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Tilted-field magneto-optical absorption in an imperfect parabolic quantum well

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We study the far-infrared optical absorption spectrum of electrons confined in an imperfect parabolic quantum well in a magnetic field tilted with respect to the growth axis. The calculations are carried out at finite temperature using a self-consistent-field approach both with and without a local exchange-correlation potential. We choose well parameters to match a real experimental sample and obtain excellent quantitative agreement over a wide range of magnetic-field strengths. We discuss the effects of possible asymmetries in the confining potential, and conclude that the infrared spectrum is dominated by depolarization and finite-temperature effects.

Remotely doped parabolic quantum wells have attracted attention in recent years as systems where an almost three-dimensional (3D) electron gas can be obtained with much weaker electron-impurity interactions than are possible in conventional doped semiconductors.[1-10] Experimental work has been done on magnetotransport,[2] on photoluminescence excitation spectroscopy,[3] and on far-infrared optical absorption[4-8] in parabolic wells grown in the $Al_xGa_{1-x}As$ system. It has been shown theoretically[9] that in the case of perfect parabolic confinement, with an applied magnetic field in a general direction, long-wavelength optical perturbations can cause transitions only at the two frequencies that correspond to exact excitations in the center-of-mass motion of the electron gas.

Recently, optical spectra have been measured for systems that have been deliberately grown so as to deviate in various ways from perfect parabolicity.[6-8] For small deviations, one might expect that nonparabolicity would have two main effects: to shift the excitation energies of the system slightly, and to redistribute the oscillator strength so that excitations other than the center-of-mass modes become visible in far-infrared optical spectra. This expectation is borne out by experiments with no magnetic field,[7] and with in-plane[6,8] and tilted[6] magnetic fields, and by calculations of optical spectra for imperfect parabolic wells at $B=0$.[10]

Intersubband optical absorption for quasi-two-dimensional electron systems in tilted magnetic fields has been studied by Ando,[11] who used the local density approximation (LDA) to include exchange and correlation effects within a self-consistent-field (SCF) framework. Because fully self-consistent calculations in tilted fields are computationally demanding, and because the "depolarization" and "excitonlike" shifts are relatively small in quasi-2D systems,[12] simple approximation schemes have been used to analyze tilted-field experiments in these systems.[12,13] Such approximation schemes are not adequate in parabolic wells, however, where the depolarization shift can be many times larger than the intersubband spacing.[10,14]

In this paper, we present self-consistent calculations of optical spectra for an imperfect parabolic well in a tilted magnetic field at finite temperature. We concentrate on a well with abrupt boundaries of the type studied experimentally in Ref. 6, where "overfilling" forces the electron gas to feel the strong nonparabolicities at the edges of the well. We make a detailed comparison with the results of Ref. 6, discussing the effects of finite temperature, Zeeman splitting, and symmetry-breaking terms in the confining potential. We obtain excellent quantitative agreement with experiment, and find that the details of the optical spectrum are controlled by depolarization and finite-temperature effects.

We follow the method of Ando,[11] and choose the growth axis in the z direction, the magnetic field $\mathbf{B}=(0,B_y,B_z)$, and the gauge $\mathbf{A}=(zB_y-yB_z,0,0)$. Ignoring for the moment the Zeeman energy, we calculate the self-consistent eigenvalues and eigenfunctions of the Hamiltonian

$$H=\frac{(p_x-m^*\omega_{cz}y+m^*\omega_{cy}z)^2}{2m^*}+\frac{p_y^2}{2m^*}+\frac{p_z^2}{2m^*}+V(z)\,, \tag{1}$$

where m^* is the electron effective mass, ω_{cy} and ω_{cz} are eB_y/m^*c and eB_z/m^*c, respectively, and $V(z)=V_c(z)+V_H(z)+V_{XC}(z)$ is the sum of the bare confining potential V_c, the Hartree potential V_H, and a local exchange-correlation potential V_{XC}.[15] The eigenfunctions can be written in the form

$$\psi_{\mu Y}(x,y,z)=\frac{e^{iYx/l_\perp^2}}{(L_x)^{1/2}}\phi_\mu(y-Y,z) \tag{2}$$

where $l_\perp=(eB_z/\hbar c)^{1/2}$ is the effective magnetic length in the xy plane, and where the eigenvalues $\{\varepsilon_\mu\}$ are independent of Y. Defining $\rho_{\mu\nu}\equiv 2\pi l_\perp^2\sum_Y\psi^*_{\mu Y}(\mathbf{r})\psi_{\nu Y}(\mathbf{r})$ and taking the limit $L_x\to\infty$, we can write the ground-state electron density as

$$n_0(z)=\frac{g_s}{2\pi l_\perp^2}\sum_\nu f(\varepsilon_\nu)\rho_{\nu\nu}(z)\,, \tag{3}$$

where $f(\varepsilon)=\{\exp[(\varepsilon-\mu)/k_BT]+1\}^{-1}$ is the Fermi function and g_s is the spin degeneracy. The chemical potential μ is fixed by the relation $n_s=(g_s/2\pi l_\perp^2)\sum_\nu f(\varepsilon_\nu)$.

