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Effect of impurities on cyclotron resonance in two-dimensional electronic systems

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We have investigated the influence of impurities on the cyclotron resonance in two-dimensional electron gases, using general sum-rule arguments. The method provides an explanation for the different behaviors observed in samples with either donor or acceptor δ-doped layers. The unique behavior of the Be-doped samples at high magnetic fields can be understood in terms of a rigid oscillation of the electron gas against the fixed impurities, which give rise to an effective harmonic restoring force. An explicit expression for the resonant frequency is obtained, whose square is equal to the square of the cyclotron frequency plus a constant shift. An expression for the resonance linewidth is also given that involves the electron density at the position of the impurity. The dramatic narrowing of the resonance observed in the Be-doped samples is due to this density vanishing for some critical filling factor less than 1.

Cyclotron resonance has been used extensively as a probe of two-dimensional electron gases (2DEG) in semiconductor heterostructures. For the ideal translationally invariant system, Kohn's theorem[1] stipulates that the resonance is infinitely sharp and that its position occurs at the classical cyclotron frequency $\omega_c = eB/m^*c$. These features are due to the fact that a transverse radiation field couples to the center-of-mass motion which itself is decoupled from the internal degrees of freedom. In this situation, electron-electron interactions play no role and the resonance corresponds to that of a free particle. With the inevitable presence of impurities in the system, the situation changes drastically since the impurity disorder couples the center-of-mass motion to the internal degrees of freedom. In particular, the driven motion of the electron gas against the impurity background will normally generate density fluctuations which are strongly affected by electron-electron interactions. These in turn would be expected to affect the character of the cyclotron resonance.

The experimental record clearly establishes the importance of these impurity related effects[2-7] but a coherent picture of how the cyclotron resonance is modified has yet to emerge. One difficulty has been the sample dependence of the behavior observed, which presumably is associated with the different kinds of impurities present and variations in their distribution throughout the region confining the 2DEG. The lack of precise information about the impurities has made it difficult to establish correlations with the various observed anomalies. Thus the recent series of experiments in which the distribution of impurities is controlled by the method of δ doping[8,9] or electron irradiation[10] are particularly important and offer the possibility of clarifying the situation. But even here the distinct behavior of donor versus acceptor δ-doped layers[8] seems to have raised more questions than it has answered.

One of the intriguing observations[8] for the Be-doped samples is the splitting of the cyclotron resonance at some intermediate field close to a filling factor $\nu=2$, followed by the strengthening of a shifted resonance, and finally its narrowing for filling factors less than unity. The Si-doped samples do not exhibit a similar behavior but retain a relatively broad resonance even to the highest fields studied. In this paper we wish to point out that much of this data can be understood on rather general theoretical grounds.

We consider an arbitrary 2DEG in the presence of a perpendicular magnetic field. The Hamiltonian of the N-electron system is

$$H = \sum_{i=1}^{N} \frac{1}{2m^*} \left(\mathbf{p}_i + \frac{e}{c}\mathbf{A}_i \right)^2 + \sum_{i=1}^{N} v_{\text{ext}}(\mathbf{r}_i) + U , \tag{1}$$

where the vector potential in the symmetric gauge is given by $\mathbf{A}(\mathbf{r}) = \frac{1}{2}\mathbf{B}\times\mathbf{r}$, $v_{\text{ext}}(\mathbf{r})$ is the *total* external potential acting on the electronic system (including both the confining and impurity potentials) and U is the electron-electron Coulomb repulsion. The experimentally measurable quantity is the power absorption for a normally incident electromagnetic wave

$$P(\omega) = \tfrac{1}{2} E_0^2 \frac{Q''_{xx}(\omega)}{\omega} , \tag{2}$$

where E_0 is the amplitude of the incident field and $Q''_{xx}(\omega)$ is the absorptive part of the current-current response function,[11]

$$Q''_{xx}(\omega) = \frac{\pi}{\hbar} \sum_n |\langle 0|J_x|n\rangle|^2 [\delta(\omega-\omega_{n0}) - \delta(\omega+\omega_{n0})] . \tag{3}$$

