Coherent and dissipative transport in aperiodic solids : an overview

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Abstract

This lecture is a review of a theoretical approach, based on Noncommutative Geometry, liable to describe transport properties of aperiodic solids. After a short introduction, the section 2 concerns a description of the experimental problems that may be covered by such a study. A special emphasis is put upon Mott's hopping conductivity in Anderson insulators and transport properties of quasicrystals. Section 3 is a heuristic description of the laws of Thermodynamics, both at equilibrium and out of equilibrium, that are needed in these lecture notes. Section 4 gives the mathematical framework that replaces Bloch theory for aperiodic solids. In particular the notion of Noncommutative Brillouin zone is defined. The section 5 is devoted to coherent transport in such solids, with emphasis upon the definition and properties of various spectral and transport exponents. Section 6 gives an account of the various kinetic approach to transport within the Relaxation Time Approximation (RTA). The main result is the *anomalous Drude formula*. A discussion of the impact of *quantum chaos* is also provided to explain the existence of residual conductivity at low temperature in quasicrystals. The last section is a short introduction to kinetic theories beyond the RTA.

1 Introduction

The theory of Solid State Physics started with the seminal paper of P. Drude [1] giving the first microscopic insight on transport properties of metals in term of the theory of electrons (see [2] for a History of Solid State Physics). It was soon followed by a series of works on phonons including the ones by A. Einstein [3], P. Debye (see [2] Section 1.1) and M. Born & von Karmann [4], before the first diffraction experiment was performed by von Laüe (see [2] Section 1.1). Still from then on, most of the subject concerned perfect crystals.

Soon after the creation of Quantum Mechanics, F. Bloch [5] developped the band theory, the main tool available since then for computing the energy spectrum of periodic crystals. Under the influence of Sommerfeld (see [2] Section 2.2), using the Pauli principle for electrons [6], the theory of metal was developped to the extend of understanding what characterized the difference between metals, insulators and semiconductors from a microscopic point of view [7].

It was not until the early seventies that disordered systems were systematically studied under the influence of P.W. Anderson [8] and D. Thouless [9]. It has been recognized that disordered media have entirely new transport properties. Anderson predicted the occurence of a metal-insulator transition depending on how strong is the disorder [10]. As a result, a residual conductivity at low temperature appears in weakly disordered systems due to quantum interferences [11, 12]. In strongly disordered ones, the Anderson localization leads to insulating behaviour through Mott's variable range hopping [13, 14].

The discovery of quasicrystals in 1984 [15] added a new step in dealing with aperiodic solids. Unlike disordered media, quasicrystals have a long range order even though non periodic. Still their transport properties at low temperature are not yet understood well [16, 17]. To make things simple how can quasicrystalline alloys, such as $Al_{62.5}Cu_{25}Fe_{12.5}$ in its icosahedral phase, behave like insulators ? In this series of lecture, a simple mechanism will be proposed, based on the complexity of quantum interferences due to Bragg reflections, as a possible explanation for such strange behaviour.

These notes report on a long standing program which started in the early eighties [18], with goal to provide a substitute to Bloch theory for aperiodic solids. The main focus however, will be on the recent developments on transport theory, such that the *anomalous Drude formula*, or various kinetic models within which a complete Kubo formula is established covering most of the situations occuring in aperiodic solids. It will be shown that, due to absence of translation invariance, Bloch theory may be replaced by *Noncommutative Geometry*. The quasimomentum space can then be defined as a *noncommutative manifold* called the Noncommutative Brillouin Zone (NCBZ). A Calculus on such manifold allows to extend most of formulæ valid for crystals to aperiodic solids. Using the full power of functional analysis and spectral theory, it will then be possible to investigate what makes the difference between periodic crystals and aperiodic solids.

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2 Experimental Aspects

2.1 Why should one revisit transport ?

Transport theory goes back to the seminal work by Boltzmann [19]. It came after the first attempt by Clausius [20] to understand why the sound velocity in gas was much smaller than the diffusion one: he got the idea that if gas were made of small particles then this could be easily understood. In his first work, he was supposing that all particles had the same velocity but with random directions. Even though the model was so elementary, it was giving good order of magnitude for the microscopic datas, such as the mean free path, the mean collision time. Moreover he was made to understand the difference between sound and diffusion at a time when the atomic hypothesis was far from being accepted. Soon after, Maxwell [21] realized that the velocity of particle was not unique but given by a distribution depending on the temperature of the gas. This was the starting point of Boltzmann who's goal was to go beyond the very nice argument of Maxwell and to offer a microscopic theory liable to provide formulæ for transport cœfficients such that the viscosity (see the Preface of the French translation of the Boltzmann book by M. Brillouin [22]).

This theory was not immediately recognized as valid. In the early twentieth century, several contributions described transport through using stochastic processes. The Drude model for electrons in metals [1] is the first example. It was not until 1905, however, that Lorentz recognized that it could also be represented by a Boltzmann equation [23]. Later, the study of the Brownian motion by Einstein [24] and then by Langevin [25], gave rise to a different description which eventually led to the foundation of Probability Theory through the notion of Stochastic Processes, thanks to the works by Markov, Levy, Wiener and eventually Kolmogorov in the late thirties. The Boltzmann equation, even though an approximation valid whenever three-body collisions can be neglected, has been used successfully in a large number of situations, including the electron transport in metals [23], the derivation of equations for fluids dynamics, the description of low density self gravitating celestial systems, or the dynamics of atomic nuclei.

These approaches were supplemented in 1931 by the Onsager approach to irreversible thermodynamics [26] and its linear response theory with the reciprocity relations. In 1948, the works by Bogoliubov, Born, Green, Kirkwood and Yvon [27] permitted to supplement the Boltzmann equation in situations for which the density of the system was higher. During the fifties, the contributions by Green [28] and Kubo [29] led to explicit formulæ for the linear response cœfficients in term of the microscopic Hamiltonians. The Green-Kubo formula is actually valid in full generality, for classical and quantum systems as well. One of the striking fact about this theory is that its derivation from first principle is still not well understood today. Since the early seventies, starting with the seminal work by Lanford [30], there has been intensive works with aim to derive the Boltzamnn equations from the first principles. It is not the aim of this work to give a full report on it.

The study of various kind of new conducting materials since the early sixties, including doped semiconductors at low temperature, disordered crystals, such as real metals, amorphous conductors, and more recently, quasicrystals, exhibited new type of transport properties that are not fully understood even today. This is because the electronic transport become sensitive to quantum interferences at low temperature. The large variety of quantum effects that can be produced, depending upon the atomic arrangement or on the chemical bonding, is a source of theoretical difficulties requiring a qualitatively new mathematical approach.

2.2 Known Mechanisms

Several mechanisms have already been identified concerning the temperature behaviour of the electric conductivity in solids.
(i) For metals, the conductivity increases as the temperature decreases. Moreover, the Landau theory of Fermi liquid predicts [31, 32]

$$\sigma(T) \stackrel{T\downarrow 0}{\sim} T^{-2}$$

over a large range of temperatures.
(ii) On the opposite side, thermally activated processes, namely whenever a gap arises in the spectrum near the Fermi level, give [14]

$$\sigma(T) \stackrel{T\downarrow 0}{\sim} e^{-\Delta/T}$$

(iii) For weakly disordered systems, such as strongly doped semiconductors or normal metals, there is a residual conductivity at low temperature, due to *quantum interferences* [14, 11]

$$\sigma(T) \stackrel{T\downarrow 0}{\sim} \sigma_0 > 0$$

(iv) In strongly disordered systems, such as for lightly doped semiconductors, and whenever the Density of States (DOS) is small at the Fermi level, one expects a *Mott variable range hopping* [14] (see Section 2.3), namely in dimension D

$$\sigma(T) \stackrel{T\downarrow 0}{\sim} \exp\left\{-\left(\frac{T_0}{T}\right)^{1/(D+1)}\right\}$$

(v) The case of quasicrystals is special and not yet completely established. Conductivity properties of QC's are rather anomalous when compared to the previous mechanisms. Even though made of good metals, like $Al, Fe, Cu, \cdots$, they behave like insulators at low temperature. Moreover, their conductivity follow a scaling law of the type [16]:

$$\sigma \sim \sigma_0 + A\,T^{\gamma} \qquad\qquad 1 < \gamma < 2$$

where σ_0, the residual conductivity, may vanish in some cases. No mechanisms are proposed in conventional books to explain such a behaviour. One of the aim of these notes is to provide a possible explanation [17, 33] (see Section 5).

2.3 Mott variable hopping transport

In 1968, Mott [13] proposed the following argument liable to explain the conductivity properties of Anderson insulators at low temperature (see also [14]).
Mott assumes that the solid is a D-dimensional Anderson insulator, namely the electrons are strongly localized. In particular, each energy level of the electron energy spectrum is associated with a position in the solid within a ball of diameter given by the localization length ξ. Moreover, he assumes that the density of states (DOS) n_F at the Fermi level is non vanishing but small enough so as to avoid overlap between electron states. In particular the mean distance between neighbouring electron states is large compare with ξ. The inverse of $n_F \cdot \xi^D$ is a measure of the mean level spacing between states within a ball of diameter ξ. The temperature will be small compare to this scale namely

$$k_B T n_F \xi^D \;=\; \frac{T}{T_0} \;\ll\; 1\,,$$

if k_B denotes the Boltzmann constant. Then (see Fig 1), within a small error, all states with energy smaller than the Fermi level E_F are occupied, whereas the ones with energy bigger are

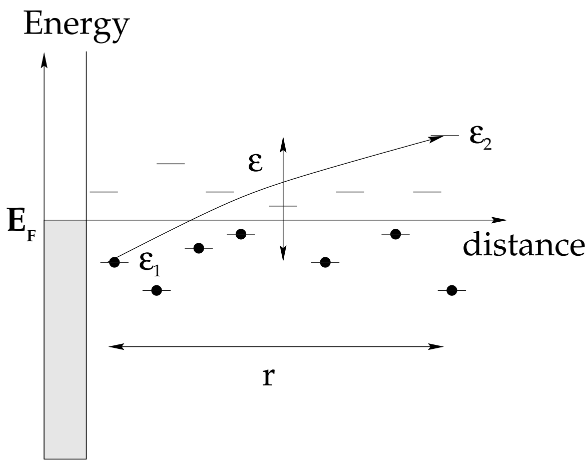

Figure 1: Mott's Variable Range Hopping

empty. The probability that a phonon of energy ε be produced is proportional to e^{ε/k_BT}. This is true provided $\varepsilon \gg k_BT$. The probability that this phonon be absorbed by an electron of the Fermi sea, with energy $\epsilon_1 < E_F$ to jump in a state of energy $\epsilon_2 > E_F$ is controlled by the tunneling effect forcing such an electron to move in space, since the two states are localized apart from each other. Let then d be the distance between such states, so that the tunneling probability be proportional to $e^{d/\xi}$. Therefore the probability P of transfer of an electron at distance d from its original location is proportional to

$$P \;\propto\; \exp - \left\{ \frac{\varepsilon}{k_BT} + \frac{d}{\xi} \right\}$$

By definition of the DOS, the product $\varepsilon \cdot n_F \cdot d^D$ represents the number of states in an energy interval of width ε localized in a ball of diameter d. This number must be at least 1 so that

$$\varepsilon \cdot n_F \cdot d^D \;\geq\; 1$$

the probability of jump P is then optimized provided d assumes its minimum value, which depends on ε. Therefore the conductivity, which is proportional to the sum of contributions of all such jumps, will be controlled by the maximal value of P. Optimizing over ε leads to

$$P \;\propto\; \exp - \left\{ \frac{T_0}{T} \right\}^{1/D+1}$$

Then, the phonon energy optimizing P is given by $\varepsilon_{opt} \approx T^{D/D+1} \gg T$, while the average distance of the jump is given by $d/\xi \approx (T_0/T)^{1/D+1} \gg 1$.
For lightly doped $3D$-semiconductors like silicon (see [14]), the localization length is given by the Bohr radius of the impurity, which is about 100Å. For a concentration of 10^{-9}, the mean distance between impurities is 1000Å which is approximately 10ξ. Then, the typical width of the impurity band is about $1meV$. Assuming the DOS to be flat on it leads to $k_BT_0 \approx 1eV$ or $T_0 \approx 1.1 \times 10^4 K$! This is huge indeed compare even to the room temperature $k_BT \approx 27meV$. However, this Mott hopping conductivity is hidden as long as the gap between the impurity and

the conduction bands is small compare to the temperature. This gap is of the order of $10meV$, requiring a temperature much smaller than $110K$. This example shows that the conductivity is multiplied by a very small factor of order 10^{-4} due to this mechanism ! It turns out that this is exactly what happens in the quantum Hall effect (QHE) [34, 35]: the Mott variable range hopping controls the fluctuation of the plateaus, leading to the amazing accuracy of this experiment.

2.4 Quasicrystals

The first quasicrystal discovered in 1984 [15] was an alloy of $AlMn$ in a metastable phase. However the transmission electron diffration picture (TEM) was exhibiting a point like spectrum with a 5-fold symmetry, a fact incompatible with the existence of a translation symmetry. It was proposed that such material had a quasiperiodic arrangement of its atoms (see [16] for a review). Since this discovery about 400 alloys have been discovered having a quasicrystalline structure. Most of them have the icosahedral symmetry, a large number a decagonal symmetry. But some other type of symmetries have been observed too. Experiments on the conductivity properties were initiated by the end of the eighties until quite recently. They were performed on high quality sample mainly on $AlFeCu$, $AlPdMn$ and $AlPdRe$ [36]. Their main properties are summarized as follows:

QC.1 Their conductivity is low to very low [16].

QC.2 Their conductivity decreases enormously with the temperature, with, in some cases

$$\frac{\sigma_{300K}}{\sigma_{4K}} \geq 300$$

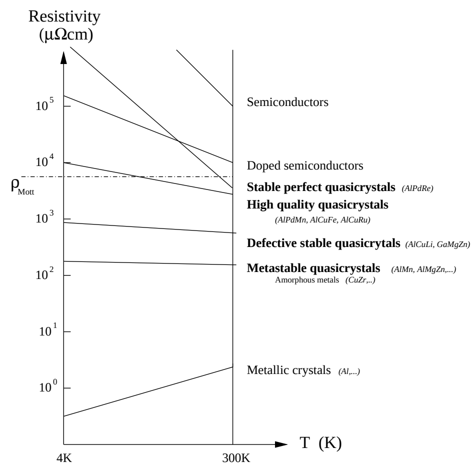

Figure 2: Typical resistivity of quasicrystals (see C. Berger in [37])

QC.3 The conductivity is not thermally activated.

QC.4 The conductivity decreases with improved sample quality.

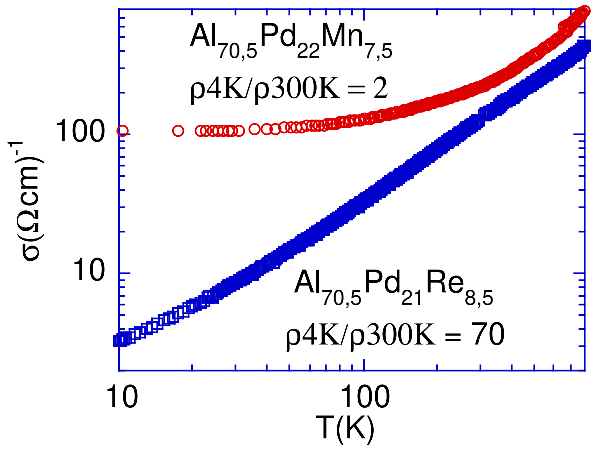

Figure 3: Conductivity for $AlPdMn$ and $AlPdRe$ [17]

QC.5 In the temperature range from $50mK$ to $1000K$, the conductivity follows a scaling law [16].

$$\sigma \sim \sigma_0 + A\,T^{\gamma} \qquad\qquad 1 < \gamma < 2$$

QC.6 For most good quality icosahedral compounds, such as $AlCuFe$ or $AlPdMn$, the conductivity flattens below $300K$ to reach a residual conductivity $\sigma(t) \approx \sigma_0 > 0$ (see Fig. 3). However, $\sigma_0 = 0$ for $i - AlPdRe$.

QC.7 In the icosahedral phase of $AlPdRe$, instead, some type of Mott variable range hopping is observed with [38, 39]

$$\sigma \propto e^{-(T_0/T)^{1/4}}$$

in a range of temperature which varies from author to author within the interval 0 to $10K$. In [39], $T_0 \sim 6mK$.

2.5 Questions

The description given in the last three sections raises several questions:

1. Is it possible to extend the Bloch theory to non periodic solids ?
2. Is there a theory for transport, at least in the one particle approximation, that provides reliable Kubo formulæ for the electric conductivity ?
3. Is there a chance to prove rigorously the Mott estimate for the variable range hopping ?
4. Is it possible to account for the scaling laws that appear in the conductivity of quasicrystals ?

The aim of these notes is to propose a mathematical framework, based upon A. Connes ideas on Noncommutative Geometry [40] which is liable to provide answers to these questions. This theory started in the early eighties [18] and developped over the years [42, 35, 43]. More recently the theory was extended to coherent [33] and dissipative transport [44, 45]. Several of the results shown at the end (see Section 6) are part of a paper in preparation [46].

3 Irreversible Thermodynamics: Heuristic

This Section is a summary of the principle of thermodynamics, whether at equilibrium or out of equilibrium. It can be found in many textbook [47, 48, 49, 50]. For a more rigorous approach of the equilibrium statistical mechanics, the reader should look at [51, 52, 53]. For reviews on nonequilibrium see [54, 55, 56, 57]. This heuristic exposition is given here for the convenience of the reader and to fix the notations and the physical frame within which this work in done.

3.1 Information Theory and Thermodynamics

The main ingredient in the foundation of statistical thermodynamics, is the notion of *information* that was defined and studied in 1948 by Shannon [58] for the purpose of transmission of messages. It turns out that the formalism he developped is very similar to what was in use at the time in Thermodynamics. To be more precise, let $\mathcal{S}$ be a classical system with N particles contained in a box Λ of the physical real space $\mathbb{R}^d$. Its phase space is $\mathfrak{F} = (\Lambda \times \mathbb{R}^d)^N$. In practice, it is not necessary to know with infinite precision the state of the system at all times. So it is convenient to divide the phase space into cells (such as Planck cells if quantum mechanics is considered in a semiclassical approximation). The number of such cells may be at most countable, but it may be convenient to ignore a large number of them on the account that their probability of being visited is very small. For instance the probability for the momentum to reach large values is usually very small. So, one cell can have infinite volume if its probability of visit is small. Let then Ω be the set of such cells. Moreover, the time can also be discretized, as is usually done in dynamical system when using a Poincaré section, and will be labelled by integers. Hence the state of the system at time $n \in \mathbb{Z}$ is a label $q_n \in \Omega$ denoting in which box of the phase space $\mathcal{S}$ is located. In this way, the evolution of the system can be seen as the transmission of a signal through a transducer exactly as Shannon describes it in his paper. Shannon proposed to consider the map $n \mapsto q_n$ as a *stochastic process*. The signal itself is a succession of *digits* namely, in the present situation, a sequence $q_1, q_2, \cdots, q_n$ of box labels through which the orbit of the system is passing. The evolution being deterministic, the evolution equation for the probability distribution of the successive q_n's can be well represented by a short time memory process. Markov processes are only the roughest approximation for such an evolution. Hence at each time $n \in \mathbb{Z}$, the state of the system is rather a *probability distribution* $\mathbb{P}_n$ on Ω. The amount of information such a state contains is measured by the *lack of information* namely its *Shanon entropy* (denoted by H in [58]) given by

$$s(\mathbb{P}) \;=\; -\sum_{q\in\Omega} \mathbb{P}(q) \ln \mathbb{P}(q)\,.$$

Quantum system are defined by following a similar chain of arguments. The phase space $\mathfrak{F}$ is then replaced by a Hilbert space $\mathfrak{H}$ as long as the system is contained in a box Λ of finite volume. The stochastic process describing the evolution is now described by a one-parameter group of unitary operators $U(t)$ (here the time may be taken as continuous) while the probability distribution is given by a *density matrix* ρ, that is a positive selfadjoint operator with $\mathrm{Tr}\{\rho\} = 1$. Its entropy is the *von Neumann entropy* given by

$$s(\rho) \;=\; -\mathrm{Tr}\{\rho \ln \rho\}\,.$$

An *observable* is either a function $\widehat{F} : q \in \Omega \mapsto \widehat{F}(q) \in \mathbb{R}$, in the classical case, or a selfadjoint operator $\widehat{F}$ on the Hilbert space $\mathfrak{H}$, in the quantum one. Its thermodynamical average is defined as

$$\langle \widehat{F} \rangle \;=\; \sum_{q\in\Omega} \mathbb{P}(q)\widehat{F}(q)\,,\ \text{(classical)} \qquad \langle \widehat{F} \rangle \;=\; \mathrm{Tr}\{\rho \widehat{F}\}\,,\ \text{(quantum)}$$

Classical or quantum systems are subjected to physical constraints, most of them coming from symmetries. The most important one, related to the time translation symmetry, is the conservation of the total energy of the system (*First Law of Thermodynamics*). In the classical case, the energy is a function $\widehat{E} : q \in \Omega \mapsto \widehat{E}(q) \in \mathbb{R}$. In the quantum case it is given by a selfadjoint operator $H = H^*$ acting on $\mathfrak{H}$ ans called the *Hamiltonian*. Because the system is contained in a finite volume, this Hamiltonian has usually a *discrete spectrum*, denoted by $\mathrm{Sp}H$, namely its spectrum is made of a discrete set of eigenvalues with finite multiplicity. In particular the Hamiltonian admits a countable orthonormal basis of eigenvectors. In very much the same way, other conservation laws, such as the total momentum, the total angular momentum, must be taken into account. Also there are other constraints of various origins, geometrical, chemical, *etc.*, such as the conservation of the volume V of the box Λ in which the system evolves, or of the particle number N of each chemical species. Throughout the evolution, these quantities are conserved whenever the system is isolated.
To fix the notation, let $\widehat{X}_1, \cdots, \widehat{X}_K$ be the list of conserved quantities associated with the system. In the classical case, each of the $\widehat{X}_\alpha$'s is a function on Ω which will be supposed to be *real valued* for convenience. If one of the conserved quantities (*e.g.* the momentum) is vectorial or tensorial, then the corresponding coordinates will correspond to some of the $\widehat{X}_\alpha$'s. Therefore, only the labels $q \in \Omega$ with prescribed values X_α of the $\widehat{X}_\alpha$'s are allowed. Let then $\Omega\{X_1, \cdots, X_K\}$ be the subset of such q's. In the quantum case, $\{\widehat{X}_1, \cdots, \widehat{X}_K\}$ is a set of commuting selfadjoint operators. Again because the system is in a finite volume, these operators have usually a discrete spectrum. In particular they have a common orthonormal basis of eigenvectors. Their *joint spectrum* is defined as

$$\mathrm{Sp}\{\widehat{X}_1, \cdots, \widehat{X}_K\} \;=\; \{x = (x_1, \cdots, x_K) \in \mathbb{R}^K\,;\, \exists \phi \in \mathfrak{H}, \widehat{X}_\alpha \phi = x_\alpha \phi\, \forall \alpha\,, \phi \neq 0\}$$

The multiplicity of a joint eigenvalue x is the dimension of the corresponding eigenspace. In most usual cases, this family is *complete* in the sense that its joint spectrum is *simple*, namely each joint eigenvalue has multiplicity one. But this is not necessarily the case. If $I \subset [1, K]$, $\mathfrak{H}\{X_\alpha\,; \alpha \in I\}$ will denote the eigensubspace of $\mathfrak{H}$ corresponding to the eigenvalues $x_\alpha = X_\alpha$ for $\alpha \in I$.

