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Spin-orbit splitting of the cyclotron resonance in GaAs

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We have studied the relevance of spin-orbit coupling to the splitting of the cyclotron resonance of electron space-charge layers in GaAs recently observed by Manger *et al.* [Phys. Rev. B **63**, 121203R (2001)]. We show that the spin-orbit interaction couples density and spin-density excitations in the long-wavelength limit and is able to explain all the features observed in the experiment.

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The influence of impurity and band-structure effects on the cyclotron resonance (CR) is an important topic that has been investigated in many experiments on space-charge layers.[1–7] These effects break the translational invariance of the system and as a consequence invalidate the Kohn theorem[8] according to which in the CR experiments a single line at the cyclotron energy $\omega_c = eB/mc$ should be observed. Indeed, in a recent CR investigation of high-mobility electron space-charge layers in GaAs,[9] a line splitting of the CR resonance due to band-structure influences was clearly observed. The main features of the experiment are the following: a well-resolved splitting of CR for filling factors $\nu=3$ and 5 ($\nu = 2\pi\ell^2 N_s$, $\ell = \sqrt{\hbar/eB}$) which increases with the electron carrier density N_s; a similar behavior, but less pronounced, for $\nu=7$; a gain in strength of the line with lower transition frequency with ncreasing N_s; and finally no significant splitting for the even filling factors.

In this Rapid Communication we argue that the Dresselhaus spin-orbit interaction,[10] which is responsible for the spin splitting of the conduction band in bulk GaAs, is also the main cause of the observed CR splitting. Moreover, assuming the presence of an additional small, but not negligible, nonlocal electron-electron interaction, it can explain all the features observed in the experiment.

The study of spin-orbit (SO) effects in semiconductor nanostructures has been the object of many experimental and theoretical investigations in the last few years.[11–23] It links the spin and the charge dynamics, hence opening the possibility of spin control by means of electric fields.[24,25] Here we show that the SO interaction strongly affects the optical properties of electron space-charge layers in GaAs by inducing a strong coupling between charge-density and spin-density excitations in the long-wavelength limit. We show that the energy splitting of the CR is a clear and quantitative signature of the Dresselhaus SO coupling in these systems. The other possible spin-orbit interaction, known as the Rashba term,[26,27] which is due to the asymmetry of the confinement potential, has been found to be negligible in all the cases we have studied for the electron space-charge layer in GaAs of Ref. 9. This does not mean that the Rashba SO interaction is always negligible. For other structures or widths of the layer the intensities of the two SO interactions can be comparable and both affect the CR energy splitting. In general any kind of SO interaction affects the CR energy splitting since it violates the Kohn theorem due to its spin and momentum dependences.

The operator describing the SO Dresselhaus contribution for the standard (001) plane of GaAs is given by

$$H_D = \frac{\lambda}{\hbar}\sum_{i=1}^{N}[P_x\sigma_x - P_y\sigma_y]_i, \tag{1}$$

where the σ's are the Pauli matrices and $\mathbf{P} = -i\hbar\boldsymbol{\nabla} + (e/c)\mathbf{A}$ represents the canonical momentum given in terms of the vector potential $\mathbf{A}$ in the Landau gauge. We ignore terms cubic in the momentum for simplicity. The Dresselhaus parameter λ is given by $\lambda \approx \gamma\langle(P_z/\hbar)^2\rangle$ where γ is a material specific constant that for GaAs is[28] $\gamma = 27.5$ eV Å^3 and $\langle(P_z/\hbar)^2\rangle$ can be related to the layer vertical width z_0[17] by $\langle(P_z/\hbar)^2\rangle \simeq (\pi/z_0)^2$, assuming that the electrons in the z direction are confined in the ground state of a square well of width z_0. This rough estimate should be taken with some care since it does not introduce any density dependence in λ. This is in disagreement with some experimental evidence;[29–33] therefore it must be taken as just giving an order of magnitude of the effect we are going to investigate, whose strength turns out to be proportional to $\lambda^2 m/\hbar^2 \simeq 0.25$ cm^{-1} for a layer width of 100 Å. For larger widths the Dresselhaus SO intensity decreases and the Rashba term may become important.

