Asymptotic localization of plasmons in a periodic array of stripes

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The plasmonic bands of a periodic array of stripes are investigated for a class of continuous equilibrium density profiles within the frictionless and dispersionless hydrodynamical model. The attention has been focused on the behavior of the frequencies at large values of parallel wave vector. In this range we have found a strong localization of plasmons at the point of minimum density in the cell. The effect of a vanishing minimum density is also studied.

I. INTRODUCTION

In the last ten years the study of the plasma excitations of a homogeneous two-dimensional (2D) electron gas in metal-oxide-semiconductor (MOS) structures or in heterostructures (GaAs-$Al_xGa_{1-x}As$) has attracted considerable attention both experimentally[1] and theoretically.[2]

More recently the role of spatial periodic modulation of the equilibrium density of a two-dimensional electron gas (2D EG) has been studied in artificial structures[3] as well as in high-Miller-index surfaces of semiconductors.[4] In the case of artificial structures, with the use of lithographic and etching techniques it is possible to modulate the electron gas in order to produce a 2D periodic array of stripes with a periodicity, L, from 300 to 1200 nm. The width as well as the equilibrium density of a strip depend on the voltage, V_g, applied between the substrate and a grating deposited on the top of the heterostructure. Some accurate self-consistent calculations of the equilibrium density have been reported[5] showing how the effective potential acting on the electrons depends on V_g: the shape and the width of the electron density can be strongly different compared with the grating structure.

Far-infrared transmission spectroscopy has been applied in order to study the excitations of these electronic systems. The radiation impinges on the heterostructures, lying in the x-y plane and modulated along x, perpendicularly to the 2D EG, along the z direction. When the radiation emerges from the structure, due to the grating periodicity, it acquires all x components of the wave vectors which are integer multiples of $2\pi/L$. The relative change of transmission $\Delta T/T=[T(n_s)-T(0)]/T(0)$, where $T(n_s)$ is the transmission in presence of 2D EG equilibrium density n_s, shows pairs of peaks which corresponds to the edges of plasmonic bands at the center of the Brillouin zone.

These plasmonic bands have been calculated within the frictionless and dispersionless linearized hydrodynamic theory by using an approximate method,[6] a perturbative technique,[7] and a numerical analysis of the associate eigenvalue problem.[8]

Our aim, here, is to discuss systematically, in the same hydrodynamic theoretical framework proposed in the previous works, how the plasmonic spectrum depends on a *continuous* equilibrium density profile. We also point out some peculiar features of these 2D systems.

The main results obtained are as follows.

(a) As the profile becomes more squared, the plasmonic bands become narrower and the frequencies lower. The effect is qualitatively relevant when the relative variation with respect to the mean value of density profile is large.

(b) In the large-k_y limit (that is the y component of the wave vector associated with the plasmons) the induced density is localized around the point of minimum density and the associated frequencies are equal to those of a homogeneous 2D EG with the minimum density.

(c) If the equilibrium density vanishes in some point, the system is no longer able to support plasmons. This result, which is in contrast with what has been found for a discontinuous density profile,[9,10] has been verified for a class of *continuous* profiles. The question arises of what is the effect of discontinuities in the equilibrium density on the plasmonic bands. In our opinion the presence of finite regions of zero density allows for accumulation of the induced charge at the edges with far-reaching consequences on dispersion relations.

II. THE MODEL

Within the electrostatic approximation the collective modes of the 2D periodic EG (PEG) are obtained by solving the Laplace equation for the electrostatic potential Φ in the two semispaces surrounding the plane containing the electron gas, and then matching the solutions according to Maxwell's condition:

$$\left.\frac{\partial\Phi}{\partial z}\right|_{0^+}-\left.\frac{\partial\Phi}{\partial z}\right|_{0^-}=4\pi e n(x,y) \ . \qquad (1)$$

The gas lies in the plane (x,y), z is the direction normal to it, and $n(x,y)$ is the areal induced electron density in the plane. The consistency of the equation for electron's motion,

$$i\mu\omega v=-e\nabla_2\Phi \ , \qquad (2)$$

with the continuity equation for the induced density gives for the time Fourier transform of Φ the following equation:

$$\left.\frac{\partial\Phi}{\partial z}\right|_{0^+}-\left.\frac{\partial\Phi}{\partial z}\right|_{0^-}=\frac{4\pi e^2}{\mu\omega^2}(\nabla_2 n_0\cdot\nabla_2+n_0\nabla_2^2)\Phi\,|_0\;, \qquad (3)$$

where n_0 is the equilibrium density for the ground state, v is the velocity, μ is the effective electronic mass, e is the electronic charge, ω is the frequency, and ∇_2 is the gradient in the plane. We note that n_0 is a function of the position in the plane. We note that this equation can be obtained in the limit of high frequencies at the lowest order from the microscopic linear-response theory of the system.[11] In this way we are choosing a classical and macroscopic approach.

