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Conductivity and thermopower of 2D Bloch electrons in magnetic fields with electron–phonon instabilities

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Abstract. The anomalies in the conductivity and thermopower associated with the charge-density-wave instabilities of 2D Bloch electrons in magnetic fields are studied. It is assumed that the electrons are scattered elastically by randomly distributed impurities. The minimum of the conductivity σ_{xx} and the maximum of the thermopower Q_{xx} are split into several minima and maxima in the same way as the Van Hove singularities after the lattice distortion takes place. If the electron scattering is anisotropic (low angle) the results are essentially the same as in the case of isotropic scattering, with the only difference being that σ_{xx} is multiplied by a large factor.

It has been shown in [1] that a system of two-dimensional electrons moving in a square lattice potential subject to a perpendicular magnetic field may undergo a periodic lattice distortion if the chemical potential μ is close to a Van Hove singularity of the density of states (situated at $\mu = 0$). The distortion affects the spectrum by shifting the energy of the saddle points of the electron dispersion relation $\varepsilon(k)$ in opposite directions causing the originally coincident logarithmic peaks of the density of states to split apart. A topological transition of the Fermi surface will also take place since an initially closed (open) Fermi surface may become open (closed) in the vicinity of a saddle point when the energy of the latter decreases (increases). It is then expected that such a transition will be associated with anomalies in the behaviour of the transport coefficients, namely the conductivity and the thermopower, as the chemical potential is varied in the vicinity of the Van Hove singularities. This paper is addressed to the study of this phenomenon.

It is assumed that the electrons are elastically scattered by randomly distributed inpurities. In the undistorted system the conductivity σ_{xx} has a minimum as $\mu \to 0$, $\sigma_{xx} \propto 1/\log|\mu|$, and the thermopower approaches a maximum $Q_{xx} \propto 1/\mu \log|\mu|$. In the distorted system the minima of σ_{xx} and the maxima of Q_{xx} are displaced to the positions of the Van Hove singularities. Curiously, the functional dependence of these quantities on μ is almost independent of whether the electron scattering by the impurities is assumed to be isotropic or anisotropic (low-angle scattering). As shown below, this is because the most important contribution for the conductivity comes from the electrons in the regions of the Fermi surface that are far from the saddle points. If the scattering is anisotropic, the inverse of the relaxation time $(1/\tau_{tr})$ in the kinetic (Boltzmann) equation still contains the contribution $\propto \log|\mu|$ (dominant as $\mu \to 0$) coming from the saddle points, simply affected by a small factor because the probability of scattering of these electrons into the the vicinity of the saddle points is small.

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In what follows, and just for the sake of definiteness, the magnetic field flux per unit cell will be set equal to half of the flux quantum ($hc/|e|$).

In the framework of linear response theory the electrical current j is related to the electric field E and temperature gradient by the tensors σ and β:

$$j = \sigma E + \beta \nabla T \tag{1}$$

with

$$\beta = -\frac{1}{eT}\int \left(-\frac{\partial f}{\partial \varepsilon}\right)(\varepsilon - \mu)\sigma(\varepsilon)\, \mathrm{d}\varepsilon \tag{2}$$

where $f(\varepsilon)$ is the Fermi–Dirac distribution function, and $\sigma(\varepsilon)$ denotes the conductivity tensor at zero temperature and chemical potential ε [2]. The component Q_{xx} of the thermoelectric tensor $Q = (1/\sigma)\beta$ is

$$Q_{xx} = \frac{\sigma_{xy}\beta_{yx} - \sigma_{yy}\beta_{xx}}{\sigma_{xy}\sigma_{yx} - \sigma_{xx}\sigma_{yy}}. \tag{3}$$

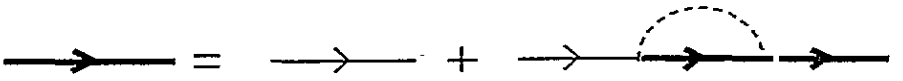

Figure 1. The self-consistent Born approximation for the electron Green's function $G = (E - H + \mathrm{i}0)^{-1}$. The thick lines represent the Green's function averaged over impurity configurations. The impurity line (dashed) is associated with a factor of $2\pi l^2\Gamma_0^2$.

