Collective electron excitations on a two-dimensional lattice

A. Latgé and J. d'Albuquerque e Castro
Instituto de Física, Universidade Federal Fluminense, Niteroi, 24020 Rio de Janeiro, Brazil
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The frequency and wave-vector-dependent dielectric function $\varepsilon(\mathbf{q},\omega)$ of a two-dimensional electron system on a square lattice is calculated within the random-phase approximation. Effects of the periodic potential on the electronic structure and dielectric properties are taken into account within the framework of the tight-binding model. Both the dispersion relation of long-wavelength plasmons and the energy-loss function $\mathrm{Im}[1/\varepsilon(\mathbf{q},\omega)]$ are numerically obtained for different values of the electronic concentration n_s. For low values of n_s, results are well described by the effective-mass approximation. As n_s increases, the Fermi level moves to regions in $\mathbf{k}$ space where the band structure strongly deviates from that of free electrons, and the appearance of structures in the energy-loss spectrum can be observed. Regarding plasmon excitations it is found that for all values of n_s the long-wavelength behavior of the plasma frequency $\omega_p(\mathbf{q})$ can be described by a two-dimensional free-electron model provided a renormalized value of the electronic effective mass is introduced.

Artificial semiconductor structures such as superlattices, quantum wells (single and multiple), quantum-well wires, and quantum dots have been intensively studied in the last two decades. Progress in this area has been possible because of the development of sophisticated techniques of material growth and characterization. The remarkable feature of those systems is the possibility of effectively confining electrons and holes to space regions of reduced dimensionality, which gives rise to a number of very interesting physical phenomena.[1]

The electronic structure of a system is largely determined by space dimensionality. As a consequence, the electronic properties of low-dimensional systems can be quite distinct of those of ordinary three-dimensional materials. One example is the dielectric response function of the system, in terms of which a number of problems such as the response to externally applied electric fields and the spectrum of plasmon excitations can be discussed. Regarding the latter, the dispersion relation of long-wavelength plasmon modes of an interacting free-electron gas in three dimensions exhibits a gap, whereas that for interacting free electrons confined to two dimensions behaves as the square root of the wave vector q (Ref. 2).

Recently, considerable interest has been concentrated in the study of spatially modulated two-dimensional (2D) electron gas. Such a system can be found in microstructured field-effect devices fabricated using high-resolution lithography.[3] The gate potential modulates the 2D electronic density along one direction in the plane, giving rise to a lateral confinement of the gas. Depending on the intensity of the gate voltage, a crossover from a 2D system to a regular arrangement of quantum wires can be observed.[3] Another interesting case is that of a two-dimensional arrangement of quantum dots.[4] In such a heterostructure, electrons are strongly confined to the quasizero dimension. Nevertheless, transport through the discrete spectrum of states has been observed, indicating the existence of resonant tunneling between quantum-dot quasibound states.

Spatial modulation of the electronic density strongly affects the excitation spectra of 2D systems. In the past few years a number of papers has appeared in the literature dealing with the problem of plasmon excitations in such systems. For the case of a planar array of quantum wires, the plasmon dispersion relation has been calculated considering electron tunneling between the wires and also in the limit of strong electron confinement.[5–8] As regards quantum-dot arrays, Que and Kirczenow[9] have considered the extreme case in which electrons are entirely confined within the dots, whereas Huang and coworkers[10,11] have discussed the cases in which electrons can tunnel between dots along only one direction and in two perpendicular directions in the plane.

A convenient framework for studying the electronic properties of modulated 2D systems is provided by the tight-binding model for electrons in a two-dimensional lattice. The limit of a regular array of isolated quantum dots is readily obtained by setting the hopping between the lattice points equal to zero. On the other hand, as the tight-binding bands are broadened, i.e., as the hopping parameters increase, the case of uniform 2D gas is approached. By using different values for the hopping parameters along perpendicular directions, the situation corresponding to a regular array of quantum wires can also be reproduced.

In the present work, we are concerned with the calculation of the dielectric response function of an electronic system on a 2D lattice described by the tight-binding model. We consider only intraband electron excitations and restrict our discussion to the one-band model. For simplicity, we assume a square lattice and keep hoppings only between nearest-neighbor sites. Our purpose is to investigate the dispersion relation of long-wavelength plasmons and the energy-loss function in the region of independent electron-hole pair excitations for different values of the 2D electronic density n_s.