We study a system in which n_0 is periodic along x, with period L, and is represented by the sum

$$n_0(x)=\nu_0+\sum_{m=1}^{M} n_m\cos\left[\frac{2\pi m x}{L}\right]. \qquad (4)$$

Given an arbitrary periodic profile n_0, at most piecewise continuous, it can be expanded in Fourier series. In general, therefore, M stands for ∞, and the n_m coincide with the Fourier coefficients.[8] In the following we shall make a different choice, that should be, in our opinion, suitable to represent a periodic step function, if a truncation of the sum is needed to perform numerical calculations.

The periodicity of n_0 suggests that one take a solution of the Laplace equation in the form

$$\Phi=\sum_n A_n e^{ik_n x}e^{ik_y y}e^{\pm k_z z},\quad k_n=\frac{2\pi n}{L}+k_x \qquad (5)$$

if we want solutions decaying both for $z\to\infty$ (+) and for $z\to-\infty$ (−). Substituting (5) in (3) we obtain the eigenvalue equation for the plasmon frequencies:

$$\sum_{p=-\infty}^{\infty}\left[\frac{z_p^2-(p-n)z_p+z_y^2}{2(z_n^2+z_y^2)}\chi_{p-n}H(p-n)-\Omega^2\delta_{pn}\right]A_p=0,\quad H(l)=0 \text{ for } |l|>M,\quad H(l)=1 \text{ for } |l|\le M\;, \qquad (6)$$

where

$$z_i=\frac{k_i L}{2\pi}(i=x,y,n),\quad \chi_0=1,\quad \chi_j=\frac{n_{|j|}}{2\nu_0}\;,$$

$$\Omega^2=\frac{\omega^2}{\omega_s^2},\quad \omega_s^2=\frac{8\pi^2 e^2\nu_0}{\mu L}\;.$$

Eliasson *et al.*[8] used Eq. (6) for a squared equilibrium profile approximated with the first seven terms of Fourier series. Because one of the aims of this paper is to point out the role of the minimum density on the plasmonic band structure, we fix the value of χ_j in a different way. Indeed the truncation of Fourier series originates the Gibbs phenomenon which does not allow one to reach the zero minimum density without having regions of unphysical negative equilibrium density. In order to overcome this problem we choose the χ_j in such a way the first $M-1$ derivatives vanish at $x=0$ and $x=L/2$. This procedure gives an alternative succession of non-negative functions approximating the step with a minimum value that can be taken as small as we want.

The effect of a dielectric substrate, due to the frequency range of the studied collective excitations, can be described through a frequency-independent dielectric constant ϵ_s whose only consequence is to redefine ω_s^2:

$$\omega_s^2=\frac{16\pi^2 e^2\nu_0}{\mu L(\epsilon_s+1)}\;.$$

This is true only in the electrostatic approximation and in a plane geometry.

III. THE CASE OF A COSINE PROFILE

We begin our analysis by taking $M=1$ in Eq. (4). Equation (6) now has the form

$$M_j^- A_{j-1}+(M_j-\Omega^2)A_j+M_j^+A_{j+1}=0\;, \qquad (7)$$

where

$$M_j^{\pm}=\frac{\chi}{2}\frac{(j+z_x)(j+z_x\pm1)+z_y^2}{[(j+z_x)^2+z_y^2]^{1/2}}\;,$$

$$M_j=[(j+z_x)^2+z_y^2]^{1/2}/2$$

in which j goes from $-\infty$ to ∞ and χ stands for χ_1. For a numerical evaluation we approximate Eq. (7) with the homogeneous system of $2N+1$ equations:

$$(M_{-N}-\Omega^2)A_{-N}+M_{-N}^+A_{-N+1}=0\;,$$
$$M_j^-A_{j-1}+(M_j-\Omega^2)A_j+M_j^+A_{j+1}=0\;, \qquad (8)$$
$$M_N^-A_{N-1}+(M_N-\Omega^2)A_N=0\;,$$

in which $|j|\le M-1$, that can be solved by taking $A_{-N}=1$ and calculating for recurrence the other coefficients so that the last equation becomes the eigenvalue equation.

