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LETTER TO THE EDITOR

The Hall coefficient of disordered electronic systems in high magnetic fields

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Abstract. We calculate the Hall resistivity in the low frequency limit for a model of independent electrons in the lower tail of the density of states of the disorder broadened lowest Landau level. It is shown that the Hall coefficient remains finite for $\omega \rightarrow 0$ even in the lowest localization regime for 2D as well as for 3D systems in contrast to the characteristics of magnetic freezing out. We relate our theoretical results to recent experiments on magnetic field induced MI transitions in doped semiconductors.

In a recent experiment Hopkins *et al* [1] studied the behaviour of the resistivities in uncompensated degenerately doped Ge : Sb slightly above the critical concentration, as a function of the magnetic field. Increasing the magnetic field beyond 4 T they observed an increase of ρ_{xx} of about 3 orders of magnitude whereas the Hall coefficient changed only by a factor of 2–4. In the same region the temperature dependence of the longitudinal resistivity changed from a metallic to an activated behaviour.

This phenomenon cannot be explained by freezing out (cf [2]) because this would imply a simultaneous reduction of the apparent carrier concentration and thus a drastic increase of the Hall coefficient.

Hopkins *et al* [1] conjectured that some magnetic field induced localization mechanism might be involved. However, to the best of our knowledge no theoretical results for the Hall resistivity in the localized regime have been presented so far.

Motivated by the above presented phenomenon we consider a simple model of non-interacting electrons in a random potential subjected to a strong magnetic field B and show that ρ_{xx} diverges in the limit of low frequencies ω but ρ_{xy} remains finite.

In fact we calculate the conductivities $\sigma_{\mu\nu}$ and only then can we find the resistivities using the relations

$$\rho_{xx} = \sigma_{xx}/(\sigma_{xx}^2 + \sigma_{yx}^2) \quad \rho_{xy} = \sigma_{yx}/(\sigma_{xx}^2 + \sigma_{yx}^2). \quad (1)$$

In the lowest localized region both σ_{xx} and σ_{yx} vanish in the limit $\omega \rightarrow 0$ and the inversion of the conductivity tensor in (1) has to be performed for finite frequencies. It is well known that the leading term in the frequency dependence of the longitudinal conductivity σ_{xx} is proportional to $i\omega$. Below we show that the Hall conductivity in the low frequency limit is proportional to ω^2 . From this proportionality together with (1) the above proposed behaviour of ρ_{xx} and ρ_{xy} follows immediately.

Since the derivation of our results is rather involved we will present in this letter only the outline of our method stressing the principle aspects.

Now let us formulate the model. The one-particle Hamiltonian of the system reads

$$\begin{aligned} H &= H_0 + V(r) \\ H_0 &= (1/2m)|\mathbf{p} - e\mathbf{A}|^2 \quad \mathbf{A} = \frac{1}{2}B(-y, x, 0). \end{aligned} \quad (2)$$

The random potential is assumed to be white noise, i.e.

$$\bar{V}(\mathbf{r}) = 0 \quad \overline{V(\mathbf{r}_1)V(\mathbf{r}_2)} = \lambda\delta(\mathbf{r}_1 - \mathbf{r}_2). \quad (3)$$

Our calculations are based on the Kubo formula and it has turned out to be convenient to use the following decomposition of the conductivities at finite frequencies

$$\begin{aligned} \sigma_{\mu\nu}(\omega) &= \sigma_{\mu\nu}^{(-)}(\omega) + \sigma_{\mu\nu}^{(+)}(\omega) \\ \sigma_{\mu\nu}^{(\mp)}(\omega) &= \frac{e^2\omega^2}{4\pi V} \int \mathbf{r}_\nu(\mathbf{r}'_\mu - \mathbf{r}_\mu) \frac{f(E + \omega/2) \mp f(E - \omega/2)}{\omega} K^{(\mp)}(\mathbf{r}, \mathbf{r}'; E, \omega) d\mathbf{r} d\mathbf{r}' dE \end{aligned} \quad (4a)$$

with

$$\begin{aligned} K^{(-)}(\mathbf{r}, \mathbf{r}'; E, \omega) &= \overline{2G^+(\mathbf{r}, \mathbf{r}'; E + \omega/2)G^-(\mathbf{r}', \mathbf{r}; E - \omega/2)} \\ &\quad - \overline{G^+(\mathbf{r}, \mathbf{r}'; E + \omega/2)G^+(\mathbf{r}', \mathbf{r}; E - \omega/2)} \\ &\quad - \overline{G^-(\mathbf{r}, \mathbf{r}'; E + \omega/2)G^-(\mathbf{r}', \mathbf{r}; E - \omega/2)} \\ K^{(+)}(\mathbf{r}, \mathbf{r}'; E, \omega) &= \overline{G^+(\mathbf{r}, \mathbf{r}'; E + \omega/2)G^+(\mathbf{r}', \mathbf{r}; E - \omega/2)} \\ &\quad - \overline{G^-(\mathbf{r}, \mathbf{r}'; E + \omega/2)G^-(\mathbf{r}', \mathbf{r}; E - \omega/2)} \end{aligned} \quad (4b)$$