The response of a system to an external potential $\varphi_{\mathrm{ext}}(\mathbf{q},\omega)$ is given by the dielectric response function

$[\varepsilon(\mathbf{q},\omega)]^{-1}$, which is related to the polarizability tensor $\Pi(\mathbf{q},\omega)$ by the equation

$$\varepsilon(\mathbf{q},\omega)=1-v(\mathbf{q})\pi(\mathbf{q},\omega)\ . \tag{1}$$

Here $\mathbf{q}$ is a vector in the x-y plane, $v(\mathbf{q})=2\pi e^2/\varepsilon_0 q$ is the 2D Fourier transform of the interacting potential, and ε_0 is the background dielectric constant. Within the random-phase approximation (RPA),[12,13] the polarizability can be calculated in terms of the one-electron wave functions and energies. On calculating $\pi(\mathbf{q},\omega)$, we follow Ehrenreich and Cohen[13] and neglect local-field corrections and hence umklapp processes. Such a procedure is valid in the present case, in which we are considering intraband electron excitations only and restricting our calculation to the long-wavelength regime $q\rightarrow 0$ (Ref. 8). Thus we get

$$\varepsilon(\mathbf{q},\omega)=1-\frac{2\pi e^2}{q\varepsilon_0}\sum_{\mathbf{k}}\frac{f_{\mathbf{k}+\mathbf{q}}-f_{\mathbf{k}}}{E_{\mathbf{k}+\mathbf{q}}-E_{\mathbf{k}}-\hbar\omega^+}\ , \tag{2}$$

where $E_{\mathbf{k}}$ is the single-particle energy, $\omega^+=\omega+i\eta$ ($\eta=0^+$), $f_{\mathbf{k}}$ is the Fermi distribution, and $\mathbf{k}$ runs over the 2D Brillouin zone (BZ). Here we consider the system in its ground state ($T=0$). The dispersion relation $E_{\mathbf{k}}$ for a square lattice is given by

$$E_{\mathbf{k}}=E_s-2t[\cos(k_x a)+\cos(k_y a)]\ , \tag{3}$$

where E_s corresponds to an s-type atomic-orbital energy, k_x and k_y are the components of the 2D wave vector $\mathbf{k}$, a is the lattice parameter, and t is the two-center hopping integral.

The difficulty in evaluating the sum over $\mathbf{k}$ in Eq. (2) resides in the fact that for small q values the region in k space contributing to the sum becomes very small due to the Fermi factors in the numerator. Therefore a very fine mesh in the BZ is necessary in order to achieve convergence. In addition, for a finite q the integrand does not have the symmetry of the BZ, so that sum cannot be restricted to the irreduceable wedge of the zone. In this paper, the summation over the wave vector k was performed using Cunninghan's[14] special points. In our calculations we have generated up to 10^9 points in the BZ. However, depending on the value of q, only a few thousand of them contribute to the sum.

Our results are presented for $\mathbf{q}$ along the x direction. We have calculated the energy-loss function $\mathrm{Im}[1/\varepsilon(\mathbf{q},w)]$ as a function of ω for different $\mathbf{q}$ values. By determining the position of the poles of $1/\varepsilon$ in the (q,ω) plane, we were able to obtain the plasmon dispersion relation $\omega_p(\mathbf{q})$.

Figure 1 shows the plasmon dispersion relation as a function of the wave vector $\mathbf{q}=(q,0)(2\pi/q)$ for different values of the number of electrons per site n_s. Each value of n_s corresponds to distinct positions of the Fermi energy within the band. All results are presented in reduced atomic units (a.u.*), which correspond to a length unit of an effective Bohr radius $a_B^*=\hbar^2\varepsilon_0/(m^*e^2)$ and an energy unit of an effective Rydberg $\mathrm{Ry}^*=e^2/(2\varepsilon_0 a_B^*)$. The value of the hopping parameter t was chosen so that $m^*=\hbar^2/\nabla^2 E_{\mathbf{k}}$ calculated at $k=0$ is equal to the GaAs bulk effective mass. We find that in the long-wavelength limit all curves behave as $\alpha q^{1/2}$, where α is a prefactor depending on n_s. Such behavior is characteristic of a two-dimensional free-electron gas, the case in which the dependence of α on n_s is given by[2]

