A Kinetic Theory for Quantum Transport in Aperiodic Media

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Abstract

Transport theory is reinvestigated in a one-particle model including dissipation mechanisms through a phenomenological time dependent part. Using the description of an aperiodic crystal in terms of non-commutative geometry, it is then possible to rigorously derive Kubo formulæ for the electric conductivity. Within the framework of the relaxation time approximation, a fractal analysis applied to the spectral measures entering in the Kubo formula allows to examine anomalous transport owing to quantum interferences. This leads to anomalies in Drude's formula.

Keywords: Kubo formula in aperiodic media, anomalous transport

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1 Introduction

The purpose of this work is to explore the mathematical properties of a model introduced in [11] to describe dissipation mechanisms leading to the linear response theory for electronic transport in periodic or aperiodic homogeneous media. Once this model is accepted, Kubo's formula can be proved rigorously and the linear response theory justified. In this work, we will describe the general formalism and restrict further investigations to the case of the relaxation time approximation (RTA). We will leave the more detailed descriptions needed at low temperature for a forthcoming work.

The main idea is the following: in first approximation, the conduction electrons in a solid are considered to be individual particles (electrons or holes), with no interactions between them, neither with any other type of particles, except for the quenched potential created by the fixed nuclei. This approximation led in the late twenties to the band theory for perfect crystals that was very successful in understanding the electronic properties of solids. Here we just add the possibility of having the electron moving in some aperiodic crystal. This is what happens in quasicrystals [17, 54, 14, 38, 53, 27], in slightly disordered systems [3, 57, 58, 1, 34] such as amorphous metals and strongly doped semiconductors and also in strongly disordered systems such as impurity bands in lightly doped semiconductors at low temperature [52]. This latter situation occurs on the plateaus of the integer quantum Hall effect (IQHE) [33, 59, 7, 5, 11, 42]. Instead of introducing a many-body theory to describe the exchange of energy with other type of excitations, the charge carriers are supposed to experience some *random quantum jumps*, called *collisions* in this article, at *random times*. We will just give few examples of possible choices for such processes here, leaving a more systematic description for a forthcoming work. The linear response theory is recovered by a time average of the instantaneous quantum evolution. This averaging introduces a loss of information liable to describe dissipation.

The idea behind this model is not new. As early as 1900, Drude [20] introduced it in a classical kinetic theory describing the electron gas. Since then it was used in many works such as the Kubo-Toyabe model for nuclear magnetic resonance [24]. It is also very similar to Boltzmann's kinetic theory (see [29] for instance). This method has recently been the focus of attention in quantum optics because it provides a convenient tool for numerical calculations of optical response by means of Monte-Carlo simulations [40, 22]. In this context, it is related to the old idea of Einstein [21] according to which individual quantum systems experience quantum jumps from one state to another when absorbing or emitting energy. In solid state physics, by analogy, electrons or holes are absorbing or emitting other excitations present in the solid, especially phonons.

The RTA consists in summarizing all dissipative effects into a unique parameter, the *relaxation time*, describing the effective average time separating two consecutive collisions [4].
Despite the coarseness of this approach, one can already say something non trivial with it. In particular, one can derive Kubo's formula on a rigorous mathematical ground and justify the validity of the linear response. Applied to the IQHE [11], it gives a rough estimate of the plateaus accuracy and provides a qualitative explanation of the interplay between the strong localization and the mobility of the sample. In the case of aperiodic media, the quantum evolution of an individual electron or hole may cause the usual Drude formula to fail even in the RTA [12, 50, 51]. The reason is that quantum interferences may slow down the wave packet in an unusual way. This has been used recently as a test of Aubry's duality for two dimensional Bloch electrons in a uniform magnetic field [6].
The RTA is, however, too rough to take into account low temperature effects. This is the main criticism against the RTA in [11] to estimate the accuracy of the Hall plateaus in the IQHE. For indeed, the variable range hopping mechanism [52], proposed by Mott [39] to describe the low temperature conductivity of insulators, introduces a prefactor in the direct conductivity decreasing the error by at least four orders of magnitude. This is crucial to explain why the Hall conductance measurement provides a new standard of resistance [56]. To go beyond the RTA, we must consider that the test particles undergoes several kinds of quantum jumps, each of which with its own time delay. This will be developed elsewhere.

The article is organized as follows. In this chapter, we motivate the model for transport as well as the mathematical description of aperiodic homogeneous media and then present the main results of the article, that is the Kubo formula with dissipative term and the anomalous Drude formula. In Chapter 2, we give a more detailed mathematical description of the model and discuss its physical validity. In order to make the physical content of the chapter more transparent, we again only give elementary and short arguments of some crucial points. In Chapter 3, the mathematical formalism needed for treating time dependent external fields is described and the main results are proved.

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1.1 No-go theorems

When trying to compute the current of a system of independent charged classical or quantum particles submitted to an external electric field $\vec{\mathcal{E}}$ without possibility to dissipate, one immediately runs into the following dichotomy: the conductivity is either zero or infinite. If the one-particle Hamiltonian H is given by $\vec{p}^{\,2}/2m$, then every particle is continuously accelerated and the current is infinite. If the Hamiltonian is bounded, then the time averaged current projected in the direction of the electric field vanishes (see [11] and Proposition 6 below). For indeed, the current is defined as $\vec{\jmath} = q\, d\vec{x}/dt$ where q and $\vec{x}$ are the charge and the position of the carrier. Let $\mathcal{L}_A(B) = \{A, B\}$ define the Liouville operator acting on observables by means of the Poisson bracket. Then $\vec{\jmath}(t) = e^{t\mathcal{L}_{H-q\vec{\mathcal{E}}\cdot\vec{x}}}(\vec{\jmath})$ if a DC electric field $\vec{\mathcal{E}}$ is added. The time average of the current is given by

$$\langle \vec{\jmath} \rangle \;=\; \lim_{t\to\infty} \int_0^t \frac{dt'}{t}\, \vec{\jmath}(t') \;=\; \lim_{t\to\infty} \int_0^t \frac{dt'}{t}\, e^{t'\mathcal{L}_{H-q\vec{\mathcal{E}}\cdot\vec{x}}}(\vec{\jmath}) \tag{1}$$

Noting that $\vec{\mathcal{E}} \cdot \vec{\jmath}(t') = -\mathcal{L}_{H-q\vec{\mathcal{E}}\cdot\vec{x}}(H(t')) = -dH/dt'$, we get

$$\vec{\mathcal{E}} \cdot \langle \vec{\jmath} \rangle \;=\; \lim_{t\to\infty} \frac{H - H(t)}{t} \;=\; 0\;, \tag{2}$$

whenever H is bounded. When transposed to quantum mechanics ($\{A, B\}$ is replaced by $\imath[A, B]/\hbar$), the same argument shows that the conductivity computed in this way should always vanishes for a lattice Hamiltonian no matter whether it is periodic or not! For a periodic Hamiltonian, this phenomenon is well known in solid state physics as Bloch oscillations [28]. An extension of this result to AC fields is proved in Proposition 6 in Chapter 3.

The reason for these results to hold is the absence of dissipation mechanisms. In solids, dissipation is due to exchange of energy and momentum with other type of excitations, mainly with phonons. These interactions will be modeled by a random collisional process. In order to motivate our approach and to explain its kinetics, we recall next the Drude model of classical.

1.2 Drude's kinetic theory

We consider a model of classical, non relativistic, free particles of mass m and charge q. The Hamiltonian of such a particle is $H = \vec{p}^{\,2}/2m$ where $\vec{p}$ is its momentum. We assume that a test particle is scaterred at random times $(t_l)_{l\in\mathbf{Z}}$ with $t_l < t_{l+1}$ such that the time delays $t_l - t_{l-1}$ between collisions be independent, identically distributed random variables with common distribution $dt/\tau \exp(-t/\tau)$ on $[0, \infty)$. At each collision, the direction of the momentum is changed randomly according to the uniform distribution on the $(d-1)$-sphere, but its modulus is conserved. Each collision is stochastically independent from the others. If we denote by R_l the random rotation acting on $\vec{p}$ at the time t_l, the phase space orbit of a test particle is computable entirely in terms of the random sequence $\xi = (t_l, R_l)_{l\in\mathbf{Z}}$. We will denote by $\mathbf{E}_\xi$ the ergodic average over the random variable ξ. Using Birkhoff's ergodic theorem, the time averaged current can be computed as in (1) to give:

$$\mathbf{E}_\xi(\langle \vec{\jmath} \rangle) \;=\; \lim_{\delta\to 0} \delta \int_0^\infty dt\, e^{-\delta t}\, \mathbf{E}_\xi(\vec{\jmath}(t)) \;=\; \frac{q^2 \vec{\mathcal{E}} \tau}{m}\,. \tag{3}$$

Let n be the particle density. The conductivity σ is defined as the linear coefficient of the current density $n\mathbf{E}_\xi(\langle \vec{\jmath} \rangle)$ with respect to the electric field. As a consequence, it is given by the

Drude formula

$$\sigma \;=\; \frac{q^2 n\tau}{m} \;. \tag{4}$$

Note that, during each collision, there is a momentum transfer from the particle to the scatterer, but no energy transfer in this model (elastic collisions). Although this is sufficient to calculate the mean current, a closer look shows that the particle gets faster and faster, namely $\mathbf{E}_\xi(\vec{p}^{\,2}(t)) \approx 2q^2\vec{\mathcal{E}}^2\tau t$. This undesired feature goes along with the impossibility to treat the Joule effect in the present model. Actually, Drude's formula results from the limit and averaging procedure in (3).

We can take the Joule effect into account if we allow for energy transfer from particles to scatterers during each collision. The scatterers are supposed to form a bath at temperature T. We suppose that the outcome of the collision at time t_l is characterized by a momentum transfer $\delta\vec{p}_l$ distributed according to Maxwell's law with temperature T. One obtains the same Drude formula. But the energy of the particle is bounded and there is Joule heating of the scatterers with an energy transfer per unit time given by $W = q^2\vec{\mathcal{E}}^2\tau/m$. This second model was proposed by Drude in 1900 [20], whereas the model with elastic collisions could be referred to as the simplified Lorentz model [35].

A complementary way to look at the collision process above is to study the diffusion of a particle in absence of an external electric field. One then considers the mean square displacement:

$$\mathbf{E}_\xi((\vec{x}(t)-\vec{x}(0))^2) \;=\; 2dD\left(t-\tau\left(1-e^{-\frac{t}{\tau}}\right)\right) \;, \tag{5}$$

where $D = k_B T\tau/m$ is the diffusion coefficient and k_B is the Boltzmann constant. In other words, the motion is diffusive, a necessary condition to get the Ohm law. In this case the Einstein relation $\sigma = q^2 nD/k_B T$ between conductivity and diffusion coefficient is satisfied.

A generalized version of the Drude model allowing to study the kinetics of anomalous transport was considered in [49]. There it is shown, in particular, that replacing the exponential law for the time delays by another law only changes some numerical constants in the above formulæ as long as this law has a finite second moment.

1.3 A kinetic quantum model in a perfect crystal

If one considers electrons in a perfect crystal, the Drude kinetic theory leads to several problems when compared to experimental results (see [4] chap 1-3 for a complete discussion). Right after the discovery of Pauli's principle, Sommerfeld introduced the quantization of free electrons to improve upon Drude's theory. However, electrons in metals are not free and band theory, developped by Bloch and Brillouin, is necessary[16]. This theory leads to the notion of "holes" playing the rôle of a positively charged particle carrying the current. Furthermore, the current is carried only by electrons or holes with energies within $\mathcal{O}(k_B T)$ from the Fermi level E_F. Hence the effective Hamiltonian describing the current carrying particles can be seen as a matrix of operators $H_{\text{eff}} = (H_{n,n'})_{n,n'\in B}$ in which B is the (finite) set of bands intersecting this energy interval. Each matrix element can then be seen as a bounded self-adjoint operator acting on the ℓ^2-space of the lattice describing the equilibrium positions of the atomic nuclei. This is the so-called *tight-binding representation.* A complete mathematically rigorous justification of this approach can be found iis available (see [8] for instance).

Following closely the Drude approach, one can construct a kinetic model for quantum transport as a first step towards a more accurate description of the interactions. The various sources of interactions, such as impurity, electron-phonon or electron-electron scattering, are then described through collisions occuring at random times $(t_l)_{l\in\mathbf{Z}}$ with $\cdots t_{l-1} \leq t_l \leq \cdots$. **This description is valid provided the number of collisions per unit of time is small enough**, namely the interaction with the corresponding particles can be considered as a small perturbation.