The states $|n\rangle$ are the exact eigenstates of H with eigenvalues ε_n and $\omega_{n0} = (\varepsilon_n - \varepsilon_0)/\hbar$. The operator J_x is given by

$$J_x = -e\sum_i v_{ix} = -\frac{e}{m^*}\sum_i \left(p_{ix} + \frac{e}{c}A_{ix} \right) \equiv -\frac{e}{m^*}P_x . \tag{4}$$

Here we have introduced the total center-of-mass mechanical momentum $\mathbf{P}$.

Motivated by the observation that the cyclotron resonance in the Be-doped samples is a narrow line for high magnetic fields,[8] we adopt a procedure which exploits sum-rule arguments as applied to the current-current response function $Q''_{xx}(\omega)$. In the following we consider $\omega Q''_{xx}(\omega)$ to be a spectral distribution and define a squared frequency by the ratio of frequency moments

$$\Omega^2 = \frac{\int_0^\infty \omega^3 Q''_{xx}(\omega)d\omega}{\int_0^\infty \omega Q''_{xx}(\omega)d\omega} . \tag{5}$$

The extent to which Ω^2 reflects the actual resonant frequency depends on the width of the distribution. For the ideal situation of a δ-function-like response $Q''_{xx}(\omega) \propto \delta(\omega - \Omega)$, Ω^2 is indeed the square of the resonant frequency. However, for more realistic distributions the width plays an important role in determining the value of Ω^2.

Using Eq. (3), the frequency moments can be expressed in terms of commutators and Eq. (5) becomes

$$\Omega^2 = \frac{1}{\hbar^2} \frac{\langle 0|[[H,[P_x,H]],[P_x,H]]|0\rangle}{\langle 0|[[P_x,H],P_x]|0\rangle} . \tag{6}$$

The various commutators can be worked out exactly using the Hamiltonian H and the definition of P_x in Eq. (4). Taking the ground-state expectation values of the indicated quantities, Eq. (6) becomes

$$\Omega^2 = \omega_c^2 \left(\frac{1 - 1/M\omega_c^2 \int d\mathbf{r}[\nabla_\parallel v_{\text{ext}} \cdot \nabla_\parallel n_0 + \nabla_x v_{\text{ext}} \nabla_x n_0] + 1/m^* M\omega_c^4 \int d\mathbf{r}(\nabla \cdot \nabla_x v_{\text{ext}})^2 n_0}{1 - 1/M\omega_c^2 \int d\mathbf{r} \nabla_x v_{\text{ext}} \nabla_x n_0} \right) , \tag{7}$$

where $M = m^* N$ is the total electron mass and $\nabla_\parallel$ denotes the components of the gradient operator perpendicular to $\mathbf{B}$. $n_0(\mathbf{r})$ is the exact ground-state density in the presence of impurities and implicitly includes the effect of electron-electron interactions.

The expression for Ω^2 is an exact property of the experimental absorption spectrum and in the limit $v_{\text{ext}}(\mathbf{r}) \to 0$, we recover the expected result $\Omega = \omega_c$. To infer more from this formal expression we shall make use of various pieces of experimental information and consider some limiting situations. In the extreme high-field limit ($B \to \infty$), the last term in the numerator can be neglected and we find

$$\Omega^2 = \omega_c^2 - \frac{1}{M} \int d\mathbf{r} \nabla_\parallel v_{\text{ext}}(\mathbf{r}) \cdot \nabla_\parallel n_0(\mathbf{r}) \equiv \omega_c^2 + \omega_0^2 . \tag{8}$$

To the extent that $n_0(\mathbf{r})$ is a relatively weak function of B in the limit of low filling factors ($\nu < 1$), this is precisely of the form of the shifted resonance observed in the case of the Be-doped samples.[8] Since the resonance line in this limit is sharp, we shall argue that Eq. (8) gives an accurate expression for the resonance position.