where $\hbar = 1$. V denotes the volume and f is the Fermi-distribution function. Equation (4) can be obtained from the current-current correlation by using the equation of motion for the velocity operators, i.e. $v_\mu = i(H, r_\mu)$, and performing the trace in coordinate representation. Both kernels in (4b) contribute to the Hall conductivity. Since $K^{(+)}$ in contrast to $K^{(-)}$ is non-singular for $\omega \rightarrow 0$ we perform the calculation of $\sigma_{yx}^{(+)}$ first. When expanding $K^{(+)}$ with respect to ω the zeroth term depends on $(x - x')^2 + (y - y')^2$, $z - z'$ only and thus cannot contribute to $\sigma_{yx}^{(+)}$. To the lowest non-vanishing order in ω we obtain

$$\sigma_{yx}^{(+)}(\omega) = \frac{e^2\omega^2}{6\pi V} \int f(E)\Delta(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3)I(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3; E) d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3 dE \quad (5)$$

where

$$\Delta(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = \frac{1}{2}(\mathbf{r}_1 \times \mathbf{r}_2 + \mathbf{r}_2 \times \mathbf{r}_3 + \mathbf{r}_3 \times \mathbf{r}_1)_z \quad (6)$$

denotes the orientated area of the triangle spanned by $\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3$ and

$$I(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3; E) = \text{Re}[\overline{G^+(\mathbf{r}_1, \mathbf{r}_2; E)G^+(\mathbf{r}_2, \mathbf{r}_3; E)G^+(\mathbf{r}_3, \mathbf{r}_1; E)} - (\mathbf{r}_2 \leftrightarrow \mathbf{r}_3)]. \quad (7)$$

For the calculation of I in (7) it is convenient to represent it as a functional integral over commuting and anticommuting variables

$$\begin{aligned} I(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3; E) &= \text{Re}(J(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3; E) - J(\mathbf{r}_1, \mathbf{r}_3, \mathbf{r}_2; E)) \\ J(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3; E) &= i \int [d\bar{\Phi}][d\Phi] \chi(\mathbf{r}_1)\bar{\chi}(\mathbf{r}_2)s(\mathbf{r}_2)s^*(\mathbf{r}_3)\chi(\mathbf{r}_3)\bar{\chi}(\mathbf{r}_1) \exp(-S) \end{aligned} \quad (8)$$

where the action

$$S = -i \int \bar{\Phi}(E - H_0 + i\eta)\Phi \, dr + \frac{\lambda}{2} \int (\bar{\Phi}\Phi)^2 \, dr \tag{9}$$

is given in terms of the supervector $\Phi = (s, \chi)$ with s being commuting and χ anti-commuting. We calculate the functional integral of (8) using the saddle-point method. The instanton solution corresponding to the action of (9) in the limit of high magnetic fields, when only the tail of the lowest Landau level (LLL) is occupied, has already been studied in previous works [3, 4]. In the functional integral representation the density of states reads $\rho(E) = - (1/\pi) \text{Im } G^+(\mathbf{r}, \mathbf{r}; E)$ with

$$\overline{G^+(\mathbf{r}, \mathbf{r}; E)} = -i \int [d\bar{\Phi}][d\Phi] \chi\bar{\chi}(\mathbf{r}) \exp(-S). \tag{10}$$

For later use we repeat the results

$$\rho(E) = \begin{cases} \frac{2}{\sqrt{\pi}} \frac{1}{2\pi l^2} \frac{1}{\Gamma_2} \left(\frac{|\varepsilon|}{\Gamma_2}\right)^2 \exp\left(-\left(\frac{|\varepsilon|}{\Gamma_2}\right)^2\right) & \text{for } d = 2 \\ \text{constant} \frac{1}{2\pi l^2} \sqrt{\frac{2m}{\Gamma_3}} \left(\frac{|\varepsilon|}{\Gamma_3}\right)^{5/2} \exp\left(-\left(\frac{|\varepsilon|}{\Gamma_3}\right)^{3/2}\right) & \text{for } d = 3 \end{cases} \tag{11}$$

with $\varepsilon = E - \omega_c/2$, $\Gamma_2 = (2\pi l^2/\lambda)^{-1/2}$, $\Gamma_3 = (32\pi l^2/3\lambda \sqrt{2m})^{-2/3}$, and l denotes the magnetic length. Of course, for $d = 2$, this agrees with Wegner's exact result [5, 6] in the limit of large $|\varepsilon|/\Gamma_2$.

