Strength of dipolar backflow patterns around slow protons in three- and two-dimensional electron gases

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The familiar dipolar backflow in an electron gas around a slowly moving massive impurity represents, in linear response, the averaged induced current far from the impurity and is proportional to the density response function and the forward scattering amplitude within the Born approximation. Here, we calculate the strength of the dipolar density modulation around a slow proton in three- and two-dimensional paramagnetic electron gases, beyond the perturbative linear-response treatment, by using scattering phase shifts at the Fermi energy which satisfy the Friedel-sum rule. These are determined by solving self-consistently the ground-state Kohn-Sham equations for screening. A sign-changing effect, as a function of the electron gas density, is found in the strength in both dimensions. Using the self-consistent phase shifts, a recently proposed expression for the so-called direct charge in three-dimensional electromigration is also investigated.

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I. INTRODUCTION AND MOTIVATION

In linear-response theory,[1] the strength of the dipolar backflow around a slowly moving impurity is proportional with the Fourier transform of the electron-impurity interaction at zero momentum, i.e., with the forward limit of the two-body scattering amplitude treated in first-order Born approximation. In the charged-impurity case, it is, therefore, proportional with Z due to complete dielectric screening of a point charge (Z) in a metallic environment. The dielectric description corresponds, in the case of a heavy charged particle, to the linearized limit ($Z \to 0$) of a self-consistent-field treatment.[2] Such a treatment rests on the independent particle picture, in which the screening can immediately be seen to be expressible in terms of quantum mechanics of scattering of a single electron from an effective potential $[V_{eff}(r)]$ determined self-consistently. The statistical mechanics of the system then follows[2] by filling up the new set of energy levels according to the *whole* Fermi distribution. These levels are doubly occupied in a paramagnetic gas.

A recent reconsideration[3] of the problem of backflow in three- and two-dimensional electron gases shows that the strength, denoted as $h(D) \equiv h^{(1)}(D) + h^{(2)}(D)$, of the *dipolar* backflow is expressible, beyond linear-response theory, in terms of scattering phase shifts $[\delta_m(k_F)]$ *solely* at the Fermi surface. The leading term is given by

$$h^{(1)}(D) = \frac{1}{\pi} \sum_{l=0}^{\infty} a_l \sin(2\delta_l), \tag{1}$$

where $a_l = 2l+1$ in $3D$. In $2D$, one has $a_0 = 1$ and $a_l = 2$ for all $l \geqslant 1$. The perturbatively higher-order, so-called next-to-leading term

$$h^{(2)}(D) = \frac{4}{\pi} \sum_{l=0}^{\infty} c_l \sin\delta_l \sin\delta_{l+1} \sin(\delta_l - \delta_{l+1}) \tag{2}$$

is based on an interference between the first and next-to-leading contributions in the outgoing waves. In Eq. (2), $c_l = (l+1)^2$ in $3D$ and $c_l = 2l+1$ in $2D$. The host densities (n_0) determine k_F in standard way in $3D$ and $2D$ dimensions; $k_F = (3\pi^2 n_0)^{1/3}$ and $k_F = (2\pi n_0)^{1/2}$, respectively. Hartree atomic units, $e^2 = \hbar = m_e = 1$, are used throughout this work.

To the best of our knowledge, a calculation of $h(D)$ based on phase shifts at k_F which are obtained from the self-consistent-field treatment is not performed yet. It is an important question, since the complete dielectric screening of the point charge *implies*[3] a rule with $h(D) = Z$, which could give a nontrivial constraint on phase shifts (solely) at k_F. Apart from this intrinsic theoretical interest, the relevance of a detailed study of $h(D)$ can be motivated further by the following observation.

