Classification
Physics Abstracts
71.45G

New plasma waves and soft modes in narrow gap inversion layers

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(Reçu le 22 mars 1981, révisé le 10 août, accepté le 29 septembre 1981)

Résumé. — Une interaction électron-électron dans des couches d'inversion des semi-conducteurs, à bande interdite étroite a été considérée. Nous obtenons des nouvelles excitations collectives comme résultat de l'occupation simultanée de plus d'une zone de surface. Une des solutions est du type d'un mode mou $\omega(|\mathbf{k}|) = v \cdot (p_1 - p_2 - |\mathbf{k}|)$ où p_1 et p_2 sont des impulsions de Fermi pour les deux zones de surface. L'autre mode est semblable aux excitations interbandes qui sont créées par les transitions d'une bande d'énergie plus élevée vers une autre, qui a une énergie inférieure.

Abstract. — The influence of the electron-electron interaction is considered in the inversion layers of narrow gap semiconductors. Due to the simultaneous filling of more than one surface level new collective modes are created. One of the new excitations is of the soft mode type at a wave vector $|\mathbf{k}| = p_1 - p_2$, where p_1 and p_2 are the two surface subband Fermi wave vectors. The other mode is similar to the interband excitations being created by transitions from the higher energy subband to the lower energy one.

Over the last few years the electronic structure of inversion layers has been intensively studied. In view of the electronic properties of two-dimensional systems the inversion layers offer unique conditions for investigation. The applied electric field is screened on lengths of order of L_D causing band-bending. The electron wave length is of the same order of magnitude as L_D . Hence, the motion perpendicular to the surface is quantized [1]. The periodicity parallel to the surface transforms these electronic levels into surface subbands. In narrow gap semiconductors the structure of the inversion layers is more complicated, because of the simultaneous filling of more than one surface band [2-4]. The electron gas in these two-dimensional bands is degenerate as in the case of metals. The Fermi surface for parabolic dispersion is a circle. In narrow gap semiconductors the electron-electron interaction is of special importance and may lead to a more complicated plasmon spectrum and other collective phenomena such as CDW, Wigner crystallization commensurate or incommensurate with the lattice parameter. Experimental work on narrow gap inversion layers in InSb and PbTe demonstrated clear differences from the Si and Ge inversion layers. For instance, the FIR spectra as obtained in [5] shows an additional peak, not seen in Ge and Si. In the present work a two-band model of the inversion layer taking into account the effects of electron-electron interaction is considered. It is worth noting

that in the case of degenerate layers the electron-electron interaction leads to an instability of the two-dimensional electronic liquid resulting in CDW or other structures.

1. Elementary excitation in non-interacting 2-d electron gas. — The wave function of the exact ground state of the interacting system is a superposition of the wave functions of the ground state of the non-interacting particles and of its excitations, constituting a complete set. The low energy elementary excitations will dominate such a perturbation expansion because of the small energy denominators for these excitations. In narrow gap semiconductors the degenerate 2-d electron gas has interband elementary excitations [6, 7] generating the above mentioned instability. Therefore we concentrate our attention on the excitations of an ideal system of this type. For the sake of simplicity we use a model with : (i) two neighbouring surface subbands and (ii) a circular Fermi surface (Fermi-line). The Fermi energy is denoted by μ . The relations $\varepsilon_1(\mathbf{p}_1) = \varepsilon_2(\mathbf{p}_2) = \mu$ (Fig. 1) determine both the Fermi momenta p_1 and p_2 . The first band is filled up to momentum p_1 and the second up to p_2 . Since $p_1 \neq p_2$, the Fermi « surface » consists of two sheets S_1 and S_2 , one fitting inside the other. This specific property of the Fermi « surface » is reflected in the electron-hole excitation spectrum. In this situation, creation of interband pairs with zero energy transfer is possible.

Fig. 1. — Dispersion relation of the surface subband (up). The corresponding Fermi « surface » is shown below.

