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Screening and oscillations in a spatially modulated 2D electron gas

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Abstract. The screening of a one-dimensional potential relief by a 2D electron gas and plasma oscillations is investigated for the case of cosine-like external potentials. The analytical solution of the screening problem provides an opportunity for the development of qualified numerical procedures for linear oscillations within the framework of the hydrodynamical model. A simple analytical expression is obtained for the frequency of a zero-wave vector plasmon as a function of electron concentration and potential amplitude. A strong frequency drop at the critical point of concentration between linear and non-linear screening regimes, which was observed experimentally, is explained. In the vicinity of the critical concentration the asymptotical expressions are derived, which hold for any smooth periodical potential.

1. Introduction

In recent years experiments have been developed extensively on two-dimensional systems with artificial periodicity in one direction [1–5]. The potential relief in the plane of the 2D electron channel in MOS devices or heterostructures is produced by a specially shaped electrode or by photoionized impurities. The present work was stimulated by far infrared absorption (FIR) experiments [4, 5], in which the zero-wave vector odd modes of plasma oscillations with non-zero spatially averaged current density are observed. The dependence of resonant frequencies on the averaged areal density \bar{n} in the device was investigated, and the most specific feature was found in a sharp frequency drop at some value of \bar{n} . This value did not depend on the transverse magnetic field also present in the experiment and was considered to be the critical concentration, below which the redistribution of electron density fails to screen the external potential completely and the modulated continuous charge distribution is transformed into a periodic array of isolated stripes.

This transition and its effect on the plasma resonance spectrum is the subject of the present work. The period and amplitude of the external potential in the experiment were usually 100 nm and 1 eV, respectively. One may, therefore, assume that the quantum effects are negligible. The approximations and method of calculation do not greatly differ from those used in [6–8], where the dispersion law of plasmons (mainly along the stripes) for different profiles of equilibrium electron concentration was studied.

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In the present work the cosine-like external potential is considered, for which, as is shown below, the analytical expression for equilibrium distribution and plasma resonance frequencies at zero-wave vector along the plane in the whole range of concentration can be obtained. The screening effect of a gate electrode in real devices is not taken into account.

2. General considerations

The external potential $U(x)$ is assumed to depend only on one of the coordinates along the plane, so the equilibrium distribution of electron density $n_0(x)$ and electrostatic potential $\varphi_0(x, z)$ are determined through the 2D Poisson equation

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2} \right) \varphi_0(x, z) = -4\pi e \varepsilon^{-1} n_0(x) \delta(z) \quad (1)$$

(e is electron charge, ε is dielectric constant) and the constancy of the potential combined with the external potential $U(x)$ is

$$\varphi_0(x, 0) + U(x) = \text{constant}. \quad (2)$$

The latter condition must hold over the whole plane if the concentration does not vanish anywhere. In this case ideal screening of the external potential takes place. In the opposite case the electron concentration is insufficient for complete screening, so the equipotentiality (2) takes place only within the 'metal' regions of the plane with the positive electron concentration $n_0 > 0$. In the remaining 'dielectric' regions with the absence of electrons, the full potential exceeds its level in metal regions. Thus the non-linear screening problem (see [9]) appears in a 2D variant. A very similar problem was treated in the theory of the charged surface of liquid helium and in [10], but the present case is much simpler due to the 1D nature of the external potential. The note by Shikin [11] is also of some interest.

In order to describe the small plasma oscillations, which generally differ in symmetry from the equilibrium distribution, one needs the equations of the oscillating part of electron density $n(x, y) e^{-i\omega t}$ and electrostatic potential $\varphi(x, y, z) e^{-i\omega t}$. The first of these equations is the 3D (in contrast with (1)) Poisson equation

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \varphi(x, y, z) = -4\pi e \varepsilon^{-1} n(x, y) \delta(z). \quad (3)$$

The second equation

$$i\omega n(x, y) = \nabla[\hat{\sigma}(x)\nabla\varphi(x, y, 0)] \quad (4)$$

is the kinetic one and follows from the continuity equation combined with Ohm's law $\mathbf{j} = \hat{\sigma}\mathbf{E}$. The 2D conductivity tensor $\hat{\sigma}$ has the form

$$\begin{aligned} \sigma_{xx} &= \sigma_{yy} = i\omega n_0(x) e^2 / m(\omega^2 - \omega_c^2) \\ \sigma_{xy} &= -\sigma_{yx} = -\omega_c n_0(x) e^2 / m(\omega^2 - \omega_c^2). \end{aligned} \quad (5)$$

