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Two-dimensional space-charge layer in a tilted magnetic field

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Combined intersubband cyclotron resonances in a quasi-two-dimensional space-charge layer with a magnetic field tilted with respect to the surface are studied through a simple single-electron model. Two alternative basis sets have been pointed out which enable one to obtain analytical matrix elements of the Hamiltonian for all values of the magnitude and the angle of tilt of the magnetic field. The effect of the coupling between electronic motions normal and parallel to the layer has been investigated in detail and is found to give rise to deviations in the expected values of the Landau spacings as functions of the tilt angle of the B field. Optical spectra for such systems show some features in qualitative agreement with experiments and other calculations. The system is a prototype of nonseparable problems in two dimensions.

I. INTRODUCTION

In recent years, the study of two-dimensional space-charge layers (as can be found in metal-oxide—semiconductor sandwiches) under a tilted magnetic field has been of increasing theoretical and experimental interest.[1-3] Following a report[2] on combined intersubband cyclotron resonances, Ando[1] performed a detailed numerical calculation with a large basis set that includes many-body corrections which account for many features of the observations. We present here a simple one-electron model for a two-dimensional space-charge layer under a tilted magnetic field. This is not to say that many-body effects are unimportant; in fact, they are important, particularly in the silicon system which is the system most extensively studied.[1,2] However, use of a model potential,[4] in which the electron in the space-charge layer is assumed to be held in the z direction (normal to the interface) by a "triangular" potential well due to the applied electric field, is not uncommon in the literature.[3,5] This is because the model seems to be quite adequate for certain systems like PbTe (Ref. 3) and, because it serves as a common backdrop against which new many-body effects can be viewed, the model continues to be used for this purpose.[5] The motivation for our study of the tilted magnetic field problem in this model is that it seems desirable to be able to explore which and how much of the observed phenomena can arise out of the single-particle description. Such a complete study of single-particle effects will serve to point out more clearly features which are due solely to many-body aspects of the problem. Since we neglect many-body aspects, we make no claim for a complete description of a space-charge layer in a tilted field. The merit of our study, as we will see, is that we get results qualitatively similar to those hitherto attributed to many-body effects. In this way, our study points to another possible origin of some of the observed features of the combined resonances, namely the coupling between the motions parallel and perpendicular to the interface induced by the tilted magnetic field. A further and important feature of the simple model is that it is a prototype of problems[6] involving motions in more than one dimension (here two perpendicular directions) when the nonseparability of the motions is essential for the phenomena under study. Being simple enough, this prototype may serve to give insights into the general quantum mechanical problem of nonseparable motions.

The electric field normal to the oxide-semiconductor interface (x-y plane) groups the electrons into quantized energy levels called electric subbands. An additional magnetic field along the z direction further quantizes the electronic motion in the x-y plane. Since there is no coupling between the cyclotron motion in the x-y plane and the subband motion along the z direction, such a problem is trivial. A more interesting case results when the B field is tilted from the normal so that a component B_y is present as well. As shown in Sec. II, the Hamiltonian, when reduced to its simplest form, contains a term coupling the y and z

motions. Because of this coupling between the cyclotron and subband motions, transitions between energy levels involving a simultaneous change in the subband index as well as the Landau quantum number become possible under an external radiation field. These are the combined intersubband cyclotron resonances. Depending on the strength of the magnetic field relative to the electric one and on the angle of tilt of the B field, the coupling can modify the optical spectrum considerably. In most of the experiments done so far, particularly on Si-MOSFET (metal-oxide—semiconductor field-effect transistor) devices, the quantization of the z motion has been dominated by the electric field. However, situations where even the z motion is governed mainly by the B field have appeared recently in the literature.[3] Thus the model Hamiltonian we consider proves to be even more interesting in that it contains a nontrivial coupling between two competing modes (the y and z motions) and such systems may prove to be a fertile ground where one may expect to find features due to the strong mixing phenomenon as has been suggested in the literature.[7] This provides a further motivation for investigating such systems. The Hamiltonian as given in Sec. II represents a simple (in that all the dependences are either linear or quadratic in the coordinate variables) prototype of two-dimensional nonseparable systems.

We employ two alternative basis sets to diagonalize the Hamiltonian. The matrix elements obtained are in closed form and easily calculable. Section II describes briefly the model Hamiltonian and the methods for calculating the energy levels as well as the optical spectrum for a weak z-polarized radiation. Section III then proceeds to describe the numerical results and their discussions. Section IV contains a summary and conclusions.

II. CALCULATION OF ENERGY LEVELS AND OPTICAL SPECTRUM

As our model[4] for the space-charge layer in metal-oxide—semiconductor (MOS) devices, we consider it to be effectively a two-dimensional electron gas. Each electron describes free motion in the x-y plane (assumed parallel to the oxide-semiconductor interface) but is held in the z direction (normal to the interface) by an infinite potential barrier at $z=0$ on the oxide side and a linear electric field potential $e\epsilon z$ on the other side. The electric subband levels are then considered to be the quantized energy levels in such a triangular potential well. The strength of the electric field is proportional to the sum N_s of the number density of the space-charge layer and that in the depletion layer: $\epsilon=kN_s$. The constant of proportionality k is regarded as an adjustable parameter and can be chosen to reproduce the experimental value for the energy separation of the ground and the first excited subband. In this way, through the empirical choice of k, the many-body aspects may be thought to be included to some extent in our model. But, apart from that, we consider the system as one of a single electron moving in a triangular potential well. This approximation is reasonably justified for inversion layers as well as for low-doped semiconductors (quasi-accumulation-layers). We do emphasize, however, that this is an oversimplication, because the actual effective potential for an electron, especially in an excited state or in accumulation layers, departs considerably over some ranges from the triangular one.[8]

