Far-IR absorption of short-period quantum wires and the transition from one to two dimensions

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(Received 27 May 1997)

We investigate the far-IR absorption of short-period parallel quantum wires in a perpendicular quantizing magnetic field. The external time-dependent electric field is linearly polarized along the wire modulation. The mutual Coulomb interaction of the electrons is treated self-consistently in the ground state and in the absorption calculation within the Hartree approximation. We consider the effects of a metal gate grating coupler, with the same or with a different period as the wire modulation, on the absorption. The evolution of the magnetoplasmon in the nonlocal region where it is split into several Bernstein modes is discussed in the transition from narrow to broad wires and isolated to overlapping wires. We show that in the case of narrow and not strongly modulated wires the absorption can be directly correlated with the underlying electronic band structure. [S0163-1829(98)11203-1]

I. INTRODUCTION

Parallel quantum wires can be produced in $Al_xGa_{1-x}As$-GaAs heterostructures by a periodically modulated metal gate on top of the $Al_xGa_{1-x}As$ insulator. By applying a voltage bias between the gate and the two-dimensional electron gas (2DEG) at the insulator-semiconductor interface the properties of a 2DEG can be studied in the entire range from a homogeneous system to isolated wires.

The theory of far-infrared (FIR) absorption of the *homogeneous* 2DEG in the presence of the metal gate acting as a *grating coupler* has been developed by Zheng, Schaich, and MacDonald[1] and Liu and Das Sarma.[2] In those papers the FIR response has been calculated semiclassically, allowing the presence of a weak magnetic field. The FIR absorption of a *modulated* system, for instance due to the presence of a gate potential, has been extensively studied experimentally for a simple unidirectional modulation[3] and calculated self-consistently for a sinusoidal potential and strong magnetic fields.[4,5] Modes specific to more structured modulation such as parallel pairs of wires have been identified as well.[6]

The well-known magnetoplasmon dispersion law for a homogeneous 2DEG with density ρ_0 in a strong magnetic field is

$$\omega^2=\omega_c^2+2\pi\rho_0 e^2 q/\kappa m, \tag{1.1}$$

which is valid in the lowest order in the wave vector q, i.e., as long as the second term is much smaller than the first one. For shorter wavelengths or for lower magnetic fields the magnetoplasma oscillations have higher branches, around harmonics of the cyclotron frequency $n\omega_c$, $n=2,3,\ldots$, known as Bernstein modes.[7] The Bernstein modes are likewise known in single wires and dots.[8,9]

In this paper we want to focus our attention on the FIR absorption of a periodically modulated 2DEG in a perpendicular quantizing magnetic field, in the regime where the Bernstein modes are a prominent feature of the frequency dispersion. Furthermore, we take into account the grating coupler effects of the metal gate on the incident FIR radiation.[10,11] The external time-dependent electric field is hence modulated with a large wave vector, the lowest inverse lattice vector of the gate structure. This is an approximation to the leading order compared to the studies of the grating coupler effects mentioned above.[1,2] In principle, the 2DEG can be modulated by an independent method, i.e., not by the gate structure.

We calculate the FIR absorption fully quantum mechanically with the help of the inverse dielectric function. The mutual Coulomb interaction of the electrons is treated within the Hartree approximation both in the ground state and in the absorption calculation, i.e., the absorption is obtained in the framework of the random-phase approximation. The intra- or interwire Coulomb interactions thus enter the model on equal footing.

We show that as the width of the wires is reduced the resulting Landau band structure can be identified through the effects of its van Hove singularities (VHS) on the FIR absorption. The evolution of the FIR absorption is traced from the case of weakly coupled wires to the case of a weakly modulated 2DEG by increasing the electron density but keeping the modulation strength constant. We systematically use the induced density to sort out the complex hierarchy of absorption modes caused by the modulation of the electron gas or by the electric coupling between wires.

