

Lecture notes: semiclassical dynamics and kinetic theory

Léo Mangeolle

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References

Textbooks:

- J. Ziman, *Electrons and Phonons: The Theory of Transport Phenomena in Solids*.
A very detailed, most deep, quite pedagogical and sometimes humorous textbook covering most of sections I, II, III and part of section IV of this course.
- N. Pottier, *Nonequilibrium Statistical Physics: Linear Irreversible Processes*.
A very pedagogical book, with a mostly classical and thermodynamical focus, which can be useful to understand sections I, II, III as well as some of the implicit prerequisites of this course.
- R. Peierls' *Quantum theory of solids* and E. Lifshitz & L. Pitaevskii's *Physical kinetics* are always good references to be able to cite religiously in a conversation with educated people.
- A. Kamenev, *Field Theory of Non-Equilibrium Systems*, and J. Rammer, *Quantum field theory of non-equilibrium states* are useful references for the general field theory methods hinted at in section VI.
These are modernized and updated versions of Kadanoff & Baym's *Quantum statistical mechanics*.

Review papers:

- D. Xiao, M. Chang and Q. Niu, *Berry phase effects on electronic properties*. A review of topology in semiclassical dynamics with lots of references and ramifications, which covers parts of section V.
- N. Sinitsyn, *Semiclassical theories of the anomalous Hall effect*. A general, theory-oriented review which discusses various topological effects in combination with scattering, useful for section V.
- J. Rammer and H. Smith, *Quantum field-theoretical methods in transport theory of metals*. A quite pedagogical review which predates the field theory books mentioned above.
- L. Fritz and T. Scaffidi, *Hydrodynamic electronic transport*. A recent, very easy to read and fairly hand-waving review paper upon which part of section IV is based.

Introduction

Kinetic theory has played an important role in the development of modern physics, by providing an appropriate mathematical framework to describe the emergence of thermodynamic quantities (temperature, pressure, flow velocity, etc) out of the individual properties of a huge number of elementary constituents (molecules, atoms, etc) away from equilibrium. While this theory applied originally to gases and liquids, which it describes as an ensemble of molecules governed by the laws of *classical* mechanics, it was soon applied with tremendous success to solid state physics, where it describes properties now emerging from an assembly of *quantum* particles which behave very non-classically – electrons in metals would not do much were it not for Pauli exclusion, and phonons are non-conserved bosons which keep appearing and disappearing all the time. Yet kinetic theory, and its core engine Boltzmann's equation, seems to describe very well all sorts of classical and quantum systems, basically as long as there are particles to be described. This lecture aims at illustrating which uses can be made of Boltzmann's equation in the context of solid state physics, and we will see how it can be complemented by quantum corrections to describe some very quantum phenomena. But since this equation was derived from, and first applied to, classical physics, let us start from there.

1 Physical structure of Boltzmann's kinetic theory

In this section, we introduce the Boltzmann equation as a description of the statistical properties of a gas of classical particles governed by hamiltonian mechanics. We discuss the meaning of equilibrium, local equilibrium and detailed balance, and the emergence of thermodynamics and irreversibility. We show how the latter can be understood mathematically as a manifestation of a variational principle obeyed by Boltzmann's equation.

1.1 From Liouville to Boltzmann

Let us start with a system of N classical, possibly interacting particles. Their classical density in $6N$ -dimensional phase space is $f_N(r_i, p_i, t)$, a function of $6N + 1$ variables normalized such that $\int \prod_{i=1}^N d^3r_i d^3p_i f_N = 1 \forall t$. Because f_N is a globally conserved quantity, it satisfies a conservation equation:

$$\partial_t f_N + \partial_{\mathbf{r}_i}(\dot{\mathbf{r}}_i f_N) + \partial_{\mathbf{p}_i}(\dot{\mathbf{p}}_i f_N) = 0, \quad (1)$$

where summation over $i = 1..N$ is implicit. Since the system of N particles obeys the classical laws of mechanics, namely Hamilton's equations $\dot{\mathbf{p}}_i = -\partial_{\mathbf{r}_i} H$ and $\dot{\mathbf{r}}_i = \partial_{\mathbf{p}_i} H$ with H the hamiltonian, one gets a simplification and the conservation equation takes the form

$$\partial_t f_N + \dot{\mathbf{r}}_i \partial_{\mathbf{r}_i} f_N + \dot{\mathbf{p}}_i \partial_{\mathbf{p}_i} f_N = 0 \quad (2)$$

which is the statement of Liouville's theorem, $\partial_t f_N + \{f_N, H\} = 0$, where $\{\cdot, \cdot\}$ are Poisson brackets.

The above equation is a complicated many-body problem. We could be happy with finding a stationary solution, i.e. with $\partial_t f_N = 0$: it is then clear that any $f_N(r_i, p_i)$ function of $H(r_i, p_i)$ will be a solution, because its Poisson bracket with H would straightforwardly vanish. For instance we would like to choose $f_N \propto e^{-\beta H}$, which is the natural solution that comes from thermalization. This, however, is not satisfactory for at least two reasons. First, fundamentally, why should one choose this solution instead of any other? There must be some extra assumptions about the system and the form of $H(r_i, p_i)$ which make this solution "more plausible" than others, in some sense yet to be defined. Second, practically, H is a function of $6N$ variables which is a very large number, so this solution is anyway useless in practice.

Instead, the idea is to reduce the problem to an effective one-particle equation for the one-particle reduced density

$$f_1(r_1, p_1, t) = N \int \prod_{i=2}^N d^3r_i d^3p_i f_N(r_i, p_i, t), \quad (3)$$

which now is a function of only $6 + 1$ variables, normalized such that $\int d^3r_1 d^3p_1 f_1 = 1 \forall t$. By integrating Liouville's equation we obtain

$$\partial_t f_1 = N \int \prod_{i=2}^N d^3r_i d^3p_i \partial_t f_N = N \int \prod_{i=2}^N d^3r_i d^3p_i \{H, f_N\}. \quad (4)$$

The rhs is in fact very simple because, upon integration by parts (ibp), all the terms with derivatives wrt r_i, p_i for $i \geq 2$ cancel against each other (if the integration also included $i = 1$, note this ibp-induced cancellation would ensure the global conservation of probability, $\partial_t 1 = 0$). Only the $i = 1$ Poisson bracket remains, and we have

$$\partial_t f_1 = N \int \prod_{i=2}^N d^3r_i d^3p_i (\partial_{\mathbf{r}_1} H \partial_{\mathbf{p}_1} f_N - \partial_{\mathbf{p}_1} H \partial_{\mathbf{r}_1} f_N). \quad (5)$$

Now let us write $H = H_1 + H'$ where $H_1(\{r_i\}, \{p_i\}) = \sum_j h_1(r_j, p_j)$ is the free part (h_1 being a function of only 6 variables), and H' is the interaction part. This leads us to Boltzmann's equation:

$$\boxed{(\partial_t + \mathbf{v} \cdot \partial_{\mathbf{r}_1} + \boldsymbol{\xi} \cdot \partial_{\mathbf{p}_1}) f_1(r_1, p_1, t) = (d_t f_1)_{\text{coll}}(r_1, p_1, t)} \quad (6)$$

where $\mathbf{v} = \partial_{\mathbf{p}_1} h_1$ is the one-particle velocity, $\boldsymbol{\xi} = -\partial_{\mathbf{r}_1} h_1$ is the one-particle force, and the right-hand side,

$$(\mathrm{d}_t f_1)_{\mathrm{coll}} = N \int \prod_{i=2}^N \mathrm{d}^3 r_i \mathrm{d}^3 p_i \{H', f_N\} = N \int \prod_{i=2}^N \mathrm{d}^3 r_i \mathrm{d}^3 p_i (\partial_{\mathbf{r}_1} H' \partial_{\mathbf{p}_1} f_N - \partial_{\mathbf{p}_1} H' \partial_{\mathbf{r}_1} f_N) \quad (7)$$

is the collision integral, which accounts for the effect of particle interactions. Here we can claim at least a partial victory, because we have separated the one-particle semiclassical dynamics (lhs) from the many-body interactions (rhs). This is not yet fully satisfactory, though, because this is not yet a closed equation for f_1 , as the rhs still depends on f_N the full density for the whole system. This could be expected, since until now all our manipulations were *exact*. Now we will make some approximations.

Let us consider that H' contains only two-body interactions, which we will describe as local two-particle collisions with a rate $\Gamma(p'_1, p'_2 | p_1, p_2)$ of transition from momenta $(p_1, p_2) \mapsto (p'_1, p'_2)$. This allows us to write

$$(\mathrm{d}_t f_1)_{\mathrm{coll}}(p_1) = \int \mathrm{d}^3 p_2 \mathrm{d}^3 p'_1 \mathrm{d}^3 p'_2 [\Gamma(p_1, p_2 | p'_1, p'_2) f_2(r, p'_1, r, p'_2) - \Gamma(p'_1, p'_2 | p_1, p_2) f_2(r, p_1, r, p_2)], \quad (8)$$

where $f_2 = N(N-1) \int \prod_{i=3}^N \mathrm{d}^3 r_i \mathrm{d}^3 p_i f_N(r_i, p_i, t)$ is the two-particle reduced density function. The problem is not yet closed: to compute f_1 we need f_2 ; now to compute f_2 we can again integrate Liouville's equation over phase space variables $i \geq 3$ and see that we need f_3 ; etc. We need to truncate this series (the ‘‘BBGKY hierarchy’’) at some order. Let's do it at order one: we can assume

$$f_2(r, p_1, r, p_2) \approx f_1(r, p_1) f_1(r, p_2) \quad (9)$$

which is called the molecular chaos assumption. A comment about this later, when we discuss the second law of thermodynamics.

Although it is not needed to close the problem, we can assume that the collision rates satisfy the ‘‘micro-reversibility property’’,

$$\Gamma(p_1, p_2 | p'_1, p'_2) = \Gamma(p'_1, p'_2 | p_1, p_2), \quad (10)$$

which for instance is necessarily true if both inversion and time reversal are symmetries of the system.

With this necessary truncation and this simplifying assumption, and dropping the index $f_1 \equiv f$, we obtain:

$$(\partial_t + \mathbf{v} \cdot \partial_{\mathbf{r}} + \boldsymbol{\xi} \cdot \partial_{\mathbf{p}_1}) f(r, p_1, t) = \int \mathrm{d}^3 p_2 \mathrm{d}^3 p'_1 \mathrm{d}^3 p'_2 \Gamma(p_1, p_2 | p'_1, p'_2) [f(r, p'_1) f(r, p'_2) - f(r, p_1) f(r, p_2)], \quad (11)$$

which is the historical form of Boltzmann's equation for a system of classical particles with two-body interactions.

The molecular chaos assumption means that the statistics of collisions depends solely from the state of the system before a collision event, but not after. Now, for quantum particles (bosons or fermions) the population factors should really be thought of as $\langle a_{\mathbf{p}}^\dagger a_{\mathbf{p}} \rangle$ for incoming particles and $\langle a_{\mathbf{p}} a_{\mathbf{p}}^\dagger \rangle$ for outgoing ones, instead of $f_{\mathbf{p}}$ for incoming and 1 for outgoing. Thus the collision integral reads

$$\begin{aligned} (\partial_t + \mathbf{v} \cdot \partial_{\mathbf{r}} + \boldsymbol{\xi} \cdot \partial_{\mathbf{p}_1}) f(r, p_1, t) = & \int \mathrm{d}^3 p_2 \mathrm{d}^3 p'_1 \mathrm{d}^3 p'_2 \Gamma(p_1, p_2 | p'_1, p'_2) \\ & \times \left(f(r, p'_1) f(r, p'_2) [1 \mp f(r, p_1)] [1 \mp f(r, p_2)] - f(r, p_1) f(r, p_2) [1 \mp f(r, p'_1)] [1 \mp f(r, p'_2)] \right), \end{aligned} \quad (12)$$

where $+$ is for bosons and $-$ for fermions. The interpretation as a Bose/Fermi enhancing/blocking factor is straightforward. In this section we will still mostly discuss the classical particle gas, and deal with the fermionic and bosonic cases in the next sections.

1.2 Local equilibrium and detailed balance

A *stationary* solution to our problem is a function f such that $\partial_t f = 0$, in other words $\{f, h\} = (\mathrm{d}_t f)_{\mathrm{coll}}$. This means that the system has reached a state where the free evolution (the lhs) is exactly compensated by the collisions (the rhs) and the statistical quantities do no longer evolve. More restrictively, an *equilibrium* solution is a distribution f such that *both* the lhs and the rhs cancel separately. This excludes cases, which we will longly

study in section 2, where the stationary solution has a steady current flowing as a result of a compensation between e.g. free fall acceleration by an applied electric field (on the lhs) and scattering along the way which slows down the motion (on the rhs).

As mentioned before, any f that is a function of h_1 only will cancel the lhs. Now, a particular circumstance under which the rhs vanishes as well is the “detailed balance condition”:

$$f(r, p'_1)f(r, p'_2) = f(r, p_1)f(r, p_2) \quad \forall p_1, p'_1, p_2, p'_2, r \quad (13)$$

which is a sufficient but not necessary condition. It means that $\log f$ is a conserved quantity through a collision event. Because our conserved quantities are energy ($E = h_1$) and momentum, we can build a detailed-balance enforcing f as a linear combination of these,

$$\log f = \beta(\mu - E(p, r) + \mathbf{u} \cdot \mathbf{p}) \quad (14)$$

which in the particular case $E(p, r) = \frac{p^2}{2m} + U(r)$ is the Maxwell-Boltzmann distribution in a confining potential $U(r)$ with an advection velocity \mathbf{u} . Note that eq.(14) does not necessarily provide a solution to Boltzmann’s equation, we still have to check that it makes the lhs vanish. For $U(r) = 0$ any value of \mathbf{u} provides a solution, but for a more general $U(r)$ only $\mathbf{u} = \mathbf{0}$ works, which physically seems to make perfect sense – think of $U(r)$ as a quadratic well for instance: in a stationary state, particles just stay motionless (on average!) at the bottom of the well. In any case, we have learned that the condition under which $f_1 \propto e^{-\beta h_1}$ is preferred to any other stationary solution is the detailed balance condition.

This was in a uniform case where the statistical quantities μ, β, \mathbf{u} are the same at every point in space (and time). Now, in non-uniform settings, one can want to look for functions f which cancel the rhs exactly but only approximately the lhs. For instance this is what one gets if detailed balance is enforced with local parameters $\mu(r), \beta(r), \mathbf{u}(r)$: then the rhs still vanishes (which means that microscopically the collisions exactly balance each other), however the lhs cancels only to zeroth order in $\nabla\mu, \nabla\beta, \nabla\mathbf{u}$. Such a “solution” will be called a *local equilibrium* solution, because at microscopic scales where μ, β, \mathbf{u} are almost uniform this is a good enough equilibrium solution.¹

1.3 From kinetics to thermodynamics

An important property of Boltzmann’s equation as given by eq.(11) is that it implies the second law of thermodynamics (this result is known as the H-theorem). To prove this, start from the expression for the classical entropy, $S = - \int d^3r d^3p f \log f$, whose time derivative is

$$\begin{aligned} d_t S &= - \int d^3r d^3p \partial_t f (\mathcal{L} + \log f) \\ &= \int d^3r d^3p \log f (\mathbf{v} \cdot \partial_r f + \boldsymbol{\xi} \cdot \partial_p f - (d_t f)_{\text{coll}}), \end{aligned} \quad (15)$$

where the first cancellation comes from the global conservation of probability, and the second cancellation can be obtained after a few integrations by parts, using the definitions of \mathbf{v} and $\boldsymbol{\xi}$ as derivatives of h_1 . Physically it makes sense of course that the growth of entropy does not depend on the free dynamics but only on interactions. We see that an equilibrium solution, or indeed a *local equilibrium* solution, because it nullifies $(d_t f)_{\text{coll}}$, has stationary entropy $d_t S = 0$.

There is in fact an H-theorem for each form of the collision integral. Here we use that of eq.(11): after doubly symmetrizing the integrand wrt $1 \leftrightarrow 2$ and $p_i \leftrightarrow p'_i$, and using the micro-reversibility property, one obtains

$$\begin{aligned} d_t S &= \int d^3r \int d^3p_1 d^3p_2 d^3p'_1 d^3p'_2 \Gamma(p_1, p_2 | p'_1, p'_2) \\ &\quad \times \frac{1}{2} [f(r, p'_1)f(r, p'_2) - f(r, p_1)f(r, p_2)] [\log(f(r, p'_1)f(r, p'_2)) - \log(f(r, p_1)f(r, p_2))]. \end{aligned} \quad (16)$$

¹Let me emphasize that a local equilibrium, or even a global equilibrium, solution can perfectly well host a steady current \mathbf{u} , or any other “flowing” quantity traditionally associated with non-equilibrium physics. What is prohibited is that this current be the result of a compromise between an acceleration tendency on the lhs and a braking tendency on the rhs.

The integrand is a positive function, so we have obtained $d_t S \geq 0$ which is the second law of thermodynamics.

That irreversibility arises from hamiltonian dynamics might seem either miraculous or more accurately dubious, and indeed it's something we have brought in the equations by hand when we wrote eq.(8). Should we decide that the f_2 functions depend on the momenta *after* the collision event rather than *before* it, this would result in an overall minus sign in front of the collision integral, ensuring the decrease of entropy.

One may wonder what happens in the quantum case, because whereas the molecular chaos assumption is an assumption, the Bose/Fermi enhancing/blocking factors are imposed by quantum mechanics. We will discuss this as an exercise.

1.4 Variational formulation of Boltzmann's equation

Solving Boltzmann's equation is an applied mathematics problem, and we may want to use the traditional recipes of integro-differential equations solving. Among these are variational methods, which can be applied to those equations that are endowed with a variational principle – we will now see that Boltzmann's equation is of this kind.

Let us consider for simplicity a system where, instead of colliding with each other, the classical particles collide elastically with unspecified objects which deviate their momentum but do not change their energy. This means that we consider now the collision integral

$$(d_t f_{\mathbf{k}})_{\text{coll}} = \int d^3 \mathbf{k}' [\Gamma(\mathbf{k}|\mathbf{k}') f_{\mathbf{k}'} - \Gamma(\mathbf{k}'|\mathbf{k}) f_{\mathbf{k}}] = \int d^3 \mathbf{k}' \Gamma_{\mathbf{k}, \mathbf{k}'} [f_{\mathbf{k}'} - f_{\mathbf{k}}], \quad (17)$$

where in going to the rightmost expression we also assumed micro-reversibility $\Gamma(\mathbf{k}|\mathbf{k}') = \Gamma_{\mathbf{k}, \mathbf{k}'} = \Gamma(\mathbf{k}'|\mathbf{k})$, and it is implicit that $\Gamma_{\mathbf{k}, \mathbf{k}'}$ is nonzero only for momenta \mathbf{k}, \mathbf{k}' with the same energy.

Then a standard expansion around (local) equilibrium is to write

$$f_{\mathbf{k}} = f_{\mathbf{k}}^{\text{eq}} - \phi_{\mathbf{k}} \partial_E f_{\mathbf{k}}^{\text{eq}}, \quad (18)$$

where now $\phi_{\mathbf{k}}$ is the unknown of the problem. Since the latter is already order one in forces and gradients, in the lhs of Boltzmann's equation it is sufficient, to the order of linear response, to consider gradients and forces acting on the local equilibrium solution $f_{\mathbf{k}}^{\text{eq}}$. Also because of elasticity $f_{\mathbf{k}}^{\text{eq}} = f_{\mathbf{k}'}^{\text{eq}}$, and in the classical Maxwell-Boltzmann case we just have $\partial_E f_{\mathbf{k}}^{\text{eq}} = -f_{\mathbf{k}}^{\text{eq}}/T$, so one can write the stationary Boltzmann's equation in the approximate form $(\mathbf{v} \cdot \partial_{\mathbf{r}} + \boldsymbol{\xi} \cdot \partial_{\mathbf{k}}) f_{\mathbf{k}}^{\text{eq}} = (d_t f_{\mathbf{k}})_{\text{coll}}$ with

$$(d_t f_{\mathbf{k}})_{\text{coll}} = \frac{1}{T} \int d^3 \mathbf{k}' [\phi_{\mathbf{k}'} - \phi_{\mathbf{k}}] P_{\mathbf{k}, \mathbf{k}'} \quad (19)$$

where $P_{\mathbf{k}, \mathbf{k}'} = f_{\mathbf{k}}^{\text{eq}} \Gamma_{\mathbf{k}, \mathbf{k}'}$ is again symmetric because we assumed elastic scattering.

Formally, Boltzmann's equation has the general form $\Xi_k = \mathcal{K}_{k, k'} \phi_{k'}$ with implicit k' summation, where $\mathcal{K}_{k, k'}$ is an integral kernel (here in particular $\mathcal{K}_{k, k'} = \delta_{k, k'} \sum_q P_{k, q} - P_{k, k'}$) and Ξ_k is just a known function of k (here in particular $\Xi_k = -T (\mathbf{v} \cdot \partial_{\mathbf{r}} + \boldsymbol{\xi} \cdot \partial_{\mathbf{k}}) f_{\mathbf{k}}^{\text{eq}}$).

Denoting the standard scalar product between real functions, $\langle \varphi; \psi \rangle_1 = \int_k \varphi_k \psi_k$, we can notice that

$$\langle \varphi; \mathcal{K} \psi \rangle_1 = \frac{1}{2} \int d^3 \mathbf{k} d^3 \mathbf{k}' [\varphi_{\mathbf{k}} - \varphi_{\mathbf{k}'}] P_{\mathbf{k}, \mathbf{k}'} [\psi_{\mathbf{k}} - \psi_{\mathbf{k}'}] = \langle \mathcal{K} \varphi; \psi \rangle_1 \quad (20)$$

and obviously we also have $\langle \varphi; \mathcal{K} \varphi \rangle \geq 0$ so this defines a good scalar product, $\langle \varphi; \psi \rangle_{\mathcal{K}} \equiv \langle \varphi; \mathcal{K} \psi \rangle_1$, in the space of functions. The solution ϕ to Boltzmann's equation satisfies

$$\Xi = \mathcal{K} \phi \quad \Rightarrow \quad \langle \Xi; \phi \rangle_1 = \langle \phi; \phi \rangle_{\mathcal{K}}. \quad (21)$$

This is an implication but of course not an equivalence, as any function can be made to satisfy the rhs up to a global rescaling factor. In fact we will now prove that among all the trial functions φ that verify the rhs, the actual solution ϕ is the one with maximal \mathcal{K} -norm. Indeed let φ be such that $\langle \Xi; \varphi \rangle_1 = \langle \varphi; \varphi \rangle_{\mathcal{K}}$. Then write

$$0 \leq \langle (\phi - \varphi); (\phi - \varphi) \rangle_{\mathcal{K}} = \dots = \langle \phi; \phi \rangle_{\mathcal{K}} - \langle \varphi; \varphi \rangle_{\mathcal{K}}, \quad (22)$$

where at some stage in the calculation one has to use the lhs of eq.(21) of course.

This variational principle provides us with a practical tool to (e.g. numerically) find approximate solutions to Boltzmann's equation. It may look like we are lucky that such a variational principle exists without us asking for it, but in fact implicitly we did – by ensuring that Boltzmann's equation implies the growth of entropy. Let us see why this is the case. Combining eqs.(18) and (15), we get

$$d_t S = -\frac{1}{T} \int d^3 \mathbf{k} (d_t f_{\mathbf{k}})_{\text{coll}} \phi_{\mathbf{k}} + \frac{1}{T} \int d^3 \mathbf{k} \cancel{(d_t f_{\mathbf{k}})_{\text{coll}}} \epsilon_{\mathbf{k}} \quad (23)$$

where the second term cancels because energy is globally conserved. Plugging in eq.(19), we see that

$$\boxed{d_t S = \frac{1}{2T} \langle \phi; \phi \rangle_{\mathcal{K}} \geq 0.} \quad (24)$$

This proves again the H-theorem, and draws a link between the variational principle and the second law of thermodynamics. Note that here I considered a simple case where the “potential” functional is the norm built out of a scalar product, which was possible because eq.(17) is linear; with more complicated collision integrals one gets more complicated norms, but the principle still works.