In practical situations, no system is totaly isolated. $\mathcal{S}$ may exchange part of the information contained in the conserved quantities with the outside world. However, because these quantities are *extensive*, namely their average value is proportional to the volume V of the box Λ in which the system evolves, the exchange with the outside world can only occur on the boundary $\partial\Lambda$ of this box, so that the relative fluctuation varies like the ratio surface-to-volume S/V of the box, which is very small for large boxes. Therefore, let I_{fluc} be the list of α's corresponding to conserved quantities liable to fluctuate in this manner and let I_{fix} the other labels: the first group of conserved quantities will be called *fluctuating* the other will be *fixed*. It is then equally convenient to consider such a system as defined by the phase space $\Omega\{X_\alpha\,;\alpha\in I_{\mathit{fix}}\}$ in the classical case and by the Hilbert space $\mathfrak{H}\{X_\alpha\,;\alpha\in I_{\mathit{fix}}\}$ in the quantum one, on which the variables $\widehat{X}_\beta\,,\ \beta\in I_{\mathit{fluc}}$ are defined. The data of a subset $I_{\mathit{fluc}}\subset[1,K]$ defines a *Gibbs ensemble*. The *microcanonical ensemble* is defined by setting $I_{\mathit{fluc}}=\emptyset$, namely it describes an isolated system.

3.2 Equilibrium Statistical Mechanics

The Second Law of Thermodynamics can be very roughly summarized as follows:

> **Second Law of Thermodynamics:** *During an evolution the total information contained in an isolated system cannot increase*

In other words, the entropy of the system cannot decrease. So the evolution will change the state as long as the entropy increases. But if the state has already reached a maximum of its entropy, its state cannot change anymore. This is precisely the definition of a *Gibbs state* or *equilibrium state*. Its is usual to apply this principle to Gibbs ensembles. This is because, even though they describe partially open systems, such systems are seen as a representative sample of a large isolated system. However, because of the conservation laws, such partially open systems will be subjected to conservation of the variables $\widehat{X}_\alpha$ in the mean whenever $\alpha\in I_{\mathit{fluc}}$

$$\langle\widehat{X}_\alpha\rangle \;=\; X_\alpha\,, \qquad\qquad \forall\alpha\in I_{\mathit{fluc}} \tag{1}$$

To compute Gibbs states in the classical case, it is therefore enough to find, among all probabilities on $\Omega_{I_{\mathit{fix}}}=\Omega\{X_\alpha\,;\alpha\in I_{\mathit{fix}}\}$ satisfying eq. (1), the one which maximizes the entropy. This a problem of maximizing the functional $s(\mathbb{P})$ with constraints. Because $\mathbb{P}$ is a probability, $\sum_q\mathbb{P}(q)=1$ gives an extra constraint too. The solution is given in term of *Lagrange multipliers*, namely it is enough to find the critical points of the functional:

$$G(\mathbb{P}) \;=\; s(\mathbb{P})-\lambda_0\sum_{q\in\Omega_{I_{\mathit{fix}}}}\mathbb{P}(q)-\sum_{\alpha\in I_{\mathit{fluc}}}\lambda_\alpha\langle\widehat{X}_\alpha\rangle\,.$$

Since Ω is a finite set, $\mathbb{P}$ is defined as a vector on $\mathbb{R}^{\Omega_{I_{\mathit{fix}}}}$ and G as a unique maximum because it is strictly concave. This maximum can be computed by solving the equation $\partial G/\partial\mathbb{P}(q)=0$ which gives:

$$\mathbb{P}(q) \;=\; \frac{e^{-\sum_{\alpha\in I_{\mathit{fluc}}}\lambda_\alpha\widehat{X}_\alpha}}{\mathcal{Z}} \qquad\qquad \mathcal{Z} \;=\; \sum_{q\in\Omega_{I_{\mathit{fix}}}} e^{-\sum_{\alpha\in I_{\mathit{fluc}}}\lambda_\alpha\widehat{X}_\alpha}\,. \tag{2}$$

The normalization constant $\mathcal{Z}$ is called the *partition function*. A very similar result is obtained in the quantum case, provided $\mathbb{P}$ is replaced by ρ and the sum over the q's by the trace over the corresponding Hilbert space.
The other Lagrange multipliers are, in principle, computable through the constraints (1). However, it is usual to proceed differently and to give them a thermodynamical meaning. To do so, the main hypothesis is provided by the *Boltzmann formula*

$$S \;=\; k_{\scriptscriptstyle B}\, s(\mathbb{P})\,, \qquad\qquad k_{\scriptscriptstyle B} \;=\; 1.38\times 10^{-23}\, J\cdot K^{-1}\,, \tag{3}$$

where S is the *Clausius entropy*. The Thermodynamics of the 19th century was dealing with infinitesimal changes of equilibrium. In the language defined before, the equilibrium is entirely defined by the data of $\{X_\beta\,;\,\beta\in I_{\mathit{fix}}\}$ and by the Lagrange multipliers. Equivalently, if the Lagrange multipliers are uniquely defined by (1), the equilibrium is entirely defined by the data of $\{X_1,\cdots,X_K\}$. It is traditional to denote by $U=\langle\widehat{E}\rangle$ the average of the total energy of the system, which will be identified with the variable $\widehat{E}=\widehat{X}_1$ in the sequel. Then $dU, dX_2,\cdots,dX_K$ will denote the infinitesimal variation of the X's under this infinitesimal change of equilibrium. The Clausius entropy was defined as a quantity S, the variation of which being given by

$$T\,dS \;=\; dU + \sum_{\alpha=2}^{K} F_\alpha\, dX_\alpha\,, \tag{4}$$

where T is the *temperature* and the F_α's are called the *conjugate quantities*. The Table 3.2 below gives a list of such quantities.
If the infinitesimal variation is computed directly from the formula (2) , it leads to the following relation

$$\lambda_\alpha \;=\; \frac{F_\alpha}{k_{\scriptscriptstyle B} T} \qquad\qquad \forall\alpha\in I_{\mathit{fluc}}\,. \tag{5}$$

By convention, the conjugate variable to the energy will be given by $F_1=1$. Then the *thermodynamical potentiel* associated with I_{fluc} is defined as

$$A=-k_{\scriptscriptstyle B}T\ln\mathcal{Z}=\sum_{\alpha\in I_{\mathit{fluc}}} F_\alpha X_\alpha\,-TS\;\Rightarrow\; dA=\sum_{\alpha\in I_{\mathit{fluc}}} dF_\alpha X_\alpha-\sum_{\alpha\in I_{\mathit{fix}}} F_\alpha dX_\alpha - SdT \tag{6}$$

3.3 The Local Equilibrium Approximation

If now the system under study is put out of equilibrium, the situation changes because the state describing it will evolve in time. In general, the evolution equation is difficult to describe, but even when this is possible, it is practically too hard to solve and becomes useless. The most common approximation that is used to deal with real systems is called the *Local Equilibrium Approximation*. It is based upon the observation that in most systems, there are various *scales* in space or time. In the simplest possible case there are three main scales called respectively *microscopic, macroscopic* and *mesoscopic*. For example the length and the time scales will be

$$\ell\;\ll\;\delta L\;\ll\;L\,, \qquad\qquad \tau_{\mathit{rel}}\;\ll\;\delta t\;\ll\;t\,. \tag{7}$$

Name of X	*Notation* $\widehat{X}$	*Average*	*Conjugate Variable F*	*Name of F*
Energy	$\hat{E}(q)$	U	1	T = temperature
Local momentum	$\hat{p}_i(q)$ $i = x, y, z$	$\vec{p} = (p_x, p_y, p_z)$	$-\vec{v}$	$\vec{v}$ = local velocity
Angular momentum	$\hat{L}_i(q)$ $i = x, y, z$	$\vec{L} = (L_x, L_y, L_z)$	$-\vec{\omega}$	$\vec{\omega}$ = local angular velocity
Volume	$\hat{V}(q)$	V	P	P = pressure
Number of particles of species a	$\hat{N}_a(q)$	N_a	$-\mu_a$	μ_a = chemical potential of species a
Magnetization	$\hat{M}_i(q)$ $i = x, y, z$	$\vec{M} = (M_x, M_y, M_z)$	$-\vec{B}$	$\vec{B}$ = magnetic field
Electric charge	$\hat{Q_{el}}(q)$	Q_{el}	$-\mathcal{V}$	$\mathcal{V}$ = Electric potential
Deformation tensor *(in solids)*	$\hat{\Sigma}_{i,j}(q)$ $i, j \in \{x, y, z\}$	$\Sigma_{i,j}$	$\Pi_{i,j}$	Π = stress tensor

Table 1: Conserved quantities and their conjugate variables in 3D (classical systems)

Here ℓ, τ_{rel} are the typical scales at the microscopic level for which the microscopic evolution is computable through, say, perturbation theory. In the case of a gas, for instance, ℓ is of the order of magnitude of the *mean free path*, namely the average length within which no collisions between particles occur, whereas τ_{rel} is the average time between two consecutive collisions experienced by one particle. For electrons in a conductor, ℓ is also the *inelastic mean free path*, namely the average length within which no collisions with phonon occur and τ_{rel} is the average time between two such collisions. The macroscopic scale L is the typical system size whereas t is the observation time. The *mesoscopic length* δL is defined as follows: on the one hand it is large enough so that a cell of size δL can be considered as a Thermodynamical system within Statistical Mechanics; but on the other hand, it is small enough to be considered as infinitesimal compared to L. Similarly the time scales δt is large enough so as

> **Local Equilibrium Approximation:** (LEA) *A cell of mesoscopic size has returned to equilibrium after a mesoscopic period of time.*

On the other hand, δt is small enough to be considered as an infinitesimal if compared to t.

In practice, the typical microscopic time involved in conductors varies between $\tau_{rel} \approx 10^{-12} - 10^{-14}s$ [59]. In the case of copper (Cu), it is $\tau_{rel} = 21 \times 10^{-14}s$([59] p.10). To compute the mean free path, it is sufficient to have an estimate of the conduction electron velocity. In a metal, the conduction electrons have an energy given by the Fermi level E_F. For Cu, the Fermi temperature is $\Theta_F = E_F/k_B = 8.16 \times 10^4 K$ (it varies between $11,000$ and $130,000K$ in metals [59] p.38). An estimate of the velocity is given by $m_* v_F^2/2 = k_B\Theta_F$ where m_* is the effective electron mass. In copper $m_* = 1.3m_e$, if m_e is the free electron mass. This gives $v_F = 1.7 \times 10^6 m.s^{-1}$ leading to a mean free path $\ell = v_F\tau_{rel} = 3,600$Å. Thus already in a cell of size 10 times bigger, 1000 collisions occur per collision time. Such a cell can be considered as mesoscopic. In much the same way, if one assumes that the mixing properties of the collision holds, a time 100 times bigger than τ_{rel} should be sufficient to produce a complete loss of memory of the initial condition of a typical electron. This mesoscopic times can be taken as small as $\delta t = 10^{-11}s$ in copper. Hence as long as the measurement process is much slower than δt, the LEA should apply.
The counterpart of the previous arguments is that in modern experiments involving femtosecond lasers, the LEA is clearly violated. This is why such measurement permits to track the details of the particle motion. Morever, using the paradox of quantum mechanics, it is possible to maintain a system in a given state, otherwise unstable, by a constant measurement. This is used today to control coherently some chemical reactions.
Note also that in biological systems, there may be more than three scales. For instance the folding of a protein takes about 1 s to be compared with the typical relaxation time for electronic motion $10^{-14}s$. It turns out that every two orders of magnitude gives rise to a new type of physics, leading to 6 or 7 type of time scales. The spatial structure of such protein is also involved and can be hierarchically described in term of primary, secondary, *etc.* structures [60, 61]. Still the (LEA) may give usually an acurate description of biological systems [62].

Thanks to the LEA, the box Λ containing the system $\mathcal{S}$ can be partitioned into cells $\Delta_{\vec{r}}$ of mesoscopic size centered at points $\vec{r}$, while the time axis will be also partitioned into intervals $[t, t+\delta t]$ of mesoscopic size. The subsystem $\mathcal{S}(\vec{r}, t)$ corresponding to the part of $\mathcal{S}$ contained in $\Delta_{\vec{r}}$ during times in $[t, t+\delta t]$, can be therefore considered at equilibrium. However $\mathcal{S}(\vec{r}, t)$

is totally opened, namely all $\widehat{X}_\alpha$'s are exchanging information with the neighbouring cells. Therefore such cell requires to be described with the largest possible Gibbs ensemble for which $I_{fluc} = [1, K]$. Thanks to the Section 3.2, the state describing it will be given by a family of conjugate variables, including the temperature, depending on $(\vec{r}, t)$, leading to the local Gibbs state (see eq. (2),(5))

$$\mathbb{P}_{(\vec{r},t)} \;=\; \frac{e^{-\beta(\vec{r},t)\left(\widehat{E}+\sum_{\alpha=2}^{K} F_\alpha(\vec{r},t)\widehat{X}_\alpha\right)}}{\mathcal{Z}(\vec{r},t)} \qquad\qquad \beta(\vec{r},t) = \frac{1}{k_B T(\vec{r},t)} \,. \tag{8}$$

A very similar formula holds for quantum systems. In much the same way, the average value of the conserved quantity $\widehat{X}_\alpha$ in the cell will depend on $(\vec{r}, t)$. But since it is extensive it is proportional to the volume of the cell so that it is itself mesoscopic, hence

$$\delta X_\alpha \;=\; \sum_{q\in\Omega(\vec{r},t)} \mathbb{P}_{(\vec{r},t)}(q)\, \widehat{X}_\alpha(q)\,,$$

where $\Omega(\vec{r}, t)$ represents the state space of the cell. The volume $\delta V(\vec{r}, t)$ is itself liable to fluctuate, however it will be convenient to choose cells of fixed volume δV. Thus the *local density* of $\widehat{X}_\alpha$ is well defined by

$$\rho_\alpha(\vec{r},t) \;=\; \frac{\delta X_\alpha(\vec{r},t)}{\delta V}\,. \tag{9}$$

3.4 Currents and transport

Considering the partition into mesoscopic cells as described in Section 3.3, it becomes clear that, on the one hand, the value of the $\widehat{X}_\alpha$'s may vary in time and space, namely from cell to cell. But due to the conservation law, this is possible only if the variation in one cell is compensated by an equal variation of opposite sign outside of this cell. Figure 4 shows an oversimplified situation in which two cells have been isolated from the rest of the world, but can exchange through an hypothetical membrane separating them.

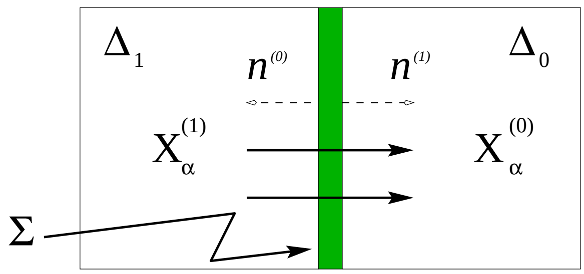

Figure 4: Transfer, fluxes and currents

Considering this example, let $\delta X_\alpha(\vec{r}, t)$ be the variation of $\widehat{X}_\alpha$ in the cell $\Delta^{(1)}$ over a mesoscopic time interval δt. Using the convention of Figure 4 above, it can be written as

$$\delta X_\alpha(\vec{r},t) \;=\; -\delta\Phi_\alpha(\vec{r},t)\delta t \;=\; -\vec{j}_\alpha(\vec{r},t)\cdot\vec{n}^{(1)}\,\delta\Sigma\,\delta t\,,$$

where $\vec{n}^{(1)}$ is the unit vector normal to the membrane and oriented from the cell $\Delta^{(1)}$ toward the cell $\Delta^{(0)}$, whereas $\delta\Sigma$ is the (mesoscopic) area of the membrane. $\delta\Phi_\alpha(\vec{r},t)$ represents the *flux* of the variable $\widehat{X}_\alpha$ through the membrane, namely the loss of $\widehat{X}_\alpha$ in the cell $\Delta^{(1)}$ per unit time. The vector $\vec{j}_\alpha(\vec{r},t)$ is called the *local current* flowing between the two cells.

Remark 1 *It is important to notice that this definition of the current is* mesoscopic*. There may be contributions to the current that have no microscopic counterpart. An important example in solids is provided by the* phonon drag*: phonons are like waves on the ocean on top of which electrons can surf, producing a charge transfer, thus a contribution to the electric current. Such contribution cannot be defined microscopically.*

Proceeding in much the same way with a more realistic situation where a cell is surrounding by more than one other cell, the current vector can be define accordingly. Summing all the contributions from all faces of the cell leads to the usual *continuity equation*

$$\frac{\partial \rho_\alpha}{\partial t}(\vec{r},t) + \vec{\nabla}\cdot\vec{j}_\alpha(\vec{r},t) \;=\; 0\,. \tag{10}$$

In much the same way there is a (Clausius) *entropy density* defined as before by

$$s(\vec{r},t) \;=\; \frac{\delta S(\vec{r},t)}{\delta V}\,,$$

in each mesoscopic cell. In view of the eq.(4), thanks to the LEA, its variation in time is given by

$$\frac{\partial s}{\partial t}(\vec{r},t) \;=\; \sum_{\alpha=1}^{K}\frac{F_\alpha(\vec{r},t)}{T}\;\frac{\partial \rho_\alpha}{\partial t}(\vec{r},t)\,,$$

By analogy with the previous definition of a flux, the local entropy current will be defined as

$$\vec{j}_S(\vec{r},t) \;=\; \sum_{\alpha=1}^{K}\frac{F_\alpha(\vec{r},t)}{T}\;\vec{j}_\alpha(\vec{r},t)\,.$$

Hence the total *entropy production rate* is given by

$$\frac{ds}{dt} \;=\; \frac{\partial s}{\partial t} + \vec{\nabla}\cdot\vec{j}_S \;=\; \sum_{\alpha=1}^{K}\vec{\nabla}\left(\frac{F_\alpha}{T}\right)\vec{j}_\alpha \;\geq\; 0\,, \tag{11}$$

where the positivity comes from the Second Law of Thermodynamics !

3.5 The Linear Response Theory

The main consequence of the previous Section 3.4 is that currents and fluxes occur because the conjugate variable are not constant in space. Through the LEA, the changes of equilibrium state is slow enough to allow constant return to equilibrium, hence leading to

> **Response theory:** *Each current is a smooth function of the gradient of the conjugate variables.*

Proving such a statement from first principle is still today an open challenge for a Mathematical Physicist. But on the basis of experiment, it is quite acceptable and provides a good frame to interpret the data. Since there should be no current at equilibrium, developing the functionnal relationship between currents and conjugate variables to first order leads to

$$\vec{j}_\alpha = \sum_{\beta=1}^{K} L_{\alpha,\beta}\, \vec{\nabla}\left(\frac{F_\beta}{T}\right) + O\left\{\left|\frac{F_\beta}{T}\right|^2\right\} . \tag{12}$$

Linear Response Theory (LRT) consists in neglecting higher order terms in this expansion. In most of the situation this is an excellent approximation.

