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The evolution of Bernstein modes in quantum wires with increasing deviation from parabolic confinement

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Abstract. We investigate the evolution of the interaction of the magnetoplasmon resonance with the harmonics of the cyclotron resonance as the confinement of an electron gas in a quantum wire increasingly deviates from the parabolic case. The occurrence of the Bernstein modes is observed in a time-dependent Hartree model of a two-dimensional electron gas in a single quantum wire.

1. Introduction

Quantum wires are interesting for probing the electron–electron interaction in the transition regime from quasi-two-dimensional systems to quasi-one-dimensional systems. These systems can be fabricated starting from two-dimensional semiconductor microstructures (2DES), for example in AlGaAs–GaAs heterostructures. The wires may be created by a gate structure or by etching techniques. The presence of a magnetic field is manifested by many interesting quantum features, most notably the quantum Hall effect and the fractional quantum Hall effect. The far-infrared response provides a powerful method for determining the charge-density spectra in the transverse direction. For transverse parabolic potentials, the motion of the electrons may be separated into centre-of-mass motion and relative motion. The centre-of-mass motion is decoupled from the relative motion of the electrons, and takes place in a transverse potential with the effective frequency $(\omega_0^2 + \omega_c^2)^{1/2}$, where $\hbar\omega_0$ is the confinement energy and ω_c is the cyclotron frequency. The time-dependent external potential ϕ_e representing the long-wavelength far-infrared radiation only couples to the centre-of-mass motion causing a single peak in the FIR spectrum at the plasmon frequency $\Omega_p = (\omega_c^2 + \omega_0^2)^{1/2}$ equal to the effective transverse frequency [1, 2]. Therefore, according to Kohn's theorem [1], although a rich spectrum would be expected, there is only a single resonance. For small systems with general confinement potentials deviating strongly from the parabolic case, the single-particle excitations may overlap with the collective excitations causing a fine structure in the plasmon peak [3, 4]. Any deviation from parabolic confinement will couple the internal and collective motion.

Bernstein showed [5] that in 3D homogeneous systems the dispersion of the magnetoplasmon as a function of the magnetic field will have anticrossings at finite wave vectors ($\boldsymbol{k} \perp \boldsymbol{B}$) around $\Omega_p = n\omega_c$ where $n = 2, 3, \ldots$. The calculation was based

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on solving the classical Boltzmann equation and Maxwell's equations self-consistently. The strength of the anticrossings depends on temperature, wavelength and magnetic field in a complex way and decreases for the higher harmonics. An interaction between the magnetoplasmon resonance and the harmonics of the cyclotron resonance, a so-called Bernstein mode [5], have been observed in 3DES [6], 2DES [7, 8], 1DES (wires) and 0DES (dots) [4]. For confined electron systems in reduced dimensions the breakdown of Kohn's theorem in nonparabolic potentials is sufficient for observing Bernstein modes instead of considering absorption at finite wave vector.

We study the far-infrared absorption in the integer quantum Hall regime. Here we consider a broad range of deviations from parabolic wires in the time-dependent Hartree approximation. Increasing deviations give richer excitation spectra when the magnetoplasmon resonance starts to couple to increasingly higher harmonics of the cyclotron resonance. We systematically investigate how the splitting and its location depend on the strength of the deviation from the parabolic confinement.

2. The model

We consider a strictly two-dimensional electron system lying in the x–y plane. The motion in the z-direction is neglected since the electrons are confined to the lowest subband at the low temperature attained in experiments. We use the Hartree approximation (HA) to reduce the many-particle Hamiltonian to a single-particle Hamiltonian for each electron in an effective potential approximating the electron–electron interaction. For the FIR absorption we use the corresponding time-dependent approximation describing the self-consistent linear response of the 2DES to an external homogeneous time-varying electrical field (the random-phase approximation, RPA). In a constant perpendicular magnetic field B the cyclotron frequency and the magnetic length are $\omega_c = eB/(m^*c)$ and $l_c = [\overline{h}/(m^*\omega_c)]^{1/2}$, respectively, where m^* is the effective mass. The dielectric constant of the surrounding medium is denoted by κ. It is convenient to introduce the constant perpendicular magnetic field with the vector potential in the Landau gauge $\boldsymbol{A}(\boldsymbol{r}) = (-By, 0)$.