(The cyclotron frequency $\omega_c = eH/mc$ equals zero in the absence of the magnetic field H .) Naturally, equation (4) has sense only within the 'metal' regions, where $n_0(x)$ and $n(x, y)$ exist. Equations (1-5) give the full description of the equilibrium state and the

small oscillations of an electron gas with 1D inhomogeneity under the classical cold plasma approximation (the hydrodynamical model).

If the solution of the equilibrium part of the problem has already been found, the direct way to find the spectrum of plasma oscillations is to expand n and φ in the orthogonal bases N_k and Φ_k with elements satisfying pairwise (at every value of index k) the Poisson equation (3)

$$\varphi(x, y, z) = \sum_k \psi_k \Phi_k(x, y, z) \quad n(x, y) = \sum_k \psi_k N_k(x, y).$$

When using this expansion, the determination of the ω spectrum is reduced to the generalized eigenvalue problem

$$(\omega^2 - \omega_c^2)\hat{A}\psi = \hat{B}(\omega)\psi \tag{6}$$

with symmetric matrix components

$$A_{kk'} = \int \Phi_k(x, y, 0)N_{k'}(x, y) dx$$

$$B_{kk'} = -ie^{-1}(\omega^2 - \omega_c^2)\omega^{-1} \int (\nabla\Phi_k^*)\hat{\sigma}(\nabla\Phi_{k'}) dx. \tag{7}$$

3. Specification of the problem

The following consideration deals mostly with the cosine-like profile of the external potential energy

$$U(x) = -U_0 \cos(Qx)$$

which simplifies the problem dramatically and has at least qualitative bearing on the real experimental situation. The most remarkable feature of this kind of potential is that the problem of screening can be solved analytically over the whole range of concentrations. For example, in the case of high concentration the equilibrium solution is trivial

$$n_0(x) = \bar{n} + (U_0 Q \epsilon / 2\pi e^2) \cos(x). \tag{8}$$

The border of the ideal screening regime corresponds to vanishing of $n_0(x)$ at the maxima of the potential $U(x)$. For the case considered this gives the critical value of concentration

$$\bar{n} = n_c = U_0 Q \epsilon / 2\pi e^2.$$

It is convenient to rewrite equations (1)–(5) in a dimensionless form taking U_0 as the unit for potential energy, n_c as the unit for concentration, and Q^{-1} as a unit for length. The optimal unit for frequency is found to be the frequency $\omega_p = (2\pi e^2 n_c Q / m \epsilon)^{1/2}$ of a plasmon with wave vector Q in a homogeneous electron gas of concentration n_c . Another simplification of the equations is possible by restricting the treatment to the case of a plasmon wavevector directed along the x axis. These modes are uniform in the y direction, so that $n(x, y)$ and $\varphi(x, y, z)$ can be regarded as independent of y . The general case is not much more complicated, but of principal interest here are modes with zero wave vector, so we only consider the case $q_y = 0$ below, and the coordinate y is omitted in the formulae.

Thus the system of equations to be solved takes the form

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial}{\partial z^2}\right)\varphi_0(x, z) = -4\pi n_0(x)\delta(z) \quad (9)$$

$$\varphi_0(x, z) - \cos(x) = \text{constant} \quad (10)$$

for x where $n_0(x) > 0$,

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2}\right)\varphi(x, z) = -4\pi n(x)\delta(z) \quad (11)$$

$$(\omega^2 - \omega_c^2)n(x) = -\frac{\partial}{\partial x}\left(n_0(x)\frac{\partial\varphi(x, 0)}{\partial x}\right) \quad (12)$$

and the matrices $\hat{\mathbf{A}}$ and $\hat{\mathbf{B}}$ entering the eigenvalue problem (6) for calculation of resonant frequencies have components

$$A_{kk'} = \int_{-\pi}^{\pi} \Phi_k(x, 0)N_{k'}(x) dx, \quad (13)$$

$$B_{kk'} = \int_{-\pi}^{\pi} \left(\frac{\partial}{\partial x}\Phi_k(x, 0)\right)n_0(x)\left(\frac{\partial}{\partial x}\Phi_{k'}(x, 0)\right)\frac{dx}{2\pi}$$

Since $\hat{\mathbf{B}}$ is independent of ω , the equation (6) is equivalent to the diagonalization of an asymmetric matrix $\hat{\mathbf{A}}^{-1}\hat{\mathbf{B}}$. The diagonalization of the matrix is a standard problem of numerical methods and can be solved very precisely (the matrix must of course be truncated at sufficiently high indices).

