

Nonlinear Screening in Two-Dimensional Electron Gases

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We have performed self-consistent calculations of the nonlinear screening of a point charge Z in a two-dimensional electron gas using a density functional theory method. We find that the screened potential for a $Z = 1$ charge supports a bound state even in the high-density limit where one might expect perturbation theory to apply. To explain this behavior, we prove a theorem to show that the results of linear response theory are in fact correct even though bound states exist.

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Screening is a fundamental property of an electron gas in arbitrary dimensions. The example of two dimensions is of particular interest because of the possible realization of quasi-two-dimensional systems in a variety of contexts: semiconductor heterostructures [1], image or band-gap surface states at metal surfaces [2], electrons on the surface of liquid helium [3], and layered materials [4]. In all of these cases, the interaction of external charges with the two-dimensional electron gas (2DEG) is a problem of both fundamental and practical interest. For example, the transport of electrons in a 2DEG is often limited by charged impurity scattering and a detailed knowledge of the scattering potential is needed for an accurate determination of the electron mobility [1]. Scanning tunneling microscopy offers an even more direct means of determining the screening response of a quasi-2DEG through the observation of adsorbate-induced Friedel oscillations [5]. Still another class of problems involves the interaction with *moving* charges as might arise in low-energy electron scattering [6] or tunneling experiments [7]. In this case, the dynamic response of the 2DEG is important in that electronic excitation, and, hence, energy loss, will occur.

A charged impurity or projectile typically represents a strong perturbation and a nonlinear screening theory is in general needed to account for the modifications of the local electronic structure. However, in certain situations the *screened* impurity potential may be relatively weak and therefore amenable to a perturbative treatment. This is usually the method adopted to deal with donor impurities that are spatially removed from the 2DEG within a heterostructure [1], although it is rare to find quantitative agreement between theory and experimentally measured mobilities [8]. The situation of acceptor impurities *within* the gas is a much more severe perturbation, and quite dramatic effects can arise as a result of the modified electronic structure [9,10]. In such situations, the screening response has to be determined nonlinearly.

One of our objectives in this Letter is to provide a fully self-consistent description of the nonlinear screening in an ideal 2DEG within the context of density functional theory. A second objective is to use these calculations to establish the range of validity of linear response theory. Somewhat surprisingly, this latter objective is more subtle than anticipated as a result of a peculiarity of potential scattering in 2D, namely, the fact that any purely attractive potential always has at least one bound state [11], in marked contrast to the situation in 3D. For a positively charged impurity, we in fact encounter a situation in which the screened potential supports a bound state even in the high-density limit where one would intuitively expect a perturbative treatment to be valid. To resolve this apparent paradox, we prove what will be referred to as the high-density screening theorem which states that the screening charge can indeed be calculated perturbatively *even when bound states exist*. In this way, we are able to justify the use of perturbation theory when at first sight it would seem inapplicable.

The problem we address is the nonlinear screening of a stationary point charge, Z , located in the plane of a 2DEG. The latter is treated as ideal in the sense that the electrons are confined to the plane. Of course in real applications, such as a heterostructure, a more accurate treatment of the electronic states is required. We ignore these complications in order to focus on those aspects of nonlinear screening which are expected to be independent of these details. To stabilize the system, the electrons move in the presence of a uniform neutralizing positive background. In addition, we assume the electrons to have an isotropic effective mass m^* and to be immersed in an extended dielectric with permittivity ϵ . We use the effective Bohr radius, $a_0 = \epsilon \hbar^2 / m^* e^2$, as the unit of length and the effective Hartree, $H = e^2 / \epsilon a_0$, as the unit of energy. The density of the gas, n_0 , is characterized by the density parameter $r_s = 1 / \sqrt{\pi n_0}$.

The static screening response of the 2DEG is determined by solving self-consistently the two-dimensional Kohn-Sham equations:

$$-\frac{1}{2}\nabla^2\psi_i(\mathbf{r}) + \Delta v_{\text{eff}}(\mathbf{r})\psi_i(\mathbf{r}) = E_i\psi_i(\mathbf{r}), \quad (1)$$

where the effective potential is given by

$$\Delta v_{\text{eff}}(\mathbf{r}) = v_{\text{ext}}(\mathbf{r}) + \Delta v_H(\mathbf{r}) + \Delta v_{\text{xc}}(\mathbf{r}). \quad (2)$$

Here, $v_{\text{ext}} = -Z/r$ is the external potential and Δv_H is the Hartree potential due to the electronic screening density, $\Delta n(\mathbf{r}) = n(\mathbf{r}) - n_0$. The change in the exchange-correlation potential, $\Delta v_{\text{xc}}(\mathbf{r}) = v_{\text{xc}}[n(\mathbf{r})] - v_{\text{xc}}[n_0]$, is defined in the local density approximation using the parametrization of the 2D exchange-correlation energy given in Ref. [12].