In Fig. 1(a) we sketch the form of $v_{\text{ext}}(\mathbf{r})$ and $n_0(\mathbf{r})$ in the vicinity of a single negatively charged impurity immersed in an ideal 2DEG. It is clear from Fig. 1(a) that the gradients of $v_{\text{ext}}(\mathbf{r})$ and $n_0(\mathbf{r})$ have opposite sign so that the sign of the integral in Eq. (8) is negative, i.e., the impurity potential gives a *positive* frequency shift. One arrives at a similar conclusion in the case of the positively charged donor impurity sketched in Fig. 1(b), however this situation is more complex as will become clearer later.

If the mean distance between impurities d is large compared to a typical impurity screening length, it is clear that each impurity contributes independently to the integral in Eq. (8). However the contribution of each is different depending on its position relative to the 2DEG. To simplify the discussion we assume a δ-doped layer so that each impurity contributes the same amount. We then find

$$\Omega^2 = \omega_c^2 + \frac{c}{m^*} \int d\mathbf{r} \nabla_\parallel^2 v_{\text{ext}}(\mathbf{r}) n_0(\mathbf{r}) , \tag{9}$$

where $c = N_i/N$ is the concentration of impurities and v_{ext} is now the external potential in the vicinity of a single impurity; we have performed an integration by parts in order to display a positive sign in the frequency shift. The proportionality of the frequency shift to c is consistent with the experimentally observed dependence.[12]

As stated previously, provided the resonance is sharp, the value of Ω obtained from the sum-rule argument actually represents the resonance position and corresponds to the frequency of the collective mode. This mode can be given a simple physical interpretation already alluded to in the paper of Antoniou, MacDonald, and Swihart.[13] Consider the effect of both a rigid displacement of the ground-state wave function through a distance $\mathbf{a}$ and a gauge transformation, the combined transformation being defined by the operator

$$T(\mathbf{a}) = \exp\left(-i \sum_i \mathbf{p}_i \cdot \mathbf{a}/\hbar \right) \exp\left[i \frac{e}{2\hbar c} \sum_i \mathbf{r}_i \cdot \mathbf{a} \times \mathbf{B} \right] . \tag{10}$$

Defining the wave function $|\Psi(\mathbf{a})\rangle = T(\mathbf{a})|0\rangle$, a variational estimate of the energy is given by

$$\varepsilon(\mathbf{a}) \equiv \langle \Psi(\mathbf{a})|H|\Psi(\mathbf{a})\rangle$$
$$= \varepsilon_0 + \int d\mathbf{r}\, n_0(\mathbf{r})[v_{\text{ext}}(\mathbf{r}+\mathbf{a}) - v_{\text{ext}}(\mathbf{r})] . \tag{11}$$

The transformation therefore preserves the total kinetic energy and total Coulomb energy of the electrons and

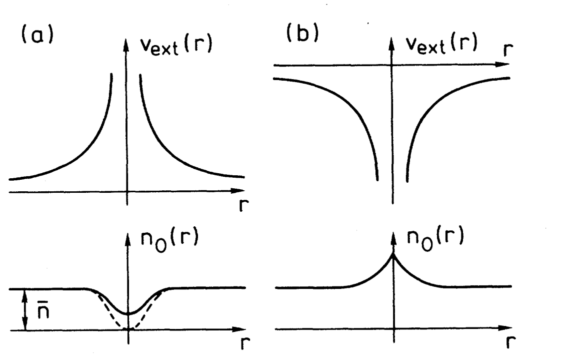

FIG. 1. (a) Schematic representation of an acceptor impurity potential in a 2DEG $v_{\text{ext}}(r)$, and the corresponding screening charge density, $n_0(r)$, as a function of the distance from the impurity, r. The dashed line is for some filling factor $\nu < 1$ for which $n_0(0) = 0$. (b) As in (a) but for a positively charged donor impurity.