If a magnetic field is applied to such a system tilted with respect to the normal to the interface by an angle α, let B_z and B_y be its components perpendicular and parallel to the surface, respectively. Choosing a gauge $\vec{A}=(zB_y-yB_z,0,0)$ as in Ref. 2 to describe this field, the Hamiltonian for the electron can be written as

$$H=\frac{p_y^2}{2m_t}+\frac{p_z^2}{2m_l}+\frac{1}{2m_t}\left[p_x+\frac{e}{c}(zB_y-yB_z)\right]^2 +e\epsilon z\ ,$$

$$-\infty\leq y\leq\infty,\ 0\leq z\leq\infty \tag{1}$$

where m_t and m_l are the effective masses of the electron parallel and perpendicular to the interface, respectively. With H as given in Eq. (1) the x part of the wave function is described by plane waves and translating y by cp_x/eB_z, the x coordinate can be removed. This transformation is legitimate for all $B_z\neq 0$. Equation (1) then becomes

$$H=\left[\frac{p_y^2}{2m_t}+\frac{e^2B_z^2}{2m_tc^2}y^2\right]+\left[\frac{p_z^2}{2m_l}+e\epsilon z+\frac{e^2B_y^2}{2m_tc^2}z^2\right] -\frac{e^2B_yB_z}{m_tc^2}yz\ . \tag{2a}$$

One obtains the same Hamiltonian as above for the parametric choice $\langle p_x \rangle = 0$. We note that while this choice of $\langle p_x \rangle$ does not affect the eigenvalue structure when B_z is nonzero (because of the admissible translation in y), it does *not* give the true ground-state energy when $B_z = 0$. The value of $\langle p_x \rangle$ which minimizes the energy in this case is seen from Eq. (1) to be $(-eB_y/c)\langle z \rangle$ and then the appropriate Hamiltonian becomes

$$H = \frac{p_y^2}{2m_t} + \frac{p_z^2}{2m_l} + e\epsilon z + \frac{e^2 B_y^2}{2m_t c^2}(z - \langle z \rangle)^2 \,. \tag{2b}$$

For $B_z = 0$, the difference between the two Hamiltonians given by Eqs. (2a) and (2b) is due to the presence of the $\langle z \rangle$ terms in the latter. We, however, attempt in this paper to solve for the Hamiltonian given by Eq. (2a), after noting that this is *singular* at $B_z = 0$, and that its eigenvalues have a jump discontinuity at $B_z = 0$, the magnitude of the "jump" being equal to the difference in the eigenvalues of the Hamiltonian (2a) from the corresponding ones of the Hamiltonian (2b).

Thereby, for $B_z \neq 0$, the effect of the magnetic field is to quantize further the y motion of the electron. Note that the last term, which denotes the coupling between the y and the z motions, vanishes in either Faraday ($\alpha = 0°$) or Voigt ($\alpha = 90°$) geometry. Further, for $\alpha = 90°$, B_z is zero and the electron becomes free in the y direction and is assumed to carry zero momentum in that direction in the subsequent discussions.

If the effect of the B field is weak, a Born-Oppenheimer- (BO-) type solution is possible wherein one starts with the undisturbed electric subbands and evaluates the z^2 and the z terms in the magnetic part in terms of the undisturbed wave functions. One can then solve for the y motion. Such a procedure leads to a positive correction

$$\Delta E_n^{\mathrm{BO}} = (e^2 B_y^2 / 2m_t c^2)(\langle z^2 \rangle_{nn} - \langle z \rangle_{nn}^2) \tag{3}$$

to the nth subband energy and the appearance of substructure in the form of equally spaced Landau levels for y motion on each subband with spacing $\hbar\omega_z$ where $\omega_z = eB_z/m_t c$. It may be interesting to note that when $B_z = 0$, the BO-type approach leads to the same correction when applied to the Hamiltonian (2b) but to a different and larger correction when applied to the Hamiltonian (2a). The difference between these, viz., $(e^2 B_y^2/2m_t c^2)\langle z \rangle_{nn}^2$ is roughly equal to the magnitude of the "jump" at the singular point $B_z = 0$ for the Hamiltonian (2a), as mentioned before. We will return to this point again in Sec. III. With regard to the Landau substructure formed on each subband, the experimental results,[2,3] however, showed substantial departure from the expected pattern of equispaced Landau levels, particularly at large tilt angles. As an example, the Landau-level spacings were not given solely in terms of B_z. We regard this as a crucial point. Within an adiabatic separation of y and z motions, the Landau-level spacing is unequivocally a function of B_z alone. However, proper treatment of the coupling between the two motions can, even within a single particle description, account for additional dependences of the spacings on B_y as well.