If an electric field ($\mathbf{E}$) is applied to a metal or semiconductor, the phenomenon of electromigration[4,5] may occur. The technological importance of this current-driven phenomenon is in its possible failure influence, especially at miniaturization.[6] According to a recent[7] derivation, which is based also on one-electron scattering states at k_F, the direct charge (Z_d) to the total force

$$\mathbf{F} = (Z_d + Z_w)\mathbf{E} \tag{3}$$

is given (in $3D$) by the following expression:

$$Z_d = \frac{2}{\pi}\left[F^0(k_F) + \frac{1}{3}k_F^2 \frac{d}{dk_F}\left(\frac{1}{k_F} F^0(k_F) \right) \right]. \tag{4}$$

In this equation, $2F^0(k_F) = \Sigma_{l=0}^{\infty}(2l+1)\sin[2\delta_l(k_F)]$. Therefore, the first term for the direct charge has the *same* form as $h^{(1)}(3D)$ in Eq. (1). There is an agreement between theories of electromigration that the wind (w) force $Z_w\mathbf{E}$ is described via the transport cross section. Thus, the electron-wind term is at least of order of Z^2. On the other hand, there are conceptual uncertainties in the theoretical magnitude of the direct charge.[5]

TABLE I. Phase shifts at the Fermi level $\delta_l(k_F)$ for proton, $Z=1$, embedded in $2D$ electron gases with selected r_s values.

	$\delta_l(k_F)$						
r_s	$l=0$	$l=1$	$l=2$	$l=3$	$l=4$	$l=5$	$l=6$
0.5	0.765577	0.165566	0.071559	0.040944	0.025981	0.018308	0.013707
1.0	1.154110	0.115585	0.032537	0.018592	0.009020	0.006952	0.004761
2.0	1.575694	−0.000683	−0.007204	0.003724	−0.002086	0.001460	0.000048
3.0	1.780856	−0.075585	−0.017898	0.000252	−0.004024	−0.000326	0.000546
4.0	1.875719	−0.116874	−0.017275	−0.005233	−0.002954	−0.004692	−0.002056
5.0	1.907727	−0.138777	−0.016339	−0.005588	−0.003475	−0.004263	0.000171
6.0	1.914537	−0.148908	−0.013374	−0.006827	−0.002840	−0.004869	0.000282
7.0	1.915041	−0.149949	−0.007571	−0.009738	0.000102	−0.003224	0.000168
8.0	1.906250	−0.151205	−0.005618	−0.012838	0.001045	−0.003853	−0.002088
9.0	1.902759	−0.145352	0.004626	−0.016408	0.002476	−0.000004	−0.001318
10.0	1.867959	−0.171308	0.034339	−0.007462	−0.003574	−0.000480	−0.000036

II. RESULTS

We use standard local approximation local-density approximation for the exchange-correlation part in the Kohn-Sham (orbital) approximation[9] to obtain effective potentials $[V_{eff}(r)]$ at ground-state embedding conditions. This approximation treats the screening action, a fundamental property of the electron gas, by using a grand-canonical ensemble for the electron gas with constant chemical potential. The scattering phase shifts generated satisfy[10–12] the appropriate Friedel-sum rules,

$$Z = \frac{2}{\pi}\sum_{l=0}^{\infty} a_l \delta_l(k_F), \tag{5}$$

at self-consistency of iterations in both dimensions. The corresponding (negative) sums of phase shifts at $k=0$ cancel the number of occupied bound states in agreement with the Levinson's theorem. This number depends, of course, on the details of $V_{eff}(r)$, for example, on the input exchange-correlation chemical potential for electron-electron interaction. More importantly, a *charge state* and Eq. (5) are inherently interconnected.[3]

The Friedel condition in Eq. (5) ensures the charge neutrality of the *entire* system in the presence of a static charged impurity. It does not tell us where an extra electron is located.[13] This comes from a concrete screening calculation, as the present one. Notice that if the screening problem were perturbative ($Z\rightarrow 0$), all phase shifts would be small and Eqs. (1) and (5) would be numerically equivalent. Since Eq. (2) is at least of order Z^3 in this weak potential limit, the dipolar backflow strength would be given by $h(D)\simeq Z$.