Both results have been obtained by Ioffe and Larkin [3] using the optimal fluctuation method and for 2D Affleck [4] rederived it using supersymmetry. We perform the calculation of the integral in (8) starting from the same one-instanton approximation underlying (11). As in Affleck's calculation for the density of states (cf [4]) there is no contribution from the trivial saddle-point $s = 0$ and the leading term in (8) is given for s being the instanton solution

$$s_{\text{cl}}(\mathbf{r}) = A\varphi^{(0)}(\mathbf{r}) \quad \text{with } A^2 = \begin{cases} \frac{4\pi l^2}{\lambda} |\varepsilon| & \text{for } d = 2 \\ \frac{16\pi l^2}{\lambda} \sqrt{\frac{|\varepsilon|}{2m}} & \text{for } d = 3. \end{cases} \tag{12}$$

In the two-dimensional case $\varphi^{(0)}(\mathbf{r})$ is the $m = 0$ eigenfunction of the unperturbed Hamiltonian in the symmetrical gauge; in 3D it has to be multiplied by the function $g(z) = (m|\varepsilon|/2)^{1/4} \cosh^{-1}(\sqrt{2m|\varepsilon|}z)$. The functional integrations are performed after expanding the involved fields with respect to the set of eigenfunctions of H_0 , which for the LLL reads

$$\begin{aligned} \varphi^{(m)}(\mathbf{r}) &= g(z)u^{(m)}(x, y) \\ u^{(m)}(x, y) &= (1/\sqrt{2\pi l^2 m!})[(x + iy)/2l]^m \exp[-(x^2 + y^2)/4l^2]. \end{aligned} \tag{13}$$

The integral over all field configurations are calculated by integrating over the set of commuting and anticommuting coefficients. Since the coefficients of the fermionic $m = 0$ mode cannot come from expanding the action, a non-vanishing result for $J(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3; E)$ can only be obtained if in one pair of Grassmann fields in (8) the variable χ as well as $\bar{\chi}$ is a fermionic zero-mode. Using the same notation as in [4] we thus obtain

$$\begin{aligned}
I(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3; E) &= e^{-S_0} \left| \det' \frac{\partial^2 S}{\partial s_i \partial s_j} \right|^{-1/2} \det' \frac{\partial^2 S}{\partial \bar{\chi} \partial \chi} \left(\prod_i \frac{\Delta_i}{\sqrt{\pi}} \right) A^2 \\
&\times 4\pi \operatorname{Im} \left\{ \int d\mathbf{r}_0 \sum_{m=1}^{\infty} \frac{1}{\lambda_F^{(m)}} [\varphi^{(m)}(\mathbf{r}_1 - \mathbf{r}_0) \varphi^{(m)*}(\mathbf{r}_2 - \mathbf{r}_0) \varphi^{(0)}(\mathbf{r}_2 - \mathbf{r}_0) \right. \\
&\left. \times \varphi^{(0)*}(\mathbf{r}_3 - \mathbf{r}_0) \varphi^{(0)}(\mathbf{r}_3 - \mathbf{r}_0) \varphi^{(0)*}(\mathbf{r}_1 - \mathbf{r}_0) - (\mathbf{r}_2 \leftrightarrow \mathbf{r}_3) - (\mathbf{r}_1 \leftrightarrow \mathbf{r}_3) \right\} \quad (14)
\end{aligned}$$

where S_0 is the saddle-point value of the action corresponding to the solution of (9), the primes denote the omission of zero-modes in the determinants and Δ_i are the Jacobians originating from the transformations of the bosonic zero-modes to the continuous parameters ϑ , \mathbf{r}_0 . $\varphi^{(m)}$ are the normalised eigenfunctions of H_0 in the symmetrical gauge and $\lambda_F^{(m)}$ denote the corresponding diagonal elements of the operator $\partial^2 S / \partial \bar{\chi} \partial \chi$. Each term occurring in the above sum is proportional to $\sin(m(\alpha_i - \alpha_j))$ where α_i is the polar angle of \mathbf{r} . Since the sine-functions for different positive integers m are orthogonal on the one hand and the oriented area $\Delta(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3)$ contains only terms proportional to $\sin(\alpha_i - \alpha_j)$ on the other hand, the Hall conductivity is just determined by the contribution $I^{(1)}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3; E)$ originating from the $m = 1$ modes.