II. MODEL

We consider a modulated 2DEG located in the plane $\mathbf{r}=(x,y)$ and describe it with the Hamiltonian

$$H=H_0+V_{\rm mod}+V_H. \tag{2.1}$$

$H_0=(\mathbf{P}+e\mathbf{A})^2/2m$ is the Hamiltonian of the noninteracting system. We employ the Landau gauge for the vector potential $\mathbf{A}=(0,Bx)$. $V_{\rm mod}(x)=V\cos(Kx)$ is the simplest model of an electrostatic potential modulation varying in only one

direction. V_H is the Hartree potential ''felt'' by each electron, self-consistently with the particle density,

$$\rho(x)=\sum_{p\geqslant 0}\rho_p\cos(pKx), \tag{2.2}$$

$$V_H(x)=\frac{e^2}{\kappa}\int d\mathbf{r}'\,\frac{\rho(x')}{|\mathbf{r}-\mathbf{r}'|}=\frac{e^2}{\kappa}\frac{2\pi}{K}\sum_{p\geqslant 1}\frac{\rho_p}{p}\cos(pKx), \tag{2.3}$$

where κ is the dielectric constant of the semiconductor host of the 2DEG. We assume the electrical neutrality to be ensured by a uniform background of positive charges, of density $-e\rho_0$. The eigenstates of the Hamiltonian (2.1) are calculated numerically, within an iterative scheme, by successive diagonalization in the basis of the wave functions corresponding to H_0, known as Landau wave functions. The resulting single-particle energies $E_{n,X_0}=E_{n,X_0+a}$, $a=2\pi/K$, have a one-dimensional periodic band structure, where $n=0,1,2,\ldots$ is the Landau quantum number and X_0 is the center coordinate. We assume spin degeneracy. The eigenfunctions of H have the form $L^{-1/2}\exp(-iX_0y/l^2)\psi_{n,X_0}(x)$, where L is a normalization length and $l=(\hbar c/eB)^{1/2}$ is the magnetic length.

We consider a time-dependent electric field incident to the 2DEG, linearly polarized in the direction of the modulation x with only one Fourier component, of wave vector $\mathbf{q}=(q,0)$ and frequency ω. This field is supposed to be sufficiently small, within the linear-response regime. We denote by $\phi_{\rm ext}(q,\omega)$ the associated electric potential.

In order to evaluate the absorption due to plasma oscillations we need to calculate first the dielectric matrix $\varepsilon_{GG'}(q,\omega)$, where G and G' are vectors in the reciprocal space, of the form mK, $m=0,\pm1,\pm2,\ldots$. We use the random-phase approximation, as described, e.g., in the paper by Wulf *et al.*,[4] in which

$$\varepsilon_{GG'}(q,\omega)=\delta_{GG'}-\frac{2\pi e^2}{\kappa|q+G|}\chi_{GG'}(q,\omega).$$

The dielectric susceptibility $\chi_{GG'}$ is given by the Lindhard formula, which in our case reads

$$\chi_{GG'}(q,\omega)=\frac{1}{a\pi l^2}\sum_{n,n'}\int_0^a dX_0\,\frac{\mathcal{F}(E_{n,X_0})-\mathcal{F}(E_{n',X_0})}{E_{n,X_0}-E_{n',X_0}-\hbar\omega-i\eta}\times\mathcal{J}_{nn';X_0}(q+G)\mathcal{J}^*_{nn';X_0}(q+G'), \tag{2.4}$$

where $\mathcal{F}$ is the Fermi function, $\eta\to0^+$, and $\mathcal{J}_{nn';X_0}(q)=\langle\psi_{n',X_0}|e^{iqx}|\psi_{n,X_0}\rangle$.

The absorption power can be calculated from the Joule law of heating, which may be written as[12]

$$P(q,\omega)=-\frac{\omega}{4\pi}\,\mathrm{Im}\,\varepsilon^{-1}_{GG}(q_1;\omega)q|\phi_{\rm ext}(q,\omega)|^2, \tag{2.5}$$

where $q=q_1+G$. Due to the periodicity of the system $\varepsilon_{GG'}(q,\omega)=\varepsilon_{G-K,G'-K}(q+K,\omega)$ and we can take $0\leqslant q_1\leqslant K$. We will be mostly interested in the case when the wavelength of the incident field is identical to that of the modulation, as in the absorption experiments with grating-coupler devices, that is, $q=q_1=K$ and $G=0$. For simplicity, we will normalize the external potential in Eq. (2.5) such that $(1/4\pi)q|\phi_{\rm ext}(q,\omega)|^2=1$.