Figures 1 and 2 show the plasmonic bands for two different values of χ. We note that for the lowest value of χ our results are very similar to those obtained by Eilasson *et al.*[8] for a square equilibrium profile represented by the first seven Fourier components. Of course, increasing χ the effect of the other Fourier components modifies the spectrum, even if the change is not dramatic.

One of the aims of this work is to discuss the asymptotic behavior for large values of z_y. We note that the numerical technique we have used allows this analysis. Fig-

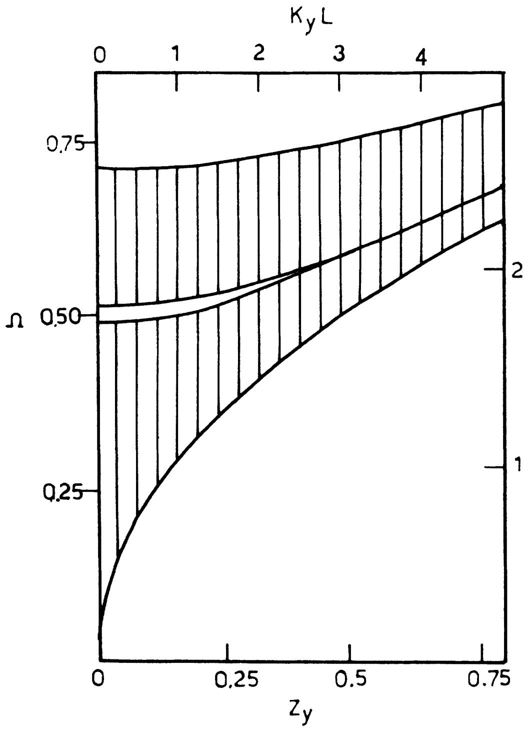

FIG. 1. The first two plasmonic bands for the cosine profile. $\mathcal{X}=0.05$. On the right-hand side we report the units of Ref. 8 for comparison.

ure 3 exhibits the first two bands at $\mathcal{X}=0.05$ for large values of z_y. Increasing z_y the bands become narrower and narrower around the value of $z_x=0$, and the squared frequencies lean on straight lines so that

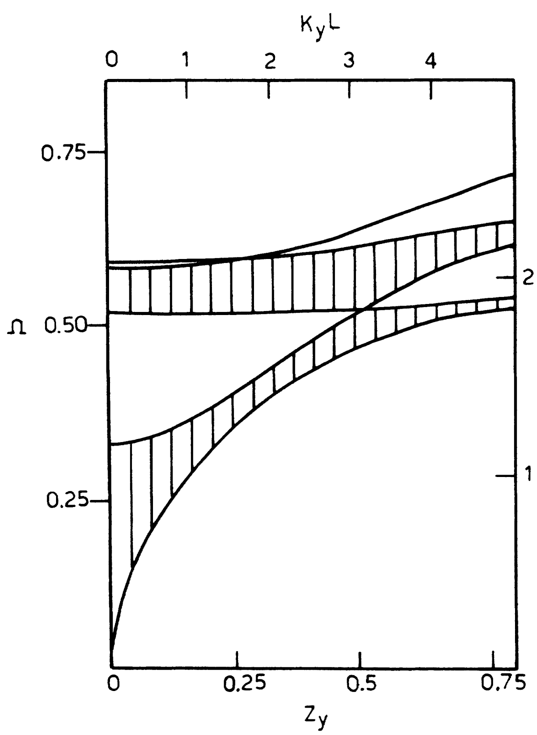

FIG. 2. The same as Fig. 1 with $\mathcal{X}=0.375$.