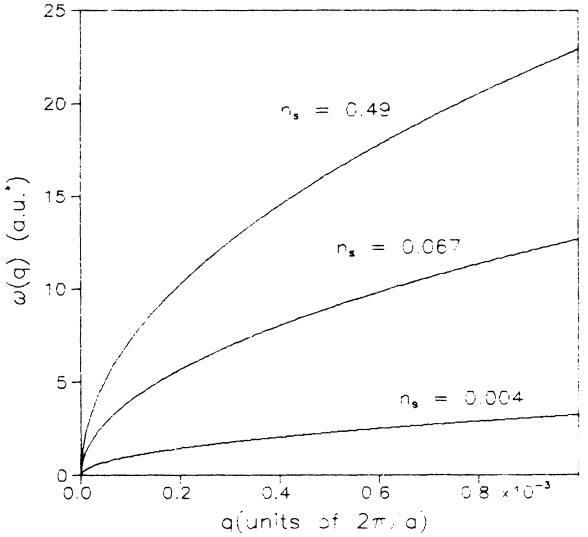

FIG. 1. The plasmon dispersion relation as a function of the wave vector $\mathbf{q}=(q,0)$, for three electronic surface densities, namely $n_s=0.49$, 0.067, and 0.004.

$$\alpha(n_s)=\left[\frac{2\pi e^2 n_s}{\varepsilon_0}\right]^{1/2}\left[\frac{1}{m^*}\right]\ . \tag{4}$$

We observe that for values $n_s \ll 1$ the relation between α and n_s is well described by Eq. (4). However, as n_s in-

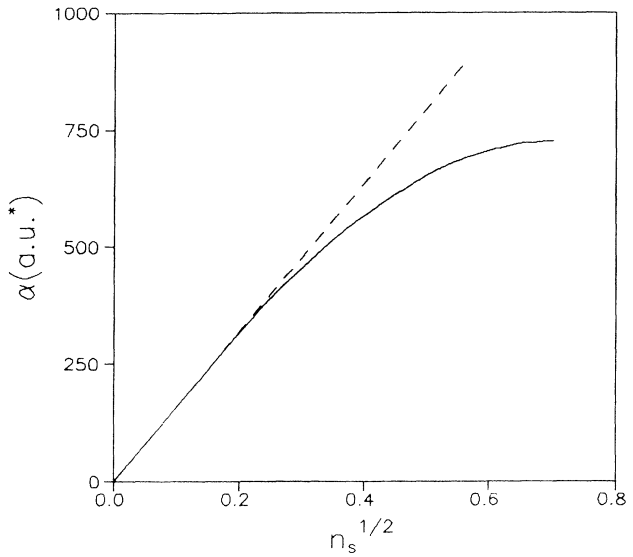

FIG. 2. The coefficient α, in effective atomic units, as a function of the electronic density n_s for two-dimensional systems described by the tight-binding (solid line) and free-electron-gas (dashed line) models.

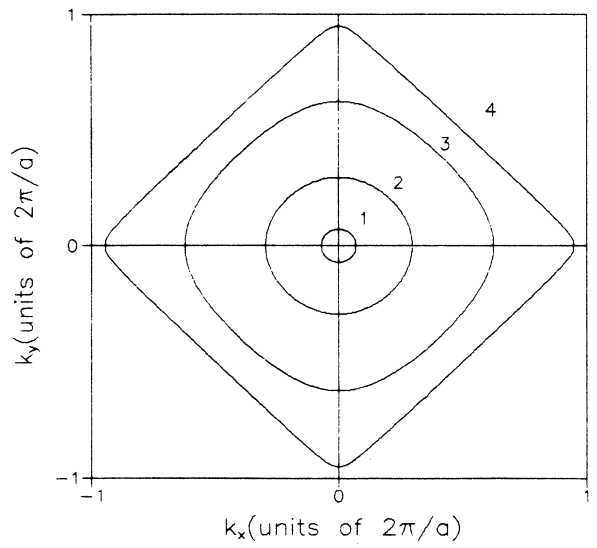

FIG. 3. Fermi surfaces for different electronic densities $n_s = 0.004$ (1), 0.067 (2), 0.27 (3), and 0.49 (4).

creases and the situation of a half-filled band is approached, the dependence of α on n_s deviates significantly from that in Eq. (4). This is clearly shown in Fig. 2, which presents the coefficient α as a function of $n_s^{1/2}$ in the range $0 \leq n_s \leq 0.5$. The dashed line corresponds to the 2D free-electron behavior.

