Quantum Hall effect in a two-dimensional electron-impurity system

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The contribution of quasilocalized states to the Hall conductivity produced by thermal excitation in a two-dimensional electron-impurity system is calculated in the approximation of sparse impurity centers. It is proved that a solitary axisymmetric impurity center does not give rise, in all perturbation-theory orders, to corrections to the ideal value of the Hall current of occupied Landau levels. In the case of an arbitrary scattering potential the corresponding correction is zero up to third-order perturbation theory.

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1. INTRODUCTION

Experiments on the quantum Hall effect in inversion layers on silicon surface have shown[1,2] that in a strong magnetic field B, in the region of the minima of the Shubnikov–de Haas oscillations, the Hall component σ_{xy} of the electric conductivity tensor is close to the Hall component of a free two-dimensional electron gas $\sigma_{xy}^{(0)} = ecN_e/BS$, where e is the electron charge, c is the speed of light, N_e is the number of electrons in the system, and S is the sample area. It is known that no minimum of the Shubnikov–de Haas oscillations occurs when several Landau levels in the systems are fully occupied, i.e., when $N_e = pN_0$, where p is an integer, $N_0 = S/2\pi\lambda^2$ is the number of possible electronic states on the Landau level, and $\lambda = (c\hbar/eB)^{1/2}$ is the magnetic length. Therefore the quantity $\sigma_{xy}^{(0)} = pe^2/2\pi\hbar$ depends only on a combination of fundamental constants. Recent precise measurements of the components σ_{xy} have shown[3] that in this situation the correction $\delta\sigma_{xy} = \sigma_{xy} - \sigma_{xy}^{(0)}$ is exceedingly small, $|\delta\sigma_{xy}/\sigma_{xy}^{(0)}| < 10^{-5}$. It was proposed in Ref. 3 to use this fact to produce a quantum standard for resistance.

A theoretical analysis of the situation raises two fundamental questions: (a) How can the chemical potential of the system be fixed periodically in a manner that satisfies the condition $N_e = pN_0$? (b) What is the theoretical value (if not equal to zero) of the correction $\delta\sigma_{xy}$ to the ideal value $\sigma_{xy}^{(0)}$? These questions are considered from various points of view in the current literature.[3–10]

The answer to the first question is relatively simple.[10] The position of the chemical potential can be fixed on the tail of any of the broadened Landau levels in the region of the localized states produced by a perturbing random potential $V(\mathbf{r})$. In Ref. 10 we considered a simple model of a two-dimensional system, wherein the perturbing potential is produced by random disposition of charged impurity centers in a dielectric near the inversion layer. In a strong magnetic field $\hbar\omega_c^* \gg V_0$, where ω_c^* is the cyclotron frequency and V_0 is the characteristic value of the impurity-center potential, a two-dimensional impurity band is produced on the tail of each Landau level, and all the electronic states of the band are localized provided that $n_{0x}\lambda^2 \ll 1$, where n_{0x} is the surface density of the impurity centers. The two-dimensional impurity band contains then only a small fraction of the total number of Landau levels, since it follows from the condition $n_{0x}\lambda^2 \ll 1$ that $n_{0x}S \ll N_0$. If the chemical potential of the system is located at a sufficiently low temperature in the two-dimensional impurity band of the level numbered N, ($N \sim 1$), all the states of the lower Landau levels with $N' < N$ are completely filled with electrons and are separated by a gap $\sim\hbar\omega_c^*$ from the unfilled states of the N-th Landau level. In addition, the localized states of the two-dimensional impurity band of the N-th level are separated from the lower edge of the mobility threshold of this level by a gap $\sim V_0 \ll \hbar\omega_c^*$.