The electrons in these pairs are from the first Fermi sheet S_1 and the holes are from the second Fermi sheet S_2 (or *vice versa*). Of course, these interband excitations are only part of the total excitation spectrum. There are also the typical Fermi-liquid excitations when the electron and the hole are on one and the same surface subband. Figure 2 represents the spectrum of the interband electron-hole excitations. It is seen from the figure that, when the momentum $|\mathbf{k}|$ is in the region between $p_1 - p_2$ and $p_1 + p_2$, the excitation energy can be arbitrarily small approaching zero. In the region $|\mathbf{k}| < p_1 - p_2$ and $|\mathbf{k}| > p_2 + p_1$ the excitation energy is always finite. Near such points, according to the 3-d Fermi liquids theory, the dielectric constant has a singularity—a Kohn anomaly. In our 2-d model this singularity is also present. In the case of almost equal Fermi sheets ($p_1 \approx p_2$) the anomaly near the point $p_1 - p_2$ is even stronger, being proportional to $(p_1 - p_2)^{-3/2}$. It will be shown that this leads to an instability producing a surface charge density wave.

The interband excitations can be described more clearly from the physical point of view in real space. The electronic z -envelope wave functions, from one and the same surface band with equal number of zeros, are similar. Therefore, the electrons from

Fig. 2. — The interband elementary excitation spectrum - full lines. In comparison, the intraband excitations are shown with dashed line.

different surface bands are spaced at different mean distances from the surface. In this sense it is possible to consider the inversion layer on a narrow gap semiconductor as consisting of two electronic « sheets ». Interband excitations with a hole from one band and an electron from the other correspond in real space to an electron and a hole from different « sheets ». It is clear that the interband excitations give rise to a dipole moment.

2. Evaluation of the excitation spectrum. — We consider a simple model with two parabolic bands. This straightforward calculation confirms the simple picture considered in section 1. The dispersion relations for the two filled bands are the following :

$$\varepsilon_1(\mathbf{p}) = \mathbf{p}^2/2m, \quad \varepsilon_2(\mathbf{p}) = \varepsilon_0 + \mathbf{p}^2/2m. \quad (1)$$

Here $\mathbf{p}$ is 2-d momentum. The wave functions are of the type

$$\begin{aligned} \psi_1(x, y, z) &= \exp(i\mathbf{p} \cdot \boldsymbol{\rho}) f_1(z), \\ \psi_2(x, y, z) &= \exp(i\mathbf{p} \cdot \boldsymbol{\rho}) f_2(z) \end{aligned} \quad (2)$$

where $\boldsymbol{\rho} = (x, y)$, and the envelope functions f_1 and f_2 are orthogonal to each other, decreasing exponentially inside the crystal ($z \rightarrow \infty$). The non-interacting Hamiltonian of the electrons in the layer is :

$$H_0 = \sum_{|\mathbf{p}| < p_1} \varepsilon_1(\mathbf{p}) a_{1\mathbf{p}}^\dagger a_{1\mathbf{p}} + \sum_{|\mathbf{p}| < p_2} \varepsilon_2(\mathbf{p}) a_{2\mathbf{p}}^\dagger a_{2\mathbf{p}} \quad (3)$$

where $a_{n\mathbf{p}}^\dagger$, $a_{n\mathbf{p}}$ are the creation and destruction operators for electrons with momentum $\mathbf{p}$ in the n -th band with an envelope function $f_n(z)$. The electron-electron interaction term is :

$$H_{\text{int}} = \sum_{n, \mathbf{p}_1, \mathbf{p}_2, \mathbf{k}} \left\langle f_{n_1}(z_1) f_{n_2}(z_2) \left| \frac{2\pi e^2}{|\mathbf{k}| \kappa_\infty} \exp(-|\mathbf{k}| \cdot |z_1 - z_2|) \right| f_{n_3}(z_1) f_{n_4}(z_2) \right\rangle a_{n_1, \mathbf{p}_1 + \mathbf{k}}^\dagger a_{n_2, \mathbf{p}_2 - \mathbf{k}}^\dagger a_{n_4, \mathbf{p}_2} a_{n_3, \mathbf{p}_1}. \quad (4)$$