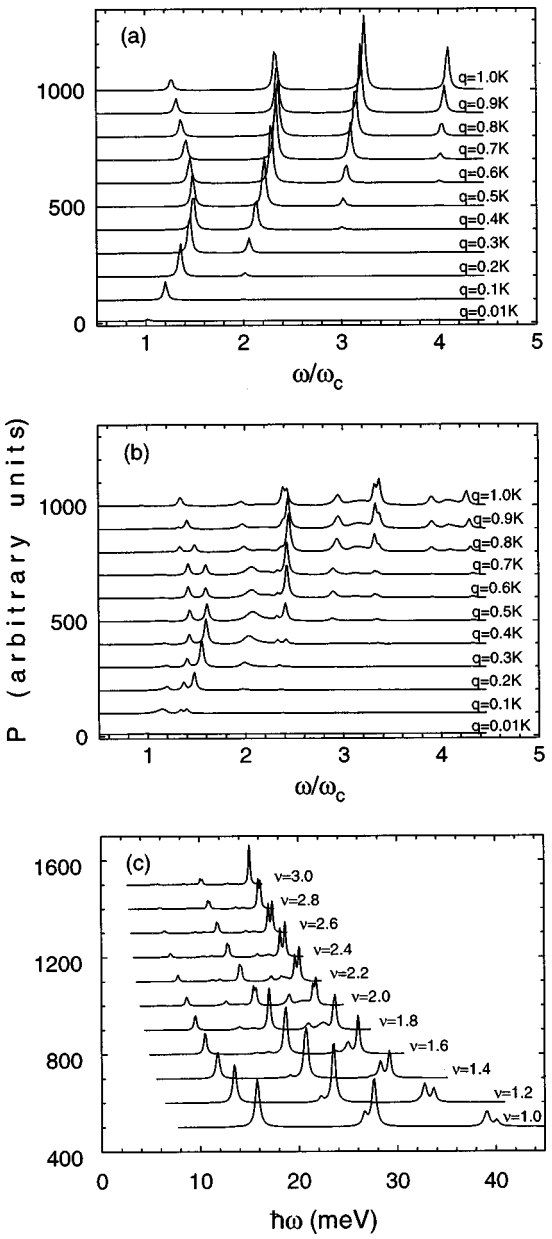

FIG. 1. (a) Absorption spectra for a homogeneous system. $K=2\pi/a$, $a=50$ nm. The filling factor is 2 and the density $\rho_0=1.8\times10^{11}$ cm^{-2}. (b) Same as (a), but with a modulation of period $a=50$ nm and amplitude $V=5$ meV. (c) Same modulation as (b), with a variable magnetic field such that the filling factor evolves between 1 and 3. $q=K$.

In order to avoid calculation of the plasma poles of the dielectric matrix, we assume a finite $\eta=\hbar\omega_c/50$ in Eq. (2.4). In other words, we assume an unspecified dissipation mechanism, which leads us directly to the oscillator strength of the collective modes and thus to measurable results.

III. RESULTS

The parameters of our model are those for GaAs: the electron mass $m=0.067m_0$ and $\kappa=12.4$. The temperature will

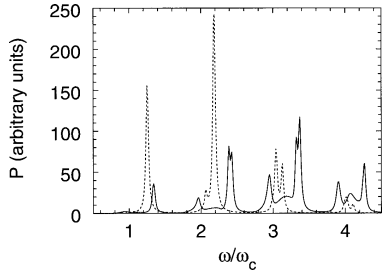

FIG. 2. Curves of Fig. 1(c) corresponding to $\nu=2$ (full line) and $\nu=1.2$ (dashed line), magnified.

be fixed to 1 K. We truncate the Fourier series such that $|mK|\leqslant MK$ and we achieve numerical convergence for $5\leqslant M\leqslant 15$.

As has been mentioned in the Introduction, the magnetoplasmon dispersion at low magnetic fields and short wavelengths splits into Bernstein modes due to the interaction with harmonics of the cyclotron resonance. In Fig. 1(a) we show the absorption power in the regime of the Bernstein modes, for the homogeneous system, for wave vectors varying from $0.01K$ to K, with $K=2\pi/a$ and $a=50$ nm. The electron density is fixed to $\rho_0=1.8\times10^{11}$ cm^{-2} and the magnetic field is $B=3.74$ T, which corresponds to the filling factor $\nu=2$. Equation (1.1) holds only for wave vectors below $q=0.2K$ for the present choice of parameters. In Fig. 1(b) we display the results for a modulated system, with a modulation period $a=50$ nm and a modulation amplitude $V=5$ meV. As we observe, each peak corresponding to a Bernstein mode splits into several subpeaks. The same modulation effect is evidenced in Fig. 1(c), where we have fixed the wave vector of the incident field $q=K$, but we sweep the magnetic field such that the filling factor varies between 1 and 3. The traces for $\nu=1.2$ and $\nu=2$ are magnified in Fig. 2. Each Bernstein mode has up to four subpeaks.