Note: the form eq.(23) can be convenient to compute dissipative quantities. For instance, if we know $\phi_{\mathbf{k}}$ (or have an ansatz for it) we can rely on the fact that $d_t S = \mathbf{j}_c \boldsymbol{\sigma}^{-1} \mathbf{j}_c / T$, or $d_t S = \mathbf{j}_q \boldsymbol{\kappa}^{-1} \mathbf{j}_q / T^2$, to obtain an expression for the symmetric part of $\boldsymbol{\sigma}, \boldsymbol{\kappa}$ without having to write down $\phi_{\mathbf{k}}$ as a function of \mathbf{E} or ∇T . This can sometimes be useful, as we will illustrate for instance in sec.4.3.

2 Transport theory in the relaxation time approximation

In this section, we show how the collision integral can be derived formally by means of standard quantum-mechanical scattering theory. This means, we will be using the most classical Boltzmann's equation for *quantum* particles with *quantum-mechanical* collisions. We then introduce the relaxation time approximation of the collision integral, which can also be understood as just a convenient ansatz which captures correctly most of the physics. Thus doing, we will review some of the most basic results of out-of-equilibrium solid state physics, namely the transport of charge and heat in usual metals and insulators. We derive these by finding stationary solutions to Boltzmann's equation for electrons and phonons in the relaxation time approximation. In subsection 3.3 we go beyond the relaxation time approximation and introduce some useful concepts that will pave the way to hydrodynamics in section 4.

2.1 The relaxation time approximation

In (local) equilibrium, the collision integral vanishes. Therefore, away from equilibrium it should look, as a first-order approximation, like $f - f_{\text{eq}}$ where f_{eq} is the (local) equilibrium solution. This allows us to identify a relaxation time $\tau(r, p)$ such that, approximately,

$$(\partial_t + \mathbf{v} \cdot \partial_{\mathbf{r}} + \boldsymbol{\xi} \cdot \partial_{\mathbf{p}}) f(r, p, t) = -\frac{f(r, p, t) - f_{\text{eq}}(r, p)}{\tau(r, p)} \quad (25)$$

This is the relaxation time approximation. An important feature is that the rhs is now linear and has no phase space integral – compare it with eq.(11). As a result, we can now solve the equation perturbatively. We write $f(r, p, t) = f_{\text{eq}}(r, p) + g(r, p, t)$ where now g is the unknown, and g is already order one in forces and gradients. So in the lhs it is sufficient, to the order of linear response, to consider gradients and forces acting on the local equilibrium solution, and one gets

$$\partial_t g(r, p, t) + (\mathbf{v} \cdot \partial_{\mathbf{r}} + \boldsymbol{\xi} \cdot \partial_{\mathbf{p}}) f_{\text{eq}}(r, p) \approx -\frac{g(r, p, t)}{\tau(r, p)} \quad (26)$$

and the stationary solution is then just $g(r, p) = -\tau(r, p) [\mathbf{v} \cdot \partial_{\mathbf{r}} + \boldsymbol{\xi} \cdot \partial_{\mathbf{p}}] f_{\text{eq}}(r, p)$.

2.2 Conductivity and other transport responses

We will now review briefly the transport properties of metals, using Boltzmann's equation in the relaxation time approximation. We consider application of an electric field and a gradient of temperature. Then the out-of-equilibrium distribution function is

$$g(\mathbf{k}) = -\tau(\mathbf{k}) v_{\mathbf{k}}^{\nu} \left(\nabla_{\nu} T \left(-\frac{\epsilon_{\mathbf{k}}}{T} \right) - e E^{\nu} \right) n'_{\text{F}}(\epsilon_{\mathbf{k}}). \quad (27)$$

Then we can plug it into the intuitive expression for the heat and charge currents:

$$\begin{bmatrix} j_c^{\mu} \\ j_q^{\mu} \end{bmatrix} = 2 \int \frac{d^3 \mathbf{k}}{(2\pi)^3} v_{\mathbf{k}}^{\mu} \begin{bmatrix} -e \\ \epsilon_{\mathbf{k}} \end{bmatrix} g(\mathbf{k}) = \begin{bmatrix} \text{L}_{11} & \text{L}_{12} \\ \text{L}_{21} & \text{L}_{22} \end{bmatrix}_{\mu\nu} \begin{bmatrix} E^{\nu} \\ -\nabla_{\nu} T \end{bmatrix}, \quad (28)$$

where the factor of 2 is for spin degeneracy, and we have obtained

$$\text{L}_{11} = e^2 I_0, \quad \text{L}_{21} = T \text{L}_{12} = -e I_1, \quad \text{L}_{22} = (1/T) I_2, \quad I_p^{\mu\nu} := -2 \int \frac{d^3 \mathbf{k}}{(2\pi)^3} v_{\mathbf{k}}^{\mu} v_{\mathbf{k}}^{\nu} \tau(\mathbf{k}) n'_{\text{F}}(\epsilon_{\mathbf{k}}) \epsilon_{\mathbf{k}}^p. \quad (29)$$

The fact that $\text{L}_{21} = T \text{L}_{12}$ is an Onsager's relation.

Reducing $\tau(\mathbf{k}) \rightarrow \tau(\epsilon_{\mathbf{k}})$, and also assuming that $\tau(\epsilon)$ is a much slowly varying function than n_{F} and its derivatives (we will come back to this disputable assumption later) so that $\tau(\epsilon_{\mathbf{k}}) \rightarrow \tau(\epsilon_{\text{F}})$, we can then expand around the FS in the limit of small temperatures, and using the density of states $D(\epsilon_{\text{F}})$ to trade integrals from momentum to energy, we can compute the integrals – for the I_1, I_2 integrals one needs to use the Sommerfeld expansion. Then we get the familiar results

$$\text{L}_{11}^{\mu\nu} = \delta^{\mu\nu} e^2 \tau(\epsilon_{\text{F}}) v_{\text{F}}^2 D(\epsilon_{\text{F}}) / 3, \quad \text{L}_{22} = \frac{\pi^2 T^2}{3 e} \text{L}_{11}. \quad (30)$$

This second identity is the Wiedemann-Franz law, and the first result is the Sommerfeld law.

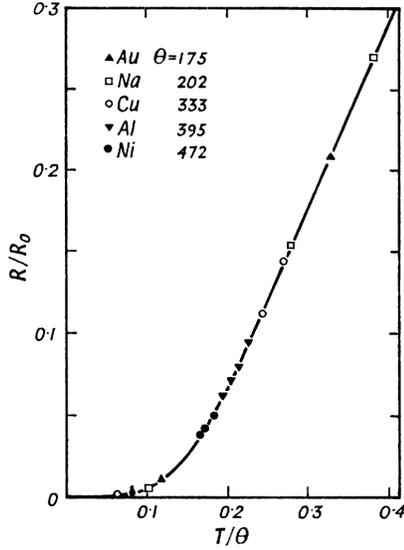


FIG. 115. The Grüneisen-Bloch formula fitted to experimental data on the resistivity of metals (Meissner, 1935).

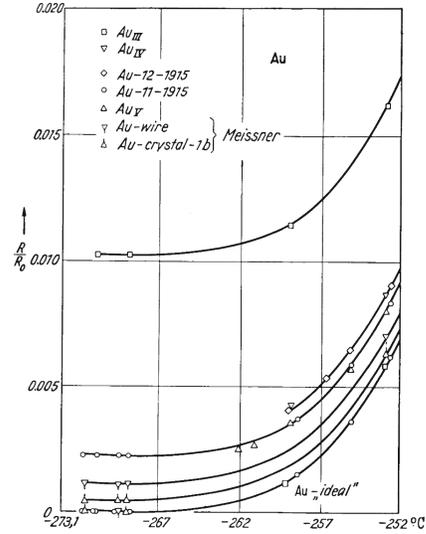


Fig. 3. Electrical resistance of gold samples of varying purity at low temperatures illustrating MATTHIESSEN'S RULE (from VAN DEN BERG).

Figure 1: © MacDonald, *Electrical Conductivity of Metals and Alloys at Low Temperatures*, Handbuch der Physik (1956).

More familiar forms: To connect with the more familiar Drude expression for the electrical conductivity $\sigma = L_{11}$ in the quadratic band case, where $\epsilon_{\mathbf{k}} = k^2/2m$, one just has to remember than in the latter case $D(\epsilon_F) = mk_F/\pi^2$, and the particle density is just the volume of the FS divided by the elementary phase space volume of a particle, namely $n = \frac{4}{3}\pi k_F^3/(2\pi)^3$, which finally gives $\sigma = 2ne^2\tau/m$.

Because the thermal conductivity $\kappa = L_{22} - L_{21}L_{11}^{-1}L_{12}$ actually amounts to L_{22} up to corrections $O(T/\epsilon_F)^2$ which is anyway the amount of accuracy we have achieved here, and because the electrical conductivity is just $\sigma = L_{11}$, we can just as well formulate the Wiedemann-Franz law as the more familiar

$$\frac{\kappa}{T\sigma} = \frac{\pi^2}{3} \frac{k_B^2}{e^2}. \quad (31)$$

Note that it is in fact a matrix identity, which holds even in the presence of a magnetic field – provided the above assumptions still hold. We will probably come back to this later.

As a side remark, the thermal capacity of electrons in a metal is $c_v = \frac{\pi^2}{3}TD(\epsilon_F)$, so that by writing $v = v_F$ and $\ell = v\tau$ the mean free path we have obtained $\kappa = \frac{1}{3}c_v v\ell$. This is a phenomenological relation which works very well in much broader generality, basically as soon as there are quasiparticles carrying heat.

Shortcut: There is a way to derive much more simply the Drude result for the electrical conductivity, by taking inspiration from hydrodynamics (or from solid state physics 101). The trick is to integrate Boltzmann's equation over momentum against $\mathbf{v}_{\mathbf{k}} = \mathbf{k}/m$. The corresponding hydrodynamical equation is

$$\partial_i \bar{v} + \bar{v}/\tau + e\mathbf{E}/m = 0, \quad \bar{v} \equiv \int \frac{d^3\mathbf{k}}{(2\pi)^3} \mathbf{v}_{\mathbf{k}} [f(\mathbf{k}) - f_{\text{eq}}(\mathbf{k})], \quad (32)$$

where the $e\mathbf{E}/m$ bit required an integration by parts. Then one can just solve for stationary \bar{v} and plug this into $\mathbf{j}_c = -ne\bar{v}$: this gives the Drude result. I'm not aware that this trick generalizes to the other transport coefficients, unfortunately.

2.3 Competition between scattering mechanisms and temperature dependence

When different scattering processes $i = 1, \dots$, happen in parallel, each with its own associated scattering time τ_i , their scattering rates add up to the total scattering rate $\tau^{-1} = \tau_1^{-1} + \tau_2^{-1} + \dots$. This is sometimes known as

Matthiessen's rule. As a side note, this excludes complicated events where different scattering processes happen *together*, which diagrammatically would correspond to complicated events with crossing lines. So this is not a law of nature but it is sufficient in the vast majority of cases. Because scattering rates of different processes can have different temperature dependences, they can lead to different behaviours of the transport properties as a function of temperature.

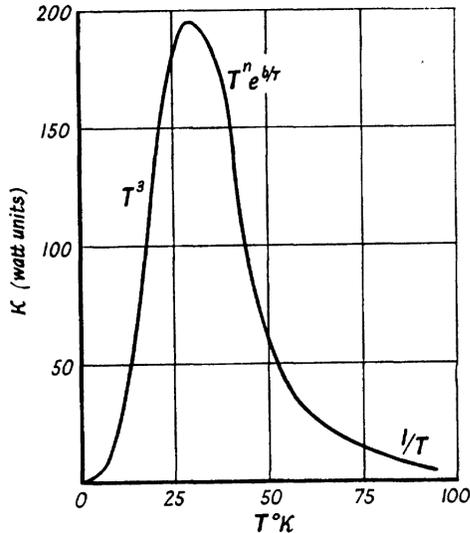


FIG. 83. Thermal conductivity of Al_2O_3 (Berman, 1958).

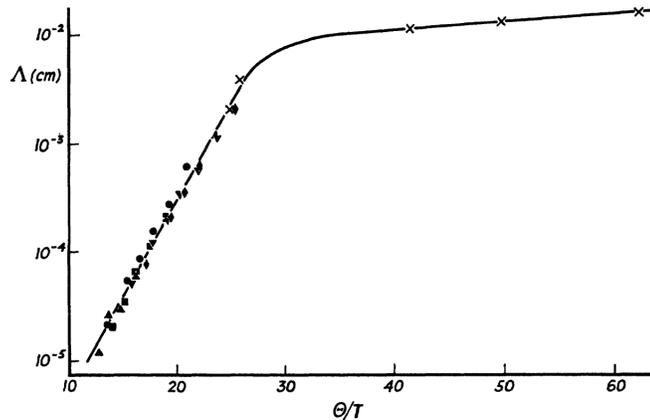


FIG. 87. Mean free path of phonons in solid He, as a function of reduced temperature (Webb, Wilkinson & Wilks, 1952).

Figure 2: © Ziman, *Electrons and Phonons*, Clarendon Press (1960).

Electrical resistivity of metals: For instance, we have seen that the scattering rate associated to elastic disorder scattering, τ_{dis}^{-1} , does not depend on temperature. Meanwhile, one can (and we will as an exercise) show that the electron-phonon scattering rate, under some assumptions, takes the form

$$\tau_{\text{e-ph}}^{-1}(\mathbf{k}) = \frac{m}{2\pi k^3} \left(\frac{T}{v_s}\right)^5 A^2 \int_0^{2v_s k/T} \frac{x^4}{e^x - 1} dx, \quad (33)$$

where v_s is the sound velocity and A (whose explicit expression is known but does not matter) quantifies the electron-phonon interaction. We are interested in $k \approx k_F$, and there are two regimes depending on temperature wrt $\Theta_R = 2v_s k_F$: for low $T \ll \Theta_R$, one gets $\tau_{\text{e-ph}}^{-1}(k_F) \propto T^5$, while for high $T \gg \Theta_R$, one gets $\tau_{\text{e-ph}}^{-1}(k_F) \propto T^1$. With also the disorder scattering at sufficiently low temperatures, this gives us three different temperature behaviours of the resistivity $\rho(T)$, which are commonly referred to as the Bloch-Grüneisen law for $\rho(T)$, cf Fig.1.

Thermal conductivity of insulators: In most insulators, acoustic phonons are the main carriers of energy. We then have 3 branches of bosonic modes $i = 1..3$ with linear dispersion $\omega_{i,\mathbf{q}}$. As usual we get from the relaxation time approximation $g_{i,\mathbf{q}} = -\tau_{i,\mathbf{q}}(\mathbf{v}_{i,\mathbf{q}} \cdot \nabla T) \partial_T n_B(\omega_{i,\mathbf{q}})$, which we can plug into the energy current to get

$$j_{\mathbf{q}}^{\mu} = \sum_{i,\mathbf{q}} g_{i,\mathbf{q}} \omega_{i,\mathbf{q}} v_{i,\mathbf{q}}^{\mu} = -\frac{1}{3} \sum_{i,\mathbf{q}} \omega_{i,\mathbf{q}} v_{i,\mathbf{q}}^2 \tau_{i,\mathbf{q}} \partial_T n_B(\omega_{i,\mathbf{q}}) \nabla_{\mu} T. \quad (34)$$

Now assume $\omega_{i,\mathbf{q}} = v|\mathbf{q}|$ with the same velocity for all three modes, also $\tau_{i,\mathbf{q}} = \tau(q)$, and replace $\sum_{i,\mathbf{q}} \rightarrow$

$3 \int \frac{q^2 dq}{2\pi^2}$, whence

$$\kappa_L(T) = \frac{T^3}{2\pi^2 v} \int_0^{\Theta_D/T} dx \tilde{\tau}(x) \frac{x^4 e^x}{(e^x - 1)^2}, \quad (35)$$

where Θ_D is the Debye temperature and $\tilde{\tau}(x) = \tau(xT/v)$. This formula eq.(35) is basically the equivalent to the Bloch-Grüneisen formula for $\rho(T)$.

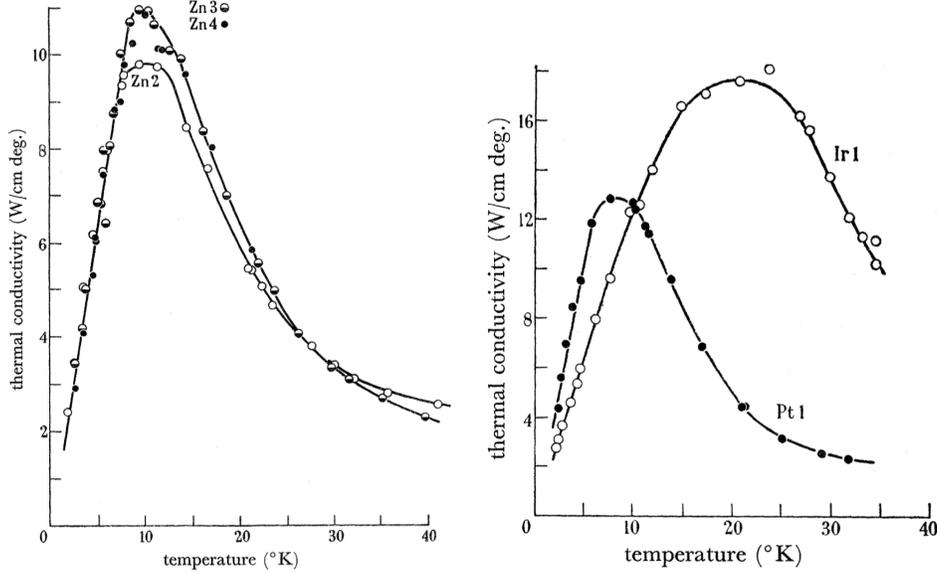


Figure 3: © Rosenberg, *The Thermal Conductivity of Metals at Low T*, Royal Society Publishing (1955).

At low enough temperatures where constant τ is dominant (cf Fig.2 for an experimental justification) and the integral can be extended to infinity, it yields $\kappa_L \propto T^3$, which turns out to be consistent with a simple and elegant argument by Casimir relying on black-body radiation. The explanation for the rest of the curve, and the temperature dependence of the mean free path, will have to wait until Sec.4.2.

Note that the differential thermal capacity of a gas of bosons (with one polarization) is $C(x)dx = \frac{T^3}{2\pi^2 v^3} \frac{x^4 e^x}{(e^x - 1)^2} dx$, so that we have (now counting all three acoustic branches)

$$\kappa_L = \frac{1}{3} \int_0^{\Theta_D/T} dx C(x) v \tilde{\ell}(x), \quad \tilde{\ell}(x) = v \tilde{\tau}(x). \quad (36)$$

We have already encountered this relation in the case of thermal transport by electrons in the relaxation time approximation. It is in fact quite general, at least as a good estimate. Indeed, a rough estimate of the longitudinal thermal conductivity in a solid can be obtained for a gas well-defined energy-carrying particles with total specific heat c_v . Indeed their total increase of internal energy U through displacement in a temperature gradient is $d_t U = c_v v^\mu \partial_\mu T$, and the corresponding average energy current density is $j_q^\mu = -c_v \tau \frac{v^2}{3} \partial_\mu T$, where τ is the typical scattering time of a particle. This indicates the longitudinal thermal conductivity $\kappa_L \approx \frac{1}{3} \sum_i c_{v,i} v_i \ell_i$, where i indexes the different particle flavors involved in energy transport. Here $\ell_i = v_i \tau_i$ is the mean free path with τ_i the average scattering time of the i particles. Note that if different momenta contribute differently, i can index momentum too – so in fact eq.(36) was already obvious at the stage of eq.(35).

Thermal conductivity of metals: For electrons in a metal, the formula $\kappa_L \approx \frac{1}{3} c_v v_F \ell$, with $c_v = \frac{\pi^2}{3} TD(\epsilon_F)$, tells us that at low temperatures where $\ell_{\text{imp}} \approx \text{cst}$ we should have $\kappa \propto T^1$, and at large temperatures where $\ell_{\text{e-ph}} \propto 1/T$ we should have $\kappa \simeq \text{cst}$ (cf Fig.4). This is what is seen experimentally (cf Fig.3).

3 Actually deriving the collision integral

3.1 Scattering rates from microscopic (quantum) interactions

Fermi's golden rule and Born's expansion: The transition rates $\Gamma(\mathbf{f}|\mathbf{i})$ appearing in the collision integral can be evaluated using scattering theory. The latter is a particular instance of time-dependent perturbation theory, i.e. the problem of solving $H = H_0 + V$ where H_0 is soluble and V is an (arguably small) interaction term, where the interaction is a collision. This last statement means that the system is assumed to be non-interacting at $t \rightarrow \pm\infty$, and only at intermediate times (i.e. when the ‘‘collision’’ happens) does the interaction manifest itself. This assumption achieves considerable simplification of the perturbation problem. The scattering rate $\Gamma(\mathbf{f}|\mathbf{i})$ between the initial $|\mathbf{i}\rangle$ and final $|\mathbf{f}\rangle$ states (defined in the *unperturbed* theory of H_0 alone) is expressed using Fermi's golden rule,

$$\Gamma(\mathbf{f}|\mathbf{i}) = \frac{2\pi}{\hbar} |T_{\mathbf{f}\mathbf{i}}|^2 \delta(E_{\mathbf{f}} - E_{\mathbf{i}}). \quad (37)$$

In this formula, $E_{\mathbf{f}}$ and $E_{\mathbf{i}}$ are the unperturbed energies of the \mathbf{i}, \mathbf{f} states, and $T_{\mathbf{f}\mathbf{i}}$ are matrix elements of the T -matrix. The latter is defined from the S -matrix via the formula $S_{\mathbf{f}\mathbf{i}} = \delta_{\mathbf{f},\mathbf{i}} - 2\pi i \delta(E_{\mathbf{f}} - E_{\mathbf{i}}) T_{\mathbf{f}\mathbf{i}}$. The S -matrix, in the interaction picture, reads $S_{\mathbf{f}\mathbf{i}} = \langle \mathbf{f} | U(+\infty, -\infty) | \mathbf{i} \rangle$, with $U(t, t')$ the quantum evolution operator in the interaction picture. The central result of scattering theory is the Lippman-Schwinger equation, which formulated in terms of the T -matrix reads:

$$T_{\mathbf{f}\mathbf{i}} = \langle \mathbf{f} | V | \mathbf{i} \rangle + \frac{1}{\hbar} \sum_{\mathbf{n}} \frac{\langle \mathbf{f} | V | \mathbf{n} \rangle T_{\mathbf{n}\mathbf{i}}}{E_{\mathbf{i}} - E_{\mathbf{n}} + i\eta}, \quad (38)$$

where $\eta \rightarrow 0^+$ is a regularization keeping track of the time-ordering of the evolution operator U . By iterating the formula, one obtains the Born's expansion of the T -matrix:

$$T_{\mathbf{f}\mathbf{i}} = \langle \mathbf{f} | V | \mathbf{i} \rangle + \frac{\langle \mathbf{f} | V | \mathbf{n} \rangle \langle \mathbf{n} | V | \mathbf{i} \rangle}{E_{\mathbf{i}} - E_{\mathbf{n}} + i\eta} + \sum_{l=2}^{\infty} \langle \mathbf{f} | V \left(\frac{1}{E_{\mathbf{i}} - H_0 + i\eta} V \right)^l | \mathbf{i} \rangle. \quad (39)$$

The initial assumptions of scattering theory thus appear to considerably simplify the perturbation expansion. Indeed, the form Eq.(39) is both much simpler than the usual Rayleigh-Schrödinger expansion, and much more tractable than the seemingly simple Brillouin-Wigner expansion, since here all the energies appearing in the denominators are *unperturbed* energies. In practice the first two orders of the expansion are usually sufficient.