We start from the quantum-well Hamiltonian in the effective-mass, dielectric constant approximation:

$$H = H_0 + V, \tag{2}$$

where H_0 is the one-body part of the Hamiltonian consisting of the kinetic, Dresselhaus, and Zeeman terms, i.e.,

$$H_0 = \sum_{i=1}^{N}\left[\frac{P^+P^- + P^-P^+}{4m} + \frac{\lambda}{2\hbar}(P^+\sigma_+ + P^-\sigma_-) + \frac{1}{2}g^*\mu_B B\sigma_z\right]_i, \tag{3}$$

where $m = m^* m_e$ ($m^* = 0.067$ for GaAs) is the effective electron mass in units of the bare electron mass m_e, $P^\pm = P_x \pm iP_y$, and $\sigma_\pm = \sigma_x \pm i\sigma_y$. The Zeeman term $H_Z = \Sigma_i g^*\mu_B B\sigma_z^i$ depends on the total vertical spin $\Sigma_i\sigma_z^i$, the Bohr magneton μ_B, and the effective gyromagnetic factor g^*, which for bulk GaAs is -0.44. In Eq. (2), V is the usual Coulomb interaction,

$$V = \sum_{i<j}^{N} \frac{e^2}{\epsilon|\mathbf{r}_i - \mathbf{r}_j|}, \tag{4}$$

where ϵ is the dielectric constant of the semiconductor ($\epsilon = 12.4$ for GaAs).

By using the unitary transformation[20,34]

$$U = \exp\left[- i\lambda \frac{m}{\hbar^2} \sum_{i=1}^{N} (x\sigma_x - y\sigma_y)_i \right], \tag{5}$$

the Schrödinger equation $(H_0+V)|n\rangle = E_n|n\rangle$ is transformed into

$$(\tilde{H}_0 + V)|\tilde{n}\rangle = E_n|\tilde{n}\rangle, \tag{6}$$

where $|\tilde{n}\rangle = U|n\rangle$, $\tilde{H}_0 = U^{-1}H_0U$, and the interaction V and the energies E_n remain unchanged. At the leading order in λ, one gets for $\tilde{H}_0$ in the transformed system (to simplify the expressions, in the following we shall use effective atomic units $\hbar = e^2/\epsilon = m = 1$, where the length unit is the effective Bohr radius $a_0^* = a_0\epsilon/m$ and the energy unit is the effective Hartree $H^* = Hm^*/\epsilon^2$; for GaAs one gets $a_0^* = 97.9$ Å and $H^* \simeq 11.9$ meV $\simeq 95.6$ cm^{-1})

$$\tilde{H}_0 = \sum_{i=1}^{N} \left[\frac{P^+P^- + P^-P^+}{4} - i\frac{\lambda^2}{2}(Q^-P^+ - Q^+P^-)\sigma_z + \frac{1}{2} g^* \mu_B B \sigma_z \right]_i, \tag{7}$$

where $Q^{\pm} = x \pm iy$. The advantage of using transformation (5) lies in the fact that in the transformed system the states $|\tilde{n}\rangle$ are eigenstates of S_z and calculations can be performed using the usual spinorial formalism. The unitary transformation (5) can be used to evaluate expectation values of physical observables other than the energy in the laboratory frame. In particular the quantity of interest, i.e., the dipole strength, transforms into itself since the operator U of Eq. (5) commutes with the dipole operator $\Sigma_{i=1}^{N} Q_i^+$.

The spin-orbit term in Eq. (7) mixes density excitations induced by the operator $\Sigma_{i=1}^{N} P_i^+$ with the spin-density excitations induced by $\Sigma_{i=1}^{N} P_i^+ \sigma_z^i$ since

$$\left[\tilde{H}_0, \sum_{i=1}^{N} P_i^+ \right] = \omega_c \sum_{i=1}^{N} P_i^+ + \lambda^2 \sum_{i=1}^{N} (P_i^+ \sigma_z^i + i\omega_c Q_i^+ \sigma_z^i), \tag{8}$$

and violates the Kohn theorem for which $[H, \Sigma_{i=1}^{N} P_i^+] = \omega_c \Sigma_{i=1}^{N} P_i^+$.