Example 1 Thermoelectric effects. In the case of a conductor in which only thermal and electric current are considered, the Table 3.2 gives

$$dQ = T\, dS = dU - \mathcal{V}\, dQ_{el} \tag{13}$$

The left hand side defines the *variation of the heat* produced by the infinitesimal change of equilibrium. But the heat itself *is not* a conserved quantity, while both the energy U and the electric charge Q_{el} are conserved quantities. Here $\mathcal{V}$ is the electric potential. Correspondingly there will be an energy current $\vec{j}_U$ and an electric current $\vec{j}_{el}$. Thanks to eq. (13) it is convenient to define the *heat current* as

$$\vec{j}_{th} := \vec{j}_U - \mathcal{V}\,\vec{j}_{el} \tag{14}$$

On the other hand, the Onsager relations become

$$\begin{aligned} \vec{j}_U &= L_{u,u}\vec{\nabla}(\frac{1}{T}) + L_{u,q}\vec{\nabla}(\frac{-\mathcal{V}}{T}) \\ \vec{j}_{el} &= L_{q,u}\vec{\nabla}(\frac{1}{T}) + L_{q,q}\vec{\nabla}(\frac{-\mathcal{V}}{T}) \end{aligned} \tag{15}$$

For simplicity, let the conductor be isotropic, namely let the Onsager cœfficients above be multiple of the identity matrix. Then, if there is no current, namely if $\vec{j}_{el} = 0$ so that $\vec{j}_{th} = \vec{j}_U$,

$$\vec{j}_{th} := -\lambda\vec{\nabla}T\,, \qquad \lambda = \frac{L_{u,u}L_{q,q} - L_{u,q}L_{q,u}}{T^2 L_{q,q}}\,, \qquad \textbf{(Fourier's law)} \tag{16}$$

where λ is called the *thermal conductivity.* Moreover, there is a potential difference created due to the temperature gradient (Seebeck effect)

$$-\vec{\nabla}\mathcal{V} = \epsilon\vec{\nabla}T\,, \qquad \epsilon = \frac{L_{q,u} - \mathcal{V}L_{q,q}}{TL_{q,q}}\,, \tag{17}$$

where ϵ is called the *thermopower.* At last if the temperature gradient vanishes

$$\vec{j}_{el} = \sigma\,\vec{\mathcal{E}}\,, \qquad \vec{\mathcal{E}} = -\vec{\nabla}\mathcal{V}\,, \qquad \sigma = \frac{L_{q,q}}{T}\,, \qquad \textbf{(Ohm's law)} \tag{18}$$

where σ is the *conductivity.* In thermoelectric experiments, the linear response theory is barely violated. It requires the very high electric field found in lasers to start seeing second order effects that are used in nonlinear optics. □

In dimension d, each current takes on values in $\mathbb{R}^d$ so that the $L_{\alpha,\beta}$'s are $d \times d$ real valued matrices, called the *Onsager cœfficients*. The gradient $\vec{\nabla}(F_\alpha/T)$ plays the rôle of a generalized force and is called an *affinity*. It is quite convenient to consider the Onsager cœfficients as a matrix of blocks, namely as an element of $M_K(\mathbb{R}) \otimes M_d(\mathbb{R})$

$$\mathbb{L} \;=\; ((L_{\alpha,\beta}))_{\alpha,\beta=1}^{K} \,.$$

It is remarkable that the Second Law of Thermodynamics, as expressed in eq.(11) implies the following positivity property

$$\textbf{Second Law of Thermodynamics} \qquad \Longrightarrow \qquad \mathbb{L} + \mathbb{L}^t \;\geq\; 0\,. \tag{19}$$

This relation suggests that the only the symmetric part of the matrix $\mathbb{L}$ participates to the dissipation mechanisms responsible for the information loss during the evolution. The antisymmetric part of this matrix contains *nondissipative* response.

In 1931, Onsager [26] published a paper in which he investigated the consequences of the microscopic time reversibility on this cœfficients. The time reversal symmetry is generated by a transformation T_R such that ${T_R}^2 = 1$. There are two irreducible representations corresponding to either the character $\varepsilon = 1$ or to the character $\varepsilon = -1$. In particular, each conserved quantity $\widehat{X}_\alpha$ transforms according to one of this character under T_R denoted by ε_α. Onsager showed that, if the system is submitted to external forces through a set of parameters $\mathcal{P}$, then

$$L_{\beta,\alpha}(\mathcal{P}) \;=\; \varepsilon_\alpha\, \varepsilon_\beta\, L_{\alpha,\beta}(T_R\,\mathcal{P}) \qquad\qquad \textbf{Onsager's reciprocity relations} \tag{20}$$

The meaning of this formula is that while the affinity of type α can produce a current of type β, conversely the β-affinity produces an α-current with the same Onsager cœfficients up to a sign given by the corresponding characters of the time-reversal symmetry. In the example 1 of thermoelectric effects, it simply means that $L_{u,q} = L_{q,u}$. Then using the positivity (19) leads to $\sigma \geq 0\,, \lambda \geq 0$. Due to the existence of parameters that can change sign under time reversal symmetry, the matrix $\mathbb{L}$ may have non dissipative parts. We infer that these non dissipative contributions are related to toplogical invariants, such as what happens for the Quantum Hall Effect [35, 63].

4 Aperiodic Systems

The main problem in transport theory, is to have access to the computation and properties of the transport cœfficients from the microscopic properties of the system. In Solid State physics, most of the theory available in textbooks concern periodic crystal in which the Bloch theory applies. Since the mid-sixties, however, physicists started wondering about what happens for non periodic materials. In this section we propose a formalism developped in various papers since the early eighties [18, 64, 42, 35, 43, 65], that is a substitute to Bloch theory, whenever Bloch theory fails to apply.

4.1 The Hull

The starting point of the theory consists in considering the set of atomic positions in the ideal case where the atoms are fixed at their equilibrium position at zero temperature. This is a set of points in the ambient space $\mathbb{R}^d$. This set will be considered in the idealized situation for which the solid has infinite volume and is homogeneous in space. This is a convenient approximation that fails only for submicronic samples. Let $\mathcal{L}$ denote this set. It is clear that atoms cannot be too close from each others, due to nucleus repulsion at short distance. Moreover, since the system is idealized at zero temperature, except for special situations, like for zeolites, no lacuna is expected to occur so that there is a maximal size to holes between these points. This can be axiomatized in the following way [66]

Definition 1 *1)- A subset $\mathcal{L}$ of $\mathbb{R}^d$ is* uniformly discrete *if there is $r > 0$ such that every open ball of radius r meets $\mathcal{L}$ at most on one point. Then $\mathcal{L}$ will be called r-discrete.*
2)- A subset $\mathcal{L}$ of $\mathbb{R}^d$ is relatively dense *if there is $R > 0$ such that every closed ball of radius R meets $\mathcal{L}$ at least on one point. Then $\mathcal{L}$ will be called R-dense.*
3)- A subset $\mathcal{L}$ of $\mathbb{R}^d$ is a Delone set *(or also Delaunay) if it is both uniformly discrete and relatively dense. $\mathcal{L}$ will be called (r, R)-Delone if it is r-discrete and R-dense.*
4)- A Delone set $\mathcal{L}$ has finite type whenever $\mathcal{L} - \mathcal{L}$ is locally finite
5)- A Delone set is a Meyer set *whenever $\mathcal{L} - \mathcal{L}$ is itself a Delone set.*

Example 2

1. A random subset $\mathcal{L}$ of $\mathbb{R}^d$ distributed according to the Poisson distribution with a finite positive density is almost surely discrete, but with probability one, it is neither uniformly discrete nor relatively dense.

2. Let $\mathcal{L}_0$ be a *lattice* in $\mathbb{R}^d$, namely a discrete cocompact subgroup of $\mathbb{R}^d$. Let $\mathcal{L}$ be a random subset of $\mathcal{L}_0$ distributed according to the Bernoulli law on each sites. Then with probability one $\mathcal{L}$ is uniformly discrete (obvious) but not relatively dense. This situation occurs precisely for the distribution of impurity sites in a lightly doped semiconductor [14].

3. Most solids are described, at zero temperature by Delone sets. This is the case for amorphous materials (silicon), glasses, crystals.

4. The cut-and-project method to describe quasicrystals [16] shows that the set of atomic sites of such a material is a Meyer set.

□

In order to represent a uniformly discrete set $\mathcal{L}$, it is convenient to consider its *counting measure* which is the Radon measure on $\mathbb{R}^d$

$$\nu^{(\mathcal{L})} = \sum_{y \in \mathcal{L}} \delta(. - y)\,. \tag{21}$$

Recall that a Radon measure μ on $\mathbb{R}^d$ is an element of the dual space to the space $\mathcal{C}_c(\mathbb{R}^d)$ of continuous functions with compact support. Since it is not the aim of this paper to give all technical details, the reader should look at [67] to learn more about the natural topology on this space. Thus μ becomes a linear map $\mu : f \in \mathcal{C}_c(\mathbb{R}^d) \mapsto \mu(f) \in \mathbb{C}$ which is continuous. Here

$\nu^{(\mathcal{L})}(f) = \sum_{y\in\mathcal{L}} f(y)$ and this sum is finite since f has compact support and since $\mathcal{L}$ is discrete. The measure $\nu^{(\mathcal{L})}$ has the following properties

1. Any ball $B \subset \mathbb{R}^d$ has an integer measure, that is $\nu^{(\mathcal{L})}(B) \in \mathbb{N}$.

2. If B is an open ball of radius less than or equal to r then $\nu^{(\mathcal{L})}(B) \leq 1$, due to the uniform discreteness.

3. If, in addition, $\mathcal{L}$ is relatively dense any closed ball B of radius larger than or equal to R as a measure $\nu^{(\mathcal{L})}(B) \geq 1$.

It is not difficult to check that these three properties characterize $\mathcal{L}$ which is nothing but the support of the measure $\nu^{(\mathcal{L})}$. In other words, there is a one-to-one correspondance between discrete sets and their related measures so that each property of such set can be read on the associated measure and vice versa.

Representing the atomic set by a measure is a convenient tool to describe topologies. The space $\mathfrak{M}(\mathbb{R}^d)$ of Radon measures on $\mathbb{R}^d$ will be endowed with the weak* topology over $\mathcal{C}_c(\mathbb{R}^d)$. This means that a sequence $(\mu_n)_{n\in\mathbb{N}}$ of Radon measures converges to μ if and only if given any continuous function f with compact support on $\mathbb{R}^d$, then $\lim_{n\to\infty} \mu_n(f) = \mu(f)$. Thanks to this language, to say that a sequence $\mathcal{L}_n$ of discrete sets converges to the discrete set $\mathcal{L}$ means that in each open ball B the sets $\mathcal{L}_n \cap B$ converges to $\mathcal{L} \cap B$, say for the Hausdorff distance. Note however, that this convergence needs not being uniform *w.r.t.* B. So it is convenient to denote by $UD_r(\mathbb{R}^d)$ the set of Radon measures on $\mathbb{R}^d$ with support given by an r-discrete set. In very much the same way let $Del_{r,R}(\mathbb{R}^d)$ be the set of Radon measures on $\mathbb{R}^d$ with support given by an (r, R)-Delone sets. Then [43]:

Proposition 1 *1)- The spaces $UD_r(\mathbb{R}^d)$ and $Del_{r,R}(\mathbb{R}^d)$ are closed and compact in $\mathfrak{M}(\mathbb{R}^d)$.*
2)- The closure $QD(\mathbb{R}^d)$ of the union $\bigcup_{r>0} UD_r(\mathbb{R}^d)$ in $\mathfrak{M}(\mathbb{R}^d)$, is nothing but the set of measures with discrete support such that each point in the support has an integer positive mass.
3)- $UD_r(\mathbb{R}^d)$ is the closure of the union $\bigcup_{R>r} Del_{r,R}(\mathbb{R}^d)$.

Remark 2 1)- means that from any sequence of r-discrete sets it is possible to extract a convergent subsequence that converges to an r-discrete set. In particular the limit of a convergent sequence of r-discrete sets is itself r-discrete.
2)- a measure of $QD(\mathbb{R}^d)$ can be seen as an atomic set in which a finite number of atoms can sit on top of each other.
3)- means that each r-discrete set can be approximated by a sequence of r-discrete Delone sets. $\square$

Remark 3 In much the same way, a Meyer set is an (r, R)-Delone set such that $\mathcal{L}-\mathcal{L}$ is (r', R')-Delone for some $0 < r < R\,, 0 < r' < R'$. If $Mey_{r,R;r',R'}(\mathbb{R}^d)$ denote such set of measures, it is also compact in the weak* topology. $\square$

Remark 4 The property for $\mathcal{L}$ of having finite type is not preserved under limits. $\square$

Given now $a \in \mathbb{R}^d$, the translation $\mathrm{T}^a : x \in \mathbb{R}^d \mapsto x + a \in \mathbb{R}^d$ acts on $\mathcal{C}_c(\mathbb{R}^d)$ through $\mathrm{T}^a f(x) = f(x-a)$ whenever $f \in \mathcal{C}_c(\mathbb{R}^d)$. Therefore it also acts on the space of Radon measures through $\mathrm{T}^a \mu(f) = \mu(\mathrm{T}^{-a} f)$ whenever $f \in \mathcal{C}_c(\mathbb{R}^d)$ and $\mu \in \mathfrak{M}(\mathbb{R}^d)$. It is elementary to check that these maps are continuous and invertible. Hence the translation group $\mathbb{R}^d$ acts on $\mathfrak{M}(\mathbb{R}^d)$ in a continuous way and

Proposition 2 *The spaces $QD(\mathbb{R}^d)$, $UD_r(\mathbb{R}^d)$ and $Del_{r,R}(\mathbb{R}^d)$ are $\mathbb{R}^d$-invariant.*

Remark 5 In much the same way $Mey_{r,R;r',R'}(\mathbb{R}^d)$ is translation invariant. □

Remark 6 If $\mathcal{L}$ has finite type, then all its translated have finite type. □

This last result allows to define the *Hull* of a uniformly discrete set as follows

Definition 2 *Let $\mathcal{L}$ be a uniformly discrete subset of $\mathbb{R}^d$. Then its Hull is the dynamical system $(\Omega, \mathbb{R}^d, \mathrm{T})$ where Ω is the closure of the $\mathbb{R}^d$-orbit of $\nu^{(\mathcal{L})}$ in $\mathfrak{M}(\mathbb{R}^d)$.*

Remark 7 1)- Since $\mathcal{L}$ is uniformly discrete there is $r > 0$ such that $\nu^{(\mathcal{L})} \in UD_r(\mathbb{R}^d)$. Hence, by Prop. 2 its orbit is contained in $UD_r(\mathbb{R}^d)$. By Prop. 1 then, Ω is a compact subset of $UD_r(\mathbb{R}^d)$. In particular, any measure $\omega \in \Omega$ defines an r-discrete set $\mathcal{L}_\omega$, namely its support.
2)- The closure of the orbit of any point is obviously translation invariant, so that $\mathbb{R}^d$ acts on Ω through T.
3)- If in addition $\mathcal{L}$ is (r, R)-Delone, the same argument implies that all $\mathcal{L}_\omega$'s are (r, R)-Delone.
4)- If $\mathcal{L}$ has finite type, then so does any elements of the Hull. Actually then $\mathcal{L}_\omega - \mathcal{L}_\omega \subset \mathcal{L} - \mathcal{L}$ for any $\omega \in \Omega$. In particular if $\mathcal{L}$ is Meyer, so does any element of the Hull. □

4.2 Properties of the Hull

Let $\mathcal{L}$ be a uniformly discrete set in $\mathbb{R}^d$ and let Ω its Hull. Then the *canonical transversal* is the subset of $X \subset \Omega$ defined by

$$X = \{\omega \in \Omega \,;\, 0 \in \mathcal{L}_\omega\} \qquad \textbf{(Canonical transversal)} \tag{22}$$

Each orbit meets this transversal on the corresponding atomic set, namely

$$\mathrm{T}^{-x}\omega \in X \qquad \Leftrightarrow \qquad x \in \mathcal{L}_\omega \,.$$

Since $\mathcal{L}$ is uniformly discrete, so does $\mathcal{L}_\omega$, so that there is a minimum distance from one point of X to any other along the orbit. In this sense the orbits are transversal.

Example 3 Let $\mathcal{L}$ be periodic with period group $\mathbb{G}$. If $\mathbb{G}$ is a lattice, namely a discrete subgroup of $\mathbb{R}^d$ that generates $\mathbb{R}^d$ as a vector space, then the Hull is homeomorphic to the torus $\mathbb{R}^d/\mathbb{G}$. Moreover, the transversal is the finite set $X = \mathcal{L}/\mathbb{G}$. □

Example 4 A quasicrystal can be constructed by mean of the *cut-and-project method*. For $N > d$ let $\mathcal{R}$ be a lattice in $\mathbb{R}^N$ and let Δ be a polyhedral fundamental domain. Let then $\mathcal{E}_{\|}$ be a d-dimensional subspace of $\mathbb{R}^N$ meeting $\mathcal{R}$ only at the origin. Then project all points of the strip $\Delta + \mathcal{E}_{\|}$ on $\mathcal{E}_{\|}$ to get $\mathcal{L}$. By identifying $\mathcal{E}_{\|}$ with $\mathbb{R}^d$, $\mathcal{L}$ becomes a Meyer set that is a model for all known quasicrystals [16].
Let $W = \pi_\perp(\Delta)$, where $\pi_\perp$ denote the projection operator on the orthogonal subspace of $\mathcal{E}_{\|}$. Let W be endowed with the coarsest topology such that $W \cap (W + \pi_\perp(a_1)) \cap \cdots \cap (W + \pi_\perp(a_n))$ becomes closed and open for any family $\{a_1, \cdots, a_n\} \subset \mathcal{R}$. Then W is homeomorphic to the transversal [43]. $\square$

In the following it will be convenient to introduce the Hausdorff distance of two sets A, B in $\mathbb{R}^d$, namely $d_H(A, B) = \max\{\sup_{x\in A} \inf_{y\in B} |x - y|\, , \sup_{x\in A} \inf_{y\in B} |x - y|\}$.

The first property of such system is given as follows [43]. It is necessary to recall that a dynamical system is *minimal* if every orbit is dense

Proposition 3 *If $\mathcal{L}$ is uniformly discrete but not relatively dense, then Ω admits a fixpoint the orbit of which does not meet X. In particular the Hull is not minimal.*

Consequently, $\mathcal{L}$ must be Delone to have a minimal Hull.

Definition 3 *Let $\mathcal{L}$ be a Delone set in $\mathbb{R}^d$. Then $\mathcal{L}$ is repetitive if for any finite subset $p \subset \mathcal{L}$, and any $\epsilon > 0$, there is $R > 0$ such that any ball of radius R contains a translated of a finite subset p' such that $d_H(p, p') < \epsilon$.*

The following can be found in [66, 68, 43]

Theorem 1 *Let $\mathcal{L}$ be a Delone set. Then its Hull is minimal if and only if it is repetitive.*

Associated with the transversal X of the Hull, is a *groupoid* $\Gamma(X)$ [69]. This groupoid plays a rôle similar to the notion of *Poincaré map* or *first return map* in the theory of dynamical systems [70, 71]. This groupoid is defined as follows. The set of unit $\Gamma^{(0)}$ coincides with X. The set of arrows $\Gamma(X)$ is the set of pairs $(\omega, a) \in X \times \mathbb{R}^d$ such that $\mathrm{T}^{-a}\omega \in X$. Then the range, the source and the composition maps are defined by

$$r(\omega, a) \;=\; \omega\,, \qquad s(\omega, a) \;=\; \mathrm{T}^{-a}\omega\,, \qquad (\omega, a) \circ (\mathrm{T}^{-a}\omega, b) \;=\; (\omega, a + b)$$

The fiber $\Gamma^{(\omega)}$ is $r^{-1}(\{\omega\})$. Endowed with the topology induced by $\Omega \times \mathbb{R}^d$, this is a locally compact groupoid. If $\mathbb{P}$ is an $\mathbb{R}^d$-invariant ergodic measure on Ω, then it induced on $\Gamma(X)$ a *transverse measure* represented by a probability measure $\mathbb{P}_{tr}$ on X [72].

From Def. 1 a uniformly discrete set $\mathcal{L}$ has finite type whenever $\mathcal{L} - \mathcal{L}$ is discrete, thus closed. In such case the following is true

Proposition 4 *A uniformly discrete subset $\mathcal{L}$ of $\mathbb{R}^d$ with finite type admits a Cantorian transversal.*

A characterization of the Hull of a finite type repetitive Delone set has been given in [65]

Theorem 2 *Let $\mathcal{L}$ be a repetitive Delone set with finite type in $\mathbb{R}^d$. Then its Hull is conjugate by homeomorphisms to the projective limit of an inverse sequence of branched oriented flat compact manifolds without boundaries, in which the $\mathbb{R}^d$-action is induced by parallel transport of constant vector fields.*

4.3 Atomic Gibbs groundstates

In realistic solids, the atomic positions are also determined by their thermodynamical properties. This is because atoms can vibrate around their equilibrium position and can also diffuse through the solid. This motion creates both acoustic waves (phonons) and lacunæ. Nevertheless, the atomic position can still be described by a discrete set, thus an element of $QD(\mathbb{R}^d)$. Hence this last space plays the rôle of the *configuration space* that is needed in Statistical Mechanics. Nevertheless, it is very convenient to describe the atomic motion in solids as a perturbation of the equilibrium position. The acoustic wave are usually treated as phonon degrees of freedom, whereas lacunæ can be seen as impurities. Still, the atomic positions can be seen as typical configurations for the Gibbs measure describing the thermal equilibrium of atoms. Neglecting the atomic motion is equivalent to considering the $T \downarrow 0$ limit $\mathbb{P}$ of the Gibbs measure for the atoms. Then $\mathbb{P}$ can be seen as a *probability measure on* $QD(\mathbb{R}^d)$.

From the mathematical point of view, there is a difficulty. For indeed, $QD(\mathbb{R}^d)$ is not a locally compact space, so that the notion of Radon measure is meaningless. Nevertheless, the weak* topology makes this space a *Polish space* [67]. That is, the topology can be described through a distance for which the space is complete (the choice of such a distance is actually not unique and certainly not canonical). But the beauty of Polish spaces is that there is a genuine theory of probabilities [73] using the Borel approach through σ-additive functions on the σ-algebra of Borel sets. In particular, since the translation group acts on $QD(\mathbb{R}^d)$ in a continuous way, it transforms Borel sets into Borel sets so that it also acts on the space of probabilities by $\mathrm{T}^a\mathbb{P}(A) = \mathbb{P}(\mathrm{T}^{-a}A)$ for A a Borel set. The Prokhorov theorem gives also a very useful criterion for compactness of a family of such probabilities. It turns out that describing the atomic configurations through such probabilities gives rise to several interesting results for physicists [43].

If the solid under consideration is homogeneous, then its Gibbs measure $\mathbb{P}$ is expected to be translation invariant. Moreover, standard results of Statistical Mechanics [51] show that a translation invariant pure phase is described by a Gibbs measure that is ergodic under the translation group. In addition with such consideration, the analysis proposed in Section 4.1 shows that typical configurations of atoms at zero temperature should be at least uniformly discrete, but also Delone unless in very special cases. This is why the following definition can be useful

Definition 4 *An atomic grounstate is a probability measure $\mathbb{P}$ on $QD(\mathbb{R}^d)$ such that*

1. *$\mathbb{P}$ is $\mathbb{R}^d$-invariant;*
2. *$\mathbb{P}$ is $\mathbb{R}^d$-ergodic;*
3. *the space of uniformly discrete sets has $\mathbb{P}$-probability one.*

In addition, $\mathbb{P}$ is called Delone (resp. Meyer) if it gives probability one to the space of Delone (resp. Meyer) sets.