Micro-reversibility relations: We already see that if we keep only the first order in Born's expansion, the T -matrix we obtain is hermitian, $T_{\mathbf{f}\mathbf{i}} = T_{\mathbf{i}\mathbf{f}}^*$. Then if we plug this into Fermi's golden rule, we obtain $\Gamma(\mathbf{f}|\mathbf{i}) = \Gamma(\mathbf{i}|\mathbf{f})$. At this stage this is not a micro-reversibility, let alone a detailed balance, relation because we do not assume anything about the quantum states $|\mathbf{i}\rangle, |\mathbf{f}\rangle$ in terms of particles, and momentum is not yet a thing, but we will soon introduce these. Let us just comment briefly on the case where one splits the system into a ‘‘carriers’’ part and a ‘‘scatterers’’ part, and writes $|\mathbf{n}\rangle = |\mathbf{n}_c\rangle \otimes |\mathbf{n}_s\rangle$, and assumes the energy of a state is $E_{\mathbf{n}} = E_{\mathbf{n}_c} + E_{\mathbf{n}_s}$. Then one can define $\Gamma(\mathbf{f}_c|\mathbf{i}_c) = \sum_{\mathbf{i}_s} p(\mathbf{i}_s) \sum_{\mathbf{f}_s} \Gamma(\mathbf{f}|\mathbf{i})$, and assuming thermal probabilities $p(\mathbf{i}_s) = e^{-\beta E_{\mathbf{i}_s}} / Z_s$ and using the conservation of energy $E_{\mathbf{i}_s} - E_{\mathbf{f}_s} = E_{\mathbf{i}_c} - E_{\mathbf{f}_c}$ imposed by Fermi's golden rule, one arrives to the result

$$\Gamma(\mathbf{f}_c|\mathbf{i}_c) e^{-\beta E_{\mathbf{i}_c}} = \Gamma(\mathbf{i}_c|\mathbf{f}_c) e^{-\beta E_{\mathbf{f}_c}}. \quad (40)$$

As we just saw this is not a fully general property, but it happens often enough in practical cases. Unfortunately it often goes under the name of ‘‘detailed balance’’ (because it usually *implies* detailed balance in the collision integral, since as we can see it means that transition rates weighted by probabilities compensate each other), but to avoid confusion let us call it inelastic micro-reversibility relation, or Kubo-Martin-Schwinger relation.

To see why this is related, and how this works concretely in practice, let us now label the carrier states by momentum $|\mathbf{n}_c\rangle \equiv |\mathbf{k}\rangle$, and the scatterer states by a generic label $|\mathbf{n}_s\rangle \equiv |n\rangle$. Here we neglect interactions between carriers, so that the energy of the system of carriers is just the sum of the energies of independent carriers, otherwise we could not describe a many-body quantum state by just the momentum of the particle

which is being scattered. The matrix elements of the scattering process are $\langle \mathbf{k}' | \hat{Q} | \mathbf{k} \rangle = \hat{Q}(\mathbf{k}' - \mathbf{k})$. Then, the scattering rate is

$$\Gamma(\mathbf{k}' | \mathbf{k}) = 2\pi \sum_{n, n'} p_n \left| \langle n' | \hat{Q}(\mathbf{k}' - \mathbf{k}) | n \rangle \right|^2 \delta(\epsilon_{\mathbf{k}'} + E_{n'} - \epsilon_{\mathbf{k}} - E_n) \quad (41)$$

which, by writing $\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dt e^{i\omega t}$ and using $1 = \sum_n |n\rangle \langle n|$, can be cast into the form of the dynamical structure factor,

$$\Gamma(\mathbf{k}' | \mathbf{k}) = S(\mathbf{k} - \mathbf{k}', \epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}'}), \quad S(\mathbf{q}, \omega) \equiv \int_{-\infty}^{+\infty} dt \left\langle \hat{Q}(\mathbf{q}, t) \hat{Q}(-\mathbf{q}, 0) \right\rangle_{\beta} e^{i\omega t}, \quad (42)$$

as is very familiar for instance from the theory of experimental techniques such as X-ray or neutron scattering. Here $\langle \cdot \rangle$ means the equilibrium correlation function of the \hat{Q} system at finite temperature. Such equilibrium correlation functions can be easily shown (for instance in the Lehmann representation) to satisfy the important relation

$$S(\mathbf{q}, \omega) = S(-\mathbf{q}, -\omega) e^{\beta \hbar \omega}, \quad (43)$$

known as the Kubo-Martin-Schwinger relation. The latter is just an occurrence of the quantum fluctuation-dissipation theorem. These identities between *two-point equilibrium correlators*, once plugged into Fermi's golden rule at first Born's order, become relations about *scattering rates*, as we have discussed above, and manifest themselves in the form of micro-reversibility and detailed balance properties.

Examples: we will probably see as an exercise the actual derivation of these, but let me just briefly mention two relevant cases, which are scattering of electrons by static impurities, and scattering of electrons by phonons. In both cases we will use a collision integral with the same physical content as eq.(17) except that we are now working with fermions so we include a Pauli blocking factor for the final states:

$$(\partial_t f_{\mathbf{k}})_{\text{coll}} = \int \frac{d^d \mathbf{k}'}{(2\pi)^d} [\Gamma(\mathbf{k} | \mathbf{k}') f_{\mathbf{k}'} (1 - f_{\mathbf{k}}) - \Gamma(\mathbf{k}' | \mathbf{k}) f_{\mathbf{k}} (1 - f_{\mathbf{k}'})]. \quad (44)$$

In the case of impurity scattering, we just get $\Gamma(\mathbf{k}' | \mathbf{k}) = 2\pi |\langle \mathbf{k}' | V_{\text{imp}} | \mathbf{k} \rangle|^2 \delta(\epsilon_{\mathbf{k}'} - \epsilon_{\mathbf{k}})$. This scattering is clearly elastic, it verifies micro-reversibility, and if we plug it into eq.(44) at equilibrium we can see easily it implies detailed balance.

In the case of electron-phonon scattering, after a little bit of work one gets

$$\Gamma(\mathbf{k}' | \mathbf{k}) = \sum_n \left(\Gamma(\mathbf{k}', n+1 | \mathbf{k}, n) p_n - \Gamma(\mathbf{k}', n | \mathbf{k}, n+1) p_{n+1} \right), \quad (45)$$

where n counts the number of phonons with momentum $\mathbf{k} - \mathbf{k}'$. Because of the micro-reversibility relation $\Gamma(\mathbf{k}', n+1 | \mathbf{k}, n) = \Gamma(\mathbf{k}, n | \mathbf{k}', n+1)$ and of $p_{n+1}/p_n = e^{-\beta(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}'})}$, one gets the inelastic micro-reversibility relation

$$\Gamma(\mathbf{k}' | \mathbf{k}) e^{-\beta \epsilon_{\mathbf{k}}} = \Gamma(\mathbf{k} | \mathbf{k}') e^{-\beta \epsilon_{\mathbf{k}'}} \quad (46)$$

which, when plugged into eq.(44) at equilibrium, again implies detailed balance.

Hopefully these two examples provide a clear picture of the relation between micro-reversibility, Kubo-Martin-Schwinger relation, and detailed balance.

3.2 Actually deriving the relaxation time approximation

We still consider the collision integral for fermions scattering with other objects, eq.(44). Again we assume micro-reversibility, $\Gamma(\mathbf{k} | \mathbf{k}') = \Gamma_{\mathbf{k}, \mathbf{k}'} = \Gamma(\mathbf{k}' | \mathbf{k})$, and we will make a stronger assumption that the fermion dispersion and the scattering rate are isotropic, and that the scattering rate is elastic: we write

$$\Gamma_{\mathbf{k}, \mathbf{k}'} = \Gamma(\epsilon, \hat{\mathbf{k}} \cdot \hat{\mathbf{k}'}) \delta(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}'}) / D(\epsilon) \quad (47)$$

where $D(\epsilon)$ the density of states just serves as a normalization.

Looking for the response to an applied electric field, and expanding around the equilibrium solution, namely $f_{\mathbf{k}} = f_{\mathbf{k}}^{\text{eq}} + g_{\mathbf{k}}$, we can use this to simplify and write Boltzmann's equation in the form

$$-e\mathbf{E} \cdot \mathbf{v}_{\mathbf{k}} n'_{\text{F}}(\epsilon_{\mathbf{k}}) = \int \frac{d^d \mathbf{k}'}{(2\pi)^d} \Gamma_{\mathbf{k}, \mathbf{k}'} [g_{\mathbf{k}'} - g_{\mathbf{k}}]. \quad (48)$$

We can express $g_{\mathbf{k}} = g(\epsilon, \hat{\mathbf{k}})$ as a function of energy and direction of momentum, and considering momenta \mathbf{k}' close to the FS and collapsing the delta function we get

$$-e\mathbf{E} \cdot \hat{\mathbf{k}} v_{\text{F}} n'_{\text{F}}(\epsilon) = \frac{k_{\text{F}}^{d-1}}{v_{\text{F}} D(\epsilon)} \int \frac{d\hat{\mathbf{k}}'}{(2\pi)^d} \Gamma(\epsilon, \hat{\mathbf{k}} \cdot \hat{\mathbf{k}}') [g(\epsilon, \hat{\mathbf{k}}') - g(\epsilon, \hat{\mathbf{k}})]. \quad (49)$$

The lhs transforms as a vector under rotations of $\hat{\mathbf{k}}$, so the same must hold for the rhs, and the only way to possibly achieve this is to have $g(\epsilon, \hat{\mathbf{k}}) = \hat{\mathbf{k}} \cdot \mathbf{E} g(\epsilon)$. We can then factorize \mathbf{E} out of the integral, and in the first term in brackets clearly only the component of $\hat{\mathbf{k}}'$ that is parallel to $\hat{\mathbf{k}}$ contributes, so we can replace $\mathbf{k}' \rightarrow (\hat{\mathbf{k}} \cdot \mathbf{k}') \hat{\mathbf{k}}$ and this yields

$$-e(\mathbf{E} \cdot \hat{\mathbf{k}}) v_{\text{F}} n'_{\text{F}}(\epsilon) = g(\epsilon) \frac{k_{\text{F}}^{d-1} S_d}{v_{\text{F}} D(\epsilon) (2\pi)^d} (\mathbf{E} \cdot \hat{\mathbf{k}}) \int \frac{d\hat{\mathbf{k}}'}{S_d} \Gamma(\epsilon, \hat{\mathbf{k}} \cdot \hat{\mathbf{k}}') [(\hat{\mathbf{k}} \cdot \hat{\mathbf{k}}') - 1], \quad (50)$$

where we extracted S_d the surface of the d -sphere so that now the integral is precisely an angular average, which we can call $-2\tau_{\text{tr}}^{-1}(\epsilon)$ – in principle it is still a function of \mathbf{k} , through its energy ϵ only because we assumed isotropy. Recognizing also the density of states at the Fermi energy $\frac{2k_{\text{F}}^{d-1} S_d}{v_{\text{F}} (2\pi)^d} = D(\epsilon_{\text{F}}) \approx D(\epsilon)$, we can now solve eq.(50), and we find

$$g(\epsilon) = e v_{\text{F}} n'_{\text{F}}(\epsilon) \tau_{\text{tr}}(\epsilon), \quad \tau_{\text{tr}}(\epsilon)^{-1} = \frac{1}{2} \int \frac{d\hat{\mathbf{k}}'}{S_d} \Gamma(\epsilon, \hat{\mathbf{k}} \cdot \hat{\mathbf{k}}') [1 - (\hat{\mathbf{k}} \cdot \hat{\mathbf{k}}')]. \quad (51)$$

We have thus *derived* the relaxation time approximation, in a particular case where the relaxation rate τ^{-1} depends only on the magnitude of momentum, and can be called the “transport relaxation rate” τ_{tr}^{-1} . The latter visibly gets more contributions from backward-scattering than from forward-scattering events, which is of course physically reasonable (and happens in practice).

Aside: it would be instructional to compare the relative simplicity with which we obtained this $[1 - (\hat{\mathbf{k}} \cdot \hat{\mathbf{k}}')]$ factor in the transport scattering rate to the somewhat involved vertex resummation required to get the same effect from a Kubo-type approach. Not sure I'll have time to touch upon this.

3.3 Application: breakdown of the Wiedemann-Franz law

At intermediate temperatures something new happens. Let us look at the typical behaviour depicted in Fig.4. The Wiedemann-Franz does not apply there. Can we understand why?

This seems annoying at first because the derivation of the Wiedemann-Franz law seems quite general. There is no restriction of symmetry, nor even of the existence of a single simple relaxation time. All that is really necessary is that the Boltzmann equation should have a solution of the general form eq.(27), which follows from the relaxation time approximation.

If we come back to sec.3.2 where we *derived* the relaxation time approximation, we see that a key ingredient was that scattering should be *elastic*. Let us see, however, what happens when this assumption is broken.

When we measure the thermal conductivity of a metal, we set up an electron distribution in which there is a flow of heat without any net flow of charge. Let us come back to eq.(27) without an electric field. Now $g(\mathbf{k}) = \tau(\mathbf{k}) v_{\mathbf{k}}' (\nabla_{\nu} T / T) \epsilon_{\mathbf{k}} n'_{\text{F}}(\epsilon_{\mathbf{k}})$ is a function whose sign changes as we go through the Fermi surface. It also depends on the relative orientations of $\mathbf{v}_{\mathbf{k}}$ and ∇T . The situation is depicted in Fig.5.

In charge transport, the important distinction is between “forward” and “backward” electrons, whereas in energy transport the difference is between “hot” and “cold” electrons. If the scattering is through a large angle,

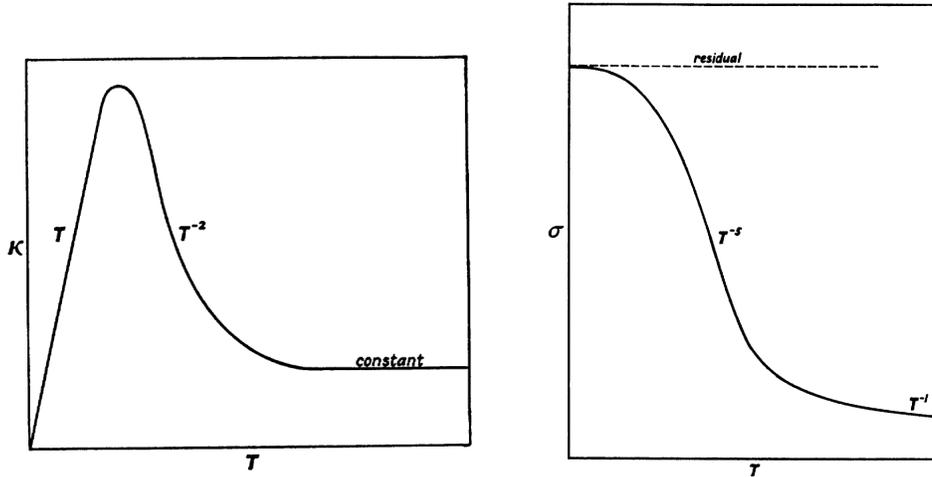


FIG. 101. Thermal conductivity of a typical metal. FIG. 100. Electrical conductivity of a typical metal.

Figure 4: © Ziman, *Electrons and Phonons*, Clarendon Press (1960).

and is approximately elastic (“horizontal scattering”), it will tend to have the same effect in both diagrams, namely restoring equilibrium. This is the type of scattering we have considered in sec.3.2, which can be put into the form of the relaxation time approximation, and does not break WF. On the other hand, scattering through small angles (elastic or inelastic) makes only a small change to the electric current – cf the $(1 - \hat{\mathbf{k}} \cdot \hat{\mathbf{k}}')$ factor –, but inelastic scattering through a small angle (“vertical scattering”) may be very effective in reducing the heat current, for it can change a “hot” electron into a “cold” one. In short, we must expect serious deviations from the Wiedemann-Franz law when “vertical” inelastic transitions dominate the resistivity.²

Because inelastic scattering is much harder to cast into a simple form such as the relaxation time approximation, the way this is usually dealt with is to replace eq.(27) by the phenomenological form

$$g(\mathbf{k}) = v_{\mathbf{k}}' (\tau_{\kappa}(\mathbf{k}) (\nabla_{\nu} T/T) \epsilon_{\mathbf{k}} + \tau_{\sigma}(\mathbf{k}) e E_{\nu}') n_{\mathbf{F}}'(\epsilon_{\mathbf{k}}), \quad (52)$$

with two different scattering rates. There is no reason why eq.(51) should no longer apply for $\tau_{\sigma}(\mathbf{k})$, but for $\tau_{\kappa}(\mathbf{k})$ one must look for something else. Sometimes people solve self-consistently for $\tau_{\kappa}, \tau_{\sigma}$ by plugging back $g(\mathbf{k})$ into the collision integral and solving “again” Boltzmann’s equation. This leads to

$$\tau_{\sigma}^{-1}(\epsilon_{\mathbf{k}}) = \int \frac{d^3 \mathbf{k}'}{(2\pi)^3} \frac{1 - n_{\mathbf{F}}(\epsilon_{\mathbf{k}'})}{1 - n_{\mathbf{F}}(\epsilon_{\mathbf{k}})} \left(1 - (\hat{\mathbf{k}} \cdot \hat{\mathbf{k}}')\right) \Gamma(\mathbf{k}'|\mathbf{k}), \quad \tau_{\kappa}^{-1}(\epsilon_{\mathbf{k}}) = \int \frac{d^3 \mathbf{k}'}{(2\pi)^3} \frac{1 - n_{\mathbf{F}}(\epsilon_{\mathbf{k}'})}{1 - n_{\mathbf{F}}(\epsilon_{\mathbf{k}})} \Gamma(\mathbf{k}'|\mathbf{k}) \quad (53)$$

where we see the difference lies in the $[1 - (\hat{\mathbf{k}} \cdot \hat{\mathbf{k}}')]$ factor, which is what makes the physical difference between charge and energy transport. Thus the “naïve” relaxation time approximation overestimates the efficiency of charge current relaxation, and thus overestimates the Lorentz ratio.

Can we understand simply the T^2 discrepancy, at intermediate temperatures, between the actual thermal conductivity of metals and what would be expected from Wiedemann-Franz and Bloch-Grüneisen (cf Fig.4)? That is to say the fact that $\tau_{\sigma}^{-1}(\epsilon_{\mathbf{F}}) = (T/\epsilon_{\mathbf{F}})^2 \tau_{\kappa}^{-1}(\epsilon_{\mathbf{F}})$? There is a very nice picture. Let us focus on one electron. To relax the heat current, one needs only to change the momentum of this electron by roughly T .

²Experimentally, horizontal scattering is almost certainly true for scattering by all sorts of static objects, so that whenever the resistance is mainly due to impurities or imperfections we expect the Wiedemann-Franz law to be valid. However, the resistance of a relatively pure metal comes mainly (as we have seen with the experimental test of the Bloch-Grüneisen law) from the scattering of the electrons by the lattice vibrations, which are certainly not elastic processes. They are mostly inelastic (so “vertical”) at low temperatures, where phonon momenta are small. The effect cannot be negligible, for the change of electron energy in a typical electron-phonon transition is of the order of T , and this is the same as the width of the electron distribution function. Thus, we expect the thermal conductivity to be always less than predicted by the Wiedemann-Franz law, and especially so at low temperatures. What determines a “low” temperature is the Bloch temperature $\Theta_{\mathbf{R}}$, and there are arguments showing that the WF must be asymptotically correct for $T \gg \Theta_{\mathbf{R}}$. For instance, it is very well verified in metals at room temperature.

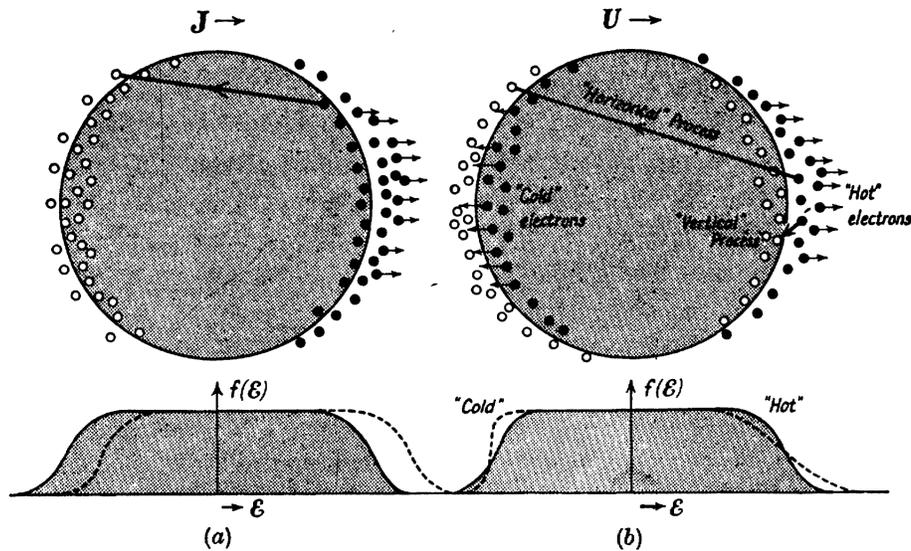


FIG. 122. The Fermi surface and distribution functions: (a) in electrical conduction; (b) in thermal conduction.

- extra electron ——— equilibrium distribution.
- electron deficiency - - - - - steady state transport distribution.

Figure 5: © Ziman, *Electrons and Phonons*, Clarendon Press (1960).

This can be done in one blow by absorbing one phonon. Now, to relax the charge current, one needs to change the momentum of this electron by roughly ϵ_F . We will need multiple collisions with phonons. The momentum of the electron will make a random walk in momentum space, following a diffusion equation with typical step length T , and hence reaching a distance ϵ_F from its original point after typically a quite large number of $(\epsilon_F/T)^2$ steps. There is also a much more mundane argument which is just that the factor $1 - \cos(\theta_{\mathbf{k},\mathbf{k}'}) \approx \theta_{\mathbf{k},\mathbf{k}'}^2/2 \sim (T/\epsilon_F)^2$. One can see things the other way round: the fact that electron momentum relaxation obeys a diffusion equation *imposes* that the angular factor should be $O(\theta^2)$ at small θ , instead of any other possible function of angle.

4 Relaxational dynamics beyond the diffusive regime

In section 3.3, we have seen that because the electron momentum is almost conserved through a collision with a phonon at low temperature, the effective scattering time to be used in charge transport is much larger than the naïve relaxation time. Here we will explore this concept much more extensively, and see that the divergence of the relaxation time of a conserved quantity (momentum, energy) characterizes the transition from the diffusive to the hydrodynamic regime.

4.1 Hydrodynamics: definition

Hydrodynamics here means the differential equation(s) obeyed by a coarse-grained quantity, function of (r, t) , that is conserved by collisions, such as particle number, energy, momentum. Let $\chi(r, p)$ be one such collisional invariant (for particle number $\chi = 1$). This means, by assumption,

$$\int d^3p \chi(r, p) (d_t f)_{\text{coll}} = 0 \quad \forall (r, t). \quad (54)$$

Then we can integrate Boltzmann's equation against $\chi(r, p)$ over momentum (but not position), and after ibp this yields

$$\partial_t \langle n\chi \rangle + \langle \mathbf{v} \partial_r \chi \rangle - \langle n \xi \partial_p \chi \rangle = 0, \quad (55)$$

where we use the shorthand $\langle Q \rangle = (\int d^3p Q f) / n$ with $n = \int d^3p f$. Eq.(55) is a local conservation equation in real space and time: it's a hydrodynamical equation.

4.2 Example: lattice thermal conductivity and Umklapp processes

We have already seen that although there is one relaxation time, basically τ_κ in eq.(53), it can be different from the useful (for instance “transport”) relaxation time for the problem at hand, depending on which quantity is relaxing and the phase space constraints imposed by the dynamics.

An extreme example of this is given by the thermal conductivity of a pure phonon system in an otherwise completely boring crystal (say, diamond). We go beyond linear elasticity and include phonon anharmonicity, which means collision vertices with three phonons or more.

Because of translational invariance, all collisions preserve momentum, then it seems that any local equilibrium distribution

$$f_{\text{eq}}[\mathbf{u}(r)](p) = \left(e^{\beta(\omega_p - \mathbf{u}(r) \cdot \mathbf{p})} - 1 \right)^{-1} \quad (56)$$

is an *exact* solution to the phononic Boltzmann's equation, and in such a distribution, momentum flows according to a hydrodynamical equation of the type of eq.(55) for the average local velocity $\mathbf{u}(r)$.

That momentum be allowed to flow hydrodynamically across the whole sample is an issue, especially insofar as phonons are not conserved particles. Therefore, if energy is given to one end of the system and absorbed at the other end, phonons are just created at the first end, carry momentum (and energy) hydrodynamically down to the other end, and there disappear and give back their energy. In other words, there is a hydrodynamical flow with conserved global momentum, which implies a steady energy current. The fact that conserved momentum implies conserved energy current is always true (as we will show below), and this is particularly obvious if we consider phonons with a linear dispersion: then,

$$\mathbf{j}_q = \int d^d p \omega_p f_{\text{eq}}(\mathbf{p}) \mathbf{v}_p = v^2 \int d^d p f_{\text{eq}}(\mathbf{p}) \mathbf{p} = v^2 \langle \mathbf{p} \rangle, \quad (57)$$

and there is infinite thermal conductivity. But we know that the thermal conductivity of diamond is finite, so there must be a loophole.

