Time-dependent screening in a two-dimensional electron gas

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Abstract

Transient effects during the evolution in time of the screening process are studied for the particular case of a suddenly created charge in a two-dimensional (2D) electron gas. The response of the medium is described using linear theory and the random-phase approximation to the dielectric function. The distinctive peculiarities of the excitation spectra for a two-dimensional electron gas provide a time behaviour different from the one obtained for a three-dimensional (3D) medium. We find that, for \( r_s = 2 \), the transition to the steady-state regime takes place in less than 0.5 fs, without showing the long-time oscillations characteristic of the 3D system. The results are explained in terms of the different nature of the 2D and 3D plasmons.

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1. Introduction

A charged impurity immersed in a metal induces a rearrangement of the conduction electrons around it creating the so-called induced screening charge. This dressing process is not instantaneous. With the development of ultrashort-pulse laser spectroscopic techniques now it is possible to probe electron scattering mechanisms at timescales below femtoseconds [1–3]. This is the timescale in which the electrons of a metal dress an initially bare charged particle. Apart from its fundamental interest, the study of screening transients is important in a variety of situations. For instance, it has been shown their effects in the high-energy tail of soft X-ray emission spectra [4]. More recently, in order to explain lifetime measurements of excited electrons in crystalline copper, it has been proposed the existence of transient excitonic states during the short-time in which the screening of the hole left behind by the excited electron, takes place [5,6]. In a somewhat different context, Huber et al. [7] have monitored the temporal evolution of charge–charge interactions after ultrafast excitations of an electron-hole plasma in a semiconductor material. In this way, they observed the formation of charge screening in a nonequilibrium system with low electronic density on a
femtosecond timescale. Their findings were consistent with calculations based on quantum kinetic theories for nonequilibrium dynamics of Coulomb interactions [8] that predict a delayed build-up of the screening.

In this article, we study for the first time, the building up of the electronic screening in a two-dimensional (2D) jellium below the femtosecond scale. Canright [9] calculated the transient screening response to a suddenly created point charge in a three-dimensional (3D) jellium. The method, based on a linear screening approximation, allowed a decomposition of the response of the system into a part due to plasmons and a part due to electron-hole pair excitation. Here, we follow a similar approach to study transient screening effects in a 2D electron gas. The study of 2D systems is relevant in connection to the properties of thin films and surfaces. More precisely, quasi-2D systems are realized in the cases of electrons on the surface of liquid helium, electrons at the interfaces of semiconductor heterojunctions, image states at metal surfaces and layered materials. Concerning our study of screening transients in a 2D electron gas, an interesting feature is the different nature of the plasmon mode as compared to that of the 3D case. In the latter, the plasmon frequency tends to a constant value \( \omega_0 \) with \( \omega_0^3 = 4\pi n \) (\( n \) is the electronic density of the 3D system) in the small wave vector limit and, as a consequence, \( 2\pi/\omega_0 \) represents a characteristic timescale of the system [9,10]. In a typical metal such as Al this time is of the order of 0.1 fs. In this respect, it is worth to mention that for the evolution of the image potential when a charged particle is suddenly created in front of a metal surface this role is played by the surface plasmon frequency \( \omega_0/\sqrt{2} \) [11]. On the contrary, for a 2D electron gas, the plasmon frequency goes to zero in the small wave vector limit and shows a stronger dispersion. These properties make difficult to assign a unique frequency in order to characterize the response of the 2D system to an external perturbation. Due to this, qualitative differences between the 2D and the 3D electron gas are found.