We will assume again that the collision times are Poisson distributed with an averaged collision time $\tau = \langle t_l - t_{l-1}\rangle$. At each collision, the charge carrier is randomly kicked with some energy and quasi-momentum exchange. Between collisions, however, the charge carriers evolvs according to the perfect crystal Hamiltonian, with possibly the addition of the potential energy $V_{\text{ext}}(t)$ created by (possibly time-dependent) external forces such as an electromagnetic field. In the Schrödinger picture, this leads to a Hamiltonian of the form

$$H_{\text{tot}} \;=\; H_{\text{eff}} + V_{\text{ext}}(t) + \sum_{l=-\infty}^{\infty} \delta(t-t_l) W_l \;. \tag{6}$$

Here, the W_l's will be a set of random operators, that one can assume to be selfadjoint, bounded, stochastically independent and identically distributed. This kinetic model was proposed in [11] in order to derive rigorously the Kubo formula for the IQHE. The evolution of wave packets is easily computable: the wave function immediately after a kick is given by

$$\psi(t_l + 0) \;=\; e^{-\imath W_l/\hbar}\psi(t_l - 0) \;.$$

Therefore, it is easy to compute the current in the limit of small external forces (linear response theory) and to control the correction terms.

The outcome of this model depends essentially upon the assumptions made on the common distribution of the W_l's. More precisely, the collision term should enforce the thermal equilibrium if no external forces are present. This leads to the requirement that the equilibrium density matrix ρ, given by the Fermi function $\rho = f_{\beta,\mu}(H_{\text{eff}})$ where $\beta = 1/k_B T$ and μ is the chemical potential, should not be changed in the average before and after a collision. More precisely, if $\mathbf{E}_W$ denotes the expectation value with respect to the W-distribution,

$$\hat{\kappa}^*(\rho) \;:=\; \mathbf{E}_W\left(e^{-\imath W_l/\hbar}\rho e^{\imath W_l/\hbar}\right) \;=\; \rho \;.$$

This condition is quite strong since in many cases it forces the W_l's to commute almost surely with H_{eff}. In particular, the stationnary distribution obtained from this stochastic evolution may be any function of H and not necessarily the Fermi distribution! In addition, it is not always possible to describe the outcome of the collision on the density matrix through a Hamiltonian formulation (*cf.* Section 2.5 III). Thus it is better to abandon the Schrödinger point of view and adopt the Heisenberg point of view of *observables* and *states*. Namely, we will introduce a C^*-algebra of observables $\mathcal{A}$ on which states are acting as positive linear forms. The density matrix will be represented by such a state. The quantum evolution is no longer described by unitaries, but by automorphisms of this algebra. However, it is still possible to describe kicks easily by introducing at times t_l's a sudden automorphism modifying instantly the instanteneous state describing the system. This will be done in Section 2.2.

1.4 Bloch theory for aperiodic media

It turns out that in many cases a perfect crystal is a rather bad approximation to describe the impurity scattering. This is what happens for lightly doped semiconductors at low temperature, whenever the current is carried by the impurity band [52]. The effective Hamiltonian is closer to an Anderson type model at high disorder than to the one of a perfect crystal. This is also the case for quasicrystals for which there is definitely no translation invariance left so that there is no chance to use efficiently Bloch theory. Other systems like amorphous materials may require a special description, too.

In these cases, it is better to replace H_{eff} by the one-particle Hamiltonian describing independent particles in such an aperiodic medium, so that *impurity scattering* is treated exactly without any approximation. The kinetic model that we have designed previously can be used again, **but the collisions now concern every collision processes other than the impurity scattering**. Therefore our model is more accurate if the other sources of dissipation can be considered as perturbations.

Even though Bloch theory does not apply, these crystals are macroscopically translation invariant. This can be expressed in terms of *homogeneity* [7, 9]. Let us describe the formalism whenever the system under consideration admits an underlying translation invariant lattice (such as it is for doped semiconductors). The Hilbert space $\mathcal{H}$ of quantum states is usually isomorphic to the ℓ^2-space of the lattice, possibly tensorized with $\mathbf{C}^p$ for some p if one includes several bands or spin. Hence we place ourself at the thermodynamic limit from the very beginning. Then, the effective Hamiltonian gives rise to a family $(H_\omega)_{\omega\in\Omega}$ of (bounded) selfadjoint operators indexed by a parameter ω representing the possible *configurations of disorder*. It has been shown that the set Ω of such parameters has a natural structure of compact metrizable toplogical space [7, 9]. Moreover, the translation group acts in a natural way by means of a group of homeomorphisms. At last, this family satisfies two properties:

1. the map $\omega \mapsto H_\omega$ is strongly continuous;
2. if $U(a)$ is the unitary representing the translation a in the Hilbert space and if T^a is the homeomorphism representing the action of a in Ω, then

$$U(a)H_\omega U(a)^{-1} \;=\; H_{T^a\omega}\;, \qquad \text{(covariance)}.$$

In other cases (impurity band in doped semiconductors, quasicrystals, amorphous systems), the description is more involved and requires the use of a *groupoid* (see [43, 18, 13] for the case of a quasicrystal). We will not consider this case here, but the extension of our approach is straightforward.

The observable algebra $\mathcal{A}$ is the C^*-algebra defined by the family $(H_\omega)_{\omega\in\Omega}$. In general, $\mathcal{A}$ is not abelian, it is not even of type I (namely, the tensor product of an abelian C^*-algebra by a matrix algebra). It is however possible to describe this algebra without reference to any Hilbert space (see Section 2.1). For a perfect crystal, this construction leads to the algebra $\mathcal{C}(\mathbf{B})\otimes\mathcal{K}$ where $\mathcal{K}$ is the algebra of compact operator (*i.e.*, the C^*-algebra generated by the finite dimensional matrices) and $\mathbf{B}$ is the *Brillouin zone*, namely the group dual to the translation group [7, 9]. In this sense, one can see $\mathcal{A}$ as the *non-comutative analog of the Brillouin zone* (NCBZ). It turns out that, given any $\omega \in \Omega$, there is a *-representation π_ω of $\mathcal{A}$ in $\mathcal{H}$ such that for $A \in \mathcal{A}$, $\pi_\omega(A)$ satisfies the strong continuity and the covariance conditions. In addition there is $H = H^* \in \mathcal{A}$ such that $H_\omega = \pi_\omega(H)$.

This analogy goes along with the geometry of this NCBZ, namely one can integrate and differentiate observables with respect to quasimomenta. The integral of A is given by the *trace per unit volume* of $\pi_\omega(A)$. This requires the data of a probability measure $\mathbf{P}$ on Ω which is translation invariant and ergodic. Then:

$$\mathcal{T}(A) \;=\; \lim_{|\Lambda|\uparrow\infty} \frac{1}{|\Lambda|}\,\mathrm{Tr}_\Lambda(\pi_\omega(A)), \qquad \text{for } \mathbf{P}\text{-almost all } \omega\text{'s},$$

where Λ is a sequence of boxes of finite volume $|\Lambda|$, and Tr_Λ is the trace of the restriction to Λ of the operator inside the brackets. There is also a set of *-derivations $(\partial_i)_{i=1}^d$ (where d is the dimension of the underlying lattice), generalizing the $\partial/\partial k_i$'s of the Bloch theory, defined in such a way as to give

$$\pi_\omega(\partial_i A) \;=\; \imath[X_i, \pi_\omega(A)]\;,$$

where $X_1, \cdots, X_d$ are the components of the *position operator*. This framework is the proper generalization of Bloch theory whenever the underlying system is homogeneous, but not microscopically translation invariant.

1.5 Main results

Our first result, after having defined the kinetic model, will be the derivation of Kubo's formula.

Theorem 1 *Let $\mathcal{L}_H$ be the operator $\imath[H, .]/\hbar$ acting on $\mathcal{A}$. The conductivity tensor at frequency $\hat{\omega}$, inverse temperature β and chemical potential μ, is given by $(i, j = 1, \ldots, d)$:*

$$\sigma_{i,j}(\beta,\mu,\hat{\omega}) \;=\; \frac{q^2}{\hbar^2}\,\mathcal{T}\left(\partial_i H\,\frac{1}{\frac{\mathbf{1}-\hat{\kappa}^*}{\tau} + \mathcal{L}_H - \imath\hat{\omega}}(\partial_j f_{\beta,\mu}(H))\right)\;, \tag{7}$$

provided the operator $(\mathbf{1}-\hat{\kappa}^*)/\tau + \mathcal{L}_H - \imath\hat{\omega}$ be invertible (see Section 2 *for more details) and the various derivative exists.*

The RTA now consists in replacing the operator $(\mathbf{1}-\hat{\kappa}^*)/\tau$ by $\mathbf{1}/\tau_{\mathrm{rel}}$. Note that in practice, τ_{rel} depends upon the temperature in a non trivial way.

As an illustration, let us consider the periodic case within a one-band approximation. Then $\mathcal{A} = C(\mathbf{T}^d)$. $H \in C^1(\mathbf{T}^d)$ is given by the function $E(k)$, $k \in \mathbf{T}^d$, and $\vec{J}(k) = \vec{\nabla}E(k)/\hbar$. Moreover, $\mathcal{T}(A) = \int_{\mathbf{T}^d} d^dk\; A(k)/(2\pi)^d$. The RTA conductivity tensor is given by

$$\sigma_{i,j}(\beta,\mu,\hat{\omega},\tau_{\mathrm{rel}}) \;=\; -\frac{1}{\frac{1}{\tau_{\mathrm{rel}}} - \imath\hat{\omega}}\,\frac{q^2}{\hbar^2}\int_{\mathbf{T}^d}\frac{d^dk}{(2\pi)^d}\,\frac{\partial f_{\beta,\mu}}{\partial E}(E(k))\;\partial_i E(k)\partial_j E(k)\;,$$

which is the usual Drude formula in the form obtained by semi-classical analysis [16, 4].

If p bands are needed, $\mathcal{A} = C(\mathbf{T}^d) \otimes M_p(\mathbf{C})$. H becomes a $p \times p$ self-adjoint matrix valued smooth function $H(k)$ on $\mathbf{T}^d$. Let $E_1(k) \leq \ldots \leq E_p(k)$ be the corresponding eigenvalues, notably the band functions. Let us assume, for simplicity, that no pair of bands is touching (but they may overlap) and let $P_r(k)$ be the eigenprojection corresponding to $E_r(k)$, then

$$\begin{aligned}\sigma_{i,j}(\beta,\mu,\hat\omega,\tau_{\rm rel}) \;&=\; -\frac{1}{\frac{1}{\tau_{\rm rel}}-\imath\hat\omega}\,\frac{q^2}{\hbar^2}\,\sum_{r=1}^{p}\int\frac{d^dk}{(2\pi)^d}\,\frac{\partial f_{\beta,\mu}}{\partial E}(E_r(k))\;\partial_iE_r(k)\partial_jE_r(k)\\ &+\sum_{r\neq s=1}^{p} q^2\int\frac{d^dk}{(2\pi)^d}\,\frac{f_{\beta,\mu}(E_s(k))-f_{\beta,\mu}(E_r(k))}{E_r(k)-E_s(k)}\,\frac{{\rm Tr}_p(P_r(k)J_i(k)P_s(k)J_j(k))}{\frac{1}{\tau_{\rm rel}}-\imath(\frac{E_r(k)-E_s(k)}{\hbar}+\hat\omega)}.\end{aligned}$$

Note that interband transitions are taken into account. This is ignored in the semiclassical approach [4, Chapter 12]. See [6] for an application to 2D Bloch electrons in a magnetic field.

The effects of quantum interferences in a disordered or quasiperiodic potential on the motion of an electron can be characterized by diffusion exponents [25, 23, 38, 41, 12, 32, 45, 27, 51]. Diffusion exponents characterize the behavior of the Kubo formula in the zero dissipation limit $\tau_{\rm rel}\to\infty$. Let us summarize the main results contained in [12, 51] about these exponents. Let $\Delta\subset\mathbf{R}$ be a Borel subset considered as a spectral subset of the energy space. Let $\Pi_\omega(\Delta)$ be the associated spectral projection of the Hamiltonian $H_\omega=\pi_\omega(H)$. The diffusion exponent $\sigma_{\rm diff}(\Delta)$ measures the growth of the matrix elements of the disorder averaged mean square displacement operator

$$\delta X^2_\Delta(t)\;=\;\int_0^t\frac{dt'}{t}\int_\Omega d\mathbf{P}(\omega)\;\langle 0|\Pi_\omega(\Delta)(\vec X_\omega(t')-\vec X)^2\Pi_\omega(\Delta)|0\rangle\;\underset{t\uparrow\infty}{\sim}\;t^{2\sigma_{\rm diff}(\Delta)}\;, \tag{8}$$

where $\vec X_\omega(t)$ is the time evolution of the position operator with respect to H_ω. Here, if f is a measurable function, $f(t)\underset{t\uparrow\infty}{\sim}t^\alpha$ means

$$\alpha\;=\;\inf\left\{\gamma\in\mathbf{R}\;|\;\exists\;0<a<\infty:\;\int_a^\infty\frac{dt}{t}\,\frac{f(t)}{t^\gamma}\;<\;\infty\right\}\;. \tag{9}$$

If $H\in\mathcal{C}^1(\mathcal{A})$ (namely the set of differentiable elements of $\mathcal{A}$), the diffusion exponent takes values in the interval $[0,1]$ and the state $|0\rangle$ in (8) may be replaced by any other state $\phi\in\ell^1(\mathbf{Z}^d)$ [51].