The answer is that translation invariance in a lattice only imposes conservation of momentum *up to a reciprocal lattice vector*. Collision events where this vector is not zero are called Umklapp processes (as opposed to Normal processes). For instance, for three-phonon interactions, they look like $\mathbf{p} + \mathbf{p}' = \mathbf{p}'' + \mathbf{G}$, where \mathbf{G} is a

reciprocal lattice vector.³ Once U-processes are included, momentum is no longer conserved by the collisions, and only $\mathbf{u}(r) = \mathbf{0}$ in eq.(56) provides a solution to Boltzmann's equation (namely, the global equilibrium solution), as we have already mentioned in sec.1.2.

Let me emphasize that there is nothing mysterious or phenomenological about these processes, they can be computed very accurately given sufficient time and work. Nonetheless here we'll just estimate roughly for the interest of time, so as to come back to figure 2. At large temperatures beyond the Debye temperature where Umklapp processes dominate the scattering rate, there is really only one time scale which is $\tau \sim 1/T$, and besides the thermal capacity saturates at $c_v \sim \text{cst}$ which yields $\kappa \sim 1/T$ as is indeed observed. At smaller temperatures $T \leq \Theta_D$, the thermal capacity looks more and more like $c_v \sim T^3$, meanwhile Umklapp processes are thermally activated with a rate $\tau^{-1} \sim e^{-\Theta_D/T}$, which yields the complicated intermediate behavior in figure 2. Eventually, then $\tau^{-1}U$ becomes so small that it is no longer relevant in Matthiessen's rule, impurities start playing the relevant role. The theory of impurity scattering of phonons is very rich and complicated, but the experimental outcome seems to be that "boundary scattering" with constant τ dominates, and since $c_v \sim T^3$ one gets the universal $\kappa \sim T^3$ at very low temperatures.

As a final remark, normal processes still play an important role, as we'll see in an exercise. Such processes, which are responsible for relaxing the distribution to *local* equilibrium but not to global equilibrium, are responsible for the viscosity term in the hydrodynamic equation obeyed by quasiparticles in the hydrodynamic regime (i.e. when momentum is poorly relaxed), which for phonons would be at low temperatures in a pure crystal, when Umklapp is exponentially suppressed and there is little to no impurity scattering.

4.3 Conservative laws against diffusive behaviors

Let us now see more formally how conservation of momentum implies infinite conductivity, among other things. Also let us now consider the case of electron-electron collisions. Then, Boltzmann's equation with an electric field can be recast into the form

$$e\mathbf{v}_{\mathbf{k}} \cdot \mathbf{E} = - \int_{\mathbf{q}, \mathbf{k}', \mathbf{q}'} \Gamma(\mathbf{k}', \mathbf{q}' | \mathbf{k}, \mathbf{q}) (\phi_{\mathbf{k}} + \phi_{\mathbf{q}} - \phi_{\mathbf{k}'} - \phi_{\mathbf{q}'}) K(\mathbf{k}, \mathbf{q}, \mathbf{k}', \mathbf{q}') \quad (58)$$

where $K(\dots)$ is some combination of Fermi distributions and derivatives thereof whose precise form is not important, $\Gamma(\dots)$ ensures that $\mathbf{k} + \mathbf{q} = \mathbf{k}' + \mathbf{q}'$, and we recall $f_{\mathbf{k}} = f_{\mathbf{k}}^{\text{eq}} - \phi_{\mathbf{k}} \partial_E f_{\mathbf{k}}^{\text{eq}}$. The point here is: if $\phi_{\mathbf{k}}$ is a solution, then so is $\phi_{\mathbf{k}} + \boldsymbol{\lambda} \cdot \mathbf{k}$ for any constant $\boldsymbol{\lambda}$, and here in particular, $\phi_{\mathbf{k}} = \boldsymbol{\lambda} \cdot \mathbf{k}$ is a solution. This implies that the current $\mathbf{j}_c = e \int_{\mathbf{k}} \mathbf{v}_{\mathbf{k}} \phi_{\mathbf{k}} \partial_E f_{\mathbf{k}}^{\text{eq}}$ does not relax to zero and can be made as large as one wants by changing the value of $\boldsymbol{\lambda}$. So the conductivity is infinite.

An even more formal and straightforward way to show this is provided by the variational principle. Let us for a change consider thermal conductivity of phonons, although this always works. Then the entropy production rate is both

$$d_t S = -\frac{1}{T} \int_{\mathbf{k}} (d_t f_{\mathbf{k}})_{\text{coll}} \phi_{\mathbf{k}} = \frac{1}{T^2} \int_{\mathbf{k}, \mathbf{k}', \mathbf{q}} \Gamma(\mathbf{q} | \mathbf{k}, \mathbf{k}') (\phi_{\mathbf{k}} + \phi_{\mathbf{k}'} - \phi_{\mathbf{q}})^2 n_{\text{eq}}(\mathbf{k}) n_{\text{eq}}(\mathbf{k}') [1 + n_{\text{eq}}(\mathbf{q})], \quad (59)$$

$$d_t S = -\mathbf{j}_q \frac{1}{\boldsymbol{\kappa}} \mathbf{j}_q / T^2 = \frac{1}{T^2} \left(\int_{\mathbf{k}} \mathbf{v}_{\mathbf{k}} \epsilon_{\mathbf{k}} \phi_{\mathbf{k}} \partial_{\epsilon} f_{\mathbf{k}}^{\text{eq}} \right)^2 \frac{1}{\boldsymbol{\kappa}} \quad (60)$$

where I write carelessly $1/\boldsymbol{\kappa}$ instead of the matrix inverse of the symmetric part of $\boldsymbol{\kappa}$. From this we can readily extract

$$\frac{1}{\boldsymbol{\kappa}} = \frac{T^2 \int_{\mathbf{k}, \mathbf{k}', \mathbf{q}} \Gamma(\mathbf{q} | \mathbf{k}, \mathbf{k}') (\phi_{\mathbf{k}} + \phi_{\mathbf{k}'} - \phi_{\mathbf{q}})^2 n_{\text{eq}}(\mathbf{k}) n_{\text{eq}}(\mathbf{k}') [1 + n_{\text{eq}}(\mathbf{q})]}{\left(\int_{\mathbf{k}} \mathbf{v}_{\mathbf{k}} \epsilon_{\mathbf{k}} \phi_{\mathbf{k}} \partial_{\epsilon} f_{\mathbf{k}}^{\text{eq}} \right)^2}. \quad (61)$$

We see directly that the ansatz $\phi_{\mathbf{k}} = \boldsymbol{\lambda} \cdot \mathbf{k}$ makes the numerator vanish, and since it is indeed a solution to the Boltzmann equation, this proves undoubtedly that the thermal conductivity is infinite.⁴

³It seems a bit hard to believe that energy can be preserved with such a collision, and indeed if one has only one phonon band with physically reasonable dispersion it is not really possible. But remember that the three phonons involved can belong to different bands with different velocities, and so an U-process to a faster band followed by a cascade of N-processes to e.g. slower bands can efficiently relax momentum while also conserving energy at every step.

⁴Note we can also directly check that the numerator and denominator in Eq.(61) are precisely those quantities appearing in

Now an important property is that such problems are mostly a feature of DC conductivity. Indeed, if we come back to eq.(58) but now in the AC case, there is an extra $-i\Omega\phi_{\mathbf{k}}$ on the lhs, and now $\phi_{\mathbf{k}} = \boldsymbol{\lambda} \cdot \mathbf{k}$ is no longer a solution for all $\boldsymbol{\lambda}$; instead one has to solve perturbatively for $\phi_{\mathbf{k}}$. To zeroth order, $\phi_{\mathbf{k}}^{(0)} = (i\Omega)^{-1} e\mathbf{v}_{\mathbf{k}} \cdot \mathbf{E}$ is a finite quantity in the AC regime. We have found a divergent imaginary (i.e. non-dissipative) part of the conductivity, $\sigma''(\Omega) \sim 1/\Omega$. Now to first order,

$$\phi_{\mathbf{k}}^{(1)} = -\frac{e}{\Omega^2} \int_{\mathbf{q}, \mathbf{k}', \mathbf{q}'} \Gamma(\mathbf{k}', \mathbf{q}' | \mathbf{k}, \mathbf{q}) \mathbf{E} \cdot (\mathbf{v}_{\mathbf{k}} + \mathbf{v}_{\mathbf{q}} - \mathbf{v}_{\mathbf{k}'} - \mathbf{v}_{\mathbf{q}'}) K(\mathbf{k}, \mathbf{q}, \mathbf{k}', \mathbf{q}') \quad (62)$$

which, if nonzero, provides a divergent real (i.e. dissipative) part of the conductivity, $\sigma'(\Omega) \sim \tau_{ee}^{-1}/\Omega^2$. With this reasoning, we have obtained

$$\sigma(\Omega) = C' \frac{i}{\Omega} + C'' \frac{\tau_{ee}^{-1}}{\Omega^2} \quad (63)$$

which happens to coincide with the relaxation time approximation result for $\Omega \rightarrow +\infty$, but of course not in the DC limit where $\sigma(\Omega)$ diverges whereas the relaxation time approximation predicts a constant (real) conductivity.

One notable exception to the above is the case where galilean invariance is preserved, which here just means $\mathbf{v}_{\mathbf{k}} = \mathbf{k}/m$. Then precisely eq.(62) vanishes, and this is found to be the case to any higher order in the expansion, simply because then the steady current $\mathbf{j}_c^{\text{eq}} = -e \int d\mathbf{k} \mathbf{v}_{\mathbf{k}} f_{\mathbf{k}}^{\text{eq}} = -(e/m) \int_{\mathbf{k}} \mathbf{k} f_{\mathbf{k}}^{\text{eq}} = -(e/m) \mathbf{K}$ is conserved since \mathbf{K} is conserved.⁵

4.4 The hydrodynamical limit

Now that we have seen in some detail how conserved quantities lead to hydrodynamic transport, at the technical level of the collision integral in Boltzmann's equation, we can take a step back and think more phenomenologically about complex problems with *several* coupled Boltzmann's equations. Let us thus consider the case of an electron-phonon-hole plasma, which can happen when the chemical is close to a band touching point and temperature is sufficiently high. There are three Boltzmann equations, one for each species of particles:

$$(\partial_t + \mathbf{v}_+(\mathbf{k}) \partial_{\mathbf{r}} + \boldsymbol{\xi}_+(\mathbf{k}) \partial_{\mathbf{k}}) f_+ = C_+^{ee} + C_+^{eh} + C_+^{\text{ph}} + C_+^{\text{dis}}, \quad (64)$$

$$(\partial_t + \mathbf{v}_-(\mathbf{k}) \partial_{\mathbf{r}} + \boldsymbol{\xi}_-(\mathbf{k}) \partial_{\mathbf{k}}) f_- = C_-^{hh} + C_-^{he} + C_-^{\text{ph}} + C_-^{\text{dis}}, \quad (65)$$

$$(\partial_t + \mathbf{v}_{\text{ph}}(\mathbf{k}) \partial_{\mathbf{r}} + \boldsymbol{\xi}_{\text{ph}}(\mathbf{k}) \partial_{\mathbf{k}}) n = C_{\text{ph}}^+ + C_{\text{ph}}^- + C_{\text{ph}}^{\text{rel}}. \quad (66)$$

Here electrons are "+", holes are "-", and collision terms are labeled according to $C_{\text{part}}^{\text{coll}}$, where the lower index indicates which particle's kinetic equation the term belongs to, and the upper index indicates which type of process is described.

We will be particularly interested in the relaxation of the three hydrodynamic variables (particle number, momentum and energy) by each collision term,

$$\{N_{\text{part}}^{\text{coll}}, \mathbf{P}_{\text{part}}^{\text{coll}}, E_{\text{part}}^{\text{coll}}\} = \int \frac{d^3\mathbf{k}}{(2\pi)^3} \{1, \mathbf{k}, \epsilon_{\text{part}}(\mathbf{k})\} C_{\text{part}}^{\text{coll}}. \quad (67)$$

Each collision term preserves some quantities and relaxes some others: collisional invariants are $Q_{\pm}^{ee} = 0 = Q_{\pm}^{hh}$ for all three $Q \in \{N, \mathbf{P}, E\}$, as well as $N_{\pm}^{\text{dis}} = 0 = E_{\pm}^{\text{dis}}$ because we assume elastic disorder scattering which nonetheless does not preserve momentum, and all the other collisional integrals are potentially not zero. In particular $C_{\text{ph}}^{\text{rel}}$ relaxes all three phonon quantities since it includes phonon N-processes, U-processes, and any kind of disorder.

the variational formulation of Boltzmann's equation, namely we have $\frac{1}{\kappa} \propto \frac{(\phi, \phi)_{\mathcal{K}}}{|(\mathbf{E}, \phi)_1|^2}$ in that language. And we know from the variational theorem that this quantity is *minimized* by the solutions of the kinetic equation. So the local zero it reaches for our ansatz is a global zero, and our ansatz is actually a solution to the equation – in case we did not already know it.

⁵This is directly related to the quite nontrivial cancellation of the “Maki-Thompson” diagrams and the “Aslamazov-Larkin” diagrams for the optical conductivity of a circular Fermi surface. This is a relevant point for a spinon Fermi surface coupled to an emergent photon, and pioneering calculations thereof missed the subtle cancellation between diagrams, leading to incorrect predictions. There are many cases where Boltzmann-based calculations provide intuitive insight on a problem whereas Kubo-based calculations make it a tricky business, and we have here a very good illustration.

The quantities associated to electrons and holes are not always separately conserved (not even the particle number because one “species” of fermion can be changed into the other), however for the combined system of fermions we have extra sum rules:

$$Q_+^{eh} + Q_-^{he} = 0, \quad (68)$$

$$Q_+^{\text{ph}} + Q_-^{\text{ph}} + Q_{\text{ph}}^+ + Q_{\text{ph}}^- = 0, \quad (69)$$

for $Q \in \{N, \mathbf{P}, E\}$ ⁶. Collision terms enforcing such a sum rule but not conserving each hydrodynamic variable independently are often referred to as drag terms. These are particularly relevant when discussing thermopower experiments, because particles which are good at carrying charge (like electrons) can “drag” particles which are good at carrying energy (like phonons).

We have already discussed quite extensively phonon hydrodynamics in the previous two sections, and electron-phonon (or hole-phonon) hydrodynamics already in Sec.3.3. Here we will consider the electron-hole plasma, focusing on the charge neutrality point, because this is where the Fermi liquid behaviors are most inapplicable. Following the same idea we have introduced when discussing the Wiedemann-Franz law, we can

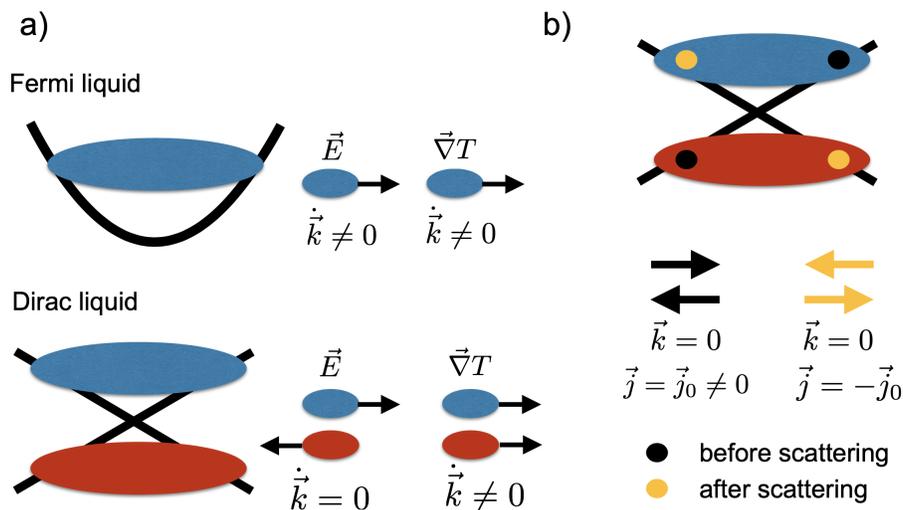


Figure 6: © Fritz & Scaffidi, *Hydrodynamic Electronic Transport*, Annual Reviews (2021).

write a generalized relaxation time approximation for the two coupled equations:

$$\partial_t f_+ - \{(\nabla T/T) \epsilon_+(\mathbf{k}) + e\mathbf{E}\} \partial_{\mathbf{k}} f_+^{\text{eq}} = -\frac{g_+}{\tau_{+-}} + \frac{g_-}{\tau_{-+}} - \frac{g_+}{\tau_{\text{rel}}}, \quad (70)$$

$$\partial_t f_- - \{(\nabla T/T) \epsilon_-(\mathbf{k}) - e\mathbf{E}\} \partial_{\mathbf{k}} f_-^{\text{eq}} = -\frac{g_-}{\tau_{-+}} + \frac{g_+}{\tau_{+-}} - \frac{g_-}{\tau_{\text{rel}}}. \quad (71)$$

It is necessary to use the same relaxation times τ_{\pm} and τ_{\mp} in both equations so that the sum rule $Q_+^{eh} + Q_-^{he} = 0$ is obeyed. Meanwhile we use the same τ_{rel} just for notational convenience, accounting for both disorder and maybe some amount of phonon scattering.

Contrarily to sec.3.3, there is no need to distinguish between τ_{σ} and τ_{κ} type times, because electrons and holes have similar momenta and the Fermi momentum is no longer large. However, and crucially, this does not mean the Wiedemann-Franz law is obeyed. Recall that in the case of a Fermi liquid, both electrical and thermal transport were governed by momentum relaxation, just it did not happen on the same timescales for both, whence an overestimated Lorentz ratio in the relaxation time approximation. In the case of an electron-hole plasma, the violation is more obvious, because although thermal transport is still governed by momentum

⁶The $Q = N$ case in eq.(69) above is not completely obvious; it comes from the fact that phonons are real bosons, so for each process which emits a phonon there is another process, occurring with the same rate, which destroys a phonon.

relaxation, electrical transport is completely decoupled therefrom, cf Fig.6 (left panel). You can also look at the parity of the relaxation terms in the rhs of eq.(70) and compare to the parity of the \mathbf{E} and ∇T terms on the lhs. Thus we can expect, and we will check straightaway, that thermal conductivity should be governed by τ_{diss} and electrical conductivity by $\tau_{\pm, \mp}$.

For clarity let us consider the hydrodynamic limit, which is

$$\frac{1}{\tau_{\text{rel}}} \ll \frac{1}{\tau_{\text{drag}}} = \frac{1}{\tau_{+-}} + \frac{1}{\tau_{-+}}, \quad (72)$$

and for simplicity also assume particle-hole symmetry together with inversion, $\epsilon(\mathbf{k}) = \epsilon_+ = \epsilon_-$ and $\mathbf{v}(\mathbf{k}) = \partial_{\mathbf{k}}\epsilon_+ = \partial_{\mathbf{k}}\epsilon_-$ so the only difference between holes and electrons is their charge, $\pm e$.

For the DC electrical conductivity, we get

$$\sigma = e^2 \tau_{\text{drag}} \int_{\mathbf{k}} \mathbf{v}(\mathbf{k}) \partial_{\mathbf{k}} (f_+^{\text{eq}} - f_-^{\text{eq}}), \quad (73)$$

which confirms intuition – in particular, we see that only the difference between populations matters. For the thermal conductivity, we get

$$\kappa = -\tau_{\text{rel}} \int_{\mathbf{k}} \epsilon_{\mathbf{k}}^2 \mathbf{v}_{\mathbf{k}} \partial_{\mathbf{k}} (f_+^{\text{eq}} + f_-^{\text{eq}}), \quad (74)$$

which again confirms intuition – in particular, we see that only the sum of populations matters. Thus, the Lorentz ratio $L = \frac{\kappa}{\sigma T} \propto \tau_{\text{rel}}/\tau_{\text{drag}}$ is possibly much larger in the hydrodynamic regime than in the diffusive regime we considered thus far. In this hydrodynamic electron-hole plasma scenario, the “usual” relaxation time approximation would considerably *underestimate* the Lorentz ratio.

4.5 Separation of scales from collisional constraints

Let us come back to the familiar problem of a Fermi surface, and explore the hydrodynamic limit where electron-electron collision is the main source of scattering. Let us consider a contact interaction with potential $U \delta(\mathbf{r} - \mathbf{r}')$, to first Born’s order, to express the rhs in eq.(58):

$$\begin{aligned} (\partial_t + \mathbf{v}_{\mathbf{k}} \cdot \partial_{\mathbf{r}}) f_{\mathbf{k}} = & -\frac{1}{T} \int_{\mathbf{q}, \mathbf{k}', \mathbf{q}'} 2\pi |U|^2 f_{\mathbf{k}}^{\text{eq}} f_{\mathbf{q}}^{\text{eq}} [1 - f_{\mathbf{k}'}^{\text{eq}}] [1 - f_{\mathbf{q}'}^{\text{eq}}] (\phi_{\mathbf{k}} + \phi_{\mathbf{q}} - \phi_{\mathbf{k}'} - \phi_{\mathbf{q}'}) \\ & \times \delta(\epsilon_{\mathbf{k}} + \epsilon_{\mathbf{q}} - \epsilon_{\mathbf{k}'} - \epsilon_{\mathbf{q}'}) (2\pi)^2 \delta(\mathbf{k} + \mathbf{q} - \mathbf{k}' - \mathbf{q}'). \end{aligned} \quad (75)$$

We see that the combination of the population factors with energy and momentum conservation, at low temperatures $T \ll E_{\text{F}}$, imposes that all four momenta should lie very close to the FS – actually exactly on the FS, to lowest order in (T/E_{F}) .

Let us now consider the problem in 2D, and in particular a circular Fermi surface. Then, the scattering $\mathbf{k} + \mathbf{q} = \mathbf{k}' + \mathbf{q}'$ has exactly two solutions: $(\mathbf{k} = \mathbf{k}', \mathbf{q} = \mathbf{q}')$, or $(\mathbf{k} = \mathbf{q}', \mathbf{q} = \mathbf{k}')$.

There is one exception to the above: for $\mathbf{k} + \mathbf{q} = \mathbf{0} = \mathbf{k}' + \mathbf{q}'$, all deflection angles are allowed. This is actually important. Indeed, if we now look at the combination of ϕ in eq.(75), we find that it always vanishes in the cases we mentioned previously, but in the “head-on” case it does not have to. Instead, it makes a strong distinction between the modes of the Fermi surface that are to be relaxed. Namely, we can distinguish between even modes, where $\phi_{-\mathbf{k}} = \phi_{\mathbf{k}}$, and odd modes, where $\phi_{-\mathbf{k}} = -\phi_{\mathbf{k}}$ (cf fig 7).

For even modes, the collision integral is finite, whereas for odd modes it again vanishes. Thus we must expect a much smaller relaxation rate for odd modes, which will be provided by relaxing the momentum constraint at higher temperatures, and since the next order in the Sommerfeld expansion has an extra $(T/E_{\text{F}})^2$ power we can expect $\tau_{\text{odd}}^{-1} \sim (T/E_{\text{F}})^2 \tau_{\text{even}}^{-1}$, which is indeed what is shown by detailed careful calculations.

For practical purposes in bulk transport we are only interested in the relaxation of the first mode (momentum relaxation) which gives us σ and the zeroth mode (particle number relaxation) in the case of an electron-hole plasma which gives us κ . So it is not obvious that we should care about higher harmonics. It turns out they becomes relevant in constrained geometries, where one can study (even experimentally with local probes) the transition between ballistic, hydrodynamic and dissipative electron flow.

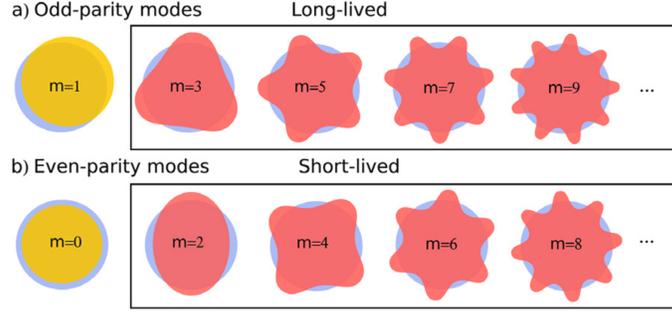


Figure 7: © Ledwith et al., *The hierarchy of excitation lifetimes in 2D Fermi gases*, Annals of Physics (2019).