As discussed in [1], the Fermi surface of the electron system before the distortion takes place has two equal sheets and passes near the saddle points at which the dispersion relation may be written as

$$\varepsilon(k) = \frac{\hbar^2}{2m_-}\Delta k_x{}^2 + \frac{\hbar^2}{2m_+}\Delta k_y{}^2 \qquad \varepsilon(k) = \frac{\hbar^2}{2m_+}\Delta k_x{}^2 + \frac{\hbar^2}{2m_-}\Delta k_y{}^2$$

with the effective masses $m_+ > 0$ and $m_- < 0$. Δk measures the departure from the saddle points. The density of states is then given by

$$D(E) = \frac{\sqrt{-m_+m_-}}{\pi^2\hbar^2}\log\left|\frac{W}{E}\right| \tag{4}$$

where W is of the order of the bandwidth. The transport coefficients will be calculated for values of the chemical potential at which the density of states is given by equation (4). Owing to the disorder, the logarithmic form of the density of states is destroyed for energies too close to zero. The validity of equation (4) can be studied by considering the imaginary part ($\Sigma''(E)$) of the self-energy ($\Sigma(E) = \Sigma'(E) + \mathrm{i}\Sigma''(E)$) of an electron moving in a random potential. In the self-consistent Born approximation, expressed in figure 1, Σ'' is obtained from the relation [3]

$$\frac{2\pi}{l^2\Gamma_0^2} = \sum_n \int \mathrm{d}^2k\, \frac{1}{(E - \varepsilon_n(k) - \Sigma'(E))^2 + (\Sigma''(E))^2} \tag{5}$$

where the index n denotes the Bloch band, l is the magnetic length and Γ_0 is an energy characterizing the strength of disorder. If there was no periodic potential, equation (5) would predict a Landau level broadening of $4\Gamma_0$ [4]. Since our aim is to study the singular part of the density of states, with E inside a certain band, the sum over n may be discarded. Replacing the integral over k by an integral over energy, equation (5) may be re written as

$$\frac{1}{2\pi l^2\Gamma_0^2} \simeq \frac{2\sqrt{-m_+m_-}}{\pi^2\hbar^2}\int_{-W}^{W} \mathrm{d}\varepsilon \frac{\log|W/\varepsilon|}{(E - \varepsilon - \Sigma'(E))^2 + (\Sigma''(E))^2}.$$

For weak enough disorder, $\Sigma''(E) \ll W$ and the limits of integration can be extended to infinity. The result is

$$\frac{|\Sigma''|}{2\pi l^2 {\Gamma_0}^2} = \frac{\sqrt{-m_+m_-}}{\pi^2\hbar^2} \log \frac{W^2}{(E - \Sigma'(E))^2 + (\Sigma''(E))^2}.$$

Since [3]

$$D(E) = \frac{|\Sigma''(E)|}{2\pi^2 l^2 {\Gamma_0}^2}$$

equation (4) is recovered when $\Sigma''(E) \ll E$ or, equivalently,

$$\frac{|E|}{W} \gg \left(\frac{\Gamma_0}{W}\right)^2 \log \frac{W}{|E|} \tag{6}$$

where $W \simeq \hbar^2/l^2\sqrt{-m_+m_-}$ was used. Since we need the logarithm to be large, this may be viewed as a condition for weak disorder. Similarly, the density of states of the distorted system is

$$D(E) = \frac{\sqrt{-m_+m_-}}{\pi^2\hbar^2} \left(\log \frac{W}{|E - v|} + \log \frac{W}{|E + v|}\right) \tag{7}$$

as long as E stays sufficiently far from each of the peaks (the condition is the same as equation (6) with E replaced by $E \pm v$) [5].