The total screening charge is given by

$$\Delta n(\mathbf{r}) = \sum_b |\psi_b(\mathbf{r})|^2 + \sum_i [|\psi_i(\mathbf{r})|^2 - |\psi_i^0(\mathbf{r})|^2], \quad (3)$$

where the first sum extends over all bound states of the effective potential, and the second extends over all occupied continuum states up to the Fermi level E_F . We assume that each spatial orbital is doubly occupied for spin. The scattering states $\psi_i(\mathbf{r})$ are shifted asymptotically relative to the free-particle solutions $\psi_i^0(\mathbf{r})$ by a phase $\eta_m(E)$. These scattering phase shifts are related to the total screening charge according to the 2D Friedel sum rule (FSR) [13]

$$Z_{\text{FSR}} = \frac{2}{\pi} \sum_{m=-\infty}^{\infty} \eta_m(E_F). \quad (4)$$

Details of the self-consistent solution of Eqs. (1) and (2) will be presented elsewhere.

We begin by considering the case of a negatively charged impurity ($Z = -1$), such as an antiproton or acceptor state in a semiconductor. Figure 1 presents the

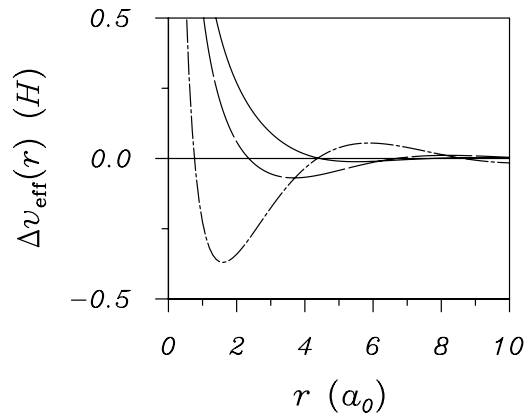


FIG. 1. Comparison of nonlinear and linear screened potentials: nonlinear with exchange correlation (solid), nonlinear Hartree potential (short-dashed), linear Hartree potential with LFC (chain); $Z = -1$, $r_s = 4$.

self-consistent effective potential Δv_{eff} for $r_s = 4$ (solid curve) as a function of the distance from the impurity. This potential repels electrons almost completely from the impurity's vicinity, leaving exposed a positively charged disk of radius $R \simeq r_s$ which neutralizes the impurity charge. As is the case in 3D, this behavior cannot be reproduced in a linear theory. The screened $Z = -1$ potential does not support bound states for any r_s value, as might have been expected. We mention this since it has been claimed [14] that the introduction of a negative test charge into a 2D gas can give rise to a potential which is sufficiently strong to bind an electron.

To make contact with this earlier work, we compare in Fig. 1 the nonlinearly screened potentials with those obtained on the basis of linear response theory. The chain curve shows the linear response Hartree potential ($v_{\text{ext}} + \Delta v_H$) as obtained when local field corrections (LFC) are included in the determination of the electron screening density [14]. This potential has a large attractive region in real space and supports a bound state for a unit negative test charge of one electron mass. This observation led to the suggestion of a possible pairing mechanism that could be responsible for a correlation-induced instability at low densities [14]. Such a conclusion, however, is invalid on two counts. First, the screening of the impurity is *strongly nonlinear*. The dashed curve in Fig. 1 shows the corresponding Hartree potential when the nonlinear screening density is used. It has a much shallower attractive region. But more importantly, an electron, as opposed to a negative test charge, also feels the effect of the induced xc potential. With this contribution included in the full nonlinear potential Δv_{eff} (solid curve), there is no tendency for bound state formation, as confirmed numerically.

The results for a positive impurity are quite different in that the attractive screened potential supports bound states for all densities of physical interest (including $r_s \rightarrow 0$). For $Z = 1$ there is one $m = 0$ bound state that is doubly occupied. Since the total screening density integrates to unity to satisfy the FSR, the continuum screening density must itself contribute a total charge of $+1$ in order to compensate for the overscreening provided by the bound states. In other words, the $Z = 1$ impurity with two bound electrons can be viewed as an H^- ion which acts as a $Z = -1$ impurity. This was confirmed by comparing the $Z = 1$ and $Z = -1$ *continuum* screening densities. For $r_s = 10$, the two are virtually the same.

In Fig. 2, we show the $Z = 1$ bound state energy as a function of r_s . The behavior seen is surprising in view of the corresponding behavior in 3D. There, the bound state energy *increases* with decreasing r_s since the impurity potential is screened more effectively with increasing density and, as a result, the bound state eventually ceases to exist [15]. Beyond this point, the accuracy of perturbation theory improves with increasing density. The contrary behavior exhibited in Fig. 2 calls into question the applicability of perturbation theory in the 2D case.