The important point is that as it follows from the equation (6) that the magnetic field enters the mathematical part of the problem in a trivial way, and so does not require special consideration, so only the case $\omega_c = 0$ will be discussed below. This simplification is only justified when dealing with plasmon dispersion along the y direction.

4. Ideal screening

In this region of average concentration \bar{n} , described by the condition $\bar{n} > 1$, the equilibrium solution is given by equation (8) and has the dimensionless form

$$n_0(x) = \bar{n} + \cos(x). \quad (14)$$

One can hardly invent anything better than the usual Fourier expansion used in [6–8] for the oscillating parts of the potential and concentration

$$\begin{aligned} \Phi_k(x, z) &= \exp(ikx + iq_x x + iq_y y - |kz|) \\ N_k(x) &= [(k - q_x)^2 + q_y^2]^{1/2} \exp(ikx + iq_x x + iq_y y) \end{aligned} \quad (15)$$

where k is an integer index and \mathbf{q} is an arbitrary directed 2D wave vector.

In line with the assumptions adopted in deriving the equations (9–12), only the plasmon dispersion law transverse to stripes $\omega^2(q_x)$ will be studied. When setting $q_y = 0$, the basis (15) gives for matrices $\hat{\mathbf{A}}$ and $\hat{\mathbf{B}}$ the expressions

$$\begin{aligned} A_{kk'} &= |k + q_x|\delta_{kk'} \\ B_{kk'} &= |(k + q_x)(k' + q_x)|(\bar{n}\delta_{kk'} + \frac{1}{2}\delta_{k \pm 1, k'}). \end{aligned}$$

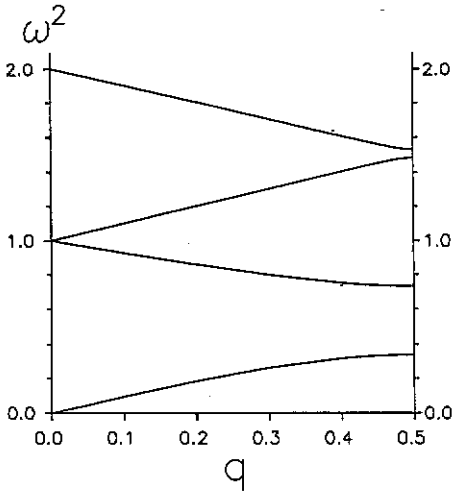


Figure 1. Dispersion curves $\omega^2(q_x)$ for dimensionless density $\bar{n} = 1.5$. The unit $(\bar{n}^2 - 1)^{1/2}$ for ω^2 is chosen to demonstrate the simple rule for the resonant frequencies at $q = 0$.

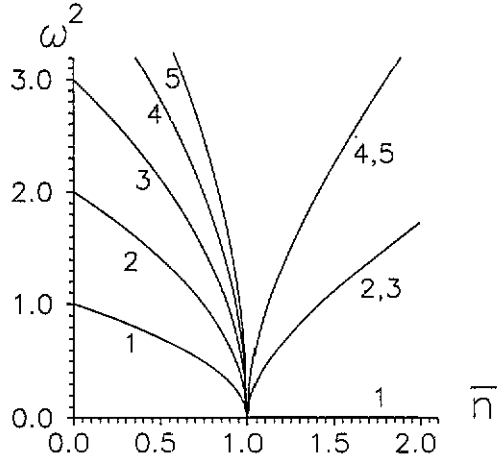


Figure 2. The resonance position at $q = 0$ as a function of dimensionless density \bar{n} . Modes are numerated in the ascending order of frequency (taking into consideration the doubling at $\bar{n} > 1$). The parity of the number corresponds to the mode parity.