For completeness, we present in Table I self-consistent phase shift values as a function of the density parameter $r_s = \sqrt{2}/k_F$; Eq. (5) is properly satisfied at iterative convergency in $2D$. For a detailed Table in $3D$, we refer to the work of Puska and Nieminen.[11] In $3D$, a bound state appears at about $r_s \geqslant 2$, which is occupied by two electrons in a paramagnetic system. In the $2D$ case, the doubly occupied bound state appears already at the $r_s=0$ value of the density parameter.[12] For related detailed mathematical investigations on the problem of bound-state appearance in $2D$, we refer to Refs. 14 and 15. Note that all-electron quantities, such as the total physical densities, are analytical (smooth) functions in our Hartree-like mean-field treatment, even at the appearance of a normalizable (doubly populated) bound state.[16–18]

Since the total screening charge must integrate to unity according to Eq. (5) in both dimensions, the continuum states must themselves contribute a total charge of +1 in order to compensate for the overscreening provided by the two bound electrons. These charge arrangements represent the ground states in the applied effective one-electron method. The obvious differences of $h(D)$ or $Z_d(3D)$ from Eq. (5) suggest that deviations from $Z=1$ (proton) are expected beyond the perturbative limit.

The strengths of the dipolar part, calculated by Eqs. (1) and (2) for $Z=1$ in $2D$ by using self-consistent phase shifts, are exhibited in Fig. 1. The open circles refer to the leading term, Eq. (1) for $h^{(1)}(2D)$, while the filled ones to the complete $h(2D)=h^{(1)}(2D)+h^{(2)}(2D)$ expression. The $3D$ equivalents, based on the corresponding self-consistent phase shifts, are plotted on Fig. 2 for a similar range of the density parameter r_s. The open squares in Fig. 2 refer to Eq. (4) for the direct charge. As we mentioned earlier in this Brief Report, only the leading terms (open circles) are equal in the scattering description of $h(3D)$ and the direct charge $Z_d(3D)$.

In our ground-state modeling, $Z_d(3D)$ becomes negative at about $r_s\approx 3$, while $h(3D)$ only at about $r_s\approx 4$. Clearly, the role of the next terms, beyond the common first one, is different. Indeed, via the derivative term for $Z_d(3D)$, a weighted change in the density of states gives a strong effect already at a relatively high density of the host system. For a free-electron metal, Al with $r_s\simeq 2$, the deviations from unity are notable and the difference between $h(3D)$ and $Z_d(3D)$ is transparent.

We can conclude that an "effective-antiproton" nature of the screened proton potential (with doubly populated bound

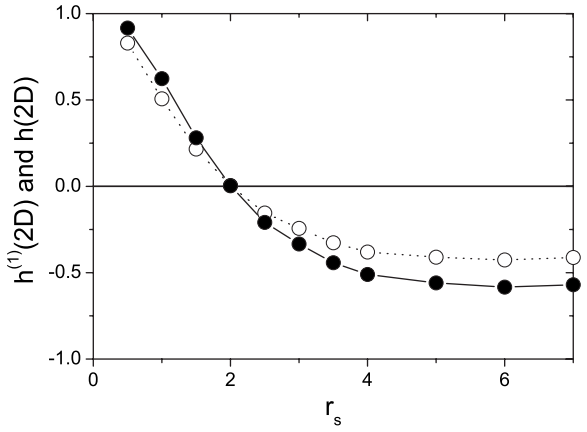

FIG. 1. Strengths of the dipolar backflow around a slow proton $Z=1$ in a $2D$ gas for $r_s \in [0.5,7]$. The leading term, denoted by $h^{(1)}(2D)$, and the complete expression, denoted by $h(2D)$, are based on Eqs. (1) and (2) and are represented by open and filled circles, respectively. The density parameter (r_s) is calculated from the host density as $\pi r_s^2 = 1/n_0$.