The motion is called ballistic whenever $\sigma_{\rm diff}(\Delta)=1$. This is what happens for a periodic Hamiltonian. The motion will be called diffusive if $\sigma_{\rm diff}(\Delta)=1/2$. An example of diffusive motion is Wegner's n-orbital model [60, 31, 51]. A diffusive behavior is expected, but not yet proved, in the Anderson model in $d\geq3$ at low disorder and at energies near the band center. Localization is characterized by $\delta X^2_\Delta(t)<\infty$ [10, 11] which implies $\sigma_{\rm diff}(\Delta)=0$ (but the converse is false [45]). Localization holds in the Anderson model for $d=1$, and at any d on band edges or at high disorder (see [2] and references therein). If $0<\sigma_{\rm diff}(\Delta)<1/2$, the motion is called subdiffusive, whereas for $1/2<\sigma_{\rm diff}(\Delta)<1$ it is called overdiffusive. There are numerical and analytical evidences for anomalous (over- or sub-) diffusion in quasiperiodic structures [25, 55, 41, 37].

Variants of the formula below already appeared in [54, 38, 12, 49], a proof in the present formalism is given in [51].

Theorem 2 (Anomalous Drude formula) [12, 51] *The isotropic direct conductivity $\sigma=\sum\sigma_{i,i}$ at zero frequency of a homogeneous electron system given by* (7) *satisfies* (*with $\beta<\infty$ fixed*)

$$\sigma(\beta,\mu,\hat\omega=0,\tau_{\rm rel})\;\underset{\tau_{\rm rel}\uparrow\infty}{\sim}\;\tau_{\rm rel}^{2\sigma_{\rm diff}(\mathbf{R})-1}\;. \tag{10}$$

Remark 1 In most physical situations, temperature and relaxation time are usually linked by a powerlaw relation $\tau_{\rm rel}\sim\beta^\alpha$ with $\beta>0$. Hence the limit $\tau_{\rm rel}\to\infty$ should be taken together with the zero temperature limit. One then expects the relation $\sigma(\beta, \mu, \tau_{\text{rel}} = \beta^\alpha) \sim \beta^{\alpha(2\sigma_{\text{diff}}(\mu)-1)}$ as $\beta \to \infty$ where $\sigma_{\text{diff}}(\mu)$ is the diffusion exponent at the Fermi level. $\diamond$

Remark 2 For a ballistic motion, $\sigma_{\text{diff}} = 1$, leading to the usual Drude formula. More generally, for $\sigma_{\text{diff}} > 1/2$, dissipation lowers the wave packet velocity so as to give a classical diffusion at large times. As the dissipation is removed, the conductivity increases and diverges, namely the systems behaves like a conductor. On the opposite, for $\sigma_{\text{diff}} < 1/2$, the interference effects slow down the wave packet, hence the conductivity is enhanced by dissipation. So as the dissipation is removed, the conductivity decreases to zero, namely the system behaves as an insulator. This is a possible mechanism explaining why quasicrystalline materials such as the $AlCuFe$ are insulators at low temperature [38]. As $\sigma_{\text{diff}} = 1/2$, the dissipation just adds up to the quantum diffusion so that, as $\tau_{\text{rel}} \to \infty$, a residual conductivity may remain. $\diamond$

Remark 3 In contrast with the absence of current whenever the Hamiltonian is bounded and the dissipation is absent (see [11] and Proposition 6 below), the conductivity diverges in the limit $\tau_{\text{rel}} \to \infty$ whenever $\sigma_{\text{diff}}(\mu) > 1/2$. It shows that the limits of small dissipation and large volume (or large measurement time) do not commute (see for instance [57, Section 3.1]). $\diamond$

Let η be the spectral measure of the Liouville operator $\mathcal{L}_H$ defined by:

$$\int d\eta(l)\, f(l) \;=\; \mathcal{T}(\vec{\nabla} H \cdot f(\mathcal{L}_H)(\vec{\nabla} H)) \; . \tag{11}$$

Its local spectral exponent $\alpha_\eta(\hat{\omega})$ at $\hat{\omega}$ is defined by $\eta([\hat{\omega}+\epsilon, \hat{\omega}-\epsilon]) \sim \epsilon^{\alpha_\eta(\hat{\omega})}$ as $\epsilon \to 0$. Note that $\alpha_\eta(0) = 2(1 - \sigma_{\text{diff}}(\mathbf{R}))$ [51]. The proof of the following result is similar to the one of Theorem 2 in [51] and is omitted.

Theorem 3 *For the electric conductivity at fixed frequency $\hat{\omega}$ and temperature $\beta < \infty$, the behavior in the zero dissipation limit is*

$$|\sigma(\beta, \mu, \hat{\omega}, \tau_{\text{rel}})| \underset{\tau_{\text{rel}}\uparrow\infty}{\sim} \tau_{\text{rel}}^{1-\alpha_\eta(\hat{\omega})} \; . \tag{12}$$

2 Quantum transport in aperiodic media

2.1 The non-commutative Brillouin zone

In order to fix notations, we briefly review from [7, 9, 11, 51]the mathematical description of independent charged particles in homogeneous media as motivated in Section 1.4. Let us consider first the case for which there is only one band and no spin. Then we will indicate how one can describe the case for which several bands and the spin may enter into this mathematical framework.

The underlying crystal will be identified with $\mathbf{Z}^d$ with $d = 1, 2, 3, \ldots$. In the tight binding representation [7], the one-particle Hilbert space describing the electronic quantum states is $\mathcal{H} = \ell^2(\mathbf{Z}^d)$. The *position operator* $\vec{X} = (X_1, \ldots, X_d)$ is defined by $X_j\psi(n) = n_j\psi(n)$, $\psi \in \mathcal{H}$. If there is a magnetic field, it is given by an antisymmetric real matrix $\mathcal{B} = (B_{i,j})_{i,j=1\ldots d}$ with $B_{i,j} = -B_{j,i}$. The magnetic translations

$$U(a)\psi(n) = e^{\frac{iq}{2\hbar}\mathcal{B}.a\wedge n}\psi(n-a) \; , \tag{13}$$

define a projective unitary representation of the *translation group* $\mathbf{Z}^d$ on $\mathcal{H}$. The one-particle Hamiltonian H_0 is a bounded selfadjoint operator on $\mathcal{H}$ which may or may not be translation invariant. Its *hull* Ω is the strong closure of the set $\{U(a)H_0U(a)^{-1}; a \in \mathbf{Z}^d\}$. We have proposed in [7] to call *homogeneous* the Hamiltonians with compact hull. For each $\omega \in \Omega$, we will denote by H_ω the operator acting on $\mathcal{H}$ associated to ω. The translation group acts on Ω by homeomorphisms denoted by T^a so that the covariance relation holds

$$U(a)H_\omega U(a)^{-1} = H_{T^a\omega} \ , \qquad a \in \mathbf{Z}^d \ .$$

The C^*-algebra of observable $\mathcal{A}$ is the algebra generated by the translated of H_0. It has been argued in [7] that, under suitably mild conditions on H_0, $\mathcal{A}$ is given by the crossed-product of the action of $\mathbf{Z}^d$ on Ω through the magnetic translations. Its construction goes as follows: we endow the topological vector space $\mathcal{C}_\kappa(\Omega \times \mathbf{Z}^d)$ of continuous functions with compact support on $\Omega \times \mathbf{Z}^d$ with the following structure of $*$-algebra:

$$AB(\omega,n) \ = \ \sum_{l\in\mathbf{Z}^d} A(\omega,l)B(T^{-l}\omega,n-l)e^{\frac{\imath q}{2\hbar}\mathcal{B}.n\wedge l} \ , \qquad A^*(\omega,n) \ = \ \overline{A(T^{-n}\omega,-n)} \ , \tag{14}$$

where $A,B \in \mathcal{C}_\kappa(\Omega\times\mathbf{Z}^d)$, $\omega \in \Omega$, $n \in \mathbf{Z}^d$ and $\mathcal{B}.n\wedge l = \sum_{i,j} B_{i,j}n_il_j$. For $\omega \in \Omega$, a representation of this $*$-algebra on $\mathcal{H} = \ell^2(\mathbf{Z}^d)$ is given by

$$\pi_\omega(A)\psi(n) = \sum_{l\in\mathbf{Z}^d} A(T^{-n}\omega,l-n) \ e^{\frac{\imath q}{2\hbar}\mathcal{B}.l\wedge n} \ \psi(l) \ , \qquad \psi \in \ell^2(\mathbf{Z}^d) \ . \tag{15}$$

The representations π_ω are related by the covariance relation

$$U(a)\pi_\omega(A)U(a)^{-1} = \pi_{T^a\omega}(A) \ , \qquad a \in \mathbf{Z}^d \ .$$

Now $\|A\| = \sup_{\omega\in\Omega}\|\pi_\omega(A)\|$ defines a C^*-norm on $\mathcal{C}_\kappa(\Omega \times \mathbf{Z}^d)$ and the observable C^*-algebra $\mathcal{A} = C^*(\Omega \times \mathbf{Z}^d, \mathcal{B})$ is defined as the completion of $\mathcal{C}_\kappa(\Omega \times \mathbf{Z}^d)$ under this norm. Given a T-invariant, ergodic probability measure $\mathbf{P}$ on Ω, a normalized trace $\mathcal{T}$ on $\mathcal{A}$ is defined by

$$\mathcal{T}(A) \ = \ \int_\Omega d\mathbf{P}(\omega) \ A(\omega,0) \ , \qquad \Longrightarrow \qquad \mathcal{T}(\mathbf{1}) \ = \ 1 \ . \tag{16}$$

Using the bra-ket notations, let $|n\rangle$ be the unit vector in $\mathcal{H}$ supported by $n \in \mathbf{Z}^d$. For any increasing sequence $(\Lambda_l)_{l\in\mathbf{N}}$ of cubes centered at the origin, Birkhoff's ergodic theorem implies

$$\mathcal{T}(A) \ = \ \int_\Omega d\mathbf{P}(\omega) \ \langle 0|\pi_\omega(A)|0\rangle = \lim_{l\to\infty}\frac{1}{|\Lambda_l|}\sum_{n\in\Lambda_l}\langle n|\pi_\omega(A)|n\rangle \ , \tag{17}$$

for $\mathbf{P}$-almost all $\omega \in \Omega$ showing that $\mathcal{T}$ is the trace per unit volume.

For $p \in [1,\infty)$, the Banach space $L^p(\mathcal{A},\mathcal{T})$ is the closure of $\mathcal{A}$ under the norm $\|A\|_{L^p} = (\mathcal{T}(|A|^p))^{1/p}$. If $\pi_{\rm GNS}$ denotes the GNS representation of $\mathcal{T}$ on $L^2(\mathcal{A},\mathcal{T})$, $L^\infty(\mathcal{A},\mathcal{T})$ denotes von Neumann algebra $\pi_{\rm GNS}(\mathcal{A})''$ where $''$ is the bicommutant. By a theorem of Connes [11], $L^\infty(\mathcal{A},\mathcal{T})$ is canonically isomorphic to the von Neumann algebra of $\mathbf{P}$-essentially bounded, weakly measurable and covariant families $(A_\omega)_{\omega\in\Omega}$ of operators on $\mathcal{H} = \ell^2(\mathbf{Z}^d)$ endowed with the norm

$$\|A\|_{L^\infty} \ = \ \mathbf{P}\text{-}\operatorname*{essinf}_{\omega\in\Omega}\|A_\omega\|_{\mathcal{B}(\mathcal{H})} \ .$$

Consequently, the family of representations π_ω extends as a family of weakly measurable representations of $L^\infty(\mathcal{A},\mathcal{T})$. Moreover, the trace $\mathcal{T}$ extends to $L^\infty(\mathcal{A},\mathcal{T})$ as a normalized normal trace.