Note that if the coupling is neglected, the y and z part of the wave functions are described by the well-known harmonic oscillator and Weber functions, respectively. However, Weber functions are, in general, more cumbersome to handle. Depending on whether the electric field or the magnetic one dominates the subband structure, however, either Airy functions or harmonic oscillator wave functions (of odd order, since the wave function must vanish at $z = 0$ for all y) provide us with two suitable alternative choices of the basis functions to diagonalize H. We define a parameter

$$\Theta = (e^2 \epsilon^2 \hbar^2 / 2m_l)^{1/3} / \hbar\omega_0, \quad \omega_0 = eB_0/m_t c \,, \qquad B_0 = (B_y^2 + B_z^2)^{1/2} \,, \tag{4}$$

which gives a measure of the strength of the ϵ field relative to the B field. $\Theta \sim 0.57$ implies a situation where the energy separation between the ground electric subband and the next higher one equals the Landau separation for $\alpha = 0°$. It may be interesting to note that Θ, as defined above, can also be written as the ratio $m_t l_B^2 / m_l l_E^2$, where l_B and l_E are the characteristic lengths associated with the magnetic and the electric fields and are equal to $(\hbar/2m_t\omega_0)^{1/2}$ and $(\hbar^2/2m_l e\epsilon)^{1/3}$, respectively. In most of the space-charge layers studied so far, Θ is large. However, a situation where the B field dominates the z quantization (i.e., Θ small and α large) has also been reported.[3] Accordingly, we proceed to obtain the matrix elements of H in two alternative basis sets.

(i) Electric field dominating the z quantization. We

write

$$H = H_{01} + H_1' \ , \tag{5}$$

where

$$H_{01} = \left[-\frac{\hbar^2}{2m_t}\frac{d^2}{dy^2} + \frac{e^2B_z^2}{2m_tc^2}y^2 \right] + \left[-\frac{\hbar^2}{2m_l}\frac{d^2}{dz^2} + e\epsilon z \right] , \tag{6}$$

and

$$H_1' = \frac{e^2B_y^2}{2m_tc^2}z^2 - \frac{e^2B_yB_z}{m_tc^2}yz \ . \tag{7}$$

The orthonormal basis is provided by the eigenfunctions $|nN\rangle$ of H_{01}, which satisfy

$$H_{01}|nN\rangle = \epsilon_{nN}^1 |nN\rangle \ , \tag{8}$$

where

$$\epsilon_{nN}^1 = (N+\tfrac{1}{2})\hbar \left[\frac{eB_z}{m_tc} \right] + \beta_n \left[\frac{e^2\epsilon^2\hbar^2}{2m_l} \right]^{1/3} , \tag{9}$$

β_n being the negative of the nth zero of the Airy function and $n,N = 0,1,2,\ldots$. The wave functions are written as

$$\langle y,z|nN\rangle = U_N(y)\mathrm{Ai}_n(z) \ , \tag{10}$$

where U_N and Ai_n are the usual harmonic-oscillator wave function and the Airy function, respectively, and are assumed to be properly normalized. In this basis, the matrix elements of the full Hamiltonian can now be written[9] in dimensionless form (after being scaled to $\hbar\omega_0$) as

$$\langle n'N'|H|nN\rangle/\hbar\omega_0 = [\beta_n\Theta + (N+\tfrac{1}{2})\cos\alpha]\delta_{nn'}\delta_{NN'} + \left[\frac{l_E}{2l_B}\right]^2 \sin^2\alpha \left[\frac{z^2}{l_E^2}\right]_{nn'} \delta_{NN'} - \left[\frac{l_E}{2l_B}\right] \sin\alpha(\cos\alpha)^{1/2} \left[\frac{z}{l_E}\right]_{nn'} (y\cos^{1/2}\alpha/l_B)_{NN'} \ , \tag{11}$$

where $B_z = B_0\cos\alpha$, $B_y = B_0\sin\alpha$,

$$\left[\frac{y\cos^{1/2}\alpha}{l_B}\right]_{NN'} = (N')^{1/2}\delta_{N,N'-1} + (N'+1)^{1/2}\delta_{N,N'+1} \ , \tag{12}$$

$$\left[\frac{z}{l_E}\right]_{nn'} = \begin{cases} \frac{2}{3}\beta_n & \text{if } n=n' \\ \dfrac{-2}{(\beta_n-\beta_{n'})^2} & \text{if } n\neq n' \end{cases} , \tag{13}$$

and

$$\left[\frac{z^2}{l_E^2}\right]_{nn'} = \begin{cases} \frac{8}{15}\beta_n^2 & \text{if } n=n' \\ \dfrac{-24}{(\beta_n-\beta_{n'})^4} & \text{if } n\neq n' \end{cases} . \tag{14}$$

Notice that the last term in (11) represents the coupling of the y and z motions with the ratio $l_E/2l_B$ appearing as the coupling constant. The matrix given by (11) can be cast into another form, convenient for situations where the z component of the magnetic field, B_z, is kept fixed while the tilt angle is changed so that B_y is now given by $B_z\tan\alpha$. As in (4), defining

$$\Theta_z = \frac{(e^2\epsilon^2\hbar^2/2m_l)^{1/3}}{\hbar\omega_z} \ , \tag{15}$$

the matrix elements of H after being scaled to $\hbar\omega_z$ are now given by

$$\langle n'N'|H|nN\rangle/\hbar\omega_z = [\beta_n\Theta_z + (N+\tfrac{1}{2})]\delta_{nn'}\delta_{NN'} + \left[\frac{l_E}{2l_B}\right]^2 \tan^2\alpha\cos\alpha \left[\frac{z^2}{l_E^2}\right]_{nn'} \delta_{NN'} - \left[\frac{l_E}{2l_B}\right] \tan\alpha\cos^{1/2}\alpha \left[\frac{z}{l_E}\right]_{nn'} \left[\frac{y\cos^{1/2}\alpha}{l_B}\right]_{NN'} . \tag{16}$$