The effective Hamilton operator for a single electron in the confining potential $V_c(y)$ is

$$H = -\frac{\overline{h}^2}{2m^*}\left(\nabla^2 - \frac{2\mathrm{i}}{l_c^2}y\frac{\partial}{\partial x}\right) + \frac{1}{2}m^*\omega_c^2 y^2 + V_c(y) + V_H(\boldsymbol{r}) \tag{1}$$

where $V_H(\boldsymbol{r})$ is the self-consistent Hartree potential representing the direct Coulomb interaction between one electron and the total charge density of the 2DES. The periodic boundary condition in the longitudinal direction of the wire gives a Bloch-type single-particle wave function:

$$\Psi_{nk}(x, y) = \frac{1}{\sqrt{L_x}}\mathrm{e}^{\mathrm{i}kx}\psi_{nk}(y) \tag{2}$$

where the longitudinal wave vector $k = p\,2\pi/L_x$ with $p \in \mathbb{Z}$ and n is the transverse quantum number. The length of the wire, L_x, is assumed to be much larger than the effective width of the wire; therefore the Hartree potential only depends on the transverse coordinate [9]:

$$V_H(y) = -\frac{2e^2}{\kappa}\int_{-\infty}^{\infty}\mathrm{d}y'\; n_s(y')\ln\left|\frac{y-y'}{L}\right| \tag{3}$$

with L given below. It has been assumed that a neutralizing background charge exists. For noninteracting electrons in a simple one-dimensional parabolic potential $V(y) = \frac{1}{2}m^*\omega_0^2 y^2$,

the single-particle eigenfunctions are

$$\phi_{nk}(y) = \frac{1}{\sqrt{L}} \frac{1}{\sqrt{2^n n! \sqrt{\pi}}} H_n\left(\frac{y - y_k}{L}\right) \exp\left[-\frac{(y - y_k)^2}{2L^2}\right] \tag{4}$$

where $y_k = k l_c^2 l_0^4/(l_0^4 + l_c^4)$ is the centre coordinate, which generally does not equal the expectation value of the transverse coordinate y [10]. The nth Hermite polynomial is denoted by H_n. The confinement length is defined as $l_0 = [\hbar/(m^*\omega_0)]^{1/2}$. The electron is localized within the effective length $L = [\hbar/(m^*\Omega)]^{1/2}$, replacing the magnetic length l_c, and the cyclotron frequency ω_c is replaced by an effective frequency defined by $\Omega = (\omega_0^2 + \omega_c^2)^{1/2}$. The eigenenergies corresponding to the eigenstates (4) are

$$E_{nk} = \hbar\Omega(n + 1/2) + (\hbar^2 k^2/2m^*) l_c^4/(l_c^4 + l_0^4).$$

In the case of vanishing confinement (2DES), $l_0 \to \infty$, the energy bands reduce to the familiar dispersionless Landau levels. The effective single-particle Hamiltonian is diagonalized using the wave functions of the noninteracting electrons (4) as a functional basis and the self-consistent solutions are obtained by iteration.

The response to a time-dependent perturbation may be found by using the RPA where exchange and correlation effects are neglected. In this mean-field approximation the noninteracting Hartree quasi-particles move in a self-consistent potential given by the external perturbation and the response of the charge density of the electrons n_s. The self-consistent potential, $\phi_s(\boldsymbol{r}, \omega)$, may be found from the external potential $\phi_e(\boldsymbol{r}, \omega)$:

$$\langle\alpha|\phi_s(\omega)|\beta\rangle = \langle\alpha|\phi_e(\omega)|\beta\rangle + \sum_{\delta\gamma} \frac{H_{\alpha,\beta;\gamma,\delta}(f_\gamma - f_\delta)}{\hbar\omega + (\epsilon_\gamma - \epsilon_\delta) + \mathrm{i}0^+} \langle\delta|\phi_s(\omega)|\gamma\rangle \tag{5}$$

where α denotes the longitudinal and transverse quantum numbers n and k. f_α is the Fermi occupation factor and the Hartree matrix elements are defined in terms of the Hartree ground-state wave functions:

$$H_{\alpha,\beta;\gamma,\delta} = \frac{e^2}{\kappa} \int \mathrm{d}\boldsymbol{r} \int \mathrm{d}\boldsymbol{r}' \, \frac{\psi_\gamma^*(\boldsymbol{r}')\psi_\delta(\boldsymbol{r}')\psi_\alpha^*(\boldsymbol{r})\psi_\beta(\boldsymbol{r})}{|\boldsymbol{r} - \boldsymbol{r}'|} \,. \tag{6}$$