As an example, the dispersion curves $\omega^2(q_x)$ for $\bar{n} = 1.5$ are shown in figure 1. The first point demonstrated by this figure is the absence of gaps in a plasmon spectrum at zero-wave vector point. It should be emphasized that this degeneracy is not trivial and takes place only for the sinusoidal external potential. Secondly, one peculiar mode exists whose frequency goes to zero at $q = 0$. This mode is of Goldstonian origin and corresponds to spatially uniform constant current. It is odd in terms of the electron density distribution and manifests itself in the FIR experiments as a cyclotron resonance (in the presence of the magnetic field).

Note that the results of the work [8] considering in detail the cosine-like potential with $\bar{n} > 1$ are suspicious. They do not contain any trace of degeneracy at $q = 0$ and give very strange dispersion curves $\omega^2(q_x)$ with extrema in an intermediate region of q_x (between $q_x = 0$ and $q_x = \pm \frac{1}{2}$). Such a discrepancy can hardly be treated in any positive sense and appears to come from numerical mistakes in [8].

For the modes with zero wave vector q , which are the main object of the present consideration, the full basis (15) is not the optimal one from the numerical accuracy point of view. In this case the symmetry of the equations invites us to classify the solutions by the parity of charge distribution and use two alternative bases: the even

$$\Phi_k(x, z) = \cos(kz) \exp(-k|z|) \quad N_k(x) = k \cos(kx) \quad (k = 1, 2, \dots)$$

and the odd

$$\Phi_k(x, z) = \sin(kx) \exp(-k|z|) \quad N_k(x) = k \sin(kx) \quad (k = 1, 2, \dots).$$

Both bases result in the same pair of matrices $\hat{\mathbf{A}}$ and $\hat{\mathbf{B}}$

$$A_{kk'} = (k/2)\delta_{kk'}$$

$$B_{kk'} = (\bar{n}k^2/2)\delta_{kk'} + (kk'/4)\delta_{k\pm 1, k'}$$

in agreement with the dispersion law degeneracy noted above.

The diagonalization of matrix $\hat{\mathbf{A}}^{-1}\hat{\mathbf{B}}$ gives a rather curious result for the case $q = 0$: within the accuracy of calculation (better than five digits for $|\bar{n} - 1| > 0.01$) the spectrum is ideally described by a simple analytical formula

$$\omega^2 = Z(\bar{n}^2 - 1)^{1/2} \tag{16}$$

where $Z = 0, 1, 2, \dots$ for odd modes and $Z = 1, 2, 3, \dots$ for even ones.

5. Non-linear screening

This area of consideration is somewhat more involved, so only the case $q_x = 0, q_y = 0$ is considered here. The basic ideas are taken from the conformal transformations technique, which is a well known and very powerful tool in 2D electrostatics problems. The complex variable $\xi = x + iz$ is introduced, and the main point is to construct a suitable full set of functions of this variable, analytic outside the cuts, corresponding to the 'metal' regions. For any such function, its real and imaginary parts will both give some solution of the Laplace equation outside the cuts, and give the corresponding charge distribution along the cuts through the boundary conditions.

For the particular problem considered here one needs the periodic solutions $\Phi(x, z)$. As is usual in the conformal transformations technique, the solution is found by guess-work rather than by regular methods, so it is only worthwhile to present the result, which can be checked if necessary. The appropriate full set of functions for solving the equilibrium problem and the expansion of oscillating perturbations consists of two subsets of different parity. The even one is

$$\begin{aligned} \Phi_1(x, z) &= \text{Re}[\ln\{F[\sin(\xi/2)/\sin(d/2)]\}] \\ \Phi_k(x, z) &= \text{Re}[\{F[\sin(\xi/2)/\sin(d/2)]\}^{2k-2}] \quad k = 2, 3, \dots \end{aligned} \tag{17a}$$

where $F(\xi) \equiv \xi - (\xi^2 - 1)^{1/2}$ (obviously the logarithm corresponds to the zero power). The odd subset is constructed in a similar manner

$$\Phi_k(x, z) = \text{Re}[\cos(\xi/2)\{F[\sin(\xi/2)/\sin(d/2)]\}^{2k-1}] \quad k = 1, 2, \dots \tag{17b}$$