To see this, let us start from a generic form of Boltzmann's equation,

$$\partial_t \phi_{\mathbf{k}} + \mathbf{v}_{\mathbf{k}} \cdot \partial_{\mathbf{r}} \phi_{\mathbf{k}} - \frac{e\mathbf{E}}{mv_{\text{F}}} \cdot \mathbf{v}_{\mathbf{k}} = \mathcal{C}[\phi], \quad (76)$$

in terms of $\phi(\mathbf{k})$ parameterizing the deviation from equilibrium. Now, expanding around a 2D circular Fermi surface, one can decompose $\phi(\mathbf{k}) \rightarrow \phi(\theta)$ into angular harmonics:

$$\phi(\theta) = \phi_0 + \sum_{n>0} \{\phi_{1,n} \cos(n\theta) + \phi_{2,n} \sin(n\theta)\}. \quad (77)$$

From eq.(76), we see that the components affected by the electric field are the ϕ_n defined as $\phi_{i,n}$ where i has the same parity as n . For the collision integral, let us assume the relaxation time approximation for each ϕ_n independently, i.e. each excitation decays at its own rate, $\mathcal{C}[\phi] = -\sum_{n>0} \gamma_n \phi_n$.

Now, to see how constrained geometry can highlight hydrodynamic behavior, consider a channel infinite along x (the direction of the electric field), and narrow along y , so that $\partial_y f$ is no longer negligible on the rhs of Boltzmann's equation. Then eq.(76) becomes

$$\partial_t \phi_n - \frac{1}{2}(-1)^n v_{\text{F}} \partial_y (\phi_{n+1} - \phi_{n-1}) = -\gamma_n \phi_n + \frac{eE}{m} \delta_{n,1}. \quad (78)$$

Because γ_1 is by definition momentum-relaxing, whereas relaxation rates for higher harmonics are momentum-conserving, in the hydrodynamic regime we have $\gamma_1 \ll \gamma_{n>1}$, and we can decouple the first two equations from the others: by plugging the second equation $\frac{1}{2}v_{\text{F}}\partial_y\phi_1 = -\gamma_2\phi_2$ into the first one $\partial_t\phi_1 + \frac{1}{2}v_{\text{F}}\partial_y\phi_2 = -\gamma_1\phi_1 + (e/m)E$, one obtains

$$\partial_t \phi_1 + \eta \partial_{yy}^2 \phi_1 = -\gamma_1 \phi_1 + (e/m)E \quad (79)$$

which is the Stokes equation (or diffusion equation for momentum), with the viscosity $\eta = \gamma_2 v_{\text{F}}^2 / 4$ proportional to the momentum-*conserving* relaxation rate. We will encounter a similar phenomenon as an exercise with the Callaway model for phonon conductivity with normal processes. Compared to the usual Stokes equation there is an extra momentum-relaxing diffusive term $-\gamma_1 \phi_1$, which can be made negligible wrt the hydrodynamic term by narrowing the channel.

5 Semiclassical corrections – as a user

In this section, we will talk about Hall effects, starting from the classical Hall effect and the skew-scattering-induced anomalous Hall effect. We will then delve more seriously into the semiclassical equations of motion for an electron wavepacket, including quantum effects related to the topology of electron bands. We will see that by including such quantum corrections into Boltzmann’s equation, we can derive some unquestionably quantum phenomena such as the integer quantum Hall effect and even the $d = 3 + 1$ chiral anomaly.

5.1 Semiclassical dynamics and the anomalous velocity

We will now go beyond the “classical” kinetic equation by now caring not only about the particle populations, but also about the actual shape of the Bloch eigenfunctions, defined by the equation $\mathcal{H}_{\mathbf{k}}|u_{n,\mathbf{k}}\rangle = \epsilon_{n,\mathbf{k}}|u_{n,\mathbf{k}}\rangle$.

There is always a gauge choice in the definitions of the eigenfunctions, $|u_{n,\mathbf{k}}\rangle \rightarrow e^{i\theta_{n,\mathbf{k}}}|u_{n,\mathbf{k}}\rangle$. One can define an associated vector potential $\mathcal{A}_{n,\mathbf{k}} = i\langle u_{n,\mathbf{k}}|\partial_{\mathbf{k}}u_{n,\mathbf{k}}\rangle$, which is the Berry connection. This quantity is defined to be gauge-dependent, and transforms as $\mathcal{A}_{n,\mathbf{k}} \rightarrow \mathcal{A}_{n,\mathbf{k}} - \partial_{\mathbf{k}}\theta_{n,\mathbf{k}}$. This connection defines a curvature, $\Omega_{n,\mathbf{k}} = \partial_{\mathbf{k}} \times \mathcal{A}_{n,\mathbf{k}}$, which is the Berry curvature and is gauge invariant.

Instead of point-like particles in phase space (which do not satisfy Heisenberg’s uncertainty relation) we will consider a wavepacket built out of the Bloch eigenfunctions. Because these functions can have a nontrivial structure imposed by $\mathcal{H}_{\mathbf{k}}$, it seems that we should worry that our classical equations of motion are no longer the correct ones. Indeed, they are modified by the Berry curvature, and the correct semiclassical equations for an electron wavepacket are

$$\begin{aligned} \dot{\mathbf{x}} &= \mathbf{v}_{n,\mathbf{k}} - \dot{\mathbf{k}} \times \Omega_{n,\mathbf{k}}, \\ \dot{\mathbf{k}} &= -e\mathbf{E} - e\dot{\mathbf{x}} \times \mathbf{B}, \end{aligned} \quad (80)$$

where $\mathbf{v}_{n,\mathbf{k}} = \partial_{\mathbf{k}}\epsilon_{n,\mathbf{k}}$ up to an extra subtlety.⁷ One must understand eqs. (80), (81) as a set of $2N$ first-order equations, where N is the number of electron bands, because $\Omega_{n,\mathbf{k}}$ is a band-dependent quantity (and so both equations are in fact band-dependent).

How does one prove eqs.(80), (81)? One way to approach this question is to view the equation of motion for the position as arising from taking the expectation value of the *operator* equation of motion for the position operator. Since we are discussing motion within a band, we want to consider the position operator projected into a single band. From now on, let us work in a given band n . The projected wavefunction expanded into the Bloch eigenfunctions of this band reads $\psi(\mathbf{x}) = \int d^d\mathbf{k}\psi(\mathbf{k})e^{i\mathbf{k}\mathbf{x}}u_{n,\mathbf{k}}(\mathbf{x})$, and (using orthonormality of the Bloch eigenfunctions as well as their invariance upon translation by a Bravais lattice vector) it is not difficult to show that its Fourier transform reads $\psi(\mathbf{k}) = \int d^d\mathbf{x}\psi(\mathbf{x})e^{-i\mathbf{k}\mathbf{x}}u_{n,\mathbf{k}}^*(\mathbf{x})$.

In the following, we will work with wavefunctions belonging to one given band n , with basis the plane waves at momentum \mathbf{k} , namely $\psi_{n,\mathbf{k}}(\mathbf{x}) = e^{i\mathbf{k}\mathbf{x}}u_{n,\mathbf{k}}(\mathbf{x})$. Now we consider the action of the position operator $\hat{\mathbf{x}}$, with matrix elements

$$\int_x \psi_{n',\mathbf{k}'}^* x^\mu \psi_{n,\mathbf{k}} = -i\partial_{k_\mu} \delta(k - k') \delta_{nn'} + \delta(k - k') \int_x i u_{n',\mathbf{k}'}^* \partial_{k_\mu} u_{n,\mathbf{k}}. \quad (82)$$

In other words,

$$\hat{\mathbf{x}}|\psi_{n,\mathbf{k}}\rangle = i\partial_{\mathbf{k}}|\psi_{n,\mathbf{k}}\rangle + i\langle u_{n,\mathbf{k}}|\partial_{\mathbf{k}}u_{n,\mathbf{k}}\rangle|\psi_{n,\mathbf{k}}\rangle = i(\partial_{\mathbf{k}} - i\mathcal{A}_{n,\mathbf{k}})|\psi_{n,\mathbf{k}}\rangle. \quad (83)$$

We have thus identified $\hat{\mathbf{x}}_n = i(\partial_{\mathbf{k}} - i\mathcal{A}_{n,\mathbf{k}})$, the band-projected position operator. This operator produces gauge invariant observables: any change in the phase of the wavefunction $\psi(k) \rightarrow e^{i\alpha_n(k)}\psi(k)$ can be compensated by a change in the phase of the Bloch eigenbasis, which does $\mathcal{A}_{n,\mathbf{k}} \rightarrow \mathcal{A}_{n,\mathbf{k}} + \partial_{\mathbf{k}}\alpha_n(k)$.

Crucially, the band-projected coordinate operators have nontrivial commutation relations. While $[x_n^\mu, k_n^\nu] = i\delta_{\mu\nu}$ and $[k^\mu, k^\nu] = 0$ remain unchanged (in the absence of a magnetic field), we now have $[x_n^\mu, x_n^\nu] = i\epsilon_{\mu\nu\lambda}\Omega_\lambda$. We can now compute the equation of motion for the position operator $\hat{\mathbf{x}}_n$. We can use the band-projected

⁷In fact, the proper velocity to be used in eq. (80) is $\mathbf{v}_{n,\mathbf{k}} = \partial_{\mathbf{k}}(\epsilon_{n,\mathbf{k}} - \mathbf{B} \cdot \mathbf{m}_{n,\mathbf{k}})$, where

$$m_{n,\mathbf{k}}^\mu = -i(e/2)\epsilon_{\mu\nu\lambda}\langle\partial_k^\nu u_{n,\mathbf{k}}|\mathcal{H}_{\mathbf{k}} - \epsilon_{n,\mathbf{k}}|\partial_k^\lambda u_{n,\mathbf{k}}\rangle$$

is the “orbital magnetic moment”. We will mention this later.

hamiltonian which (when there is no magnetic field) reads $\hat{H}_n = \epsilon_{n,\mathbf{k}} + e\mathbf{E}\hat{x}_n$. The Heisenberg equation of evolution is

$$\begin{aligned}\frac{dx_n^\mu}{dt} &= -i \left[x_n^\mu, \hat{H}_n \right] \\ &= -i [x_n^\mu, \epsilon_{n,\mathbf{k}}] - i [x_n^\mu, eE_\nu x_n^\nu] = \partial_k^\mu \epsilon_{n,\mathbf{k}} + eE_\nu \Omega_{\lambda} \epsilon_{\mu\nu\lambda}.\end{aligned}\quad (84)$$

This gives us the first equation eq.(80), which is the new piece of physics. This derivation follows the original approach by Karplus and Luttinger. Now we would still need to include the magnetic field contribution in the Lorentz force; we can still loosely argue that the replacement $\mathbf{E} \rightarrow \mathbf{E} + \mathbf{v} \times \mathbf{B}$ is imposed by galilean invariance in the laboratory frame, but anyway, we still have to prove that it's $\frac{dx_n^\mu}{dt}$ and not $v_{n,\mathbf{k}}^\mu$ that appears in the Lorentz force. To prove everything properly, one needs to work more carefully in a magnetic field, and this was done much later by Niu and collaborators.

5.2 Consequences for the kinetic equation and the quantum Hall effect

Using that $\dot{\mathbf{x}} \cdot \Omega_{n,\mathbf{k}} = \mathbf{v}_{n,\mathbf{k}} \cdot \Omega_{n,\mathbf{k}}$ and similarly $\dot{\mathbf{k}} \cdot \mathbf{B} = -e\mathbf{E} \cdot \mathbf{B}$, as well as $(a \times b) \times c = (c \cdot a)b - (b \cdot c)a$, one can easily solve the ‘‘Hamilton’’ equations explicitly, which yields

$$\dot{\mathbf{x}} = \frac{\mathbf{v}_{n,\mathbf{k}} + e\mathbf{E} \times \Omega_{n,\mathbf{k}} + e(\mathbf{v}_{n,\mathbf{k}} \cdot \Omega_{n,\mathbf{k}})\mathbf{B}}{1 + e\mathbf{B} \cdot \Omega_{n,\mathbf{k}}}, \quad (85)$$

$$\dot{\mathbf{k}} = -e \frac{\mathbf{E} + \mathbf{v}_{n,\mathbf{k}} \times \mathbf{B} + e(\mathbf{E} \cdot \mathbf{B})\Omega_{n,\mathbf{k}}}{1 + e\mathbf{B} \cdot \Omega_{n,\mathbf{k}}}. \quad (86)$$

It was already apparent in eqs. (80), (81), and perhaps it is even more so in eqs. (85), (86), that the Berry curvature is very much like a magnetic field defined in momentum space. Now we will make a guess that these corrected semiclassical $\dot{\mathbf{x}}$ and $\dot{\mathbf{k}}$ are the correct ones which should be used on the lhs of Boltzmann's equation. This will lead to new physical predictions, so that we can test this statement (we will do it theoretically below).

An interesting new ingredient is the denominator appearing in both of these equations. It indicates a correction to the phase space density of states, $D_n(\mathbf{k}) = \frac{1}{(2\pi)^d} (1 + e\mathbf{B} \cdot \Omega_{n,\mathbf{k}})$. That's because $d^d\mathbf{k}$, the volume element in momentum space occupied *classically* by one quasiparticle, is *not* invariant under the semiclassical evolution including Berry curvature effects. This means that Liouville's theorem needs corrections when we include the Berry curvature effects.

Indeed, let us follow an infinitesimal momentum space volume along a semiclassical path, $d^d\mathbf{k} \rightarrow d^d\mathbf{k}'$ where

$$d^d\mathbf{k}' = \left\| \frac{d^d\mathbf{k}'}{d^d\mathbf{k}} \right\| = d^d\mathbf{k} \det \left[\delta_{\mu\nu} + \frac{\partial \dot{k}_\mu}{\partial k_\nu} dt \right]_{\mu\nu} = d^d\mathbf{k} \left(1 + \frac{\partial \dot{k}_\mu}{\partial k_\mu} dt \right). \quad (87)$$

Notice the analogy with a compressible fluid in real space, this dilation factor is analogous to $(1 + \nabla \cdot \mathbf{v} dt)$.

It is easy to check that the numerator of eq.(86) is divergenceless, but the denominator yields a contribution:

$$\frac{\partial \dot{k}_\mu}{\partial k_\mu} = -\dot{k}_\mu \frac{e\mathbf{B} \cdot \partial_k^\mu \Omega_{n,\mathbf{k}}}{1 + e\mathbf{B} \cdot \Omega_{n,\mathbf{k}}} = -\frac{d}{dt} \ln(1 + e\mathbf{B} \cdot \Omega_{n,\mathbf{k}}). \quad (88)$$

This can still be written $d^d\mathbf{k}' = (1 - dD_n(\mathbf{k})/D_n(\mathbf{k})) d^d\mathbf{k}$, or better:

$$\boxed{d^d\mathbf{k}' D_n(\mathbf{k}') = d^d\mathbf{k} D_n(\mathbf{k})} \quad (89)$$

This means that $d^d\mathbf{k} D_n(\mathbf{k})$ is the correct invariant to be used in Liouville's theorem for instance. It means also a correction to Luttinger's theorem, because the volume in momentum space occupied by a quasiparticle is no longer $(2\pi)^d$ but instead $1/D_n(\mathbf{k}) = (2\pi)^d / (1 + e\mathbf{B} \cdot \Omega_{n,\mathbf{k}})$.

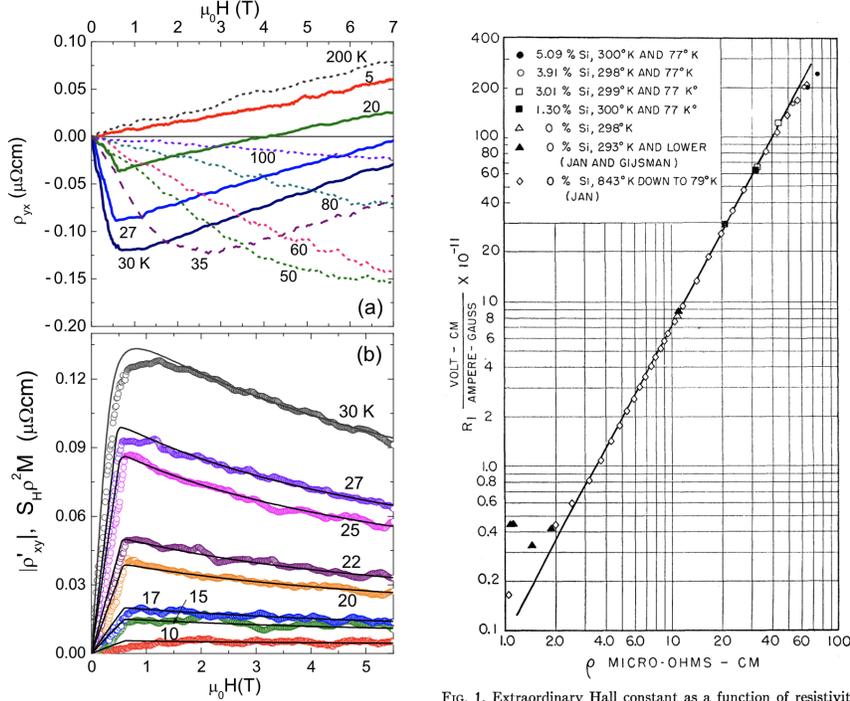


FIG. 1. Extraordinary Hall constant as a function of resistivity.

Figure 8: © Nagaosa et al., *Anomalous Hall effect*, Rev. Mod. Phys. (2010). Left: MnSi. Right: $\text{Fe}_{1-x}\text{Si}_x$.

Consequence: the correct local particle number is $n(\mathbf{x}, t) = 2 \sum_n \int d^d \mathbf{k} D_n(\mathbf{k}) f_n(\mathbf{k}, \mathbf{x}, t)$. Now we can plug this, at equilibrium, into Středa's formula⁸ for the intrinsic Hall conductivity:

$$\sigma_{xy} = -e \left. \frac{\partial n}{\partial B_z} \right|_{\mu} = -2e \sum_n \int d^d \mathbf{k} n_F(\epsilon_{n,\mathbf{k}}) \frac{1}{(2\pi)^d} \frac{\partial}{\partial B_z} (e\mathbf{B} \cdot \Omega_{n,\mathbf{k}}) = -2e^2 \sum_n \int \frac{d^d \mathbf{k}}{(2\pi)^d} n_F(\epsilon_{n,\mathbf{k}}) \Omega_{n,\mathbf{k}}^z. \quad (90)$$

This is precisely the famous Karplus-Luttinger formula for the anomalous quantum Hall effect. In particular, for fully filled (Chern) bands this recovers the IQHE result, but this formula is much more general and applies equally well to systems with much larger electron density at much lower fields, for instance itinerant ferromagnets, where it is now accepted that this “intrinsic” contribution dominates the response: see Fig.8.

Alternatively: instead one can also look at the current, with the proper velocity and density of states:

$$\mathbf{j}_c(\mathbf{x}, t) = -2e \sum_n \int d^d \mathbf{k} D_n(\mathbf{k}) \dot{\mathbf{x}}_n(\mathbf{k}) f_n(\mathbf{k}, \mathbf{x}, t). \quad (91)$$

Note that the two dilation factors cancel against each other in the current. For the dominant contribution at not too large fields, just take $\mathbf{B} = \mathbf{0}$, so that $\dot{\mathbf{x}}_n(\mathbf{k}) = \mathbf{v}_{n,\mathbf{k}} + e\mathbf{E} \times \Omega_{n,\mathbf{k}}$. The only correction to the classical formula comes from the anomalous velocity $e\mathbf{E} \times \Omega_{n,\mathbf{k}}$. For $f_n(\mathbf{k})$ we can just use the equilibrium distribution, which yields

$$\mathbf{j}_c = -2e \sum_n \int \frac{d^d \mathbf{k}}{(2\pi)^d} (\mathbf{v}_{n,\mathbf{k}} + e\mathbf{E} \times \Omega_{n,\mathbf{k}}) n_F(\epsilon_{n,\mathbf{k}}) \Rightarrow \sigma_{xy} = -2e^2 \sum_n \int \frac{d^d \mathbf{k}}{(2\pi)^d} n_F(\epsilon_{n,\mathbf{k}}) \Omega_{n,\mathbf{k}}^z. \quad (92)$$

⁸Consider a 2D material with a magnetic flux going through a disk-shaped area with radius R . There is a circulating electric field around the disk given by Faraday's law, $\oint \mathbf{E} \cdot d\mathbf{l} = -\pi R^2 \partial_t B^z$, which means a tangent electric field $\mathbf{E}_\theta = -(R/2) \partial_t B^z$. This in turn generates an incoming charge current $\mathbf{j}_{c,\text{in}} = -\sigma_{xy} \mathbf{E}_\theta$, and the charge contained in the disk-shaped area increases by $\partial_t Q = 2\pi R j_{c,\text{in}} = \pi R^2 \sigma_{xy} \partial_t B^z$. We have thus obtained $\sigma_{xy} = (1/\pi R^2) (\partial Q / \partial B^z) = -e (\partial n / \partial B^z)$.

Conclusion: We have recovered the Karplus-Luttinger formula by two different methods, which maybe is a good clue that using (85), (86) in the kinetic theory is the correct thing to do. As a quick experimental remark, under time reversal $\Omega_{n,\mathbf{k}} \rightarrow -\Omega_{n,-\mathbf{k}}$, so even without a field, time reversal breaking is needed to get an intrinsic Hall effect from the Berry curvature. This is just a manifestation of the Onsager-Casimir-Büttiker relations.

5.3 Orbital magnetization and the energy shift

Here we discuss the correction to the energy mentioned above in an intuitive way. We will derive it more rigorously in the next section. For now, starting from a hamiltonian for electrons in a magnetic field, $H(\mathbf{p}, \mathbf{r}) \rightarrow H(\mathbf{p} + e\mathbf{A}(\mathbf{r}), \mathbf{r})$, we want to describe the effective hamiltonian felt by a wavepacket centered at position \mathbf{r}_c , due to its spatial extension in the field $\mathbf{A}(\mathbf{r}) = \frac{1}{2}\mathbf{B} \times \mathbf{r}$. To first order in gradients,

$$\Delta H = \frac{1}{2}e(\mathbf{A}(\mathbf{r}) - \mathbf{A}(\mathbf{r}_c)) \cdot \partial_{\mathbf{k}}H + \text{h.c.} = \frac{e}{2}\mathbf{B} \cdot \mathbf{L}, \quad (93)$$

with $\hat{\mathbf{L}} = \frac{1}{2}[(\hat{\mathbf{r}} - \mathbf{r}_c) \times \partial_{\mathbf{k}}\hat{H} + \text{h.c.}]$. Note that \mathbf{L} is just an effective quantity, defined relatively to the wavepacket. Then we can evaluate the energy shift of a given Bloch wavefunction,

$$\Delta\varepsilon_{n,\mathbf{k}} = \frac{e}{2}\mathbf{B} \cdot \langle \psi_{n,\mathbf{k}} | \hat{\mathbf{L}} | \psi_{n,\mathbf{k}} \rangle = -\frac{e}{2}\mathbf{B} \cdot \frac{1}{2} \langle \psi_{n,\mathbf{k}} | \partial_{\mathbf{k}}\hat{H} \times (\hat{\mathbf{r}} - \mathbf{r}_c) | \psi_{n,\mathbf{k}} \rangle + \text{h.c.} \quad (94)$$

To define \mathbf{r}_c , in principle one should be careful and define some reasonable wavepacket. Here let me not do that in the interest of time, and just write crudely $\mathbf{r}_c = \langle \psi_{n,\mathbf{k}} | \hat{\mathbf{r}} | \psi_{n,\mathbf{k}} \rangle$.

