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1982 J. Phys. C: Solid State Phys. 15 L717

(http://iopscience.iop.org/0022-3719/15/22/005)

J. Phys. C: Solid State Phys., **15** (1982) L717–L721. Printed in Great Britain

LETTER TO THE EDITOR

Theory of quantised Hall conductivity in two dimensions

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Received 10 December 1981

Abstract. On the basis of linear response theory, the Hall conductivity is expressed as a sum of two contributions: one corresponding to the classical Drude–Zener formula, and a second which has no classical analogy. The developed theory is applied to the Hall effect, thermopower and thermal conductivity in two-dimensional systems. The periodic potential is taken into account.

Several recent experiments made by von Klitzing, Dorda and Pepper (1980) and by Tsui and Gossard (1981) lead to the remarkable conclusion that the Hall conductivity of a two-dimensional system in its quantum limit is quantised to better than one part in 10^5 to integral multiples of e^2/h. Theoretical explanation of this effect was originally given by the renormalised weak-scattering calculations of Ando (1974). Later, several papers appeared in which the more advanced derivations were presented (Prange 1981, Thouless 1981). Nevertheless all these theories are based on simple model calculations or only particular aspects of the problem are taken into account. The apparent insensitivity of experimental results (von Klitzing *et al* 1980, Tsui and Gossard 1981) to the type or location of impurities and also to the type of the host material suggests that the effect is due to a fundamental principle, especially due to the long-range phase rigidity characteristic of a supercurrent as was pointed out by Laughlin (1981). Since the results are simple and general, the existence of an equilibrium quantity might be intuitively supposed, which would allow us to deduce them in a straightforward manner. In this Letter we shall prove that the Hall conductivity is closely connected to the derivative of the number of electrons with respect to the magnetic field taken at Fermi energy. The thermopower and thermal conductivity will also be discussed.

To derive the expression for the conductivity, we shall use the linear response theory based on the following assumptions:

(i) The electron system can be described as a Fermi–Dirac assembly of independent quasiparticles.

(ii) Only elastic scattering is admissible.

(iii) A two-dimensional solid is formed by a layer in the (x, y) plane and magnetic field $\boldsymbol{B}$ is perpendicular to the layer ($\boldsymbol{B} \equiv (0, 0, B)$).

(iv) There are gaps in the energy spectrum of the one-electron Hamiltonian describing the system

$$H = (1/2m)[\boldsymbol{P} - (e/c)\boldsymbol{A}]^2 + V(x, y) \tag{1}$$

0022-3719/82/220717 + 05 $02.00

where m and e are electron mass and charge respectively, $\boldsymbol{A}$ is the vector potential ($\boldsymbol{B} = \operatorname{curl} \boldsymbol{A}$) and $V(x, y)$ is an arbitrary fixed potential.

(v) An electric field $\boldsymbol{E}$ established in the solid results in an electric current $\boldsymbol{I}$ linearly related to the field through Ohm's law

$$\boldsymbol{I} = \boldsymbol{\sigma E} \tag{2}$$

where $\boldsymbol{\sigma}$ is the conductivity tensor.

Under the above assumptions, the components of the conductivity tensor $\boldsymbol{\sigma}$ are given by the expressions derived for example by Smrčka and Středa (1977):

$$\sigma_{ij}(T) = -\int \frac{\mathrm{d}\rho_0(\eta)}{\mathrm{d}\eta}\,\sigma_{ij}(\eta, 0)\,\mathrm{d}\eta \tag{3}$$

where $\rho_0(\eta)$ is the equilibrium Fermi–Dirac distribution function and $\sigma_{ij}(E_\mathrm{F}, 0)$ are components of the conductivity tensor at zero temperature T (E_F denotes the Fermi energy). The diagonal components are given by the following expression (Kubo *et al* 1965):

$$\sigma_{ii} \equiv \sigma_{ii}(E_\mathrm{F}, 0) = \pi\hbar e^2\,\mathrm{Tr}[v_i\delta(E_\mathrm{F} - H)v_i\,\delta(E_\mathrm{F} - H)] \tag{4}$$

and non-diagonal components by (Bastin *et al* 1971)

$$\sigma_{ij} \equiv \sigma_{ij}(E_\mathrm{F}, 0) = e^2\int_{-\infty}^{E_\mathrm{F}} A_{ij}(\eta)\,\mathrm{d}\eta \tag{5}$$

$$A_{ij}(\eta) = \mathrm{i}\hbar\,\mathrm{Tr}[v_i(\mathrm{d}G^+/\mathrm{d}\eta)\,v_j\delta(\eta - H) - v_i\delta(\eta - H)\,v_j\,\mathrm{d}G^-/\mathrm{d}\eta] \tag{6}$$

where the Green function is defined by

$$G^\pm(\eta) = (\eta - H \pm \mathrm{i}0)^{-1} \qquad \delta(\eta - H) = -\frac{1}{2\pi\mathrm{i}}(G^+ - G^-) \tag{7}$$

and velocity operator is given by the commutation relation

$$v_i = \frac{1}{\mathrm{i}\hbar}[r_i, H] = -\frac{1}{\mathrm{i}\hbar}[r_i, G^{-1}] = \frac{1}{m}\left(p_i - \frac{e}{c}A_i\right). \tag{8}$$

