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The effect of combination of magnetic field and low temperature on doped quantum wells

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Abstract

In this work, we study in the optical absorption of lightly doped and compensated GaAs–GaAlAs quantum wells in the presence of applied magnetic field at low temperatures. The maximum values of magnetic field and temperature are chosen to be 10 T and 5 K, respectively. The wave functions and energies of electrons bound to impurities are calculated variationally using hydrogen-like functions. The absorption coefficient is computed through the use of Fermi golden rule and the statistics of this system is made by a self-consistent calculation of the electrostatic potential generated by ionized impurities, while the convergence parameter is the electronic chemical potential. We focus our attention on $1s \rightarrow 2p_{\pm}$ transitions. The results show that the range of frequency absorbed by the system stays unaltered in $1s \rightarrow 2p_{-}$ transition and changes for the $1s \rightarrow 2p_{+}$ transition, presenting a shift to higher frequencies as the magnetic field increases. Another important result is the decrease of the absorption coefficient for the lowest part of the frequency range as the temperature decreases, turning the material almost transparent for those frequencies. This kind of information may be useful for further diagnosis of quantum well systems. © 2001 Elsevier Science B.V. All rights reserved.

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1. Introduction

The use of heterostructures in electronics experienced a real growth in the previous decade, mainly in opto-electronic devices. One of the most important heterostructures is the quantum well formed by

GaAs–GaAlAs that is generated by several techniques, for example the molecular beam epitaxy (MBE), in which layer by layer of the crystal are deposited on a substrate. When this system is doped it presents an infrared optical coefficient, which varies with the geometry, density of impurities, the ratio of acceptor and donor densities, and applied magnetic field. As the distribution of electrons in donors depend on the temperature, this coefficient and other properties such as the electronic specific heat present

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a temperature-dependent behavior. Serra et al. [1] showed an anomaly in the electronic specific heat of doped quantum well of the Schottky type. There are several calculations of infrared optical coefficient [2–5]. Recently, Baldan et al. [6] calculated the absorption coefficient at zero magnetic field.

In this paper, we study a doped quantum well in the presence of a magnetic field under various conditions of temperature, impurity density and compensation. Depending on the kind of transition, there is a change on the range of absorbed frequency as the magnetic field varies. As the temperature decreases there is a weakening of the absorption coefficient in the lowest part of the frequency range.

2. The model

We study a lightly doped and compensated quantum well with shallow impurities. Being N_A and N_D the acceptor and donor densities, respectively, we define the compensation as

$$k = \frac{N_A}{N_D}. \quad (1)$$

Due to the low concentration of donors, we neglect the superposition of electron wave functions and consider only the electrostatic interaction between ionized impurities. Since we treat donors as major impurities, we have at low temperatures a distribution of neutral donors and an equal number of ionized donors and acceptors. We make use of the semiclassical impurity band model developed by Andrada e Silva and da Cunha Lima [7], which treats ionized impurities classically, while considering the interaction between bound electrons and donor quantum mechanically.

The Hamiltonian of one electron bound to a donor in the presence of a magnetic field is given by

$$H = -\frac{\hbar^2}{2m^*} \nabla^2 - \frac{e^2}{Ku} + V(z) + \frac{e^2 B^2}{2m^* c^2} + \frac{eB}{2m^* c} L_z, \quad (2)$$

where e , m^* and L_z are the absolute value of the charge, effective mass and the z -component of the angular momentum of the electron, respectively, $u = \sqrt{x^2 + y^2 + (z - z_i)^2}$ is the distance between the electron and the donor situated at $(0, 0, z_i)$, K is the dielectric constant, B is the magnetic field, c is the

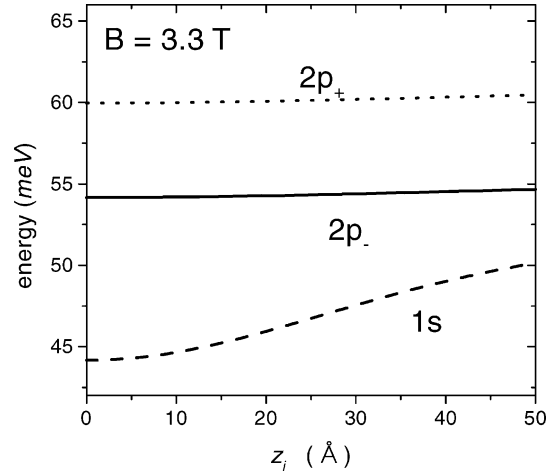


Fig. 1. Electronic energy of the states 1s, 2p₋, and 2p₊, for a quantum well with a width of 100 Å, and intensity of magnetic field $B = 3.3$ T.

light velocity, and $V(z)$ is the confining quantum well potential energy defined by

$$V(z) = \begin{cases} 0 & \text{if } |z| < L/2, \\ \infty & \text{if } |z| > L/2, \end{cases} \quad (3)$$

L being the well width.