The conductivity of Bloch electrons in a magnetic field as given by the Kubo formula has two contributions $\sigma = \Delta\sigma + \sigma^s$ [3]. The 'intra-band' conductivity $\Delta\sigma$ vanishes if $W \to 0$ and diverges as $\Gamma_0 \to 0$. Since it involves only the matrix elements of the velocity operator between states in the same Bloch band, it is analogous to the conductivity of Bloch electrons in the absence of magnetic field. The 'inter-band' conductivity σ^s_{xx} involves matrix elements of the velocity operator between different bands. It remains finite as $W \to 0$ and its diagonal component σ^s_{xx} vanishes as $\Gamma_0 \to 0$. An estimation of σ^s_{xx} based on the Kubo formula shows that $\sigma^s_{xx} \ll \Delta\sigma_{xx}$ if the condition (6) is satisfied and, for that reason, it may be neglected.

The band conductivity may be obtained from the Boltzmann equation [6]:

$$\Delta\sigma_{xx} = \frac{e^2}{(2\pi)^2} \int d^2k \left(-\frac{\partial f}{\partial\varepsilon(k)}\right) v_x^2 \tau_{tr}(k) = \frac{e^2}{(2\pi)^2} \oint \frac{d\zeta_k}{|\nabla_k \varepsilon|} v_x^2 \tau_{tr} \tag{8}$$

where $d\zeta_k$ denotes the line element along the Fermi surface, $v_x = \partial\varepsilon(k)/\partial k_x$ and the approximation $\partial f/\partial\varepsilon = \delta(\varepsilon - \mu)$ was used. The relaxation time is given by

$$\frac{1}{\tau_{tr}(k)} = \frac{1}{2\pi\hbar} \oint \frac{d\zeta_k}{|\nabla_k \varepsilon|} (1 - \cos\theta_{k,k'}) \, |V_{k,k'}|^2 \tag{9}$$

where $\theta_{k,k'}$ is the angle between the vectors k and k'.

If the scattering is isotropic, the square of the matrix element of the random potential between k-states is a constant $|V_{k,k'}|^2 = u^2$ (with $u^2 = 2\pi l^2 \Gamma_0^2$) and $\tau_{tr}(k)$ becomes essentially independent of k. Before the lattice distortion takes place we have

$$\frac{1}{\tau_{tr}} = \frac{4u^2\sqrt{-m_+m_-}}{\pi\hbar^3} \log \frac{W}{|\mu|}. \tag{10}$$

Consequently, equation (8) gives

$$\Delta\sigma_{xx} \simeq \sigma_{xx} \simeq \frac{e^2\hbar W}{2\pi u^2} \left(\frac{1}{m_+} - \frac{1}{m_-}\right) \frac{1}{\log(W/|\mu|)}. \tag{11}$$

Using $u^2 = 2\pi l^2 \Gamma_0^2$ and $W \simeq \hbar^2/l^2\sqrt{-m_+m_-}$ together with the condition (6) it is easy to see that

$$\sigma_{xx} \gg \frac{e^2}{\hbar}\frac{W}{|\mu|}. \tag{12}$$

As the chemical potential is swept through the Bloch bands the non-diagonal conductivity σ_{xy} interpolates smoothly between the quantized values that occur when the bands are completely filled [3, 7]. Therefore, σ_{xy} is always of the order of $e^2/\hbar$ and, in view of equation (12), we assume $\sigma_{xx} \gg \sigma_{xy}$. From equations (2) and (3) it is seen that Q_{xx} may be calculated from the Mott relation:

$$Q_{xx} \simeq \frac{\pi^2 T}{3\,e}\frac{\mathrm{d}}{\mathrm{d}\mu}\log\sigma_{xx} = \frac{\pi^2 T}{3\,e}\frac{1}{\mu\log(W/|\mu|)}. \tag{13}$$