(ii) Magnetic field dominating the subband structure (Θ small and α large). As before, we write

$$H = H_{02} + H_2' \ , \tag{17}$$

where

$$H_{02} = \left[-\frac{\hbar^2}{2m_t}\frac{d^2}{dy^2} + \frac{e^2B_z^2}{2m_tc^2}y^2 \right] + \left[-\frac{\hbar^2}{2m_l}\frac{d^2}{dz^2} + \frac{e^2B_y^2}{2m_tc^2}z^2 \right] , \tag{18}$$

and

$$H_2' = e\epsilon z - \frac{e^2B_yB_z}{m_tc^2}yz \ . \tag{19}$$

The basis is provided by the orthonormal eigenfunctions of H_{02},

$$\langle y,z \mid pP \rangle = U_p(y)U_{2P+1}(z), \quad p,P = 0,1,2,\ldots \tag{20}$$

which satisfy

$$H_{02} \mid pP \rangle = \epsilon_{pP}^2 \mid pP \rangle \ , \tag{21}$$

where

$$\epsilon_{pP}^2 = (p + \tfrac{1}{2}) \left[\frac{\hbar eB_z}{m_tc} \right] + (2P + \tfrac{3}{2})\hbar \left[\frac{m_t}{m_l} \right]^{1/2} \left[\frac{eB_y}{m_tc} \right] , \tag{22}$$

and U_p and U_{2P+1} are the usual harmonic-oscillator wave functions. Note the occurence of only the odd functions for the z motion because of the boundary conditions at $z = 0$.

The integral $\int_0^\infty U_{2P+1}^*(z)zU_{2P'+1}(z)dz$ can easily be calculated,[10,11] and the matrix elements of H are obtained as (when scaled to $\hbar\omega_0$)

$$\frac{\langle p'P' \mid H \mid pP \rangle}{\hbar\omega_0} = \left[(p + \tfrac{1}{2})\cos\alpha + \left[2P + \frac{3}{2} \right] \left[\frac{m_t}{m_l} \right]^{1/2} \sin\alpha \right] \delta_{pp'}\delta_{PP'} + \left[\frac{2}{\sin\alpha} \right]^{1/2} \left[\frac{l_B}{l_E} \right]^3 \left[\frac{m_t}{m_l} \right]^{5/4} \delta_{pp'}I_{PP'} - \left[\frac{m_t}{m_l} \right]^{1/4} \left[\frac{\sin\alpha\cos\alpha}{2} \right] \left[\frac{y\cos^{1/2}\alpha}{l_B} \right]_{pp'} I_{PP'} \ , \tag{23}$$

where $(y\cos^{1/2}\alpha/l_B)_{pp'}$ is given by Eq. (12) and

$$I_{PP'} = \frac{2}{\sqrt{\pi}} \frac{2^{P+P'}}{\sqrt{(2P+1)!(2P'+1)!}} \frac{\Gamma(P+\tfrac{3}{2})\Gamma(P'+\tfrac{3}{2})}{\Gamma(P-P'+\tfrac{3}{2})\Gamma(P'-P+\tfrac{3}{2})} \ . \tag{24}$$

Note the presence of the $\sin\alpha$ term in the denominator of the second term in (23) which, as expected, implies that this basis is not suitable for small tilt angles. Any of the large symmetric matrices given by (11), (16), or (23) can be diagonalized for appropriate values of the parameters to obtain energy eigenvalues E_μ and the corresponding eigenfunctions ψ_μ.

In order to see what information can be obtained regarding the strengths of various transitions from the ground to an excited subband in the presence of a magnetic field, we have calculated the optical-absorption spectrum of the system under a weak z-polarized radiation, using linear response and the dipole approximation. Following Ando,[12] the absorption can be seen to be proportional to the real part of the two-dimensional conductivity $\sigma_{zz}(\omega)$ given by

$$\mathrm{Re}\sigma_{zz}(\omega) \propto \omega^2\Gamma \sum_\mu \sum_\nu \frac{f_{\mu\nu}}{[(E_\mu - E_\nu)^2 - \hbar^2\omega^2]^2 + 4\hbar^2\omega^2\Gamma^2} \tag{25}$$

for which a phenomenological width parameter Γ has been assumed. $f_{\mu\nu}$ is the oscillator strength between states μ and ν, given by

$$f_{\mu\nu} = \frac{2m_l}{\hbar^2}(E_\mu - E_\nu) \mid \langle \Psi_\mu \mid z \mid \psi_\nu \rangle \mid^2 \ , \tag{26}$$

and satisfies the sum rule

$$\sum_\mu f_{\mu\nu} = 1 \ . \tag{27}$$

It should be noted that according to (25), resonances occur when the incident photon energy $\hbar\omega$ equals the energy differences between the unoccupied levels and the occupied levels. A main modification, due to the many-body aspects, is expected to shift this energy, particularly for transitions with a large amplitude, through the depolarization effect.[1]

III. RESULTS AND DISCUSSION

For calculations of energy levels and the corresponding wave functions the matrices given by Eqs. (11) and (16) have been diagonalized. Twenty Landau levels and 15 subband levels are included in the basis. For effective masses we used values appropriate to the silicon (100) surface, viz., $m_t=0.1905m$, $m_l=0.916m$, m being the free-electron mass. Most of the calculations were performed using Θ or Θ_z as defined in Eqs. (4) and (15) as parameters and the energies expressed in units of $\hbar\omega_0$ and $\hbar\omega_z$, respectively. $E_n^N(\alpha)$ denotes energy levels on the nth ($n=0,1,2,\ldots$) subband and Nth ($N=0,1,2,\ldots$) Landau level. $E_{10}(\alpha)$ denotes the energy corresponding to the transition from the ground ($n=0$) to the first ($n=1$) excited subband level involving no change in the Landau quantum number, while $E_{10}^{\Delta N}(\alpha)$ corresponds to similar transitions involving a simultaneous change ΔN ($\neq 0$) in the Landau index. We should emphasize that the wave function belonging to $E_n^N(\alpha)$ may contain as much or even more of the original $|n, N\pm 1\rangle$ character than of the $|nN\rangle$ function, especially at large tilt angles.