only the external potential energy of the system is affected. By the variational theorem $\varepsilon(\mathbf{a})$ is a minimum at $\mathbf{a}=0$, so that

$$-\frac{\partial\varepsilon(\mathbf{a})}{\partial a_\mu}=-\int d\mathbf{r}\, n_0(\mathbf{r})\frac{\partial^2 v_{\text{ext}}(\mathbf{r})}{\partial x_\mu \partial x_\nu}a_\nu \tag{12}$$

can be interpreted as the restoring force for this rigid displacement of the 2DEG. For a random distribution of impurities in the system one would not expect a component of the force in a direction transverse to the displacement, i.e., we retain only the $\mu=\nu$ part of $\partial^2 v_{\text{ext}}/\partial x_\mu \partial x_\nu$ and by symmetry, these two diagonal contributions are equal. Including the Lorentz force on the electrons, the classical equations of motion for the center of mass become

$$\ddot{a}_x=-\omega_c\dot{a}_y-\tfrac{1}{2}\omega_0^2 a_x\,,\quad \ddot{a}_y=\omega_c\dot{a}_x-\tfrac{1}{2}\omega_0^2 a_y\,, \tag{13}$$

which have harmonic solutions whose frequencies for large magnetic fields ($\omega_c \gg \omega_0$) are $\Omega_+^2=\omega_c^2+\omega_0^2$ and $\Omega_-^2=\omega_0^4/4\omega_c^2$. The upper mode frequency is precisely the result obtained with the sum-rule argument, Eq. (8). Thus the latter is consistent with the picture that the many-electron system oscillates rigidly against the background impurity potential. To the extent that the observed resonance is sharp and that the sum-rule argument gives the correct resonance frequency, we can infer that the 2DEG is indeed oscillating as a coherent, rigid whole, which is clearly possible only if electron-electron correlations are sufficiently strong to lock the electrons into this kind of motion. The narrowness of the observed resonance is indicative of the lack of dissipation to be expected in a situation where internal excitations are suppressed.

So far in this discussion there is nothing to distinguish the donor from acceptor-doped systems. However we have tacitly assumed that the last term in the numerator of Eq. (7) can be neglected at the fields of interest. In fact, this is not really the case but we can argue that this additional term is directly related to the width of the resonance. This term allows one to distinguish naturally between donors and acceptors and can be used to explain the different behaviors observed experimentally.

We first give an argument for the interpretation of the term in question based on the assumption that the dynamics of the electrons is consistent with the picture developed above. In analogy with Eq. (5), we define the resonant frequency by the equation

$$\overline{\Omega}=\frac{\int_0^\infty \omega Q''_{xx}(\omega)d\omega}{\int_0^\infty Q''_{xx}(\omega)d\omega}=\frac{1}{2\hbar}\frac{\langle 0|[[P_x,H],P_x]|0\rangle}{\langle 0|P_x^2|0\rangle}\,, \tag{14}$$

which should give a result equivalent to Eq. (8) if our interpretation is correct. The main difficulty with using Eq. (14) to obtain the resonance position in the first place, is the evaluation of the denominator. If the ground state $|0\rangle$ represents an ideal system without impurities it is easy to show that $\langle 0|P_x^2|0\rangle_{\text{ideal}}=\frac{1}{2}M\hbar\omega_c$. The situation with impurities is more complex and an equivalent general expression for the matrix element cannot be given. However, if we accept the physical picture described above and assume the center of mass to be bound harmonically in accord with Eq. (13), the ground-state energy of the oscillator is $\varepsilon_0=\hbar\Omega_0\equiv\hbar(\omega_0^2/2+\omega_c^2/4)^{1/2}$. In this case,

$$\begin{aligned}\langle 0|P_x^2|0\rangle &= M\langle 0|H|0\rangle-\tfrac{1}{2}M^2\omega_0^2\langle 0|X^2|0\rangle\\ &= M\hbar\Omega_0-M\hbar\omega_0^2/(4\Omega_0)\\ &= \tfrac{1}{2}M\hbar\omega_c+O(\omega_0^4)\,.\end{aligned} \tag{15}$$