Density matrices are positive elements ρ of $L^1(\mathcal{A},\mathcal{T})$ with $\mathcal{T}(\rho)=n$ if n is the particle density. $L^1(\mathcal{A},\mathcal{T})$ can be identified with the predual of $L^\infty(\mathcal{A},\mathcal{T})$, namely the linear space spanned by the set of normal states on $L^\infty(\mathcal{A},\mathcal{T})$. $L^1(\mathcal{A},\mathcal{T})_+$ will denote the positive part of $L^1(\mathcal{A},\mathcal{T})$. Any trace preserving *-automorphism $\alpha\in\mathrm{Aut}(\mathcal{A})$ acts on $L^1(\mathcal{A},\mathcal{T})$ by duality as $\mathcal{T}(\rho\,\alpha(A))=\mathcal{T}(\alpha^*(\rho)A)$. In particular if $\rho\in\mathcal{A}\cap L^1(\mathcal{A},\mathcal{T})$ then $\alpha^*(\rho)=\alpha^{-1}(\rho)$.
We will denote by $\mathcal{F}$ the convex set of linear operators on $L^1(\mathcal{A},\mathcal{T})$ preserving the positivity and the trace. We endow $\mathcal{F}$ with the weak topology, namely the one defined by the seminorms $p_{\rho,B}(\mathcal{K})=|\mathcal{T}(\mathcal{K}(\rho)B)|$ with $\rho\in L^1(\mathcal{A},\mathcal{T})_+$, $\mathcal{T}(\rho)=1$ and $B\in L^\infty(\mathcal{A},\mathcal{T})$, $\|B\|\le 1$. Any *-automorphism of $\mathcal{A}$ defines, by duality, an element of $\mathcal{F}$.

The C^*-algebra $\mathcal{A}$ admits also a differential structure given by the family of *-derivations $\vec{\nabla}=(\partial_1,\ldots,\partial_d)$ defined by

$$\partial_j A(\omega,x)=\imath x_j A(\omega,x)\ . \tag{18}$$

This family generates a d-parameter group $\rho_k=\exp\{\sum_j k_j\partial_j\}$, $\ k\in\mathbf{T}^d$, of *-automorphisms [7]. Moreover, $\pi_\omega(\partial_j A)=\imath[\pi_\omega(A),X_j]$. We denote by $\mathcal{C}^1(\mathcal{A})$ the dense sub*-algebra of $\mathcal{A}$ of differentiable elements A, namely such that $\partial_j A\in\mathcal{A}$ for all j's, endowed with the norm $\|A\|_{\mathcal{C}^1}=\|A\|+\sum_j\|\partial_j A\|$. The following result is proved in [47]

Proposition 1 *Let $H=H^*$ be an element of $\mathcal{C}^1(\mathcal{A})$ and let $\Sigma\subset\mathbf{R}$ be its spectrum. Then for any $f\in\mathcal{C}^2(\mathbf{R})$, the operator $f(H)$ belongs to $\mathcal{C}^1(\mathcal{A})$ and*

$$\|\partial_j f(H)\|\le const.\|f\|_{\mathcal{C}^2}\|\partial_j H\|\ .$$

We also have (see in particular [48])

Proposition 2 *Let $H=H^*$ be an element of $\mathcal{C}^1(\mathcal{A})$ with spectrum $\Sigma\subset\mathbf{R}$. Then*

1. *For any $j=1,\ldots,d$ there exists a positive Radon measure m_j on $\Sigma\times\Sigma$ defined by*

$$\int_{\Sigma\times\Sigma}dm_{j,j}(E,E')f(E)g(E')=\mathcal{T}\left(\partial_j H f(H)\partial_j H g(H)\right)\qquad\forall f,g\in\mathcal{C}(\Sigma)\ . \tag{19}$$

The sum $m=\sum_{j=1}^d m_{j,j}$ is called the current-current correlation *measure* [31, 51].

2. *Let $f\in\mathcal{C}^1(\Sigma)$. Then*

$$\mathcal{T}\left(|\ \partial_j f(H)\ |^2\right)=\int_{\Sigma\times\Sigma}dm_{j,j}(E,E')\left|\frac{f(E)-f(E')}{E-E'}\right|^2\ , \tag{20}$$

where $(f(E)-f(E'))/(E-E')$ is replaced by $f'(E)$ if $E=E'$.

Proof. The mapping $(f,g)\in C(\Sigma)\times C(\Sigma)\to\mathcal{T}(\partial_j H\,f(H)\partial_j H\,g(H))\in\mathbf{C}$ defines a positive and continuous bilinear form. By the Riesz-Markov theorem [44] $m_{j,j}$ exists and its mass is $\mathcal{T}(|\partial_j H|^2)$.
For $m,n\in\mathbf{N}$, using the Leibniz rule we get:

$$\mathcal{T}\left(\partial_j(H^m)\partial_j(H^n)\right) = \sum_{k=1}^{m}\sum_{l=1}^{n} \mathcal{T}\left(\partial_j H H^{m-k+l-1}\partial_j H H^{n+k-l-1}\right) \ .$$

Thanks to eq. (19) it gives

$$\mathcal{T}\left(\partial_j(H^m)\partial_j(H^n)\right) = \int_{\Sigma\times\Sigma} dm_{j,j}(E,E')\frac{(E^m - E'^m)(E^n - E'^n)}{(E-E')^2} \ .$$

Therefore, by linearity, eq. (20) holds for polynomials and, by density, for all differentiable functions. □

By the Radon-Nykodym theorem, there exists a non-negative matrix valued function $M_{i,j} \in L^1(\mathbf{R}^2, dm)$ such that

$$\int_{\mathbf{R}^2} dm(E,E')M_{i,j}(E,E')\ f(E)g(E') \ = \ \mathcal{T}(\partial_i H\, f(H)\partial_j H\, g(H)) \ .$$

We will set $m_{i,j} = M_{i,j}m$. Let us note that if $H_\omega = H_0 + V_\omega$ with H_0 translation invariant and V_ω commuting with $\vec{X}$, these measures can be expressed in terms of the 4-point Green's function (see [51]).

For a selfadjoint element H of $\mathcal{A}$, we denote by $\mathcal{L}_H$ the operator acting on $\mathcal{A}$ by

$$\mathcal{L}_H(A) = \frac{\imath}{\hbar}[H, A] \ . \tag{21}$$

It is a bounded *-derivation of $\mathcal{A}$ generating a one-parameter group of *-automorphisms called the *time evolution*. For $\omega \in \Omega$, the operator $H_\omega = \pi_\omega(H)$ acts on $\mathcal{H}$ and describes the physical Hamiltonian acting on a lattice with disorder ω. In particular the current is given by the operator $\vec{J}_\omega = q d\vec{X}_\omega/dt$, notably by the Heisenberg equation of motion, $\vec{J}_\omega = \pi_\omega(q/\hbar\vec{\nabla}H)$. Hence the current can be seen as an element of $\mathcal{A}$ whenever H is differentiable, namely

$$\vec{J} = \frac{q}{\hbar}\vec{\nabla}H \ . \tag{22}$$

Let $\mathcal{A}_H$ denote the commutative C^*-algebra spanned by the continuous functions of the Hamiltonian $H \in \mathcal{A}$. Then

Proposition 3 *Let $H = H^*$ be an element of $\mathcal{C}^1(\mathcal{A})$. Let $\mathcal{A}_H^\perp$ be the subspace of $L^2(\mathcal{A},\mathcal{T})$ orthogonal $\mathcal{A}_H$.*

1. *$\mathcal{L}_H$ extends as a bounded anti-selfadjoint operator on $L^2(\mathcal{A},\mathcal{T})$ leaving $\mathcal{A}_H^\perp$ invariant.*

2. *Let f, g be the restrictions to the spectrum of H of continuously differentiable function on $\mathbf{R}$. Then $\partial_j f(H) \in \mathcal{A}_H^\perp$ for all j's, namely*

$$\mathcal{T}(\partial_j f(H) g(H)) = 0 \ . \tag{23}$$

3. *Let Γ be a bounded positive operator on $L^2(\mathcal{A},\mathcal{T})$ leaving $\mathcal{A}_H^\perp$ invariant and bounded from below on $\mathcal{A}_H^\perp$ by $\gamma\mathbf{1}$ with $\gamma > 0$. Then the operator $\Gamma + \mathcal{L}_H - \imath\hat{\omega}$ is invertible on $\mathcal{A}_H^\perp$ for any $\hat{\omega} \in \mathbf{R}$.*

4. *Let Γ be a bounded positive operator on $L^2(\mathcal{A},\mathcal{T})$ bounded from below by $\gamma\mathbf{1}$ with $\gamma > 0$. Then the operator $\Gamma + \mathcal{L}_H - \imath\hat{\omega} - \vec{\mathcal{E}}\cdot\vec{\nabla}$ has a bounded inverse for any $\hat{\omega} \in \mathbf{R}$ and any $\vec{\mathcal{E}} \in \mathbf{R}^d$. This inverse is strongly continuous with respect to $\vec{\mathcal{E}} \in \mathbf{R}^d$.*

Proof. Since H is bounded, its norm as an operator acting on $L^2(\mathcal{A},\mathcal{T})$ by left or right multiplication is bounded by $\|H\|$. Therefore $\mathcal{L}_H$ is bounded. An explicit calculation, using the trace property, shows that it is anti-selfadjoint. At last, $\mathcal{L}_H(H^n) = [H, H^n] = 0 \; \forall n \geq 0$. Thus $\mathcal{L}_H$ leaves $\mathcal{A}_H^{\perp}$ invariant.
We note that $\mathcal{T}(\partial_j A) = 0$ for all j's and $A \in \mathcal{A}$. Using the Leibniz rule and the trace property, it follows that $\mathcal{T}(\partial_j(H^m)H^n) = 0$ for $m \geq 0, n \geq 0$. Thus for any polynomial p on $\mathbf{R}$, we get

$$\mathcal{T}\left(\partial_j p(H) H^n\right) = 0 \;, \qquad \forall\, n \geq 0 \;.$$

By density and thanks to Proposition 2, this is still true for f Lipshitz continuous, namely $\partial_j f(H) \in \mathcal{A}_H^{\perp}$, and (23) follows.
Since both Γ and $\mathcal{L}_H - \imath\hat{\omega}$ leave $\mathcal{A}_H^{\perp}$ invariant, so does their sum. Since $\Gamma \geq \gamma \mathbf{1} > 0$ on $\mathcal{A}_H^{\perp}$ and since $\mathcal{L}_H - \imath\hat{\omega}$ is antiselfadjoint, the real part of the sum is bounded from below by a positive number, implying the invertibility of $\Gamma + \mathcal{L}_H - \imath\hat{\omega}$.
We know that $\vec{\nabla}$ is the set of infinitesimal generators of an automorphism group ρ_k. This automorphism group extends obviously as a unitary group on $L^2(\mathcal{A},\mathcal{T})$. Therefore, for all $\vec{\mathcal{E}} \in \mathbf{R}^d$, $\vec{\mathcal{E}} \cdot \vec{\nabla}$ is well defined as an anti-selfadjoint (unbounded) operator on $L^2(\mathcal{A},\mathcal{T})$ with domain defined through this unitary group. The same kind of arguments as before shows that the operator $\Gamma + \mathcal{L}_H - \imath\hat{\omega} - \vec{\mathcal{E}} \cdot \vec{\nabla}$ has a bounded inverse. Moreover, the strong continuity is a standard result of spectral theory [44]. □

If the fermion particles have spin or if several bands are needed to describe the system around its Fermi level, $\mathcal{A}$ must be replaced by $\mathcal{A} \otimes M_r(\mathbf{C})$, namely the C^*-algebra of $r \times r$ matrices with entries in $\mathcal{A}$. The matrix indices represent both the spin and band indices. The new trace includes the sum over the indices of the diagonal terms, while every other result described above still holds.

H fixes the grand-canonical equilibrium state. If T is the temperature and μ the chemical potential, the grand canonical Gibbs states is given by the Fermi-Dirac one-particle density matrix $f_{\beta,\mu}(H) = (1 + e^{\beta(H-\mu)})^{-1}$, where $\beta = 1/k_B T$. Usually, μ is fixed by the condition $n = \mathcal{T}(f_{\beta,\mu}(H))$ where n is the charge carrier density. Given any density matrix ρ as an initial state, its one-particle time evolution is given by the Liouville-von Neumann equation

$$\frac{d\rho}{dt} \;=\; -\mathcal{L}_H(\rho) \;. \tag{24}$$

This is the dual action of $\mathcal{L}_H$ on $L^1(\mathcal{A},\mathcal{T})$. Let us point out that the observable algebra of a quasicrystal constructed by the cut and projection method is generally given by the C^*-algebra associated to a groupoid [9, 30] and not necessarily by a crossed-product as above. However, all results of this section extend to this case.

2.2 A model for quantum transport

The previous section was devoted to the description of a formalism liable to describe systems of independant fermions. In this section interactions are taken into account through a phenomenological description of dissipation similar to the one given in Section 1.2. This formalism will be valid only if the interactions with other particles can be treated as a noise. In this approach, a test particle evolves according to an Hamiltonian $H \in \mathcal{A}$. At random times, it is scattered in a random way. At this level of description the precise nature of the scatterer will not be important. Only its density matrix is modified instantaneously into another one. This collision process should enforce the equilibrium. For this reason we will demand this collision process to leave the thermal equilibrium invariant if no external force acts upon the system. More explicit models for the collision operators will be given in Section 2.5.