Several results have been obtained in [43] from such a definition.

Theorem 3 *Let $\mathbb{P}$ be an atomic groundstate. Then*

1. *there is $r > 0$ such that $\mathbb{P}$-almost every atomic configuration $\mathcal{L}$ is r-discrete an not r'-discrete for $r' > r$;*

2. *there is a compact subset $\Omega \subset UD_r(\mathbb{R}^d)$ such that for $\mathbb{P}$-almost all atomic configuration $\mathcal{L}$, the Hull of $\mathcal{L}$ is Ω; Ω coincides with the topological support of $\mathbb{P}$;*

3. *if, in addition, $\mathbb{P}$ is Delone (resp. Meyer), there is a unique pair (r, R) (resp. family $(r, R; r', R')$) such that $\mathbb{P}$-almost every configuration is (r, R)-Delone and not $(r", R")$-Delone for $r < r"$ and $R" < R$ (resp. $(r, R; r', R')$-Meyer and not $(r_1, R_1; r'_1, R'_1)$ for $r < r_1\,, R > R_1\,, r' < r'_1\,, R' > R'_1$).*

The next result concerns the notion of *diffraction measure*. Let $\mathcal{L}$ be a point set representing the position of atoms in the solid. Then, the diffraction pattern seen on a screen, in an X-ray diffraction experiment or in a transmission electronic microscope (T.E.M.), can be computed from the Fourier transform of $\mathcal{L}$ restricted to the domain Λ occupied by the sample in $\mathbb{R}^d$. More precisely, the intensity seen on the screen is proportional to

$$I_\Lambda(k) \;=\; \frac{1}{|\Lambda|}\left|\sum_{x\in\mathcal{L}\cap\Lambda} e^{\imath\langle k|x\rangle}\right|^2 \tag{23}$$

where $k \in \mathbb{R}^d$ represents the wave vector of the diffraction beam, the direction of which gives the position on the screen. The Fourier transform of $I_\Lambda(k)$ is given by the following expression: if $f \in \mathcal{C}_c(\mathbb{R}^d)$, with Fourier transform denoted by $\tilde{f}$, then

$$\int_{k\in\mathbb{R}^d} dk\tilde{f}(k)I_\Lambda(k) \;=\; \frac{1}{|\Lambda|}\sum_{x,y\in\mathcal{L}\cap\Lambda} f(x-y) \;=\; \rho_{\mathcal{L}}^{(\Lambda)}(f) \tag{24}$$

where $\rho_{\mathcal{L}}^{(\Lambda)}$ will be called the *finite volume diffraction measure*. From eq. (24), it follows that $\rho_{\mathcal{L}}^{(\Lambda)} \in \mathfrak{M}(\mathbb{R}^d)$ is a positive measure with a Fourier transform being also a positive measure. The main problem is whether such quantity converges as $\Lambda \uparrow \mathbb{R}^d$. The next theorem gives conditions under which convergence holds

Theorem 4 *Let $\mathbb{P}$ be an atomic groundstate. Then:*

(i) For $\mathbb{P}$-almost every $\mathcal{L}$ the family $\rho_{\mathcal{L}}^{(\Lambda)}$ of measures on $\mathbb{R}^d$ converges to a positive measure $\rho_{\mathbb{P}} \in \mathfrak{M}(\mathbb{R}^d)$.

(ii) The distributional Fourier transform of $\rho_{\mathbb{P}}$ is also a positive measure on $\mathbb{R}^d$.

In other words, $\mathbb{P}$ determines in a unique way the diffraction pattern. □

4.4 Bloch Theory

If the solid is a perfect crystal, the set $\mathcal{L}$ is invariant under a *translation group* $\mathbb{G}$. $\mathbb{G}$ is a *lattice* in $\mathbb{R}^d$ namely a discrete subgroup generating $\mathbb{R}^d$ as a vector space. Bloch theory deals with the Schrödinger equation with a $\mathbb{G}$-periodic potential. More precisely, let $\mathcal{H} = L^2(\mathbb{R}^d)$ be the Hilbert space of quantum states. The groups $\mathbb{G}$ is unitarily represented in $\mathcal{H}$ through

$U(a)\psi(x) = \psi(x-a)$ whenever $a \in \mathbb{G}$. The Schrödinger operator is a selfadjoint operator $H = H^* = -\Delta + V$ with dense domain, where Δ is the Laplacian on $\mathbb{R}^d$ and V is a locally L^1 $\mathbb{G}$-periodic real valued function. In particular

$$U(a)\, H\, U(a)^{-1} \;=\; H \qquad\qquad \forall a \in \mathbb{G}\,.$$

Therefore H and the $U(a)$'s can be simultaneously diagonalized. Since $\mathbb{G}$ is Abelian, diagonalization of the $U(a)$'s is performed through its character group $\mathbb{G}^*$. Standard results in Pontryagin duality theory imply that $\mathbb{G}^*$ is isomorphic to the quotient $\mathbb{B} = \mathbb{R}^{d*}/\mathbb{G}^\perp$ of the dual group of $\mathbb{R}^d$ (isomorphic to $\mathbb{R}^d$) by the orthogonal $\mathbb{G}^\perp$ of $\mathbb{G}$ in this group. It is a well known fact that $\mathbb{G}^\perp$ is a lattice in $\mathbb{R}^d$ (called *the reciprocal lattice* in Solid State Physics [74]) so that $\mathbb{B} = \mathbb{R}^{d*}/\mathbb{G}^\perp$ is a compact group homeomorphic to a d-torus. $\mathbb{B}$ will be called the *Brillouin zone* (strictly speaking this is slightly different from what crystallographers call Brillouin zone). The concrete calculation of $\mathbb{B}$ goes as follows: any character of $\mathbb{R}^d$ is represented by an element $k \in \mathbb{R}^{d*}$. Since $\mathbb{R}^{d*}$ and $\mathbb{R}^d$ can be identified canonically, by using the usual Euclidean structure, k can be seen as a vector $k = (k_1, \cdots, k_d) \in \mathbb{R}^d$. The corresponding character is given by the map

$$\eta_k : x \in \mathbb{R}^d \mapsto e^{\imath\langle k|x\rangle} \in U(1)\,, \qquad \langle k|x\rangle \;=\; k_1x_1 + \cdots + k_dx_d\,.$$

In particular η_k restricts to a character of $\mathbb{G}$, with the condition that $\eta_k\restriction_{\mathbb{G}} = \eta_{k'}\restriction_{\mathbb{G}}$ if and only if $k - k' \in \mathbb{G}^\perp$, where

$$\mathbb{G}^\perp \;=\; \{b \in \mathbb{R}^d\,;\; \langle b|a\rangle \in 2\pi\mathbb{Z},\; \forall a \in \mathbb{G}\}\,.$$

Since $\mathbb{B}$ is a compact group, the diagonalization of the $U(a)$'s requires the use of a direct integral decomposition of $\mathcal{H}$ over $\mathbb{B}$, so that

$$\mathcal{H} \;=\; \int_{k\in\mathbb{B}}^{\oplus} d^dk\, \mathcal{H}_k \qquad\qquad H \;=\; \int_{k\in\mathbb{B}}^{\oplus} d^dk\, H_k\,.$$

Here, $\mathcal{H}_k$ is the space of measurable functions ψ on $\mathbb{R}^d$ such that $\psi(x+a) = e^{\imath\langle k|x\rangle}\psi(x)$ for all $a \in \mathbb{G}$ and that $\int_{\mathbb{V}} d^dx|\psi(x)|^2 = \|\psi\|^2_{\mathcal{H}_k} < \infty$, where $\mathbb{V} = \mathbb{R}^d/\mathbb{G}$. H_k is then the partial differential operator formally given by the same expression as H, but with domain $\mathcal{D}_k$ given by the space of elements $\psi \in \mathcal{H}_k$ such that $\partial_i\psi/\partial x_i \in \mathcal{H}_k$, for $1 \le i \le d$, and $\Delta_x\psi \in \mathcal{H}_k$. Then H_k is unitarily equivalent to an elliptic operator on the torus $\mathbb{R}^d/\mathbb{G} = \mathbb{V}$. In solid state physics, $\mathbb{V}$ is called the *Wigner-Seitz cell*, whereas it is called the *Voronoi cell* in tiling theory.
Consequently, for each $k \in \mathbb{B}$, the spectrum of H_k is discrete and bounded from below. If $E_i(k)$ denotes the eigenvalues, with a convenient labelling i, the maps $k \in \mathbb{B} \mapsto E_i(k) \in \mathbb{R}$ are called the *band functions*. The spectrum of H is recovered as $\mathrm{Sp}(H) = \bigcup_{i,k\in\mathbb{B}} E_i(k)$ and is called a *band spectrum*. A discrete spectrum is usually liable to be computable by suitable algorithms, since it restricts to diagonalizing large matrices.

This is a short summary of *Bloch theory*. Strutt first realized the existence of band functions [75], but soon after Bloch wrote his important paper [76]. In 1930, Peierls gave a perturbative treatment of the band calculations [77] and Brillouin discussed the $2D$ and $3D$ cases [78]. The reader is invited to look at [74, 59] to understand why this theory has been so successful in solid state physics. Let us simply mention that the first explicit calculations of bands in $3D$ were performed in 1933 by Wigner & Seitz [79] on sodium using the cellular method that holds their names. The symmetry properties of the wave function were explicitly used in an important paper by Bouckaert, Smoluchowski & Wigner [80] leading to noticeable simplifications of the band calculation.

4.5 The noncommutative Brillouin zone

In Section 4.1 it has been shown that an aperiodic solid is well described by its Hull $(\Omega, \mathbb{R}^d, \mathrm{T})$, namely a dynamical system with group $\mathbb{R}^d$ acting by homeomorphisms on a compact metrizable space Ω. With any dynamical system, there is a canonical C^*-algebra namely the *crossed product* $\mathcal{C}(\Omega) \rtimes \mathbb{R}^d$ [81]. In a similar way, such system can also be described through its canonical transversal X, and its related groupoid $\Gamma(X)$. With any locally compact groupoid Γ, endowed with a *transverse function* [72], and with any *module* δ on Γ, is associated a C^*-algebra $C^*(\Gamma, \delta)$ [69]. In this section, it will be shown that, after a slight modification if the solid is submitted to a magnetic field, $\mathcal{C}(\Omega) \rtimes \mathbb{R}^d$ is the smallest C^*-algebra generated by the electronic Schrödinger operator and all its translated. Moreover, it will be shown that, $C^*(\Gamma(X))$ is also generated by the matrix of phonon modes that appears in the equations of motion for phonons or by the *effective Hamiltonian* derived form the so-called *tight binding representation* [64, 42]. It will also be shown that, for periodic crystals, this algebra is nothing but the set of continuous functions on the Brillouin zone.

Given a uniform magnetic field $B = (B_{\nu\mu})$, namely a real-valued antisymmetric $d \times d$-matrix, the C^*-algebra $C^*(\Omega \times \mathbb{R}^d, B)$ is defined as follows. Let $\mathcal{A}_0$ be the topological vector space $\mathcal{C}_c(\Omega \times \mathbb{R}^d)$ of continuous functions with compact support in $\Omega \times \mathbb{R}^d$. It becomes a topological *-algebra when endowed with the following structure

$$\begin{aligned} fg\,(\omega, x) &= \int_{\mathbb{R}^d} dy\, f(\omega, y)\, g(T^{-y}\omega, x-y)\, e^{i\pi(e/h)\, B\cdot x\wedge y}\,, && (25)\\ f^*(\omega, x) &= \overline{f(T^{-x}\omega, -x)}\,, && (26)\end{aligned}$$

where $f, g \in C_c(\Omega \times \mathbb{R}^d)$, $B \cdot x \wedge y = \sum B_{\nu\mu} x_\nu y_\mu$ and $\omega \in \Omega$, $x \in \mathbb{R}^d$. Here e is the electric charge of the particle and $h = 2\pi\hbar$ is Planck's constant. This *-algebra is represented on $L^2(\mathbb{R}^d)$ by the family of representations $\{\pi_\omega;\ \omega \in \Omega\}$ given by

$$\pi_\omega(f)\psi\,(x) = \int_{\mathbb{R}^d} dy\, f(T^{-x}\omega, y-x)\, e^{-i\pi(e/h)\, B\cdot x\wedge y}\psi(y), \qquad \psi \in L^2(\mathbb{R}^d)\,, \qquad (27)$$

where π_ω is linear, $\pi_\omega(fg) = \pi_\omega(f)\pi_\omega(g)$ and $\pi_\omega(f)^* = \pi_\omega(f^*)$. In addition $\pi_\omega(f)$ is a bounded operator and the representations $(\pi_\omega)_{\omega\in\Omega}$ are related by the covariance condition:

$$U(a)\, \pi_\omega(f)\, U(a)^{-1} = \pi_{\mathrm{T}^a\omega}(f)\,, \qquad (28)$$

where the U's are the so-called *magnetic translations* [82] defined by:

$$U(a)\psi(x) = \exp\left\{(ie/\hbar) \int_{[x-a,x]} dy^\mu A_\mu(y)\right\} \psi(x-a)\,, \qquad (29)$$

where $\vec{A} = (A_1, ..., A_d)$ is a vector potential defined by $B_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$, $a \in \mathbb{R}^d$, $\psi \in L^2(\mathbb{R}^d)$ and $[x-a, x]$ is the line segment joining $x-a$ to a in $\mathbb{R}^d$. A C^*-norm on $\mathcal{A}_0$ is defined by

$$\|f\| = \sup_{\omega\in\Omega} \|\pi_\omega(f)\|\,. \qquad (30)$$

Definition 5 *The non-commutative Brillouin zone is the topological manifold associated with the C^*-algebra $\mathcal{A} = C^*(\Omega \rtimes \mathbb{R}^d, B)$ obtained by completion of $\mathcal{A}_0 = \mathcal{C}_c(\Omega \times \mathbb{R}^d)$ under the norm $\|\cdot\|$ defined by eq. (30).*

For $B = 0$ this construction gives the definition of the C^*-crossed product $\mathcal{C}(\Omega) \rtimes \mathbb{R}^d$ [81, 83]. In the case of a perfect crystal (see Section 4.4), with lattice translation group $\mathbb{G}$, the hull $\Omega = \mathbb{R}^d/\mathbb{G}$ is homeomorphic to $\mathbb{T}^d$ (see Example 3) and

Theorem 5 *[84, 42] The C^*-algebra $C^*(\mathbb{R}^d/\mathbb{G} \rtimes \mathbb{R}^d, B = 0)$ associated with a perfect crystal with lattice translation group $\mathbb{G}$, is isomorphic to $\mathcal{C}(\mathbb{B}) \otimes \mathcal{K}$, where $\mathcal{C}(\mathbb{B})$ is the space of continuous functions over the Brillouin zone and $\mathcal{K}$ the algebra of compact operators.*

Even though the algebra $\mathcal{C}(\mathbb{B}) \otimes \mathcal{K}$ is already non-commutative, its non-commutativity comes from $\mathcal{K}$, the smallest C^*-algebra generated by finite rank matrices. It describes the possible vector bundles over $\mathbb{B}$. Theorem 5 is the reason to claim that $\mathcal{A}$ generalizes the Brillouin zone for aperiodic systems.

The groupoid C^*-algebra of $\Gamma(X)$ can be defined very similarly. Here $\mathcal{B}_0 = \mathcal{C}_c(\Gamma(X))$ and the structure of *-algebra is given by

$$fg\,(\omega, x) = \sum_{y \in \Gamma^{(\omega)}} f(\omega, y)\, g(T^{-y}\omega, x - y)\, e^{i\pi(e/h)\, B\cdot x\wedge y}\,, \tag{31}$$

$$f^*(\omega, x) = \overline{f(T^{-x}\omega, -x)}\,, \tag{32}$$

Setting $\mathfrak{H}_\omega = \ell^2(\Gamma^{(\omega)})$, there is a representation $\widehat{\pi}_\omega$ on $\mathfrak{H}_\omega$ defined by

$$\widehat{\pi}_\omega(f)\psi\,(x) = \sum_{y \in \Gamma^{(\omega)}} f(T^{-x}\omega, y - x)\, e^{-i\pi(e/h)\, B\cdot x\wedge y}\psi(y), \qquad \psi \in \mathfrak{H}_\omega\,, \tag{33}$$

Giving $\gamma = (\omega, a) \in \Gamma(X)$, there is a unitary operator $U(\gamma) : \mathfrak{H}_{\mathrm{T}^{-a}\omega} \mapsto \mathfrak{H}_\omega$ defined by

$$U(\gamma)\psi(x) = \exp\left\{(ie/\hbar)\int_{[x-a,x]} dy^\mu A_\mu(y)\right\}\psi(x - a)\,, \qquad \psi \in \mathfrak{H}_{\mathrm{T}^{-a}\omega}\,, \tag{34}$$

such that the covariance condition holds

$$U(\gamma)\,\widehat{\pi}_{\mathrm{T}^{-a}\omega}(f)\,U(\gamma)^{-1} = \pi_\omega(f)\,, \tag{35}$$

A C^*-norm on $\mathcal{B}_0$ is defined by

$$\|f\| = \sup_{\omega \in X} \|\widehat{\pi}_\omega(f)\|\,. \tag{36}$$

The C^*-algebra $\mathcal{B} = C^*(\Gamma(X), B)$ is the completion of $\mathcal{B}_0$ under this norm. The main result is the following [84]

Theorem 6 *1)- The C^*-algebras $\mathcal{B} = C^*(\Gamma(X), B)$ and $\mathcal{A} = C^*(\Omega \rtimes \mathbb{R}^d, B)$ are Morita equivalent, namely $\mathcal{A}$ is isomorphic to $\mathcal{B} \otimes \mathcal{K}$.*
2)- For $B = 0$ and for a crystal $\mathcal{L}$ with period group $\mathbb{G}$ and transversal $X = \mathcal{L}/\mathbb{G}$, the C^*-algebra $\mathcal{B}$ is isomorphic to $\mathcal{C}(\mathbb{B}) \otimes M_N(\mathbb{C})$ if N is the cardinality of X.

In order to see the Noncommutative Brillouin zone as a manifold, rules of Calculus are required. Integration is provided by using a transverse measure. Let $\mathbb{P}$ be an $\mathbb{R}^d$-invariant ergodic probabilty measure on $\mathbb{R}^d$ and let $\mathbb{P}_{tr}$ be the probability induced on X. Then traces are defined on $\mathcal{A}$ and $\mathcal{B}$ as follows

$$\mathcal{T}_{\mathbb{P}}(f) \;=\; \int_{\Omega} d\mathbb{P}(\omega)\, f(\omega,0)\,, \quad f\in\mathcal{A}_0\,, \qquad \hat{\mathcal{T}}_{\mathbb{P}}(f) \;=\; \int_{X} d\mathbb{P}_{tr}(\omega)\, f(\omega,0)\,, \quad f\in\mathcal{B}_0\,, \tag{37}$$

$\mathcal{T}_{\mathbb{P}}$ and $\hat{\mathcal{T}}_{\mathbb{P}}$ are traces in the sense that $\mathcal{T}_{\mathbb{P}}(fg) = \mathcal{T}_{\mathbb{P}}(gf)$, and that $\mathcal{T}_{\mathbb{P}}(ff^*) > 0$. Whereas $\mathcal{T}_{\mathbb{P}}$ is not bounded, $\hat{\mathcal{T}}_{\mathbb{P}}$ is actually normalized, namely $\hat{\mathcal{T}}_{\mathbb{P}}(\mathbf{1}) = 1$. Moreover, using the Birkhoff ergodic theorem [70, 71], these traces can be seen as *trace per unit volume* in the following sense

$$\mathcal{T}_{\mathbb{P}}(f) \;=\; \lim_{R\uparrow\infty} \frac{1}{|B(0;R)|}\, \mathrm{Tr}\left(\pi_\omega(f)\restriction_{B(0;R)}\right)\,,$$

where $B(x;R)$ denotes the ball of radius R centered at $x\in\mathbb{R}^d$. A similar formula holds for $\hat{\mathcal{T}}_{\mathbb{P}}$. In particular in the crystalline case,

$$\mathcal{T}_{\mathbb{P}}(f) \;=\; \int_{\mathbb{B}} dk\; \mathrm{Tr}\left(\tilde{f}(k)\right)\,,$$

if $\tilde{f}(k)$ denotes the representative of f in $\mathcal{C}(\mathbb{B})\otimes\mathcal{K}$ and dk is the normalized Haar measure on $\mathbb{B}\simeq\mathbb{T}^d$. A similar formula holds for $\hat{\mathcal{T}}_{\mathbb{P}}$ provided $|B(0;R)|$ is replaced by the number of points in $\mathcal{L}_\omega\cap B(0;R)$. Therefore, these traces appears as the noncommutative analog of the integration over the Brillouin zone.
A positive measure on a topological space defines various spaces of measurable functions, such as the L^p-spaces. In much the same way, a positive trace on a C^*-algebra defines also L^p-spaces [85]. Whenever $1\leq p<\infty$, $L^p(\mathcal{A},\mathcal{T}_{\mathbb{P}})$ is the separation-completion of $\mathcal{A}_0$ with respect to the seminorm $\|A\|_p = \mathcal{T}_{\mathbb{P}}\{(A^*A)^{p/2}\}^{1/p}$ for $A\in\mathcal{A}_0$. A similar definition is given for $\mathcal{B}$. In particular, $L^2(\mathcal{A},\mathcal{T}_{\mathbb{P}})$ coincides with the Hibert space of the GNS-representation π_{GNS} of $\mathcal{A}$ associated with $\mathcal{T}_{\mathbb{P}}$ [86, 87]. Then $L^\infty(\mathcal{A},\mathcal{T}_{\mathbb{P}})$ denotes the von Neumann algebra generated by (namely the weak closure of) $\pi_{GNS}(\mathcal{A})$.

