Holes at GaAs-$Al_xGa_{1-x}As$ heterojunctions in magnetic fields

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The effects of anisotropy of the valence-band structure and of the mixing of the heavy and light holes on the Landau levels of the hole inversion layer in a normal magnetic field are studied. Some of the crossings of the Landau levels which occur when anisotropy is neglected are removed when it is included. While the measured multiple cyclotron-resonance frequencies are explained qualitatively by our calculation, there is quantitative disagreement.

I. INTRODUCTION

Recently, the Landau levels for the topmost valence subband in a p-channel inversion layer at a GaAs-$Al_xGa_{1-x}As$ heterojunction under a normal magnetic field have been calculated independently by Bangert and Landwehr[1] and by Broido and Sham.[2] Both theories are based on the Luttinger effective Hamiltonian for the spin-orbit split valence bands.[3] The interaction of the heavy- and light-hole bands gives rise to Landau levels that are unequally spaced and have a very nonlinear magnetic-field dependence such that some levels actually cross. The unequal level spacings give rise to a multiplet of cyclotron frequencies at a particular value of the field which are qualitatively similar to observation,[4] but the calculated frequencies are generally too high compared with the measured ones. Broido and Sham[2] have suggested that the discrepancy may be due to many-body interaction.

In a calculation of the hole subbands, both groups include the band anisotropy between the normal direction and the directions parallel to the interface, and the anisotropy in the plane of the interface itself. Inclusion of the in-plane or subband anisotropy results in the warped Fermi surfaces shown in Fig. 2 of Ref. 1 and Fig. 3 of Ref. 2. In determining the Landau levels, both groups, for simplicity, neglect the terms which produce this anisotropy. In this paper, we study the effect of the subband anisotropy on the Landau levels. In Sec. II the $\mathbf{k}\cdot\mathbf{p}$ method with the subband basis is used to determine the energy levels in magnetic field, with the anisotropy effect included. In Sec. III the calculated Landau levels are presented together with a discussion of the effect of anisotropy. The resultant cyclotron frequencies are compared with experiment. Section IV presents our conclusions.

II. THE SUBBAND $\mathbf{k}\cdot\mathbf{p}$ METHOD

The 4×4 Luttinger Hamiltonian[3] is used to describe the four uppermost valence bands. If the normal to the interface and the direction of magnetic field are taken to be along the z axis, $\hat{k}_z$ stands for the operator $(1/i)\partial/\partial z$, and the in-plane components, $\hat{k}_x$ and $\hat{k}_y$, stand for the operators,

$$\hat{k}_\alpha=\frac{1}{i}\frac{\partial}{\partial x_\alpha}+\frac{e}{\hbar c}A_\alpha\ , \tag{1}$$

where the $\{A_\alpha\}$ are the components of the vector potential.

Following Luttinger, we define the creation and annihilation operators for the harmonic oscillator with frequency $\omega_c=eB/mc$ and cyclotron radius $R_c=\sqrt{\hbar c/eB}$:

$$a^\dagger=\frac{R_c}{\sqrt{2}}\hat{k}_+,\ a=\frac{R_c}{\sqrt{2}}\hat{k}_-,\ \ \hat{k}_\pm=\hat{k}_x\pm i\hat{k}_y\ . \tag{2}$$

Note that m is the free electron mass.

The effective Hamiltonian in the presence of the self-consistent inversion layer potential $V(z)$ and the magnetic field is given by

$$H_{\rm eff}=H_I+H_A\ . \tag{3}$$

H_I is the "isotropic" part of the Hamiltonian used in Refs. 1 and 2:

$$H_I=H_0(a,a^\dagger,\hat{k}_z)+V(z)\ , \tag{4}$$

with

$$H_0(a,a^\dagger,\hat{k}_z)=\begin{bmatrix} -P-Q-\frac{3}{2}\kappa B & -R_I & S & 0 \\ -R_I^\dagger & -P+Q+\frac{1}{2}\kappa B & 0 & -S \\ S^\dagger & 0 & -P+Q-\frac{1}{2}\kappa B & -R_I \\ 0 & -S^\dagger & -R_I^\dagger & -P-Q+\frac{3}{2}\kappa B \end{bmatrix}. \tag{5a}$$