These hypothesis are formulated more precisely as follows

A The time evolution of the particle is governed by the Liouville-von Neumann equation (24) with $H \in \mathcal{A}$. External forces such as an electric field may be added. At random times t_l, $l \in \mathbf{Z}$ with $t_l < t_{l+1}$, the particle is scattered instantaneously.

B The time delays $s_l = t_l - t_{l-1}$ between two collisions are independent random variables identically distributed according to the exponential law of rare events $dt/\tau \exp(-t/\tau)$. Hence the collision process is a Poisson process [15]. τ is called the *collision time*.

C For each $l \in \mathbf{Z}$, the density matrix ρ of the system just before the l-th collison is transformed into $\mathcal{C}_l(\rho)$ just after the collision where $(\mathcal{C}_l)_{l\in\mathbf{Z}}$ is a sequence of independent, identically distributed, random variables with values in $\mathcal{F}$ and common distribution p.

D The probability measure p on $\mathcal{F}$ is such that the element $\hat{\kappa}^* \in \mathcal{F}$, defined as the weak integral $\hat{\kappa}^* = \int_{\mathcal{F}} dp(\mathcal{K})\ \mathcal{K}$, preserves the Fermi-Dirac distribution $f_{\beta,\mu}(H)$. $\hat{\kappa}^*$ will be called the *collision efficiency operator.*

The probability space used here can be constructed as follows. The set $\Xi_0 = \mathbf{R}_+ \times \mathcal{F}$ becomes a probability space if endowed with the σ-algebra of Borel sets and the probability $d\mathbf{M}_0(s,\mathcal{K}) = \exp-(s/\tau)\ ds/\tau \otimes dp(\mathcal{K})$. Then Ξ_d is the cartesian product $\Xi_0^{\mathbf{Z}}$ endowed with the product σ-algebra and the product measures $d\mathbf{M}_d(\tilde{\xi}) = \bigotimes_{l\in\mathbf{Z}} d\mathbf{M}_0(s_l,\mathcal{K}_l)$ if $\tilde{\xi} = (s_l,\mathcal{K}_l)_{l\in\mathbf{Z}}$. The *shift* S acts on Ξ_d by $S(s_l,\mathcal{K}_l)_{l\in\mathbf{Z}} = (s_{l-1},\mathcal{K}_{l-1})_{l\in\mathbf{Z}}$. It is a bimeasurable bijection leaving the probability $\mathbf{M}_d$ invariant. Moreover, $\mathbf{M}_d$ is S-ergodic. Here S is a *discrete* time translation. Let g be the non-negative measurable function on Ξ_d given by $g((s_l,\mathcal{K}_l)_{l\in\mathbf{Z}}) = s_0$. The probability space Ξ is then the suspension of Ξ_d by this map [19]. Namely one defines on the product $\Xi_d \times \mathbf{R}$ the maps $\phi_s(\tilde{\xi},t) = (\tilde{\xi},t+s)$ and $G(\tilde{\xi},t) = (S\tilde{\xi},t-g(\tilde{\xi}))$ for $\tilde{\xi} \in \Xi_d$ and $s,t \in \mathbf{R}$. Then ϕ_s defines a one-parameter group of bimeasurable bijections leaving the positive measure $d\mathbf{M}_d \otimes dt$ invariant. Moreover, G is also a bimeasurable bijection leaving the positive measure $d\mathbf{M}_d \otimes dt$ invariant. Therefore the quotient space $\Xi = \Xi_d/G$ obtained by identifying $(\tilde{\xi},t)$ and $G(\tilde{\xi},t)$, endowed with the quotient σ-algebra Σ becomes a probability space on which ϕ_s still acts as a bimeasurable bijection and preserving the probability measure $d\mathbf{M} = d\mathbf{M}_d \otimes (dt/g)_{[0,g]}$. This gives the desired probability space $(\Xi,\Sigma,d\mathbf{M})$ with a $\mathbf{R}$-action ϕ. Using the standard results on the suspension, $d\mathbf{M}$ is ϕ-ergodic [19]. The collision time t_l is recovered as the second coordinate of $G^{-l}(\tilde{\xi},t)$, namely $t_l = t + s_1 + \ldots + s_l$ if $l > 0$ and a similar formula for $l \leq 0$.

Given $\xi \in \Xi$ and using the assumption above, the instantaneous evolution of the density matrix between times t' and t is given by the operator:

$$U_\xi(t,t') \;=\; e^{-\mathcal{L}_H(t-t_l)} \left(\prod_{r=l'}^{l-1} \mathcal{C}_r\ e^{-\mathcal{L}_H(t_r-t_{r-1})}\right) \mathcal{C}_{l'}\ e^{-\mathcal{L}_H(t_{l'}-t')}\ , \tag{25}$$

whenever $t_{l'-1} < t' < t_{l'} < \ldots < t_l < t < t_{l+1}$. This evolution operator belongs to $\mathcal{F}$ and satisfies the following causality equations

$$U_\xi(t,t') \;=\; U_\xi(t,t")U_\xi(t",t')\ , \qquad \text{if } t' \leq t" \leq t\ , \qquad U_\xi(t,t) \;=\; \mathbf{1}\ ,$$

together with the time-covariance condition

$$U_{\phi_s\xi}(t+s,t'+s) \;=\; U_\xi(t,t')\;, \qquad \forall s\in\mathbf{R}\;.$$

For any $\xi \in \Xi$ and $\rho \in L^1(\mathcal{A},\mathcal{T})_+$, $U_\xi(t,t')\rho$ is continuous with respect to t and t' except possibly when they coincide with a collision time. Thanks to the Birkhoff ergodic theorem and the time-covariance condition, the time-average of the evolution coincides with the ergodic average:

$$\lim_{T\to\infty}\int_{-T}^{T}\frac{ds}{2T}\,U_\xi(t+s,t'+s) \;=\; \mathbf{E}_\xi(U_\xi(t,t')) \;=\; U(t-t') \qquad \text{for } \mathbf{M}\text{-almost all } \xi\;.$$

Again the integral must be understood in the weak sense in $\mathcal{F}$. That U depends only upon the difference $t-t'$ is a consequence of the time-covariance. Moreoever, the causality gives $U(t+t') = U(t)U(t')$ provided $t\geq 0,\ t'\geq 0$. In addition, the averaging smooths out the discontinuity in time so that for $\rho\in L^1(\mathcal{A},\mathcal{T})_+$, $\rho(t) = U(t)\rho \in L^1(\mathcal{A},\mathcal{T})_+$ is continuous in time. So the averaged evolution gives a strongly continuous trace preserving semigroup. The Laplace transform of the mean evolution can be calculated explicitly as in [24, 11] and gives the generator of this semigroup, namely (see Section 3.3 for the proof):

Proposition 4 *The time-averaged evolution is governed by the quantum Boltzmann equation*

$$\frac{d\rho}{dt}+\mathcal{L}_H(\rho) \;=\; -\frac{1-\hat{\kappa}^*}{\tau}(\rho)\;. \tag{26}$$

The right hand side of this equation is called the collision term and will be denoted by $-\Gamma(\rho)$.

In absence of external forces such as an electric field, the Fermi-Dirac equilibrium distribution is a fixed point of the dynamics of (26). Depending upon the explicit form of Γ, this dynamic may or may not have a unique fixpoint. If there is a unique fixpoint, it may or may not be stable, that is produce thermalization or the return to equilibrium.

2.3 Kubo's formula with a dissipative term

In order to get a non vanishing current with such a dissipative evolution, an external electric field must be added. In this section, only DC electric fields are considered. AC fields are technically more involved and treated in the Section 3, giving similar results. $\vec{\mathcal{E}}$ will be assumed uniform in space.
In practical situations, however, the electric field may not be uniform even at microscopic scales (due to Coulomb interaction, for instance [52]). But then it is the superposition of a uniform external field and of a fluctuating one. The fluctuating field may be treated as an extra potential in the Hamiltonian, with the cost of modifying the hull Ω if necessary and adding a field dependent term to the Hamiltonian H. So that, in the worst case, the effective Hamiltonian becomes $\pi_\omega(H(\vec{\mathcal{E}}))-q\vec{\mathcal{E}}\vec{X}$ for some $H(\vec{\mathcal{E}})\in\mathcal{A}$. But the mathematical difficulties are exactly the same as if the fluctuating field were absent.

Here is the main argument to derive Kubo's formula (see Section 3 for the proofs). H is assumed to be in $\mathcal{C}^1(\mathcal{A})$ in order that the current $\vec{J}$ be defined in $\mathcal{A}$ (see eq. (22)). Starting from a thermal equilibrium at time $t=0$, an external electric field $\vec{\mathcal{E}}$ is turned on for $t>0$.

The generator of the new evolution in $\mathcal{A}$ is $\mathcal{L}_H - q/\hbar\vec{\mathcal{E}}\cdot\vec{\nabla}$. The initial state is the density matrix $\rho(t=0) = f_{\beta,\mu}(H)$. The time-averaged current density becomes

$$\vec{\jmath}_{\beta,\mu,\vec{\mathcal{E}}} = \lim_{\delta\to 0}\delta\int_0^\infty dt\, e^{-\delta t}\,\mathcal{T}(\vec{J}\rho(t)) \;=\; \lim_{\delta\to 0}\delta\,\mathcal{T}\left(\vec{J}\;\frac{1}{\delta+\Gamma+\mathcal{L}_H-\frac{q}{\hbar}\vec{\mathcal{E}}\cdot\vec{\nabla}}(f_{\beta,\mu}(H))\right)\;.$$

Thanks to Proposition 3, the current carried by the equilibrium state vanishes and therefore we can subtract $0 = \delta\,\mathcal{T}(\vec{J}\frac{1}{\delta}f_{\beta,\mu}(H))$. This leads to:

$$\vec{\jmath}_{\beta,\mu,\vec{\mathcal{E}}} \;=\; \lim_{\delta\to 0}\,\mathcal{T}\left(\vec{J}\;\frac{1}{\delta+\Gamma+\mathcal{L}_H-\frac{q}{\hbar}\vec{\mathcal{E}}\cdot\vec{\nabla}}\;\frac{q}{\hbar}\vec{\mathcal{E}}\cdot\vec{\nabla}\;\frac{\delta}{\delta+\Gamma+\mathcal{L}_H}(f_{\beta,\mu}(H))\right)\;.$$

Because $\Gamma(f_{\beta,\mu}(H)) = 0 = \mathcal{L}_H(f_{\beta,\mu}(H))$, the previous formula simplifies to give

$$\vec{\jmath}_{\beta,\mu,\vec{\mathcal{E}}} \;=\; \frac{q}{\hbar}\sum_{j=1}^{d}\mathcal{E}_j\;\mathcal{T}\left(\vec{J}\,\frac{1}{\Gamma+\mathcal{L}_H-\frac{q}{\hbar}\vec{\mathcal{E}}\cdot\vec{\nabla}}(\partial_j f_{\beta,\mu}(H))\right)\;. \tag{27}$$

The linear coefficients $\sigma_{i,j}(\beta,\mu)$, $i,j = 1\ldots d$, of $(\vec{\jmath}_{\beta,\mu,\vec{\mathcal{E}}})_i$ with respect to the electric field, define the conductivity tensor. The case of an oscillating external electric field of frequency $\hat{\omega}$ is treated in Section 3 and the following result is proved in Section 3.3.