Our study has application in problems in which a charge is created in a polarizable medium that can be approximated by a 2D electron gas, on a timescale much shorter than the characteristic screening times obtained here. In this respect, recent experiments performed for atomic coverage adlayers on semiconductors have revealed the 2D collective excitations of the overlayers [12,13]. The response of a well-defined surface state band that is not strongly coupled to the bulk modes, such as the surface state at the Be(0001) surface [14], is also characterized by its 2D nature. In all these systems, processes such as the creation of an inner-shell hole in an adsorbate located at these surfaces, or the excitation of an electron from an image or a surface state will induce the 2D-like response of the electrons in the medium, trying to screen the external charge created. In these cases, a natural question arising in view of the recent development of time-resolved techniques is which time resolution is needed to probe the transient regime or under which conditions this transient behaviour can be neglected.

The paper is organized as follows. In Section 2 we explain the theoretical model to calculate the induced density when a charge is suddenly created in a 2D electron gas. In Section 3 a comparative analysis of the transients effects occurring during the screening process in a 2D and in a 3D electron gas is presented. Our concluding remarks are summarized in Section 4. In order to avoid an extensive use of variables, we indistinctly refer to the space and wave vectors for the 2D and the 3D cases as \( r \) and \( q \), although the meaning is obviously different. Atomic units (a.u.) are used unless it is otherwise stated. In this system, the unit of time corresponds to \( 2.42 \times 10^{-2} \) fs, the unit of energy to \( 27.21 \) eV, and the unit of density to \( 3.57 \times 10^{16} \) cm\(^{-2}\) in the 2D case and to \( 6.75 \times 10^{24} \) cm\(^{-3}\) in the 3D case.

2. Model

Let us consider that a charge \( Z_1 \) is suddenly created in a 2D electron gas at time \( t = 0 \). The impurity charge density is \( \rho_{\text{ext}} = Z_1 \delta(r) \theta(t) \), where \( \theta(t) \) is the Heaviside function. Our purpose is to model, using linear response theory (LRT), the evolution in time of the charge density fluctuation.
induced by the impurity charge. Linear response theory fails in reproducing quantitatively key features such as the absolute values of the induced density at the origin and the presence of a bound state for any positive charge in 2D [15]. Nevertheless, in 3D comparison between recent nonlinear calculations [10] and the linear results of [9] shows that the time evolution of transients is well reproduced by LRT. The reason for this is that LRT describes correctly the plasmon frequency which defines the characteristic timescale for transients. Since the same is true in 2D, our results for the time evolution are meaningful, though they are presumably more reliable for negative charges due to the problems that may be associated with the presence of the bound state.

In LRT the potential induced by an external charge \( \rho_{\text{ext}} \) can be easily obtained in Fourier space as

\[
\phi_{\text{ind}}(q, \omega) = \rho_{\text{ext}}(q, \omega) \frac{2\pi}{q} \left[ \frac{1}{\varepsilon_{\text{2D}}(q, \omega)} - 1 \right],
\]

where \( \varepsilon_{\text{2D}}(q, \omega) \) is the dielectric response function of the 2D electron gas; the Coulomb potential is \( v_c(q) = 2\pi/q \), and the Fourier transform of the suddenly created external charge density is

\[
\rho_{\text{ext}}(q, \omega) = \frac{iZ_1}{\omega + i\eta},
\]

with \( \eta \) a positive infinitesimal. The induced density is obtained as \( \rho_{\text{ind}}(q, \omega) = \phi_{\text{ind}}(q, \omega)/v_c(q) \). Hence,

\[
\rho_{\text{ind}}(q, \omega) = \rho_{\text{ext}}(q, \omega) \left[ \frac{1}{\varepsilon_{\text{2D}}(q, \omega)} - 1 \right].
\]