A method for finding ϕ_s based on a Fourier transformation of the position coordinates and repeatedly solving (5) for all the values of ω needed is given in [4]. Here we present an alternative method, transforming (5) such that $\phi_s(\omega)$ can be simultaneously obtained for all values of ω from a matrix eigenvalue problem. The latter method considerably speeds up numerical calculations and we have checked that they deliver exactly the same results. The equation for the self-consistent potential (5) simplifies for transverse external fields. The longitudinal quantum number k is conserved in the transition, so each single electron transition may be labelled by k and two transverse quantum numbers n and m. On applying a time-dependent but spatially constant electric field, $\boldsymbol{E}_e(\boldsymbol{r}, t) = -\hat{y}\mathcal{E}_e \exp(-\mathrm{i}\omega t)$, the Fourier component of the external potential is $\phi_e(\boldsymbol{r}, \omega) = -e\mathcal{E}_e y$, where $-e$ is the electron charge. In the basis (2) the interband matrix elements of the external potential

$$\{\phi_e(\omega)\}_{n,m}^k = \int \mathrm{d}y \; \psi_{nk}(y)\phi_e(\boldsymbol{r}, \omega)\psi_{mk}(y)$$

are real and symmetric. Since the Hartree potential is local, the matrix elements of the self-consistent potential are also symmetric with respect to the transverse quantum numbers $\{\phi_s(\omega)\}_{n,m}^k = \{\phi_s(\omega)\}_{m,n}^k$. This is also the case for local-density approximations, but not for

the Hartree–Fock approximation, since the Fock potential is nonlocal [11]. The equation for the self–consistent potential may then be written as an eigenvalue problem:

$$(\hbar^2\omega^2 - (\epsilon^k_{n,m})^2)\,\{\eta(\omega)\}^k_{n,m} = \sqrt{2f^k_{n,m}\epsilon^k_{n,m}}\,\{\phi_e(\omega)\}^k_{n,m} \\ -2\sum_{n',m',k'}^{\epsilon^{k'}_{n',m'}>0} H^{k;k'}_{n,m;n',m'}\sqrt{f^k_{n,m}\epsilon^k_{n,m}}\sqrt{f^k_{n',m'}\epsilon^{k'}_{n',m'}}\,\{\eta(\omega)\}^{k'}_{n',m'} \tag{7}$$

where $\epsilon^k_{n,m} = \epsilon^k_n - \epsilon^k_m$ are the quasi-particle excitation energies, and $f^k_{n,m} = f^k_m - f^k_n$ are the differences in occupation between initial and final states. For convenience we have introduced the variable

$$\{\eta(\omega)\}^k_{n,m} = \{\phi_s(\omega)\}^k_{n,m}(2f^k_{n,m}\epsilon^k_{n,m})^{1/2}/(\hbar^2\omega^2 - (\epsilon^k_{n,m})^2).$$

The resonances in the FIR spectrum are the eigenvalues of the symmetric matrix:

$$A^{k;k'}_{n,m;n',m'} = (\epsilon^k_{n,m})^2\delta^{k;k'}_{n,m;n',m'} - 2H^{k;k'}_{n,m;n',m'}(f^k_{n,m}\epsilon^k_{n,m}f^{k'}_{n',m'}\epsilon^{k'}_{n',m'})^{1/2}. \tag{8}$$

The power absorption may be found from the Joule heating:

$$P(\omega) = \frac{1}{2}\int \mathrm{d}\boldsymbol{r}\ \mathrm{Re}\left\{\delta\boldsymbol{J}(\boldsymbol{r},\omega)\cdot\boldsymbol{E}^*_s(\boldsymbol{r},\omega)\right\} \tag{9}$$

where $\delta\boldsymbol{J}(\boldsymbol{r},\omega)$ is the induced current in the wire and $\boldsymbol{E}_s$ is the self-consistent electric field. For our system it is

$$P(\omega) = -\frac{\omega}{2}\sum_{n,m,k}^{\epsilon^k_{n,m}>0}\{\phi_e(\omega)\}^k_{n,m}\ \mathrm{Im}\left[\frac{2f^k_{n,m}\epsilon^k_{n,m}}{(\hbar\omega)^2 - (\epsilon^k_{n,m})^2}\,\{\phi_s(\omega)\}^k_{n,m}\right] \\ = -\frac{\omega}{2}\sum_{n,m,k}^{\epsilon^k_{n,m}>0}\sqrt{2f^k_{n,m}\epsilon^k_{n,m}}\{\phi_e(\omega)\}^k_{n,m}\,\mathrm{Im}\{\eta(\omega)\}^k_{n,m}. \tag{10}$$