In Luttinger's notation, P, Q, R_I, and S have the following expressions (in atomic units with hole energy measured as negative):

$$P=\frac{\gamma_1}{2}(\hat{k}_z^2+2\omega_c a^\dagger a+\omega_c),$$
$$Q=\frac{\gamma_2}{2}(-2\hat{k}_z^2+2\omega_c a^\dagger a+\omega_c)\,, \tag{5b}$$
$$R_I=-\sqrt{3}\bar{\gamma}\omega_c a^2,\quad S=\sqrt{6}\gamma_3\hat{k}_z\omega_c a\,,$$
$$\bar{\gamma}=\tfrac{1}{2}(\gamma_2+\gamma_3)\,.$$

$V(z)$ enters along the diagonal of matrix H_I. The Luttinger parameters, γ_1, γ_2, and γ_3, and κ are taken to be:[5] $\gamma_1=6.85$, $\gamma_2=2.1$, $\gamma_3=2.9$, and $\kappa=1.2$. H_A contains the previously neglected anisotropy terms

$$H_A(a,a^\dagger)=\begin{bmatrix} 0 & -R_A & 0 & 0 \\ -R_A^\dagger & 0 & 0 & 0 \\ 0 & 0 & 0 & -R_A \\ 0 & 0 & -R_A^\dagger & 0 \end{bmatrix},$$
$$R_A=\sqrt{3}\mu\omega_c a^{\dagger 2},\quad \mu=\tfrac{1}{2}(\gamma_3-\gamma_2)\,. \tag{6}$$

In general, the four-component effective-mass wave function has the form

$$\Psi^s=\sum_j F_j^s v_j\,. \tag{7}$$

The $\{v_j\}$ are the (J,m_J) basis states for $J=\frac{3}{2}$ (see Appendix of Ref. 2), and j stands for the branch index of the valence band complex, $m_J=\frac{3}{2},-\frac{1}{2},\frac{1}{2},-\frac{3}{2}$. The F_j^s are the components of the column vector solution of $H_{\rm eff}$. The index s represents all the quantum numbers needed to specify a state in the Landau level spectrum; i.e., it labels an eigenstate of $H_{\rm eff}$, and it consists of the set $\{i,\nu,n,k\}$. Here, i characterizes the nature of the subband as one of two heavy-hole $(h+,h-)$ and two light-hole $(l+,l-)$ solutions. If the band mixture (i.e., the off-diagonal elements) were reduced to zero, i would be identical to j, and the characterization would be exact. ν ranks the subband for each i, n identifies one of an infinite set of Landau levels for each (i,ν), and k specifies one of the N-fold degenerate states within each Landau level (i,ν,n).

In the subband $\mathbf{k}\cdot\mathbf{p}$ method, the set of eigenstates at $k_x=k_y=0$ is chosen to be the basis set for motion along z. Denote these functions by $\psi_{\nu,j}(z)$. The motion parallel to the interface is expressed in terms of products of harmonic oscillator functions and plane waves, which take the form

$$\phi_{n_r k}(x,y)=e^{ikx}u_{n_r}(y-R_c^2k)$$

if we choose the gauge $\mathbf{A}=(-By,0,0)$. ν_r and n_r label the subbands and Landau levels of the product basis $\phi_{n_r k}\psi_{\nu_r j}$. Then, expanding the envelope functions in terms of $\phi_{n_r k}\psi_{\nu_r j}$ gives

$$F_j^s=\sum_{\nu_r n_r} A^s_{\nu_r n_r j}\phi_{n_r k}\psi_{\nu_r j}\,. \tag{8}$$

Taking the matrix element $\langle \underline{F}^s\,|\,H_{\rm eff}\,|\,\underline{F}^s\rangle$, where $\underline{F}^s$ is the four-component vector, $(F^s_{3/2},F^s_{-1/2},F^s_{1/2},F^s_{-3/2})$, we obtain a matrix equation for the $A^s_{\nu_r n_r j}$. The energy values and eigenstates are found by diagonalizing this matrix. Note that Ψ^s is a linear combination of the products of $\psi_{\nu_r j}$, $\phi_{n_r k}$, and v_j. Therefore, i,ν,n, which label an eigenstate s are not to be confused with the labels of the basis functions ν_r,n_r,j.