In order to describe in real space, the time evolution of the induced density, we just substitute Eq. (2) in Eq. (3) and take the inverse Fourier transform of it. Thus, after some manipulation one gets

\[
\rho_{\text{ind}}(r, t) = \frac{Z_1}{2\pi^2} \int_0^\infty dq q J_0(qr)
\]

\[
\times \int_{-\infty}^{\infty} \frac{d\omega}{\omega} \times \text{Im}\left\{ \frac{1}{\varepsilon_{\text{2D}}(q, \omega)} \right\}
\]

\[
\times [1 - \cos(\omega t)] \theta(t),
\]

where \( J_0(x) \) is the Bessel function of order zero. In deriving this final equation, we follow the same procedure applied by Canright to the 3D problem [9]. Briefly, the differences in the analytical expressions of the charge density induced in a 2D electron gas and in a 3D electron gas are the following. The dependence on space is given by the Bessel function \( J_0(qr) \) in the former and by a \([\sin(qr)])/r \) term in the latter. In both cases, the result is an oscillatory behaviour with the distance to the external charge. Formally, the time dependence is ruled in both systems by the same oscillatory term \([1 - \cos(\omega t)]\), which multiplies the corresponding spectral function, \( \text{Im}\{1/\varepsilon_{\text{2D,3D}}(q, \omega)\}\).

In this work, we use the dielectric response function derived by Stern [16] in the random-phase approximation (RPA), \( \varepsilon_{\text{RPA}}^{\text{2D}} \). In this approach, the excitations contributing to the spectral function \( \text{Im}\{1/\varepsilon_{\text{RPA}}^{\text{2D}}\} \) include two kinds of processes, single particle or electron-hole (e-h) pair creation and collective or plasmon excitation. On the one hand, the e-h pair formation occurs for those \((q, \omega)\)-values at which \( \text{Im}\{\varepsilon_{\text{2D}}(q, \omega)\} \neq 0 \). For \( \omega > 0 \), that condition is verified in the region limited by the curves \( \omega = -q q_F + q^2/2 \) and \( \omega = q q_F + q^2/2 \), where \( q_F = (2\pi n)^{1/2} \) is the Fermi wave vector for a 2D electron gas with electronic density \( n \). On the other hand, a plasmon excitation is characterized by the condition \( \varepsilon_{\text{2D}}(q, \omega) = 0 \), which defines a single curve \( \omega_p(q) \) in the \((q, \omega)\)-plane. The spectrum of excitations is plotted in Fig. 1(a) for a 2D electron gas with \( r_s = 2 \) (defined as \( n = 1/(\pi r_s^2) \)). The shadow region corresponds to e-h pair excitations and the curve \( \omega_p(q) \) accounts for the plasmon excitation. For comparison, Fig. 1(b) shows the spectrum of excitations obtained in the RPA for a 3D electron gas with \( r_s = 2 \) [now defined as \( n = 3/(4\pi r_s^3) \)]. Here, the plasmon excitation takes place along the curve \( \omega_p(q) \), whereas the shadow region limited by the curves \( \omega = -q q_F + q^2/2 \) and \( \omega = q q_F + q^2/2 \) indicates the e-h pair contribution \((q_F = (3\pi^2 n)^{1/3} \) is the Fermi wave vector in a 3D electron gas). The plasmon curves show a different behaviour in both systems. In a 3D electron gas, the plasmon mode takes a finite value \( \omega_0^2 = 4\pi n \) at \( q = 0 \) and shows a smooth dispersion given by

\[
\omega_p^2 \simeq \omega_0^2 + 3/5 q_F^2 q^2.
\]
In the 2D case however, the plasmon frequency behaves as
\[ \omega_p^2 \approx q^2 \] for small values of \( q \)
and as
\[ \omega_p^2 \approx q^2 + \frac{3}{4}q^2 \] for larger values of \( q \).

There are two distinctive features for the 2D-plasmon frequency as compared to the 3D one: \( \omega_p \) is zero for \( q = 0 \) and the \( q \)-dispersion is stronger.