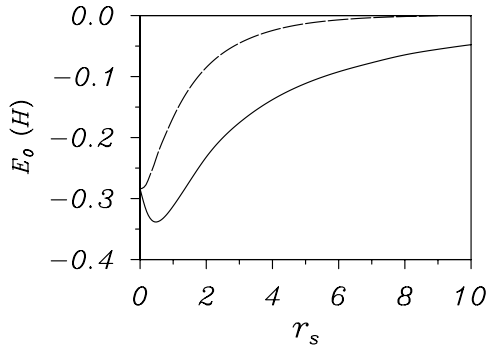


FIG. 2. Bound state eigenvalue vs r_s ; nonlinear DFT with (solid) and without (dashed) exchange correlation.

To address this question, we now prove a theorem regarding electronic screening in the high-density limit. We consider the introduction of an external potential $\lambda V(\mathbf{r})$ into a uniform *noninteracting* Fermi gas for arbitrary dimension D . The parameter λ is a coupling constant whose physical value is unity. The problem is to determine the induced density $\Delta n(\mathbf{r})$ due to the introduction of $\lambda V(\mathbf{r})$; the effect of interactions will be dealt with afterwards. By making use of Dyson's equation, $G_{\lambda+\delta\lambda} = G_\lambda + \delta\lambda G_\lambda V G_{\lambda+\delta\lambda}$, for the single particle Green function $G_\lambda(\mathbf{r}, \mathbf{r}', z)$, one can show that the screening density satisfies

$$\frac{\partial \Delta n(\mathbf{r}; \lambda)}{\partial \lambda} = -\frac{1}{\pi} \int d\mathbf{r}' V(\mathbf{r}') \int_{-\infty}^{E_F} dE \times \text{Im}[G_\lambda(\mathbf{r}, \mathbf{r}', E + i\epsilon) G_\lambda(\mathbf{r}', \mathbf{r}, E + i\epsilon)]. \quad (5)$$

The crucial next step in the argument is to use the analytic properties of the Green functions to change the energy integral from $(\int_{-\infty}^{E_F})$ to $(-\int_{E_F}^{\infty})$. In the $E_F \rightarrow \infty$ limit, it is then permissible to replace G_λ by the free-particle Green function G_0 since the energy E can now be assumed to be much larger than the strength of the (bounded) potential $|V(\mathbf{r})|$. Once this is done, the energy integration can be changed back to its original range, and, after integrating with respect to the coupling constant, we obtain

$$\Delta n(\mathbf{r}) \simeq -\frac{1}{\pi} \int d\mathbf{r}' V(\mathbf{r}') \lim_{E_F \rightarrow \infty} \int_{-\infty}^{E_F} dE \times \text{Im}[G_0(\mathbf{r}, \mathbf{r}', E + i\epsilon) G_0(\mathbf{r}', \mathbf{r}, E + i\epsilon)]. \quad (6)$$

This asymptotic result is valid for any D and applies even when the potential $V(\mathbf{r})$ supports bound states. It can also be seen to apply to a singular Coulomb potential in a limiting sense. If the impurity is moved slightly out of the plane, the potential is bounded and the theorem applies. The screening density in this case will differ from that of the singular potential only within a small distance of the impurity.

An alternative expression for (6) is

$$\Delta n(\mathbf{r}) \simeq -\lim_{E_F \rightarrow \infty} \frac{1}{L^D} \sum_{\mathbf{q}} \chi_0(\mathbf{q}) V(\mathbf{q}) e^{i\mathbf{q} \cdot \mathbf{r}}, \quad (7)$$

which is the result of linear response theory. Here, $\chi_0(\mathbf{q})$ is the noninteracting static density response function of the system. In the high-density limit, $q \ll k_F$ for all wave vectors for which $V(\mathbf{q})$ is finite, and we have $\Delta n(\mathbf{r}) \simeq -\chi_0(0)V(\mathbf{r})$. In 2D, $\chi_0(0) = \pi^{-1}$ and

$$\Delta n(\mathbf{r}) \simeq -\frac{1}{\pi} V(\mathbf{r}). \quad (8)$$

Thus, we arrive at the interesting conclusion that in 2D the screening density takes on a *density-independent* form in the high-density limit, and is simply proportional to the perturbing potential.