At this point, let us consider the degeneracy N associated with each Landau level, (i,ν,n). Since $\phi_{n_r k}$ is an eigenstate of $a^\dagger a$ with an eigenvalue that is independent of k, i.e., $a\phi_{n_r k}=(n_r)^{1/2}\phi_{(n_r-1)k}$, and $a^\dagger\phi_{n_r k}=(n_r+1)^{1/2}\phi_{(n_r+1)k}$, the eigenvalues of $H_{\rm eff}$ must also be independent of k. Each k specifies a unique orbit center $y_0=R_c^2k$ which must lie within the y dimensions of the interface. By the same argument used for the equally spaced free-electron Landau levels, the degeneracy per unit area of each level is then just the free-electron factor $N=eB/hc$.

Luttinger[3] has found that when the anisotropy is neglected (i.e., $\mu=0$), the solution simplifies considerably. Then, the coefficient $A^s_{\nu_r n_r j}$ has, for a given j and ν_r, only one nonzero component in the whole range of n_r values. For example, at a particular value of ν_r and $j=-\frac{1}{2}$, the only nonzero component is for $n_r=n$. Then, for the same ν_r, at $j=\frac{3}{2}$ the nonzero component is at $n_r=n-2$. At $j=\frac{1}{2}$, $n_r=n-1$ and at $j=-\frac{3}{2}$, $n_r=n+1$. Each n then specifies a unique set of four running indices $\{n_r\}$ and ranges from -1 to ∞. The $\mu=0$ envelope functions can be expressed in place of Eq. (8) as the vector

$$\underline{G}^s=\begin{bmatrix} u_{n-2}\psi_{1,n} \\ u_n\psi_{2,n} \\ u_{n-1}\psi_{3,n} \\ u_{n+1}\psi_{4,n} \end{bmatrix}, \tag{9}$$

with $\psi_{1,n}=\sum_{\nu_r}A^s_{\nu_r,n-2,3/2}\psi_{\nu_r j}$, etc.

For $\mu\neq 0$, the anisotropy terms in H_A introduce more nonzero n_r components and consequently mix the unperturbed states $\underline{G}^s$. In particular,

$$\langle \underline{G}^{i\nu m}\,|\,H_A\,|\,\underline{G}^{j\nu n}\rangle\sim\delta_{m,n\pm 4} \tag{10}$$

so that only states whose Landau indices differ by multiples of four are connected in a perturbation expansion of the G^s. Note that this coupling is independent of i and j. H_A has been treated in second-order perturbation theory in the three-dimensional case.[6] In our calculation, we find it easier simply to diagonalize a sufficiently large matrix for the expansion coefficients in Eq. (8). We use perturbation theory only to examine qualitatively the splitting of the crossed Landau levels.

Consider the effect of H_A treated as a perturbation on the eigenstates of H_I given by Eq. (8). From Eq. (10), H_A has no diagonal elements in the H_I representation. The strongest coupling of two nondegenerate levels then occurs between states whose Landau indices differ by 4. A second-order energy shift of each level results. Nondegenerate states whose Landau indices differ by 0, 8, 12, 16, etc., are coupled in higher order. The nonlinear char-

acter of the unperturbed Landau levels results in many level crossings. At a crossing, if the degenerate states have Landau indices which differ by 4, then, by degenerate perturbation theory, a first-order energy shift lifts the degeneracy. We expect that levels corresponding to these states will be the most strongly mixed by the anisotropy. For other coupled levels that cross, the energy shift is of higher order.

III. LANDAU LEVELS OF THE HOLE INVERSION LAYER

As in Ref. 2, we consider the topmost hole level $\nu=0$, $i=h\pm$ occupied to a hole layer density of 5×10^{11} cm^{-2}. The dopent in the GaAs is taken to be n type with a density of 10^{15} cm^{-3}. Bangert and Landwehr, in contrast, take the GaAs to be pure. Also, they do not use the $\mathbf{k}\cdot\mathbf{p}$ subband basis set. We use the same subband basis as in Ref. 2, consisting of two heavy-hole and two light-hole bands. Our result for the Landau level energies is valid to three significant figures. Typically 12–17 harmonic oscillator functions are used. The $\mu=0$ energy levels check with those of Ref. 2.