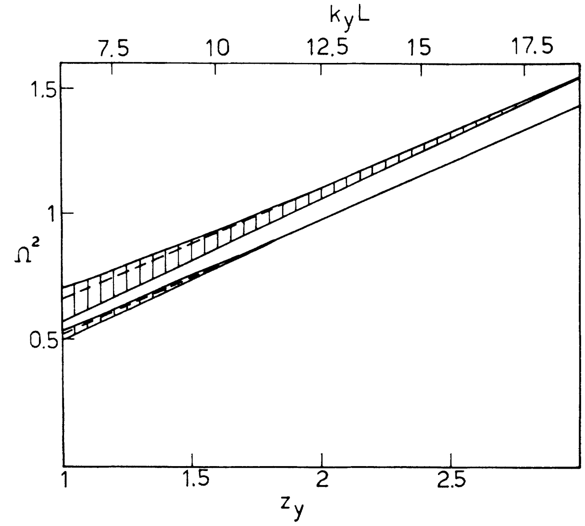

FIG. 3. The asymptotic behavior of the first two bands at $\mathcal{X}=0.05$. The dashed lines give the linear asymptotic dependence of Ω^2 on z_y.

$$\Omega^2 \sim (\tfrac{1}{2}-\mathcal{X})z_y+\alpha_i \quad (z_y \to \infty)\ . \tag{9}$$

Here the index i labels the different bands at the increasing of the frequency, and the dependence of the coefficients α_i on $\mathcal{X}$ is shown in Fig. 4. Equation (9) implies that the asymptotic behavior is that of a uniform density at the minimum value of n_0. When the minimum

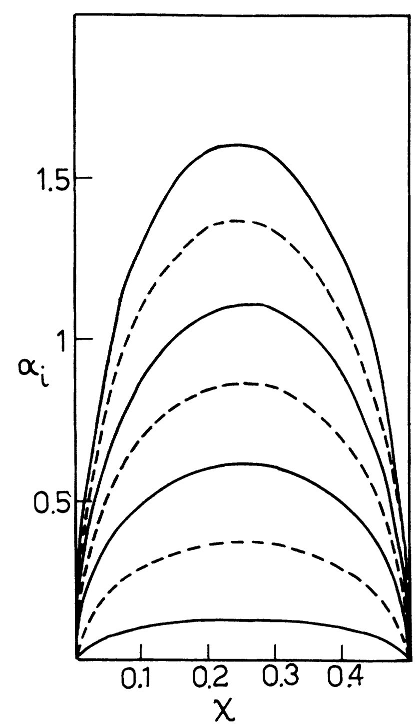

FIG. 4. The dependence of α_i [Eq. (9)] on $\mathcal{X}$ for the first seven bands. The solid (dashed) lines refer to the even (odd) modes at $z_x=0$.

density is zero ($\mathcal{X}=\frac{1}{2}$) all the bands collapse towards zero frequency. However, this happens not only at a large value of z_y but at *any* value of the y component of the wave vector. We will return later to this point, and, for the moment, we focus our attention on the asymptotic region. We note that the gaps for large z_y are all equal and they are of the same order of magnitude or even greater than those appearing in the $z_y=0$ spectrum.

When $z_x=0$ the A_i solution of the system (8) can be classified in even $A_i=A_{-i}$ or odd $A_i=-A_{-i}$. Using this property of symmetry we build up two recurrence relations for the succession of determinants D_N obtained by (8). For the even modes we get

$$\begin{aligned} D_0&=z_y/2-\Omega^2 ,\\ D_1&=(M_1-\Omega^2)D_0-2\mathcal{X}^2a_1M_1M_0 ,\\ D_n&=(M_n-\Omega^2)D_{n-1}-\mathcal{X}^2a_nM_nM_{n-1}D_{n-2} , \end{aligned} \tag{10}$$

where

$$a_n=\frac{[n(n-1)+z_y^2]^2}{[(n-1)^2+z_y^2](n^2+z_y^2)},\quad M_n=\frac{(n^2+z_y^2)^{1/2}}{2} .$$

The corresponding relation for the odd modes is obtained by simply changing the initial conditions for the difference equation (10):

$$\begin{aligned} D_1&=M_1-\Omega^2 ,\\ D_2&=(M_2-\Omega^2)D_1-\mathcal{X}^2a_2M_2M_1 . \end{aligned} \tag{11}$$

Redefining D_n as

$$\mathcal{D}_n=\frac{D_n}{\mathcal{X}^{n+1}\prod_{i=1}^{n}M_i}$$

the difference equation (10) becomes

$$\mathcal{D}_n=\frac{1}{\mathcal{X}}\left[1-\frac{\Omega^2}{M_n}\right]\mathcal{D}_{n-1}-a_n\mathcal{D}_{n-2} . \tag{12}$$