The Coulomb interaction may shift the poles of the matrix $\{\eta(\omega)\}^k_{n,m}$ from the Hartree single-particle excitations $\epsilon^k_{n,m}$ as can be seen from the eigenequation (7). The new poles will show up as resonances in the FIR absorption (10). Here a phenomenological broadening should be inserted to give the lifetime of the excitations. In a Fermi liquid the scattering cross-section decreases for lower-energy one-particle excitations. Hence, one should expect that at least for low-energy one-particle excitations this broadening is small. The power absorption may be expanded in the eigenfunctions of the matrix A. The oscillator strengths can then be found and the whole FIR spectrum determined. Since the Hartree RPA is a conserving approximation [12], the longitudinal f-sum rule for the oscillator strengths is satisfied for arbitrary electron–electron interaction strengths.

We study quantum wires with confining potentials of the form

$$V_c(y) = \frac{1}{2}\hbar\omega_0\left[\left(\frac{y}{l_0}\right)^2 + a\left(\frac{y}{l_0}\right)^4 + b\left(\frac{y}{l_0}\right)^6\right] \tag{11}$$

where a and b are parameters that determine the higher-order deviations from parabolic confinement. By the method described above, we are able to find the FIR spectra arising from this confining potential.

3. Numerical results

The functional basis of the Hartree ground state has been chosen large enough that a further expansion or iteration of the Hartree equations does not result in visible changes in the single-particle energy spectra or the electron density $n_s(\boldsymbol{r})$ of the ground state. To attain sufficient accuracy in the calculation of the absorption the size of the functional basis for the excited states has been chosen such that further refinement results in changes to the location of the absorption peaks that are smaller than a typical linewidth in experiments, 0.1 meV.

For the calculations we employ the usual GaAs parameters, $m^* = 0.067m_0$, and $\kappa = 12.4$, where m_0 is the free-electron mass. The absorption is only weakly dependent on T in the temperature range $T \leqslant 4$ K for the parameters that we use. The calculations have thus been performed for $T = 1.0$ K.

The FIR spectra have been calculated for the range of magnetic fields $B = 0$–3 T. For a strict parabolic confinement, $a = 0$ and $b = 0$, we have checked that the generalized Kohn theorem is satisfied with a high degree of accuracy. We consider pure fourth-order deviations, $a = 0.01$ to $a = 0.40$, and pure sixth-order deviations, $b = 0.001$ to $b = 0.030$. Mixed deviations of fourth and sixth order do not give significant new qualitative information.

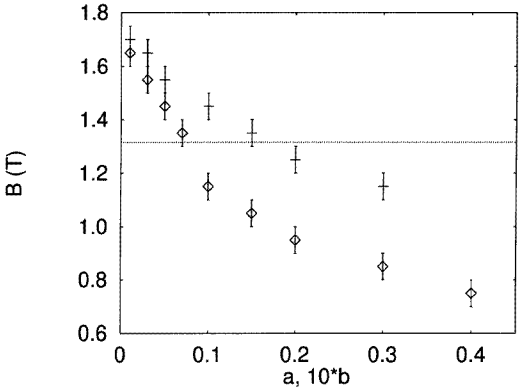

Figure 1. The location of the first anticrossing as a function of the magnetic field B and the fourth-order deviation, $a \neq 0$, $b = 0$ ($\diamond$), or the sixth-order deviation, $a = 0$, $b \neq 0$ (+). The horizontal line shows where $\Omega_p = 2\omega_c$. 30 states are occupied, $L_x = 240$ nm, $\hbar\omega_0 = 3.94$ meV, $T = 1.0$ K, $m^* = 0.067m_0$, $\kappa = 12.4$.

For small deviations, with either $a \neq 0$ or $b \neq 0$, a single anticrossing close to the $2\omega_c$-line appears. The position of the anticrossing as a function of the deviation a or b is shown in figure 1. The horizontal line shows where $\Omega_p = 2\omega_c$, i.e. where a possible resonance between the magnetoplasmon and the cyclotron frequency should appear. The calculated anticrossing is to the right of the $2\omega_c$-line for small deviations, but is shifted quite strongly to the left with increasing deviation. This is due to the interaction of the collective oscillations, the magnetoplasmons, with the first harmonic of the cyclotron resonance, $2\omega_c$, a so-called Bernstein mode [5].