Figure 1 shows the difference of the ground-state energy $E_0^0(\alpha)$ from the unperturbed ground subband energy $\beta_0\Theta$ as a function of the tilt angle α for various values of Θ. Except at regions very close to $\alpha=90°$, the curves approximate the expected "$\cos\alpha+$ diamagnetic shift" type of behavior. Because of their large diamagnetic shifts, the curves corresponding to lower Θ values lie above the ones corresponding to larger Θ. The minimum of each curve and the steep rise beyond it is believed to be caused by the smoothing out of the singularity at $\alpha=90°$ due to an inadequate basis set. However, close proximity of such a minimum to the point $\alpha=90°$ shows that for a very wide range of angles of tilt, and especially for large Θ, convergence has been adequate. Once again, we note that the energy values at $\alpha=90°$ are higher than the true ground-state energies by about $(e^2B_y^2/2m_tc^2)\langle z\rangle_{00}^2$. One can obtain the approximate ground-state energies at $\alpha=90°$ by extrapolating to 90° the portion of each curve just to the left of the minimum.

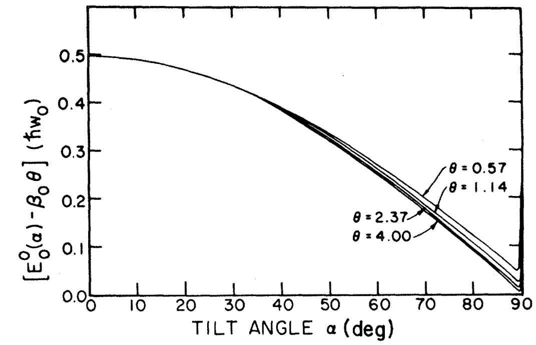

FIG. 1. Plots of ground-state energy $E_0^0(\alpha)$ relative to ground unperturbed electric subband level $\beta_0\Theta$ as a function of the tilt angle α. The ordinate is expressed in units of $\hbar\omega_0$.

Figure 2 shows $E_{10}(\alpha)-E_{10}(\alpha=0)$, i.e., the difference between the main transition energy in the presence of a magnetic field and that when the B field is absent (or normal to the interface) as a function of the tilt angle α and for several values of Θ. Note again the sharp rise near $\alpha\simeq 90°$ whose origin is explained in the above paragraph. For angles below which the sharp rise takes place, the curves can be well approximated by the Born-Oppenheimer value $(e^2/2m_tc^2)B_y^2(\langle z^2\rangle_{11}-\langle z^2\rangle_{00}-\langle z\rangle_{11}^2+\langle z\rangle_{00}^2)$.

In Fig. 3 the inverse of the quantity $E_{10}^{+1}-E_{10}$ $(\alpha=0)$ is plotted as a function of tilt angle

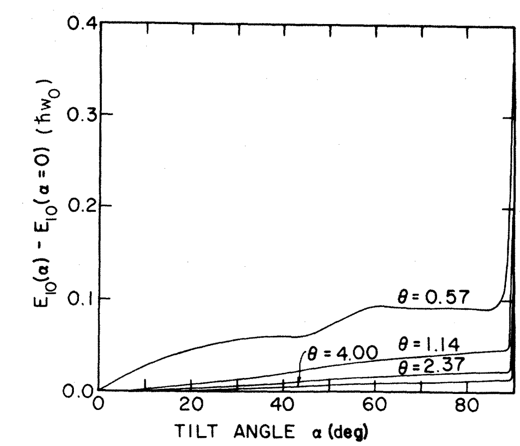

FIG. 2. Shift of the main resonance energies from the values corresponding to Faraday geometry plotted as a function of the tilt angle α. The additional structure for $\Theta\sim 0.57$ is due to strong mutual interaction among the unperturbed states brought about by the coupling term.

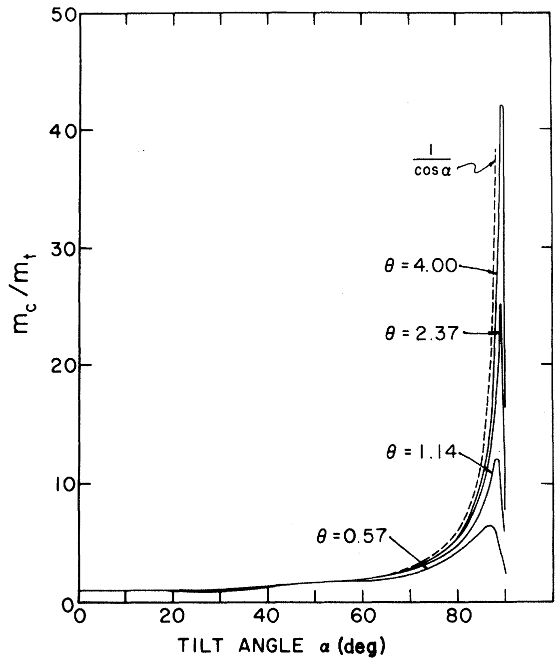

FIG. 3. Effective cyclotron mass normalized with respect to m_t: m_c/m_t corresponding to transitions from $|n=0,N=0\rangle$ state to $|n=1,N=1\rangle$ state. m_c/m_t is equivalent to $[E_{10}^{+1}(\alpha)-E_{10}(\alpha=0)]^{-1}$. Note the deviation from the $(\cos\alpha)^{-1}$ curve given by the dashed line.