Having calculated the self-consistent single-particle states, we can calculate the absorption spectrum. Because the radiation in the experiment of Ref. 6 is normally incident, we calculate the yy component[16] of the modified

two-dimensional conductivity $\tilde{\sigma}_{yy}$, obtaining[11,16]

$$\tilde{\sigma}_{yy} = -i\omega e^2 \left[\frac{\hbar^2}{2m^*}\right] \sum_{\eta} \frac{f_\eta}{\tilde{\varepsilon}_\eta^2 - (\hbar\omega)^2 - 2i\hbar\omega(\hbar/\tau)} \quad (4)$$

where

$$f_\eta \equiv \left[\sum_{\mu,\nu} U_{\mu\nu,\eta} \left[\frac{2m\varepsilon_{\mu\nu}}{\hbar^2}\right]^{1/2} \left[\frac{g_s}{2\pi l_\perp^2}\right]^{1/2} \times [f(\varepsilon_\nu) - f(\varepsilon_\mu)]^{1/2} \langle \mu | y | \nu \rangle\right]^2 . \quad (5)$$

In these expressions, $\varepsilon_{\mu\nu} \equiv \varepsilon_\mu - \varepsilon_\nu$, τ is a phenomenological relaxation time, and $\{\tilde{\varepsilon}_\eta^2\}$ and $\{U_{\mu\nu,\eta}\}$ are the eigenvalues and eigenvectors of the matrix

$$\Lambda_{\mu\nu,\mu'\nu'} = \varepsilon_{\mu'\nu'}^2 \delta_{\mu\mu'}\delta_{\nu\nu'} + \frac{g_s}{2\pi l_\perp^2} \varepsilon_{\mu\nu}^{1/2} [f(\varepsilon_\nu) - f(\varepsilon_\mu)]^{1/2} \times (\alpha_{\mu\nu,\mu'\nu'} - \beta_{\mu\nu,\mu'\nu'}) [f(\varepsilon_{\nu'}) - f(\varepsilon_{\mu'})]^{1/2} \varepsilon_{\mu'\nu'}^{1/2} . \quad (6)$$

Depolarization ($\alpha_{\mu\nu,\mu'\nu'}$) and excitonlike ($\beta_{\mu\nu,\mu'\nu'}$) effects are included through

$$\alpha_{\mu\nu,\mu'\nu'} = -\frac{4\pi e^2}{\varepsilon_{sc}} \int_{-\infty}^{\infty} dz\, \rho_{\mu\nu}(z) \int_{-\infty}^{z} dz' \times \int_{-\infty}^{z'} dz''\, \rho_{\mu'\nu'}(z'') \quad (7)$$

and

$$\beta_{\mu\nu,\mu'\nu'} = -\int_{-\infty}^{\infty} dz\, \rho_{\mu\nu}(z) \frac{\delta V_{XC}}{\delta n} \rho_{\mu'\nu'}(z) . \quad (8)$$

We calculate optical spectra for two wells: one well designed to be identical to the nominally 750-Å-wide well in the sample of Ref. 6, and one well with the same curvature but with perfect parabolicity. The experimental sample used in Ref. 6 was cut from a wafer grown to have a well width of 750 Å and an Al concentration that varied quadratically from $x=0$ at the center of the well to $x=0.1$ at the well boundary, where the concentration jumped discontinuously to $x=0.3$. Thick Si-doped layers were set back 200 Å from the well on both sides.[17] Because the Al profile in unrotated molecular-beam-epitaxy samples like that used in Ref. 6 can vary across the wafer,[18] and because the conduction band offset in $Al_xGa_{1-x}As$ is somewhat uncertain, the potential profile for the experimental sample is not known precisely. To obtain a quantitative match between theory and experiment, we use well parameters that lie within the various uncertainties: width 787.5 Å, parabolic height 70 meV, and additional potential discontinuity 150 meV. The sheet density of carriers is $n_s = 4.7\times10^{-1}$ cm^{-2}, which we assume to come equally from the donors on each side of the well.[19] We use the tilt angle 23° specified in Ref. 6 and an effective mass $m^* = 0.07m_e$, which represents an average over the width of the well.