By fixing the chemical potential in a two-dimensional impurity band we satisfy the fundamental relation $N_e = pN_0$ only approximately, accurate to a small number of electrons situated in the impurity band. By assumption, however, all the electronic states in a two-dimensional impurity band are localized. In this case the impurity-band electrons contribute only to the temperature-dependent correction to $\sigma_{xy}^{(0)}$, due to thermal excitation to the mobility threshold of the nearest Landau level. We show in the present paper that this correction is exponentially small at sufficiently low temperature. We are still left with the question of how the impurity potential influences the Hall current of the occupied lower Landau levels at $T = 0$. It is clear from physical consideration that the corresponding correction $\delta\sigma_{xy}$ cannot be large, since the wave function of the occupied Landau level is nondegenerate and the perturbing potential is relatively weak: $V_0 \ll \hbar\omega_c^*$. So far it has not been proved that $\delta\sigma_{xy} = 0$. On the other hand, nor is a rigorous estimate of this quantity been given, although this question is of importance for a theoretical estimate of the accuracy of the possible resistance standard.

By way of a particular result, it was shown in Ref. 11 that in the so-called SCBA approximation one obtains $\delta\sigma_{xy} = 0$. The approximations used in the derivation, however, do not make it possible to estimate the accuracy of this result. An attempt to prove that $\delta\sigma_{xy} = 0$ was made for the particular case of a perturbing potential in the form $V = \delta(\mathbf{r})$. The calculations in Ref. 4 show only that the main contribution to $\delta\sigma_{xy}$ is cancelled out and are not convincing. Results close to ours were obtained in Ref. 9. There, however, the important role of localized states at $T \neq 0$ was not investigated and only the lowest order of perturbation theory was considered.

In §2 we investigate in detail the contribution of the localized states to the Hall mobility on account of thermal

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excitation to the mobility threshold, and show that for a short-range impurity potential this contribution is exponentially small if the temperature is low enough. In addition, we prove rigorously that a solitary axisymmetric impurity centers does not necessitate at $T=0$, for all orders of perturbation theory, corrections to the ideal value of the Hall current of occupied lower Landau levels.

In the case of an arbitrary impurity potential, we prove in §3 that for a filled Landau level the correction $\delta\sigma_{xy}$ is zero in third- and fourth-order perturbation theory in the small parameter $V_0/\hbar\omega_c^* \ll 1$, and estimate the possible value of the correction in fourth order in this parameter. The estimate shows that even if the correction $\delta\sigma_{xy}$ for an occupied Landau level is not zero, it is small enough to account for the experimental data.[3]

2. CONTRIBUTION OF SOLITARY IMPURITY STATES TO THE HALL CONDUCTIVITY

We consider the case of sparse impurity centers and a strong magnetic field, $n_{0x}\lambda^2 \ll 1$, when the influence of the surrounding impurity center on the electronic states of a given solitary impurity center can be neglected. To calculate the contribution of the electronic states of the solitary impurity center to the Hall component of the conductivity tensor of the system we use the Kubo formula in the form[12]

$$\sigma_{xy}=-\frac{ecN_e}{BS}+\frac{e^2}{S}\lim_{\varepsilon\to 0}\int_0^\infty dt\, e^{-\varepsilon t}\int_0^\beta dz\,\mathrm{Sp}\{\hat\rho\hat Y(-i\hbar z)\hat X(t)\}, \tag{1}$$

where $\hat X$ and $\hat Y$ are the operators of the center of the cyclotron motion of the electron, $T=\beta^{-1}$ is the temperature, and $\hat\rho$ is the operator of the equilibrium density matrix of the system with Hamiltonian $\hat H=\hat H_0+\hat V$, where $\hat H_0$ is the Hamiltonian of the free two-dimensional electrons in a magnetic field. The use of the Kubo formula in the form (1) is particularly convenient for our problem, since the first term of (1) is equal to the Hall component of a free electron gas, and the second term is the correction to be calculated.