For a fixed value of z_y and for any value of Ω^2 an $\bar{n}$ exists such that $M_n \gg \Omega^2$ for any $n>\bar{n}$; furthermore, for z_y large enough we can take $a_n \sim 1$. In other words the asymptotic form of Eq. (12) is

$$\mathcal{D}_n=\frac{1}{\mathcal{X}}\mathcal{D}_{n-1}-\mathcal{D}_{n-2}\quad (n>\bar{n}) , \tag{13}$$

whose solution is

$$\mathcal{D}_n=R_{\pm}^n \quad\text{with } R_{\pm}=\frac{1\pm(1-4\mathcal{X}^2)^{1/2}}{2\mathcal{X}} . \tag{14}$$

As we want $\mathcal{D}_\infty=0$ we have the unique solution R_-^n. We note that when $\mathcal{X}=\frac{1}{2}$, Eq. (13) does not have vanishing solutions for n going to infinity.

The explicit calculation of the asymptotic dependence of Ω^2 on z_y implies both the limit $z_y\to\infty$ and the limit $n\to\infty$. We have to find the values of Ω^2 for which the initial conditions on the first values of $\mathcal{D}$ allow matching with the unique vanishing asymptotic solution. When z_y is large at low values of n, Eq. (12) coincides with the succession of polynomials

$$\begin{aligned} P_0&=y ,\\ P_1&=y^2-2 ,\\ P_n&=yP_{n-1}-P_{n-2} , \end{aligned} \tag{15}$$

where

$$y=\frac{1}{\mathcal{X}}\left[1-\frac{2\Omega^2}{z_v}\right] .$$

In other words for large z_y Eq. (12) reduces to Eqs. (15), while low values of n Eq. (12) reduces to Eqs. (13) for large n. Going with n to infinity the roots of polynomials (15) converge to $y=2,-2$, accumulating towards these limit points. We note that $y=2$ gives the frequency corresponding to the minimum density of Eq. (9), while $y=-2$ gives the frequency corresponding to the maximum density. There is strong evidence from the numerical calculations that only $y=2$ is the unique correct solution at the highest order in z_y of Eqs. (12), while $y=-2$ is a spurious one that arises from extending the low-n approximation (15) to infinity. For odd modes the initial conditions $P_1=y$ and $P_2=y^2-1$ have to be substituted in Eq. (15), but the above conclusions are still valid.

This asymptotic behavior implies that the plasmonic modes are localized around the point of minimum equilibrium density. In fact, when the eigenfrequencies have been calculated, we can obtain the corresponding electrostatic potential, and from it the induced density, summing up the Fourier series (5). In Fig. 5 the potential is

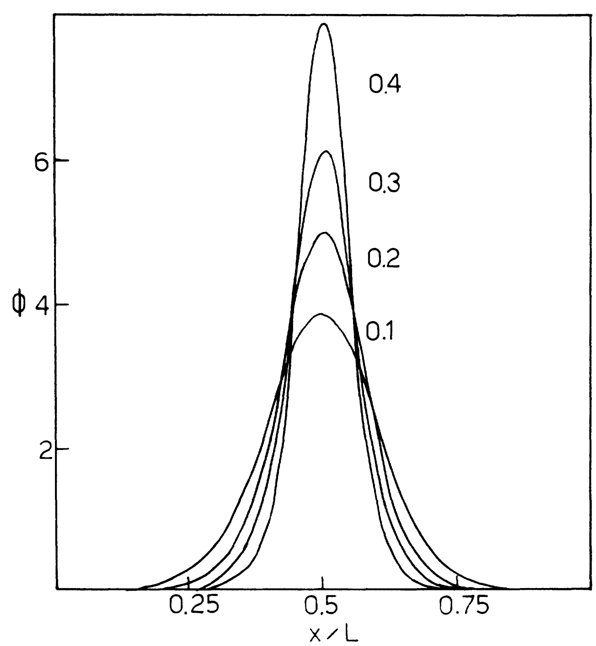

FIG. 5. The electrostatic potential Φ vs the position within the cell x/L at $z_y=5$. The curves are normalized in such a way that their area is equal to 2π, and they are labeled by the value of $\mathcal{X}$.

shown within a cell in the asymptotic region ($z_y = 5$) for the lowest band. For such a large value of z_y we have a very slight dependence on z_x for both the frequency and the potential. The localization increases with both z_y and $\mathcal{X}$. When $\mathcal{X} \to \frac{1}{2}$ or $z_y \to \infty$ the potential shrinks around $x = L/2$ approaching a δ function. This happens because the integral of Φ over the cell is constant, and it is equal to 2π if we choose $A_0 = 1$. Furthermore, when $\mathcal{X} \to 0.5$, the frequency goes to zero. Therefore the system does not support density fluctuations any longer, due to this dramatic localization and to the vanishing of the minimum density. As shown in Fig. 6 the induced density follows the same behavior of the potential. The number of its nodes increases with the band index. The appearance of these oscillations is compatible with the localization property previously discussed however.