Let us make a final comment on the expression we derived for the induced density in Eq. (4). In the limit \( t \to \infty \), since the \( \cos(\omega t) \) term integrates to zero, the \( \omega \)-integral can be analytically evaluated using the Kramers–Kroning relations. Hence, one gets

\[
\rho_{\text{ind}}(r) = \frac{Z_1}{2\pi} \int_0^\infty dq q J_0(qr) \text{Re}\left\{ \frac{1}{\epsilon_{2\text{D}}(q,0)} - 1 \right\},
\]  

which correspond to the stationary expression for the density induced by an external charge density \( \rho_{\text{ext}}(r) = Z_1 \delta(r) \). We checked that the results obtained by omitting the cosine term in Eq. (4) reproduce well those obtained with Eq. (5). Notice, however, that in order to achieve this agreement it was necessary to use the exact \( \omega_p(q) \) instead of the analytical approximations.

3. Results and discussion

In this section we show results for an external charge created in an electron gas with \( r_s = 2 \). Calculations were also carried out for different metallic densities (\( r_s = 3, 4 \)). In general, we observe that for lower densities, the response of the medium to screen the external impurity is slower. Except for this fact, the comparative analysis between the 2D and the 3D electron gas presented in this section can be qualitatively generalized to those densities.

In Fig. 2 we plot the electronic density \( n_{\text{ind}}(t) \) induced at the position of the suddenly created charge as a function of time \( t \) for a 2D (Fig. 2(a), upper panel) and a 3D (Fig. 2(b), lower panel) electron gas. Since the spectral functions \( \text{Im}\{1/\epsilon_{2\text{D.3D}}(\omega)\} \) consist of a continuum part (e-h pair) and a plasmon mode, we calculate the induced density as \( \rho_{\text{ind}} = \rho_{\text{ch}} + \rho_{\text{pl}} \), where \( \rho_{\text{ch}} \) and \( \rho_{\text{pl}} \) take into account the contribution to the screening process coming from e-h and plasmon excitation, respectively. Accordingly in Fig. 2, \( n_{\text{ind}} \) (bold-solid line) is the sum of \( n_{\text{ch}} \) (long-dashed line) and \( n_{\text{pl}} \) (dotted line). The stationary value (\( t \to \infty \)) is indicated by a thin-solid line. As it may be seen from the figure, \( n_{\text{ind}}(0,t) \) is dominated by the e-h part that rises quite fast within the first 2–3 a.u. of time. This behaviour is observed for both the 2D and the 3D medium. Nevertheless, an important difference arises between both cases. Whereas in a 2D electron gas \( n_{\text{ind}} \) reaches the stationary value at \( t \approx 8–9 \) a.u., in the 3D case \( n_{\text{ind}} \) oscillates around its stationary value even for the longest time.
shown in the figure. Comparison between Fig. 2(a) and (b) reveals that the origin of this discrepancy is, precisely, the different time dependence of \( n_{pl} \). As it was already pointed out by Canright for a 3D electron gas [9], the long-term transient is provided by the plasmon part. The existence of a quite well-defined frequency at which the spectral function takes the highest values gives rise to the oscillatory behaviour with frequency \( \omega_{pl} \). The absence of this oscillatory term at long times in the 2D case is thus related to the special character of the 2D plasmon mode. The two features remarked in the previous section make difficult to find a unique characteristic frequency as in the 3D case. As a consequence, its contribution to the induced density at \( r = 0 \) is very different from the 3D result, and does not show an oscillatory behaviour.

In Fig. 3, we show the interpolated images of the radial densities, i.e., \( 2\pi r n_{ind}(r,t) \) in 2D (Fig. 3(a)) and \( 4\pi r^2 n_{ind}(r,t) \) in 3D (Fig. 3(b)). The corresponding stationary limit is represented on the right part of each panel. We observe the Friedel oscillations appearing in both stationary limits that scale as \( \sin(q_F r)/r \) for \( r \to \infty \). The images provide a valuable information on the propagation of the response of the medium to an external perturbation. In view of these figures, the evolution in time of the screening process can be described in two steps: the switching on process or propagation of the shock-wave along the medium and the stabilization to the steady behaviour. We define the switching on process at a given distance as the interval going from the arrival of the first perturbation up to the instant at which the induced density reaches its highest value. This wave-front can be easily identified in each image as the first band growing upwards from the left-bottom corner of the figure.