Similarly, a differential structure is provided in the following way

$$\vec{\nabla} f\;(\omega,x) \;=\; \imath\vec{x} f(\omega,x)\,, \qquad\qquad f\in\mathcal{A}_0 \text{ or } \mathcal{B}_0\,. \tag{38}$$

Here $\vec{x}$ denotes the vector $x\in\mathbb{R}^d$. It is easy to check that $\vec{\nabla}$ defines a *-derivation namely it obeys Leibniz rule $\vec{\nabla}(fg) = \vec{\nabla}(f)g + f\vec{\nabla}(g)$ and $\vec{\nabla}(f)^* = \vec{\nabla}(f^*)$. Moreover $\vec{\nabla}$ is the infinitesimal generator of a norm pointwise continuous d-parameter group of automorphisms defined by [81]

$$\eta_{\vec{k}}(f)\;(\omega,x) \;=\; e^{\imath\vec{k}\cdot\vec{x}}\; f(\omega,x)\,, \qquad\qquad f\in\mathcal{A}_0 \text{ or } \mathcal{B}_0\,.$$

Let $\vec{X}$ be the position operator on $L^2(\mathbb{R}^d)$, (resp. on $\mathfrak{H}_\omega$), defined by $\vec{X}\psi(x) \;=\; \vec{x}\psi(x)$. Then

$$\pi_\omega\left(\vec{\nabla} f\right) \;=\; \imath[\vec{X},\pi_\omega(f)]\,, \quad f\in\mathcal{A}_0\,, \qquad \widehat{\pi}_\omega\left(\vec{\nabla} f\right) \;=\; \imath[\vec{X},\widehat{\pi}_\omega(f)]\,, \quad f\in\mathcal{B}_0\,,$$

In the crystalline case, it is easy to show that $\vec{\nabla}$ coincides with $\partial/\partial k$ in $\mathbb{B}$ [42]. Hence $\vec{\nabla}$ appears as the noncommutative analog of the derivation in momentum space.

In the philosophy of A.Connes, a noncommutative Geometry for a compact maniflod is given by a spectral triplet $(\mathfrak{A}, \mathcal{H}, D)$ where $\mathfrak{A}$ is a dense subalgebra of a unital C^*-algebra , invariant by holomorphic functional calculus, $\mathcal{H}$ a $\mathbb{Z}_2$-graded Hilbert space on which $\mathfrak{A}$ is represented by degree 0 operators and D is a degree 1 selfadjoint operator with compact resolvent, such that $[D, A] \in \mathcal{B}(\mathcal{H})$ for all $A \in \mathfrak{A}$. Then D plays the rôle of a Dirac operator on the noncommutative space associated with $\mathfrak{A}$, giving both a differential structure and a Riemannien metric corresponding to $ds^2 = D^{-2}$ [40]. Then the dimension spectrum is provided by the set of poles of the ζ-function

$$\zeta_D(s) \;=\; \mathrm{Tr}\left(\frac{1}{|D|^s}\right) .$$

If s_0 denote the maximum real pole, then the residue ats_0 provides an integral over the manifold given by

$$\int T \;=\; \lim_{s\downarrow s_0} (s - s_0)\, \mathrm{Tr}\left(\frac{1}{|D|^s} T\right) \;=\; \mathrm{Tr}_{\mathrm{Dix}}\left(\frac{1}{|D|^{s_0}} T\right) ,$$

where $\mathrm{Tr}_{\mathrm{Dix}}$ denotes a *Dixmier trace* on $\mathcal{H}$ [40, 41]. Such a structure is also present on the noncommutative Brillouin zone $\mathcal{B}$. For indeed, let $\gamma_1, \cdots, \gamma_d$ be an irreducible representation of the Clifford algebra of $\mathbb{R}^d$ by Dirac matrices satisfying $\gamma_\mu\gamma_\nu + \gamma_\nu\gamma_\mu = 2\delta_{\mu,\nu}$ and $\gamma_\mu^* = \gamma_\mu$ in the finite dimensional Hilbert space Cliff(d). Then Cliff(d) is graded by the matrix $\gamma_0 = \gamma_1\gamma_2\cdots\gamma_d$, so that setting $\mathcal{H} = \mathfrak{H}_\omega \otimes \mathrm{Cliff}(d)$, $G = \mathbf{1} \otimes \gamma_0$, this gives a graded Hilbert space where G defines the graduation. Moreover $\mathfrak{A} = \mathcal{B}_0$ and $D = \sum_{\mu=1}^d \gamma_\mu X_\mu$ give a spectral triplet for which $s_0 = d$. In particular, the Dixmier trace $\mathrm{Tr}_{\mathrm{Dix}}(|D|^{-d})$ exist for $\mathbb{P}_{tr}$-almost every $\omega \in X$ and its common value is given by

$$\mathrm{Tr}_{\mathrm{Dix}}(|D|^{-d}) \;=\; \mathrm{Dens}_{\mathbb{P}}(\mathcal{L}_\omega)\, \frac{\pi^d}{\Gamma(1 + d/2)} ,$$

where $\mathrm{Dens}_{\mathbb{P}}(\mathcal{L}_\omega)$ is the density of $\mathcal{L}_\omega$ which exists for $\mathbb{P}$-almost all ω's (see [43] see proof of Theorem 1.12). The numerical factor represents the volume of the unit ball of $\mathbb{R}^d$. Moreover, if $f \in \mathcal{B}_0$ this gives

$$\int f \;=\; \mathrm{Tr}_{\mathrm{Dix}}(|D|^{-d}\, \widehat{\pi}_\omega(f)) \;=\; \hat{\mathcal{T}}_{\mathbb{P}}(f)\, \frac{\pi^d}{\Gamma(1 + d/2)} , \qquad \mathbb{P}_{tr} - a.e.\ \omega \in X ,$$

showing that the Connes integral and the integral over the Brillouin zone coincide modulo normalization.

4.6 Electrons and Phonons

The formalism developped in the previous sections will eventually be useful to describe the quantum motion of electrons and phonons in an aperiodic solid, within the one particle approximation. The interacting case is more involved [88] and will not been considered in these notes.

The quantum motion of an electron in a monoatomic aperiodic solid represented by a uniformly discrete set $\mathcal{L}$ of atomic positions, and submitted to a uniform magnetic field B, is well described by a covariant family of Schrödinger operators of the type

$$H_\omega \;=\; \frac{1}{2m}\left(\frac{\hbar}{\imath}\vec{\nabla} - e\vec{A}\right)^2 \;+\; \sum_{y\in\mathcal{L}_\omega} v(X-y)\,, \qquad\qquad \text{on } L^2(\mathbb{R}^d)\,, \tag{39}$$

where $\hbar$ is the Planck constant, m is the electron mass, $\vec{A}$ is a vector potential and v is an effective atomic potential, that represents the binding forces acting on the valence electron. In practice, an aperiodic solid contains more than one species of atoms, so that $\mathcal{L}$ must be replaced by a family $\mathcal{L}^1, \cdots, \mathcal{L}^r$ of uniformly discrete subsets representing the position of each atomic species, supposing that r species are present. Then each species i acts via an effective potential v_i. Moreover, the number of valence electrons involved in the conduction may be more than one per atom, so that it should be necessary to consider instead an l-body problem if l valence electrons are involved. This latter case will not be considered either, even though its treatment does not represent a major difficulty. In these notes the model described in eq. (39) will be sufficient.

The Schrödinger operator (39) is not well defined as long as no assumption is given on the nature of the atomic potential v. For the sum over the atomic sites to converge, it is necessary that v decay fast enough at infinity. Also local regularity is necessary. A sufficient condition has been given in [43] (Lemma 2.22), namely let

$$L^1_{K,r}(\mathbb{R}^d) \;=\; \{f\in L^1(\mathbb{R}^d);\, |f(x)| \leq \frac{K}{r^d}\int_{|x-y|<r/2} d^dy\; |f(y)|, \;\; \text{for a.e. x}\}$$

be the set of integrable K-subharmonic functions on $\mathbb{R}^d$. Then

Lemma 1 *Let $v \in L^1_{K,r}(\mathbb{R}^d)$ and $\nu \in UD_r(\mathbb{R}^d)$. Then $\nu * v \in L^\infty_{\mathbb{R}}(\mathbb{R}^d)$ and the map $v \in L^1_{K,r}(\mathbb{R}^d) \mapsto \nu * v \in L^\infty_{\mathbb{R}}(\mathbb{R}^d)$ is continuous.*

The following Proposition is a consequence of [42] Section 2, Theorem 4 and [43] Theorem 2.23

Proposition 5 *1)- For any $\mathcal{L}$ an r-discrete subset of $\mathbb{R}^d$, let $H_{\mathcal{L}}$ be the Schrödinger operator given by eq. (39). Then, if $v \in L^1_{K,r}(\mathbb{R}^d)$ the map $\mathcal{L} \in UD_r(\mathbb{R}^d) \mapsto H_{\mathcal{L}}$ is strong resolvent continuous.*
2)- If Ω is the Hull of $\mathcal{L}$, the map $\omega \in \Omega \mapsto H_\omega$ is strong resolvent continuous and covariant.

As a consequence, thanks to [42] Theorem 6,

Theorem 7 *Let $\mathcal{L}$ be a uniformly discrete set in $\mathbb{R}^d$ with Hull Ω. Let $\mathcal{A} = C^*(\Omega \rtimes \mathbb{R}^d, B)$ be the C^*-algebra of the corresponding Noncommutative Brillouin zone. Let $\{H_\omega;\, \omega\in\Omega\}$ be the strong resolvent continuous and covariant family of Schrödinger operators defined by eq. (39) with $v \in L^1_{K,r}(\mathbb{R}^d)$. Then there is a holomorphic family $z \in \mathbb{C}\setminus\mathbb{R} \mapsto R(z) \in \mathcal{A}$ such that*

$$\pi_\omega(R(z)) \;=\; (z - H_\omega)^{-1}\;, \qquad \forall \omega\in\Omega\,.$$

As a consequence, it can be said that the Schrödinger oeprator is *affiliated to* the C^*-algebra $\mathcal{A}$: a covariant family (A_ω) of selfadjoint operators is affiliated to $\mathcal{A}$ if, for all $f \in \mathcal{C}_0(\mathbb{R})$, the bounded operator $f(A_\omega)$ can be represented as $\pi_\omega(A_f)$ for some $A_f \in \mathcal{A}$ such that the map $A : f \in \mathcal{C}_0(\mathbb{R}) \mapsto A_f \in \mathcal{A}$ is a bounded $*$-morphism [89, 90, 91]. The resolvent map $R(z)$ is then given by A_{r_z} if $r_z : s \in \mathbb{R} \mapsto 1/(z-s) \in \mathbb{C}$ for $z \in \mathbb{C} \setminus \mathbb{R}$. Conversely the resolvent map permits to reconstruct the map A through a contour integral. It has been argued in [42] that the C^*-algebra $\mathcal{A}$ above can be actually reconstructed from the Schrödinger operator $H_{\mathcal{L}}$ itself.

In Solid State Physics the conduction electrons are commonly described through the so-called *tight binding approximation.* This is because only those electrons with energy within $O(k_B T)$ from the Fermi level do contribute to the current. There is no need then to consider the full range of energy to describe these electrons. In particular, the Schrödinger operator can be replaced by its restriction to an energy interval of size $O(k_B T)$ around the Fermi level. However this is not practically accessible in most cases. The method to perform such a reduction goes as follows [64, 92, 93]. The single atom Schrödinger equation

$$H_1 \;=\; \frac{1}{2m}\left(\frac{\hbar}{\imath}\vec{\nabla} - e\vec{A}\right)^2 \;+\; v(X)\,, \qquad\qquad \text{on } L^2(\mathbb{R}^d)\,,$$

has usually a non empty discrete spectrum, described by *quantum numbers.* The valence electron occupy a given eigenstate, denoted by $\phi_v \in L^2(\mathbb{R}^d)$ corresponding to the energy E_v. If the potential v decays fast enough to zero at infinity, ϕ_v decays exponentially fast away from the origin. Then an approximate basis of eigenstate of H_ω is provided by the family $\{U(y)\phi_v;\, y \in \mathcal{L}_\omega\}$ whenever U is the magnetic translation group. Denoting by P_ω the projection on the subspace generated by such family in $L^2(\mathbb{R}^d)$, it is possible to check that $P_\omega = \pi_\omega(P)$ for some projection $P \in \mathcal{A}$. Thanks to an orthonormalization procedure, the family $U(y)\phi_v$ gives rise to an orthonormal basis $\{\psi_y;\, y \in \mathcal{L}_\omega\}$ indexed by the atomic sites, where each ψ_y is exponentially localized near y. By using either the Schur complement (or Feshbach) method [94] or a Grushin method [95] there exists an effective Hamiltonian in the form of a function $z \mapsto H_{eff}(z)$ holomorphic in a neighbourhood of E_v with values in covariant matrices over $\mathcal{L}_\omega$. Moreover, the spectrum of the original problem is given by the implicit equation $E \in \mathrm{Sp}H \Leftrightarrow E \in \mathrm{Sp}H_{eff}(E)$. The advantage of this method is that $H_{eff}(z)$ can be seen as an element of the groupoid C^*-algebra $\mathcal{B}$ [64, 42], with matrix elements decreasing exponentially fast away from the main diagonal. In practice only a finite number of such diagonals are kept to compute the spectrum, giving rise to *tight-binding models.* Such a method is actually commonly used also in computer software for the purpose of band calculations in crystals. The various *ab initio* methods of Quantum Chemistry or the functional density calculations (Kohn-Sham method), may lead to an accurate calculation of the parameters involved in such effective Hamiltonian. It is not the purpose of these notes to explain these methods. However, they lead to effective Hamiltonian described by elements of the groupoid C^*-algebra $\mathcal{B}$.

Phonons can also be described in a similar way through $\mathcal{B}$ with zero magnetic field. This is because phonons are the harmonic approximation of the atomic motion around their equilibrium positions. If the atom located at $x \in \mathcal{L}$ is moving around x, let $\vec{x} + \vec{u}_x(t)$ be its position at time t. Since x is an equilibrium position for the atom, the potential energy created by its neigbours increases away from x, hence it is expected that $\vec{u}_x(t)$ stay small at all time. Moreover, the lowest order expansion of the potential energy around x gives rise to a quadratic potential, namely harmonic forces, tending to force the atom back to its position x. Therefore, within this *harmonic approximation*, the classical equation of motion for the atom has the form

$$M \frac{d^2\vec{u}_x}{dt^2} \;=\; \sum_{y\in\mathcal{L}_\omega} \kappa_\omega(x,y)\,(\vec{u}_y - \vec{u}_x)\;, \tag{40}$$

where M is the atomic mass and $\kappa_\omega(x,y)$ is the matrix of spring constants between atoms located at y and x. So $\kappa_\omega(x,y) \in M_d(\mathbb{R})$. Phonons are just the quantized degrees of freedom associated with this classical motion. In practice however, the influence of atoms far apart is negligible so that $\kappa_\omega(x,y)$ decays fast enough as $|x-y| \to \infty$. Moreover, the action-reaction principle implies that $\kappa_\omega(x,y) = \kappa_\omega(y,x)^t$. In addition, since it describes an attracting force, $\kappa_\omega(x,y)$ is a positive matrix for any (x,y). Also, the translation invariance of interactions between atoms leads to the covariance condition

$$\kappa_{\mathrm{T}^a\omega}(x+a, y+a) \;=\; \kappa_\omega(x,y)\,.$$

In very much the same way, the translation invariance of interactions between atoms leads to the continuity of $\kappa_\omega(x,y)$ with respect to ω. Hence the map $(\omega,x) \in \Gamma(X) \mapsto \kappa_\omega(0,x) \in M_d(\mathbb{R}^d)$ defines an element κ of $C^*(\Gamma(x)) \otimes M_d$. The equation of motion (40) is usually solved by looking at the stationnary solutions, namely solutions for which

$$\frac{d^2\vec{u}_x}{dt^2} \;=\; -\tilde{\omega}^2\vec{u}_x\,,$$

leading to the eigenmode equation

$$\sum_{y\in\mathcal{L}_\omega} \langle x|\widehat{\pi}_\omega(K)y\rangle \vec{u}_y \;=\; \tilde{\omega}^2\vec{u}_x\,, \qquad K(\omega,x) \;=\; \delta_{x,0}\sum_{y\in\mathcal{L}_\omega}\frac{\kappa(\omega,y)}{M} - (1-\delta_{x,0})\frac{\kappa(\omega,x)}{M}\,. \tag{41}$$

It is easy to check that this K defines a positive element of $\mathcal{B}$ so that the eigenmodes are given by the spectrum of $K^{1/2}$. This modes are the plane waves that are allowed to propagate through the crystal. Historically, Einstein [3] was the first to propose a quantized version of these oscillations, supposing that only one mode was propagating. Then he could compute the heat capacity of the solid and shown that it saturates at high temperature leading to the Dulong an Petit law. Soon after, Debye ([2] Section 1.1) introduced a distribution of eigenmodes together with a density of eigenmodes, namely the number of eigenmodes per unit volume and unit of frequency at a given value of $\tilde{\omega}$. He also introduced a cut-off to take into account the uniform discreteness of the crystal, in the form of the *Debye Temperature* Θ_D. In 1912, Born and von Karman [4] performed the first explicit calculation of the eigenmodes in a cubic crystal and discovered the existence of *optical modes*, explaining a small discrepancy between the Debye predictions and the measurements of the heat capacity.

In both cases, whether electrons or phonons, the *density of states* (DOS) is defined in a similar way. In the phonon case, the relevant operator is $K \in \mathcal{B}$, whereas for electrons it is its Hamiltonian H, namely either the Schrödinger operator, in the continuum case, or the effective Hamiltonian in the tight binding representation. Let then H be the name of such an operator. In both cases it is given by a strong resolvent continuous family $(H_\omega)_\omega$ of selfadjoint operators, bounded from below, indexed either by the Hull Ω or by the transversal X. It acts either on $L^2(\mathbb{R}^d)$ or on $\ell^2(\mathcal{L}_\omega)$. In both cases, given a bounded box $\Lambda \subset \mathbb{R}^d$, it is meaningfull to restrict H_ω to Λ provided boundary conditions are prescribed. Let $H_{\omega,\Lambda}$ be this restriction. Then its spectrum is discrete in both cases so that there is only a finite number of eigenvalues (counted with their multiplicities), below $E \in \mathbb{R}$. This allows to define the *integrated density of states* (IDS) as

$$\mathcal{N}(E) \;=\; \lim_{\Lambda\uparrow\mathbb{R}^d} \frac{1}{|\Lambda|}\,\#\{E' \in \mathrm{Sp}(H_{\omega,\Lambda});\, E' \leq E\}$$

The existence of the limit depends upon the choice of an invariant ergodic probability measure $\mathbb{P}$ on the Hull so that the limit exists only $\mathbb{P}$-almost surely (resp. $\mathbb{P}_{tr}$-almost surely) with respect to ω [64, 96, 97, 98]. Let then $\mathcal{N}_{\mathbb{P}}$ denote this common limit. The *Shubin formula* [64, 42] expresses it in term of the noncommutative Brillouin zone as

$$\mathcal{N}_{\mathbb{P}}(E) \;=\; \mathcal{T}_{\mathbb{P}}\left(\chi\{H \leq E\}\right)\,, \qquad\qquad \textbf{(Shubin formula)} \qquad (42)$$

with a similar formular in the tight-binding case. Here $\chi\{\cdot \leq E\}$ denotes the characteristic function of the interval $(-\infty, E] \subset \mathbb{R}$. Then $\chi\{H \leq E\}$ is the spectral projection of H seen as an element of the von Neumann algebra $L^\infty(\mathcal{A}, \mathcal{T}_{\mathbb{P}})$. It is then clear from the definition, that $\mathcal{N}_{\mathbb{P}}$ is a non decresing non negative function of E. It vanishes below $E_0 \inf \mathrm{Sp}\{H\}$. It is constant on spectral gaps (see Fig 5). In particular, its derivative $d\mathcal{N}_{\mathbb{P}}/dE$ exists in the sense of a Stieljes-Lebesgue measure and is called the *density of states* (DOS).

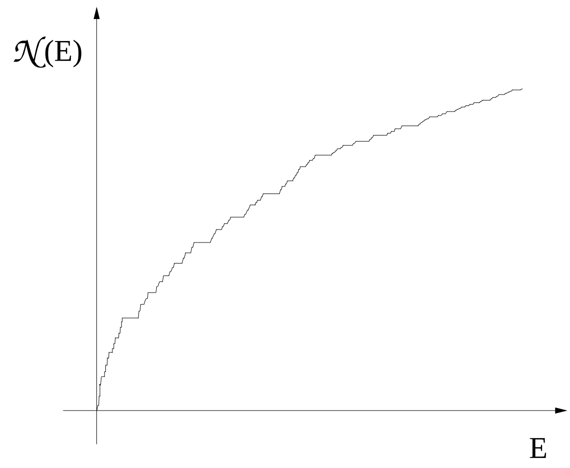

Figure 5: An example of electronic integrated density of states in 1D

The DOS is usually used to expressed thermodynamical quantities such as the *heat capacity*. In the case of phonons, the DOS is given by

$$d\mathcal{N}_\phi(\tilde{\omega}) \;=\; \rho_{\mathbb{P}}\; d\;\hat{\mathcal{T}}_{\mathbb{P}}(\chi(K \leq \tilde{\omega}^2))\,,$$

where $\rho_{\mathbb{P}}$ is the atom density (in number of particle per unit volume) in order to get a number of modes per unit volume, and the factor d in front account for the d possible choice of polarization of the acoustic wave. The Debye formula for the phonon contribution to heat capacity per unit volume leads to

$$C_v^{ph} \;=\; k_{\scriptscriptstyle B} \int_0^{\tilde{\omega}_D} d\mathcal{N}_\phi(\tilde{\omega}) \, \left\{ \frac{\hbar\tilde{\omega}/2k_{\scriptscriptstyle B}T}{\sinh\left(\hbar\tilde{\omega}/2k_{\scriptscriptstyle B}T\right)} \right\} , \tag{43}$$

where $\tilde{\omega}_D$ is the Debye cut-off frequency of the solid. If $T \uparrow \infty$, eq. (43) gives the Dulong-Petit law, namely

$$C_V^{ph} \stackrel{T\uparrow\infty}{\longrightarrow} \rho\, k_{\scriptscriptstyle B}\, d\,, \qquad\qquad \textbf{(Dulong \& Petit)} \tag{44}$$

As $T \downarrow$, only the low frequencies contribute, so that it is enough to consider the asymptotic of the DOS at $\tilde{\omega} \downarrow 0$. Since low frequencies correspond to large wave lengths, the corresponding phonons do not see the fine structure of the solid and behave like acoustic waves with sound velocity c_α for the polarisation α. In particular $d\mathcal{N}_\phi(\tilde{\omega})$ behaves like $\tilde{\omega}^{d-1}d\tilde{\omega}$, so that

$$C_v^{ph} \propto T^d\,, \qquad\qquad \text{as} \quad T \downarrow 0\,.$$

For $d = 3$ this gives the usual T^3 law discovered by Debye.