The solitary-impurity-center potential acting on the two-dimensional electrons will be assumed to be axisymmetric, $V=V(\rho), \rho=(x^2+y^2)^{1/2}$. The problem can then be solved exactly. We determine the systematics of the states of the Hamiltonian $\hat H$. In view of the axial symmetry of the problem, the angular quantum number m is an exact quantum number of this Hamiltonian. The second quantum number n_ρ describes the radial motion. If the potential $V(\rho)$ is bounded at infinity, the wave functions of the Hamiltonian H can be described in the limit of a strong magnetic field $\hbar\omega_c^* \gg V_0$, in place of the quantum number n_ρ, also by the Landau quantum number N. We shall therefore designate exact wave functions and energy eigenvalues of the Hamiltonian H by $|Nm\rangle$ and E_{Nm}, respectively. Although $|Nm\rangle$ and E_{Nm} are unknown, in the limit of a strong magnetic field they can be calculated by perturbation theory, using as the basis the wave functions $|Nm\rangle^{(0)}$ of a free electron in a magnetic field.[13]

With the aid of the equations of motion

$$\hat{\dot X}=\frac{1}{i\hbar}[\hat X,\hat H]=\frac{\lambda^2}{\hbar}\frac{\partial V}{\partial y},\quad \hat{\dot Y}=\frac{1}{i\hbar}[\hat Y,\hat H]=-\frac{\lambda^2}{\hbar}\frac{\partial V}{\partial x} \tag{2}$$

expression (1) can be rewritten in the basis $|Nm\rangle$ in the form

$$\sigma_{xy}=-\frac{ecN_e}{BS}+i\frac{e^2\lambda^4}{\hbar S}\hat P \times\sum_{N,m}\sum_{N',m'}\frac{\langle Nm|\partial V/\partial y|N'm'\rangle\langle N'm'|\partial V/\partial x|Nm\rangle}{(E_{N'm'}-E_{Nm})^2} \times(f_{Nm}-f_{N'm'}), \tag{3}$$

where $\hat P$ is the principal-value symbol and f_{Nm} are the occupation numbers of the state $|Nm\rangle$. In the derivation of (3) we have left out a term containing $\delta(E_{N'm'}-E_{Nm})$, since it does not contribute to σ_{xy} in the considered case of a solitary impurity center. It can be next verified that the matrix elements of the operators $\hat X$ and $\hat Y$ on the basis functions $|Nm\rangle$ are nonsingular. Therefore, using (2), we can simplify Eq. (3):

$$\sigma_{xy}=-\frac{ecN_e}{BS}-i\frac{e^2}{\hbar S} \times\sum_{Nm}\sum_{N'm'}\langle Nm|\hat X|N'm'\rangle\langle N'm'|\hat Y|Nm\rangle(f_{Nm}-f_{N'm'}). \tag{4}$$

Reasoning formally, the second term in (4) can be written in the form

$$-i\frac{e^2}{\hbar S}\sum_{Nm}f_{Nm}\langle Nm|[\hat X,\hat Y]|Nm\rangle. \tag{5}$$

Using next the value of the commutator $[\hat X,\hat Y]=i\lambda^2$ and the normalization condition

$$\sum_{Nm}f_{Nm}=Sp\,\hat\rho=N_e,$$

we can formally "prove" that the second term of (4) always cancels the first and $\sigma_{xy}=0$. The foregoing arguments can be justified, however, only for a potential that is not bounded at infinity [$V(\rho)\to\infty$ as $\rho\to\infty$], when the occupation numbers $f_{Nm}\to 0$ as $m\to\infty$. In this case the result, $\sigma_{xy}=0$, is obvious beforehand, since the potential that is unbounded at infinity localizes all the electronic states, and their contribution to the Hall current is zero. For potentials of the type $V(\rho\to\infty)=0$ the values of f_{Nm} tend to a nonzero constant as $m\to\infty$. We shall show below that the transformation is not valid in this case.

Using the axial symmetry of the problem and the equations of motion (2), we can show that the matrix elements of the operators $\hat X$ and $\hat Y$ differ from zero only for transitions $m'=m\pm 1$ and are, in addition connected by the relations

$$\langle Nm|\hat Y|N',m+1\rangle=-i\langle Nm|\hat X|N',m+1\rangle. \tag{6}$$

We examine now the behavior of the matrix elements (6) at $m\gg 1$. In the state $|Nm\rangle$ with $m\gg 1$ the electron is located at large distances from the center, where the potential $V(\rho)$ can be neglected. Therefore at $m\gg 1$ the wave functions $|Nm\rangle\approx|Nm\rangle^{(0)}$. The matrix elements of the operator $\hat X$ with respect to the unperturbed wave functions $|Nm\rangle^{(0)}$ are equal to

$$|(Nm|^{(0)}\hat{X}|N',\ m+1)^{(0)}|=2^{-1/2}\Delta_{N,N'}\lambda(N+m+1)^{1/2}. \quad (7)$$