The interaction in the 2-d layer, in a similar way to the 3-d Fermi systems, leads to collective modes in the excitation spectrum, which for charged fermions are plasma waves. In order to obtain the collective modes of the degenerate inversion layer we have to study the poles of the scattering amplitude Γ . In RPA the equation for Γ is :

(5)

with the following correspondence rule :

$$\begin{aligned} \overline{n, p} &= iG_n(p) \equiv (p_0 - \varepsilon_n(\mathbf{p}) + i\delta p_0) \quad \delta \rightarrow +0 \quad (\text{electronic propagator for } T=0) \\ \begin{array}{c} n_2, p_2 - \mathbf{k} \leftarrow n_4, p_2 \\ \vdots \\ n_1, p_1 + \mathbf{k} \leftarrow n_3, p_1 \end{array} &= -i \frac{2\pi e^2}{|\mathbf{k}| \kappa_\infty} \langle f_{n_1}(z_1) f_{n_2}(z_2) | e^{-|\mathbf{k}| \cdot |z_1 - z_2|} | f_{n_3}(z_1) f_{n_4}(z_2) \rangle \equiv -iV_{13,24}^k. \end{aligned} \quad (6)$$

Substituting these expressions in (5) we obtain the equation for Γ in the form :

$$\Gamma_{n_1, n_3; n_2, n_4}^{p_1, p_2; k} = V_{n_1, n_3; n_2, n_4}^{p_1, p_2; k} - i \sum_{n', n''} \int \frac{d^3 p'}{(2\pi)^3} V_{n_1, n_3; n', n''}^{p_1, p'; k} G_{n'}(p' + k) G_{n''}(p') \Gamma_{n', n''; n_2, n_4}^{p', p_2; k}. \quad (7)$$

Here $p = (p_0, \mathbf{p})$, $k = (\omega, \mathbf{k})$,

$$\Gamma_{n_1, n_3; n_2, n_4}^{p_1, p_2; k} = \Gamma(n_1, p_1 + k; n_2, p_2 - k; n_3, p_1; n_4, p_2)$$

and similar notation for V is used.

In the particular case of the Coulomb interaction, equations (7) are easily reduced to algebraic equations, because the interband matrix element depends only on the momentum transfer and not on $\mathbf{p}$ and $\mathbf{p}'$ separately. For this reason the kernel of the integral equation is independent of $\mathbf{p}_1$ and Γ also. The integration over $\mathbf{p}'$ is carried out by introducing the polarization operator P :

$$P_{n''n'}^k = -i \int \frac{d^3 p'}{(2\pi)^3} G_{n''}(p' + k) G_{n'}(p'). \quad (8)$$

The algebraic system is

$$\Gamma_{n_1, n_3; n_2, n_4}^k = V_{n_1, n_3; n_2, n_4}^k + \sum_{n', n''} V_{n_1, n_3; n', n''}^k P_{n'', n'}^k \Gamma_{n', n''; n_2, n_4}^k. \quad (9)$$

It can be written in the form

$$\Gamma = \kappa^{-1} V \quad (10)$$

where κ is the matrix of the dielectric susceptibility. From (10) it is clear that Γ has poles only if the matrix κ is degenerate i.e. when its determinant vanishes,

$$\text{Det } \kappa = 0. \quad (11)$$

Equation (11) determines the dispersion relation of the collective excitations in a 2-d electronic liquid of the type considered here. The roots of this equation are easily found in two cases :

i) For $|\mathbf{k}| \rightarrow 0$ the interband polarization operators are of little importance and (11) reduces to :

$$\text{Det} \begin{bmatrix} 1 - V_{11,11}^k P_{11}^k & -V_{11,22}^k P_{22}^k \\ -V_{22,11}^k P_{11}^k & 1 - V_{22,22}^k P_{22}^k \end{bmatrix} = 0. \quad (12)$$