We start to analyze this complicated internal structure by showing in Fig. 3 the energy spectra corresponding to Fig. 2. The periodic Landau bands are displayed in half of a Brillouin zone, i.e., for $0\leqslant KX_0\leqslant\pi$. Due to the short period, in the absence of the Coulomb interaction the energy bands are not parallel. This is seen here only for $\nu=2$, where the Fermi level is in an energy gap and thus the screening effects are small and the energy dispersion large [Fig. 3(a)]. For $\nu=1.2$ [Fig. 3(b)] the Hartree screening reduces the energy dispersion to very narrow bands.

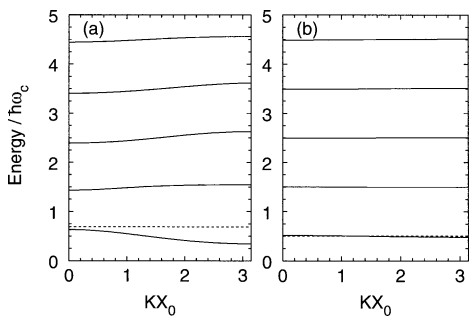

FIG. 3. Energy spectra for (a) $\nu=2$ and (b) $\nu=1.2$ in half of the Brillouin zone. The dashed horizontal lines show the Fermi level.

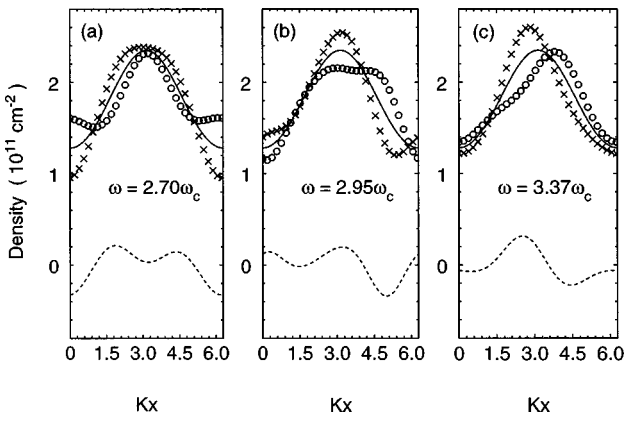

FIG. 4. Density profiles for various indicated frequencies taken from the absorption spectrum of Fig. 2, $\nu=2$. The full lines show the ground-state density, the dashed lines the maximal induced density, and the marked curves the extreme density configurations.

The absorption peaks of Fig. 2 reflect the nonparallel Landau bands or, equivalently, a certain dispersion in the center-coordinate space of the energy interval between pairs of Landau bands. This is best seen for $\nu=2$, where for each Bernstein mode we can energetically relate the lowest and the highest subpeaks to the inter-Landau-level transitions around the center and around the edges of the Brillouin zone, i.e., $X_0=0$ and $X_0=\pi/K$, respectively. The energy dispersion is locally flat in those regions or, in other words, the density of states has van Hove singularities, such that the single-particle transitions may turn into collective excitations with a slightly different energy.

For instance, for $2.8\omega_c<\omega<3.6\omega_c$, the peak at $\omega=2.95\omega_c$ corresponds to the energy interval $E_{3,0}-E_{0,0}=2.77\omega_c$, plus a blueshift determined in part by the increased energy distance between the adjacent levels, $E_{3,X_0}-E_{0,X_0}$, with, say, $0<X_0<0.5/K$, and in part by the external electric field, similarly to the second term of Eq. (1.1). The highest peaks, at $\omega=3.32\omega_c$ and $\omega=3.37\omega_c$, apart from this small splitting, can be related to the energy interval between the other pair of VHS's, $E_{3,\pi/K}-E_{0,\pi/K}=3.27\omega_c$. The small splitting of the highest mode cannot be explained only in terms of the energy spectrum. The middle peak, at $\omega=3.18\omega_c$, may be put in correspondence with the average energy interval and thus considered as a combination of the two types of VHS modes. Qualitatively, the same structure is obtained for the Bernstein modes around the other multiples of ω_c.