Using (7) we can verify by perturbation theory that the sums at $N\neq N'$ the matrix elements $\langle Nm|\hat{X}|N,\ m+1\rangle$ decrease rapidly as $m\to\infty$, so that the sums over m in (4) converge well at $N\neq N'$. The contributions to the sum (4) that are diagonal in N can converge, obviously, only if the difference $f_{Nm}-f_{N,m+1}\to 0$ decreases rapidly enough as $m\to\infty$. Taking (6) into account and separating in (4) the diagonal and off-diagonal ($N\neq N'$) parts of the sum, we obtain ultimately

$$\sigma_{xy}=-\frac{ecN_e}{BS}-i\frac{e^2}{\hbar S}F,\quad F=F_d+F_{nd}, \quad (8a)$$

$$F_d=2i\sum_{N=0}^{\infty}\sum_{m=-N}^{\infty}|\langle Nm|\hat{X}|N,m+1\rangle|^2(f_{Nm}-f_{N,m+1}), \quad (8b)$$

$$F_{nd}=2i\sum_{N=0}^{\infty}\sum_{m=-N}^{\infty}\left\{\frac{\lambda^2}{2}-|\langle Nm|\hat{X}|N,m+1\rangle|^2 +|\langle N,m-1|\hat{X}|N,m\rangle|^2(1-\Delta_{m,-N})\right\}f_{Nm}, \quad (8c)$$

where $\Delta_{m,m'}$ is the Kronecker delta.

Using (8), we consider now several particular cases. Let the system contain only one electron, $N_e=1$. Clearly, if the impurity center is attracting, the electron is localized at sufficiently low temperature on the impurity center and does not contribute to the Hall current. Indeed, let the state $|0,0\rangle$ be the ground state of the Hamiltonian $\hat{H}$. Assuming at $T=0$ an occupation $f_{Nm}=\Delta_{N,0}\Delta_{m,0}$, we get from (8) $F=i\lambda^2$ and $\sigma_{xy}=0$. It can be easily seen that there is likewise to contribution to the Hall current from an electron localized in an arbitrary metastable state $|N_0,m_0\rangle$, when $f_{Nm}=\Delta_{N,N_0}\Delta_{m,m_0}$. At finite temperatures $T\ll\hbar\omega_c^*$ we obtain from (8) in the lowest order of perturbation theory

$$F=i\lambda^2\sum_{m=0}^{\infty}(m+1)(f_{0,m}-f_{0,m+1}); \quad (9)$$

it suffices here to calculate the energies $E_{0,m}$ in (9) in first order perturbation theory, putting, $E_{0,m}=\hbar\omega_c^*/2-V_m$, where $V_m=|(0,m|^{(0)}\hat{V}|0,m)^{(0)}|$. For potentials that decrease rapidly at infinity, the sum in (9) converges well. It diverges, however, say for an unscreened Coulomb potential $V(\rho)=e^2/\rho$. The approximation of a solitary impurity center cannot be used in this case, and it is apparently necessary to take into account the screening by the surrounding impurity centers.

Let us consider in greater detail the case of a short-range potential of the δ-function type, when $V_m=V_0\Delta_{m,0}$. We determine the chemical potential from the condition

$$\sum_{m=0}^{M-1}f_{0,m}=1,$$

where M is the average number of the Landau-level states per impurity center, with $M\gg 1$ in the approximation in which the centers are sparse and the magnetic field is strong. From (9) we get

$$F=i\lambda^2[1-\sqrt{M}\exp\{-V_0/2T\}]\approx i\lambda^2,\quad T\ll V_0/\ln M,$$
$$F=i\lambda^2/M\ll i\lambda^2,\quad T\gg V_0/\ln M. \quad (10)$$

In the limit of low temperatures the contribution of an electron localized on an impurity center is thus exponentially small.[1)] In the opposite limit of high temperatures, the electron is in fact ionized and the impurity center affects its motion little.