For small $|\mathbf{k}|$ we hence obtain the 2-d dispersion relation

$$\omega^2 = \frac{2\pi(n_1 + n_2)}{m} |\mathbf{k}|; \quad n_i = \frac{P_i^2}{2\pi\hbar^2}, \quad (13)$$

with the expected square root dispersion [8, 9].

ii) For $|\mathbf{k}| \rightarrow p_1 - p_2$ the polarization is related to the interband excitations. Therefore the diagonal elements P_{11} and P_{22} of the polarization operator can be neglected. Equation (11) becomes similarly

$$1 - V_k(P_{12}^k + P_{21}^k) = 0, \quad (14)$$

where

$$V_k \equiv \frac{2\pi e^2}{|\mathbf{k}| \kappa_\infty} \iint dz_1 dz_2 f_1(z_1) f_2(z_1) \times e^{-|\mathbf{k}| \cdot |z_1 - z_2|} f_1(z_2) f_2(z_2). \quad (15)$$

To estimate the interband interaction matrix element we use typical values of $|z_1 - z_2|$ of the order of $L_D \sim p_{\text{Fermi}}^{-1}$, $|\mathbf{k}| \sim 0.1 p_{\text{Fermi}}$, so that

$$|\mathbf{k}| \cdot |z_1 - z_2| \sim 0.1.$$

Hence, we can expand the exponent in (15). Due to the orthogonality of the envelope functions f_1 and f_2 the leading term in the expansion is

$$V_k = -\frac{2\pi e^2}{\kappa_\infty} \iint dz_1 dz_2 f_1(z_1) f_2(z_1) |z_1 - z_2| \times f_1(z_2) f_2(z_2). \quad (16)$$

Using the approximation $\langle \dots | (z_1 - z_2)^2 | \dots \rangle^{1/2}$ for the expression $\langle \dots | |z_1 - z_2| | \dots \rangle$, we obtain the result

$$V_k = \frac{2\sqrt{2}}{\kappa_\infty} e^2 z_{12} \quad (17)$$

with $z_{12} = \langle f_1(z) | z | f_2(z) \rangle$ being the interband matrix element. The total operator $P = P_{12} + P_{21}$ can be rewritten in the form

$$P = (m/4 \pi \hbar^2) \tilde{P}, \quad (18)$$

where $\tilde{P}$ is the dimensionless polarization operator. For the excitation spectrum near the singular point $|\mathbf{k}| = p_1 - p_2$ from (14), (16) and (18) we obtain the equation :

$$1 - \tilde{P} z_{12}/a_B \sqrt{2} = 0. \quad (19)$$

In (19) a_B is the material's Bohr radius. The solution of (19) can be obtained as the crossing point of the straight line $\tilde{P} = \sqrt{2} a_B/z_{12}$ and the curve $\tilde{P}(\omega, \mathbf{k})$. The behaviour of $\tilde{P}(\omega, \mathbf{k})$ is shown in figure 3 for five different values of the momentum $|\mathbf{k}|$ in the vicinity of the singular point $p_1 - p_2$. For parameters of the inversion layers

$$\begin{aligned} (n_1 = 2 \times 10^{12} \text{ sm}^{-2}, \quad n_2 = 1.58 \times 10^{12} \text{ sm}^{-2}, \\ \varepsilon_0 = 10 \text{ meV}, \quad m = 0.1 m_e, \\ \kappa_\infty = 5, \text{ i.e. } a_B = 26 \text{ \AA}, \end{aligned}$$

and if $z_{12} = 24.5 \text{ \AA}$ the ratio $\sqrt{2} a_B/z_{12} = 1.5$) the dispersion relation is obtained as the crossing point of $\tilde{P}$ and the line $\tilde{P} = 1.5$.