Now we can use the two (rigorous) formulae

$$\langle \psi_{n,\mathbf{k}} | \partial_{\mathbf{k}}\hat{H} | \psi_{n',\mathbf{k}'} \rangle = \delta_{\mathbf{k},\mathbf{k}'} \delta_{n,n'} \partial_{\mathbf{k}}\varepsilon_{n,\mathbf{k}} + \delta_{\mathbf{k},\mathbf{k}'} (\varepsilon_{n,\mathbf{k}} - \varepsilon_{n',\mathbf{k}}) \langle \partial_{\mathbf{k}}u_{n,\mathbf{k}} | u_{n',\mathbf{k}} \rangle, \quad (95)$$

$$\langle \psi_{n,\mathbf{k}} | \partial_{\mathbf{k}}\hat{H} \otimes \hat{\mathbf{x}} | \psi_{n,l} \rangle = \partial_{\mathbf{k}}\varepsilon_{n,\mathbf{k}} \otimes \langle \psi_{n,\mathbf{k}} | \hat{\mathbf{x}} | \psi_{n,l} \rangle + i\delta_{\mathbf{k},\mathbf{l}} \langle \partial_{\mathbf{k}}u_{n,\mathbf{k}} | \otimes (\varepsilon_{n,\mathbf{k}} - \hat{H}) | \partial_{\mathbf{l}}u_{n,l} \rangle, \quad (96)$$

from which

$$\begin{aligned} -\mathbf{L}_{n,\mathbf{k}} &= -\langle \psi_{n,\mathbf{k}} | \hat{\mathbf{L}} | \psi_{n,\mathbf{k}} \rangle = \frac{1}{2} \left(\partial_{\mathbf{k}}\varepsilon_{n,\mathbf{k}} \times \langle \psi_{n,\mathbf{k}} | \hat{\mathbf{r}} | \psi_{n,\mathbf{k}} \rangle + i \langle \partial_{\mathbf{k}}u_{n,\mathbf{k}} | \times (\varepsilon_{n,\mathbf{k}} - \hat{H}) | \partial_{\mathbf{k}}u_{n,\mathbf{k}} \rangle - \partial_{\mathbf{k}}\varepsilon_{n,\mathbf{k}} \times \mathbf{r}_c \right) + \text{h.c.} \\ &= \frac{1}{2} i \langle \partial_{\mathbf{k}}u_{n,\mathbf{k}} | \times (\varepsilon_{n,\mathbf{k}} - \hat{H}) | \partial_{\mathbf{k}}u_{n,\mathbf{k}} \rangle + \text{h.c.} = -\text{Im} \langle \partial_{\mathbf{k}}u_{n,\mathbf{k}} | \times (\varepsilon_{n,\mathbf{k}} - \hat{H}) | \partial_{\mathbf{k}}u_{n,\mathbf{k}} \rangle \end{aligned} \quad (97)$$

whence the energy shift for a given band n ,

$$\Delta\varepsilon_{n,\mathbf{k}} = -\mathbf{B} \cdot \mathbf{M}_{n,\mathbf{k}}, \quad \mathbf{M}_{n,\mathbf{k}} = -\frac{e}{2} \text{Im} \langle \partial_{\mathbf{k}}u_{n,\mathbf{k}} | \times (\varepsilon_{n,\mathbf{k}} - \hat{H}) | \partial_{\mathbf{k}}u_{n,\mathbf{k}} \rangle. \quad (98)$$

This can be interpreted as the Zeeman energy due to the orbital amagnetization $\mathbf{M}_{n,\mathbf{k}}$.

One consequence: the Bohr-Sommerfeld quantization of semiclassical orbits of electrons in a magnetic field involves the full Berry phase accumulated around the orbit, whereas (at least in several cases of interest) the quantization of energy levels (Landau levels) picks up only the topological part of that phase, i.e. the winding number. We will see this in an exercise.

5.4 Bonus: the chiral anomaly from Boltzmann's equation

Now consider a collection of Weyl points, characterized by their winding number $w_i = \frac{1}{2\pi} \oint_{\partial V_i} d^2\mathbf{p} \cdot \boldsymbol{\Omega}_{\mathbf{p}}^i \in \mathbb{Z}$ where V_i is any volume encompassing the Weyl point (w_i is a topological property i.e. the integral does not depend on the choice of V_i). Let us call $n_{\mathbf{p}}^i$ (which implicitly also depends on \mathbf{x}, t) the distribution of electrons at momentum \mathbf{p} defined relatively around the i th Weyl point. Then, Boltzmann's equation with the semiclassical corrections reads

$$\begin{aligned} \frac{\partial}{\partial t} n_{\mathbf{p}}^i + (1 + e\mathbf{B} \cdot \boldsymbol{\Omega}_{\mathbf{p}}^i)^{-1} \left[-e(\mathbf{E} + \mathbf{v}_{\mathbf{p}}^i \times \mathbf{B} + e(\mathbf{E} \cdot \mathbf{B}) \boldsymbol{\Omega}_{\mathbf{p}}^i) \frac{\partial}{\partial \mathbf{p}} n_{\mathbf{p}}^i \right. \\ \left. + (\mathbf{v}_{\mathbf{p}}^i + e\mathbf{E} \times \boldsymbol{\Omega}_{\mathbf{p}}^i + e(\mathbf{v}_{\mathbf{p}}^i \cdot \boldsymbol{\Omega}_{\mathbf{p}}^i) \mathbf{B}) \frac{\partial}{\partial \mathbf{r}} n_{\mathbf{p}}^i \right] = (d_i n_{\mathbf{p}}^i)_{\text{coll}}. \end{aligned} \quad (99)$$

Traditionally, the collision integral is decomposed in terms of the “transport” and “intervalley” relaxation times, $\tau_{\text{tr}} \ll \tau_{\text{iv}}$. Here we are interested in timescales where the electron distribution shows no anisotropy within one valley, $n_{\mathbf{p}}^i = n_i(\epsilon_{\mathbf{p}}^i)$. Then $\partial_{\mathbf{p}} n_{\mathbf{p}}^i = \mathbf{v}_{\mathbf{p}}^i \partial_{\epsilon} n_i(\epsilon_{\mathbf{p}}^i)$, and (very much like for the classical Hall effect) the $\mathbf{v} \times \mathbf{B}$ term drops out of the first term, so we have

$$\frac{\partial}{\partial t} n_i(\epsilon_{\mathbf{p}}^i) + (1 + e\mathbf{B} \cdot \boldsymbol{\Omega}_{\mathbf{p}}^i)^{-1} [-e(\mathbf{E} + e(\mathbf{E} \cdot \mathbf{B})\boldsymbol{\Omega}_{\mathbf{p}}^i) \mathbf{v}_{\mathbf{p}}^i \partial_{\epsilon} n_i(\epsilon_{\mathbf{p}}^i) + (\dots)] = (d_t n_{\mathbf{p}}^i)_{\text{coll}} \quad (100)$$

(I did not write again the gradient term because it is unchanged).

Let us define the density of states in the i valley,

$$\rho_i(\epsilon) = \int_{V_i} \frac{d^3 \mathbf{p}}{(2\pi)^3} (1 + e\mathbf{B} \cdot \boldsymbol{\Omega}_{\mathbf{p}}^i) \delta(\epsilon - \epsilon_{\mathbf{p}}^i) \simeq \frac{\epsilon^2}{2\pi^2 v_i^3} + \dots, \quad (101)$$

which will prove useful. By integrating eq.(100) against $(1 + e\mathbf{B} \cdot \boldsymbol{\Omega}_{\mathbf{p}}^i) \delta(\epsilon - \epsilon_{\mathbf{p}}^i)$, one gets

$$\partial_t n_i(\epsilon) - \frac{w_i}{\rho_i(\epsilon)} \frac{e^2}{4\pi} (\mathbf{E} \cdot \mathbf{B}) \partial_{\epsilon} n_i(\epsilon) + \frac{1}{\rho_i(\epsilon)} \partial_{\mathbf{r}} \mathbf{j}_i(\epsilon) = -\frac{1}{\tau_{\text{iv}}} (n_i(\epsilon) - n_i^{\text{eq}}(\epsilon)), \quad (102)$$

where in the rhs we finally wrote explicitly the relaxation time approximation, where $n_i^{\text{eq}}(\epsilon) = \frac{1}{e^{\beta(\epsilon - \mu_i)} + 1}$ with μ_i the valley-dependent chemical potential (because Weyl nodes can be shifted in energy). We also defined

$$\mathbf{j}_i(\epsilon) = \int_{V_i} \frac{d^3 \mathbf{p}}{(2\pi)^3} \delta(\epsilon - \epsilon_{\mathbf{p}}^i) (\mathbf{v}_{\mathbf{p}}^i + e\mathbf{E} \times \boldsymbol{\Omega}_{\mathbf{p}}^i + e(\mathbf{v}_{\mathbf{p}}^i \cdot \boldsymbol{\Omega}_{\mathbf{p}}^i) \mathbf{B}) n_{\mathbf{p}}^i = \frac{e w_i}{4\pi^2} n_i(\epsilon) \mathbf{B} \quad (103)$$

which is the particle current of fermions from the i th valley (and as mentioned earlier, the momentum space dilation factors cancel against each other in the current).

We can eventually integrate eq.(102) against $\rho_i(\epsilon) d\epsilon$, and defining

$$N_i(\mathbf{x}, t) = \int d\epsilon (n_i(\epsilon) - n_i^{\text{eq}}(\epsilon)) \rho_i(\epsilon), \quad \mathbf{J}_i(\mathbf{x}, t) = \int d\epsilon \mathbf{j}_i(\epsilon) \quad (104)$$

the local density and current of particles from the i th valley, and using $\int d\epsilon \partial_{\epsilon} n_i(\epsilon) = -1$, one gets

$$\partial_t N_i + \nabla \cdot \mathbf{J}_i = w_i \frac{e^2}{4\pi^2} (\mathbf{E} \cdot \mathbf{B}) - N_i / \tau_{\text{iv}}. \quad (105)$$

The first term on the rhs is the chiral anomaly term, which has exactly the same form as what we found in the “ultra-quantum regime” as an exercise.⁹

Practical implications:

- *The chiral magnetic effect* – Let us say that the magnetic field is along the z axis, so the local charge current $\mathbf{J}_c = -e \sum_i \mathbf{J}_i$ is purely along z . It’s not obvious a priori that we don’t get a current in equilibrium, because $\mathbf{J}_c^{\text{eq}} = -\frac{e^2}{4\pi^2} \mathbf{B} \sum_i w_i \mu_i$ does not seem to vanish (note that this expression is independent of the choice of lower integration bound because $\sum_i w_i = 0$). In fact, the vanishing of the charge current in equilibrium *defines* equilibrium, and one solution is when all μ_i are equal (when there are two Weyl cones, it’s the only one). This means that when the Weyl nodes are shifted in energy, there is not one global chemical potential for all electrons in the Brillouin zone: each Weyl node has its own chemical potential μ_i defined by the equilibrium condition $\mathbf{J}_c^{\text{eq}} = \mathbf{0}$. This is the chiral magnetic effect.

⁹It is to be expected that this term does not depend on the regime where it is derived, as it really is a universal field-theoretical result. Just to mention quickly why this is an *anomaly*, that’s because it breaks a conservation equation imposed by Noether’s theorem. Indeed, consider the limit $\tau_{\text{iv}} \rightarrow \infty$ so that there is no coupling between different valleys, and the lagrangean is free, namely

$$\mathcal{L}(t) = \sum_i \int d^d x \psi_i^\dagger(x, t) (i\partial_t - \hat{h}_i(x)) \psi_i(x, t).$$

The action is invariant under the global symmetry $\psi_i(x, t) \rightarrow e^{i\alpha_i} \psi_i(x, t)$ where crucially α_i is valley-dependent. So by Noether’s theorem, classically $N_i = \int d^d x \psi_i^\dagger(x, t) \psi_i(x, t)$ is conserved independently for each valley i . But here, because of the anomaly term, it is not, whence the name.

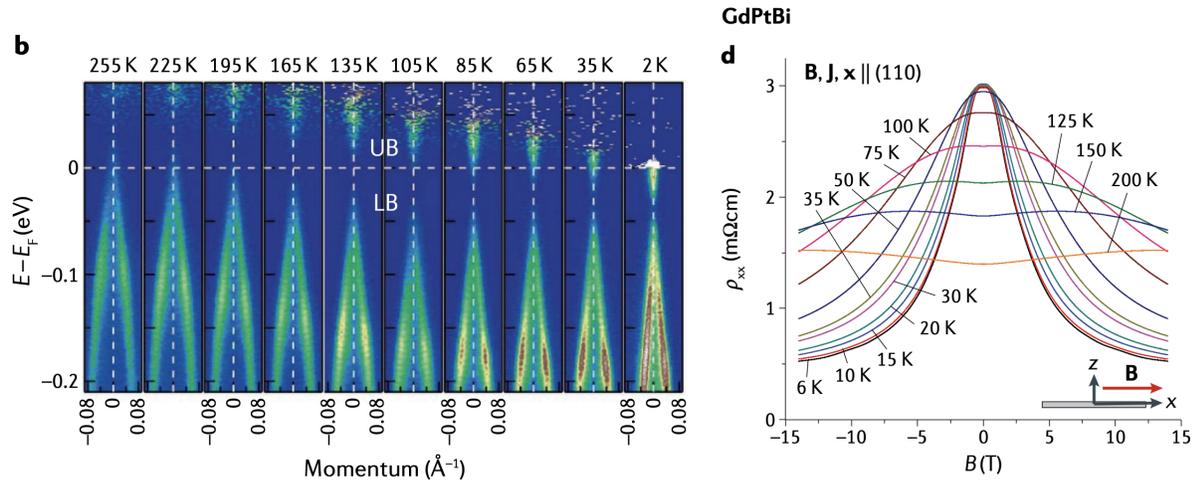


Figure 9: © Ong and Liang, *Exp. signatures of the chiral anomaly in Dirac–Weyl semimetals*, Nat. Rev. (2021)

- *The negative magnetoresistance* – It is straightforward to solve eq.(102) in the stationary and uniform case, exactly as usual. One finds

$$n_i(\epsilon) = n_i^{\text{eq}}(\epsilon) + \tau_{\text{iv}} \frac{w_i}{\rho_i(\epsilon)} \frac{e^2}{4\pi} (\mathbf{E} \cdot \mathbf{B}) \partial_\epsilon n_i^{\text{eq}}(\epsilon) \quad (106)$$

which we can then plug into the current to obtain the conductivity.

Its only nonzero component is

$$\sigma_{zz} = \tau_{\text{iv}} \frac{e^2 (eB)^2}{8\pi^2} \sum_i \frac{v_i^3 w_i^2}{\mu_i^2}, \quad (107)$$

which we can see is an increasing function of B – in other words, σ_{zz} displays a negative magnetoresistance. Expert experimentalists claim that this is what we see in Fig.9.

6 Semiclassical corrections – hardware viewpoint

In sec.2, we have treated electrons and phonons as essentially classical particles, writing the collision integral almost classically in terms of transition *rates* as a functional of particle *numbers*, whereas in principle everything should be formulated in terms of wavefunctions and propagators.

Then in sec.5 we have computed the semiclassical equations of motion for a free wavepacket, and declared without proof that these should now be the \dot{x} and \dot{p} appearing on the lhs of Boltzmann's equation (which turned out to recover correct known physical results).

Now we come back to these assumptions and justify them more carefully.

6.1 The case of free particles

We have already encountered in the previous lecture a derivation of the kinetic equation from the time evolution of the density matrix, in the particular case of a quadratic dispersion for bosons in one dimension. Here I want to take a different perspective and formulate the problem quite generally.

Let us start from a set of fields, which can be bosons or fermions, obeying the canonical (anti-)commutation relation $[\Psi_a(r_1), \Psi_b^\dagger(r_2)]_\pm = \delta_{ab}\delta(r_1 - r_2)$, where $[\cdot, \cdot]_\pm$ is an anticommutator (+) for fermions and a commutator (−) for bosons. We consider free particles, and we assume that the hamiltonian has the form ¹⁰

$$\mathbf{H} = \int_{r_1, r_2} \sum_{a, b} \mathbf{H}_{ab}(r_1, r_2) \Psi_a^\dagger(r_1) \Psi_b(r_2), \quad (108)$$

and the equation of motion for the fields is $\partial_t \Psi_a(r) = -i[\Psi_a(r), \mathbf{H}]$.

For bosons this calculation is straightforward, and for fermions it is useful to remember that $[ab, c] = a[b, c]_\mp \pm [a, c]_\mp b$ to turn the commutator into an anticommutator. The resulting equation turns out to be the same for bosons and fermions, it reads

$$\partial_t \Psi_a(r) = -i(\mathbf{H} \circ \Psi)_a(r) \quad (109)$$

in both cases, where \circ is the convolution of real space coordinates and flavor indices, defined as

$$(\hat{\mathbf{O}}_1 \circ \hat{\mathbf{O}}_2)_{ab}(r_1, r_2) \equiv \int_r \sum_c \hat{\mathbf{O}}_{1,ac}(r_1, r) \hat{\mathbf{O}}_{2,cb}(r, r_2). \quad (110)$$

We now want to look at the density matrix $\mathbf{F}_{ab}(r_1, r_2) = \langle \Psi_a^\dagger(r_1) \Psi_b(r_2) \rangle$, whose time evolution can be readily obtained and is $\partial_t \mathbf{F} = -i(\mathbf{H} \circ \mathbf{F} - \mathbf{F} \circ \mathbf{H})$. The next step is to formulate the problem in phase space, which can be done by means of the Wigner transform

$$\mathbf{O}(X, p) = \int_x e^{-ipx/\hbar} \mathbf{O}\left(X + \frac{x}{2}, X - \frac{x}{2}\right), \quad (111)$$

where $p, X, x \in \mathbb{R}^d$ (we can identify $X = \frac{1}{2}(r_1 + r_2)$ and $x = r_1 - r_2$). This generalizes the Fourier transform, which is the particular case where $\mathbf{O}(r_1, r_2) = \mathbf{O}(r_1 - r_2)$.

Just like the convolution product in real coordinates becomes the usual product in Fourier coordinates, the Wigner transform of the convolution product is the so-called Moyal product, represented by a \star :

$$\boxed{(\mathbf{O}_1 \circ \mathbf{O}_2)(r_1, r_2) \xrightarrow{\text{WT}} \mathbf{O}_1(X, p) \star \mathbf{O}_2(X, p)}. \quad (112)$$

It is a bilinear differential operator defined as

$$\mathbf{O}_1 \star \mathbf{O}_2 = \mathbf{O}_1 \exp\left[i\frac{\hbar}{2}\left(\vec{\partial}_X^\mu \vec{\partial}_p^\mu - \vec{\partial}_p^\mu \vec{\partial}_X^\mu\right)\right] \mathbf{O}_2 \approx \mathbf{O}_1 \mathbf{O}_2 + i\frac{\hbar}{2}\{\mathbf{O}_1, \mathbf{O}_2\}_P + O(\hbar^2), \quad (113)$$

¹⁰While this is the general form for free fermions, it is *not* the most general for bosons, because one can have terms that do not conserve particle number in the hamiltonian, namely $\Psi^\dagger \Psi^\dagger$ and $\Psi \Psi$, while still having free bosons. Such terms generate many interesting complications and nice physics, but are not part of the discussion I want to have here, so let us not consider them.

where the expansion of the exponential can be thought of intuitively as an expansion in powers of \hbar as a small parameter controlling the semiclassical expansion. To the zeroth order (i.e. disregarding completely the X dependence) it's just the normal product and eq.(112) is just the Fourier transformation of the convolution product. To the first order there appears the Poisson bracket $\{\cdot, \cdot\}_P$.

So the time evolution of the density matrix in phase space is

$$\partial_t F(X, p) = -i(H \star F - F \star H), \quad (114)$$

and all the dynamics is contained in the fact that \star is not a commutative product.

To see this even more clearly, assume $H(X, p)$ is already diagonal in the basis that we had chosen, so we don't have to worry about the matrix structure and we have, to the order $O(\hbar^1)$: $\partial_t F(X, p) - \{H, F\}_P = 0$ which is exactly Boltzmann's equation in the free case. It is even clearer if we say for simplicity $H(X, p) = \epsilon(p) + V(X)$, then we see this gives us exactly the lhs of Boltzmann's equation.

6.2 Including the Lorentz force

Now back to the case of free particles. For clarity I'm still considering the case where H, F are diagonal, so we don't have to bother about the matrix structure. What we want to understand now is what happens to sec.6.1 when a magnetic field is applied.

Then, momentum is no longer a good quantum number and instead of (X, p) we will want to use coordinates (R, Π) with $R = X$ and $\Pi = p + eA(X)$. This is not new of course, it's just because under gauge changes $\psi(X) \rightarrow e^{ie\alpha(X)}\psi(X)$ the canonical momentum operator $p = -i\partial_X$ is not preserved, $p \rightarrow p + e\partial_X\alpha$, while the covariant momentum operator $\Pi = p + eA(X)$ is preserved provided the gauge change $A(X) \rightarrow A(X) - \partial_X\alpha$ is simultaneously performed.

For now let us focus on the consequences of such a change of variables in phase space: we will see that it modifies the Poisson bracket. Let us indeed consider two functions $F(X, p), H(X, p)$ and their transformed versions $\tilde{F}(\Pi, R) = F(\Pi - eA, X), \tilde{H}(\Pi, R) = H(\Pi - eA, X)$. Then we can see

$$\begin{aligned} \{F, H\}_P &= \partial_X F \partial_p H - \partial_p F \partial_X H = \partial_X \tilde{F}(p + eA) \partial_p \tilde{H}(p + eA) - \partial_p \tilde{F}(p + eA) \partial_X \tilde{H}(p + eA) \\ &= (\partial_R + e\partial_X A \partial_\Pi) \tilde{F} \partial_\Pi \tilde{H} - \partial_\Pi \tilde{F} (\partial_R + e\partial_X A \partial_\Pi) \tilde{H} \\ &= \partial_R \tilde{F} \partial_\Pi \tilde{H} - \partial_\Pi \tilde{F} \partial_R \tilde{H} + e(\partial_X^\mu A^\nu - \partial_X^\nu A^\mu) \partial_\Pi^\nu \tilde{F} \partial_\Pi^\mu \tilde{H}, \end{aligned} \quad (115)$$

in other words

$$\{F, H\}_P = \{\tilde{F}, \tilde{H}\}_\Pi - e\mathbf{B} \cdot (\partial_\Pi \tilde{F} \times \partial_\Pi \tilde{H}). \quad (116)$$

Now we can apply this directly to the kinetic equation, $\partial_t F - \{H, F\}_P = 0$, which in the covariant coordinates and in terms of these new tilde functions just becomes

$$\partial_t \tilde{F} - \left\{ \tilde{H}, \tilde{F} \right\}_\Pi + e\mathbf{B} \cdot (\partial_\Pi \tilde{H} \times \partial_\Pi \tilde{F}) = 0, \quad (117)$$

or, defining $\tilde{\mathbf{v}} = \partial_\Pi \tilde{H}$ and $\tilde{\boldsymbol{\xi}} = -\partial_X \tilde{H}$:

$$\partial_t \tilde{F} + \tilde{\mathbf{v}} \partial_X \tilde{F} + (\tilde{\boldsymbol{\xi}} - e\tilde{\mathbf{v}} \times \mathbf{B}) \partial_\Pi \tilde{F} = 0. \quad (118)$$

We see that by transforming to the covariant momentum Π we have included the Lorentz force in the kinetic equation. Note that if we had not been able to already include the electric field as a gradient of chemical potential, we could still have done the same as here, but also including gauge transformations of the energy variable ω (and a generalized Moyal product for all of space-time, momentum-energy phase space). I prefer not to do it here for clarity, as the point of the semiclassical approximation is precisely to drop the energy variable.

We can apply exactly the same reasoning to derive the anomalous velocity term. I was not doing it here-inabove just for the sake of efficiency, but since the Berry connection is very much like a vector potential in momentum space, associated to gauge transformations of the Bloch wavefunctions $\psi_{n,\mathbf{k}} \rightarrow e^{i\theta_{n,\mathbf{k}}}\psi_{n,\mathbf{k}}$, this is straightforward. There is one significant difference though, which is that the vector potential of electromagnetism is the same for every electron in every band, and actually does not require to define a band, whereas

the Berry connection is a band-dependent quantity, determined only from knowing the eigensystem of the diagonalised Bloch hamiltonian. Explicitly, define the adapted covariant position operator $R_{n,\mathbf{k}} = X + \mathcal{A}_{n,\mathbf{k}}$, redo all the above steps, and the upshot is

$$\partial_t \tilde{F} + \left(\tilde{v} - \tilde{\xi} \times \Omega \right) \partial_X \tilde{F} + \left(\tilde{\xi} - e\tilde{v} \times \mathbf{B} \right) \partial_{\Pi} \tilde{F} = 0 \quad (119)$$

which recovers, that is to say proves rigorously, the result from the wavepacket analysis.