Considering this switching on process, we find similarities between the 2D and the 3D cases. The wave-front is characterized by strong variations of the induced density that achieves values much larger than those of its steady-state limit. The propagation velocity can be roughly estimated from the slope of the wave-front as \( v \sim (1 - 2) v_F \) (\( v_F \) is the Fermi velocity in each case). Main differences appear in the transition to the stationary value. In the 2D case, the screening transients last roughly the passage of this wave-front. As a consequence, after a limited short-time interval since the arrival of the initial perturbation (\( \Delta t \sim 8 - 10 \) a.u.), the steady-state value is basically reached. Furthermore, the transient regime does not show any oscillatory behaviour. Note that after 20 a.u. of time the stationary regime has been achieved for all the distances shown in the figure. On the contrary, in the 3D case the screening transients last for very long times. After the passage of the first wave-front the radial density continues oscillating around its steady-state value.

In order to get information on the efficiency of the medium to screen the external charge, we also...
calculate the integrated screening density $Q(R, t)$, defined in 2D as
\[
Q_{2D}(R, t) = \int_0^R dr 2\pi r n_{\text{ind}}(r, t),
\] (6)

and in 3D as
\[
Q_{3D}(R, t) = \int_0^R dr 4\pi r^2 n_{\text{ind}}(r, t). \tag{7}
\]

This quantity shows the range of distances in which the external charge is basically screened, i.e. the value of $R$ at which $Q(R) \sim 1$. Therefore, the study of its evolution in time allows us to extract the time needed by the system to efficiently screen the external charge.

In Fig. 4 we compare the time evolution of $Q(R)$ with the steady-state limit (bold-solid lines) in the 2D electron gas (left panels) and in the 3D electron gas (right panels). The value $Q(R) = 1$, i.e., the value of the external charge to be screened, is indicated by a thin-solid line. Lower plots show the evolution of $Q(R)$ at short times, when the switching on process is taking place in the region close to the external charge. In both systems, the dressing mechanism evolves from the incomplete screening at the beginning of the process ($t = 1–2$ a.u.) to overscreening phases around $t = 3–5$ a.u.

In the upper plots, we show the evolution of $Q(R)$ at longer times, i.e., during the stabilization period. The differences observed between the 2D and the 3D radial densities are also reproduced here. In 3D, $Q(R, t)$ strongly oscillates around the stationary value with a slowly decreasing amplitude. Note that for the longest time shown in the figure ($t = 25$ a.u.) the steady value has only been achieved up to $R = 5$ a.u. On the contrary, in 2D this transition to the stationary regime is smoother, and no strong oscillations are observed.

In the important region close to the external charge ($R < 10$ a.u.), the dressing process is already completed after the first 16–20 a.u. (0.4–0.5 fs).

4. Conclusion

In summary, we have studied using linear response theory the screening transients when a charge is suddenly created in a 2D electron gas. Perturbations in the medium propagate with a velocity of the order of $(1 - 2)\nu_F$. The steady-state is achieved after the passage of the first wave-front. For $r_s = 2$, in the important region close to
the external charge, the stationary regime is basically reached after the first 0.4–0.5 fs. This behaviour is very different from the 3D case in which the screening transients, characterized by strong oscillations of the induced density, last for much longer times. The differences between the two behaviours are due to the different nature of the 2D and 3D plasmons in the long wavelength limit.

Finally, in connection with the experimental situations mentioned in the introduction (creation of holes in inner-shells of adsorbates and excitation of electrons from image and surface states) our results show that, in principle, one should expect a reduced importance of screening transients compared to the bulk situation. Nevertheless, we also point out that the actual duration of transients will increase for lower values of the surface electronic density.

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