If the Landau level is not fully occupied, $1\ll N_e<N_0$, it is necessary to take into account at low temperatures the restructuring of the ground state of the system under the influence of the Coulomb interaction between the electrons, i.e., the formation of a Winger lattice[15] or of a charge-density wave.[16,17] Calculation of the electric-conductivity tensor components under these conditions calls for a separate analysis. If, however, the Landau level is completely filled, $N_e=N_0$, the wave function of the ground state is nondegenerate and the Coulomb interaction between electrons in a strong magnetic field $e^2/\varkappa\lambda\ll\hbar\omega_c^*$ can be regarded as a perturbation. Let, for example, the lower Landau level be fully occupied at $T=0$, so that $f_{Nm}=\Delta_{N,0}$. It can be easily seen that the diagonal contribution $F_d=0$. We shall show that the nondiagonal component F_{nd} is also zero. Indeed, the partial sum of the first l terms of the series for F_{nd} is

$$F_{nd}(l)=2i\{{}^1/_2\lambda^2 l-|\langle 0,l-1|\hat{X}|0,l\rangle|^2\}. \quad (11)$$

Taking the relation (7) into account, it can be shown that $F_{nd}(l)\to 0$ as $l\to\infty$. Thus, the presence of a solitary impurity center in the system does not influence the Hall current of the occupied lower Landau level at $T=0$. This result can be easily generalized to the case of occupation of several Landau levels.

We can treat analogously the case when several lower Landau levels in the system are occupied at $T=0$, while the next level has a small number of electrons in localized states on sparsely disposed impurity centers. The chemical potential of the system is in this case on the tail of the partly occupied Landau level. It can be verified with the aid of (8) that the localized electrons of the partly occupied Landau level do not contribute to the Hall current of the system. The presence of solitary impurity centers does not influence in this case the Hall current of the occupied lower Landau level, which is equal to its ideal value. Clearly, in this situation the temperature correction to this ideal current are determined primarily by the contribution, considered above, of the localized electrons of the partly occupied Landau level.

§3. ARBITRARY RANDOM POTENTIAL

We have considered in §2 the case of sparse impurity centers, which admits of a rigorous analysis but is most unlikely in a real experiment.[3] We examine therefore in the present section the case of an arbitrary weak ($V_0\ll\hbar\omega_c^*$) random potential. By virtue of the statements made in §2, it suffices to calculate the possible correction to the ideal value of the Hall current of the occupied lower Landau levels at $T=0$.

To estimate the correction $\delta\sigma_{xy}$ in this case we must use Eq. (3), where $|Nm\rangle$ and E_{Nm} must be replaced by the exact wave functions $|N\alpha\rangle$ and eigenvalues $E_{N\alpha}$ of the Hamilton-

ian $\hat{H}_0 + \hat{V}$. In a strong magnetic field, $V_0 \ll \hbar\omega_c^*$, the Landau quantum number N remains a good quantum number. The quantum number α numbers the states of the specified Landau level. For the case of an arbitrary perturbing potential it is necessary to retain in the right-hand side of (3) also the term with $\delta(E_{N'\alpha'} - E_{N\alpha})$. When account is taken of the electron-phonon interaction, a term of this type introduces in $\sigma_{xy}^{(0)}$ a temperature correction due to the hopping conduction over the localized states of the two-dimensional impurity band. In the limit as $T \to 0$ this term can be left out. In the general case it is difficult to justify the transition from (3) to (4) in view of the possible singularity of the matrix elements $\langle N\alpha|\hat{X}|N'\alpha'\rangle$. To estimate the correction $\delta\sigma_{xy}$ in the case of an arbitrary random potential it is convenient to start instead directly from Eq. (3), which takes at $T = 0$, for the case of occupation of the lower Landau level, the form

$$\delta\sigma_{xy} = i\frac{e^2\lambda^4}{\hbar S}\hat{P} \times \sum_{N\geqslant 1}\sum_{\alpha,\beta}\frac{\langle 0,\alpha|\partial V/\partial y|N\beta\rangle\langle N\beta|\partial V/\partial x|0,\alpha\rangle - \text{c.c.}}{(E_{N\beta}-E_{0,\alpha})^2}. \tag{12}$$