The electronic contribution to the heat capacity must take the fermionic character of the electrons into account. Then

$$C_v^{el} \;=\; T \left(\frac{\partial S}{\partial T}\right)_{V,N} ,$$

if S is the total entropy in the volume V. The derivative is taken at constant volume and constant electron number. The computation of S is usually performed in the grand canonical ensemble. If $\mathcal{N}_{el}$ denotes the electronic IDS, the chemical potential μ is fixed by the condition

$$2 \int_{\mathbb{R}} d\mathcal{N}_{el}(E) \, \frac{1}{1+e^{-\beta(E-\mu)}} \;=\; \frac{N}{V} \;=\; 2\mathcal{N}_{el}(E_F)\,.$$

Here N is the total number of electrons in volume V and E_F is called the *Fermi energy*. The factor 2 comes from the spin degrees of freedom. Then the entropy S is given by

$$S \;=\; 2k_{\scriptscriptstyle B} V \int_{\mathbb{R}} dE\, \beta^2\, (E-\mu) \, \frac{\mathcal{N}_{el}(E)}{4\cosh^2\{\beta(E-\mu)/2\}}\,. \tag{45}$$

Here $\beta = 1/k_{\scriptscriptstyle B}T$. Setting $x = \beta(E-\mu)/2$ this gives

$$S \;=\; 2k_{\scriptscriptstyle B} V \int_0^\infty dx \, \frac{x}{\cosh^2(x)} \, \left(\mathcal{N}_{el}(\mu + 2xk_{\scriptscriptstyle B}T) - \mathcal{N}_{el}(\mu - 2xk_{\scriptscriptstyle B}T)\right)\,. \tag{46}$$

Whenever the IDS is smooth around $E = E_F$, this gives the usual electronic contribution to the heat capacity

$$C_v^{el} \propto T\,, \qquad\qquad \text{as} \quad T \downarrow 0\,.$$

If, however $\mathcal{N}_{el}$ admits some fractal behaviour near the Fermi energy, then the low temperature behaviour may be modified. It turns out that such a fractal behaviour is hardly seen in practice. This is because the disorder and the interactions as well tend to smooth out the IDS at small energy scales.

4.7 The master equation

Within the one particle approximation, it is quite convenient to consider the quantum analog of the Boltzmann approach to kinetic equations. For classical gases Boltzmann was dealing with the one particle density. In the case of electron in an aperiodic solid, this one particle density is provided by a *state* on the C^*-algebra $\mathcal{A}$. Namely a state is a linear map $\phi : \mathcal{A} \mapsto \mathbb{C}$ that is both *bounded* (that is $|\phi(A)| \leq c\|A\|$ for some $c > 0$) and *positive* (that is $\phi(AA^*) \geq 0$ for all $A \in \mathcal{A}$). This state will be normalized so that, by adjoining a unit to $\mathcal{A}$ if necessary, $\phi(\mathbf{1}) = n_{el}$ whenever n_{el} is the electron density (number of electrons per unit volume). This is equivalent to impose $\sup_{\|A\|\leq 1} |\phi(A)| = n_{el}$.

The electrons in a solid are not independent particle. They usually interact with phonons. But the electron-phonon coupling can usually be considered as a small perturbation so that it is convenient to integrate out the phonon degrees of freedom to get an effective evolution for the electrons. This new evolution is no longer unitary, because the electron-phonon interaction produces a loss of information on the electron motion. However, the evolution can always be represented by a one-parameter family of *completely positive maps* $\{\Phi_t;\, t \geq 0\}$ acting on $\mathcal{A}$ and preserving the unit $\mathbf{1}$ (see a discussion of this point in [99]). A map $\Phi : \mathcal{A} \mapsto \mathcal{A}$ is completely positive if it is linear and if for any $N \in \mathbb{N}$ and any matrix $A = ((A_{i,j}))_{i,j=1}^N$ with matrix elements $A_{i,j} \in \mathcal{A}$, the matrix $((\Phi(A^*A)_{i,j}))_{i,j=1}^N$ defines a positive element in $\mathcal{A} \otimes M_N$. By Stinespring theorem [100], if $\mathcal{A}$ is represented in a Hilbert space $\mathcal{H}$, such map is given by $\Phi(A) = V\pi(A)V^*$ where π is a representation of $\mathcal{A}$ in a different Hilbert space $\mathcal{H}'$ and V is a partial isometry from $\mathcal{H}'$ to $\mathcal{H}$ (Stinespring compression). To get the electron evolution from the interacting theory, it is always necessary to proceed to such a Stinespring compression. If in addition, the electron evolution is considered on a mesoscopic time scale, the evolution becomes *Markovian*. In particular, it can be represented by a *Markov semigroup*, namely of one parameter family of completely positive maps from $\mathcal{A}$ into itself, indexed by $t \in \mathbb{R}_+$ (positive time), and such that

$$\Phi_{t+t'} \;=\; \Phi_t \circ \Phi_{t'}\,. \tag{47}$$

To describe this evolution it is convenient to write eq. (47) as a differential equation in the form

$$\frac{d\Phi}{dt} \;=\; \mathfrak{L}\,\Phi_t\,, \tag{48}$$

in which case $\mathfrak{L}$ is called a *Lindbladian*. This is because Lindblad characterized such operators whenever $\mathcal{A}$ is the C^*-algebra of all bounded operators in a Hilbert space

Theorem 8 (Lindblad [99]) *Let Φ_t be a norm continuous Markov semigroup on $\mathcal{B}(\mathcal{H})$ where $\mathcal{H}$ is some separable Hilbert space. Then there are bounded operators H, L_i such that $H = H^*$, $\sum_i L_i^* L_i \in \mathcal{B}(\mathcal{H})$ and that*

$$\frac{d\Phi}{dt} \;=\; \mathfrak{L}\,\Phi_t\,, \qquad \text{with} \qquad \mathfrak{L}(A) \;=\; \imath[H,A] + \sum_i \left(L_i^* A L_i - \frac{1}{2}\{L_i^* L_i, A\}\right),$$

where $\{A,B\} = AB + BA$. Conversely, any such $\mathfrak{L}$ generates a norm continuous Markov semigroup.

To deal with Statistical Mechanics, it is more convenient to work with states instead of observables. In the case of $\mathcal{B}(\mathcal{H})$ the state space is the set of *density matrices*, namely the positive compact trace class operator with trace 1. Then a Markov semigroup acts on the state space by duality, namely $\rho_t = \rho \circ \Phi_t$. In such a case the Lindbladian acts as follows:

$$\mathfrak{L}^\dagger(\rho) \;=\; -\imath[H,\rho] \;+\; + \sum_i \left([L_i\rho, L_i^*] + [L_i, \rho L_i^*]\right)$$

The evolution equation $d\rho/dt = \mathfrak{L}^\dagger \rho$ is called the *master equation*, which goes back to an early work by Pauli to describe the exchange between matter and radiation (see [54]).

The Lindblad theorem is a noncommutative version of the Levy-Khintchine theorem [101]. In the commutative context, states are nothing but *probability measures* and the Markov semigroups are given by the Chappmann-Kolmogoroff equations describing the evolution of the probability distribution of a stochastic process. If (Ξ, Σ) is a Borel space, where Σ is the corresponding σ-algebra, and if $\mathbb{P}_t$ denotes the probability distribution on Ξ describing the stochastic process at time t, then, for $B \in \Sigma$ and $t > s$

$$\mathbb{P}_t(B) \;=\; \int_\Xi P(t-s; B, y)\, \mathbb{P}_s(dy)\,,$$

where the transition probabilities $P(s; \cdot, y)$ satisfy (semigroup property, or Chappmann-Kolmogoroff equations)

$$P(t; B, x) \;=\; \int_\Xi P(t-s; B, y)\, P(s; dy, x)\,, \qquad 0 < s < t\,,\; x \in \Xi\,,\; B \in \Sigma\,.$$

In the special case for which $\Xi = \mathbb{R}^d$ and the transition probabilities are given by $P(t; dx, y) = p_t(y-x)dx$, with p_t a probability density, then the Fourier transform of p_t satisfies

$$\int_{\mathbb{R}^d} dx^d\, p_t(x)\, e^{-\imath k\cdot x} = e^{-t\phi(k)}\,, \quad \phi(k) = \imath k \cdot x_0 + \int_{\mathbb{R}^d} dG(u) \left(e^{\imath k\cdot u} - 1 - \frac{\imath k \cdot u}{1+u^2}\right) \frac{1+u^2}{u^2}\,, \tag{49}$$

where dG is a positive measure of finite mass. If dG admits a mass g at $u = 0$, it contributes for a term $-gk^2/2$ in the *r.h.s.* of (49), namely a gaussian term in p_t.

The Lindblad theorem has practical use in many fields of Physics. It is especially important in Quantum Optics where the explicit computation of the L_i's is related to perturbation theory in QED. Unfortunatley, such a theorem is too restrictive in many situations. First of all, the norm continuity is not natural. In many situations indeed, the generators is not bounded. Thus the norm pointwise continuity, namely $t \in \mathbb{R}_+ \mapsto \Phi_t(A) \in \mathcal{A}$ is continuous for all $A \in \mathcal{A}$, is sufficient in practice. Moreover, the result holds for C^*-algebras in a Hilbert space and is not necessarily true for a general C^*-algebra .

Example 5 (Fokker-Planck operators) Let $\mathcal{A}$ be the abelian unital C^*-algebra obtained from $\mathcal{C}_0(\mathbb{R})$ by adjoining a unit. Hence $\mathcal{A} = \mathcal{C}(\overline{\mathbb{R}})$ where $\overline{\mathbb{R}}$ is the one point compactification of $\mathbb{R}$. Let $\mathfrak{L}$ be a differential operator. For $\mathfrak{L}$ to be the generator of a norm pointwise continuous Markov semigroup on $\mathcal{A}$ it is necessary that $\mathfrak{L}$ be of the form

$$\mathfrak{L}(f) \;=\; \frac{d}{dx}\, a^2\, \frac{d}{dx} + b\, \frac{d}{dx} - \frac{d}{dx} b + c\,,$$

where a, b, c are real continuous functions on $\mathbb{R}$. In particular $\mathfrak{L}$ has no term of degree higher than 2. This is exactly the form of generators of the Fokker-Planck equation describing stochastic processes in the real line. $\Box$

In the case studied in Section 4.5 the following example is a generalization of the Levy-Khintchine theorem

Example 6 Let ϕ satisfies eq. (49). Then, if $\vec{\nabla}$ denotes the family of *-derivations on $\mathcal{A} = C^*(\Omega \rtimes \mathbb{R}^d, B)$ or on $\mathcal{B} = C^*(\Gamma(X), B)$ (see Section 4.5) defined in eq. (38)

$$\Phi_t \;=\; e^{-t\phi(\vec{\nabla})}$$

defines a Markov semigroup. $\Box$

Example 7 (Model of quantum jumps [45]) Let $\mathcal{H}$ be a separable Hilbert space and let $H = H^*$ be a selfadjoint operator with countable spectrum $S \subset \mathbb{R}$. For $E \in S$ the corresponding eigenprojection is denoted by P_E. Let $\{|j\rangle\,; j \in J\}$ be an orthonormal basis of $\mathcal{H}$, labelled by the set J and made of eigenvectors of H, so that $H|j\rangle = E_j|j\rangle$ where $E_j \in S$ denotes the eigenvalue of H corresponding to the label $j \in J$.
A model of quantum jumps is given by a family $\{\Gamma_{j\to j'}\,; j \neq j' \in S\}$ of non negative numbers representing the probability per unit time of jump from the state j to a state of energy j'. It is assumed that $\sup_j \Gamma_j^- < \infty$ if $\Gamma_j^- = \sum_{j'} \Gamma_{j\to j'}$ is the decay rate of the state j. In much the same way, $\sup_j \Gamma_j^+ < \infty$ if $\Gamma_j^+ = \sum_{j'} \Gamma_{j'\to j}$ is the creating rate of the state j.
In order to describe the jump dynamics, let $W_{j\to j'}$ be the *jump operators* defined by

$$W_{j\to j'}\,|j_0\rangle \;=\; \begin{cases} |j_0\rangle & \text{if} \quad j_0 \neq j \\ |j'\rangle & \text{if} \quad j_0 = j \end{cases}$$

Then $W_{j\to j'} = \mathbf{1} + K_{j\to j'}$ where $K_{j\to j'} = (|j'\rangle - |j\rangle)\langle j|$ is an operator of rank 1. In particular $K^*_{j\to j'}K_{j\to j'} = 2|j\rangle\langle j|$.
The Lindbladian associated with such a model is then given by

$$\mathfrak{L}(A) \;=\; \imath[H, A] + \sum_{j\neq j'} \Gamma_{j\to j'} \left(W^*_{j\to j'} A W_{j\to j'} - \frac{1}{2}\{W^*_{j\to j'} W_{j\to j'}, A\} \right) . \tag{50}$$

It is convenient to express this formula in a basis independent way. The jump probabilities define a bounded operator Γ with matrix elements $\Gamma_{j\to j'}$. Because the decay and creating rates are uniformly bounded, Γ is a bounded operator. $\Gamma^\pm$ will denote the diagonal operators with elements given by the decay and creating rates respectively. Then it is convenient to introduce two operations on the space of operators $\mathcal{B}(\mathcal{H})$. The first one is called *averaging*

$$\langle j|\mathbb{E}(A)|j'\rangle \;=\; \delta_{j,j'}\langle j|A|j\rangle\,,$$

Hence $\mathbb{E}$ is a norm 1 projection (*a conditional expectation*). The second operator is given by

$$\langle j|\mathcal{R}(A)|j'\rangle \;=\; \delta_{j,j'} \sum_{j"\in J} \langle j|A|j"\rangle\,.$$

This operator is not defined everywhere in $\mathcal{B}(\mathcal{H})$ and is not necessarily bounded. However it is simple to check that, thanks to the properies of Γ, $\Gamma^- = \mathcal{R}(\Gamma)$ and that, if D is a bounded diagonal operator, $|\mathcal{R}(\Gamma D)| \leq \mathcal{R}(\Gamma|D|) \leq \mathcal{R}(\Gamma)\|D\|$, and $\mathcal{R}(D\Gamma) = D\mathcal{R}(\Gamma)$. An elementary algebra gives

$$\mathfrak{L}(A) \;=\; \imath\left[H + \frac{\Gamma - \Gamma^*}{2\imath}, A\right] - \frac{1}{2}\{\Gamma^-, A\} - \mathbb{E}\left(\Gamma A + A\Gamma^*\right) + \mathcal{R}\left(\Gamma\mathbb{E}(A) + \mathbb{E}(A)\Gamma\right) \tag{51}$$

Hence the *r.h.s.* defines the dissipative dynamics in which the Hamiltonian is modified by the term $-\imath(\Gamma - \Gamma^*)/2$. This term corresponds to the *Knight shift* of MNR. Moreover, the second term is a damping term giving a width to any spectral ray of H since Γ^- commutes with H. $\Box$

The Model of quantum jumps can be generalized to some examples of C^*-algebras as shown in the next example.

Example 8 (Variable range hopping on an aperiodic lattice) Here $\mathcal{L}$ denotes a uniformly discrete subset of $\mathbb{R}^d$. Then Ω is its Hull, X the corresponding transversal and $\mathcal{B} = C^*(\Gamma(X))$ the C^*-algebra of the transversal without magnetic field (see Section 4.5). For any $\omega \in X$ let $\mathcal{H}_\omega = \ell^2(\mathcal{L}_\omega)$. Here the Hamiltonian H_ω is given by multiplication operator $f(\vec{X})$ if $\vec{X}$ denotes the position operator acting on $\mathcal{H}_\omega$. In particular, eigenstates are strictly localized. Hence H_ω describes electrons in the extreme case of strongly localized regime. Here H_ω is not necessarily covariant. However the bracket $L_H(A)_\omega = \imath[H_\omega, A_\omega]$ defines a *-derivation of $\mathcal{B}$ since this is the generator of the automorphism group $\eta_t(A)(\omega, x) = e^{\imath t(f(x) - f(0))} A(\omega, x)$ whenever $A \in \mathcal{B}_0$ and $\omega \in X,\ x \in \mathcal{L}_\omega$.
Quantum jumps will be produced if phonons force the electrons to leave their initial states. Thus the jump probability per unit times will be given by a function $\Gamma_{x\to y}(\omega) \geq 0$ with the properties defined in Example 7. In addition, the translation invariance of the dynamics implies that this function be *covariant*, namely $\Gamma_{x\to y}(\omega) = \Gamma_{x-a\to y-a}(\mathrm{T}^{-a}\omega)$ for any $a \in \mathcal{L}_\omega$. Hence $\Gamma \in \mathcal{B}$. Moreover, it is expected that on similar local patches, the transition rates are close, so that $\Gamma_{0\to x}(\omega)$ should be *continuous* on the groupoid $\Gamma(X)$. Thus, $\Gamma^-(\omega) = \sum_{x \in \mathcal{L}_\omega} \Gamma_{0\to x}(\omega)$ is a continuous function on X.
The operations $\mathbb{E}$ and $\mathcal{R}$ are well defined on $\mathcal{B}_0$ since

$$\mathbb{E}(A)(\omega, x) \;=\; \delta_{0,x}\, A(\omega, 0)\,, \qquad\qquad \mathcal{R}(A)(\omega, x) \;=\; \delta_{0,x} \sum_{y \in \mathcal{L}_\omega} A(\omega, y)\,.$$

following the construction given in Example 7, the corresponding Lindbladian becomes

$$\mathfrak{L}(A) \;=\; L_H(A) + \imath\left[\frac{\Gamma - \Gamma^*}{2\imath}, A\right] - \frac{1}{2}\{\Gamma^-, A\} - \mathbb{E}\left(\Gamma A + A\Gamma^*\right) + \mathcal{R}\left(\Gamma\mathbb{E}(A) + \mathbb{E}(A)\Gamma\right) \tag{52}$$

This defines a Markov semigroup on $\mathcal{B}$. This semigroup is liable to describe the dissipative evolution of a strongly localized electron due to phonons. It is the basic example for the Mott hopping conductivity. $\Box$

5 Coherent Electronic Transport

The coherent part of the electronic transport is the contribution of the quantum interferences to the quantum transport of the electronic wave packet. This is the part of the evolution that occurs before any dissipative mechanism takes place. In practice, this evolution is valid on a time scale τ_{coh} that is the time beyond which collision processes (with phonons say) destroy the phase coherence of the wave packet. This coherence time increases as the temperature decreases, so that the coherent transport eventually dominates at low temperature. In this section it will be assumed that there is no dissipative part in the quantum evolution for the electrons. Moreover, the electrons are considered as independent particles. Should the electrons interact, the description would then be given by a dissipative mechanism beyond a time scale τ_{coll} that represents the average collision times between electrons. In a sense then, the short time dynamics is insensitive to the electron interactions. The Landau theory of Fermi liquid takes care of the interactions and show that indeed the collision time increases like T^{-2} as the temperature T decreases [32]. Therefore again, at low temperature the electron-electron interaction can be neglected.

The main remark that will be developped in this Section is that the quantum wave packet exhibits an anomalous diffusion, namely the mean distance $r(t)$ that it goes after time t follows a scaling law

$$r(t) \overset{t\uparrow\infty}{\approx} t^{\beta}\,, \qquad\qquad 0 \leq \beta \leq 1$$

This will have deep consequences for the low temperature behaviour of the transport cœfficients. In particular, the conductivity will behave like a power law in term of the relaxation time (anomalous Drude formula see Section 6.3). This Section is devoted to the definition of these exponents, the relations between them and some of their properties.

5.1 Local and fractal exponents of a Borel measure

In most spectral problems related to the electron dynamics, there are various positive measures, such as the Density of states (DOS) (see Section 4.6), the spectral measure (also called the Local Density of states, LDOS) or the current-current correlation function. In this section scaling exponents are defined for a positive measure on $\mathbb{R}$. Most of the material of this section can be found in [33, 102, 103].

Let f be a positive measurable function on $(0, b]$. The power decay exponents $\alpha^+\,, \alpha^-\,, \alpha^m$ are defined as

$$\alpha^{\pm} \;=\; \left\{ \begin{array}{c} \limsup_{\epsilon\downarrow 0} \\ \liminf_{\epsilon\downarrow 0} \end{array} \right\} \frac{\ln f(\epsilon)}{\ln \epsilon}\,, \qquad\qquad \alpha^m \;=\; \sup\{\gamma \in \mathbb{R};\; \int_0^b d\epsilon\, \frac{f(\epsilon)}{\epsilon^{1+\gamma}} < \infty\} \tag{53}$$

Therefore $\alpha^- \leq \alpha^m \leq \alpha^+$ and $\alpha^m \geq 0$. Such definition will be shortened by writing

$$f(\epsilon) \overset{\epsilon\downarrow 0}{\sim} \epsilon^{\alpha^\star}\,,$$

where $\star \in \{+, -, m\}$. It can be shown that, whenever f is non decreasing, $\alpha^- = \alpha^m$ [33].

For a positive measurable function on $[b, \infty)$ the power growth exponents $f(t) \stackrel{t\uparrow\infty}{\sim} t^{\alpha^\star}$ are defined in a similar way.