6.3 Convenient coordinates and the orbital magnetization

Now let us see how one can also obtain the semiclassical energy shift due to orbital magnetization. Here for convenience I take units where the hole charge is $e = 1$. The key step here will be to define a clever change of frame, from the canonical coordinates (\mathbf{x}, \mathbf{p}) to new coordinates (\mathbf{R}, Π) , defined as $\Pi = \mathbf{p} + \mathbf{A}$ (as usual: this is just the canonical moment) and $\mathbf{R} = \hat{\mathbf{z}} \times (\mathbf{p} - \mathbf{A})/B$, which we can interpret as a guiding-center coordinate. This is also the change of coordinate that one encounters in some treatments of the integer quantum Hall effect. Note that this change of variables is only well defined at a finite magnetic field.

It is convenient to choose the gauge $\mathbf{A}(\mathbf{x}) = \frac{1}{2}B\hat{\mathbf{z}} \times \mathbf{x}$, so that $\mathbf{R} = \hat{\mathbf{z}} \times \mathbf{p}/B + \frac{1}{2}\mathbf{x}$ and $\Pi = \mathbf{p} + (B/2)\hat{\mathbf{z}} \times \mathbf{x}$. These coordinates have the very interesting property that they separate the Moyal product: using the chain rule to express $\partial_{\mathbf{x}}, \partial_{\mathbf{p}}$ in terms of $\partial_{\mathbf{R}}, \partial_{\Pi}$, it is not difficult to show that

$$\star = \exp \left[-\frac{iB}{2} \overleftarrow{\partial}_{\Pi} \times \overrightarrow{\partial}_{\Pi} \right] \exp \left[+\frac{i}{2B} \overleftarrow{\partial}_{\mathbf{R}} \times \overrightarrow{\partial}_{\mathbf{R}} \right], \quad (120)$$

with implicit $\hat{\mathbf{z}} \cdot$ in the exponentials. Crucially, the two exponentials commute, and there are no cross-terms so the coordinates are now decoupled.

There is a somewhat subtle step here. We see that the small semiclassical parameter is B , and the semiclassical expansion is no longer in powers of spatial derivatives but instead in powers of Π . Meanwhile, the coordinate one would like to interpret as a guiding center coordinate, \mathbf{R} , is nonperturbative. However one can show that the latter can be treated as a new lattice coordinate, due to magnetic translational symmetry¹¹, so that within a given magnetic unit cell the theory is actually \mathbf{R} -independent. The semiclassical approximation of small B amounts to requiring that the magnetic length be large with respect to other typical lengths in the theory. For large magnetic unit cells i.e. small magnetic fields, this is satisfactory enough and the semiclassical expansion gives correct physical results. Now we will assume this technical step is done, so we are effectively working in momentum space with variable Π and we can forget about \mathbf{R} .

Let us now use this to derive the energy correction due to B and the orbital magnetization. The eigenvalue problem in full generality reads

$$H \star |\psi\rangle = |\psi\rangle \star \epsilon \quad (121)$$

and we will want to solve it perturbatively in powers of ∂_{Π} , starting from the zero-field solution $H|\psi_0\rangle = \epsilon_0|\psi_0\rangle$. Namely we will write $|\psi\rangle = |\psi_0\rangle + |\psi_1\rangle + \dots$ and $\epsilon = \epsilon_0 + \epsilon_1 + \dots$ and solve for $|\psi_1\rangle, \epsilon_1$. An important tool is the normalization condition for eigenstates, which in full generality in phase space will read

$$\begin{aligned} 1 &= \langle \psi | \star | \psi \rangle = \langle \psi_0 | \star | \psi_0 \rangle + 2\text{Re}\langle \psi_0 | \psi_1 \rangle + \dots \\ &= 1 - \frac{1}{2}\mathbf{B} \cdot \Omega + 2\text{Re}\langle \psi_0 | \psi_1 \rangle + \dots \end{aligned} \quad (122)$$

¹¹Let us define $\hat{\mathbf{t}}(\mathbf{l}) = \exp \left[-i\mathbf{B} \cdot (\mathbf{l} \times \hat{\mathbf{R}}) \right]$, the translation operator in the new coordinates, reminiscent of the translation operator of electrons in a lattice leading to Bloch states for instance. This will provide us with a concrete example of *non-commutative geometry*: using Hadamard's lemma one can easily prove that $\hat{\mathbf{t}}(\mathbf{l}_1)\hat{\mathbf{t}}(\mathbf{l}_2) = \exp [i(\mathbf{B}/2) \cdot (\mathbf{l}_1 \times \mathbf{l}_2)] \hat{\mathbf{t}}(\mathbf{l}_1 + \mathbf{l}_2)$. Requiring that this be $\hat{\mathbf{t}}(\mathbf{l}_2)\hat{\mathbf{t}}(\mathbf{l}_1)$, we find the constraint $|\mathbf{l}_x \times \mathbf{l}_y| = 2\pi/B$. This defines the magnetic (square) lattice and the group of magnetic translation operators, $\mathbf{T} = \left\{ \hat{\mathbf{t}}(\mathbf{l}) \mid \mathbf{l} = n_x \mathbf{l}_x + n_y \mathbf{l}_y \right\}$, where $n_i \in \left[\left[1, L_i/\sqrt{2\pi/B} \right] \right]$: the application of a magnetic field breaks continuous translational invariance into a *discrete* translational invariance (in a given gauge), and the system acquires effectively a square lattice structure. The total number of unit cells is the usual degeneracy $N_{\phi} = \frac{B}{2\pi} L_x L_y$, which should be familiar from the physics of Landau level quantization. We can now define Bloch states with given magnetic momentum \mathbf{K} in the mBZ, namely $|\mathbf{K}\rangle = e^{i\mathbf{K}\hat{\mathbf{R}}}|0\rangle$, eigenstates of the magnetic translation operators: $\hat{\mathbf{t}}(\mathbf{l})|\mathbf{K}\rangle = e^{i\mathbf{K}\cdot\mathbf{l}}|\mathbf{K}\rangle$.

where in going to the second line one expanded Eq.(120) and defined $\mathbf{\Omega} = i\langle\psi_0|\overleftarrow{\partial}_{\mathbf{\Pi}}\times\overrightarrow{\partial}_{\mathbf{\Pi}}|\psi_0\rangle$, the Berry curvature (which coincides with the usual definition to lowest order in B).

Now we are in a position to compute the energy spectrum i.e. the eigenvalues (in the generalized phase-space sense of Eq.(121)) of the Peierls-substituted hamiltonian, $H(\mathbf{\Pi})$. Let us thus compute

$$\langle\psi| \star H \star |\psi\rangle = 2\text{Re}\langle\psi_0|H|\psi_1\rangle + \langle\psi_0| \star H \star |\psi_0\rangle \quad (123)$$

$$\begin{aligned} &= \epsilon_0 \left(1 + \frac{1}{2}\mathbf{B}\cdot\mathbf{\Omega}\right) - iB\partial_{\mathbf{\Pi}}\epsilon_0 \times \langle\psi_0|\partial_{\mathbf{\Pi}}\psi_0\rangle \\ &\quad - \cancel{i(B/2)\epsilon_0\langle\partial_{\mathbf{\Pi}}\psi_0|\times|\partial_{\mathbf{\Pi}}\psi_0\rangle} - i(B/2)\langle\partial_{\mathbf{\Pi}}\psi_0|\times(\epsilon_0 - H)|\partial_{\mathbf{\Pi}}\psi_0\rangle \end{aligned} \quad (124)$$

$$\begin{aligned} &= \epsilon_0(\mathbf{\Pi}) - \mathbf{B}\cdot(\partial_{\mathbf{\Pi}}\epsilon_0 \times \mathcal{A}_{\mathbf{\Pi}}) - \mathbf{B}\cdot M \\ &= \epsilon_0(\Pi_x - B\mathcal{A}_y, \Pi_y + B\mathcal{A}_x) - \mathbf{B}\cdot M, \end{aligned} \quad (125)$$

where we identified the Berry connection $\mathcal{A} = i\langle\psi_0|\partial_{\mathbf{\Pi}}\psi_0\rangle$. This recovers the result from the wavepacket analysis, as promised.

It appears useful to define a new momentum coordinate, $\pi_{x,y} = \Pi_{x,y} \mp B\mathcal{A}_{y,x}$ (which looks both familiar and strange since we are shifting *momentum* with the Berry connection and there is this unusual factor of B). As a bonus, we note that in terms of these new coordinates the Moyal product now reads

$$\star = \exp\left[-\frac{iB}{2}\frac{\overleftarrow{\partial}_{\pi}\times\overrightarrow{\partial}_{\pi}}{1+\mathbf{B}\cdot\mathbf{\Omega}}\right], \quad (126)$$

and you recognize in the denominator the phase space jacobian which we had identified previously.

Exercises – A-side

(A.1) Collision integral for bosons and fermions: variational principle

In this exercise, $\eta = \pm$ stands for fermions (+) and bosons (−), respectively. First, as a warm-up, recall the partition function for a free quantum gas, $Z = \prod_{\mathbf{k}} (1 + \eta e^{-\beta \epsilon_{\mathbf{k}}})^\eta$, where the chemical potential is implicitly included in the definition of energies, then from it deduce the thermodynamic potential, $\Omega = -\eta \beta^{-1} \sum_{\mathbf{k}} \ln(1 + \eta e^{-\beta \epsilon_{\mathbf{k}}})$, and the entropy

$$S = \sum_{\mathbf{k}} \{(1 - \eta f_{\eta}) \ln(1 - \eta f_{\eta}) + \eta f_{\eta} \ln(f_{\eta})\}, \quad (127)$$

where f_{η} is the Fermi or Bose distribution, depending on $\eta = \pm$.

Assuming micro-reversibility, the particle-particle collision integral for bosons and fermions takes the form Eq.(12). Recover the local equilibrium bosonic and fermionic distributions, as solution of the detailed-balance condition.

Using $\phi_{\mathbf{k}}$ as defined in the lecture, Eq.(18), and assuming micro-reversibility, show that to first order in ϕ , the particle-particle collision integral takes the form

$$(\mathrm{d}_t f_{\mathbf{k}})_{\mathrm{coll}} = \frac{1}{T} \int_{\mathbf{q}, \mathbf{k}', \mathbf{q}'} \Gamma(\mathbf{k}', \mathbf{q}' | \mathbf{k}, \mathbf{q}) (\phi_{\mathbf{k}'} + \phi_{\mathbf{q}'} - \phi_{\mathbf{k}} - \phi_{\mathbf{q}}) f_{\mathbf{k}}^{\mathrm{eq}} f_{\mathbf{q}}^{\mathrm{eq}} (1 - \eta f_{\mathbf{k}'}^{\mathrm{eq}}) (1 - \eta f_{\mathbf{q}'}^{\mathrm{eq}}). \quad (128)$$

From the formula Eq.(127) for the entropy of a quantum gas, show that Eq.(23) still holds unchanged. Show then the positivity of entropy production.

(A.2) The classical Hall effect in the relaxation time approximation

We now consider the following problem:

$$\partial_t f(\mathbf{k}) - e(\mathbf{E} + \mathbf{v}_{\mathbf{k}} \times \mathbf{B}) \partial_{\mathbf{k}} f(\mathbf{k}) = -\frac{f(\mathbf{k}) - f_{\mathrm{eq}}(\mathbf{k})}{\tau(\mathbf{k})}, \quad (129)$$

in a planar geometry with $\mathbf{B} \perp \mathbf{E}$ and \mathbf{B} pointing out of plane.

First, by integrating Boltzmann's equation against $\mathbf{v}_{\mathbf{k}}$, and assuming constant τ , derive Newton's equation for $\bar{\mathbf{v}} = \int_{\mathbf{k}} \mathbf{v}_{\mathbf{k}} f(\mathbf{k})$. Then show that the (in-plane) resistivity tensor is

$$\boldsymbol{\rho} = \frac{m}{ne^2 \tau} \begin{pmatrix} 1 & \omega_c \tau \\ -\omega_c \tau & 1 \end{pmatrix} \quad (130)$$

– you will find it useful to define $\omega_c = \frac{eB}{mc}$ and $\partial_{\mathbf{k}} \mathbf{v}_{\mathbf{k}} = 1/m$. Why is the Hall resistivity “more universal” than the Hall conductivity? What is the sign of the magnetoresistance?

Now we want to solve the problem for any $\tau(\epsilon_{\mathbf{k}})$. We write $f(\mathbf{k}) = f_{\mathrm{eq}}(\mathbf{k}) + g(\mathbf{k})$ and look for $g(\mathbf{k})$ solving Boltzmann's equation Eq.(129). It is useful to look for a solution of the form $g(\mathbf{k}) = -\mathbf{v}_{\mathbf{k}} \cdot \mathbf{K}(\epsilon_{\mathbf{k}}) n_{\mathrm{F}}'(\epsilon_{\mathbf{k}})$, where $\mathbf{K}(\epsilon_{\mathbf{k}})$ is an unknown vector. Assuming $\tau(\mathbf{k}) = \tau(\epsilon_{\mathbf{k}})$, recast the equation into the form

$$-\frac{e}{mc} \mathbf{v}_{\mathbf{k}} \cdot (\mathbf{B} \times \mathbf{K}) + (\mathbf{K} \cdot \mathbf{v}_{\mathbf{k}}) / \tau(\epsilon_{\mathbf{k}}) = -e \mathbf{E} \cdot \mathbf{v}_{\mathbf{k}}, \quad (131)$$

where the dependence $\mathbf{K}(\epsilon_{\mathbf{k}})$ is implicit. Show that the out-of-equilibrium population reads

$$g(\mathbf{k}) = \frac{e \tau_{\mathbf{k}}^2}{1 + \omega_c^2 \tau_{\mathbf{k}}^2} \mathbf{v}_{\mathbf{k}} \cdot (\mathbf{E} / \tau_{\mathbf{k}} + \frac{e}{mc} \mathbf{B} \times \mathbf{E}) n_{\mathrm{F}}'(\epsilon_{\mathbf{k}}), \quad (132)$$

and conclude.

(A.3) Collision integral from electron-phonon scattering

We will compute the electrons' collision integral from electron-phonon scattering of the form

$$H_{e\text{-ph}} = \int_{\mathbf{k}, \mathbf{k}'} g(\mathbf{k}, \mathbf{k}') c_{\mathbf{k}'}^\dagger c_{\mathbf{k}} \left(a_{-\mathbf{q}}^\dagger + a_{\mathbf{q}} \right), \quad (133)$$

with the shorthand $\mathbf{q} = \mathbf{k}' - \mathbf{k}$. In the limit of quasi-elastic scattering (why?), show eq.(45) in the lecture. Then show that the collision integral reads

$$(d_t f)_{\text{coll}}(\mathbf{k}) = 2\pi \int_{\mathbf{k}'} |g(\mathbf{k}, \mathbf{k}')|^2 (f_{\mathbf{k}'} - f_{\mathbf{k}}) (2n_{\text{B}}(\omega_{\mathbf{q}}) + 1) \delta(\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}) \quad (134)$$

We will now write $g(\mathbf{k}, \mathbf{k}') = -i\gamma_{\mathbf{q}}$. Show that with acoustic phonons, the relaxation time of the electrical current, for momentum k (and any orientation) takes the form

$$\frac{1}{\tau(k)} \approx 2\pi \int_{\mathbf{q}} (1 - \cos(\theta)) |\gamma_{\mathbf{q}}|^2 (2n_{\text{B}}(\omega_{\mathbf{q}}) + 1) \delta(\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}), \quad (135)$$

with $\omega_{\mathbf{q}}$ the phonon dispersion and θ the angle between the two electronic momenta, \mathbf{k} and $\mathbf{k} + \mathbf{q}$. Solving the angular integral, by assuming that the electron dispersion is quadratic with band mass m and that temperature is low, show that

$$\frac{1}{\tau(k)} \approx \frac{m}{2\pi k^3} \int_0^{2k} dq |\gamma_{\mathbf{q}}|^2 q^3 n_{\text{B}}(\omega_{\mathbf{q}}) \quad (136)$$

Assuming a screened Coulomb form $U(r) \sim e^{-k_0 r}/r$ for the electron-ion potential, argue that one can take $|\gamma_{\mathbf{q}}|^2 = A^2 q$ with a constant $A^2 \propto (v_s M k_0^4)^{-1}$ where M is the ionic mass and v_s the sound velocity. Then prove the Bloch-Grüneisen formula eq.(33).

(A.4) Phonon transport and its hydrodynamical limit

We consider thermal transport by acoustic phonons with velocity v from both U- and N- scattering, by assuming relaxation to a local equilibrium distribution of the form

$$f_{\mathbf{k}}(\mathbf{u}) = \left(e^{(\omega_{\mathbf{k}} - \mathbf{u}(\mathbf{r}) \cdot \mathbf{k})/T} - 1 \right)^{-1} \simeq f_{\text{eq}}(\mathbf{k}) + \frac{\mathbf{k} \cdot \mathbf{u}}{T} \frac{e^{\omega_{\mathbf{k}}/T}}{[e^{\omega_{\mathbf{k}}/T} - 1]^2}. \quad (137)$$

We assume two different relaxation rates on the rhs, $\tau_N(\mathbf{k})$ and $\tau_U(\mathbf{k})$, for relaxation to $f(\mathbf{u})$ and f_{eq} , respectively. By defining the combined relaxation rate $\tau_c^{-1}(\mathbf{k}) = \tau_N^{-1} + \tau_U^{-1}$ and convenient parameters $\alpha_{\mathbf{k}}, \beta$ according to

$$f_{\text{eq}, \mathbf{k}} - f_{\mathbf{k}}(\mathbf{u}) = -\alpha_{\mathbf{k}} \frac{\omega_{\mathbf{k}}}{T^2} (\mathbf{v}_{\mathbf{k}} \cdot \nabla T) \frac{e^{\omega_{\mathbf{k}}/T}}{[e^{\omega_{\mathbf{k}}/T} - 1]^2}, \quad (138)$$

$$\mathbf{u} = -\beta v^2 (\nabla T / T), \quad (139)$$

show that the Boltzmann equation takes the simple form $\alpha_{\mathbf{k}} = \tau_c (1 + \beta/\tau_N)$. Show that it is now $\alpha_{\mathbf{k}}$ that appears as the relaxation time in the ‘‘Bloch-Grüneisen-like’’ formula eq.(35). Use the fact that momentum is a collisional invariant of the N-processes to find an equation for β . Show that

$$\beta = \left(\int_0^{\Theta_{\text{D}}/T} dx \frac{\tilde{\tau}_c}{\tilde{\tau}_N} \frac{x^4 e^x}{(e^x - 1)^2} \right) / \left(\int_0^{\Theta_{\text{D}}/T} dx \frac{\tilde{\tau}_c}{\tilde{\tau}_N \tilde{\tau}_U} \frac{x^4 e^x}{(e^x - 1)^2} \right). \quad (140)$$

Comment on the two limits $\tau_N \ll \tau_U$ and $\tau_U \ll \tau_N$.

[End of A-side.]

Exercises – B-side

(B.1) A toy model to build some intuition

We consider the effect of drag between two parabolic bands of fermions with mass m_i , charge $e_i = \pm e$, and carrier density n_i , for $i = 1, 2$. We write directly the hydrodynamic equation as

$$-i\Omega m_i \mathbf{v}_i = e_i \mathbf{E} - \eta n_{\bar{i}} (\mathbf{v}_i - \mathbf{v}_{\bar{i}}), \quad (141)$$

where $\bar{1} = 2, \bar{2} = 1$, with η the drag parameter. Argue for this choice of drag term. Compute the AC conductivity, show that it can be put into the form

$$\sigma(\Omega) = \frac{\Omega_p^2 - \Omega_0^2}{4\pi} \frac{1}{\tau_{ee}^{-1} - i\Omega} + \frac{\Omega_0^2}{4\pi} \frac{i}{\Omega}, \quad (142)$$

where Ω_p^2 , Ω_0^2 and τ_{ee}^{-1} are parameters to be determined. Show in particular that in the compensated case, $n_1 e_1 + n_2 e_2 = 0$, the conductivity takes the simple Drude-like form. Comment on the case where the two bands are just two copies of one same band.

(B.2) Hydrodynamical equations for classical particles

For a gas of classical particles with local mass density $\rho(\mathbf{r}) = m n(\mathbf{r})$, show that the hydrodynamic equation for particle number is $\partial_t \rho + \partial_r(\rho \mathbf{u}) = 0$. Show then that the equation for the momentum $p_i = m v_i$ ($i = x, y, z$) takes the form

$$\left(\partial_t + \langle \mathbf{v} \rangle \partial_r \right) \langle v_i \rangle = \frac{1}{m} \boldsymbol{\xi} - \frac{1}{\rho} \partial_{r_j} P_{ij}, \quad (143)$$

where $\langle \mathbf{v} \rangle$ is the local equilibrium velocity, $\boldsymbol{\xi}$ as usual is the external force, and we have defined the local stress tensor $P_{ij} = \rho \langle w_i w_j \rangle$, with shorthand $w_i = v_i - \langle v_i \rangle$. At this stage, the distribution f (and hence all the $\langle \cdot \rangle$ averages) is yet to be solved for. In the relaxation time approximation with constant τ , and close to local equilibrium given by

$$f_0 = \frac{\rho}{m} (2\pi m T)^{-3/2} e^{-m\omega^2/2T}, \quad (144)$$

show first that $f \approx f_0 + f_1$ with

$$f_1 = -\tau \langle \mathbf{v} \rangle f_0 \left[\frac{1}{\rho} D_t \rho + \frac{m}{T} w_j D_t \langle v_j \rangle - \frac{1}{T} \boldsymbol{\xi} \cdot \mathbf{w} \right], \quad (145)$$

where $D_t \equiv \partial_t + \mathbf{v} \partial_r$, then that $P_{ij} = nT \delta_{ij} + \Pi_{ij}$ with

$$\Pi_{ij} = -\frac{\tau m^4}{T} \Lambda_{kl} \int d\mathbf{w} f_0 w_i w_j (w_k w_l - \frac{1}{3} \delta_{kl} w^2), \quad (146)$$

where f_0 is the *local* Maxwell-Boltzmann distribution and $\Lambda_{ij} = \frac{1}{2} (\partial_i \langle v_j \rangle + \partial_j \langle v_i \rangle)$.

Why can one write $\Pi_{ij} = -2\eta (\Lambda_{ij} - \frac{1}{3} \delta_{ij} \nabla \cdot \mathbf{u})$? You can show, if you really like gaussian integrals, that $\eta = nT\tau$. Comment on the hydrodynamical equation we obtained.

(B.3) Bohr-Sommerfeld \neq Landau-Onsager: an effect of the orbital magnetization

Recall the expression of the Berry curvature, in the Lehmann representation, in terms of matrix elements of $\partial_{\mathbf{k}} \hat{H}$. Find a similar expression for the orbital magnetization. In the particular case of two bands (\pm), show that $\Omega_+ + \Omega_- = 0$ and $\Omega_+ - \Omega_- = 0$, then that in the presence of particle-hole symmetry $\epsilon_{\pm} = \pm \epsilon_0$, the relation $M_{\pm} = e \epsilon_{\pm} \Omega_{\pm}$ holds.

We now consider a metal in a magnetic field. Show that the classical phase accumulated by going around a semiclassical orbit, $\phi_{cl} = \oint \mathbf{p} \cdot d\mathbf{r}$ where $\mathbf{p} = \mathbf{k} - e\mathbf{A}$ (\mathbf{A} the vector potential) and \mathbf{k} obeys Newton's equation, is $\phi_{cl} = S_k/eB = eBS_r$, where S_k and S_r are the areas enclosed by the classical orbit in momentum space and

in real space, respectively. Show that the accumulated Berry phase, obtained from the replacement $\mathbf{r} \rightarrow \mathbf{r} - \mathcal{A}$ with \mathcal{A} the Berry connection, is $\phi_B = \iint \Omega^z d^2k$. Finally you will admit (or remember from Landau and Lifshitz volume 2 paragraph 59) that there is a Maslov phase $\phi_M = -\frac{\pi}{2}m$ where $m = 2$ is the number of turning points of the orbit. Gathering all these results, show the Roth(-Bohr-Sommerfeld) quantization rule for semiclassical orbits:

$$S_k/(eB)^2 = 2\pi \left(n + \frac{m}{4} - \frac{\phi_B}{2\pi} \right). \quad (147)$$

We will now look at the case where the semiclassical orbit is at a fixed quantized energy level $\tilde{\epsilon} = \epsilon - \mathbf{M} \cdot \mathbf{B}$. Show that under the particular assumptions given at the beginning of the exercise, the energy quantization condition reads

$$S_k(\tilde{\epsilon})/(eB)^2 = 2\pi \left(n + \frac{1}{2} \right) - \frac{d}{d\epsilon}(\epsilon \phi_B(\epsilon)). \quad (148)$$

In the very particular case of a gapped Dirac cone, it is possible to show that $\phi_B(\epsilon) = \pi W(1 - \Delta/\epsilon)$, where $W \in \{\pm\}$ is the band's winding number and Δ the gap parameter. Comment on the result.