The origin of such a deviation can be understood in terms of the tight-binding band structure underlying the present calculation. In fact, in the limit of $q \rightarrow 0$ it can be shown that the polarizability $\Pi(\mathbf{q},\omega)$ depends on some average value of $1/[(\hat{\mathbf{q}}\cdot\nabla)^2 E_{\mathbf{k}}]$ over the Fermi surface, where $\hat{\mathbf{q}} = \mathbf{q}/|\mathbf{q}|$. For small values of n_s the occupied states lay near the center of the BZ, where the band structure is approximately parabolic and the Fermi surface is isotropic. Thus the polarizability is well described by that of free electrons with effective mass m^*. However, as n_s increases the Fermi level moves to regions in $\mathbf{k}$ space where $E_{\mathbf{k}}$ strongly deviates from the parabolic behavior, which is reflected in the shape of the Fermi surface (cf. Fig. 3). Despite that, we still find ω_p depending on $q^{1/2}$ in the limit of $q \rightarrow 0$, which allows us to introduce the concept of a renormalized effective mass associated with the dispersion relation of long-wavelength plasmons and given by the expression

$$m_p^* = \left[\frac{2\pi e^2 n_s}{\varepsilon_0}\right]^{1/2} (\alpha(n_s))^{-1} . \tag{5}$$

The ratio m_p^*/m^* gives us a measure of the effects of the

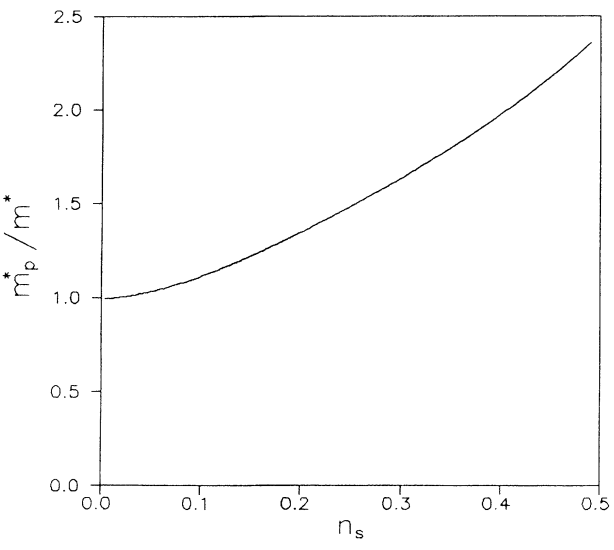

FIG. 4. The ratio between the renormalized effective mass m_p^* and the effective mass m^* as a function of the electronic density n_s.