This result can easily be checked numerically. In Fig. 3, we show $\Delta n(\mathbf{r})$ for a 2D gas with $r_s = 0.5$ for a model potential $V(r) = -V_0 \sin^2(2\pi r/r_0)\theta(r_0 - r)$ which is an axially symmetric, double-well potential. With $r_0 = 5$ a.u. and $V_0 = 0.125$ H, the potential has a single $m = 0$ bound state, while for $V_0 = 0.25$ H there are two $m = 0$ bound states. In both cases we see that the total screening density is well approximated by the asymptotic result in Eq. (8).

To include the effect of interactions, we identify Δv_{eff} in Eq. (2) with $V(r)$ and make use of Eq. (8). In the high-density limit, we then find $\Delta v_{\text{eff}}(q) = -2\pi Z/(q+2)$, which in real space gives the Thomas-Fermi potential [13]. This potential is purely attractive and has a bound state eigenvalue of $E_0 = -0.2862$ H which is the $r_s \rightarrow 0$ limit of the curves in Fig. 2. This explains why a bound state exists in the high-density limit and why, in spite of this, the result is not in conflict with the applicability of

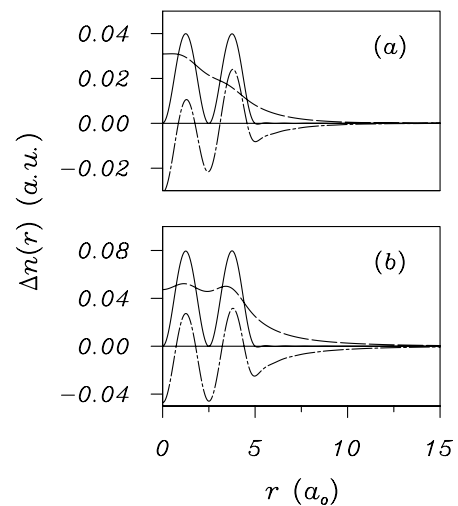


FIG. 3. Screening charge density for a model potential: bound (dashed) and continuum (chain) state contributions, total (solid). (a) $V_0 = 0.125$ H, (b) $V_0 = 0.25$ H; $r_s = 0.5$.

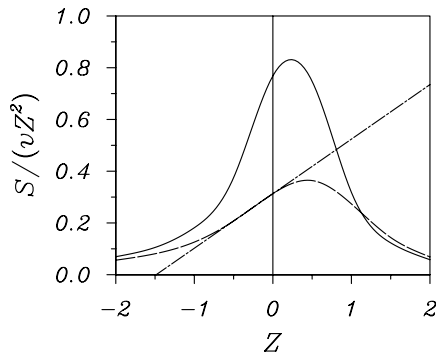


FIG. 4. Normalized stopping power as a function of the projectile charge Z , for $r_s = 2$: nonlinear screening with (solid) and without (dashed) exchange correlation. The straight chain curve gives the quadratic response result.

linear response theory. It should be emphasized that the same argument in 3D leads to the conclusion that no bound state can exist in this case.

As a final practical application, we present results of the calculation of the energy loss per unit length (or stopping power, S) for a projectile of charge Z moving with velocity v in the plane of the 2DEG. Within the so-called kinetic theory framework, the stopping power is given by the expression [16]

$$S = n_0 v v_F \sigma_{tr}(E_F), \quad (9)$$

where $\sigma_{tr}(E_F)$ is the momentum-transfer cross section defined in terms of the scattering phase shifts by [13]

$$\sigma_{tr}(E_F) = \frac{4}{v_F} \sum_{m=0}^{\infty} \sin^2[\eta_m(E_F) - \eta_{m+1}(E_F)]. \quad (10)$$

To leading order in the velocity, it is sufficient to determine the scattering phase shifts using the static nonlinearly screened potentials calculated in the present paper.

In Fig. 4, we show the stopping power as a function of the projectile charge Z . For small Z , S has the expansion $S = S_1 Z^2 + S_2 Z^3 + \dots$, where the first two terms are the linear and quadratic response results, respectively. To emphasize the deviations from linear response, we present the results in the form $S/(vZ^2)$. In this representation, the stopping power including the quadratic response correction appears as a straight line with slope S_2/v . This correction was previously calculated within the quadratic random phase approximation [17] and is shown in Fig. 4 as the straight line. We can see that corrections beyond quadratic response theory are large, especially for positive charges. Furthermore, the inclusion of xc is seen to enhance the stopping power considerably in the range $-1 \leq Z \leq 1$, even to a greater extent

than found in 3D [18]. Finally, comparison with earlier calculations [19] demonstrates that important differences arise when the self-consistently determined nonlinear screening potentials are used to evaluate the momentum scattering cross sections.

In summary, we have performed self-consistent calculations of the nonlinear screening of a point charge in a 2DEG using density functional theory. We have also proven a screening theorem which clarifies the behavior of the screening in the high-density limit. These results find application in a variety of problems, such as charged impurity scattering and the stopping power of charged projectiles.

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