Thus, even though the impurities provide a harmonic restoring force, the $\langle 0|P_x^2|0\rangle$ matrix element is not affected to $O(\omega_0^2)$. Using the result from Eq. (15) in Eq. (14) together with the denominator of Eq. (6) evaluated previously, we find $\overline{\Omega}=\omega_c+\omega_0^2/2\omega_c$ whose square is equivalent to Ω^2 as given by Eq. (8). Taking this as the center of the shifted resonance, we can define the second moment of the spectral distribution with respect to this position by

$$\Gamma^2\equiv\Omega^2-\overline{\Omega}^2=\frac{1}{m^*M\omega_c^2}\int d\mathbf{r}\,(\nabla\nabla_x v_{\text{ext}}(\mathbf{r}))^2 n_0(\mathbf{r})\,. \tag{16}$$

This contribution to Ω^2 evidently determines the width of the resonance Γ.

We now explore the implications of this interpretation. For simplicity we consider the contribution of a single impurity at the origin with potential

$$v_{\text{ext}}(\mathbf{r})=\pm\frac{e^2}{\kappa r}\,. \tag{17}$$

The integrand in Eq. (16) contains the quantity

$$(\nabla\nabla_x v_{\text{ext}}(\mathbf{r}))\cdot(\nabla\nabla_x v_{\text{ext}}(\mathbf{r}))=\left(\frac{e^2}{\kappa}\right)^2\left(\frac{1}{r^6}+\frac{3x^2}{r^8}\right). \tag{18}$$

This function is highly singular and its integral over all space, in fact, diverges for a point charge. However, in a semiconductor, the impurity charge is distributed over an atomic volume of size a which introduces a small-r cutoff. Assuming that the impurity is immersed in the 2DEG, Eq. (16) can be approximated as

$$\begin{aligned}\Gamma^2 &= \frac{c}{(m^*\omega_c)^2}\int_{r>a}d\mathbf{r}\left(\frac{e^2}{\kappa}\right)^2\left(\frac{1}{r^6}+\frac{3x^2}{r^8}\right)n_0(\mathbf{r})\\ &\simeq c\frac{8\pi}{3}\left(\frac{a^*}{a}\right)^3[a^{*3}n_0(0)]\left(\frac{H^*}{\hbar\omega_c}\right)^4\omega_c^2\,,\end{aligned} \tag{19}$$

where $a^*=\kappa\hbar^2/m^*e^2$ is the effective Bohr radius and $H^*=2\,\text{Ry}^*=e^2/\kappa a^*$ is the effective Hartree unit of energy. The ratio of this term to the square of the frequency shift is proportional to $(H^*/\hbar\omega_c)^2 \propto B^{-2}$ which will be small in the extreme high-field limit, but for the field strengths of interest (10–20 T) this ratio is of order unity. Furthermore, the ratio $(a^*/a)^3$ is typically 10^5–10^6 which represents a huge enhancement, so it is clear that Γ makes a significant contribution to the value of the ω^2 frequency moment and is why its physical interpretation is essential. The fact that the ω^2 moment is large of course does not imply that the resonance is ill defined, but only that the spectral density decreases rather slowly with increasing frequency. For example, if $\omega Q''_{xx}(\omega)$ were to have a Lorentzian line shape $\propto[(\omega-\Omega)^2+\Gamma^2]^{-1}$, the ω^2 moment would be divergent.

The final value of Γ is also dependent on the 2DEG density close to the impurity. In the case of a δ-doped layer within the 2DEG, $n_0(0)$ plays a crucial role and is ultimately what distinguishes between acceptors and donors.