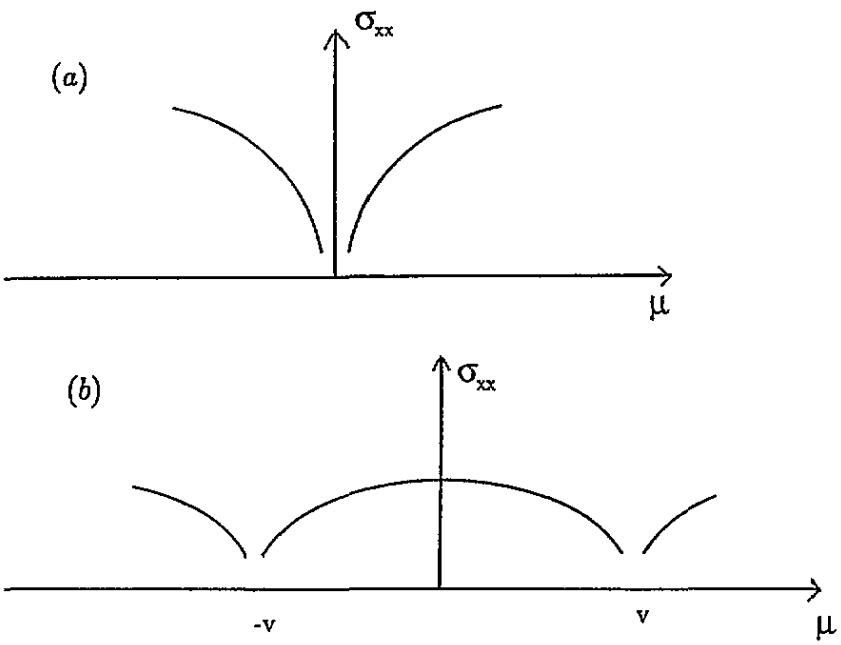

Figure 2. Conductivity with (*a*) and without (*b*) lattice distortion as a function of the chemical potential. v and $-v$ denote the positions of the Van Hove singularities in (*b*)

The result expressed in equation (11) may be understood from the following argument. The term $|\nabla_k \varepsilon|^{-1}$ contributes with a logarithmic singularity to the line integral in equation (8) in the regions close to the saddle points. But this singularity is suppressed by the term $v_x^2(k)$ which tends to zero in those regions. Then

$$\Delta\sigma_{xx} \propto e^2 \nu_{\mathrm{reg}} \langle v_x^2 \rangle \tau_{\mathrm{tr}} \tag{14}$$

where ν_{reg} is just the regular part of the density of states. The singular contribution to $\Delta\sigma_{xx}$ comes from τ_{tr}, which is proportional to the inverse of the density of states. This reasoning was applied before to three-dimensional systems in the context of electronic topological (Lifshitz) transitions [8, 9, 10, 11].

Considering the case of anisotropic (low-angle) scattering, we assume that large momentum transfers between the electrons and the inpurities have exponentially small

