Plasma modes of a two-dimensional electron gas with a two-dimensional modulation of the charge density

G. Eliasson,* P. Hawrylak, and J. J. Quinn
Department of Physics, Brown University, Providence, Rhode Island 02912
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We study the plasma modes of a two-dimensional electron gas in which the equilibrium electron density is a periodic function of both coordinates in the plane of the electron gas. The special case of a square symmetric modulation of the equilibrium density is calculated numerically. The plasmon dispersion displays a band structure similar to that found for single-particle energy bands. The results are compared with those obtained from perturbation theory valid for a weak electron-density modulation.

During the past few years there has been a considerable amount of interest in two-dimensional systems in which the equilibrium electron density is spatially varying. Mackens *et al.*[1] have fabricated metal-oxide-semiconductor devices in which the oxide thickness is a periodic function of position along one coordinate axis. The plasmons of the resulting two-dimensional electron gas (2D EG) display zone folding associated with the new periodicity. This allows direct optical excitation of the plasmon spectrum at $k=0$, as reported by Mackens *et al.*[1] and Heitmann[2] in infrared transmission. For a weak spatial modulation with period d, Krasheninnikov and Chaplik[3] have estimated the size of the induced gaps at $k=0$ and π/d by perturbation theory. They find that $\Delta\omega_m \approx |N_m/N_0|\omega_m$, where ω_m is the unperturbed plasma frequency for wave vector $k_m = m\pi/d$. $\Delta\omega_m$ is the gap induced at ω_m, and N_m is the mth coefficient in the Fourier expansion of the 2D EG equilibrium density.

For a large variation of the equilibrium density several groups have studied theoretically various limiting cases. Lai and Das Sarma[4] have investigated the lowest plasmon miniband for a periodic array of 2D EG strips separated by insulating strips. The full spectrum of two-dimensional plasmons for this system was obtained by Eliasson *et al.*[5] The generalization to systems in which the equilibrium density is an arbitrary periodic function of one coordinate, i.e., $n_0(x+d)=n_0(x)$ has also been investigated.[6,7]

Other systems displaying spatial variation of the two-dimensional electron density have been studied by Mast *et al.*[8] and by Glattli *et al.*[9] These authors have investigated edge modes of a semiinfinite 2D EG and perimeter modes of a finite 2D EG in the presence of an applied magnetic field. A number of mathematical refinements in the calculation of the dispersion relation of the edge magnetoplasmon of a single 2D EG layer,[10,11] and extensions to a periodic array of 2D EG layers[12,13] have appeared in recent literature. In addition, there has also been a considerable amount of work on thin wires.[4,14,15]

In the present article we study the plasmon spectrum of a two-dimensional electron system in which the equilibrium density $n_0(x,y)$ is an arbitrary periodic function of both coordinates. This is particularly interesting because it is, to our knowledge, the first case in which real band-structure effects (point-group symmetries and overlapping bands) occur for collective, instead of single-particle, electronic excitations. In addition, a number of groups[16,17] have been able to fabricate periodic two-dimensional arrays on a submicrometer scale, so that observation of the two-dimensional plasmon band structure discussed here via infrared spectroscopy and Raman scattering appears within reach.

We consider a two-dimensional electron gas confined to the plane $z=0$ which is embedded in a dielectric with constant ϵ. A magnetic field $\mathbf{B}=B\hat{\mathbf{z}}$ is applied perpendicularly to the electron gas. The equilibrium density $n_0(x,y,z)=n_0(x,y)\delta(z)$ is expanded in Fourier series

$$n_0(x,y)=\sum_{m,n=-\infty}^{\infty} N_{mn}e^{i\alpha_m x}e^{i\beta_n y} , \tag{1}$$

where $\alpha_m=2\pi m/d_x$, $\beta_n=2\pi n/d_y$. d_x and d_y are the periods in the x and y directions, respectively, and m,n are integers.

The equilibrium density is perturbed by a fluctuation in the density of the form

$$n_1(x,y,z,t)=n_1(x,y,\omega)\delta(z)e^{-i\omega t} . \tag{2}$$

One can find the scalar potential $\phi(x,y,z,\omega)$ due to n_1 from Poisson's equation. On the $z=0$ plane ϕ can then be written

$$\phi(x,y,z=0,\omega)\equiv\phi(x,y,\omega)=-\frac{e}{\epsilon}\int_{-\infty}^{\infty}dx'\int_{-\infty}^{\infty}dy'\frac{n_1(x',y',\omega)}{[(x-x')^2+(y-y')^2]^{1/2}} . \tag{3}$$