The functions (17) have the required periodicity with x , tend to zero at $|z| \rightarrow \infty$, and have cuts along the intervals $|x - 2\pi m| \leq d, z = 0$. As pointed out above, the main point is that they are the real parts of analytical functions, and hence satisfy the Laplace equation outside the cuts. Thus, each of the subsets may be used as a basis for the expansion of the potential. The corresponding bases for the concentration are derived from (17) through the boundary condition

$$N_k(x) = - \left. \frac{\partial \Phi_k(x, z)}{\partial z} \right|_{z=+0}$$

The equilibrium distribution is composed of a combination of the even subset's elements $\Phi_1(x, z)$ and $\Phi_2(x, z)$ with the corresponding concentrations

$$\begin{aligned} N_1(x) &= \frac{1}{2} \cos(x/2) / [\sin^2(d/2) - \sin^2(x/2)]^{1/2} \\ N_2(x) &= \frac{\cos(x/2)}{\sin^2(d/2)} \frac{2 \sin^2(x/2) - \sin^2(d/2)}{[\sin^2(d/2) - \sin^2(x/2)]^{1/2}} \end{aligned}$$

The potential $\Phi_1(x, 0)$ is zero along the interval $-d < x < d$, so the amplitude of the second harmonic

$$\Phi_2(x, 0) = [2 \sin^2(x/2) - \sin^2(d/2)]/\sin^2(d/2)$$

is determined immediately by the amplitude of the external potential, and equals $-2\pi \sin^2(d/2)$. In turn, the harmonic $N_2(x)$ does not contribute to the average concentration, so the value $4\pi\bar{n}$ follows for the amplitude of harmonic $N_1(x)$. The size d of 'metal' regions is fixed by the condition of vanishing electric field tangential components at the edges of the regions (see e.g. [10]), which takes, in the case under consideration, the form, $\sin^2(d/2) = \bar{n}$. Thus the equilibrium distribution of the concentration is obtained

$$\begin{aligned} n_0(x) &= 2 \cos(x/2)[\bar{n} - \sin^2(x/2)]^{1/2} & |\sin(x/2)| \leq \bar{n}^{1/2} \\ n_0(x) &= 0 & |\sin(x/2)| > \bar{n}^{1/2}. \end{aligned} \tag{18}$$

The calculation of matrices $\hat{\mathbf{A}}$ and $\hat{\mathbf{B}}$ is based upon the fact that at the cuts (i.e. in metal regions) the potentials (17) are expressed in terms of Chebyshev polynomials of the variable $\sin(x/2)/\sin(d/2)$. The matrices $\hat{\mathbf{A}}$ and $\hat{\mathbf{B}}$ have components

$$A_{kk'} = k\delta_{kk'} \quad B_{kk'} = (2 - \bar{n})k^2\delta_{kk'} + (\bar{n}/2)kk'\delta_{k\pm 1, k'}$$

in the odd case, and somewhat more complicated components

$$\begin{aligned} A_{kk'} &= \frac{1}{8}(2 - \bar{n})(2k - 1)\delta_{kk'} - (\bar{n}/8)(k\delta_{k+1, k'} + k'\delta_{k, k'+1}) \\ B_{kk'} &= \frac{1}{8}[(2 - 2\bar{n} + \bar{n}^2) + (8 - 8\bar{n} + 3\bar{n}^2)k(k - 1)]\delta_{kk'} \\ &\quad - [\bar{n}(2 - \bar{n})/4](k^2\delta_{k+1, k'} + k'^2\delta_{k, k'+1}) \\ &\quad + (\bar{n}^2/16)[k(k + 1)\delta_{k+2, k'} + k'(k' + 1)\delta_{k, k'+2}] \end{aligned}$$

in the even case. The result of the diagonalization matrix $\hat{\mathbf{A}}^{-1}\hat{\mathbf{B}}$ is just as remarkable as in region $\bar{n} > 1$: the resonance frequencies are exactly described by the simple formula

$$\omega^2 = Z(1 - \bar{n})^{1/2} \tag{19}$$

with $Z = 1, 2, \dots$ (no Goldstone mode). The even Z corresponds to even modes, the odd Z to odd modes. The relations (16) and (19) are plotted together in figure 2.