For a correct evaluation of the effects induced by the spin-orbit interaction on the CR resonance, it is, however, necessary to consider the effects of the electron-electron interaction too. These effects will be treated in the following in the transformed system where we consider the electron-electron interaction in the Brueckner-Hartree-Fock (BHF) approximation.[35] The reason to use BHF is that usual theories such as random-phase approximation (RPA),[36] time-dependent-Hartree-Fock,[37] and time-dependent local-density approximations[34] do not give any effect on the energies of the two modes of excitation in the long-wavelength limit, whereas nonlocal effective theories such as the Landau theory and BHF do it.

In BHF, the relevant nonlocal term in the energy functional to study the cyclotron resonance is given by[34,35]

$$\int v_0(\rho)(\rho\tau - \mathbf{J}^2) d\mathbf{r} - \int v_1(\rho) \mathbf{J}_1^2 d\mathbf{r}, \tag{9}$$

where ρ and τ are the one-body diagonal and kinetic energy densities, respectively, and the current densities $\mathbf{J}$ and $\mathbf{J}_1$ are given by

$$\mathbf{J} = \langle\Psi| \frac{1}{2} \sum_{i=1}^{N} (\mathbf{P}_i \delta(\mathbf{r} - \mathbf{r}_i) + \text{H.c.}) |\Psi\rangle$$

and

$$\mathbf{J}_1 = \langle\Psi| \frac{1}{2} \sum_{i=1}^{N} [\mathbf{P}_i \delta(\mathbf{r} - \mathbf{r}_i)\sigma_z^i + \text{H.c.}] |\Psi\rangle,$$

respectively. By taking in Eq. (9) $v_0(\rho) = k_0/2\rho$ and $v_1(\rho) = k_1/2\rho$, one gets a BHF potential

$$V = \sum_{i=1}^{N} \left[k_0 \frac{P_i^2}{2} - k_0 \mathbf{J} \cdot \mathbf{P}_i - k_1 \mathbf{J}_1 \cdot \mathbf{P}_i \sigma_z^i \right]. \tag{10}$$

The first term of this equation, added to the kinetic energy term of Eq. (7), gives rise to a constant effective mass (coming from the electron-electron interaction) $1/m_{ee}^* = (1+k_0)$. A self-consistent vibrating dipole-dipole interaction $\delta\tilde{V}(\mathbf{r},t)$, to be used in time-dependent BHF calculations, is derived from the last two terms of Eq. (10) by imposing irrotational currents $\delta\mathbf{J} = \beta(t)\rho\boldsymbol{\nabla} f$, where $f = x, y$, on both $\mathbf{J}$ and $\mathbf{J}_1$.[38–40] The irrotational nature of currents in collective motion follows naturally from the assumption that the collective state completely exhausts the excitation strength as it is the case for the CR resonance and the spin-density mode in the long-wavelength limit. By using self-consistency to determine $\beta(t)$, one gets for $\delta\tilde{V}(\mathbf{r},t)$

$$\delta\tilde{V}(\mathbf{r},t) = \sum_{i=1}^{N} \left[- \frac{k_0}{2N} \left\langle \sum_{j=1}^{N} P_j^- \right\rangle P^+ - \frac{k_1}{2N} \left\langle \sum_{j=1}^{N} \left(P_j^- \sigma_z^j - \frac{2S_z}{N} P_j^- \right) \right\rangle \left(P^+\sigma_z - \frac{2S_z}{N} P^+ \right) \right]_i + \text{H.c.}, \tag{11}$$

where $2S_z = N_\uparrow - N_\downarrow$ and $N_\uparrow$ ($N_\downarrow$) is the number of spin-up electrons (down). Note that the time dependence of $\delta\tilde{V}(\mathbf{r},t)$ is in the $\langle\cdots\rangle$ spatial foldings with the densities induced by a time-dependent external field.