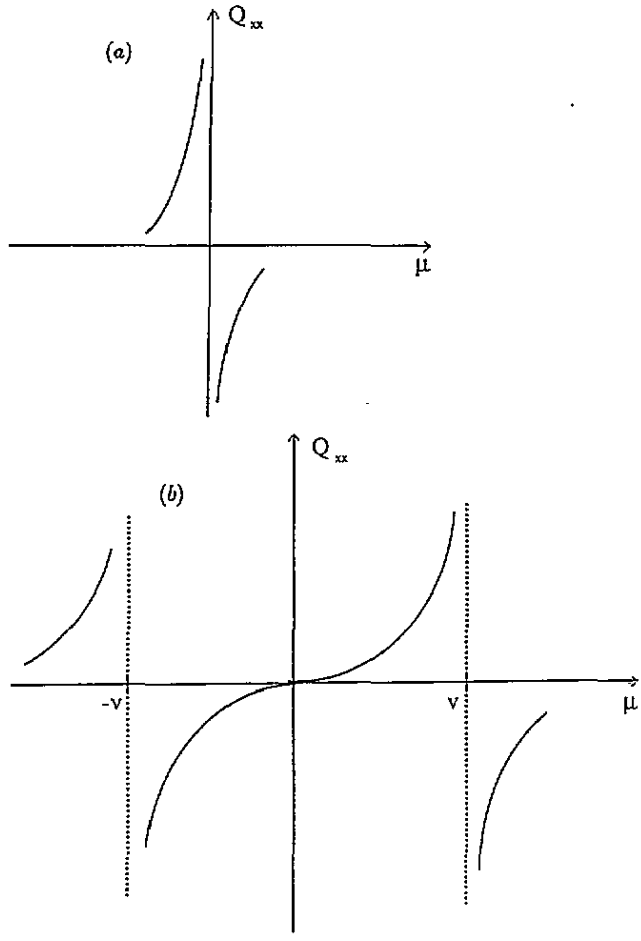

Figure 3. Thermopower with (*a*) and without (*b*) lattice distortion as a function of the chemical potential.

probability. Such a situation arises, in particular, if the scattering centres are situated far from the plane of the electrons [12]. This means that the scattering matrix element in equation (9) can be put as $|V_{k,k'}|^2 = u^2 \exp(-\rho|k-k'|)$:

$$\frac{1}{\tau_{\rm tr}(k)} = \frac{u^2}{2\pi\hbar} \oint \frac{{\rm d}\zeta_{k'}}{|\nabla_{k'}\varepsilon|} (1 - \cos\theta_{k,k'}) {\rm e}^{-\rho|k-k'|}. \tag{15}$$

If k points towards a saddle point then $1 - \cos\theta_{k,k'} \simeq \frac{1}{2}\theta^2_{k,k'}$ for k' close to k and the exponential introduces a cut-off for the contribution of that saddle point. The factor $\theta^2_{k,k'}$ suppresses the singularity in $|\nabla_{k'}\varepsilon|^{-1}$, so this saddle point does not contribute with any singular dependence on μ. Nevertheless, the saddle points for which $\theta_{k,k'} = \pm\pi/2$ and $\theta_{k,k'} = \pi$ still contribute with $\log(W/|\mu|)$ multiplied by a factor $\exp(\approx -\rho k_{\rm F})$ where $k_{\rm F}$ is the Fermi momentum (the size of the Brillouin zone in this case). Such a contribution still exists when k is in the regions of the Brillouin zone far from any saddle points. Thus the transport relaxation time becomes exponentially larger since the scattering probability into the regions that give the dominant contribution ($\log(W/|\mu|)$) is exponentially smaller. In view of the largeness of the logarithm, the conductivity is still given by equation (11)

multiplied by an exponentially large factor and the result in equation (13) remains, therefore, essentially unaffected.

When the lattice distortion occurs, the calculation of σ_{xx} and Q_{xx} is extremely similar to what has been explained above, but the density of states is now given by equation (7). The results (11) and (13) are replaced by

$$\sigma_{xx} = \frac{e^2\hbar W}{\pi\ u^2}\left(\frac{1}{m_+} - \frac{1}{m_-}\right)\ \frac{1}{\log(W/|\mu - v|) + \log(W/|\mu + v|)} \tag{16}$$

$$Q_{xx} = \frac{\pi^2 T}{3\ e}\left(\frac{1}{\mu - v} + \frac{1}{\mu + v}\right)\ \frac{1}{\log(W/|\mu - v|) + \log(W/|\mu + v|)} \tag{17}$$

respectively. A qualitative plot of these results is shown in figures 2 and 3. It is seen that the minima of σ_{xx} and the maxima of Q_{xx} follow the Van Hove singularities as they are split by the lattice distortion. The effect of finite T in the Boltzmann equation (8) is just partially to smear out these features. It must be kept in mind that v depends on temperature as well as on μ, attaining, for fixed T, its largest value at $\mu = 0$. In view of the collision broadening of the logarithmic singularities (in addition to the finite-temperature effects) both σ_{xx} and Q_{xx} remain finite as $\mu \to 0$.

In the case of arbitrary rational flux per unit cell, the initial logarithmic peak is split into various singularities by the lattice distortion. The denominator in equation (16) is then replaced by the sum of these singularities and the appropriate changes must be made in equation (17).

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