Theorem 4 *If the inverse of* $\Gamma+\mathcal{L}_H-\imath\hat{\omega}$ *contains* $\vec{\nabla}f_{\beta,\mu}(H)$ *in its domain, the conductivity tensor is given by the following Kubo formula:*

$$\sigma_{i,j}(\beta,\mu,\hat{\omega}) \;=\; \frac{q^2}{\hbar^2}\,\mathcal{T}\left(\partial_i H\,\frac{1}{\Gamma+\mathcal{L}_H-\imath\hat{\omega}}(\partial_j f_{\beta,\mu}(H))\right)\;. \tag{28}$$

Sufficient conditions for the Kubo formula to hold are given in Proposition 3. In particular, this is the case for the *relaxation time approximation* (RTA) which consists in replacing Γ in (28) by a multiple of the identity operator, namely

$$\Gamma \;=\; \frac{1}{\tau_{\rm rel}}\mathbf{1}\;, \qquad 0<\tau_{\rm rel}<\infty\;.$$

$\tau_{\rm rel}$ is then called the relaxation time. Using the current-current correlation measure m introduced in Proposition 2 and eq. (28), we get:

Theorem 5 *Within the* RTA*, the conductivity tensor is given by* $(i,j = 1,\ldots,d)$*:*

$$\sigma_{i,j}(\beta,\mu,\hat{\omega},\tau_{\rm rel}) \;=\; \frac{q^2}{\hbar^2}\int_{\mathbf{R}^2} dm_{i,j}(E,E')\;\frac{f_{\beta,\mu}(E')-f_{\beta,\mu}(E)}{E-E'}\;\frac{1}{\frac{1}{\tau_{\rm rel}}-\imath\frac{E-E'}{\hbar}-\imath\hat{\omega}}\;. \tag{29}$$

In the RTA, the error term due to the quadratic contribution in the electric field can also be estimated from (27), provided H is sufficiently smooth in $\mathcal{A}$, namely

$$\delta\sigma_{i,j} = \frac{q^3}{\hbar^3}\,\mathcal{T}\left(\partial_i H\;\frac{1}{\Gamma+\mathcal{L}_H-\imath\hat{\omega}-\frac{q}{\hbar}\vec{\mathcal{E}}\cdot\vec{\nabla}}\;\vec{\mathcal{E}}\cdot\vec{\nabla}\;\frac{1}{\Gamma+\mathcal{L}_H-\imath\hat{\omega}}(\partial_j f_{\beta,\mu}(H))\right)\;. \tag{30}$$

In the RTA, the relative size of this correction term with respect to the Kubo formula can be estimated by $q\mathcal{E}a\tau_{\text{rel}}/\hbar$ where a is the lattice spacing, giving a good measure of the effect of $\vec{\nabla}$. This ratio is very small in practice: for a typical electric field of $100V/cm$, a relaxation time of $10^{-13}s$ and a lattice constant of $a \approx 1\text{Å}$ this ratio is of the order of 10^{-6}. Actually, non linear terms are not well described by such a model, so that this estimate should not be considered too seriously for physical applications even though it shows that the linear response theory is valid.

2.4 Discussion of the model

Underlying the previous assumptions are three time scales $\tau_{\text{scat}} \ll \tau_{\text{rel}} \ll \tau_{\text{meas}}$. In our model we have set $\tau_{\text{scat}} = 0$ and $\tau_{\text{meas}} = \infty$. Here τ_{scat} is the typical time an electron or a hole (quasiparticle near the Fermi surface) spends in the interaction radius of a scatterer. τ_{rel} is the average time between two collisions renormalized by the efficiency of the collisions to lower current, whereas τ_{meas} represents the typical time needed to measure the current, namely the time over which we average the evolution.

Assuming $\tau_{\text{scat}} = 0$ is not actually a constraint. For indeed we can think of the scattering process as switching on the interaction at time t_l, letting the system evolve until at time $t_l + \varepsilon_l$ the interaction can be safely turned off. Here ε_l is of the order of τ_{scat} so that $t_l + \varepsilon_l < t_{l+1}$ with a very high probability. Therefore we can always define $\mathcal{C}_l$ such as to satisfy $U_\xi(t_l + \varepsilon_l, t_l) = \exp(-\varepsilon_l \mathcal{L}_H)\mathcal{C}_l$ and the eq. (25) still holds.
The assumption C requires, however, that τ_{scat} be small in order for the particle to interact with one scatterer at a time and in order for successive collisions to be stochastically independent. This is an important assumption made even if one starts with the many-body problem.
In order to give an order of magnitude of the ratio $\tau_{\text{scat}}/\tau_{\text{rel}}$ let us consider an electron-phonon interaction in a metal. Using Drude formula, τ_{rel} is typically of the order of $10^{-13}s$ at $77K$ [4]. On the other hand, τ_{scat} can be estimated by the quotient of the interaction radius and the relative velocity between scatterers. A reasonable estimation of the interaction radius is given by the wave length λ of the acoustic phonons of energy kT because they dominate the scattering process. For a velocity of sound of the order of $10^3\ m/s$, $\lambda \approx 5 \cdot 10^{-8}\ m/T$ with a temperature T given in Kelvin. For $T = 77\text{K}$, the interaction radius is thus of the order of 7Å. For a relative velocity given by a Fermi velocity by $10^6\ m/s$, $\tau_{\text{scat}} \approx 7 \cdot 10^{-16}s$ at 77K. The various time scales are well separated. Let us note that for systems with flat bands (such as quasicrystals and their periodic approximants [38]), the Fermi velocity may be significantly lower and hence the interaction time correspondingly bigger. But the relaxation time is also larger. In the quasicrystal $AlCuFe$, the mean free path computed from a Drude formula is typically 30Å [38] to be compared with the 7Å for the interaction radius. This is still qualitatively acceptable, but quantitative deviations are expected.

We now turn to our hypothesis B asserting that the collision times are Poisson distributed. This is a common hypothesis used to describe the emission-absorption process in quantum mechanics. The relaxation time is usually computed through a Fermi golden rule or as the inverse of the imaginary part of the self-energy in Dyson's equation (see [36], for example). However, the above characteristic time usually depends upon the initial state of the electron. In a metal, for example, formal perturbation theory usually leads to a continuous function $\tau(k)$ where k varies through the Brillouin zone. At high enough temperature, however, we may replace it by its average over the Brillouin zone. This is the argument leading to the RTA. It should also hold

in quasicrystals at high temperature. At very low temperature on the other hand, an infinite number of transitions must be taken into account during the electron-phonon collision, leading to an infinite number of collision times and making the operator Γ more involved than in (26). Nevertheless, the exponential law may be replaced by any probability distribution having a finite second moment [49]. In this case, the process on the long run looks like a Poisson one with only a renormalization of the relaxation time.
The exponential law has several nice mathematical properties. A Poisson process is characterized as the only stationary counting process satisfying the Markov property of having independent increments [15]. Furthermore, superposition of two Poisson processes with parameters τ' and τ'' respectively, gives again a Poisson process with parameter τ calculated by Mathiessen's rule:

$$\frac{1}{\tau} \;=\; \frac{1}{\tau'} + \frac{1}{\tau''} \; . \tag{31}$$

In conventional models, this relation is used in order to add the phonon-electron, the electron-electron and the impurity contributions in the calculation of the relaxation time. In our approach, however, we have already taken the impurity contribution into account in the electronic Hamiltonian H.

At last, the measurement time should be large enough as to allow the use of Birkhoff's theorem. This means that we exclude continuous measurements to produce some loss of information. A typical ratio $\tau_{\text{rel}}/\tau_{\text{meas}} \approx 100$ would require a measurement frequency not larger than $100GHz$. Beyond this frequency (laser pulses for instance), the measurement would give information on the short time behaviour of the particle only.

2.5 The collision term

The collision term in the quantum Boltzmann equation (26) is supposed to describe the interactions of the gas of independent electrons with the rest of the solid. As already pointed out in Section 2.4, it would be desirable to use perturbation theory in order to calculate it and particularly its temperature dependence from a fundamental Hamiltonian. Within the model of this article, the collision term is restricted to be given as quotient of some operator $1 - \hat{\kappa}$ and a mean collision or disintegration time τ. In this section a few simple examples of models for $\hat{\kappa}$ are described. They may be of practical interest in some cases.

I) The quantum Drude model. Each collision forces the electron system to its equilibrium. More precisely, if ρ is the density matrix just before the collision, it becomes

$$\mathcal{C}(\rho) \;=\; \hat{\kappa}^{\mathrm{D}*}_{\beta,\mu}(\rho) \;=\; f_{\beta,\mu}(H) \; , \tag{32}$$

just after the collision. So only collison times are random. If n is the charge carrier density, the density matrix is normalized according to $\mathcal{T}(\rho) = n$. Thus the collision operator acts on an observable $A \in \mathcal{A}$ by duality as

$$\hat{\kappa}^{\mathrm{D}}_{\beta,\mu}(A) \;=\; \frac{1}{n}\, \mathcal{T}(f_{\beta,\mu}(H)A)\, \mathbf{1} \; .$$

This implies $\hat{\kappa}^{\mathrm{D}}_{\beta,\mu}(A) = 0$ for any $A \in \mathcal{A}_H^{\perp}$ so that Proposition 3 applies with $\Gamma = \mathbf{1}/\tau$.

II) The quantum Lorentz model [11]. Let p be a Borel probability measure on the space $\mathrm{Aut}(\mathcal{A})$ of *-automorphisms of $\mathcal{A}$ invariant under the map $\xi \in \mathrm{Aut}(\mathcal{A}) \to \xi^{-1} \in \mathrm{Aut}(\mathcal{A})$. We assume also that p-almost surely, $\xi(H) = H$. For $\xi \in \mathrm{Aut}(\mathcal{A})$, C_ξ denotes the dual action of ξ on the space of density matrices, namely

$$\mathcal{T}\left(C_\xi(\rho)A\right) = \mathcal{T}\left(\rho\xi(A)\right) \ , \qquad \forall\, \rho \in L^1(\mathcal{A},\mathcal{T}),\ A \in \mathcal{A} \ .$$

C_ξ is the random operator of hypothesis C describing the elastic collision. Obviously $C_\xi \in \mathcal{F}$. The collision operator acting on $\mathcal{A}$ by duality is then given by

$$\hat{\kappa}^{\mathrm{L}}(A) \ = \ \int_{\mathrm{Aut}(\mathcal{A})} dp(\xi)\xi(A) \ . \tag{33}$$

It is a completely positive operator on $\mathcal{A}$ which extends as a selfadjoint contraction of $L^2(\mathcal{A},\mathcal{T})$ such that $\hat{\kappa}^{\mathrm{L}}(H^n) = H^n$ for all $n \in \mathbf{N}$. In particular, it leaves $\mathcal{A}_H^\perp$ invariant. If in addition the probability measure p is such that the restriction to $\mathcal{A}_H^\perp$ be bounded by $\kappa < 1$, then Proposition 3 still applies. This κ is a measure of the collisions' efficiency to diminish current and the relaxation time τ_{rel} is then estimated by $\tau/(1-\kappa)$. In realistic models both τ and κ may depend on temperature. Let us give an example where $\hat{\kappa}$ is contractive on $\mathcal{A}_H^\perp$.

Example: Let H be the discrete Laplacien on $\mathbf{Z}^2$. By Fourier transform, the physical Hilbert space $\mathcal{H}$ can be chosen as $L^2(\mathbf{T}^2)$ where $\mathbf{T}^2$ is the 2-torus. The observable algebra is then $\mathcal{A} = C(\mathbf{T}^2)$ acting by multiplication and the Hamiltonian is

$$H \ = \ 2\cos(k_1) + 2\cos(k_2) \ , \qquad k = (k_1,k_2) \in \mathbf{T}^2 \ .$$

It defines two open subsets of $\mathbf{T}^2$ by $D_\pm = \{k \in \mathbf{T}^2 |\ 0 < \pm H(k) < 4\}$. In each of them the constant energy sets are diffeomorphic to a circle $\mathbf{T}$. Since $\mathbf{T}^2$ is symplectic, we get action angle variables (I,ϕ) in D_+ and in D_- such that $dI \wedge d\phi = dk_1 \wedge dk_2$ and $H(k) = \pm h(I)$ when $k \in D_\pm$. Here the function h is defined by $h(I) = E$ whenever $I = \int_{E<H(k)<4} dk_1 \wedge dk_2/2\pi$ for $0 < E < 4$. Therefore $k \in D_\pm \mapsto (I,\phi) \in (0,\pi) \times \mathbf{T}$ is a symplectic diffeomorphism. Thus $L^2(\mathbf{T}^2)$ can be identified with $L^2(D_+) \oplus L^2(D_-)$, namely $\mathcal{H} \cong L^2((0,\pi)\times\mathbf{T}) \otimes \mathbf{C}^2$ and $A \in \mathcal{A}$ acts as

$$\hat{A}(I,\phi) \ = \ \left(\begin{array}{cc} A_+(I,\phi) & 0 \\ 0 & A_-(I,\phi) \end{array}\right) \ ,$$

where $A_\pm = A|_{D_\pm}$. Let p be a continuous function on $\mathbf{T}$ such that $p(\theta) = 1 + g(\theta)$ with $\int d\theta g(\theta) = 0$ and $W = -\imath d/d\phi$. Then the collision operator is

$$\hat{\kappa}_p(A) \ = \ \int \frac{d\theta}{2\pi}\, p(\theta)\, e^{\imath\theta W} A e^{-\imath\theta W} \ .$$

It satisfies $\hat{\kappa}(\mathcal{A}_H^\perp) \subset \mathcal{A}_H^\perp$ and, for $A \in \mathcal{A}_H^\perp$,

$$\hat{\kappa}_p(A_\pm)(I,\phi) \ = \ \int \frac{d\theta}{2\pi}\, g(\theta) A_\pm(I,\phi-\theta) \ .$$