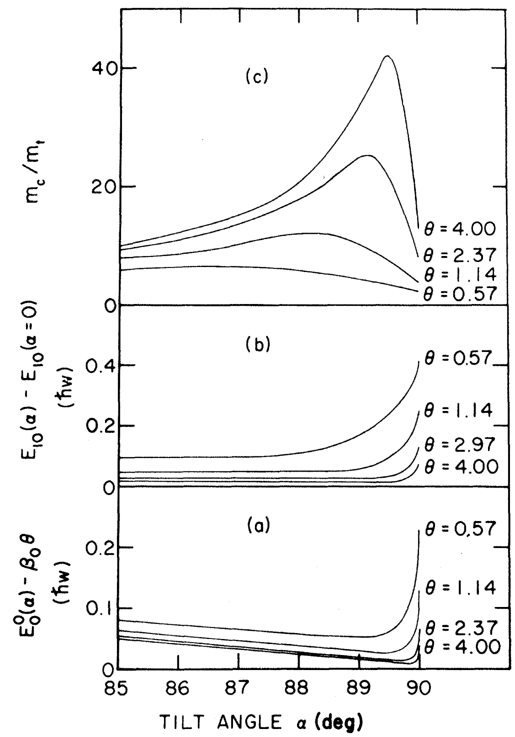

FIG. 4. Details of Figs. 1–3 from $\alpha=85°$ to $\alpha=90°$ range.

α for different values of Θ. The ordinate is equivalent to the cyclotron mass normalized with respect to m_t; that is, m_c/m_t. If the effect of finite B_y is neglected, the ratio m_c/m_t is expected to follow a $(\cos\alpha)^{-1}$ type of behavior with respect to variations in α. Finite values of m_c/m_t at $\alpha=90°$ reflect the diamagnetic shift in the Voigt geometry when $\langle p_x \rangle$ is assumed to be zero. What is interesting is the departure of the curves from the $(\cos\alpha)^{-1}$ type of behavior even for tilt angles much less than the ones where the sharp features are located. As can be noted from the figure, this departure becomes more and more prominent at large tilt angles for all Θ, but for small Θ, this departure sets in even at moderate tilt angles. The feature near $\alpha \simeq 90°$ has the same origin as in Fig. 1 discussed above.

Figure 4 displays the details of the Figs. 1–3 from $\alpha=85°$ to $\alpha=90°$ range. From this the characteristic angle of tilt where the sharp feature of each plot is located can be seen easily. It is also seen that generally for large Θ this angle is extremely close to 90° while as Θ is decreased, the characteristic angle moves towards smaller values. This figure then gives some idea about this range of the tilt angles over which our calculations can be trusted. For most experiments, Θ is greater than 1.0 and a conservative estimate for the range is $0 \le \alpha \le 85°$.

Figure 5 shows curves similar to Fig. 2, but

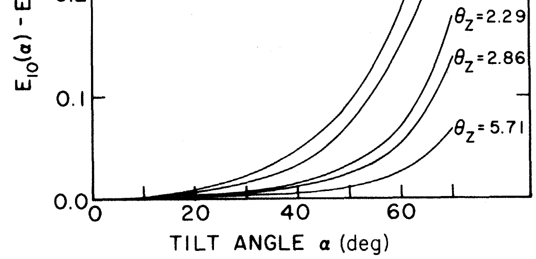

FIG. 5. Shift of the main resonance energy from the corresponding quantity in Faraday geometry plotted against different values of the tilt angle α for different values of Θ_z. The ordinate is expressed in units of $\hbar\omega_z$. B_y is related to α and is given by $B_z \tan\alpha$.

now we envisage experimental situations wherein the z component of the magnetic field, B_z, is kept fixed while the tilt angle α is changed. This implies B_y is changed and is given by $B_z \tan\alpha$. Different values of Θ_z denote different relative strengths of the ϵ field to B_z; the ordinate now is plotted in units of $\hbar\omega_z$. Here also, as in the case of the plots in Fig. 2, the curves are very well approximated by the corresponding Born-Oppenheimer values particularly for large Θ_z. For small Θ_z, Born-Oppenheimer values underestimate the actual ones, since for small Θ_z, such an argument that the y motion has little or no effect on the z quantization is not valid.

Table I displays the energies corresponding to transitions from the ground to the first excited subband with a simultaneous change ΔN $(=0,\pm1)$ in Landau quantum number for a fixed B_z $(=3.5$ T), two different electric fields corresponding to $N_s=1.0\times10^{12}$ cm^{-2} and $N_s=0.5\times10^{12}$ cm^{-2}, and for various values of B_y.[13] For these calculations, Θ_z have been determined after fixing the constant of proportionality between the ϵ field and N_s by translating 13.683 meV, the energy separation between the ground and the first excited electric subband, to an N_s value of 1.05×10^{12} cm^{-12}, as obtained from Ref. 2. The unperturbed Landau spacing $\hbar\omega_z$ for $B_z=3.5$ T is 2.127 meV. The energies are expressed in meV's. The last two columns show the energy differences between the first two Landau levels on $n=0$ and $n=1$ subbands, respectively, which are the same as the energy separations of the combined resonances $\Delta N=\mp1$ from the main $(\Delta N=0)$ one, respectively. We first note that all the transitions, the main one $(\Delta N=0)$ as well as the combined ones $(\Delta N=\pm1)$, shift to higher energies as B_y is increased from 0. We also note the B_y and subband-dependent Landau separations. For both subbands, they are smaller than the expected $\hbar\omega_z\sim2.127$ meV, though the differences are rather small until $B_y\sim10$ T. That the Landau separation on the first excited subband is smaller than that on the ground subband, as can be noted from a comparison of columns 5 and 6, implies asymmetric positioning of the $\Delta N=0$ transition with respect to the $\Delta N=\pm1$ transitions. This is in accord with the experimental findings of Beinvogl and Koch,[2] though their other observations, viz., the shift of the main $(\Delta N=0)$ resonance to the lower energy side and almost stationary positions for the combined resonances $(\Delta N=\pm1)$ with increasing B_y are in serious