To proceed further we split the Hall conductivity into two parts using an expression originally derived by Smrčka and Středa (1977):

$$A_{ij}(\eta) = \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}\eta}B_{ij}(\eta) + \frac{1}{2}\,\mathrm{Tr}\,\frac{\mathrm{d}\delta(\eta - H)}{\mathrm{d}\eta}(r_iv_j - r_jv_i) \tag{9}$$

$$B_{ij}(\eta) = \mathrm{i}\hbar\,\mathrm{Tr}[v_iG^+(\eta)v_j\delta(\eta - H) - v_i\delta(\eta - H)v_jG^-(\eta)]. \tag{10}$$

The second term on the right-hand side of equation (9) can be rewritten into the more convenient form

$$\frac{1}{2}\,\mathrm{Tr}\,\frac{\mathrm{d}\delta(\eta - H)}{\mathrm{d}\eta}(r_xv_y - r_yv_x) = \frac{c}{e}\frac{\partial}{\partial B}\,\mathrm{Tr}\,\delta(\eta - H) \tag{11}$$

if the definition of the Hamiltonian (1), the expression (8) and commutation relation

$$[r_x, v_y] = [r_y, v_x] = 0$$

are used. The expression (11) is valid for arbitrary choices of vector potential $\boldsymbol{A}$, nevertheless the simplest derivation is obtained if the circular gauge centred at the origin is

used; $\boldsymbol{A} \equiv \frac{1}{2}B(-y, x, 0)$. Introducing expressions (6), (9) and (11) into (5) we get immediately useful expression for the Hall conductivity

$$\begin{aligned} \sigma_{ij} &\equiv \sigma_{ij}^{\mathrm{I}} + \sigma_{ij}^{\mathrm{II}} \\ \sigma_{ij}^{\mathrm{I}} &= \frac{e^2}{2} \mathrm{i}\hbar \,\mathrm{Tr}[v_i G^+(E_\mathrm{F}) v_j \delta(E_\mathrm{F} - H) - v_i \delta(E_\mathrm{F} - H) v_j G^-(E_\mathrm{F})] \\ \sigma_{xy}^{\mathrm{II}} &= -\sigma_{yx}^{\mathrm{II}} = ec \frac{\partial N(E)}{\partial B}\bigg|_{E=E_\mathrm{F}} \end{aligned} \tag{12}$$

where $N(E)$ is the number of states below the energy E defined by

$$N(E) = \int_{-\infty}^{E} \mathrm{Tr}\, \delta(\eta - H)\, \mathrm{d}\eta \tag{13}$$

and the derivative with respect to the magnetic field B is taken at the Fermi energy.

The formula (12) satisfies the Onsager relations and is valid for the two-dimensional layer as well as for the three-dimensional substances.

The first term σ_{xy}^{I} depends on the structure of solid, crystallographic orientation and of course on the potential $V(\boldsymbol{r})$. The free electron model with arbitrary energy-dependent self-energy $\Sigma(E)$ leads to the classical Drude–Zener result if the vertex corrections are omitted:

$$\sigma_{xy}^{\mathrm{I}} = -\omega\tau\sigma_{xx} \tag{14}$$

where $\omega = |e|B/mc$ is the cyclotron frequency; the lifetime τ is equal to $\hbar/2\Gamma$ ($\Gamma = -\mathrm{Im}\,\Sigma(E_\mathrm{F})$).

The second term $\sigma_{xy}^{\mathrm{II}}$ has no classical analogy. In the classical limit the density of states is not a field-dependent quantity and $\sigma_{xy}^{\mathrm{II}}$ vanishes. The results for the free-electron model were obtained earlier (Středa and Smrčka 1975). Generally, $\sigma_{xy}^{\mathrm{II}}$ depends on material constants only through the number of particles. It does not depend on the crystallographic orientation and the type of scattering.

The general formulae (4) and (12) will be used to explain quantised Hall effect in the two-dimensional system. Since the influence of the bound states was recently extensively studied (Prange 1981, Thouless 1981) we shall concentrate our attention mainly on the influence of the periodic potential. According to Baraff and Tsui (1981) we shall suppose that ionised donors outside the layer serve as a reservoir of electrons. This reservoir which can produce the plateaus in the oscillations of conductivity does not contribute to the density of electron states in the two-dimensional layer.