For $\nu=1.2$, the dashed line of Fig. 2, the states around the central VHS of the Brillouin zone become empty and the corresponding subpeaks vanish. The bands are nearly flat, due to the screening effect, but the splitting of the higher subpeaks is still present. Similar results have been obtained very recently by Brataas, Zhang, and Chao *et al.*[13] for the singularities of the imaginary part of the dielectric function of modulated systems, by analytical calculations, without the inclusion of the screening in the ground state, but also related to the nonparallel Landau bands.

In order to support the above interpretation of the Bernstein subpeaks, in Fig. 4 we show the particle density at equilibrium $\rho(x)$, the induced density $\rho_{ind}(x)$, and the ex-

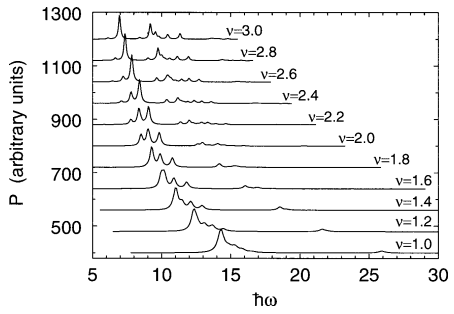

FIG. 5. Absorption spectra for a modulated system with $a=200$ nm and $V=20$ meV. The average density is $\rho_0=1.8\times10^{11}$ cm^{-2}, $q=K$.

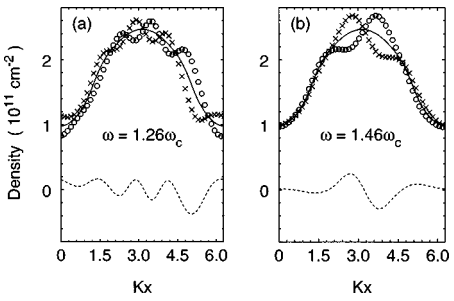

FIG. 7. Density profiles for oscillations in the absorption spectrum of Fig. 5, for $\nu=1.6$. (a) $\hbar\omega=10.2$ meV and (b) $\hbar\omega=11.8$ meV.

treme density profiles during the oscillations $\rho(x)\pm\rho_{ind}(x)$ inside a unit cell $0\leqslant x\leqslant 2\pi$ for $\nu=2$ and $q=K$. Obviously, the minima (maxima) of the equilibrium density correspond to the maxima (minima) of the modulation-potential energy. For graphical reasons we have amplified the induced density. The frequency of Fig. 4(a), $\omega=2.70\omega_c$, is chosen between two collective modes, where the absorption power is very small. The characteristic feature of such absorptionless oscillations is that the evolution of the density preserves the reflection symmetry of the unit cell, a kind of a breathing mode, attributed to single-particle excitations in the presence of a dissipation mechanism.

For the frequencies corresponding to collective peaks [Figs. 4(b) and 4(c)], we observe a global shift of the particle density inside the unit cell, i.e., we observe dipolar modes. In Fig. 4(b) both the density minima, around $Kx=0$ and $Kx=2\pi$, and the maxima, around $Kx=\pi$, have horizontal oscillations along the x direction. The amplitude for the *minima* is larger than for the maxima, which is in agreement with the domination of this mode by the transitions around the *center* of the Brillouin zone (associated with the maximum modulation-potential energy). We also observe a strong breathing component, due to the continuous spectrum of single-particle transitions of higher energies, which can be associated with the blueshift. In Fig. 4(c) we have dipolar oscillations of the density *maxima*, i.e., of frequency corresponding to the *lateral* VHS, with only a small breathing contribution, due to the excitation gap above. The neighboring mode, with $\omega=3.32\omega_c$ (Fig. 2), is very similar to that of Fig. 4(c), but has an additional node in the induced density. Also, the soft mode for $\omega=3.18\omega_c$ is similar to that of Fig. 4(b), with one node less in the induced density, but with a stronger breathing component.