We classify the levels according to their prominent character in the region of fields where the mixing is small, and label them in the manner of Ref. 2. Figure 1 illustrates the anticrossing behavior of the 1− and 5+ levels caused by anisotropy. (Here, the shorthand notation 1− refers to $i=h-$, $\nu=0$, and $n=1$, while 5+ is $i=h+$, $\nu=0$, and $n=5$. Note that an error exists in the labeling of the Landau levels of Ref. 2. Levels labeled 2− and 3− should be labeled 1− and 2−.) It is evident that the anisotropy removes the degeneracies at $B\sim3.5$ T and $B\sim8.5$ T. Note that the levels with anisotropy included are labeled according to the prominent character above the degeneracy at 8.5 T. However, between 3.5 and 8.5 T the character is reversed. Figure 2 displays several $\mu\neq0$ levels along with a trace of the Fermi level. The Fermi level jumps between Landau levels at $B=20.7$, 10.4, 6.9, 5.2, 4.1 T, etc. Note first that the anisotropy terms tend to zero as the field tends to zero, so that the $\mu\neq0$ Landau levels converge to those for $\mu=0$ in the low-field limit. Also, for a given value of B, levels with larger n shift more since the matrix element in Eq. (10) goes like n. In addition, in the region between 4 T and 8 T, the levels labeled 2−, 3−, and 4− are mixed strongly with 6+, 7+, and 8+, respectively, and below 4 T the prominent character of these levels is actually 6+, 7+, and 8+. Finally, note that levels whose indices differ by other than multiples of four still cross.

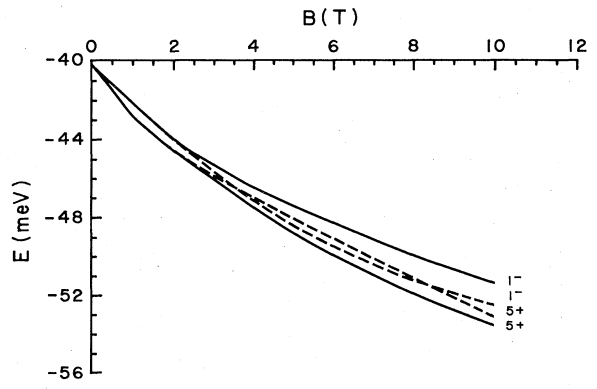

FIG. 1. Mixing of the 1− and 5+ Landau levels. Dotted (solid) lines correspond to the neglect (inclusion) of anisotropy.

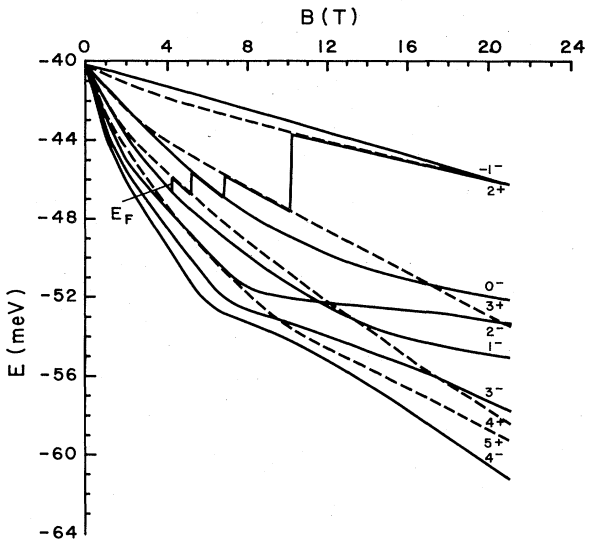

FIG. 2. Landau and Fermi levels with anisotropy effect included.