6. Asymptotic solutions

To obtain the expressions (16) and (19) in an 'honest' way, i.e. analytically, appears to be impossible. Only the asymptotic behaviour in various limiting cases can be studied analytically to confirm these results. Skipping the limits $\bar{n} \rightarrow \infty$ and $\bar{n} \rightarrow 0$, in which the off-diagonal parts of $\hat{\mathbf{A}}$ and $\hat{\mathbf{B}}$ may be considered as small perturbations, let us proceed with the region $\bar{n} \approx 1$. The analytical solution is of specific importance in this region because of the poor accuracy of the numerical calculations due to the ill-conditioned nature of matrix $\hat{\mathbf{B}}$. The asymptotic solution is based upon the assumption that the oscillating part of the concentration is localized near the external potential maxima (further consideration gives the scale $|\bar{n} - 1|^{1/2}$), where $U(x)$ can be approximated by a parabola

$$U(x) = -\cos(x) \approx 1 - x^2/2$$

x being reckoned from the maxima of $U(x)$.

For $\Delta \equiv \bar{n} - 1 \rightarrow +0$ the equilibrium distribution has, according to (14), the form $n_0(x) = \Delta + (x^2/2)$. For the oscillating parts of the potential and the concentration, the solutions can be guessed

$$\begin{aligned}\varphi(x, z) &= x / \{x^2 + [(2\Delta)^{1/2} + |z|]^2\} \\ n(x) &= 2(2\Delta)^{1/2}x / (2\Delta + x^2)\end{aligned}\quad (20)$$

which satisfy equations (11), (12) with $\omega^2 = (2\Delta)^{1/2}$ and describe the lowest non-Goldstonian mode (3 in figure 2).

For $\Delta \rightarrow -0$ the equilibrium distribution follows from (18)

$$n_0(x) = x[(x^2/4) - \Delta]^{1/2}.$$

(The width of the stripe free from electrons is $4\Delta^{1/2}$.) The lowest mode (1 in figure 2) is described by the expressions

$$\begin{aligned}\varphi(x, z) &= \text{Re}\{(\xi/2)/[\Delta^{1/2} + (\Delta - \xi^2/4)^{1/2}]\} \\ n(x) &= 2\Delta/x^2(x^2/4 - \Delta)^{1/2} \quad (|x| > 2\Delta)\end{aligned}\quad (21)$$

and has the frequency $\omega^2 = \Delta^{1/2}$.

The asymptotical dependences $\omega^2(\Delta)$ found here coincide with those given by the solutions (16) and (19) for the sinusoidal potential for $|\Delta| \ll 1$ for the lowest non-trivial modes. Note that both $\varphi(x)$ and $n(x)$ are functions of x in (20) and (21). Similarly, the solutions for all other modes can be constructed.

7. Discussion

It should be taken into account when comparing the results with experiments [4, 5], that in the latter it is not the average concentration that is directly varied, but a gate voltage. The voltage variation changes the external potential amplitude as well as \bar{n} , so the quantitative comparison is not too easy. The other complicating effect is the screening of Coulomb interactions by a gate electrode. Besides that, the real profile of potential relief is not sinusoidal and is usually closer to the smeared rectangular potential.

Nevertheless, the qualitative agreement between the results obtained here and experiment is evident. In the region of low concentration only the lowest resonance is observed experimentally. For supercritical values of concentration only a lowest finite frequency mode (3 in figure 2) is observable without the magnetic field. When a transverse magnetic field is present the mode 1, corresponding to usual cyclotron resonance, appears (the higher visible resonances are difficult to treat). One should note that the magnetic field increase causes the upward shift of the picture of resonances $\omega^2(\bar{n})$, as a whole, by ω_c^2 in agreement with equation (12).

The most delicate matter is the measurement of the frequency drop at the critical value of n between the ideal and non-linear screening regimes. The calculations presented above give the drop down to $\omega = 0$ by a square root law for $\omega^2(\bar{n})$. According to section 5 this result is unambiguously general for any smooth periodic potential and is caused by the local decrease of plasmon frequency in the regions of low concentration. The considerably weaker drop found in the experiments may come from the macroscopic spatial inhomogeneity of the system, but the more credible source of this discrepancy is the neglect of dissipative processes in the hydrodynamic model used in the present work.

The importance of dissipation is emphasized by the rather large width of the FIR peaks in the critical region of \bar{n} .

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