We now discuss the shape of the plasmonic bands as a function of z_x. In general the frequencies are increasing or decreasing functions of z_x. However, there are some particular values of $\mathcal{X}$ and z_0 for which the plasmonic bands have a minimum that is not at the center or at the border of the Brillouin zone. Therefore it is possible to find in some bands a crossing between the frequencies at $z_x = 0$ and $z_x = 0.5$. Figure 7 shows such a case in which, upon increasing $\mathcal{X}$, the width of the band goes through a minimum. When the width of the band is very small, for low values of z_y, some care has to be taken in calculating it.

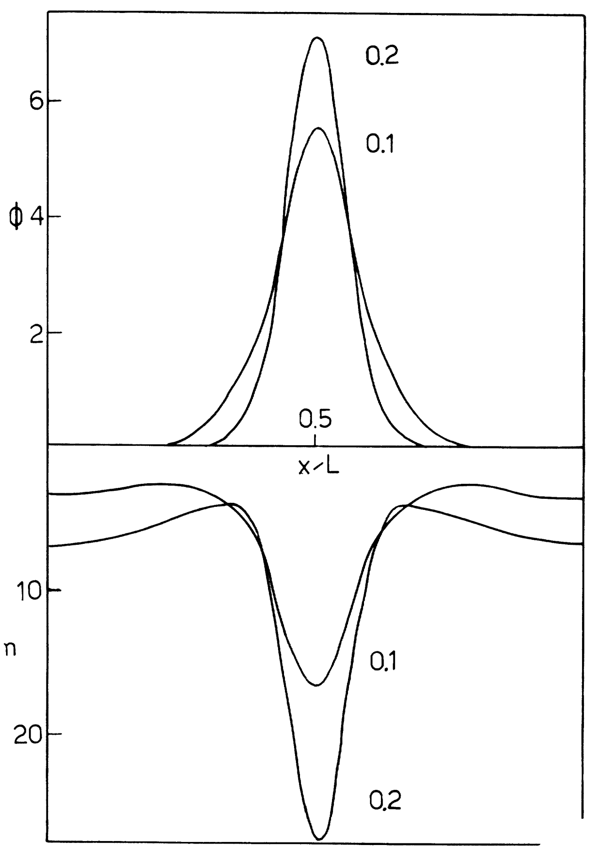

FIG. 6. The same as in Fig. 5 at $z_y = 10$. We show also the induced density n.

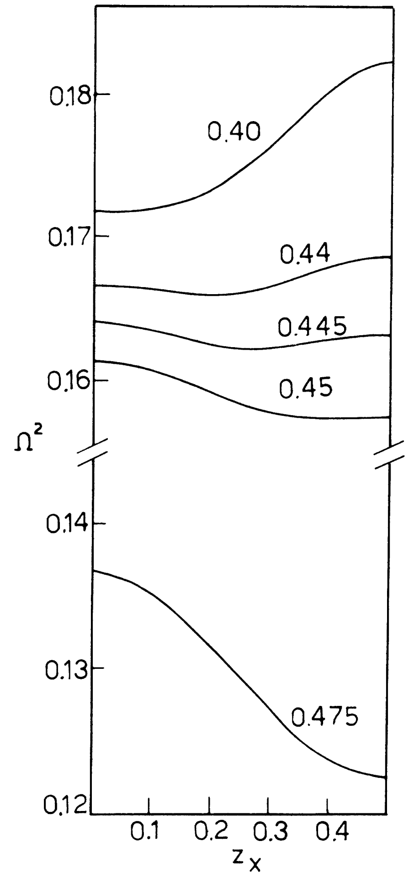

FIG. 7. We show the behavior of Ω^2 as a function of z_x varying $\mathcal{X}$ in order to show how the minimum of the bands can move from the center to the edge of the Brillouin zone. The calculations are for the first band of the cosine profile.