The most striking feature of the $\tilde{P}$, as seen from figure 3 is the sharp peak of $\tilde{P}$ appearing just above $|\mathbf{k}| = p_1 - p_2$ and not existing below it. The dispersion relation of this soft mode is of the type

$$\omega = v. (|\mathbf{k}| - p_1 + p_2) \theta(|\mathbf{k}| - p_1 + p_2) \quad p_1/m \geq v \geq p_2/m \quad (20)$$

where $\theta(x) = 1$ for $x > 0$ and $\theta(x) = 0$ for $x < 0$. When this mode is present in a certain material, an instability develops due to Coulomb interaction (in this case). The final state is inhomogeneous, the layer charge density being modulated with $|\mathbf{k}| = p_1 - p_2$. Further investigation of the nature of this instability is of great importance, because it determines the spectrum, the optical and transport properties of the layer.

Only a general description of the excitation spectrum is given here.

It should be remembered that the soft mode (20) was obtained by neglecting P_{11} and P_{22} , as well as the imaginary part of P . This approximation is valid for $|\mathbf{k}| \ll p_1, p_2$ but its range of validity can well be larger, depending on the material. This is also true for the other results obtained here. It may also be the reason for the « unphysical solutions » appearing in figure 3 for small values of the parameter a_B/z_{12} , when P_{11} and P_{22} are of the same order of magnitude, and the approximation breaks down.

Apart from the soft mode already discussed, there are also two modes obtained as a crossing point with the value $\tilde{P} = 1.5$ (in this case). The first mode has an almost constant energy, close to the level

Fig. 3. — ω dependence of the polarization operator $\tilde{P}$ for five values of $\tilde{k} = \frac{|\mathbf{k}|}{p_1 - p_2}$ near $\tilde{k} = 1$. It is remarkable that the sharp peak appears only above $\mathbf{k} = p_1 - p_2$. The crossing points of $\tilde{P}$ with the line $\tilde{P} = 1.5$ are solutions of equation (19) and the corresponding dispersion of the collective excitations is given in figure 4.

separation ε_0 . In the hydrodynamic limit $|\mathbf{k}| \rightarrow 0$ this mode has the same energy ε_0 and was considered in [6, 7, 10]. Near $|\mathbf{k}| = p_1 - p_2$ this mode shows Landau damping. The second mode with higher energy is, a new one. Whilst the second subband is not populated by electrons, only the former mode is possible. The occupation of two bands leads to a new type of transition of the electrons from the second band to the first one, with a momentum transfer larger than $p_1 - p_2$. Thus, instead of one mode, two modes are possible in narrow gap inversion layers. It is remarkable that this mode is non-damping in our model, in contrast with the others.

3. Conclusions. — The collective modes which are connected with equation (19) were obtained within the framework of a model based on plane waves instead of exact Bloch solutions. The influence of the other bands is neglected as are electron-phonon interactions. The Coulomb interaction is important and is responsible for the soft mode (20) and for the other new collective modes. The soft mode (20) is due to transitions with zero energy transfer between two subbands at the Fermi level. The transitions from the higher subband to the lower one are possible only for momentum transfer $|\mathbf{k}| > p_1 - p_2$, which leads to the soft-mode dispersion shown in figure 4.

Both subbands are occupied in our case and consequently transitions between them are possible. Therefore in this model of the narrow gap inversion layer, there are two interband excitations. Each one is

Fig. 4. — Total spectrum of excitations in the presence of two degenerated surface subbands. With dotted line is marked the mode, which in hydrodynamic limit coincides with the one, obtained in [6, 7, 10].

connected with a plasmon of the type obtained by Chen *et al.* [10]. The higher energy plasma is a new one. An important feature of this mode is the absence of Landau damping, in contrast with the other modes

Acknowledgments. — The authors would like to express their gratitude to Dr. I. Z. Kostadinov for numerous discussions of the problem. Thanks are also due to Prof. V. L. Pokrovsky for stimulating comments on the nature of the new collective excitations considered here.

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