In a check of our method, we have calculated the absorption spectrum of the perfect well as a function of magnetic field. In both the random phase approximation (RPA) (where V_{XC} and $\beta_{\mu\nu,\mu'\nu'}$ are omitted) and the LDA-SCF approximation, we obtain agreement with the results of Ref. 9 to better than 0.1% in peak positions and oscillator strengths. For the imperfect well, we find that the differences in the peak positions given by the two approximation schemes are very small for small magnetic fields and at most 3%–4% for higher fields. And while the zero-field exchange-correlation potential V_{XC} used in the LDA-SCF approach should be valid at low magnetic fields, its validity is doubtful at high magnetic fields, where the electron system can have a substantial spin polarization. For these reasons, we show only RPA results in our figures.

In Fig. 1 we compare the B-field dependence of the absorption spectra for the perfect and imperfect wells. To simplify the comparison, we show the perfect-well absorption as solid lines at the center-of-mass-mode frequencies. Absorption in the imperfect well at $T=4$ K is represented by dots, with the area of each dot proportional to the oscillator strength of the corresponding transition. The general effects of the nonparabolicity are as expected. The "center-of-mass" excitations are shifted up slightly in frequency by the increase in confinement arising from the abrupt walls. In addition, the hard walls give rise to extra peaks in the absorption spectrum that lie between the center-of-mass peaks at high fields, and to anticrossing behavior along the cyclotron-resonance curve.

Figure 2 shows the lowest few self-consistent subband energies $\varepsilon_\mu - \varepsilon_0$ (solid lines) as a function of magnetic field strength at $T=4$ K. The chemical potential is also shown (dotted line). A comparison of Figs. 1 and 2, combined with an examination of the eigenvectors $U_{\mu\nu,\eta}$ shows the importance of depolarization effects. This is seen most clearly at high fields, where only the lowest two levels have appreciable occupation. At 15 T, $\varepsilon_1 - \varepsilon_0 = 1.13$ meV and $\varepsilon_2 - \varepsilon_1 = 3.40$ meV, but the lower center-of-mass mode, which can be viewed as a coherent combination of the $0\rightarrow1$ and $1\rightarrow2$ transitions, has an energy of 9.48 meV. Similarly, $\varepsilon_3 - \varepsilon_0 = 9.30$ meV, but the lower of the two extra peaks (which is due mostly to $0\rightarrow3$ transitions) falls at 12.29 meV. The higher extra peak arises from $1\rightarrow4$ transitions and has a very small depolarization shift.

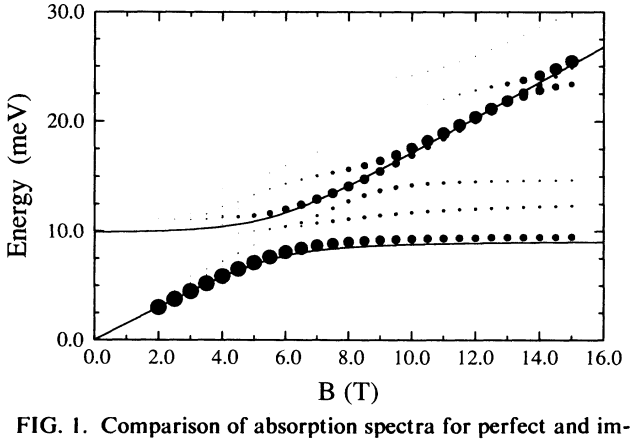

FIG. 1. Comparison of absorption spectra for perfect and imperfect parabolic wells as a function of magnetic field strength at $T=4$ K. Perfect-well absorption is indicated by lines at the center-of-mass-mode frequencies. Absorption in the imperfect well is represented by dots, with the area of each dot proportional to the oscillator strength of the corresponding transition. The magnetic field is tilted 23° with respect to the growth axis.

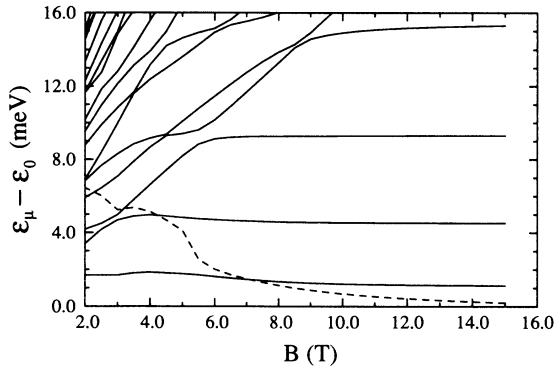

FIG. 2. Self-consistent subband energies $\varepsilon_\mu - \varepsilon_0$ (solid lines) as a function of magnetic field strength at $T=4$ K. The chemical potential (dashed line) at $T=4$ K is also shown.