By using the equation of continuity $\nabla\cdot\mathbf{J}(\mathbf{r},\omega)=-ie\omega n_1(\mathbf{r},\omega)$ and the constitutive equation $\mathbf{J}(\mathbf{r})=\underline{\sigma}(x,y)\mathbf{E}(\mathbf{r})$, where $\underline{\sigma}(x,y)$ is the local magnetoconductivity for a 2D EG,[13] one can obtain an integrodifferential equation for $\phi(x,y)$:

$$\phi(x,y)=-\frac{4\pi e^2}{\epsilon m_e(\omega^2-\omega_c^2)}\int_{-\infty}^{\infty}dx'\int_{-\infty}^{\infty}dy'\frac{1}{4\pi[(x-x')^2+(y-y')^2]^{1/2}}$$
$$\times\left\{n_0(x',y')(\nabla')^2\phi(x',y')+\nabla' n_0(x',y')\nabla'\phi(x',y') -\frac{\omega_c}{\omega}[\nabla_{x'}n_0(x',y')\nabla_{y'}\phi(x',y')-\nabla_{y'}n_0(x',y')\nabla_{x'}\phi(x',y')]\right\} . \tag{4}$$

Here $\omega_c=eB/m_ec$ is the cyclotron frequency and m_e is the effective electron mass. Since the system is periodic, $\phi(x,y)$ can be written as a Bloch function, i.e.,

$$\phi(x,y)=e^{ik_xx}e^{ik_yy}\sum_{m,n=-\infty}^{\infty}A_{mn}e^{i\alpha_mx}e^{i\beta_ny} , \tag{5}$$

where $|k_x|\le\pi/d_x$ and $|k_y|\le\pi/d_y$ are the Bloch wave vectors. We now substitute the Fourier expansions of n_0 and ϕ into Eq. (4). This results in an infinite set of equations for the Fourier coefficients A_{mn}. For the sake of simplicity we restrict our consideration to the case of zero magnetic field; then the equations can be written as

$$\bar{\omega}^2A_{mn}=\sum_{m',n'=-\infty}^{\infty}C_{mn,m'n'}A_{m'n'} , \tag{6}$$

where $\bar{\omega}=\omega/\Omega$, $\Omega^2=2\pi N_{00}e^2/\epsilon m_ed$, $N_{mn}=N_{00}\tilde{N}_{mn}$ with $\tilde{N}_{00}=1$, and

$$C_{mn,m'n'}=\sum_{l,l'=-\infty}^{\infty}D_{m,n,m'+l,n'+l'}\tilde{N}_{ll'}[(k_xd+2\pi m')^2+(k_yd+2\pi n'/\delta)^2+2\pi k_xdl+2\pi k_ydl'/\delta+4\pi^2(m'l+n'l'/\delta^2)] . \tag{7}$$

Here we have introduced $\delta=d_y/d_x$ and $d=d_x$. $D_{mn,m'n'}(k_x,k_y)$ is given by

$$D_{m,n,m'n'}=\frac{1}{2}\frac{\delta_{mm'}\delta_{nn'}}{[(k_xd+2\pi m)^2+(k_yd+2\pi n/\delta)^2]^{1/2}} . \tag{8}$$

In the case of a finite magnetic field, Eq. (6) is not a simple eigenvalue problem, since both ω and ω^2 appear. This can however be resolved by formulating the matrix equation as a generalized eigenvalue problem. We refer to Ref. 10 in this matter.

In the following we will consider only a square symmetry, i.e., $d_x=d_y=d$. When the density is uniform, i.e., $\tilde{N}_{mn}=\delta_{m0}\delta_{n0}$, then $C_{mn,m'n'}$ is diagonal. The set of equations has a nontrivial solution when the determinant of the matrix multiplying the column vector A_{mn} vanishes. In this case, $\det[\underline{1}-(\Omega^2/\omega^2)\underline{C}]=0$ gives

$$\omega^2=\omega_{mn}^2=\Omega^2[(k_xd+2\pi m)^2+(k_yd+2\pi n)^2]^{1/2} . \tag{9}$$

This is the well-known two-dimensional electron gas plasmon in the reduced zone scheme. Figure 1 shows the dispersion relation for the plasmon. The notation for the irreducible representations is the same as in Ref. 18.

We now assume that the modulation is weak, i.e., $|\tilde{N}_{mn}|\ll1$ for $(m,n)\neq(0,0)$. Equation (6) can now be solved in perturbation theory near the band edges. This was first done for a one-dimensional modulation by Krasheninnikov and Chaplik.[3] Here the problem is identical to the textbook case of an electron moving in a weak periodic potential. By using standard methods of group theory, one can easily estimate the size of the band gaps. In the general case when the modulation is not small, Eq. (6) has to be solved numerically by truncating $\underline{C}$.

We have performed calculations for a system with equilibrium density given by

$$n_0(x,y)=\begin{cases}n_s(1+a), & |x|,|y|<d/4\\ n_s(1-a) & \text{otherwise} .\end{cases} \tag{10}$$

Then, $N_{00}=(1-a/2)n_s$ and $N_{mn}=N_{nm}=N_{|m||n|}$. In the model calculation we keep terms up to $|m|,|n|=3$, and the secular equation is solved numerically. In order to achieve convergence, the order of $\underline{C}$ is larger; we truncate the matrix at $|m|,|n|=9$.