A Borel measure μ on $\mathbb{R}$ is a positive bounded measure defined as a σ-additive function on the σ-algebra of Borel sets. It can be defined through its primitive $\mathcal{N}_\mu(E) = \int_{-\infty}^{E} d\mu$ which is positive and non decreasing (Stieljes-Lebesgue theory) [104]. The set of Borel measures on $\mathbb{R}$ can also be seen (Riesz theorem) as the space dual to $\mathcal{C}_0(\mathbb{R})$ (space of continuous complex functions on $\mathbb{R}$ vanishing at infinity), with duality defined by $\langle \mu | f \rangle = \int_{\mathbb{R}} d\mu\, f$. It will then be endowed with the *vague topology*: a sequence μ_n of Borel measures converges vaguely to μ if, for all $f \in \mathcal{C}_0(\mathbb{R})$, $\lim_n \int_{\mathbb{R}} d\mu_n f \to \int_{\mathbb{R}} d\mu f$.
A positive Borel measure μ is *absolutely continuous* (*a.c.*) whenever $\mu[E-\epsilon, E+\epsilon] \leq c(E)\, \epsilon$ for almost all E's. Equivalently, the Radon-Nikodym theorem asserts that $\mu(dE) = f(E)dE$ for some Lebesgue integrable non negative function f. The measure μ is *pure-point* (*p.p.*) whenever it can be written as a linear combination of Dirac measures. If μ is neither pure-point nor absolutely continuous, it is called *singular continuous* (*s.c.*). Given two Borel measures μ, ν on $\mathbb{R}$, μ dominates ν whenever for any Borel subset Δ of $\mathbb{R}$, $\mu(\Delta) = 0 \Rightarrow \nu(\Delta) = 0$. They are equivalent if each of them dominates the other. They are orthogonal whenever there is a Borel set Δ such that $\mu(\Delta) = 0$ and $\nu(\mathbb{R} \setminus \Delta) = 0$. The Lebesgue decomposition theorem asserts that any Borel measure on $\mathbb{R}$ can be decomposed in a unique way into the sum of an *a.c.* part, a *p.p.* part and a *s.c.* one, the three contribution being orthogonal to each other.
Given a Borel measure μ on $\mathbb{R}$, its *local dimension* $d^\star_\mu(E)$ is defined by

$$\mu([E-\epsilon, E+\epsilon]) \stackrel{\epsilon\downarrow 0}{\sim} \epsilon^{d^\star_\mu(E)}\,.$$

Since $\mu([E-\epsilon, E+\epsilon])$ is a non decreasing function of ϵ, $d^m_\mu(E) = d^-_\mu(E)$, so that it is enough to consider $\star \in \{\pm\}$. An important property is the following [33]

Lemma 2 *Let μ, ν be two Borel measures on $\mathbb{R}$. Then*
(i) $d^\star_\nu(E) \leq d^\star_\mu(E)$ for ν-almost every E.
(ii) If μ dominates ν, then $d^\star_\nu(E) = d^\star_\mu(E)$, ν-almost surely.

In particular, using Lebesgue's measure, $0 \leq d^\star_\mu(E) \leq 1$ for μ-almost every E. (Note however that there may be $E \in \mathbb{R}$ for which $d^\star_\mu(E) > 1$, but such E belongs to a set of μ-measure zero.) Moreover equivalent measures have the same local dimension. Hence μ is absolutely continuous then $d^\star_\mu(E) = 1$, μ-almost everywhere. If μ is pure-point then $d^\star_\mu(E) = 0$, μ-almost surely. Thus these exponents are non trivial only for singular continuous measures. Another way to define these exponents is through potential theory [105, 106] initially proposed by Frostman [107]

$$d^-_\mu(E) \;=\; \sup\{\gamma \in \mathbb{R}\,;\, \int d\mu(E')\, \frac{1}{|E-E'|^\gamma} \;<\; \infty\}\,.$$

On the other hand [108, 109]

Lemma 3 *Let μ be a Borel measure on $\mathbb{R}$ and let $G_\mu(z) = \int_{\mathbb{R}} d\mu(E)/(z-E)$, $\Im m(z) > 0$, its Green's function. Let $\sigma^\star(E)$ be defined as*

$$\Im m\,(G_\mu(E - \imath\epsilon)) \stackrel{\epsilon\downarrow 0}{\sim} \epsilon^{\sigma^\star(E)}\,.$$

Then $\sigma^-(E) = d^-_\mu(E) - 1$ whenever $d^-_\mu(E) \in [0, 2]$.

Given a Borel subset Δ of $\mathbb{R}$, the local dimensions are defined by

$$d_\mu^{\star,\pm}(\Delta) \;=\; \left\{ \begin{array}{l} \mu - \mathrm{esssup}_{\epsilon\downarrow 0} \\ \mu - \mathrm{essinf}_{\epsilon\downarrow 0} \end{array} \right\} d_\mu^\star(E)\,.$$

Hausdorff and packing dimensions are defined in [110, 105, 111, 106]. Here are the basic definitions. Let F be a subset of $\mathbb{R}$. For $\delta \in (0,1)$, a δ-cover is a covering of F by open sets of diameter less than or equal to δ. Here $d(U)$ denotes the diameter of U. If $s > 0$ let

$$\mathcal{H}_\delta^s(F) \;=\; \inf\{\sum_{i=0}^{\infty} d(U_i)^s\,;\{U_i\} \text{ is a } \delta\text{-cover of } F\}$$

Then $\mathcal{H}_\delta^s(F)$ decreases as $\delta \downarrow 0$ so that $\mathcal{H}^s(F) = \lim_{\delta\downarrow 0}\mathcal{H}_\delta^s(F)$ exists and defines a Borel measure called the *s-Hausdorff measure* of F. The Hausdorff dimension $\dim_H(F)$ is the unique value s_0 such that $s < s_0 \Rightarrow \mathcal{H}_\delta^s(F) = \infty$ whereas $s > s_0 \Rightarrow \mathcal{H}_\delta^s(F) = 0$. In much the same way a δ-packing of F is a countable family of disjoint open balls with centers in F and diameter less than or equal to δ. Then

$$\mathcal{P}_\delta^s(F) \;=\; \sup\{\sum_{i=0}^{\infty} d(B_i)^s\,;\{B_i\} \text{ is a } \delta\text{-packing of } F\}$$

Again $\mathcal{P}_0^s(F) = \lim_{\delta\downarrow 0}\mathcal{P}_\delta^s(F)$ exists. A Borel measure $\mathcal{P}^s$, the *s-packing measure*, is defined through

$$\mathcal{P}^s(F) \;=\; \inf\{\sum_i \mathcal{P}_0^s(F_i)\,;\; F_i \text{ Borel set }\;, F \subset \bigcup_i F_i\}$$

The *packing dimension* $\dim_P(F)$ is the unique value s_0 such that $s < s_0 \Rightarrow \mathcal{P}_\delta^s(F) = \infty$ whereas $s > s_0 \Rightarrow \mathcal{P}_\delta^s(F) = 0$.

Whenever μ is a Borel measure on $\mathbb{R}$ and $\Delta \subset \mathbb{R}$ a Borel set, the Hausdorff dimensions $\dim_H^\pm(\mu,\Delta)$ and the packing dimensions $\dim_P^\pm(\mu,\Delta)$ are defined respectively as follows (where $* \in \{H,P\}$)

$$\dim_*^+(\mu,\Delta) \;=\; \inf\{\dim_*(\Delta');\; \Delta' \subset \Delta\,,\; \mu(\Delta') = \mu(\Delta)\}\,,$$

$$\dim_*^-(\mu,\Delta) \;=\; \sup\{\alpha \in \mathbb{R}; \Delta' \subset \Delta\,,\; \dim_*(\Delta') \leq \alpha \Rightarrow \mu(\Delta') = 0\}\,.$$

Then it turns out that (see [102] Appendix):

$$\dim_H^\pm(\mu,\Delta) \;=\; d_\mu^{+,\pm}(\Delta)\,, \qquad\qquad \dim_P^\pm(\mu,\Delta) \;=\; d_\mu^{-,\pm}(\Delta)\,.$$

A finer characterization of the local properties of μ are given by its *fractal exponents* defined by (for $q \neq 1$)

$$\int_\Delta d\mu(E)\; \mu([E-\epsilon, E+\epsilon])^{q-1} \;\overset{\epsilon\downarrow 0}{\sim}\; \epsilon^{(q-1)D_{\mu,\Delta}^\star(q)}\,.$$

The function $q \mapsto (q-1)D_\mu^\star(q)$ is concave and $q \mapsto D_\mu^\star(q)$ is non increasing. The fractal exponents are not measure class invariant [33].

Lemma 4 ((see [33])) *The local dimensions $d^\star_\mu(E)$ are Borel functions of (μ, E). The local dimensions $d^{\star,\pm}_\mu(\Delta)$ and the fractal exponents $D^\star_{\mu,\Delta}(q)$ are Borel functions of μ.*

The proof of this lemma for d^-_μ can be found in [33]. The same strategy applies to d^+_μ as well as for $D^\star_{\mu,\Delta}(q)$.

Lemma 5 ((see [112], Appendix)) *Let $f_\mu(\alpha)$ be the Legendre transform of the function $q \mapsto (q-1)D^\star_\mu(q)$ and let $I_\alpha(\epsilon) = \{E \in \mathbb{R};\, \mu([E-\epsilon, E+\epsilon]) < \epsilon^\alpha\}$. If $D^+_\mu(q) = D^-_\mu(q) = D_\mu(q)$ and $D_\mu(q) < \infty$ for some $q < 0$, then there are positive constants $0 < c < C$ such that*

$$c\epsilon^{\alpha - f_\mu(\alpha)} \;\leq\; \mu(I_\alpha(\epsilon)) \;\leq\; C\epsilon^{\alpha - f_\mu(\alpha)}\,.$$

□

Whenever D^+_μ and D^-_μ do not coincide, there is a weaker inequality due to Barbaroux, Germinet and Tcheremchantsev [113] : if μ has compact support then for any $0 \leq q \leq 1$ there is $\alpha = \alpha(\epsilon, q)$ such that

$$\mu(I_\alpha(\epsilon)) \;\geq\; \epsilon^{(1-q)\alpha}\,\frac{1}{|\ln \epsilon|}\int d\mu(E)\,\mu([E-\epsilon, E+\epsilon])^{q-1}\,, \qquad \textbf{(BGT estimate)}\,.$$

5.2 Spectral Exponents

Let H be a selfadjoint operator acting on the separable Hilbert space $\mathcal{H}$. The spectral theory associates with H a $\mathcal{H}$-projection-valued Borel measure Π on $\mathbb{R}$ [114] called the *spectral measure* of H. Furthermore, for any $\phi \in \mathcal{H}$, $\|\phi\| = 1$, let ρ_ϕ be the *spectral measure* of H relative to ϕ, namely for $f \in C_0(\mathbb{R})$,

$$\int d\rho_\phi(E)\; f(E) \;=\; \langle\phi|f(H)|\phi\rangle \;=\; \int \langle\phi|\Pi(dE)|\phi\rangle\; f(E)\,.$$

In physics literature, ρ_ϕ is called the *local density of states* (LDOS).

Definition 6 *Let $E \in \mathbb{R}$ and Δ be a Borel subset of $\mathbb{R}$. The spectral exponents and essential spectral exponents of Π (or H) are defined by*

$$d^{\star,+}_\Pi(\Delta) \;=\; \sup_{\phi\in\mathcal{H}} d^{\star,+}_{\rho_\phi}(\Delta)\,, \qquad d^{\star,-}_\Pi(\Delta) \;=\; \inf_{\phi\in\mathcal{H}} d^{\star,-}_{\rho_\phi}(\Delta)\,.$$

The next result shows that there are *typical* states in $\mathcal{H}$ giving the generic properties of the spectrum

Lemma 6 ([33]) *There exists $\psi \in \mathcal{H}$ with $\;d^{\star,*}_\Pi(\Delta) = d^{\star,*}_{\rho_\psi}(\Delta)$.*

Let now $\mathcal{L}$ be a uniformly discrete subset of $\mathbb{R}^d$ and let Ω its Hull and X its transversal. Let also $\mathbb{P}$ be an invariant ergodic measure on the Hull and $\mathbb{P}_{tr}$ the induced probability on X. Let then $H = (H_\omega)$ be a covariant strong resolvent continuous family of selfadjoint operators on the Hilbert space $\mathcal{H}_\omega$ corresponding to either $L^2(\mathbb{R}^d)$ (continuous case) or to $\ell^2(\mathcal{L}_\omega)$ (discrete case). Let Π_ω denote the corresponding family of spectral measures. By covariance, Π_ω and $\Pi_{\omega'}$ are equivalent measures whenever ω and ω' belong to the same orbit. Therefore their local dimension coincide. Thanks to Lemma 4 it follows that the maps $\omega \mapsto d^{\star;*}_{\Pi_\omega}(\Delta)$ is Borel and translation invariant, so that, by ergodicity, it is $\mathbb{P}$-almost surely constant ($\mathbb{P}_{tr}$-almost surely constant in the discrete case).

Definition 7 *The LDOS dimensions $d^{\star;*}_{LDOS}(\Delta)$ is the common value of the $d^{\star;*}_{\Pi_\omega}(\Delta)$'s for $\mathbb{P}$ almost all ω's.*

Remark 8 The LDOS dimensions depend on the choice of $\mathbb{P}$ in general. □

In much the same way, the DOS (see eq. (42)) $d\mathcal{N}_{\mathbb{P}}$ is a Borel measure on $\mathbb{R}$ so that it has its own local dimensions

Definition 8 *The DOS dimensions $d^{\star;*}_{DOS}(\Delta)$ are the local dimensions of the density of states $d\mathcal{N}_{\mathbb{P}}$.*

The relation between the LDOS and the DOS local dimensions is given by

Lemma 7 ([33]) *If Δ is a Borel subset of $\mathbb{R}$, then $d^{-;\pm}_{LDOS}(\Delta) \leq d^{-;\pm}_{DOS}(\Delta)$.*

In general the inequality is strict. The spectral measure may be pure point with an *a.c.* density of states. This is the case for the Anderson model in one dimension [97, 98, 96].

5.3 Diffusion exponents

Let $\mathcal{L}$ be a uniformly discrete subset of $\mathbb{R}^d$ containing the origin and let $\mathcal{H} = \ell^2(\mathcal{L})$. The position operator is defined as in Section 4.5 (see eq. (38)) by $\vec{X}\psi(x) = \vec{x}\psi(x)$, for $\psi \in \mathcal{H}$. Let also $H = H^*$ be a selfadjoint operator on $\mathcal{H}$ such that the corresponding *current operator* $\vec{J} = \imath[\vec{X}, H]$ be bounded (actually it is enough that $\vec{J}$ satisfies $f(H)\vec{J}$ bounded for all functions f continuous with compact support). For Δ a Borel subset of $\mathbb{R}$, let Π_Δ be the spectral projection of H on Δ. As time goes, the position operator evolves according to $\vec{X}(t) = e^{\imath tH}\vec{X}e^{-\imath tH}$. Thus $\vec{X}(t) - \vec{X}$ measures the distance that the particle goes between times 0 and t. The average distance the particle goes after time t, starting from an initial state located at $0 \in \mathcal{L}$ and projected on Δ can be measured through the following *transport exponents*

$$\int_{-t}^{+t} \frac{ds}{2t} \langle 0|\Pi_\Delta \, |\vec{X}(s) - \vec{X}|^q \, \Pi_\Delta|0\rangle \;\stackrel{t\uparrow\infty}{\sim}\; t^{q\,\beta^\star_q(\Delta)}\,.$$

Since the current is bounded, $\|\vec{X}(t) - \vec{X}\| \leq t\|\vec{J}\|$. it follows that $0 \leq \beta^\star_q(\Delta) \leq 1$. Even though only few specific values of q matter in practice ($q = 2$ is the most important for transport cœfficients), it may be convenient to take advantage of this varying parameter. The Cesaro mean $\int_{-t}^{+t} ds/2t$ may be replaced by a *gaussian mean* $\int_{\mathbb{R}} ds/t \exp(-s^2/t^2)$ without changing the exponents. In addition, the constant term $\vec{X}$ can also be removed without changing the exponents. Whenever $\Delta = \mathbb{R}$, Δ will be omitted.

In much the same way, the previous definition can be extended to the case of a covariant family over the Hull of $\mathcal{L}$. Then the relevant exponents are the *averaged* ones

$$
(L_{\Delta,q}(t))^q \;=\; \int_{-t}^{+t} \frac{ds}{2t} \int_X d\mathbb{P}_{tr}(\omega)\langle 0|\Pi_{\omega,\Delta}\, |\vec{X}_\omega(s)-\vec{X}|^q\, \Pi_{\omega,\Delta}|0\rangle \;\stackrel{t\uparrow\infty}{\sim}\; t^{q\overline{\beta}_q^\star(\Delta)}\,.
$$

It is interesting to notice that the last expression admits an interpretation in term of the noncommutative Brillouin zone. Namely

$$
(L_{\Delta,q}(t))^q \;=\; \int_X d\mathbb{P}_{tr}(\omega)\langle 0|\Pi_{\omega,\Delta}\, |\vec{X}_\omega(t)-\vec{X}|^q\, \Pi_{\omega,\Delta}|0\rangle \;=\; \hat{\mathcal{T}}_{\mathbb{P}}\left(|\vec{\nabla}(e^{-\imath sH})|^q\Pi_\Delta\right)\,. \tag{54}
$$

Similar definition can be given on the continuum.

The case $q=2$ is special. For indeed the corresponding diffusion exponent enters explicitely in the transport theory. To see this, let the *current-current measure* be defined as follows: let $H=H^*$ be a selfadjoint element affiliated to $\mathcal{A}$ (or to $\mathcal{B}$ in the discrete case; see 4.6). This means that $f(H)\in\mathcal{A}$ for all $f\in\mathcal{C}_0(\mathbb{R})$ [89]. In addition H is such that $\vec{\nabla}H$ is also affiliated to $\mathcal{A}$ and satisfies $f(H)\vec{\nabla}Hg(H)\in\mathcal{A}$ for all pair of functions f,g with compact support. Then, thanks to Riesz theorem, there is a Borel measure $dm_{i,j}$ on $\mathbb{R}^2$ defined by

$$
\int_{\mathbb{R}^2} dm_{i,j}(E,E')\, f(E)g(E') \;=\; \mathcal{T}_{\mathbb{P}}\left(f(H)\partial_i H\, g(H)\partial_j H\right)\,, \qquad\qquad f\;\, g\in\mathcal{C}_c(\mathbb{R})\,. \tag{55}
$$

Setting $dm=\sum_{i=1}^d dm_{i,i}$, the result is the following

Proposition 6 ([115, 33]) *The diffusion exponents $\overline{\beta}_2^\pm$ are given by*

$$
m\{(E,E'\in\Delta\times\mathbb{R}\,;\,|E-E'|\leq\epsilon\} \;\stackrel{\epsilon\downarrow 0}{\sim}\; \epsilon^{2(1-\overline{\beta}_2^\star(\Delta))}\,.
$$

Hence the diffusion exponents β_2 measure the fractal behaviour of the current-current correlation function near the diagonal.

From the definition of the diffusion exponents, if $\overline{\beta}_q^\star=0$ then particle is likely to be *localized*. Actually a stronger condition is required. Let the localization length be defined as [116, 35]

$$
l_q(\Delta)^q \;=\; \limsup_{t\to\infty}\int_{-t}^{+t}\frac{ds}{2t}\,\hat{\mathcal{T}}_{\mathbb{P}}\left(|\vec{\nabla}e^{-\imath Hs}|^q\,\Pi(\Delta)\right) \;<\; \infty\,. \tag{56}
$$

Note that this condition is stronger than $\overline{\beta}_q^\star(\Delta)=0$, because the integrand may be logarithmically divergent as $t\to\infty$ without changing the diffusion exponent. It turns out that $l_2(\Delta)$ coincides with the notion of localization length used in physics. In several examples (the Anderson model for instance) this condition has been proved to hold.

Theorem 9 *Let the localization condition* (56) *be satisfied for a Borel set $\Delta\subset\mathbb{R}$ and some $q>0$. Then, if $\vec{\nabla}H\in\mathcal{A}$, the following holds:*

i) [116, 35] $\overline{\beta}_q^\star(\Delta)=0$ *and $\pi_\omega(H)$ has pure-point spectrum in Δ for $\mathbb{P}_{tr}$-almost every $\omega\in X$.*

ii) [33] *The localization condition* (56) *is invariant by a compact perturbation of H.*

iii) [116, 35] *If $q=2$, there is a $\mathcal{N}$-measurable function l on Δ such that for every Borel subset Δ' of Δ:*

$$l_2(\Delta')^2 = \int_{\Delta'} d\mathcal{N}(E)\, l(E)^2 \,. \tag{57}$$

$l(E)$ is the localization length at the energy E.

iv) [115] *The localization length $l(E)$ is also given by*

$$l_2(\Delta')^2 \;=\; \int_{\Delta\times\mathbb{R}} dm(E,E')\,\frac{1}{|E-E'|^2}\,. \tag{58}$$

Since the current-current measure can also be expressed in term of the average of product of two Green functions, this formula gives the expression of the localization length as computed in physics literature. It justifies the claim that $l(E)$ is the localization length. Similar results are expected for the l_q's.

5.4 The Guarneri and BGT Inequalities

The main result is the so-called *Guarneri inequality* which is supplemented by the BGT one below,

Theorem 10 *Let $\mathcal{L}$ be a uniformly discrete subset of $\mathbb{R}^d$. Let H be a selfadjoint bounded operator on $\ell^2(\mathcal{L})$ such that $\vec{J} = \imath[\vec{X}, H]$ be bounded. Then for all $q > 0$*

$$\text{(i) } \beta_q^-(\Delta)\, d \geq \dim_H^+(\mu,\Delta)\,, \qquad \text{(ii) } \beta_q^+(\Delta)\, d \geq \dim_P^+(\mu,\Delta)\,, \qquad \text{(iii) } \beta_q^{\pm}(\Delta)\, d \geq D_{\mu,\Delta}^{\pm}(\frac{d}{d+q})\,,$$

The inequality (i) appeared in the original Guarneri papers [117, 118]. The form it takes above is due to Last [119]. It was extended to the continuous case by Combes [120]. The inequality (ii) first appeared in [102]. The inequality (iii) appeared in [112] with the condition that $D_\mu^+(q) = D_\mu^-(q)$, but the form given above is due to [113] without this condition. The proof is interesting in itself in that it shows where, in energy space, is concentrated the wave packet at large times.