The cyclotron frequencies are specified by the energy difference between two particular states subject to the conditions $\Delta n=\pm1$ [with anisotropy included, this condition must be relaxed because of the mixing of the states in

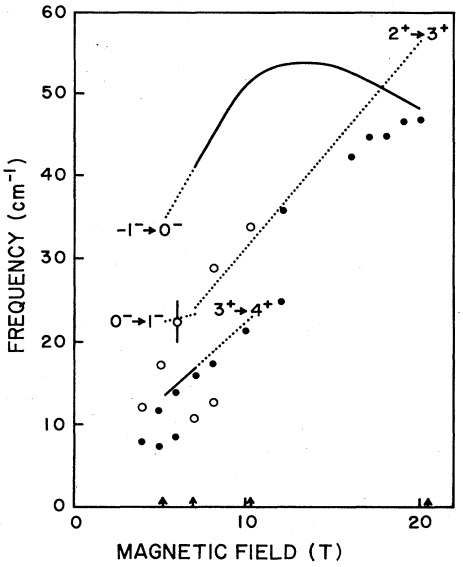

FIG. 3. Measured cyclotron frequencies compared with theory neglecting anisotropy. Experimental data from Ref. 4 shown as follows: solid circles are strong transitions, open circles are weak transitions. Theoretical results shown as follows: solid lines are strong transitions, dotted lines are weak transitions. Arrows indicate where the Fermi level jumps.

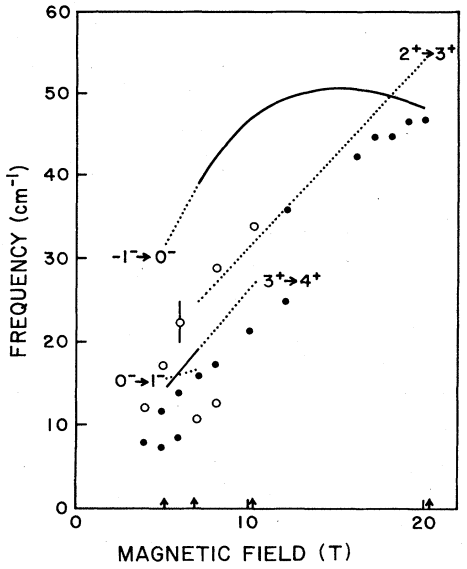

FIG. 4. Measured cyclotron frequencies compared with theory including anisotropy. Symbols are defined in Fig. 3 caption.

Eq. (10)]. Transitions from completely filled to completely empty states are designated as strong transitions. All others, some of which arise from partially filled levels, are considered weak. The measured frequencies are taken from the data of Schlesinger *et al.*[3] Figure 3 compares the measured frequencies with those of the $\mu=0$ case. In Fig. 4 the measured frequencies are compared to those obtained from the current work. Examination of Figs. 3 and 4 shows that with the inclusion of anisotropy, the $0-\rightarrow 1-$ transition exhibits the largest shift, while the shifts for the $2+\rightarrow 3+$ and $1-\rightarrow 0-$ transitions are comparably small. This is a result of the strong interaction between $1-$ and $5+$. In both cases, the theoretically determined number of transitions at a given value of magnetic field matches the experiment over the range of fields below 12 T. The calculated frequencies, however, are still much larger than the measured ones. A proper correspondence between theory and experiment requires the $2+\rightarrow 3+$ and $3+\rightarrow 4+$ transitions to be matched to the lowest two sets of points and the $1-\rightarrow 0-$ transition to be matched with the upper set of points. Also, the corresponding transition strengths do not match the data.

IV. CONCLUSIONS

The effect of subband anisotropy on the Landau levels in a *p*-channel GaAs inversion layer has been examined. This work includes a detailed study of the anticrossing of the levels which results from the inclusion of band anisotropy. This effect does not change the cyclotron frequencies significantly except when the mixing between two levels is strong. The calculated cyclotron frequencies are still too high compared with experiment. We again conjecture, as in Ref. 2, that many-body effects in the hole plasma may be the cause of this disagreement. The effect of anisotropy on the Landau levels in an undoped well is not masked by many-body effects due to the hole plasma, and may be relevant in determining exciton binding energies in finite magnetic fields. A study of this effect on excitons in the undoped quantum well in the presence of magnetic field is planned.

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