IV. THE CASE OF A SQUARE PROFILE

Following the approach discussed in Sec. II we have calculated the plasmonic bands for the profiles shown in Fig. 8 that are obtained upon adding more components in Eq. (4). They represent approximations of the density:

$$n_0 = \begin{cases} \nu_0(1+2\mathcal{X}) & \text{for } -L/4 \le x \le L/4 , \\ \nu_0(1-2\mathcal{X}) & \text{for } L/4 \le x \le 3L/4 . \end{cases}$$

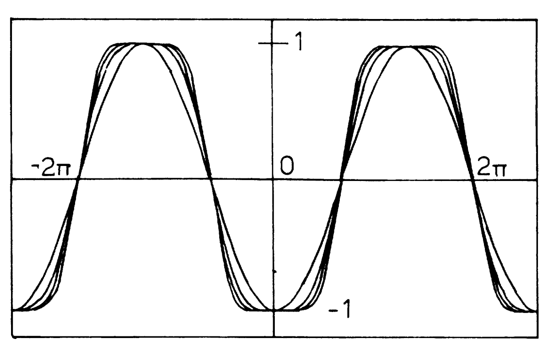

FIG. 8. The profiles used to approximate the square profile.

For the sake of completeness we report in the following table the coefficients c_i which multiplied for $\mathcal{X}$ give the $\mathcal{X}_i$.

M	c_1	c_3	c_5	c_7	c_9
3	1.125	−0.125			
5	1.172	−0.195	0.023		
7	1.196	−0.239	0.048	−0.005	
9	1.211	−0.269	0.069	−0.012	0.010

When we increase the value of M, keeping constant the value of the minimum equilibrium density, the bands show a general tendency to lower in frequency and to become narrower. This behavior has been tested going with M from 1 to 9, and the results are shown in Fig. 9. In some sense the results of calculations with only one component with a pure cosine profile give an upper bound for the frequencies of a more squared density. We remember that the calculations for $M=1$ give vanishing frequencies for $\mathcal{X}\rightarrow 0.5$ at any z_y. Hence we expect that the same happens with a more squared profile. Really the spectrum with five components exhibited in Fig. 10 confirms without a shadow of a doubt that the system is not able to support modes when the minimum density is zero. We note that [Fig. 10(a)] the numerical values are in complete agreement with those of Eliasson *et al.*[8] We emphasize that our choice for the $\mathcal{X}_i$ makes it easy to explore the neighborhood of $\mathcal{X}=0.5$, extending the previous calculations. Although we have avoided the Gibbs phenomena the convergence of the roots of the finite secular equation obtained truncating Eq. (6) gets slower and slower when $\mathcal{X}\rightarrow 0.5$. The potential associated with the eigenmodes shows large changes calculating the frequen-

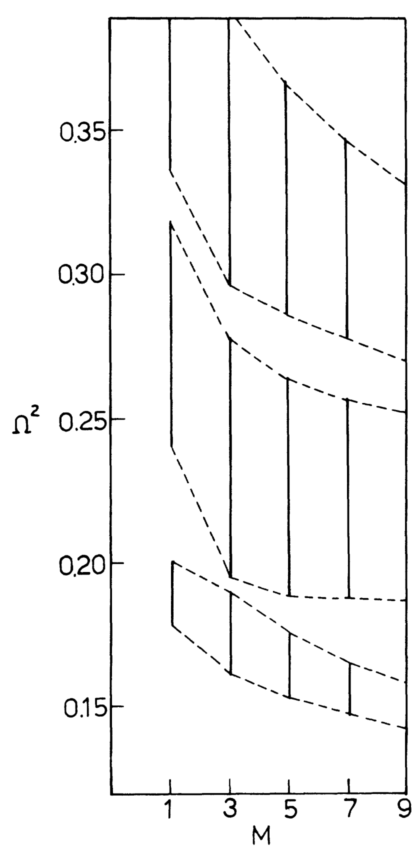

FIG. 9. The first three plasmonic bands increasing the number M of components in Eq. (4).