The absorption peaks as a function of the magnetic field for increasing fourth-order deviation, $a = 0.03$, 0.10, 0.20, 0.40, are shown in figure 2 and for increasing sixth-order deviation, $b = 0.003$, 0.005, 0.010, 0.030, in figure 3. Only absorption peaks with an

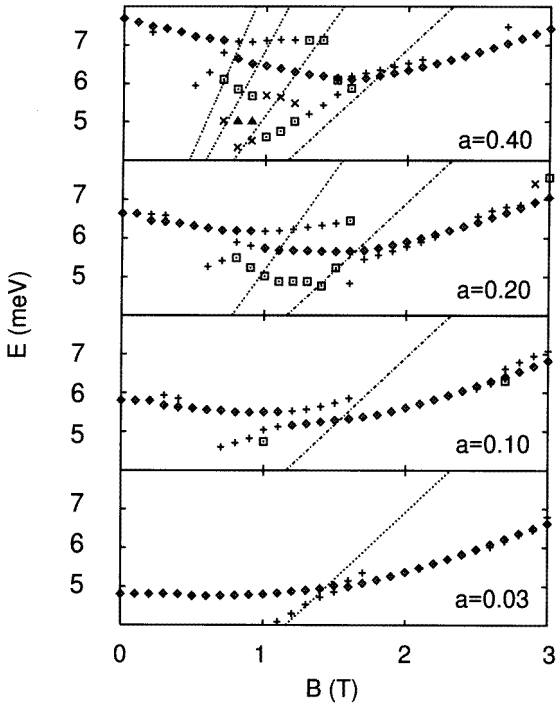

Figure 2. The location of the absorption peaks as functions of the magnetic field B and the energy $E = \hbar\omega$ supplied by ϕ_e for a pure fourth-order deviation. Only absorption peaks with an oscillator strength larger than 1% of the total oscillator strength are shown. The straight lines represent the harmonics of the cyclotron frequency, $n\omega_c$ ($n = 2, 3, 4, 5$). Strong absorption is marked by $\Diamond$, weak by $+$, very weak by $\Box$, and extremely weak by $\times$. 30 states are occupied, $L_x = 240$ nm, $\hbar\omega_0 = 3.94$ meV, $T = 1.0$ K, $m^* = 0.067m_0$, $\kappa = 12.4$.

oscillator strength that is more than 1% of the total oscillator strength are shown. The absorption peaks are labelled strong, weak, very weak and extremely weak according to their relative strength for a given magnetic field. Only excitation energies in the range 3.5–8.5 meV are shown. The location of the strong resonance at zero magnetic field increases in energy with increasing deviation, because of the stronger confinement. However, for intermediate magnetic fields the strong resonance develops a slightly negative slope with respect to the magnetic field. This softening of the mode increases with increasing deviation. For large deviations the simple splitting develops into a complex one; see figure 2 for a fourth-order deviation and figure 3 for a sixth-order deviation. We see that strong deviations from a parabolic confinement lead to interactions with higher cyclotron harmonics, $n\omega_c$, where n is larger than 2. The new modes may also interact with each other. However, it is not possible from the spectra to say which harmonics are involved, since several harmonics can be excited in a complicated way, and the anticrossing occurs at or in between the $n\omega_c$-lines. The spectrum is now very rich, because of the strong coupling of the collective motion to the internal motion in the wire. Splittings may also be seen on the weak-resonance branches for $a = 0.40$ in figure 2 and for $b = 0.030$ in figure 3.

The intensity as a function of the magnetic field and the supplied energy from the external potential is shown in figure 4 for a pure fourth-order deviation, $a = 0.20$. Only