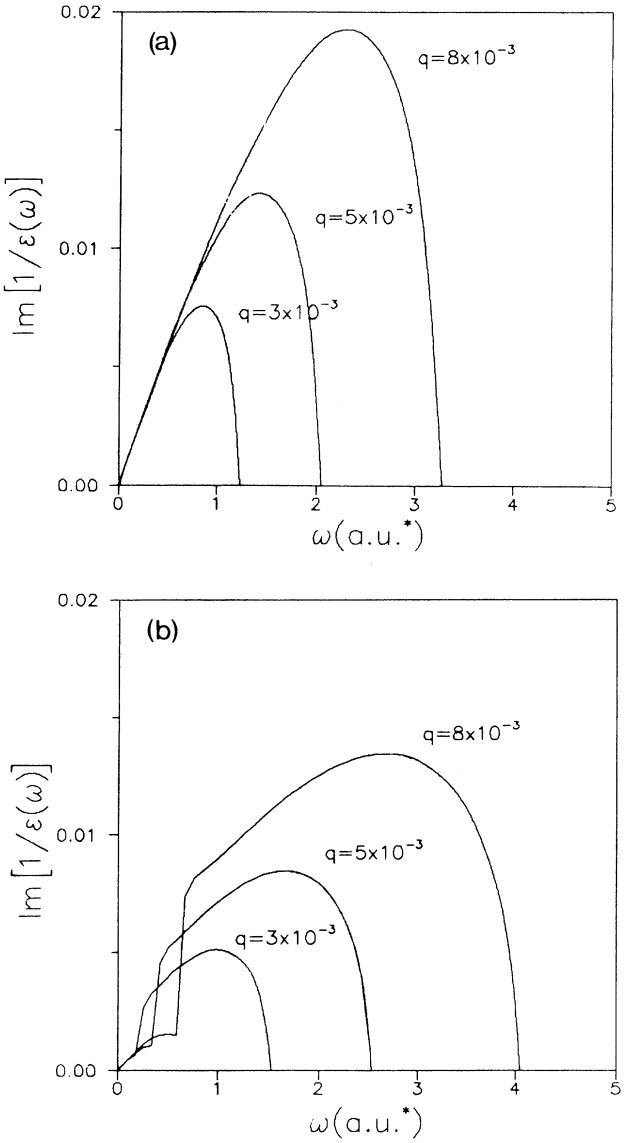

FIG. 5. The energy-loss function $\mathrm{Im}(1/\varepsilon(\mathbf{q},\omega))$ vs ω in the energy range of independent quasiparticle excitations, for different values of the wave vector q (in units of $2\pi/a$) in the x direction, and for electron densities $n_s = 0.067$ (a) and 0.49 (b).

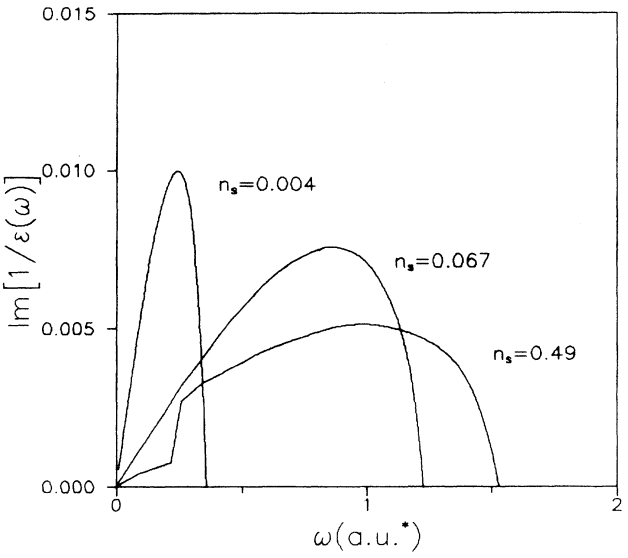

FIG. 6. The energy-loss function $\mathrm{Im}(1/\varepsilon(\mathbf{q},\omega)$ vs ω in the energy range of independent quasiparticle excitations, for $\mathbf{q}=(3\times10^{-3},0)(2\pi/a)$ and electron concentrations $n_s=0.004$, 0.067, and 0.49.

periodic potential on the plasmon excitations. Figure 4 shows the curve of m_p^*/m^* as a function of n_s in the region $0\leq n_s\leq 0.5$. As we can see, the change in m_p^* as the electronic density increases may be quite significant.

It is also interesting to study the energy-loss spectrum in the energy range of independent quasiparticle excitations. We investigate the dependence in energy of $\mathrm{Im}[1/\varepsilon(\mathbf{q},\omega)]$ for fixed values of n_s and q. In Figs. 5(a) and 5(b), we present results for values of n_s corresponding to the cases of the nearly empty band ($n_s=0.067$) and the nearly half-filled band ($n_s=0.49$), respectively. In each case three values of the q vector are considered, all in the long-wavelength limit. The curves for $n_s=0.067$ are smooth and have the behavior expected for a free-electron gas. However, as the electronic density increases the energy-loss spectra exhibit structures that are signatures of the departure from the parabolic dispersion relation due to the presence of the periodic potential. The change in the spectrum for a fixed q value with increasing n_s can be clearly seen in Fig. 6. Besides the broadening of the spectrum due to the increase of the effective Fermi wave vector, we can notice the appearance of a steplike structure in the lower-frequency region as n_s approaches the value 0.5 (the half-filled band).

Summing up, we have calculated the frequency- and wave-vector-dependent dielectric function of a two-dimensional electron system on a square lattice, taking into account the lattice periodic potential within the framework of a tight-binding model. Only intraband electron excitations are considered and calculations are restricted to the long-wavelength regime. We have found that significant deviation in the dielectric response of the system from that of free electrons may occur depending on the electronic density. For values of n_s such that the Fermi level lays near the bottom of the band, the response of the system is well described by a two-dimensional free-electron model. However, as the electronic density increases, the Fermi surface becomes anisotropic and the response of the system is markedly altered by the periodic potential, even in the small-q regime. These conclusions, although derived on the basis of a simple model, will certainly remain true in the long-wavelength regime when more complex situations (e.g., band degenerancy) are considered. In view of the potential device applications of two-dimensional structures and the interest in a proper understanding of their dielectric properties, we believe the present work represents a relevant contribution toward the understanding of the main features of the dielectric response of such systems.

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