$$\begin{aligned}
I^{(1)}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3; E) &= \rho(E) (\pi A^2 / l^2 \lambda_F^{(1)}) \Delta(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) \\
&\times \int |\varphi^{(0)}(\mathbf{r}_1 - \mathbf{r}_0)|^2 |\varphi^{(0)}(\mathbf{r}_2 - \mathbf{r}_0)|^2 |\varphi^{(0)}(\mathbf{r}_3 - \mathbf{r}_0)|^2 d\mathbf{r}_0 \quad (15)
\end{aligned}$$

with the density of states $\rho(E)$ from (11). In 2D $\lambda_F^{(1)} = |\varepsilon|/2$ and the Hall conductivity (5) finally reads

$$\sigma_{yx}^{(+)}(\omega) = (e^2 \omega^2 / \Gamma_2^2) 2l^2 n \quad (16)$$

where n is the integrated density of states. In 3D we obtain correspondingly

$$\sigma_{yx}^{(+)}(\omega) = \text{constant} \times \frac{e^2 \omega^2}{\Gamma_3} l^2 \sqrt{(\Gamma_3 / |\varepsilon|)} n. \quad (17)$$

After reviewing the arguments leading to (13)–(15) it is easy to understand that $\sigma_{yx}^{(+)}$ cannot contain a term linear in ω , because the average of the product of k retarded (advanced) Green functions at the same energy calculated from the action of (9) is rotationally invariant in the x, y -plane. For $k = 2$ this implies that the averaged product depends on $(x - x')^2 + (y - y')^2$ and $z - z'$ only, as already mentioned above. This can be seen explicitly by constructing the corresponding functional integral representation by analogy to (8); in the saddle-point approximation it just contains the bosonic instanton solution and one pairing from the fermionic zero mode in the pre-exponential.

In order to calculate the longitudinal conductivity and to justify that $\sigma_{yx}^{(-)}$ has no contributions of lower than quadratic order in ω we have to study the average of $G^+(\mathbf{r}, \mathbf{r}') G^-(\mathbf{r}', \mathbf{r})$. In the functional integral representation of $\sigma_{\mu\nu}^{(-)}$ two pairs of super-vectors have to be introduced.

In the localization regime the average $\overline{G^+ G^-}$ has a $(i\omega)^{-1}$ singularity, which can already be obtained in the one-instanton approximation, and a logarithmic singularity due to the tunnelling between two instantons. For σ_{xx} the result reads

$$\sigma_{xx}(\omega) = c_1 i\omega \rho(E_F) + c_2 \omega^2 \ln^{\nu}(1/\omega^2). \quad (18)$$

For $B = 0$ Houghton *et al* [7] derived $\nu = d + 1$ in the hydrodynamic limit. For the lower tail of the LLL Apel [8] obtained $\nu = 1$ in 2D. Both approaches were based on the optimal fluctuation method and the results could be reproduced by supersymmetry.

The kernel $K^{(-)}$ contributes to the Hall conductivity as well but it can be shown that the ω contributions to $\sigma_{yx}^{(-)}$ of the same order as those in (18) vanish.

The term of the lowest possible order originates from an expansion around the one-instanton contribution to $\overline{G^+G^-}$ and the corresponding term in $\sigma_{yx}^{(-)}$ is proportional to ω^2 . Let us briefly resume the scheme of calculation.

In the functional integral representation of the mixed two-particle Green function two pairs of supervectors are involved

$$\begin{aligned} & \overline{G^+(\mathbf{r}, \mathbf{r}')G^-(\mathbf{r}', \mathbf{r})} \\ &= \int [d\bar{\Phi}_1][d\Phi_1][d\bar{\Phi}_2][d\Phi_2] \chi_1(\mathbf{r})\bar{\chi}_1(\mathbf{r}')\chi_2(\mathbf{r}')\bar{\chi}_2(\mathbf{r}) \exp(-S_2) \\ S_2 &= -i \int \bar{\Phi}[\sigma_3(E - H_0) + \omega/2 + i\eta]\Phi \, d\mathbf{r} + \frac{\lambda}{2} \int (\bar{\Phi}\sigma_3\Phi)^2 \, d\mathbf{r} \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \\ \Phi &= (\Phi_1, \Phi_2). \end{aligned} \tag{19}$$