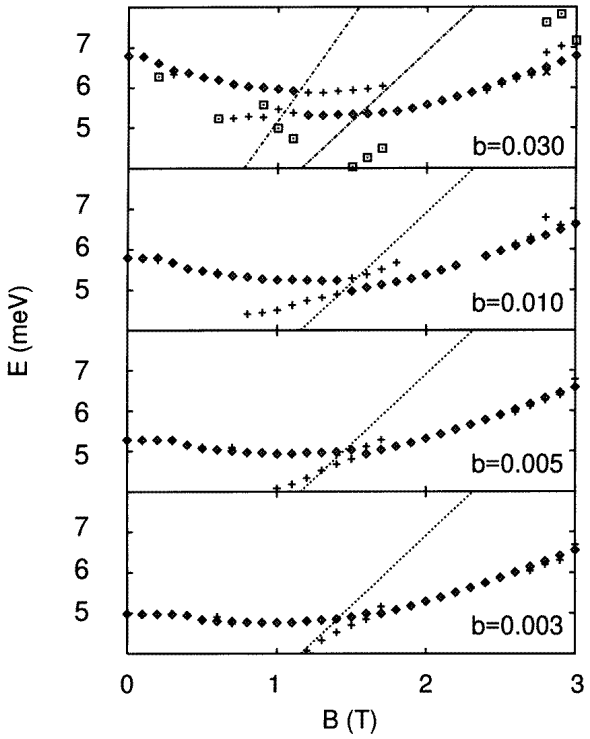

Figure 3. The location of the absorption peaks as functions of the magnetic field B and the energy $E = \hbar\omega$ supplied by ϕ_e for a pure sixth-order deviation. Only absorption peaks with an oscillator strength larger than 1% of the total oscillator strength are shown. The lines show the possible interactions of the magnetoplasmon with harmonics of the cyclotron frequency, $n\omega_c$ ($n = 2, 3$). Strong absorption is marked by $\diamondsuit$, weak by $+$, and very weak by $\square$. 30 states are occupied, $L_x = 240$ nm, $\hbar\omega_0 = 3.94$ meV, $T = 1.0$ K, $m^* = 0.067m_0$, $\kappa = 12.4$.

resonances that have a strength of more than 1% are shown. We see that for this deviation there is mainly one anticrossing; all other resonances are weak. The softening of the modes occurs as long as two main resonances are seen, i.e. as long as the modes are coupled.

The effect of the deviation is larger for a higher density of the electrons, since the chemical potential is higher and the 2DEG occupies states farther from the centre of the wire that are more affected by the fourth- and sixth-order terms of the confinement.

4. Summary

The FIR spectrum for a wire with a confining potential deviating from a parabolic one was calculated in the time-dependent Hartree approximation. The anticrossing due to interaction of the magnetoplasmon with the first harmonic of the cyclotron resonance shifts strongly from the right of the $2\omega_c$-intersection with the plasmon dispersion to the left with increasing deviation, and the simple splitting develops into a more complex one, including interactions with higher harmonics of the cyclotron resonance.

In the quantum wire $\hbar\omega_c$ is not a characteristic single-electron excitation energy, but the width of the system defines a characteristic wave vector which does not vanish with decreasing deviation from the parabolic confinement. An external perturbation does

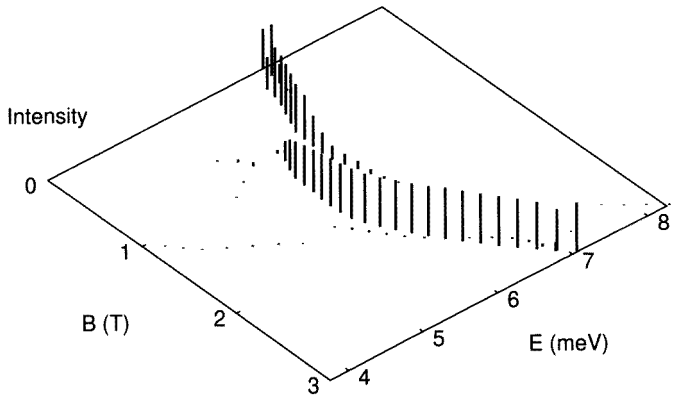

Figure 4. The intensity of the absorption peaks as a function of the magnetic field B and the energy $E = \hbar\omega$ supplied by ϕ_e for a pure fourth-order deviation, $a = 0.20$. Only absorption peaks with an oscillator strength larger than 1% of the total oscillator strength are shown. 30 states are occupied, $L_x = 240$ nm, $\hbar\omega_0 = 3.94$ meV, $T = 1.0$ K, $m^* = 0.067m_0$, $\kappa = 12.4$.

excite plasma waves with a broad range of wave vectors, but the system responds in the strongest fashion for integer multiples of the 'natural wave vector'. In a homogeneous two-dimensional electron system the response is always with the same frequency and wave vector as the external perturbation; thus the asymptotic behaviour of the split-off modes is simple. Here the asymptotic behaviour is complicated by the fact that the split-off modes again interact with higher-order plasmons. A detailed study of this phenomenon will be published elsewhere.

Acknowledgments

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