(B.4) Semiclassical dynamics with disorder: the jump-forward and side-jump effects

We now consider the anomalous Hall effect of electrons in the presence of disorder. The electric field is along x , the magnetic field along z , and the electron dispersion is quadratic. Using the semiclassical equations of motion in the case of a uniform Berry curvature pointing along z , show that the Hall current in the *absence* of impurities is $J_y^{\text{clean}} = \frac{e^2}{4\pi} E_x \Omega^z k_F^2$.

Now when electrons scatter off disorder, show that during a scattering event electrons experience a coordinate shift

$$\delta \mathbf{r} = \boldsymbol{\Omega} \times (\mathbf{k}' - \mathbf{k}) + \dots, \quad (149)$$

and argue why “+...” can be neglected. Now we consider the kinetic equation with collision integral Eq.(17), where $f_{\mathbf{k}}$ and $f_{\mathbf{k}'}$ are the distributions before and after scattering, respectively. Show that if scattering is elastic, implying $\epsilon(\mathbf{k}') - \epsilon(\mathbf{k}) = eE_x \delta r_x$, the local equilibrium solution is no longer the Fermi distribution n_F but instead undergoes a “jump-forward” distortion,

$$f_{\text{loceq}}(\mathbf{k}) = n_F(\epsilon_{\mathbf{k}}) + \partial_{\epsilon} n_F(\epsilon_{\mathbf{k}}) e E_x k_y \Omega_z. \quad (150)$$

From this deduce that there is another contribution to the anomalous Hall current, $J_y^{\text{jf}} = -\frac{e^2}{4\pi} E_x \Omega^z k_F^2$.

Besides, happening at a rate $1/\tau$, electrons undergo a side-jump shift δr_y whence a drift velocity $v_y^{\text{sj}} = \sum_{\mathbf{k}'} \Gamma_{\mathbf{k}, \mathbf{k}'} \delta r_y$. Recall why $1/\tau = \sum_{\mathbf{k}'} \Gamma_{\mathbf{k}, \mathbf{k}'} (1 - \cos \theta_{\mathbf{k}, \mathbf{k}'})$ and show that $v_y^{\text{sj}} = -\Omega^z k_x / \tau$. Solving the classical Boltzmann's equation the usual way, assuming the conditions for RTA are met, show that there is a third contribution to the anomalous Hall current, $J_y^{\text{sj}} = -\frac{e^2}{4\pi} E_x \Omega^z k_F^2$. Comment on the final result: what is the Hall conductivity? What is striking about its dependence on disorder? What are experimental implications?

[End of B-side.]

Supplementary material: classical Hall effects in the RTA

Classical Hall conductivity in the relaxation time approximation

Let us come back to an isotropic Fermi surface of electrons in the relaxation time approximation, and this time apply an electric and a magnetic field:

$$\partial_t f(\mathbf{k}) - e(\mathbf{E} + \mathbf{v}_\mathbf{k} \times \mathbf{B}) \partial_\mathbf{k} f(\mathbf{k}) = -\frac{f(\mathbf{k}) - f_{\text{eq}}(\mathbf{k})}{\tau(\mathbf{k})} \quad (151)$$

In principle one must worry that \mathbf{k} is no longer a good quantum number, but for now we can just assume that the cyclotron frequency $\omega_c = \frac{eB}{mc}$ is much smaller than temperature, $\omega_c \ll T$, so that our kinetic theory can still be relied upon.

Then there are at least two ways one can proceed. The first follows the ‘‘hydrodynamical’’ idea of integrating Boltzmann’s equation against $\mathbf{v}_\mathbf{k}$, then assuming constant τ and upon integration by parts one gets

$$\partial_t \bar{v} + \frac{\bar{v}}{\tau} = -e \int \frac{d^3 \mathbf{k}}{(2\pi)^3} f(\mathbf{k}) \partial_\mathbf{k}^\nu (E^\nu \mathbf{v}_\mathbf{k} + (\mathbf{v}_\mathbf{k} \times \mathbf{B})^\nu \mathbf{v}_\mathbf{k}) = -\frac{e}{m} (\mathbf{E} + \bar{v} \times \mathbf{B}) \quad (152)$$

where and defined $\bar{v} = \int_\mathbf{k} \mathbf{v}_\mathbf{k} f(\mathbf{k})$ and $\partial_\mathbf{k} \mathbf{v}_\mathbf{k} = 1/m$.

Let us consider a planar geometry with $\mathbf{B} \perp \mathbf{E}$ for simplicity, with \mathbf{B} pointing out of plane, then we get the (in-plane) resistivity tensor

$$\rho = \frac{m}{ne^2 \tau} \begin{pmatrix} 1 & \omega_c \tau \\ -\omega_c \tau & 1 \end{pmatrix} \quad (153)$$

which is the usual Drude-like result. Two useful physical things to notice: the Hall resistivity does not depend on the relaxation time τ , and the longitudinal conductivity $\sigma_L = \frac{ne^2 \tau}{m} (1 + \omega_c^2 \tau^2)^{-1}$ decreases with increasing magnetic field, which means there is a positive magnetoresistance.

This was the first way, now the second way is to just solve Boltzmann’s equation and plug the result into the current. We can write again $f(\mathbf{k}) = f_{\text{eq}}(\mathbf{k}) + g(\mathbf{k})$ and look for $g(\mathbf{k})$. To zeroth order (i.e. replacing f by f_{eq} on the lhs, which is what we do usually, cf sec 2.2 for instance) the Hall current vanishes, because $\partial_\mathbf{k} f_{\text{eq}}(\mathbf{k}) \propto \mathbf{v}_\mathbf{k}$ and $\mathbf{v}_\mathbf{k} \cdot (\mathbf{v}_\mathbf{k} \times \mathbf{B}) = 0$. So we expand the lhs completely:

$$-e(\mathbf{v}_\mathbf{k} \cdot \mathbf{E}) n'_F(\epsilon_\mathbf{k}) - \frac{e}{c} (\mathbf{v}_\mathbf{k} \times \mathbf{B}) \partial_\mathbf{k} g(\mathbf{k}) = -g(\mathbf{k})/\tau(\mathbf{k}). \quad (154)$$

We can look for a solution of the form $g(\mathbf{k}) = -\mathbf{v}_\mathbf{k} \cdot \mathbf{K}(\epsilon_\mathbf{k}) n'_F(\epsilon_\mathbf{k})$, where $\mathbf{K}(\epsilon_\mathbf{k})$ is an unknown vector which we can imagine will be proportional (if not parallel) to the electric field, and we will see this is the case. Assuming $\tau(\mathbf{k}) = \tau(\epsilon_\mathbf{k})$, we can recast eq.(154) into the form

$$-\frac{e}{mc} \mathbf{v}_\mathbf{k} \cdot (\mathbf{B} \times \mathbf{K}) + (\mathbf{K} \cdot \mathbf{v}_\mathbf{k})/\tau(\epsilon_\mathbf{k}) = -e\mathbf{E} \cdot \mathbf{v}_\mathbf{k}, \quad (155)$$

where $\mathbf{K}(\epsilon_\mathbf{k})$ is implicit. At given $\epsilon_\mathbf{k}$, there is only one unknown \mathbf{K} but many different equations (one for each $\hat{\mathbf{v}}_\mathbf{k}$), so in fact we must have $\frac{e}{mc} (\mathbf{B} \times \mathbf{K}) = \mathbf{K}/\tau(\epsilon_\mathbf{k}) + e\mathbf{E}$. We can solve this, again assuming $\mathbf{B} \perp \mathbf{E}$ with out-of-plane \mathbf{B} for simplicity, and this yields the out-of-equilibrium population

$$g(\mathbf{k}) = \frac{e\tau_\mathbf{k}^2}{1 + \omega_c^2 \tau_\mathbf{k}^2} \mathbf{v}_\mathbf{k} \cdot (\mathbf{E}/\tau_\mathbf{k} + \frac{e}{mc} \mathbf{B} \times \mathbf{E}) n'_F(\epsilon_\mathbf{k}). \quad (156)$$

We can then plug it into the current, and the result looks very much like eq.(153) except that we solved the problem for any $\tau(\epsilon_\mathbf{k})$ now.

Skew-scattering and the thermal Hall effect

The thermal Hall effect in insulators cannot be explained, as above, by the Lorentz force on the lhs of the equation, because in insulators all energy carriers are neutral particles and they don’t feel directly the electromagnetic field. One other way neutral particles may still carry a thermal Hall current is from skew-scattering. We will illustrate this with an example.

We consider Boltzmann's equation for bosonic neutral quasiparticles, dispersing linearly with velocity v , and for convenience we assume there are three degenerate polarizations. We focus on particle-conserving scattering. Then Boltzmann's equation in a thermal gradient reads

$$-v^2 \mathbf{k} \cdot (\nabla T/T) n'_B(\omega_{\mathbf{k}}) = \int \frac{d^3 \mathbf{k}'}{(2\pi)^3} [\Gamma(\mathbf{k}|\mathbf{k}') f(\mathbf{k}') - \Gamma(\mathbf{k}'|\mathbf{k}) f(\mathbf{k})] \quad (157)$$

We assume elastic scattering by impurities, and the essential features are then captured by

$$\Gamma(\mathbf{k}'|\mathbf{k}) = \frac{\tau^{-1}(\omega)}{4\pi} \left(1 - \gamma(\omega) \mathbf{B} \cdot (\hat{\mathbf{k}} \times \hat{\mathbf{k}}') \right), \quad (158)$$

where ω is the (incoming and outgoing) boson energy. The first term is just the relaxation time approximation, but the second term is new: we see it is odd upon exchanging incoming and outgoing momenta. Such a skew-scattering rate can only be nonzero if the impurities break time reversal symmetry, and in practical cases there are more hidden constraints, for instance disorder should be correlated, or one should instead consider *inelastic* scattering and make sure to break detailed balance (which implies to go beyond the first Born's order), etc. Let us just assume that by some subtle mechanism this term is present in the effective collision integral.

To solve Boltzmann's equation, we expand around equilibrium $f(\mathbf{k}) = f_{\text{eq}}(\omega_{\mathbf{k}}) + g_+(\mathbf{k}) + g_-(\mathbf{k})$, and intuition (by analogy with what we did in sec.6.3) dictates we must look for $g_+(\mathbf{k}) \propto \mathbf{k} \cdot \nabla T$ and $g_-(\mathbf{k}) \propto \mathbf{k} \cdot (\mathbf{B} \times \nabla T)$. It is not difficult to find the solution

$$g_+(\mathbf{k}) + g_-(\mathbf{k}) = \frac{v^2 \tau(\omega_{\mathbf{k}})}{T} n'_B(\omega_{\mathbf{k}}) \{ \mathbf{k} \cdot \nabla T - \gamma(\omega_{\mathbf{k}}) \mathbf{k} \cdot (\mathbf{B} \times \nabla T) \}. \quad (159)$$

We can now plug this solution into the current and extract the thermal conductivity, which (assuming the same planar geometry as usual) reads

$$\kappa_{xx} = \frac{T^3}{2\pi^2 v} \int_0 dx \tilde{\tau}(x) \frac{x^4 e^x}{(e^x - 1)^2}, \quad \kappa_{xy} = \frac{T^3}{2\pi^2 v} B_z \int_0 dx \tilde{\tau}(x) \tilde{\gamma}(x) \frac{x^4 e^x}{(e^x - 1)^2}, \quad (160)$$

where we defined $\tilde{\tau}(x) = \tau(Tx)$, $\tilde{\gamma}(x) = \gamma(Tx)$. The first equation is just eq.(35) again, and the second one is the thermal Hall conductivity, which as expected is proportional to B_z .

In fact, the above model is not realistic in the general case because most bosonic energy carriers (like phonons or magnons) are not conserved, and so scattering events involving them are usually strongly inelastic and not number-conserving. As mentioned above, getting eq.(158) as an effective elastic scattering rate is far from obvious for a realistic model, and only in specific cases does it provide the relevant form of the collision integral.

SM: rigorously including more effects into the QKE

Including interactions in the QKE

This section is voluntarily a bit handwaving. One may worry about something: in the above, and more generally in Boltzmann's equation, we look at the density matrix $F(r_1, r_2)$ with implicit time dependence t , which means we are looking at the specific case $t_1 = t_2 = t$ of the more general

$$\varrho_{ab}(r_1, t_1; r_2, t_2) := \langle \psi_a^\dagger(r_1, t_1) \psi_b(r_2, t_2) \rangle, \quad (161)$$

which is really the kind of objects describing the full quantum evolution of the system. In phase space, we would then look at its space-time Wigner transform $\varrho(X, p; t, \omega)$, with an extra energy variable ω which is absent in the semiclassical approaches we have been using and deriving until now. When is it safe to disregard this ω dependence?

First one can notice that this complication is nontrivial only in the interacting case, indeed if we take free particles with dispersion $\epsilon_{\mathbf{p}}$ (and if for clarity we assume a uniform, constant problem) then the Wigner transform of eq.(161) reduces to

$$\varrho(p, \omega) = \int dx dt e^{-ipx} e^{i\omega t} \langle \psi^\dagger(x, t) \psi(0, 0) \rangle = 2\pi \delta(\omega - \epsilon_{\mathbf{p}}) \langle \psi_{\mathbf{p}}^\dagger \psi_{\mathbf{p}} \rangle = 2\pi \delta(\omega - \epsilon_{\mathbf{p}}) n_{\text{eq}}(\epsilon_{\mathbf{p}}), \quad (162)$$

and we can drop the ω dependence as this energy variable is constrained to be “on-shell” and discarding it does not lose any information.

On the contrary, in interacting systems, the density matrix F does not contain all the information. For instance, we expect that the $\delta(\omega - \epsilon_p)$ in eq.(162) will be broadened, basically like the spectral function of the ψ excitations. More generally, the complete information about the time evolution of interacting quantum systems out of equilibrium cannot be accessed by means of the equation of motion for the density matrix, and instead will be given by full-fledged out-of-equilibrium quantum field theory.

The corresponding more proper way to derive the kinetic equation from a purely quantum standpoint is the Kadanoff-Baym-Keldysh method. In this method, the unknown of the kinetic equation is the distribution F , which has a precise definition but let me skip the details – roughly speaking it is defined by

$$\varrho(X, p, t, \omega) \simeq 2\pi A(p, \omega) F(X, p, t, \omega), \quad (163)$$

with $A(p, \omega)$ the spectral function.

Then the effect of interactions on the lhs is, as always, through the self-energy corrections to kinetic quantities. If we write the retarded self-energy $\Sigma = \Sigma' + i\Sigma''$, there is a correction to the quasiparticle weight $\tilde{Z}^{-1} = 1 - \partial_\omega \Sigma'$, a modification of the velocity $\tilde{v} = \partial_p(\epsilon_p + \Sigma')$ and of the force $\tilde{\xi} = -\partial_X(V + \Sigma')$, where $V(X)$ is the local potential. Then it can be shown that the quantum Boltzmann’s eqn takes the form

$$\boxed{\left(\tilde{Z}^{-1} \partial_t + \tilde{v} \partial_X - \tilde{\xi} \partial_p \right) \tilde{F} = \mathcal{I}_{\text{coll}} \left[\tilde{F}, \Sigma, \dots \right]}. \quad (164)$$

Here we defined $\tilde{F}(X, p, t, \zeta) = F(X, p, t, \omega)$ with $\zeta = \omega - \epsilon_p - V - \Sigma'$, and the dots contain another object which I have not defined here (namely, the Keldysh self-energy). At this stage, this equation is exact (it is just a rewriting of Dyson’s equation), and it is a complicated problem to solve.

The next step is where the semiclassical approximation comes in. The first part of the idea is to say that we have well-defined quasiparticles, which propagate freely without dispersion between two scattering events. In practice, this means that in the free dynamics (the lhs), we accept the energy shift given by Σ' , but we do not include the effect of the broadening by Σ'' of the propagator. That is to say, we project onto the mass shell defined by $\zeta = 0$ – and then we see that $\tilde{F}(\zeta = 0)$ plays basically the same role as F introduced in the previous section. The second part of the semiclassical approximation is to assume that the quasiparticles remain reasonably well-defined during a scattering event. This is a crucial assumption, which ensures we are allowed to talk about “collisions” between otherwise essentially free particles. In practice, this means

$$\mathcal{I}_{\text{coll}} \left[\tilde{F}(X, p, t, \zeta), \Sigma(X, p, t, \zeta), \dots \right] \rightarrow \mathcal{I}_{\text{coll}} \left[\tilde{F}(X, p, t, 0), \Sigma(X, p, t, \zeta), \dots \right]. \quad (165)$$

Why we are arguably allowed to do this is because the way F is defined (cf eq.(163)), it always multiplies a very peaked function, with a typical width Σ'' which we can argue is small. Meanwhile, if we are close to equilibrium, we have $\tilde{F} \approx \tilde{F}_{\text{eq}}$, and we know the latter is a smooth function of ζ/T . So it seems, and this is what is argued in more field-theoretical oriented books (e.g. Kamenev’s one), that as long as $\Sigma'' \ll T$, the approximation eq.(165) is reasonable – this is the Peierls criterion.

For phonons this criterion looks fine, but even for Bloch electrons in metals it is broken, $\Sigma'' \sim T$, and of course things get much worse with less well-defined quasiparticles. Therefore Landau argued that quasiparticles do not care what the equilibrium distribution is, and the only relevant scale with which to compare the self-energy is the particle energy, so instead we obtain the Landau criterion: $\Sigma'' \ll \epsilon$. The latter turns out to be the correct criterion for usual practical cases, but why this should be anything more than a leap of faith is not at all obvious. ¹²

¹²In fact the Peierls criterion is a sufficient requirement, but it is not necessary: it can also happen that we are lucky and there is another small parameter in the collision integral which ensures that $\tilde{F}(\zeta)$ is multiplied by some very peaked (possibly with width even much smaller than Σ'') function of ζ . For instance, if we consider elastic scattering by impurities, energy conservation provides us automatically with $\delta(\zeta)$. For electron-phonon interaction in metals, there is a similar argument, because phonon momentum is much smaller than electron momentum, and same for velocities. It’s a bit subtle and we don’t have time for all this, but it goes under the name of “quasi-classical approximation” and one can learn about it in chapter 7.5 of Jørgen Rammer’s book. Interesting discussions can be found in Peierls chapter 6.8 and Ziman chapter 5.12 about the Peierls and Landau conditions.

Unified phase space derivation of the semiclassical corrections

We are now going to apply roughly the same recipe as in the main text. So here we will have to re-introduce the matrix structure of \mathbf{F}, \mathbf{H} as in sec.6.1, and our first task will be to define properly what we mean by diagonalization in a system with broken translational invariance.

The proper way to define the diagonalization of the hamiltonian matrix \mathbf{H} is through the Moyal product \star . One has to find the “unitary” matrix \mathbf{U} (with inverse defined as $\mathbf{U} \star \mathbf{U}^{-1} = 1 = \mathbf{U}^{-1} \star \mathbf{U}$) such that

$$\mathbf{H}_d = \mathbf{U}^{-1} \star \mathbf{H} \star \mathbf{U} \quad (166)$$

is diagonal. One can show that the functions of (X, k) appearing on its diagonal are real functions, which we can identify as the energies. Also note that \mathbf{U} is a unitary matrix in the usual sense only to lowest order in the \hbar expansion of the Moyal product.

Then, one can rewrite $\mathbf{F} = \mathbf{U} \star \mathbf{F}_d \star \mathbf{U}^\dagger$, and look for solutions of the problem where \mathbf{F}_d is a diagonal matrix. Each of its entries is real by definition, and so it can be identified as the distribution function for the particles in the corresponding band.

In terms of these newly obtained matrices $\mathbf{H}_d, \mathbf{F}_d$ the kinetic equation reads

$$\partial_t \mathbf{F}_d(X, p) = -i (\mathbf{H}_d \star \mathbf{F}_d - \mathbf{F}_d \star \mathbf{H}_d). \quad (167)$$

We see that since \mathbf{H}_d is diagonal by construction, and since we look for solutions with \mathbf{F}_d diagonal, this equation is diagonal in the basis of bands, and the kinetic equation for the distribution in each band is independent from the others (recall that we are considering the free case, without the rhs).

The diagonalization procedure eq.(166) is not unique. Instead, there is a gauge freedom to define the phase of the eigenvectors, $\mathbf{U} \rightarrow \mathbf{U} \star e^{i\theta}$, with the diagonal matrix of phases $\theta = \text{diag}(\theta_1, \dots, \theta_N)$ where N is the number of bands (i.e. the number of entries in the vectors Ψ , i.e. the number of rows and columns of \mathbf{F}, \mathbf{H} , etc). Under such a gauge transformation, the diagonalized version of the matrix $\mathbf{Q} = \mathbf{F}, \mathbf{H}$, which is a function of $q = (X, p)$, transform as $\mathbf{Q}_d \rightarrow \mathbf{Q}'_d(q) = \mathbf{Q}_d(q) - \hbar \{ \mathbf{Q}_d, \theta \}_P + \dots = \mathbf{Q}_d(q')$, where in the last step we defined the new coordinates $X' = X - \partial_p \theta$ and $p' = p + \partial_X \theta$. This shows that a gauge transformation is equivalent to a (band-dependent!) change of coordinates in phase space.

To define covariant coordinates, we can introduce the gauge connection $\mathbf{A}_\alpha = \text{Im}(\mathbf{U}^{-1} \star \partial_\alpha \mathbf{U})^{(d)}$, where $\alpha = X_\mu, p_\mu$. This connection transforms as $\mathbf{A}_\alpha \rightarrow \mathbf{A}_\alpha + \partial_\alpha \theta$. Then, similarly to the tilde quantities we introduced in sec.6.2, we can define underlined quantities:

$$\underline{\mathbf{Q}}_d(q) = \mathbf{Q}_d(X + \mathbf{A}_p, p - \mathbf{A}_X) \quad \rightarrow \quad \underline{\mathbf{Q}}'_d(q) = \dots = \underline{\mathbf{Q}}_d(q). \quad (168)$$

These quantities are now gauge invariant (and still real), and thus describe the true physical quantities, namely energy and distribution function. This is the reason for the change of coordinates $p \rightarrow \mathbf{\Pi}$ we introduced in sec.6.2, which in the language we just introduced was the special case of $\mathbf{A}_p = 0$ and band-independent \mathbf{A}_X .

We can now redo the same calculation as eq.(115), with the modification of the Poisson brackets now being band-dependent and involving a modification of both p and X variables. Defining the generalized Berry curvature $\Omega_{\alpha, \beta} = \partial_\alpha \mathbf{A}_\beta - \partial_\beta \mathbf{A}_\alpha$, where α, β can be any X_μ, p_ν , we obtain the free kinetic equation

$$\boxed{(\partial_t + \underline{\mathbf{v}} \cdot \underline{\partial}_X + \underline{\boldsymbol{\xi}} \cdot \underline{\partial}_p) \underline{\mathbf{F}}_d = 0,} \quad (169)$$

with the proper semiclassical equations of motion appearing on the lhs,

$$\boxed{\underline{v}_\mu = \partial_{p_\mu} \underline{\mathbf{H}}_d - \Omega_{p_\mu, p_\nu} \partial_{X_\nu} \underline{\mathbf{H}}_d + \Omega_{p_\mu, X_\nu} \partial_{p_\nu} \underline{\mathbf{H}}_d} \quad (170)$$

$$\boxed{\underline{\xi}_\mu = -\partial_{X_\mu} \underline{\mathbf{H}}_d + \Omega_{X_\mu, X_\nu} \partial_{p_\nu} \underline{\mathbf{H}}_d - \Omega_{X_\mu, p_\nu} \partial_{X_\nu} \underline{\mathbf{H}}_d.} \quad (171)$$

We recognize the Berry curvature Ω_{p_μ, p_ν} and $-e$ times the magnetic field Ω_{X_μ, X_ν} . This proves that indeed, in the homogeneous case, the correct lhs in Boltzmann’s equation is given by Niu’s semiclassical equations of motion eqs.(80), (81). There is however a new ingredient: these mixed curvatures Ω_{X_μ, p_ν} , which exist only in inhomogeneous theories where Berry’s connection depends on position.