To derive the expression for the quantised Hall conductivity, we shall employ the assumption (iv) mentioned above, namely that there are gaps in the electron energy spectrum in the magnetic field and that the Fermi energy is lying just within a gap, where the density of states is zero. Since δ functions in expressions (4) and (12) describe contributions to the density at Fermi energy, diagonal elements of the conductivity tensor σ and the classical term of the Hall conductivity σ_{xy}^{I} are equal to zero and we get

$$\sigma_{xx} = \sigma_{yy} = 0, \qquad \sigma_{xy} = -\sigma_{yx} = ec(\partial N(E)/\partial B)|_{E=E_\mathrm{F}}. \tag{15}$$

For simplicity, we limit ourselves to one electron band and to the so-called 'rational' magnetic field, namely

$$\frac{|e|}{hc} \boldsymbol{B} \cdot \boldsymbol{a}_1 \times \boldsymbol{a}_2 = \frac{1}{J} \tag{16}$$

where $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$ are elementary lattice vectors and J is an integer. The electron energy structure of this system is well described for example by Rabinovitch (1969). The one-electron band is separated into J narrow bands (Landau levels) with $(J^2|\boldsymbol{a}_1 \times \boldsymbol{a}_2|)^{-1}$ states. Each state is J-times degenerate. The Landau levels are very narrow and well separated at the periphery of the electron band and broadening is increased as the centre is approached. The width of gaps is rising with increasing field intensity. Any impurities and deformations cannot change the number of states at a single Landau level without the disappearance of the gap.

We should like to point out that the limitation imposed by condition (16) to the field intensities is not essential. For example, in the case of a two-dimensional interface of $GaAs–Al_xGa_{1-x}As$ heterojunctions, J approximately equals 4000 at magnetic field 10 T. The change of J by one corresponds to the change of B by 0.0025 T. The points selected by the condition (16) form quite a dense quasicontinuum at least near the edges of an electron band. Moreover, the density of states corresponding to the 'rational' field (16) is numerically indistinguishable from that of a slightly different field which does not fulfil equation (16), although very different analytically (Wannier *et al* 1979).

Let us suppose that n narrow bands are lying below E_F. Since the magnetic field is supposed to be perpendicular to the two-dimensional layer, the number of states is given by

$$N = n \frac{1}{J^2|\boldsymbol{a}_1 \times \boldsymbol{a}_2|} J = n \frac{|e|}{hc} B. \tag{17}$$

At the bottom of the band, where broad gaps exist, the small changes in magnetic field do not change the number of Landau levels below Fermi energy and we get

$$\sigma_{xy} = -\frac{e^2}{h} n \tag{18}$$

using expressions (15) and (17). This is the result of recent experiments (von Klitzing *et al* 1980, Tsui and Gossard 1981) and can also be obtained for free electrons in a magnetic field (Ando 1974, Laughlin 1981). If the band is fully occupied, the number of states with and without magnetic field coincides and the Hall conductivity is just zero as expected. For the nearly occupied band the expression for the hole Hall conductivity is obtained:

$$\sigma_{xy}^{(h)} = \frac{e^2}{h} n \tag{19}$$

where n is now the number of empty Landau levels.

From the theoretical point of view the very interesting region is the middle of the band, where also open orbits exist. In this region the change of the magnetic field from one rational value to another can change the number of Landau levels below the Fermi energy, and simple arguments leading to expressions (18) and (19) are no longer valid. This problem will be treated in a separate paper.

The other transport coefficients also have interesting features. The thermopower S and the electronic part of the thermal conductivity K are given by following expressions

$$S = (1/T)(L_{12}L_{11}^{-1} - (E_F/e)\,\mathbf{1}) \tag{20}$$

$$K = (1/T)(L_{22} - L_{21}L_{11}^{-1}L_{12}) \tag{21}$$

where L_{ij} are the phenomenological transport coefficients (for definition see e.g. Smrčka

and Středa 1977) and **1** denotes the identity matrix. The assumptions mentioned at the beginning of this Letter lead to the expressions derived by Smrčka and Středa (1977):

$$L_{11} = \sigma \qquad L_{12} = (E_F/e)\sigma \qquad L_{22} = (E_F/e)^2\sigma. \tag{22}$$

Substituting equation (22) into equations (20) and (21) we arrive, after some algebra, at the conclusion that all components of both tensors S and K are equal to zero. This formal result reflects the obvious fact that no thermal gradient can be established in the electron gas when the Fermi energy is lying within a gap. Note also that this is the missing thermopower which makes it possible to measure the Hall voltage with unusually high accuracy.

The presented new expression (12) for the Hall conductivity is quite general and it is composed of two parts: the term σ_{xy}^{I} which corresponds to the classical expression and the purely quantum contribution σ_{xy}^{II}. It should be stressed here that it differs substantially from the well known expression derived by Kubo *et al* (1965), where the motion of centres of orbits and the relative motion of electrons are described by separate terms. Their approach can be successfully applied, e.g. in the case of closed orbits, but on the other hand it cannot explain in a simple way why a fully occupied band does not give any Hall current. It is also difficult to apply in the quasiclassical limit of weak magnetic fields.

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