The variational wave functions [3], needed for our study of light absorption, are written as

$$\psi_{1s}(\vec{r}) = A_{1s} \cos\left(\frac{\pi z}{L}\right) \exp(-[\kappa_{1s}u + \eta_{1s}\rho^2]), \quad (4)$$

$$\psi_{2p_{\pm}}(\vec{r}) = A_{2p} \cos\left(\frac{\pi z}{L}\right) \exp(\pm i\varphi) \times \exp(-[\kappa_{2p}u + \eta_{2p}\rho^2]), \quad (5)$$

where the sets $(A_{1s}, \kappa_{1s}, \eta_{1s})$ and $(A_{2p}, \kappa_{2p}, \eta_{2p})$ represent the normalization constant and variational parameters of the above wave functions and $\rho = \sqrt{x^2 + y^2}$. In Fig. 1, we show the energies of the levels 1s, 2p₊ and 2p₋ as a function of z_i for $B = 3.3$ T.

We use the self-consistent method [1] to determine the thermal properties of the system in the following way: Given an initial electric charge density (ionized impurities), the electrostatic potentials are calculated. From the knowledge of the energy of the electron bound to a donor in a quantum well, the electronic density of states are determined. After that, the chemical potential is computed by imposing the number of neutral donors which is the function of a quantum well compensation. From the chemical potential, the

charge density can be recalculated via Fermi–Dirac distribution. The procedure is performed until the convergence of the chemical potential is achieved. Finally, the system energy and the electronic specific heat are computed. These steps will be detailed as follows.

Using as initial charge density, the one obtained by Colchesqui et al. [8], corresponds to 0 K,

$$\rho(z) = \frac{eN_D}{L} (\Theta(|z| - z_m) - k),$$

$$z_m = \frac{L}{2}(1 - k),$$

where $\Theta(x)$ and z_m are the Heaviside theta function and the half-width of the distribution of neutral donors, respectively. The electrostatic potential $\phi(z)$, whose effect is only a weak perturbation ($-e\langle\psi|\phi(z)|\psi\rangle$) on the electron energy, is obtained via Poisson's equation. Next, we calculate the electronic density of states per donor

$$D(E_{1s}) = \frac{2}{L} \frac{1}{|dE_{1s}/dz|}, \quad (6)$$

where E_{1s} is the corrected energy of the 1s electron. Assuming the charge neutrality, we have

$$(1 - k) = \int D(E_{1s}) \frac{1}{\exp((E_{1s} - \mu)/k_B T) + 1} dE_{1s}, \quad (7)$$

where k_B is the Boltzmann constant. With this equation we obtain the chemical potential μ which is used to compute a new charge density

$$\rho(z) = \frac{eN_D}{L} \times \left[\left(1 - \frac{1}{\exp((E_{1s}(z) - \mu)/k_B T) + 1} \right) - k \right]. \quad (8)$$

The process continues until the convergence of the chemical potential is achieved, so that one may be able to calculate any thermal property of the system.

The time average dissipation rate of the incident electromagnetic energy (P) is computed from the Joule effect

$$P = \sigma_1 \langle \mathcal{E}^2 \rangle V, \quad (9)$$

where σ_1 is the real part of the material optical conductivity, \mathcal{E} is the intensity of the radiation electric field and V is the effective volume of a single donor

impurity which is equal to the inverse of the donor density

$$V = \frac{1}{N_D}. \quad (10)$$

The symbol $\langle \dots \rangle$ represents the time average of a physical quantity.

$\hbar\omega$ being the energy of the absorbed photon and $W(z_i)$ the transition rate per unit time between the levels of a single impurity, given by the Fermi golden rule, we have

$$P = W(z_i) \hbar\omega. \quad (11)$$

The optical conductivity for a single neutral donor impurity located at z_i inside a quantum well is then given by

$$\sigma_1(z_i, \omega) = \frac{N_D \hbar\omega W(z_i)}{\langle \mathcal{E}^2 \rangle}. \quad (12)$$

Considering the well known expression for $W(z_i)$, in the case of long wave limit, taking a plane wave of polarization \vec{u} we obtain

$$\sigma_1(z_i, \omega) = N_D e^2 \omega |\vec{u} \cdot \langle 1s | \vec{r} | m \rangle_{z_i}|^2 \delta(E_{m,1s} - \hbar\omega), \quad (13)$$

where $\langle 1s | \vec{r} | m \rangle_{z_i}$ is the matrix element of the operator \vec{r} taken between the states 1s and $m = 2p_+$, $2p_-$ of an electron bound to the impurity located in z_i . The transition takes place between the 1s and $2p_+$ or $2p_-$ donor impurity states, depending on the photon polarization. The term $E_{m,1s}$ represents the difference between these energy levels.