The right-hand side of this equation can be expanded in powers of the small parameter $V_0/\hbar\omega_c^* \ll 1$. It is convenient to carry out the calculation under the assumption that the first-approximation wave functions $|N\alpha\rangle^{(1)} = |N\alpha)$ and the energy eigenvalues $E_{N\alpha}^{(1)}$ are known as a result of formal diagonalization of the degenerate Landau level. The wave functions $|N\alpha\rangle$ are thus determined by linear combinations of the unperturbed states $|NX_0\rangle$ of the N-th Landau level:

$$|N\alpha) = \sum_{X_0} c_{NX_0}(\alpha)\,|NX_0), \quad E_{N\alpha}^{(1)} = (N\alpha|\hat{V}|N\alpha), \tag{13a}$$

$$\sum_{\alpha}|N\alpha)\,(N\alpha| = \sum_{X_0}|NX_0)\,(NX_0| = \Delta_N(\mathbf{r}_1,\mathbf{r}_2), \tag{13b}$$

where X_0 is the quantum number of the center of the cyclotron motion. The use of (13b) in the calculations for an occupied Landau level obviates the need for the complicated procedure of determining the unknown quantities $c_{NX_0}(\alpha)$ and $E_{N\alpha}^{(1)}$. It is easily seen that the expansion of (12) begins with terms of order $(V_0/\hbar\omega_c^*)^2$. In this case it is necessary to substitute the unperturbed energies $E_{N\beta}^{(0)} = \hbar\omega_c^*(N + 1/2)$, in the denominator of (12), and the first-approximation wave functions (13a) in the numerator. Using (13b), we obtain

$$\sum_{\alpha,\beta}\left(0,\alpha\left|\frac{\partial V}{\partial y}\right|N\beta\right)\left(N\beta\left|\frac{\partial V}{\partial x}\right|0,\alpha\right) = \int d\mathbf{r}_1\,d\mathbf{r}_2\,\Delta_{N'}(\mathbf{r}_1,\mathbf{r}_2)\,\Delta_N(\mathbf{r}_1,\mathbf{r}_2)\,\frac{\partial V(\mathbf{r}_1)}{\partial y_1}\,\frac{\partial V(\mathbf{r}_2)}{\partial x_2}. \tag{14}$$

The quantities $\Delta_N(\mathbf{r}_1, \mathbf{r}_2)$ can be calculated in explicit form, and it can be verified that products of the type $\Delta_N^*(\mathbf{r}_1, \mathbf{r}_2)\Delta_{N'}(\mathbf{r}_1, \mathbf{r}_2)$ are real. The second-order contribution to $\delta\sigma_{xy}$ vanishes even before the averaging over the random potential $V(\mathbf{r})$. To calculate the third-order correction we must use the second-approximation wave function and the first-approximation eigenvalues $E_{N\alpha}^{(1)}$ [Eq. (13a)]. The use of relations such as (14) makes it unnecessary to calculate $c_{NX_0}(\alpha)$ and $E_{N\alpha}^{(1)}$ explicitly. Rigorous but unwieldy calculations show that the third-order contribution to $\delta\sigma_{xy}$ is also zero.

We estimate the contribution of fourth order to $\delta\sigma_{xy}$ for the case when the potential of an individual impurity is of the form $V(\mathbf{r}) = V_0 \exp\{-\mathbf{r}^2/d^2\}$. It can be shown that in the limit $\lambda \ll d$, in the lowest order in the small parameter $n_{0x}\lambda^2 \ll 1$, a typical value of the correction is of the order of

$$\delta\sigma_{xy}^{(4)} \sim (e^2/\hbar)\,(V_0/\hbar\omega_c^*)^4 n_{0x}\lambda^2(\lambda^2/d^2). \tag{15}$$

Thus, if the correction $\delta\sigma_{xy}$ is not zero, it is small enough to account for the experimental data of Ref. 3.

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