The total Hamiltonian $\tilde{H} = \tilde{H}_0^* + \delta\tilde{V}(\mathbf{r},t)$, where $\tilde{H}_0^*$ includes the effective mass $1/m_{ee}^* = (1+k_0)$ in the kinetic energy term of Eq. (7), can now be solved analytically within the RPA by finding the operators O^+ solution of the equation of motion:

$$[\tilde{H},O^+]=\omega O^+. \tag{12}$$

We have used the methods illustrated in Ref. 34 to compute the commutators of a one-body operator F with the Hamiltonian as

$$[\tilde{H},F]=[\tilde{H}_0^*,F]+\delta\tilde{V}(F), \tag{13}$$

where $\tilde{H}_0^*$ is the static Hamiltonian [Eq. (7) with the effective mass $1/m_{ee}^*=(1+k_0)$], and $\delta\tilde{V}(F)$ is the change (linear in F) induced in the time-dependent potential by the unitary transformation e^{iF}. For the potential of Eq. (11) one gets

$$\delta\tilde{V}(F)=-\frac{k_0}{2N}\langle 0|\left[\sum_{j=1}^{N}P_j^-,F\right]|0\rangle\sum_{i=1}^{N}P_i^+-\frac{k_1}{2N}\langle 0|\left[\sum_{j=1}^{N}P_j^-\sigma_z^j-\frac{2S_z}{N}P_j^-,F\right]|0\rangle\sum_{i=1}^{N}\left(P_i^+\sigma_z^i-\frac{2S_z}{N}P_i^+\right), \tag{14}$$

where $|0\rangle$ is the static BHF ground state and analogously for the Hermitian conjugate term of Eq. (11). The two terms of Eq. (13) have a different physical meaning: the commutator $[\tilde{H}_0^*,F]$ originates from the static, one-body properties of the Hamiltonian, while the term $\delta\tilde{V}(F)$ originates from the renormalization of the self-consistent potential. The latter contribution is essential to take into account the RPA correlations. By using the basic commutation rules $[P^-,P^+]=2\omega_c$ and $[Q^-,P^+]=[Q^+,P^-]=2i$, it can be easily shown that neglecting in $\tilde{H}$ the spin-orbit term proportional to λ^2, the solutions to Eq. (12) are given by

$$O_\rho^+=\sqrt{\frac{1}{2N\omega_c}}\sum_{i=1}^{N}P_i^+,$$

$$O_\sigma^+=\sqrt{\frac{1}{2N\omega_c[1-(2S_z/N)^2]}}\sum_{i=1}^{N}\left(P_i^+\sigma_z^i-\frac{2S_z}{N}P_i^+\right), \tag{15}$$

and

$$\omega_\rho=\omega_c,\ \omega_\sigma=\omega_c(1+k), \tag{16}$$

where $k=k_0-k_1[1-(2S_z/N)^2]$ and the subscripts ρ and σ refer to density and spin-density excitations in the long-wavelength limit, respectively. The dipole strength is distributed among the above states as follows ($Q_\rho=\Sigma_{i=1}^{N}Q_i^+$):

$$|\langle 0|Q_\rho|\omega_\rho\rangle|^2=\frac{2N_s}{\omega_c},\quad |\langle 0|Q_\rho|\omega_\sigma\rangle|^2=0, \tag{17}$$

so that the Kohn's theorem is fulfilled and according to it the spin-density mode is not excited by the density operator Q_ρ and the corresponding matrix element vanishes. It is also important to note that the above results coincide with those of the Landau theory for the two-dimensional electron gas in the long wavelength limit, if one identifies the strengths k_0 and k_1 with the combinations of Landau parameters $-F_1^s/(2+F_1^s)$ and $-F_1^a/(2+F_1^s)$. This allows us to give an estimate of the strength k by using for F_1^s and F_1^a the available Monte Carlo calculation of Ref. 41. This calculation shows that k is negative, strongly density dependent (it decreases with increasing N_s), and equal to $\simeq -2\times 10^{-2}$ at $N_s=3.32\times 10^{-11}$ cm^{-2}, which is the highest value of the density reported. The CR experiment we are going to analyze covers the density regime from 2×10^{-11} to 13×10^{-11} cm^{-2}, the energy ω_c lies in some range around 100 cm^{-1}, yielding the estimate $-k\omega_c\simeq 2$ cm^{-1}, and the observed splitting is in the range $\simeq 1-4$ cm^{-1}. $k\omega_c$ is a key quantity of the model which scales as m^*/ϵ^2. Under the same conditions of density and magnetic field one can then vary this quantity by changing the material.