In particular, Proposition 3 applies if $\kappa = \int \frac{d\theta}{2\pi}|g(\theta)| < 1$. $\diamond$

III) Scattering matrix model [50]. This model is a quantum analog of a model investigated by Kac [29] for classical systems. Let $\mathcal{H}$ be the one-particle Hilbert space. As the collision process arises, the particle suddenly finds itself coupled to some thermal bath described through a one-particle Hilbert space $\mathcal{H}_{\mathrm{B}}$. The total Hilbert space becomes $\mathcal{H} \otimes \mathcal{H}_{\mathrm{B}}$ during the scattering. As long as the interaction between the particle and the bath can be neglected, the total Hamiltonian will be $H + H_{\mathrm{B}}$ where H_{B} is the Hamiltonian of the bath particles. A scattering unitary matrix S, commuting with the asymptotic Hamiltonian $H + H_{\mathrm{B}}$, describes the output of the collision process. Before the collision the density matrix of the bath is the equilibrium state $\rho_{\mathrm{B}}^{\beta}$ at inverse temperature β whereas the particle ones is ρ; we get a total density matrix $\rho \otimes \rho_{\mathrm{B}}^{\beta}$. Thus after collision the density matrix becomes $S\rho \otimes \rho_{\mathrm{B}}^{\beta} S^*$. After the collision the bath variables are integrated out by taking a partial trace leading to a new particle state

$$\hat{\kappa}_{\beta}^{*}(\rho) \;=\; \mathcal{T}_{\mathrm{B}}\left(S\left(\rho \otimes \rho_{\mathrm{B}}^{\beta}\right) S^*\right) \;. \tag{34}$$

When applied to Bloch electrons or holes, the corresponding quantum Boltzmann equation (26) is precisely the linear Boltzmann equation if the matrix elements of S are properly identified with the scattering cross section and $\mathcal{T}_{\mathrm{B}}$ is the trace per unit volume. Although possibly fruitful for the study of metals and alloys, this approach has however several inconveniences.
First of all, it does not take into account the constraints due to the Fermi-Dirac statistics. This problem can be overcome by the Uehling-Uhlenbeck proposal. The electron can only be scattered from an occupied state to an empty one. Thus the correct form of the whole collision term should be:

$$\Gamma_{\beta}^{\epsilon}(\rho) \;=\; \frac{1}{\tau}\mathcal{T}_{\mathrm{B}}\left(S(1-\rho)\otimes(1+\epsilon\rho_{\mathrm{B}}^{\beta})S^*\,\rho\otimes\rho_{\mathrm{B}}^{\beta} - S\,\rho\otimes\rho_{\mathrm{B}}^{\beta}\,S^*(1-\rho)\otimes(1+\epsilon\rho_{\mathrm{B}}^{\beta})\right) \;,$$

where ϵ equals -1,1 or 0 depending upon whether the particles of the bath are fermions, bosons or classical particles; furthermore, $\rho_{\mathrm{B}}^{\beta}$ is the corresponding Fermi-Dirac, Bose-Einstein or Boltzmann equilibrium state of the bath.
More seriously, the observable algebra of the coupled system particle-bath in the infinite volume limit has not been described. The S-matrix should leave it invariant. Moreover, the partial trace should be such as to map the coupled observables into the original one-particle observable algebra. This problem has not been solved yet and this approach will not be developed in this paper.

3 AC conductivity

In this section, the previous results are extended to time-dependent electric fields. All results contained here hold for constant electric field as well, by assuming that $\vec{\mathcal{E}}$ is constant in time. Therefore this section can be considered as the set of technical proofs of results claimed before. In Section 3.1, the evolution of observables in such a field is constructed. The method is standard in the theory of ordinary differential equations and is adapted to C^*-algebras here. In Section 3.2, the Floquet theory is adapted to C^*-algebras . In Section 3.3 the Kubo formula for the optical conductivity at frequency $\hat{\omega}$ is proved.

3.1 Evolution with a time dependent perturbations

The motion of a particle with Hamiltonian $H = H^* \in \mathcal{A}$ submitted to an external time dependent electric field, namely a continuous map $t \in \mathbf{R} \to \vec{\mathcal{E}}(t) \in \mathbf{R}^d$ is described by the Heisenberg equation of motion

$$\frac{dA}{dt} \;=\; \mathcal{L}_H(A) - \frac{q}{\hbar}\vec{\mathcal{E}}(t)\cdot\vec{\nabla}A \;. \tag{35}$$

For $H = 0$ and $q\vec{\mathcal{E}}(t)/\hbar = 1$, this equation is solved using $\rho_{\vec{k}} = \exp(\vec{k}\cdot\vec{\nabla})$ where $\vec{k} \in \mathbf{R}^d$. According to the definitions of Section 2.1 and eq. (18), it is a d-parameter group of pointwise norm continuous *-automorphisms of $\mathcal{A}$. By construction, this group is $2\pi\mathbf{Z}^d$ periodic in $\vec{k}$, so that $\vec{k}$ can be considered as an element of $\mathbf{T}^d$. The following result is elementary so that the proof will be left to the reader.

Proposition 5 *For $H = 0$, the Heisenberg equation of motion* (35) *admits the following solution*

$$A(t) = \rho_{\vec{\mathcal{G}}(t,t')}(A(t')) \ ,$$

where $\vec{\mathcal{G}}(t,t') = -q/\hbar \int_{t'}^{t} ds\, \vec{\mathcal{E}}(s)$. This evolution is a family of pointwise norm continuous *-automorphisms of $\mathcal{A}$ with respect to t, t'. It is causal, namely $\rho_{\vec{\mathcal{G}}(t,t')} = \rho_{\vec{\mathcal{G}}(t,t")}\rho_{\vec{\mathcal{G}}(t",t')}$, $\forall t, t', t" \in \mathbf{R}$ and $\rho_{\vec{\mathcal{G}}(t,t)} = id$, $\forall t \in \mathbf{R}$.

If H is non zero, a solution $A(t)$ of the Heisenberg equation (35) with initial condition $A(t_0) = A \in \mathcal{A}$ is written in the form $A(t) = \rho_{\vec{\mathcal{G}}(t,t_0)}(B(t))$ so that $B(t_0) = A$. Inserting in eq. (35) and integrating between times t' and t, B satisfies

$$B(t) = B(t') + \int_{t'}^{t} ds \mathcal{L}_{H(s)} B(s) \ , \tag{36}$$

where $H(t) = \rho^{-1}_{\vec{\mathcal{G}}(t,t_0)}(H)$, so that $\|H(t)\| = \|H\|$, $\forall t \in \mathbf{R}$. Iterating eq. (36), as in a Dyson expansion, we get

$$B(t) = B(t') + \sum_{n=1}^{N-1} \int_{t' \leq s_n \leq \ldots \leq s_1 \leq t} ds_1 \ldots ds_n \mathcal{L}_{H(s_1)} \ldots \mathcal{L}_{H(s_n)} B(t') + R_N \ , \tag{37}$$

$$R_N = \int_{t' \leq s_N \leq \ldots \leq s_1 \leq t} ds_1 \ldots ds_N \mathcal{L}_{H(s_1)} \ldots \mathcal{L}_{H(s_N)} B(s_N) \ . \tag{38}$$

The remainder is dominated by $\|R_N\| \leq (2^N (t-t')^N/N!) \|H\|^N \sup_{t' \leq s \leq t} \|B(s)\|$. This estimate shows that two solutions $B_1(t)$ and $B_2(t)$ such that $B_1(t') = B_2(t')$ actually coincide, namely there is a *unique solution* with a given initial data. Moreover, it also shows that the Dyson expansion, obtained from (37) by letting $N \to \infty$, converges for any $t' \leq t \in \mathbf{R}$. Let us write the solution in the form $B(t) = \tilde{\eta}_{t,t'}(B(t'))$ where $\tilde{\eta}_{t,t'}$ corresponds to the infinite sum appearing in Dyson's expansion. It is clearly a bounded linear operator on $\mathcal{A}$. Setting $\eta_{t,t'} = \rho_{\vec{\mathcal{G}}(t,t_0)} \circ \tilde{\eta}_{t,t'} \circ \rho_{\vec{\mathcal{G}}(t,t_0)^{-1}}$ we get

Theorem 6 *If $H = H^* \in \mathcal{A}$ and if $\vec{\mathcal{E}}(t)$ is a continuous function from $\mathbf{R}$ into $\mathbf{R}^d$, the Heisenberg equation of motion* (35) *admits a unique solution in the form*

$$A(t) = \eta_{t,t'} A(t') \ , \qquad \forall t, t' \in \mathbf{R} \ ,$$

where $\eta_{t,t'}$ is a *-automorphism of $\mathcal{A}$, norm pointwise continuous with respect to $t, t' \in \mathbf{R}$. Moreover the family η is causal, namely

1. *$\eta_{t,t} = id$ for all $t \in \mathbf{R}$*
2. *$\eta_{t,t'} = \eta_{t,t"} \circ \eta_{t",t'}$ for all $t, t', t" \in \mathbf{R}$*

If in addition $\vec{\mathcal{E}}$ is periodic in time of period $\hat{T}$, then $\eta_{t+\hat{T},t'+\hat{T}} = \eta_{t,t'}$ for all $t, t' \in \mathbf{R}$.

Proof. We only need to prove that the same properties hold for the $\tilde{\eta}_{t,t'}$'s. It is a family of *-automorphism of $\mathcal{A}$ because $\mathcal{L}_{H(t)}$ is a family of bounded *-derivations of $\mathcal{A}$. For indeed, if $B_1(t)$ and $B_2(t)$ are two solutions of eq. (36) with initial conditions $B_1(t') = B_1$ and $B_2(t') = B_2$, then $B_1(t)B_2(t)$ is also a solution with initial conditions $B_1(t')B_2(t') = B_1B_2$. Thanks to the uniqueness of the solution, $\tilde{\eta}_{t,t'}(B_1B_2) = \tilde{\eta}_{t,t'}(B_1)\tilde{\eta}_{t,t'}(B_2)$. The continuity of $\tilde{\eta}_{t,t'}$ with respect to t, t' is obvious from eq. (37). Causality follows from the uniqueness theorem. At last, if $\vec{\mathcal{E}}$ is $\hat{T}$-periodic, shifting both the initial and the final time by $\hat{T}$ does not change the equation, so that the uniqueness leads to $\eta_{t+\hat{T},t'+\hat{T}} = \eta_{t,t'}$. □

3.2 Floquet's theory

In this section, $\vec{\mathcal{E}}(t) = \vec{E}(\theta - \hat{\omega}t)$ where $\vec{E}$ is a continuous function of $\theta \in \mathbf{T} = \mathbf{R}/2\pi\mathbf{Z}$, with values in $\mathbf{R}^d$, and $H = H^* \in \mathcal{A}$. Let $\eta^\theta_{t,t'}$ denote the corresponding evolution defined as in Theorem 6. Floquet's theory can be developped in very much the same way as in Howland [26] and Yajima [61] for Hilbert spaces.

Let $\mathcal{B}$ be the C^*-algebra of continuous functions $B : \theta \in \mathbf{T} \mapsto B(\theta) \in \mathcal{A}$ endowed with the sup-norm $\|B\|_{\mathcal{B}} = \sup_{\theta\in\mathbf{T}} \|B(\theta)\|_{\mathcal{A}}$. Hence $\mathcal{B} = \mathcal{C}(\mathbf{T}) \otimes \mathcal{A}$ as C*-algebraic tensor product [46]. The evolution $\eta^\theta_{t,t'}$ satisfies $\eta^{\theta+\hat{\omega}s}_{t+s,t'+s} = \eta^\theta_{t,t'}$ for $s \in \mathbf{R}$. We introduce the map ζ_s acting on $\mathcal{B}$ by

$$\zeta_s(B) : \theta \in \mathbf{T} \mapsto \eta^\theta_{0,s}\left(B(\theta - \hat{\omega}s)\right) \in \mathcal{A} \ , \tag{39}$$

where $s \in \mathbf{R}$ and $B \in \mathcal{B}$. We denote by ∂_j the *-derivations on $\mathcal{B}$ given by $\partial_0 B(\theta) = dB(\theta)/d\theta$ whereas $(\partial_j B)(\theta) = \partial_j(B(\theta))$ for $j = 1, \ldots, d$. $\mathcal{C}^1(\mathcal{B})$ will denote the common domain of these $d+1$ derivations.