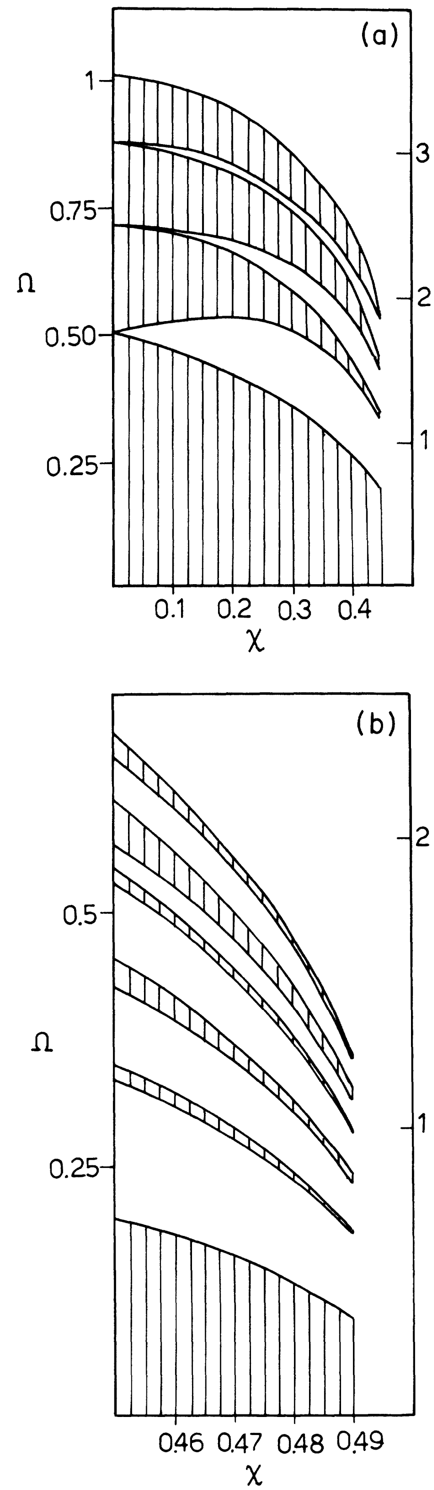

FIG. 10. We show the first plasmonic bands as a function of $\mathcal{X}$ at $z_y=0$ ($M=5$).

cies with an increasing accuracy, and it is difficult to obtain satisfactory results. In other words the Fourier series for the potential has a very slow convergence, and we need a large number of terms to stabilize it. However, the qualitative results convince us that the connection between vanishing frequencies and localization at minimum density is still present.

We emphasize that this result, which we believe to be the main result of this work, for a continuous profile, is in contrast with those obtained with a single stripe[9] or a periodic array of stripes[10] where there are infinite or finite regions of zero density. In our opinion the induced potential tends to localize around the minimum of n_0 in such a way that the induced density tries to balance the spatial variation of n_0. On the other hand, if there are forbidden regions for the electrons (which implies discontinuities on n_0) this has serious consequences on their dynamics, frustrating the basic tendency which we have found in the model studied. The possibility of accumulating charge against the boundaries dramatically changes the dispersion relation. It would be interesting to investigate what happens when, starting with a continuous profile that vanishes at one point, we move to a discontinuous one with a zero-density region of increasing width. The question remains open of what kind of profile (continuous or discontinuous) is the best one to use for applying the hydrodynamical model to the physical systems discussed in Sec. I.

V. CONCLUSIONS

We have studied the plasmonic bands of an array of 2D stripes, trying to stress the effect of the shape of the equilibrium profile assumed as a given continuous periodic function. We note that this is the only equilibrium property which enters in the equation for the induced potential (3).

We start with a cosine profile and by adding new odd components we approach a periodic step profile. The plasmonic bands of cosine profile narrow when $z_y \to \infty$ in such a way that the squared frequencies grow linearly in z_y with a slope given by the minimum density while all the gaps become equal to each other. When the minimum density goes to zero the system does not support plasmons and this happens not only in the asymptotic region but even when $z_y = 0$. The reasons for this behavior have been found in the localization of potential and density fluctuations on the point of minimum density. When the regions of zero density have a finite width the edges act as rigid barriers for the density fluctuations. This gives rise to dispersion relations which can be very different. This explains why our results are in contrast with those of Refs. 9 and 10.

The passage to more squared profiles lowers and narrows the bands and also in this more general case when the minimum density vanishes all the frequencies go toward zero. For the physical systems studied in the literature the external radiation couples only with nonradiative plasmons of zero z_y. On the other hand the localization property discussed could be of some interest for technological applications such as a truly microscopic waveguide. However, the introduction of a suitable periodicity also in the y direction could be used in order to overcome the difficulty of exciting the localized plasmons of large z_y, through the folding of the bands with respect to z_y.

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