As we have already anticipated the spin-orbit term in $\tilde{H}$ couples the density mode with the spin-density one and changes the above scenario. In particular the Kohn's theorem is violated and the spin-density mode can be excited by the dipole operator Q_ρ which is the relevant one in CR experiments. As a consequence the two strengths $|\langle 0|Q_\rho|\omega_\rho\rangle|^2$ and $|\langle 0|Q_\rho|\omega_\sigma\rangle|^2$ are both different from zero and the CR resonance splits into two lines. In this case the equations of motion (12) can be solved with the operator $O^+=\Sigma_{i=1}^{N}[aQ^+ +bP^+ +cQ^+\sigma_z+dP^+\sigma_z]_i$ yielding a homogenous system of linear equations for the coefficients a, b, c, and d from which the energies $\omega_\rho,\omega_\sigma$ are obtained by solving the secular equation (valid at the order λ^2):

$$(\omega-\omega_c)[\omega-\omega_c(1+k)]=-\frac{4S_z}{N}\lambda^2 k\omega_c. \tag{18}$$

For each energy solution, the homogenous linear system, supplemented with the normalization condition $\langle 0|[(O^+)^\dagger,O^+]|0\rangle=1$, gives the coefficients a, b, c, and d.

In the cases $\lambda=0$ or $S_z=0$ the two modes are uncoupled and one recovers the situation of Eqs. (15)–(17). This explains why in the experiments at even filling factor for which $N_\uparrow=N_\downarrow$ and $S_z=0$ no splitting of the CR line is seen. When λ, k, and S_z are different from zero, one gets two lines splitted by the energy

$$\Delta E=\frac{8S_z}{N}\lambda^2-k\omega_c, \tag{19}$$

getting the dipole strengths

$$|\langle 0|Q_\rho|\omega_\rho\rangle|^2=\frac{2N_s}{\omega_c},$$

$$|\langle 0|Q_\rho|\omega_\sigma\rangle|^2=\frac{2N_s}{\omega_c}\left|\frac{2\lambda^2}{k\omega_c}(1-(2S_z/N)^2)\right|^2. \tag{20}$$

The results (19) and (20) are able to explain all the features observed in the CR experiment if one notices that the estimates for $-k\omega_c$ and $2\lambda^2$ we have done before give for ΔE the right order of magnitude of the observed splitting and moreover if one supposes that the quantity $2\lambda^2/k\omega_c$ increases with the density. In this case the line with lower transition frequency will gain in strength with increasing N_s in agreement with the observations. Moreover at fixed density, both $(8S_z/N)\lambda^2$ and $k\omega_c$ decrease for increasing filling factors since $2S_z/N=1/\nu$ and also ω_c goes as $1/\nu$, explaining why the splitting is much better experimentally resolved at $\nu=3$

and 5 than for $\nu=7$. Finally the strength $|\langle 0|Q_\rho|\omega_\sigma\rangle|^2$ vanishes at $2S_z/N=1$, explaining why at filling factor $\nu=1$ no splitting is observed. It is also interesting to compare result (19) for CR splitting with the one of the nonparabolicity models for the GaAs conduction band. This single-particle model predicts a splitting proportional to B^2 and dipole strengths which do not reproduce the experimental results. In our theory the interaction enters in a natural and crucial way for reproducing energy splittings and strengths. In particular the splitting is linear in B.

One should note that the theory we have developed is at the lower order in λ^2 and that if λ^2 becomes comparable to $k\omega_c$, higher-order corrections might be important. However higher order terms in λ mix the CR state not only with the spin-density state but also with other modes of excitations (the spin-flip ones) which are not resolved experimentally, indicating that a first-order calculation might be sufficient at least to determine the crucial ingredients of the observed phenomena. These spin-flip modes are expected to lie in the low-energy region and carry a dipole strength of the order of some percent of the CR one. In conclusion we have found a strong indication that spin-orbit coupling is responsible for the features detected in CR experiments. A detailed experimental analysis of the CR spectrum in terms of Eqs. (19) and (20) would yield a clean determination of the Dresselhaus SO intensity and of the almost unknown Landau parameters entering k as a function of the density.

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