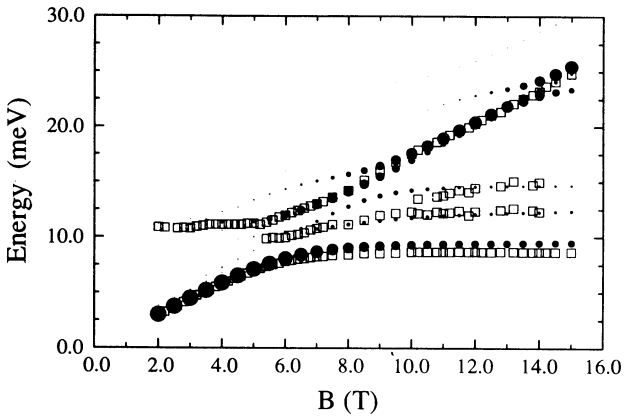

FIG. 3. Comparison of calculated (solid dots) and experimental (open squares) absorption spectra as a function of magnetic field. The area of each dot is proportional to the oscillator strength calculated at $T=4$ K. The size of the squares is arbitrary. Experimental data are from Wixforth *et al.* (Ref. 6).

We point out that the strength of the higher extra peak at high field depends on the population of electrons in the ε_1 subband and hence, within our calculation, has a strong temperature dependence. Above 10.55 T, where the ε_1 subband depopulates at zero temperature, the second extra peak owes its existence to thermal excitation across the intersubband gap $\varepsilon_1 - \varepsilon_0 \sim 1.1$ meV. At $T=4$ K, $k_B T = 0.35$ meV and a small ($\sim 10\%$) but significant fraction of the electrons are in the ε_1 subband, even at 15 T. This population drops dramatically with temperature, however, so that the second extra peak becomes essentially invisible by $T=1$ K.

In Fig. 3 we compare our calculated absorption spectrum for the imperfect well to the experimental peak locations given in Ref. 6. The theoretical resonances are again shown as dots, as in Fig. 1, while the experimental points are denoted by open squares. In the absence of experimental information on oscillator strengths, we have made all squares the same size. The agreement is excellent, with the theory reproducing all the main features of the experiment. In particular, the calculation fits the observed "extra peaks" over the whole field range, including the tail-like structure in the range from 5 to 7 T.

Our calculation predicts that the intensity of the higher-frequency "extra" resonance should be strongly temperature dependent, dropping to zero as the temperature is lowered from 4 to 1 K. On the other hand, we have so far ignored exchange effects and the Zeeman splitting. Within the RPA, inclusion of the Zeeman splitting has the simple effect of changing the subband populations. This could, in principle, have a dramatic effect on the temperature dependence of the optical spectrum, because a large Zeeman splitting might cause the ε_1 subband to be occupied above 10.55 T, even at zero temperature. Using the bare g factor ($g=-0.44$) for GaAs, we find that the Zeeman splitting at 10 T is 0.25 meV which, in view of the 1.21-meV intersubband spacing, would give only a small change in temperature dependence. We know, however, that in quasi-2D systems exchange effects can give a large enhancement to the Zeeman splitting in strong magnetic fields, so that the actual splitting in our system may be much larger than what we find using the bare g factor.[12] A more accurate calculation that includes exchange effects at arbitrary magnetic fields is required to resolve these details.

In a previous paper,[20] the authors used a hydrodynamic model to study the magnetoplasma excitations of electrons confined in a perfect parabolic well. Although one would not expect such a model to be quantitatively accurate, we found remarkable agreement between the B-field dispersion of particular hydrodynamic modes and that of the extra peaks seen in the experiments of Ref. 6. In order to achieve this agreement, however, it was necessary to associate the higher extra resonance in the experimental data (which we have here identified as the $1 \rightarrow 4$ transition) with an even-symmetry hydrodynamic mode that could be excited optically only in an asymmetric confining potential. Such an asymmetry might occur because of a voltage bias across the sample, and the forbidden mode would correspond essentially to the $0 \rightarrow 4$ transition in an RPA calculation. To investigate the question further, we have studied the absorption spectrum for a system where a term linear in z has been added to V_c. Although we find that a modest linear potential does increase the intensity of the symmetry-forbidden transitions enough to make them potentially visible, we also find that, for a well with the parameters we have used in this paper, the $0 \rightarrow 4$ transition comes markedly higher (about 20% at 15 T) than the experimental resonance frequency. The poor match of the $0 \rightarrow 4$ transition with experiment and the absence of any experimental indication of the $0 \rightarrow 2$ transition suggest that the higher extra peak does not arise from an asymmetry in the confining potential.

In summary, we have calculated the optical absorption spectrum for a realistic imperfect parabolic well in a tilted magnetic field at finite temperature. We have found only small differences between spectra calculated using the RPA and those determined using Ando's LDA-SCF approach. Our calculation gives excellent agreement with experiment over a wide range of magnetic field strengths, and suggests that the higher extra peak seen in the experiment of Ref. 6 arises from finite-temperature effects rather than from asymmetries in the confining potential.

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