Neglecting the ω and η terms the stationarity condition for $\bar{\Phi}\sigma_2\Phi$ is the same as for the calculation of the density of states. The bosonic instanton solution may be parametrised by the angles of $SU(1, 1)$. Integrating the symmetry breaking part over these angles yields in leading order a $(i\omega)^{-1}$ singularity which is characteristic for the localization regime. The leading term of the longitudinal conductivity already given in (18) is obtained from (19) for all Grassmann fields $\chi_1, \bar{\chi}_1, \chi_2, \bar{\chi}_2$ being $m = 0$ eigenmodes. However, to obtain a contribution to σ_{yx} one pair of fermions has to be built from the $m = 1$ mode whereas the other pair still has $m = 0$. Consequently (19) contributes to $\sigma_{yx}^{(-)}$ in the form

$$\frac{\pi}{2l^2} \frac{1}{|\varepsilon|} \rho(E)(\mathbf{r} \times \mathbf{r}')_z \int |\varphi^{(0)}(\mathbf{r} - \mathbf{r}_0)|^2 |\varphi^{(0)}(\mathbf{r}' - \mathbf{r}_0)|^2 \, d\mathbf{r}_0 \tag{20}$$

so that in leading order

$$\sigma_{yx}^{(-)}(\omega) = (e^2 \omega^2 / |\varepsilon|) l^2 \rho(E) \tag{21}$$

in two dimensions. Since in the deep tails of the density of states $n(E) = \rho(E)$, $\Gamma_2^2/2|\varepsilon|$ we arrive at the remarkable conclusion that $\sigma_{yx}^{(+)}$ from (16) and $\sigma_{yx}^{(-)}$ from (21) are identical and hence

$$\sigma_{yx}(\omega) = 2\sigma_{yx}^{(+)}(\omega). \tag{22}$$

The analogous result can be obtained for the 3D case.

Finally, from (19) it follows that c_1 (18) is given by $c_1 = -e^2 l^2$ and we can explicitly calculate the Hall resistivity in the localization regime

$$\rho_{xy} = -(B/en)(|\varepsilon|/\Gamma_2)^{-2} \tag{23}$$

in two dimensions and

$$\rho_{xy} = -\text{constant} \times (B/en)(|\varepsilon|/\Gamma_3)^{-3/2} \tag{24}$$

in three dimensions. Supposing the number of particles to be fixed we see that in both cases the Hall coefficient $R_H = \rho_{xy}/B$ decreases logarithmically with B in the high magnetic field limit, i.e.

$$R_H = -c(1/en) \ln^{-1}(B/B_0) \quad (25)$$

where $B_0 = n/e$ in 2D, $B_0 = n^{3/4}/e(2m)^{1/2}\lambda^{1/4}$ in 3D and c is a constant of the order of unity which depends only on the dimensionality.

We are now able to establish the relationship between our theoretical results and the experimental situation. We have shown that the finiteness of the Hall coefficient is a natural phenomenon in the localization regime where ρ_{xx} diverges. We performed our calculations for the case in which the Fermi energy is situated in the tail of the LLL. This is in agreement with the parameters characterising the experiments of Hopkins *et al* [1] who found that near the MI-transition

$$\gamma = \omega_c/2E_B = a_B^2/l^2 = 0.2 \quad \xi = \omega_c/E_F \approx 2 \quad (26)$$

where E_B is the donor binding energy, a_B the effective Bohr radius and E_F the Fermi energy at $B = 0$. The equality $\xi > 1$ means that only the LLL is occupied. For $\gamma \approx 0.2$ magnetic freezing out which is the predominant effect at $\gamma \gg 1$ does not yet play an essential role.

In our theoretical description we expect freezing out not to be important if the disorder induced level broadening largely exceeds the donor binding energy, i.e. $\Gamma_3 \gg E_B$. On the other hand a comparison with (11) shows that the Fermi energy is surely situated in the localization regime for

$$n \approx c(1/2\pi l^2) \sqrt{2m\Gamma_3} \quad (27)$$

with $c \approx 0.1$, so that the band width satisfies

$$\Gamma_3 \approx 4\pi c^2 (na_B^3)^2 \gamma^2 E_B \quad (28)$$

We adopt the Mott criterion for the critical doping concentration $na_B^3 \approx 0.02$ and deduce that for the parameters given in (23) the band width Γ_3 indeed exceeds E_B which enables us not to consider freezing out as the dominant effect.

Nevertheless a competitive influence of bound states which are not included in our model cannot be excluded. We can take this fact into account on a phenomenological level by replacing n in (23)–(25) by the apparent carrier concentration which is the concentration n diminished by the already frozen out states. With this modification of (25) we can understand the slight increase of the Hall coefficient which has been observed in the experiment.

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