We will discuss now the situation when the modulation period is much larger than the magnetic length. In this regime the Landau bands are parallel and the screening effects are stronger than before. In Fig. 5 we display the absorption for frequencies within the interval $0.5\omega_c<\omega<3\omega_c$, again with a complicated structure of the Bernstein modes. As in the case with $a=50$ nm, this structure also reflects the many branches of the magnetoplasma oscillation spectrum,[4] but now the internal peaks cannot be related to the energy spectrum as before because the excitation energies between the central and the lateral VHS coincide, e.g., like in Fig. 6. Here the energy dispersion in the vicinity of the Fermi level is flat due to the electrostatic screening.[14] Since the states around the center of the Brillouin zone are less populated than those at the edges, the active frequencies in the absorption spectrum correspond to dipolar oscillations of the density maxima, as shown in Fig. 7. The absorbant modes differ by the number of nodes in the induced density. In particular, for $\nu=1.6$, the height of the absorption peaks is lower for the modes with fewer nodes, which is somewhat contrary to the expectation.

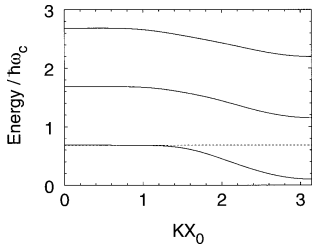

FIG. 6. Landau bands for the modulation of Fig. 5, with $\nu=1.6$.

A similar situation is shown in Fig. 8. Here we have reduced the mean particle density to $\rho_0=0.5\times10^{11}$ cm^{-2} in order to explore the limit of isolated, parallel quantum wires. The magnetic field is fixed to $B=4.67$ T. Even if the strips in between the wires are depleted to nearly zero particle density in the ground state, the wires still interact in the presence of the incident electric field. Consequently, the oscillations with a high number of nodes, capable of penetrating into the depleted strips, like in Fig. 8(b), are energetically favored with respect to those with fewer nodes, but keep a rigid wire separation [Fig. 8(c)]. Here we depict the density configurations for the middle and the right peaks in the group with three maxima of Fig. 8(a). For strictly isolated wires the induced density would be either symmetric or antisymmetric with respect to the wire center. This condition is best obeyed by the mode at $\omega=1.26\omega_c$, which is thus specific to the wire response, the other modes still being under the influence of the electric coupling between the wires.

In Fig. 9(a) we display the evolution of the absorption spectra with increasing density, from the limit of isolated wires $\rho_0=0.1\times10^{11}$ cm^{-2} up to well coupled wires $\rho_0=0.9\times10^{11}$ cm^{-2}. The wave vector of the time-dependent electric field is now small, $q=0.1K$, in order to concentrate the attention only on the effects of increasing the electron density on the absorption in a periodic system. The effect of the gate, which we neglect here, is mainly to repeat the same for each Bernstein mode. The Fermi level is always in the Landau band with $n=0$. For the lowest density the energy

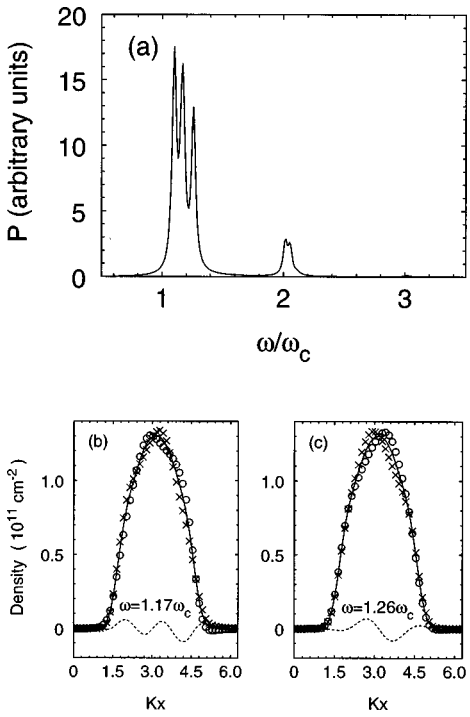

FIG. 8. (a) Absorption peaks for the same modulation as for Fig. 5, but with the average density $\rho_0 = 0.5 \times 10^{11}$ cm^{-2}. (b) and (c) are two diagrams for the induced density.

dispersion is large, but only few states are occupied at the bottom of the energy spectrum, while for the highest density the Landau band becomes very narrow, due to screening, such that the depleted strips vanish. In the limit of isolated wires the induced density at the single absorption peak has only two nodes inside each unit cell, as can be seen in Fig. 9(b). This kind of motion thus has a strong breathing component, i.e., vertical oscillations of the total charge of the type shown in Fig. 4, and only small dipolar (horizontal) components that vanish with changing frequency. Hence the internal motion of the electrons inside the wires has a strong contribution to the resonant modes or, in other words, Kohn's theorem is not obeyed here due to the nonparabolic, soft lateral confinement.