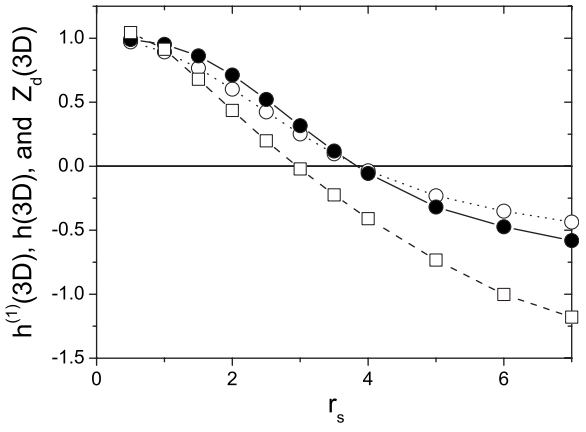

FIG. 2. Strengths of the dipolar backflow around a slow proton $Z=1$ in a $3D$ gas for $r_s \in [0.5,7]$. The leading term, denoted by $h^{(1)}(3D)$, and the complete expression, denoted by $h(3D)$, are based on Eqs. (1) and (2) and are represented by open and filled circles, respectively. The open squares, based on Eq. (4), refer to the direct charge $Z_d(3D)$. The density parameter (r_s) is calculated from the host density as $(4\pi r_s^3/3) = 1/n_0$.

and scattering states) is evident from Figs. 1 and 2, in the density dependences of $h(D)$ and $Z_d(3D)$. This already happens with the leading term. The self-consistent calculations for $h(D)$ result in a *sign-changing* effect in $2D$ and $3D$. This statement is the main result of the present study performed within a Kohn-Sham-type, ground-state mean-field approximation.

III. COMMENTS AND SUMMARY

In our mean-field method, where the independent electrons move in a common field, we cannot (apart from the high-density limit) satisfy a $h(D)=Z$ constraint proposed earlier[3] as a sum rule for the scattering phase shifts at the invariant Fermi surface. To prescribe a *different* charge arrangement for the complete screening cloud around a proton, we could force (by putting holes) a not population in the Kohn-Sham bound state but this would refer, from energetic point of view, to an excited-state configuration in our paramagnetic electron gas. This problem and a detailed modeling in a completely spin-polarized system, where a bound state is populated by one electron only, are left for future considerations. The form of the corresponding $h(D)$ will not, of course, involve a factor of 2 due to spin summation.

Finally, we outline here alternative ways for the interaction of a fixed external potential with an ideal electron gas. In many-body perturbation theory, matrix elements of the potential which connect occupied states *have no* effect on many-body wave function, since their effect cancels in a determinant wave function.[19] Due to this effect, one can use a truncated effective potential which is appreciably weaker than the original one; thus, the problem of a bound state may not appear. However, since the truncated potential is *nonlocal*, it would therefore, in practice, be inconvenient[19] to work with and, more importantly, a physical self-consistency becomes clearly nontrivial in field-theoretic methods.

A more conventional attempt based on higher-order response functions with a *linearly* screened input potential might also have relevance to the controversy found in the present work. At the level of quadratic response $(\sim Z^2)$ approximation for the forward $(q=0)$ scattering amplitude, the $h(3D)=Z$ still holds.[17] This is due to the perfect screening at the first-order $(\sim Z)$ linear level and a complete cancellation of two Z^2-order terms in a consistent amplitude. This partial observation is not in contradiction with the order[3] of Z^3 for the $h^{(2)}(3D)$ second term to the complete $h(3D)$ at $(Z/k_F) \ll 1$.

In summary, the strength of the dipolar backflow patterns around slow protons in three- and two-dimensional electron gases is calculated by using scattering phase shifts at the Fermi level. These are obtained in a self-consistent mean-field approximation, in which the Friedel-sum rule is satisfied. A sign-changing effect, as a function of the host density, is found in this strength in both dimensions, which we attribute to the doubly populated Kohn-Sham bound state. Moreover, on the same footing, we have investigated the magnitude of the so-called direct charge in $3D$ electromigration; a similar sign change is found, but at a different host density.

We pointed out few possibilities (by discussing briefly standard many-body methods) which might help to understand, beyond simple first-order perturbation theory, the classic problem of the strength of dipolar backflow pattern around a slow charged particle in a homogeneous electron gas. A combination of the present results with the above-outlined future studies could provide, in our opinion, important additional information to the existing controversy ($Z_d=1$ or not)[5,8,20] on the proper magnitude of a direct charge to the total-force expression in current-driven electromigration also. As in modern semiconductor technology, a controlled tuning of carrier densities seems to be feasible, and the sign-changing effect found here in the strength of the $2D$ dipolar backflow may become experimentally accessible.

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