 = \mathbf{q}_1 \cdot \mathbf{v}_0$. The Fourier transform of the free propagator given by Eq. (26), $D_0(\mathbf{q}, \omega)$, has been replaced by its retarded counterpart:

$$D_0^R(\mathbf{q}, \omega) = \frac{\omega_q}{(\omega + i\delta)^2 - \omega_q^2}. \quad (31)$$

The wake potential of Eq. (27) can be represented diagrammatically as in Fig. 1. The propagator of excita-

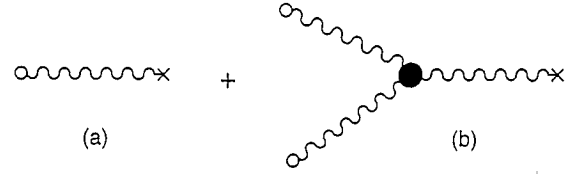


Fig. 1. Feynman diagrams representing first (a) and second (b) order contributions to the wake potential generated by a moving ion. The moving ion, considered as an external source of momentum and energy, is represented by white points, and the cross represents a test positive unit charge. Wavy lines represent plasmon propagators and the black point, joining three plasmon lines, describes the nonlinear interaction between three excitations, as given by Eq. (28).

tions in the quantum hydrodynamical system, $iD_0(\mathbf{q}, \omega)$, is represented in this figure by wavy lines. White points correspond to the external source of energy and momentum, the cross represents a test positive unit charge, and the factor $-i\Gamma(\mathbf{q}, \omega; \mathbf{q}_1, \omega_1)$, coming from the interaction between three excitations, is represented by a black dot joining three plasmon lines. Now, introduction of Eqs. (28) and (31) into Eq. (27) results in the following expression for the wake potential:

$$\begin{aligned} V_W(\mathbf{r}, t) &= Z_1 e^{-1} \int \frac{d^3 q}{(2\pi)^3} v_q (\epsilon_{q, \omega}^{-1} - 1) e^{i(\mathbf{q} \cdot \mathbf{r} - \omega t)} \\ &+ Z_1^2 e^{-1} \hbar^{-2} \int \frac{d^3 q}{(2\pi)^3} e^{i(\mathbf{q} \cdot \mathbf{r} - \omega t)} v_q \int \frac{d^3 q_1}{(2\pi)^3} v_{q_1} v_{q-q_1} \\ &\times \epsilon_{q, \omega}^{-1} \epsilon_{q_1, \omega_1}^{-1} \epsilon_{q-q_1, \omega-\omega_1}^{-1} M_{\mathbf{q}, \omega; \mathbf{q}_1, \omega_1}, \end{aligned} \quad (32)$$

where $\epsilon_{q, \omega}$ and $M_{\mathbf{q}, \omega; \mathbf{q}_1, \omega_1}$ represent plasmon |pole approximations to the exact retarded linear and quadratic response functions, as defined in Ref. [8]. The nonlinear wake potential of Eq. (32) exactly coincides with the plasmon–pole approximation to the full RPA wake potential derived by following many-body electron schemes [6], and it represents a good approximation for high velocities of the moving charged particle, as shown in Ref. [8].

Similarly, it is straightforward to conclude from Eq. (32) that the Z_1^3 correction to the electronic stopping power derived within this model coincides with the plasmon–pole approximation to the full RPA result, as described in Ref. [8].

3.2. Double plasmon excitation probability

The nonlinear quantum hydrodynamical model happens to be specially suited to calculate double plasmon excitation probabilities, recently derived in the full RPA [9]. Within this model, we first evaluate the matrix element, $\langle 0|S|f\rangle$, corresponding to the process of carrying the system from the ground state, $|0\rangle$, to a final state,

$$|f\rangle = \hat{b}_{\mathbf{q}_1, \omega_{q_1}}^+ \hat{b}_{\mathbf{q}-\mathbf{q}_1, \omega-\omega_{q_1}}^+ |0\rangle, \quad (33)$$

characterized by momentum states (q_1, ω_{q_1}) , and $(q - q_1, \omega_{q-q_1})$.

Now, this matrix element can be expanded after introduction of the perturbing Hamiltonian of Eq. (20) into Eq. (24), and Wick's theorem can be applied. Then, we focus on processes in which a single virtual excitation of the electron gas decays into two real subsequent excitations to find, up to first order in the projectile charge:

$$\begin{aligned} \langle 0 | S | f \rangle &= -iZ_1 e v_q D_0(q, \omega_q + \omega_{q-q_1}) \Gamma_{q, \omega_{q_1} + \omega_{q-q_1}; q_1, \omega_{q_1}} \\ &\quad \times 2\pi \delta(\omega_{q_1} + \omega_{q-q_1} - q \cdot v_0). \end{aligned} \quad (34)$$

Finally, the transition rate for creating a double excitation in the electron gas is derived after summing the matrix element of Eq. (34) over all final double plasmon states, and we find:

$$\begin{aligned} \gamma &= \frac{4}{\pi} Z_1^2 \int dq \, dq_1 \delta[q \cdot v_0 - (\omega_q + \omega_{q-q_1})] \\ &\quad \times |\epsilon_{q, \omega_q + \omega_{q-q_1}}|^{-2} \frac{\omega_{q_1} \omega_{q-q_1}}{q^4 q_1^2 |q - q_1|^2} \\ &\quad \times |M_{q, \omega_{q_1} + \omega_{q-q_1}; q_1, \omega_{q_1}}|^2, \end{aligned} \quad (35)$$

$\epsilon_{q, \omega}$ and $M_{q, \omega; q_1, \omega_1}$ representing, this time, time-ordered plasmon–pole linear and quadratic response functions. This result is exactly equivalent to Eq. (5) of Ref. [9], derived within the full RPA, if one replaces the full RPA linear and quadratic response functions by plasmon–pole like approximations.

4. Conclusions

Second and third order wake potential and electronic stopping powers, and, also, double plasmon excitation probabilities have been derived, within a nonlinear quantum hydrodynamical model of the electron gas, showing that the results obtained in this way coincide with plasmon–pole like approximations to the corresponding quantities evaluated recently in the full random-phase-approximation.

In future work we shall extend this model to more complex structures, such as the bounded electron gas.

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