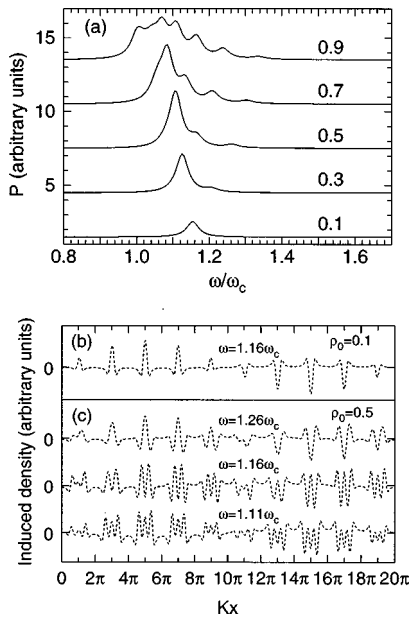

FIG. 9. (a) Absorption spectra for various electron densities, from 0.1 to 0.9 units of 10^{11} cm^{-2}, covering the transition from isolated wires to a modulated system. The magnetic field is $B = 4.67$ T and the wave vector of the incident electric field is $q = 0.1$ K. The induced electron density, in a full period of the perturbed system, is for (b) $\rho_0 = 0.1 \times 10^{11}$ cm^{-2} and (c) $\rho_0 = 0.5 \times 10^{11}$ cm^{-2}, for the frequencies corresponding to the absorption maxima.

Increasing the density, the wire coupling allows additional charge oscillations inside the unit cell [Fig. 9(c)], that may cumulate a stronger total dipolar component, thus yielding higher absorption peaks. The lower the frequency, the higher the number of nodes within each wire, as also noticed for $q = K$, in Fig. 8. The mode at $\omega = 1.26\omega_c$, with few nodes per cell, corresponds to the only mode of the isolated wire system. Such a mode is present in each trace of Fig. 9(a), being the highest in frequency but the lowest in amplitude. Instead, the new modes, with additional internal oscillations, grow rapidly at lower frequencies, when the density, and thus the wire coupling, increases.

For a given mode, the characteristic wavelength of the internal motions inside the unit cell is determined by the lateral confinement and by the wire coupling. In our periodic system both of them result self-consistently from the external modulation potential, the magnetic field, and the electron density. The evolution from a single-peak absorption around ω_c, specific to isolated wires, to the multipeak structure, specific to the modulated system, thus occurs by the progressive appearance of new modes, with richer internal motion, and accumulating larger oscillator strength. For each density, the number of nodes in the absorption maxima of Fig. 9(a) gradually increases from right to left. When the density is increased further, beyond what is shown in Fig. 9, such that more than one Landau band is occupied a stable *single peak emerges* with energy and induced density specific to the homogeneous system.

IV. SUMMARY

In the present paper we have explored the properties of the FIR absorption of a 2DEG modulated in one direction, varying the modulation and the electron density in order to cover the whole range from isolated but electrically coupled wires to a weakly modulated 2DEG. The electron-electron interaction has been treated self-consistently within the time-dependent Hartree approximation. Experimentally the transition from wires to an almost homogeneous 2DEG can be achieved in heterostructures with a modulated metal gate, which in turn also acts like a grating coupler for the incident FIR radiation. The modulation of the incident field should be determined self-consistently including effects from the gate and the three-dimensional structure of the sample.[15] To avoid this problem that is further complicated by the presence of the magnetic field we considered primarily the effects of the two lowest Fourier components in the incident field ($q \approx 0$ and $q = K$). The presence of the short-wavelength component and the magnetic field of intermediate strength place the dispersion of the magnetoplasmon in the regime of Bernstein modes.

Our calculations show that information about the nonparallel Landau bands in short-period wires can be extracted from the peak structure of the FIR absorption. The effects of the VHS of the underlying energy band structure on the dielectric function in weakly magnetically and electrically modulated system have been studied in the absence of the Coulomb interaction between electrons.[16,17]

ACKNOWLEDGMENTS

This research was supported by the Icelandic Natural Science Foundation, the University of Iceland Research Fund, and the International Center for Theoretical Physics, Trieste, Italy. We thank Detlef Heitmann and Christoph Steinebach for helpful discussions. A.M. wishes to thank both the University of Iceland and ICTP, Trieste for their hospitality.

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