TABLE I. Values of the transition energies (in meV) at which the various ΔN resonances appear as a function of B_y; $B_z=3.5$ T and $N_s=1.0\times10^{12}$ cm^{-2}. Figures in parentheses correspond to $N_s=0.5\times10^{12}$ cm^{-2}.

	Transition energies $E_{10}^{\Delta N}$ corresponding to				
B_y (T)	$\Delta N=-1$	$\Delta N=0$	$\Delta N=+1$	$E_{10}^{0}-E_{10}^{-1}$	$E_{10}^{1}-E_{10}^{0}$
0	11.118 (6.217)	13.245 (8.344)	15.372 (10.471)	2.127 (2.127)	2.127 (2.127)
2	11.130 (6.237)	13.255 (8.360)	15.379 (10.480)	2.125 (2.123)	2.124 (2.120)
4	11.164 (6.298)	13.285 (8.409)	15.401 (10.508)	2.121 (2.111)	2.116 (2.099)
6	11.121 (6.400)	13.335 (8.492)	15.439 (10.562)	2.114 (2.092)	2.104 (2.070)
8	11.302 (6.543)	13.405 (8.612)	15.492 (10.644)	2.103 (2.069)	2.087 (2.032)
10	11.406 (6.728)	13.497 (8.764)	15.563 (10.767)	2.091 (2.036)	2.066 (2.003)
20	12.228	14.277	16.228	2.049	2.001

disagreement with our calculations. However, a rigorous comparison of our calculations with the results in Ref. 2 is not possible because much of the interpretations of the latter, where the different transition frequencies and spacings are calculated by placing the resonance peaks to a common N_s value, assuming only a $N_s^{2/3}$ dependence for all the energies is affected by the N_s (or ϵ field) dependence of the transition energies as is evident from the Table I (or, so far as the main transition is concerned, from Fig. 5). Ando, in his calculations[1] based on a local-density-functional formalism, has found agreement with the experiment[2] so far as the shift of the main resonance relative to the combined ones is concerned. This effect has been attributed to excitonlike and depolarization effects. He has also found the combined resonances to show diamagnetic shifts which is in qualitative agreement with our results. In view of these, we feel that more experiments, preferably of a frequency-sweep type, will be desirable.

Figure 6 is presented as a representative example of the optical absorption spectra corresponding to a weak z polarized radiation. We have taken a Θ_z value corresponding to $B_z=5$ T and E_{10} ($\alpha=0$) $=28.0$ meV. The angle of tilt α of the B field is taken to be 75°. This implies $B_y=B_z\tan\alpha=18.7$ T. An unperturbed energy separation of 28.0 meV between the ground and the first electric subband level is typical[1] of n-type silicon inversion layers and corresponds roughly to a carrier density $N_s\sim2.1\times10^{12}$ cm^{-2}. The first four Landau levels on the ground subband ($n=0$) are assumed to be occupied. Phenomenological width parameters Γ have been assumed whose values are shown in the figure. $\hbar\omega_z$ for $B_z=5$ T is about 3.04 meV. Several combined resonances ($\Delta N\neq0$) are distinctly visible in addition to the main transition ($\Delta N=0$) and are roughly equally spaced with respect to each other. The $\Delta N=\pm1$ resonances can be seen to be placed about 3 meV away on either side of the main resonance ($\Delta N=0$) which is located at ~28.5 meV. Combined resonances $\Delta N=\pm2$ are also visible. Note the amplitude asymmetry of the $\Delta N=\pm1$ resonances. We have other calculations at other tilt angles which show how the positions, amplitudes, and amplitude asymmetries vary with α but choose not to present them here because they are substantially similar to the results in Ref. 1.[14]

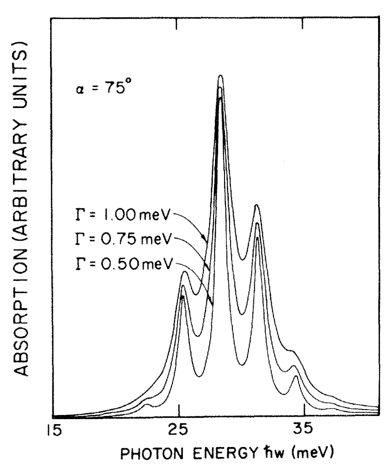

FIG. 6. Calculated optical absorption spectrum in an inversion layer on the Si(100) surface in a tilted magnetic field. Tilt angle $\alpha=75°$; $B_z=5$ T, $B_y=B_z\tan75°$; $N_s\sim2.1\times10^{12}$ cm^{-2} is assumed to correspond to $E_{10}(\alpha=0)=28.0$ meV (taken from Ref. 1).