The total absorption coefficient is obtained by summing up the contribution of all neutral donor impurities in the quantum well. For fixed N_D and k , μ is a function of temperature. ($D_j(E)$) being the joint density of states connected by the transition, given by

$$D_j^{1s \rightarrow m}(E) = \frac{2}{L} \frac{1}{|dE_{m,1s}/dz|_{E_{m,1s}=E}}, \quad (14)$$

we finally have

$$\sigma_1^{1s \rightarrow m}(\omega, T) = N_D \pi e^2 \omega \frac{1}{\exp((E_{1s}(z_0) - \mu)/k_B T) + 1} \times |\vec{u} \cdot \langle 1s | \vec{r} | m \rangle_{z_0}|^2 D_j^{1s \rightarrow m}(\hbar\omega), \quad (15)$$

where z_0 is defined as the position in which the transition energy equals the photon energy, i.e.

$$E_{m,1s}(z_0) = \hbar\omega, \quad (16)$$

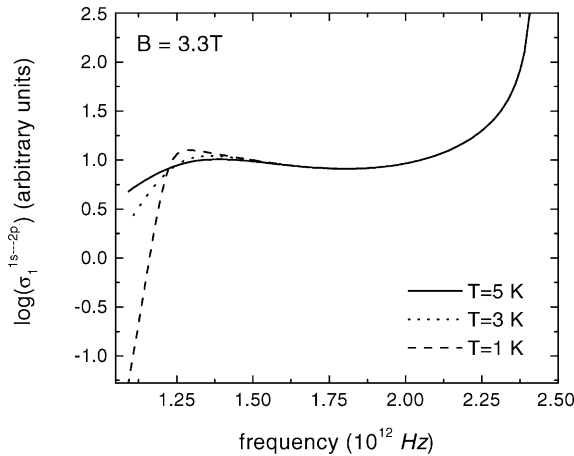


Fig. 2. Absorption coefficient for the transition $1s \rightarrow 2p_-$ with intensity of magnetic field $B = 3.3$ T, compensation $k = 0.1$, and temperatures $T = 1, 3$, and 5 K.

with m being equal to $2p_+$ or $2p_-$. It is interesting to observe the presence of the Fermi–Dirac distribution function in Eq. (15).

3. Results and conclusions

The absorption coefficient was calculated for quantum wells of 100 \AA width and concentrations of 10^9 donors/cm². The results presented here are a consequence of the neutral donor distribution that depends on the compensation, the magnetic field and temperature. At low temperatures, the neutral donors are located in the central region of the quantum well since the lowest level ($1s$) donor energy increases from the center to the border of the quantum well as shown in Fig. 1. The occupation of these levels depends on the compensation of the system, varying from the completely occupied one at $k = 0$, to a totally empty one at $k = 1$. Due to the Fermi distribution function, the occupancy of the highest levels occurs by the increase of temperature, allowing absorption of low energy photons. Fig. 2 shows the absorption coefficient at three different temperatures and one can observe that the sample is almost transparent for the lowest frequencies at a temperature of 1 K.

The effect of the magnetic field is to modify the energy levels, maintaining the absorption coefficient frequency range nearly the same for the transition

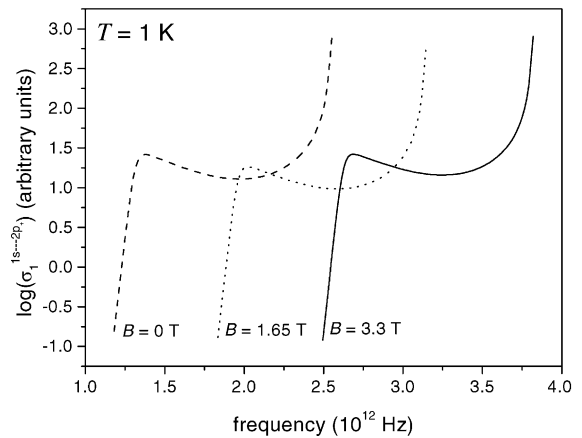


Fig. 3. Absorption coefficient for the transition $1s \rightarrow 2p_+$, with compensation $k = 0.1$, temperature $T = 1$ K, and from left to right: intensity of magnetic field $B = 0, 1.65$, and 3.3 T.

$1s \rightarrow 2p_-$, while changing those for the $1s \rightarrow 2p_+$ transitions. As the magnetic field increases, the last absorption spectrum is dislocated to higher frequencies. This effect is due to the fact that the $1s$ and $2p_-$ levels suffer almost the same changes as the magnetic field increases, while the $2p_+$ level presents a crescent increasing relatively to the other two levels. Fig. 3 shows the $1s \rightarrow 2p_+$ absorption coefficient for various magnetic fields.

As a conclusion, we can say that this is a very interesting system whose optical absorption, in the far infrared range, in principle, may be used for the diagnosis of a doped and compensated quantum well.

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