Theorem 7 *The family $(\zeta_s)_{s\in\mathbf{R}}$ defined in eq. (39) is a one-parameter group of norm pointwise *-automorphisms of $\mathcal{B}$. Its generator coincides on $\mathcal{C}^1(\mathcal{B})$ with $(-\mathcal{L}_H + q/\hbar\vec{E}(\theta)\cdot\vec{\nabla} - \hat{\omega}\partial_0)$.*

Sketch of the proof. Thanks to Theorem 6, $\zeta_s(B)$ is an element of $\mathcal{B}$ whenever $B \in \mathcal{B}$. A tedious but elementary calculation shows that ζ_s is a *-homomorphism such that $\zeta_0 = id$ and $\zeta_{s_1+s_2} = \zeta_{s_1} \circ \zeta_{s_2}$, $\forall s_1, s_2 \in \mathbf{R}$. Thus we get a one-parameter group of *-automorphisms. The norm pointwise continuity is based upon Theorem 6 and a 3ϵ-argument. The explicit computation of the generator comes from the definition (39) and the Heisenberg equation of motion. □

$\mathcal{B}$ admits a normalized trace defined by

$$\hat{\mathcal{T}}(B) \ = \ \int_{\mathbf{T}} \frac{d\theta}{2\pi}\, \mathcal{T}(B(\theta)) \ , \qquad B \in \mathcal{B} \ . \tag{40}$$

By duality, the space $L^1(\mathcal{B}, \hat{\mathcal{T}})$ is made of measurable maps $\hat{\rho} : \theta \in \mathbf{T} \mapsto \rho(\theta) \in L^1(\mathcal{A}, \mathcal{T})$ such that $\mathcal{T}(|\hat{\rho}(\theta)|)$ is integrable over $\mathbf{T}$. The evolution dual to ζ is defined by $\hat{\rho}(s) = \zeta_{-s}(\hat{\rho})$ whenever $\hat{\rho} \in \mathcal{B} \cap L^1(\mathcal{B}, \hat{\mathcal{T}})$ and extended in a unique way to $L^1(\mathcal{B}, \hat{\mathcal{T}})$. Since ζ is a group of *-automorphisms of $\mathcal{B}$, this evolution leaves the subset of density matrices invariant. Let us consider a density matrix ρ_0 over $\mathcal{A}$. Its evolution in time is given by duality by $\rho_t = (\eta^\theta_{t,0})^{-1}(\rho_0) = \eta^\theta_{0,t}(\rho_0)$. The averaged current is therefore given by $\vec{j}_\theta(t) = \mathcal{T}(\eta^\theta_{0,t}(\rho_0)\vec{J})$. It is a continuous function of $\theta \in \mathbf{T}$. Therefore one can consider its time averaged nth Fourier component defined as

$$\vec{\jmath}_n(\hat{\omega}) \;=\; \lim_{t\to\infty} \int_{-t}^{t} \frac{dt'}{2t} \int_{\mathbf{T}} \frac{d\theta}{2\pi} \exp\left(-\imath n\theta\right) \vec{j}_\theta(t') \;.$$

As in Section 1.1 and eq. (2), we get a *no-go* theorem in absence of dissipation, namely

Proposition 6 *Let $\vec{E}(\theta)$ be a continuous function on $\mathbf{T}$ with values in $\mathbf{R}^d$ and let $\vec{E}_n$ be its n-th Fourier coefficient. Then $\vec{E}_n\,\vec{\jmath}_{-n}(\hat{\omega}) = 0$ for all n's.*

Proof: Let e_n be the function $\theta \in \mathbf{T} \mapsto \exp\left(\imath n\theta\right) \in \mathbf{C}$. An elementary calculation leads to

$$\vec{\jmath}_n(\hat{\omega}) \;=\; \lim_{t\to\infty} \int_{-t}^{t} \frac{dt'}{2t}\, \hat{\mathcal{T}}\left(e_0 \otimes \rho_0 \;\; \zeta_{-t'}(e_{-n} \otimes \vec{J})\right) \;.$$

On the other hand it is simple to check that

$$\zeta_{-t'}(\vec{E} \otimes \vec{J}) \;=\; -\frac{d}{dt'}\zeta_{-t'}(e_0 \otimes H) \;.$$

Averaged over t' between $-t$ and t, the left hand side is dominated in norm by $2\|H\|/t$. This gives $\sum_{n\in\mathbf{Z}} \vec{E}_n \vec{\jmath}_{-n}(\hat{\omega}) = 0$. The same is true also if $\vec{E}(\theta)$ is replaced by $\vec{E}(\theta+\varphi)$. Then it is tedious but straightforward to check that $\vec{\jmath}_n(\hat{\omega})$ does not change, whereas $\vec{E}_n$ is multiplied by $\exp\left(\imath n\varphi\right)$. Since φ is arbitrary in $\mathbf{T}$, the proposition is proved. □

3.3 Kubo's formula for the optical conductivity

In this section, Kubo's formula (28) is derived rigorously and Proposition 4 and Theorem 4 are proved. As before, at time $t = 0$ the system with Hamiltonian $H = H^* \in \mathcal{C}^1(\mathcal{A})$ is in the equilibrium state $\rho_0 = f_{\beta,\mu}(H)$. Then for $t > 0$ an electric field $\vec{\mathcal{E}}(t) = \vec{E}(\theta - \hat{\omega}t)$ periodic in time is turned on. In particular, it can be constant in time. The average evolution of the current (or the state) will be computed. By *average* we mean both the thermal and the ergodic average. The linear response of the current at large times to the electric field $\vec{\mathcal{E}}$ gives the conductivity.

Since H is a smooth element of $\mathcal{A}$ and $f_{\beta,\mu}$ is a smooth function, ρ_0 belongs to $L^p(\mathcal{A},\mathcal{T})$ for all $p \geq 1$. In particular, it will be convenient to consider it as an element of $L^2(\mathcal{A},\mathcal{T})$. Then every *-automorphism of $\mathcal{A}$ extends to $L^2(\mathcal{A},\mathcal{T})$ as a unitary operator; so do $U_{\xi,\theta}(t,t')$ and $\eta^{\theta\,*}_{t,t'}$. By assumption D in Section 2.2 we also know that the collision efficiency operator $\hat{\kappa}^*$ must leave ρ_0 invariant. By construction it is a positivity and trace preserving operator acting on $L^1(\mathcal{A},\mathcal{T})$. For purely technical convenience, we will restrict these assumptions here as follows

D' The collision efficiency operator $\hat{\kappa}^*$ defines a bounded operator on $L^2(\mathcal{A},\mathcal{T})$ leaving the subspaces $\mathcal{A}_H^{\perp}$ and its orthogonal invariant.

According to the assumptions made in Section 2.2, the thermal average of the current at time t is given by

$$\vec{j}_{\xi,\theta}(t) = \mathcal{T}\left(\rho_0\; \eta^{\theta}_{t,t_l}\mathcal{C}_l^* \ldots \eta^{\theta}_{t_2,t_1}\mathcal{C}_1^*\eta^{\theta}_{t_1,0}(\vec{J})\right) \;, \tag{41}$$

whenever $t_0 = 0 < t_1 < \ldots < t_l < t < t_{l+1}$. Here, $\mathcal{C}_l^*$ is the adjoint of $\mathcal{C}_l$. As before, the nth Fourier coefficient of this current with respect to the phase θ of the electric field gives the response at frequency $n\hat{\omega}$. Multiplication of both sides of eq. (41) by $\exp(-\imath n\theta)$ followed by an integration over θ gives

$$\vec{\jmath}_{\xi,n}(t) \;=\; \int_{\mathbf{T}} \frac{d\theta}{2\pi} e^{-\imath n\theta} \vec{j}_{\xi,\theta}(t) \;=\; e^{-\imath n\hat{\omega}t} \hat{\mathcal{T}}\left(e_{-n}\otimes\rho_0\,\zeta_{-(t-t_l)}\mathcal{C}_l^*\ldots\zeta_{-\tau_2}\mathcal{C}_1^*\zeta_{-\tau_1}(e_0\otimes\vec{J})\right)\;.$$

We need to average this quantity over both collisions and time. A well-known tauberian theorem [44] asserts that the time average can be obtained as the limit

$$\lim_{t\uparrow\infty}\int_0^t \frac{dt'}{t} f(t') \;=\; \lim_{\delta\downarrow 0}\delta\int_0^\infty dt\, e^{-\delta t} f(t)\;.$$

Hence we need to compute the Laplace transform of $\vec{j}_{\xi,n}(t)$. It can be decomposed as follows:

$$\delta\int_0^\infty dt\; e^{-\delta t}\vec{j}_{\xi,n}(t) \;=\; \sum_{l=0}^{\infty}\delta\int_{t_l}^{t_{l+1}} dt\; e^{-(\delta+\imath n\hat{\omega})t}\;\;\hat{\mathcal{T}}\left(e_{-n}\otimes\rho_0\,\zeta_{-(t-t_l)}\mathcal{C}_l^*\ldots\zeta_{-\tau_2}\mathcal{C}_1^*\zeta_{-\tau_1}(e_0\otimes\vec{J})\right)\;.$$

Each term of the sum must be averaged over ξ. Averaging over the collison operators $\mathcal{C}_j^*$'s consists in replacing them by $\hat{\kappa}$. Averaging over the time delays $\tau_j = t_j - t_{j-1}$ can be done by using the formula

$$\int_0^\infty \frac{ds}{\tau} e^{-s/\tau} e^{-(\delta+\imath\hat{\omega})s}\zeta_{-s} \;=\; \frac{1}{\tau}\left(\frac{1}{\tau}+\delta+\imath n\hat{\omega}-\mathcal{L}_H+\frac{q}{\hbar}\vec{E}\cdot\vec{\nabla}-\hat{\omega}\partial_0\right)^{-1}\;,$$

where the operator $\mathcal{L}_H - q/\hbar\vec{E}\cdot\vec{\nabla}+\partial_0$ is the anti-selfadjoint generator of ζ_{-s} seen as acting on $L^2(\mathcal{A},\mathcal{T})$. We also need the integral

$$\int_0^{\tau_j} du\;\; e^{-(\delta+\imath\hat{\omega})u}\;\;\zeta_{-u} \;=\; \frac{1-e^{-\tau_j(\delta+\imath n\hat{\omega}-\mathcal{L}_H+q/\hbar\vec{E}\cdot\vec{\nabla}-\hat{\omega}\partial_0)}}{\delta+\imath n\hat{\omega}-\mathcal{L}_H+q/\hbar\vec{E}\cdot\vec{\nabla}-\hat{\omega}\partial_0}\;.$$

After averaging over ξ, the Laplace transform $\vec{\jmath}_n(\delta)$ of the averaged current $\mathbf{E}_\xi(\vec{\jmath}_{\xi,n}(t))$ is equal to a Neuman series that can be easily summed up and dualized to give:

$$\vec{\jmath}_n(\delta) \;=\; \delta\hat{\mathcal{T}}\left(e_0\otimes\vec{J}\;\;\frac{1}{\delta+\imath n\hat{\omega}+\frac{1-\hat{\kappa}^*}{\tau}+\mathcal{L}_H-q/\hbar\vec{E}\cdot\vec{\nabla}+\hat{\omega}\partial_0}(e_{-n}\otimes\rho_0)\right)\;.$$

Remark. This type of calculation performed for $\vec{E}=0$ and $\hat{\omega}=0$ leads immediately to Proposition 4. $\diamond$

The time average requires letting δ converge to zero. As argued in Section 2.2, this expression vanishes for $\vec{E}=0$. For indeed, $\rho_0 = f_{\beta,\mu}(H)$ so that $\{(1-\hat{\kappa}^*)/\tau+\imath n\hat{\omega}+\mathcal{L}_H+\partial_0\}e_{-n}\otimes f_{\beta,\mu}(H) = 0$. In addition, eq. (23) in Proposition 3 implies $\mathcal{T}(\vec{J}\,f_{\beta,\mu}(H))=0$. So we can safely substract the same quantity in which $\vec{E}=0$, giving

$$\vec{\jmath}_n(\delta) \;=\; \frac{q}{\hbar}\hat{\mathcal{T}}\left(e_0\otimes\vec{J}\;\;\frac{1}{\delta+\imath n\hat{\omega}+\frac{1-\hat{\kappa}^*}{\tau}+\mathcal{L}_H-q/\hbar\vec{E}\cdot\vec{\nabla}+\hat{\omega}\partial_0}\vec{E}\cdot\vec{\nabla}\,(e_{-n}\otimes f_{\beta,\mu}(H))\right)\;.$$

Due to Proposition 3, as $\vec{E}\to 0$, the term $q/\hbar\vec{E}\cdot\vec{\nabla}$ in the denominator can be ignored modulo an error of order $\vec{E}^2$. At last, $\vec{E}$ can be decomposed into its Fourier components so that only the n-th one survives inside the trace due to the integration over θ. Then the limit $\delta \downarrow 0$ can be taken. This leads to $\vec{\jmath}_n(\delta = 0) = \sigma(\beta, \mu, n\hat{\omega})\vec{E}_n$ with the matrix σ given by the eq. (28) in Theorem 4.

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