Though these spectra have been calculated for parameter values appropriate to an inversion layer, similar effects are expected to show up, in fact more strongly, for the lower values of E_{10} corresponding to accumulation layers. The asymmetry in amplitude of the combined resonances $\Delta N=\pm1$ and their enhancement relative to that of the main transition with increasing B_y essentially agree with experiments.[2] No serious conclusion should be made concerning resonances involving $\Delta N>1$ because for such resonances, particularly for accumulation layers, our simple triangular well model will be grossly inadequate. However, considering the simplified nature of our model, it is satisfying to note that the amplitude asymmetry for the combined resonances, observed in Ref. 2 and calculated with detailed many-body effects in Ref. 1, owes its origin, at least partly, to the single-electron aspects of the system. The magnetic coupling between the motions parallel and perpendicular to the layer can itself lead to such effects.

IV. CONCLUSIONS

We have calculated the energy levels and the intersubband optical spectrum of an effectively two-dimensional space-charge layer in a tilted magnetic field using a simple nonrelativistic model Hamiltonian. The coupling between two perpendicular motions introduced by the tilted magnetic field has been taken fully into account. Two alternative basis sets have been pointed out in which the matrix elements for the Hamiltonian can be obtained in closed form and are easily calculable. These two choices enable one to solve for the Hamiltonian exactly for arbitrary strengths of the magnetic field relative to the electric one for a wide range of tilt angles.

Asymmetry in amplitude and positioning of the combined resonances relative to the main one are in qualitative agreement with some recent experiment of Beinvogl and Koch and with the calculations of Ando. These point out to possible (though small) contributions from the single-electron aspects of the problem to the observed phenomena. Our calculations show, also in qualitative agreement with the calculations of Ando, diamagnetic shifts of the combined resonances as the component of the B field parallel to the surface is increased. Since the experimental results do not show this shift, it remains unexplained.

Landau spacings on different subbands are found not to be determined by the normal component of the B field alone as expected in a naive picture. Instead, they depend also on the parallel component of the B field, the relative strength of the electric to the magnetic field and on the subband index. Landau spacings are reduced for both the ground and the higher subband, the reduction being slightly more for the higher subband. However, deviations from the expected values are not appreciable unless the ratio of the parallel to the perpendicular component of the magnetic field is quite large.

We end with a couple of remarks on the general features of such problems. The first concerns the fact that the Hamiltonian we have used may be considered a prototype of nonseparable problems in two dimensions. The magnetic part itself is very interesting in that the nonseparability is due to the restriction of the coordinate space to a semi-infinite plane. The coupling term makes such problems more interesting exactly where usually they are more difficult to solve, viz., in the nonperturbative regime. Such a feature is not unique to this Hamiltonian; rather it belongs to a general class of interesting physical problems.[15]

Secondly, electron layers on a liquid-helium surface also appear to be a promising system with which to study the effects of tilted magnetic fields. Though somewhat different (because of the image Coulomb potential), such systems are more clean since the electron density is low. Despite being the first system where intersubband combined resonances were reported to be observed by Zipfel *et al.*,[16] any detailed spectroscopic investigation of the space-charge layer for different values of the appropriate parameters has not been reported in the literature. Since the lower density electron layer on liquid helium does not have the large many-body corrections of inversion layers, it is more suitably described by a single-particle model. In this system, as well as in other space-charge layers, more experiments, particularly of the frequency-sweep type, will be highly desirable.

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[1]T. Ando, Phys. Rev. B 19, 2106 (1979).

[2]W. Beinvogl and J. F. Koch, Phys. Rev. Lett. 40, 1736 (1978).

[3]H. Schaber and R. E. Doezema, Phys. Rev. B 20, 5257 (1979).

[4]F. Stern, Phys. Rev. B 5, 4891 (1972).

[5]R. E. Doezema, M. Nealon, and S. Whitmore, Phys. Rev. Lett. 45, 1593 (1980); Talat S. Rahman, D. L. Mills, and P. S. Riseborough, Phys. Rev. B 23, 4081 (1981).

[6]U. Fano, Colloq. Int. du C.N.R.S. No. 273, Aussois, France, June, 1977, p. 127; A. R. P. Rau, Bull. Am. Phys. Soc. 23, 10 (1978).

[7]A. R. P. Rau, in *Abstracts of III International Conference on Electronic Properties of Two-Dimensional Systems,* Yamada, Japan, 1979 (unpublished); Comments

At. Mol. Phys. 10, 19 (1980).
[8]T. Ando, Phys. Rev. B 13, 3468 (1976); P. Kneschaurek, A. Kamgar, and J. F. Koch, *ibid.* 14, 1610 (1976).
[9]For z integrals involving the Airy functions see Roy G. Gordon, J. Chem. Phys. 51, 14 (1969).
[10]H. Bateman, *Higher Transcendental Functions,* (McGraw-Hill, New York, 1953), Vol. 2, p. 193.
[11]I. S. Gradshteyn and I. W. Ryzhik, *Tables of Integrals, Series and Products* (Academic, New York, 1965), p. 845.
[12]T. Ando, Solid State Commun. 21, 133 (1977).
[13]This study would be of direct interest for experiments where B_z is held fixed and B_y varied independently.
[14]S. K. Bhattacharya, Ph.D. Thesis, Louisiana State University, 1982 (unpublished).
[15]A. R. P. Rau, J. Phys. B 12, L193 (1979).
[16]C. L. Zipfel, T. R. Brown, and C. C. Grimes, Surf. Sci. 58, 283 (1976).