Figures 2 and 3 show the plasmon dispersion for

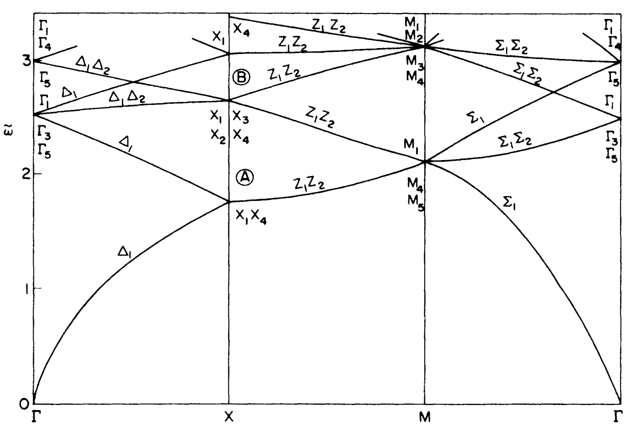

FIG. 1. Dispersion relation of a two-dimensional electron gas in the first Brillouin zone of a lattice with square symmetry. The notation for the irreducible representations is the same as in Ref. 18. $\bar{\omega}=\omega(2\pi n_se^2/\epsilon m_ed)^{-1/2}$.

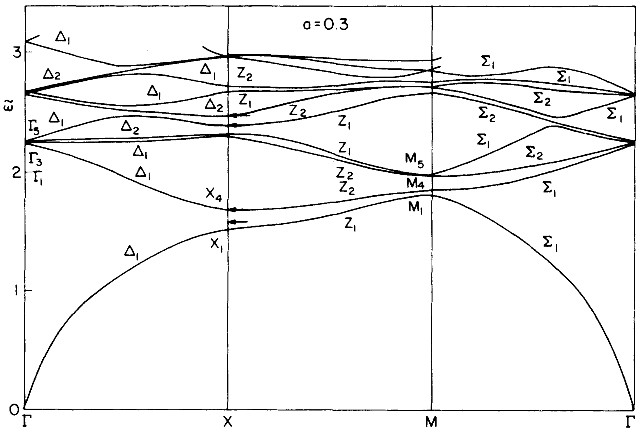

FIG. 2. Plasmon band structure for $a=0.3$. The arrows indicate the energies given by perturbation theory. The two upper arrows indicate double degenerate levels. The lower of these arrows correspond to the two levels below it and the upper arrow to the two levels closest to the arrows.

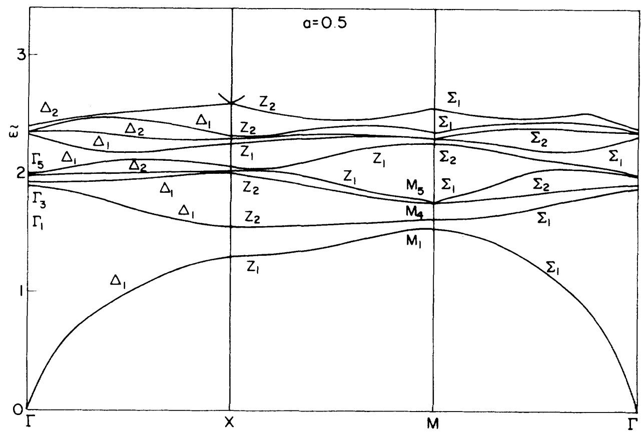

FIG. 3. Plasmon band structure for $a=0.5$.

$a=0.3$ and $a=0.5$, respectively. Since all Fourier coefficients $\tilde{N}_{mn}$ with even $m,n\neq 0$ vanish, the gaps at the Γ point are very small. We compare the results with perturbation theory at the points labeled A and B in Fig. 1. The fourfold degeneracy at B breaks up into two double-degenerate levels. The degeneracy is accidental and breaks in our numerical treatment. In Fig. 2 the result given by perturbation theory at the X point are indicated with arrows. One finds that already for $a=0.3$ the results given by perturbation theory deviate significantly from the actual frequencies. Perturbation theory gives a too high position of the band gap, and the size of the gap is too small. This effect was also noted in the case of a one-dimensional modulation.[6] A further investigation reveals that perturbation theory gives a good quantitative result for $a\leq 0.2$. We also note that as a grows, the bands become narrower and the gaps larger, as expected.

In summary, we have calculated the plasmon dispersion of a two-dimensional electron gas with a spatially periodic charge density. The equilibrium density is an arbitrary periodic function of both coordinates. We find that for a small modulation of the equilibrium density, gaps in the plasmon spectrum open up. As the modulation becomes stronger the bands become narrower and the gaps larger. For small modulations the results are well described by perturbation theory. The method used here can also be used to study the dispersion of magnetoplasmons, although this requires more computational effort. In a real system, the periodic variation of the density is induced by, for example, an external electrode with a suitable structure or an insulator whose thickness varies. The presence of a metallic gate parallel to the electron gas will affect the screening. This effect can be included by modifying the Green's function in Eq. (3), as shown in Ref. 10. This modification will, however, not change the qualitative results given here. Our results suggest the existence of "edge" modes of a semi-infinite system similar to surface states in the electron band structure. The investigation of these modes as well as the effects of a magnetic field will be reported in a later publication.

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*Present address; Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, NY 14853.

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