For acceptors, the impurity potential is repulsive and $n_0(0)$ is depleted to a value below that of the average 2DEG density (see Fig. 1). On the other hand, the charge density is enhanced for the attractive donor impurity potential. This effect can be seen in the self-consistent electronic structure calculations performed in the Hartree approximation for a finite system in a magnetic field.[14] Just on this basis we would anticipate broader lines for donor impurities as compared to acceptor impurities, all other variables such as concentration and impurity position being equal.

We now consider the interesting case of acceptor impurities in greater detail and examine the behavior of $n_0(0)$ as a function of magnetic field or filling factor, using the self-consistent Hartree calculations[14] as a guide. For a single impurity the single-particle eigenfunctions for the screened impurity potential can be classified by the Landau-level index n and the azimuthal quantum number m which lies in the range $-n \leq m \leq \infty$. The small-r behavior of these states is proportional to $r^{|m|}$ so that only the $m=0$ state for each Landau level has a finite amplitude at the origin. Conversely, because of their finite amplitude, the $m=0$ states have higher energies for a repulsive impurity than the Landau states which are further removed ($m \neq 0$). Thus, as the filling factor is reduced below 1, one expects the $m=0$ state in the lowest occupied Landau level to be depopulated first with increasing magnetic field. In other words, only states with $m \neq 0$ will be occupied and as a result $n_0(0)$ is strictly zero. Although these conclusions are based on the Hartree approximation, they should also be valid in a more rigorous treatment of the screening problem as performed, for example, using density functional theory[15] for the spin-polarized situation.

Equation (19) is not a useful result when $n_0(0)=0$. To obtain a more accurate estimate we consider the point at which the ($n=0$, $m=0$) level first becomes depopulated near $\nu=1$. The removal of one electron from this state is sufficient to screen the impurity. The effect of the impurity potential on the remaining $m \neq 0$ states is, therefore, diminished and to a first approximation these states can be chosen as ideal Landau states. The $m=1$ state has the largest amplitude near $r=0$ and contributes a density which behaves as $(r/l)^2$ where $l=(\hbar c/eB)^{1/2}$ is the magnetic length. When this form of $n_0(\mathbf{r})$ is used in Eq. (19), the final result for Γ^2 basically has $(a^*/a)^3$ replaced by $(a^*/a)(a^*/l)^2$, and since (a^*/l) is of order unity, Γ^2 is reduced by about a factor of 10^4 relative to the situation where $n_0(0)$ is finite. Such a large reduction in the ω^2 moment will have a dramatic effect on the apparent width of the resonance as observed experimentally for $\nu < 1$.[8] The situation with donor impurities is of course quite different since $n_0(0)$ is always finite and in fact enhanced above the mean 2DEG density. In view of this behavior, there is nothing particularly significant about $\nu=1$ for donor impurities, and is why the Si-doped system exhibits a much broader resonance at high fields as compared to the Be-doped samples.

In conclusion, we have presented general arguments which provide a qualitative understanding of the cyclotron resonance in Si and Be δ-doped samples. We have obtained an exact expression for the ω^2 moment of the electronic current-current response function which admits an interpretation in terms of a shift of the resonant frequency and its width. The narrow resonance observed in Be-doped samples at high magnetic fields is due to the vanishing of the contact density $n_0(0)$ for some filling factor less than 1. With the reduced dissipation implied by this result, the resonance in this limit can be thought of as a coherent cyclotron motion of the electrons in the presence of an harmonic confining potential arising from the impurity background. The fact that Si-donor impurities have a large contact density leads to qualitatively different behavior in this case. As a final comment, we should emphasize that despite their generality, sum-rule arguments are limited in what information they can provide. In particular, the detailed behavior of the cyclotron resonance observed in δ-doped samples can only be determined by a microscopic treatment of the dynamics. Nevertheless, sum-rule arguments can still provide useful constraints and, as we have shown, can elucidate the properties of both the ground and excited electronic states.

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