Sketch of the proof: (reproduced from [103]) here only the case $\Delta = \mathbb{R}$ is considered. Let $R > 0$ then

$$\langle 0||\vec{X}|^q(s)|0\rangle \;\geq\; R^q \sum_{|x|>R} |\langle x|e^{-\imath Hs}|0\rangle|^2 \;=\; R^q \left(1 - \sum_{|x|\leq R} |\langle x|e^{-\imath Hs}|0\rangle|^2\right)\,.$$

Let $|0\rangle$ be decomposed as $|\psi\rangle + |\psi^c\rangle$ so that

$$\sum_{|x|\leq R} |\langle x|e^{-\imath Hs}|0\rangle|^2 \;\leq\; 1 - \|\psi\|^2 + \sum_{|x|>R} |\langle x|e^{-\imath Hs}|\psi\rangle|^2 + \text{crossed terms}\,.$$

The crossed term can be treated as the third one on the *r.h.s.*, with a bit of technicalities. Thus

$$\langle 0||\vec{X}|^q(s)|0\rangle \;\geq\; R^q \left(\|\psi\|^2 - \sum_{|x|>R} |\langle x|e^{-\imath Hs}|\psi\rangle|^2 + \text{crossed terms}\right)\,.$$

Then ψ is chosen as $\chi(H)|0\rangle$ where χ is the characteristic function of the set $I(t) = I_\alpha(1/t)$ (see Lemma 5) if μ is the spectral measure of H relative to the state $|0\rangle$. Using the large deviation bound, $\|\psi\|^2 = \mu(I_\alpha(1/t)) \geq c\, t^{f_\mu(\alpha)-\alpha}$. To bound the oscillating terms involving $e^{-\imath Hs}$, it is simpler to use the Gaussian mean instead of the Cesaro mean. Writting $\langle 0|g(H)|x\rangle$ as $\int d\mu(E) g(E) P_x(E)$, with $\int d\mu(E)|P_x(E)|^2 = 1$, and using the Cauchy-Schwarz inequality

$$\int \frac{ds}{t}\, e^{-s^2/t^2}\, |\langle x|e^{-\imath Hs}|\psi\rangle|^2 \;\leq\; \int_{I(t)} d\mu(E)|P_x(E)|^2 \int_{I(t)} d\mu(E') e^{-(E-E')^2 t^2} \;\leq\; t^{-\alpha}\,.$$

This estimate takes care of the remaining terms. Then R is still free. If it is chosen so that $t^{f_\mu(\alpha)-\alpha} \sim R^d t^{-\alpha}$, a little algebra leads to (iii) once α is chosen in the optimal way. □

5.5 A heuristic discussion

Coherent transport has been the focus of attention of many numerical studies during the last fifteen years. Existence of models exhibiting anomalous diffusion exponents was pointed out early [121, 122, 123, 124, 125, 126, 127, 128]. Thanks to Guarneri's bounds, the following discussion follows. The meaning of the spectral exponents given by various local dimensions, is the following:

1. If the spectrum of H in the Borel set Δ is *absolutely continuous* then $d_{LDOS}(\Delta) = 1$.
2. If the spectrum of H in the Borel set Δ is *pure point* then $d_{LDOS}(\Delta) = 0$.
3. Consequently if $0 < d_{LDOS}(\Delta) < 1$ the electronic spectrum is singular continuous (or *fractal*).

One important problem is whether a singular electronic spectrum can be expected or not. The Anderson model, acting on $\ell^2(\mathbb{Z}^d)$ and defined by

$$(H\psi)(x) \;=\; \sum_{y;|y-x|=1} \psi(y) \;+\; \lambda\, V_x\, \psi(x)\,, \qquad\qquad \psi \in \ell^2(\mathbb{Z}^d)\,, \tag{59}$$

where the V_x's are real identically distributed independent random variables, with mean $\langle V_x\rangle = 0$ and covariance $\langle V_x^2\rangle = 1$, gives rise to a pure-point spectrum at large λ or near the band edges [97, 98, 96, 129, 130]. Similar result have been obtained for the analog of the Anderson model on $L^2(\mathbb{R}^d)$. Many Schrödinger operators with quasiperiodic potential also give rise to pure point spectrum for large coupling constant [97, 98].
One-dimensional Schrödinger operators on quasicrystals or with potentials given by automatic sequences, have singular continuous spectrum [131, 132, 133, 134, 135]. A systematic study of operators with singular continuous spectrum has been done by B. Simon *et al.* [109, 136, 137, 138, 139, 140, 141, 142, 143, 144].
In higher dimension there are not many results available for quasicrystals. The labyrinth model [145, 146, 147, 148, 149] is obtained as a cartesian product of one-dimensional models: it shows that as dimension grows absolutely continuous spectrum becomes more and more likely. As for the Anderson model [10], whenever the Schrödinger operator is dominated by the kinetic term, absolutely continuous spectrum becomes more likely as soon as the dimension is greater than or equal to 3. Therefore

Problem 1 *Let $\mathcal{L}$ be a uniformly discrete subset of $\mathbb{R}^d$ with $d \geq 3$. Let Ω be the Hull and $\mathbb{P}$ be an $\mathbb{R}^d$-invariant ergodic probability measure on Ω. Let $v : x \in \mathbb{R}^d \mapsto v(x) \in \mathbb{R}$ be an element of $L^1_{K,r}(\mathbb{R}^d)$ (see Section 4.6 and Lemma 1) for some K, r. Then prove or disprove that there is $E_c \in \mathbb{R}$ such that the part of the spectrum of*

$$H_\omega \; = \; -\Delta + \sum_{y \in \mathcal{L}_\omega} v(\cdot - y)$$

contained in $[E_c, \infty)$ is absolutely continuous for $\mathbb{P}$-almost every ω. □

Problem 2 *(i) Let $H = -\Delta + V$ be acting on $L^2(\mathbb{R}^d)$ where V is a bounded uniformly continuous function. Let Ω be the Hull of this operator defined as the strong resolvent closure of its translated [42, 64]. Then prove or disprove the same claim as in Problem 1*
(ii) Consider the same problem $H = -\Delta + \lambda V$ be acting on $\ell^2(\mathbb{Z}^d)$ where V is a bounded sequence on $\mathbb{Z}^d$ (including the Hull and the probability $\mathbb{P}$). Prove or disprove that for λ small enough there is an a.c. *spectrum away from the band edges* □

Remark 9 The Anderson transition problem is a special case of Problem 2(ii) whenever V is a random sequence or of Problem 1 if $\mathcal{L}$ is a chosen randomly (with Bernoulli distribution) on a regular lattice. □

Thanks to the last remark, these problems are certainly difficult to handle. Many numerical calculations in the eighties, together with the theory of mesoscopic systems have suggested that at scales of the order of λ^2 near the Fermi level, the effective Hamiltonian of the Anderson model behaves like a Gaussian random matrix [150, 151, 152, 153, 154] (see especially [153] for a review). There are many reasons to believe that the same property holds in general for potentials of the kind introduced in Problem 1 and 2, at least if the subset $\mathcal{L}$ is dense enough (say Delone) and aperiodic. In particular, the level spacing distribution of an octagonal quasicrystal belongs to the Wigner-Dyson universality class, suggesting that RMT applies [155]. Then the Random Matrix Theory (RMT) predicts a smooth DOS, a simple *a.c.* spectrum and also quantum diffusion (see below). If this is the case, the properties of this type of spectrum should be universal close to the Fermi level.

The theory of transport exponents developped in the previous Section 5.3 can also be interpreted as follows (the discussion concentrates on β_2

1. Ballistic motion implies $\beta_q = 1$. This is what happens for periodic Schrödinger operators either on the continuum or on the lattice. From the Guarneri inequality, in dimension $d = 1$, *a.c.* spectrum implies $\beta_q = 1$. Note, however, that there are examples of Hamiltonians with *a.c.* spectrum and subballistic motion [156].

2. Strong localization, on the opposite side, implies $\beta_q = 0$. However there are examples of Hamiltonian in dimension $d = 1$ with $\beta_q = 0$ and no localized states [157]. In dimension $d = \infty$ it is even possible to construct Hamiltonians with *a.c.* spectrum and $\beta_q = 0$ [158].

3. Quantum diffusion corresponds to $\beta_2 = 1/2$. This is what happens for the Anderson Hamiltonian in the Randon Phase Approximation (the so-called *Wegner N-orbital model* [33]; see Section 6.4). This type of behaviour is expected to occur every time RMT

applies, thus for the Anderson model in the weak localization regime such as low disorder for $d \geq 3$ or with spin-orbit coupling in $d = 2$ [11]. If the answer to Problem 1 is positive, then $\beta_2 = 1/2$ is expected at low energy scale near the Fermi level on any type of tiling, especially in quasicrytals. As a consequence it should produce a residual conductivity at low temperature (see Section 6.3).

4. Subballistic overdiffusive motion will correspond to $1/2 < \beta_q < 1$. This type of behaviour has been observed in many models of quasicrystals [146, 147, 159]. They are compatible with *a.c.* spectrum only if $d \geq 2$. However, these models for quasicrystals do not seem to reflect what happens in experiments.

5. Subdiffusive motion corresponds to $0 < \beta_2 < 1/2$. Many examples of models are also known to be subdiffusive [146, 147, 159]. Note that *a.c.* spectrum implies $\beta_q \geq 1/d$. In [149] examples of labyrinth models with *a.c.* spectrum and β_2 as close as possible from $1/d$ have been constructed. It is believed that in most quasicrystals (either with decagonal or icosahedral symmetry), the electronic Hamiltonian, in the one-particle approximation, should have an *a.c.* spectrum near the Fermi energy with subdiffusive behaviour. It may not be the case for the *AlPdRe* compound reported in Fig. 3 however (see Section 6.5 for a discussion). In any case, it is difficult, to produce non artificial models liable to describe faithfully the transport properties of a realistic quasicrystal.

6 Dissipative Transport in the RTA

Dissipative transport concerns what happen to electrons beyond the coherence time τ_{coh}. Then collisions with other degrees of freedom, mostly with phonons must be taken into account. In principle, the description of this regime requires giving a full account of the interactions between electrons and phonons. This means using the second quantization formalism and an effective Hamiltonian liable to represent the electron-phonon interaction or even the electron-electron interaction. In most cases, at finite volume and within the tight-binding approximation, the most common Hamiltonian that is used in Solid State Physics is the Fröhlich one given below. If Λ is a bounded open subset of $\mathbb{R}^d$, let $\Lambda_\omega = \Lambda \cap \mathcal{L}_\omega$

$$H_{\Lambda,\omega} = \sum_{x,y \in \Lambda_\omega} \left(h(\mathrm{T}^{-x}\omega, y - x)\, f^\dagger_{x,\sigma} f_{y,\sigma} + \kappa_{\alpha,\beta}(\mathrm{T}^{-x}\omega, y - x)\, b^\dagger_{x,\alpha} b_{y,\beta} \right) + \lambda \sum_{x \in \in \Lambda_\omega} (b^\dagger_x + b_x) f^\dagger_x f_x \,, \quad (60)$$

where $f^\dagger_{x,\sigma}, f_{x,\sigma}$ represent the creation-annihilation fermion operators at the site x with spin σ (electrons or holes), $b^\dagger_{x,\alpha}, b_{x,\alpha}$ represent the corresponding creation-annihilation boson operators (phonons) at x with polarization α, $h \in \mathcal{B}$ is the one-fermion Hamiltonian, $\kappa \in \mathcal{B}$ is the matrix of spring constants describing the phonon modes in the harmonic approximation, and λ is the coupling constant between phonons and fermions.

The main difficulty consists in getting a good approximation for the groundstate whenever the density of fermions is fixed and to have an efficient description of the excitation spectrum. This is usually far too complicated in comparison with the efficiency of other approximations when dealing with transport. Actually the electron-phonon coupling is very small so that the collision rate between them is often small enough so as to treat the phonon effect as an external noise. This is the essence of the kinetic models, starting with the Drude model [1], with its more elaborate version using the Boltzmann equations, as was proposed by Lorentz [23]. In this section only the so-called *Relaxation Time Approximation* (RTA) will be considered.

6.1 The Drude model

In the original Drude approach, electrons in a metal are considered as free classical particles of mass m and charge $-e$. Let n_e be the electron density. The main idea is that while moving, a typical electron experiences collisions at random times with the effect of updating its momentum. If no external forces are imposed, such as an electric field, these collisions are supposed to enforce the thermal equilibrium, so that the exchange of energy between the electrons and the metal should be described by the Maxwell-Boltzmann distribution at the metal temperature T. Namely, the momentum p_n just after the n^{th} collision is updated randomly according to the probability distribution

$$f(\vec{p}) = \frac{1}{(2\pi m k_B T)^{d/2}} \, e^{-p^2/2mk_BT} \,. \tag{61}$$

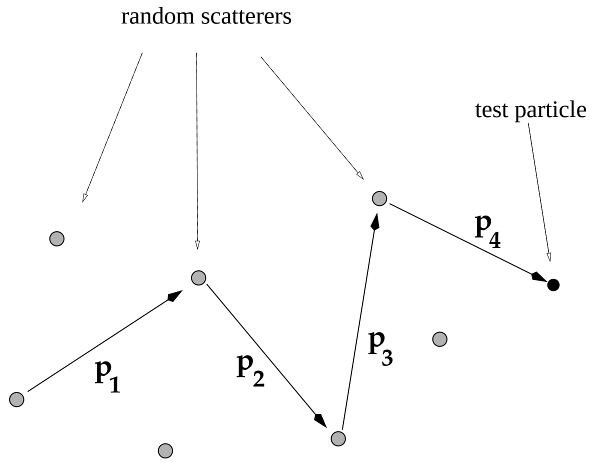

Figure 6: The Drude model for electrons in metals

A more rigorous description of this model can given as follows

1. The collisions times are distributed according to the Poisson law: given a time interval I, the probability that N collisions occur within I is given by $c^N/N!e^{-N}$ where $c = |I|/\tau_{coll}$.

2. The collisions times are labelled by $\cdots < t_1 < 0 \leq t_0 < t_1 < \cdots t_n < t_{n+1} \cdots$. The average value of the time between two consecutive collisions is $\langle t_{n+1} - t_n \rangle = \tau_{coll}$.

3. As a consequence of the Poisson law, the random variables $\tau_n = t_n - t_{n-1}$ are independent identically distributed with common probability density given by the *exponential law*

$$\nu(d\tau) \;=\; e^{-\tau/\tau_{coll}}\,\frac{d\tau}{\tau_{coll}}\,, \qquad\qquad \text{on } [0,\infty)\,.$$

4. Between two collisions times the electron motion is the free motion of a point particle of mass m and charge $-e$, possibly perturbed by external forces, with initial condition $\vec{p}(t_n+0) = \vec{p}_n$ and position $\vec{x}_n = \vec{x}(t_n+0) = \vec{x}(t_n-0)$ (continuous path).

5. The initial conditions $\vec{p}_n$ are independant random variables distributed according to the Maxwell-Boltzmann distribution (61) at temperature T.

It is an elementary calculation to compute the motion when a small constant and uniform electric field $\vec{\mathcal{E}}$ is applied to such an electron. For indeed the momentum increases between two consecutive collisions by the amount $\Delta\vec{p}_n = -\tau_n e\vec{\mathcal{E}}$. The average current is given by $\vec{j}_{el} = -en_e\langle\vec{p}/m\rangle$, so that, since the Maxwell-Boltzmann distribution is isotropic, the average comes entirely from the accelaration due to the electric field to give

$$\vec{j}_{el} \;=\; \sigma\,\vec{\mathcal{E}}\,, \qquad\qquad \sigma \;=\; \frac{n_e e^2}{m}\,\tau_{coll}\,, \qquad\qquad \textbf{(Drude)}$$

In much the same way it is also possible to compute the average energy given by the electrons to the metal through the collision process. This energy is transformed into heat. The energy gained by the metal per electron and per collision is given by the average value of the difference $(p(t_n-0)^2 - p_{n-1}^2)/2m$. Due to the isotropy of the momentum distribution, the average gain is $\tau_{coll}^2 e^2\vec{\mathcal{E}}^2/m$. To get the energy density W gained per unit time, it is enough to multiply this quantity by the electron density and to divise it by the average time between two collisions, giving

$$W \;=\; \sigma\vec{\mathcal{E}}^2 \;=\; \vec{j}_{el}\cdot\vec{\mathcal{E}}\,, \qquad\qquad \textbf{(Joules law)}$$

It is also possible to compute the heat conductivity supposing that, in a metal, the heat is transported by electrons alone, a reasonnable assumption since the conduction electron have an energy close to the Fermi energy so that their velocity is very high. To compute the heat conductivity it is necessary to assume that there is a small temperature gradient and no electric field. Considering a mesoscopic cylinder with axis parallel to $\vec{\nabla}T$ and cross-section $d\vec{\Sigma}$, the heat flux through the middle cross section located at $\vec{r}$ can be computed by remarking that the electrons arriving from the left experienced their last collision at the point $\vec{r} - \tau_{coll}\vec{p}/m$ so that their kinetic energy is given by $d/2k_BT(\vec{r} - \tau_{coll}\vec{p}/m)$. In much the same way the electron coming from the right have the energy $d/2k_BT(\vec{r} + \tau_{coll}\vec{p}/m)$. In the cylinder the number of such electrons arriving per unit time on each side is the product of the density n_e by the volume $d\vec{\Sigma}\cdot\vec{p}/m$ of the cylinder. If the cross section located at $\vec{r}$ is exactly in the middle of the cylinder, half of such electron come from each side giving a net energy flux

$$\vec{j}_U\cdot d\vec{\Sigma} \;=\; -k_B\tau_{coll}\frac{n_e\cdot d}{2}\frac{\vec{p}}{m}\cdot d\vec{\Sigma}\,\left(\vec{\nabla}T(\vec{r})\cdot\vec{p}/m)\right)\,,$$

Averaging over the momentum with respect to the Maxwell-Boltzmann distribution gives

$$\vec{j}_u \;=\; -\lambda\vec{\nabla}T\,, \qquad\qquad \lambda \;=\; \frac{d\cdot\tau_{coll}n_e}{2m}\,k_B^2T\,.$$

It is therefore remarkable that the ratio between the electric and heat conductivities be given by a universal constant, leading to the *Wiedemann-Franz law*

$$\frac{\lambda}{\sigma} = \frac{d}{2}\left(\frac{k_B}{e}\right)^2 T\,. \qquad \textbf{(Wiedemann-Franz law)}$$

The true success of the Drude theory came precisely from the microscopic explanation of this law that had been observed during the 19^{th} century in most metals without explanation. Coming two years after the discovery of the electron by J. J. Thompson, the Drude theory was giving a more solid status to the electron theory. The main criticism, however, is that this theory requires an extra parameter, the collision time τ_{coll}, which is difficult to measure directly. For a long time it was computed through the Drude formula and the measurement of the electric conductivity. For the purpose of the qualitative theory that is presented here, the question of computing τ_{coll} will barely be addressed. But it is only through the method of N-body problem that such a calculation has some chance to be performed.

6.2 The Relaxation Time Approximation

The Drude model can be extended in various ways to take into account that the electronic motion is microscopically not a classical one. In this section the simplest extension will be proposed, namely the so-called *relaxation time approximation* (RTA). Proceeding by analogy, the electron in the aperiodic solid for which the atoms sit on a uniformly discrete set $\mathcal{L}$, with Hull Ω, will be considered as a Drude particle with motion described by the one particle Hamiltonian H given either by an element of $\mathcal{B}$ in the tight-binding approximation, or by a covariant family of selfadjoint operators affiliated to $\mathcal{A}$ in the continuum case. Since these electrons are considered as independent, it is possible to take care of the fermion statistics simply by considering that, at equilibrium, the electron distribution is the Fermi-Dirac density matrix

$$\rho_{\beta,\mu} = \frac{1}{1+e^{\beta(H-\mu)}}\,,$$

where $\beta = 1/k_BT$ and μ is the chemical potential defined by the normalization condition

$$\mathcal{T}_{\mathbb{P}}\left(\frac{1}{1+e^{\beta(H-\mu)}}\right) = n_e\,.$$

In the tight-binding case, the formula is similar provided n_e is replaced by the number of electron per atomic site. The previous formula is meaningful when H is bounded from below. The evolution equation concerns the state of the electron. Since the electron is in the thermal bath created by the atoms (the atomic motion is described by phonons), it cannot be a pure state. Therefore let $\rho(t)$ be the state at time t. Then the motion will be described as follows

1. As in the Drude model, the collisions times are distributed according to the Poisson law with average collision time τ_{coll}.

2. Between two collisions times the evolution of the electron state is given by the Heisenberg equation associated with the one particle Hamiltonian H belonging to the relevant algebra of the Brillouin zone.

3. After each collision the particle state is updated to its equilibrium, namely $\rho(t_n+0) = \rho_{\beta,\mu}$.

In such a simple model, the computation of the electric conductivity is straightforward. Let $\vec{\mathcal{E}}$ be a uniform constant electric field be applied to the system (on a mesoscopic scale $\vec{\mathcal{E}}$ can be considered as uniform indeed). Then the new Hamiltonian is given by $H_{\vec{\mathcal{E}}} = H - e\vec{\mathcal{E}}\cdot\vec{X}$. Unfortunately, the second term has no meaning as an element of the algebra $\mathcal{A}$. However, the equation of motion for the state involves only the commutator with $H_{\vec{\mathcal{E}}}$. If $\mathcal{L}_H$ denote the *Liouville operator* associated with H, namely $\mathcal{L}_H(A) = \imath[H,A]/\hbar$ for $A\in\mathcal{A}$, where $\hbar$ is the Planck constant, then $\mathcal{L}_{H_{\vec{\mathcal{E}}}} = \mathcal{L}_H + (e/\hbar)\vec{\mathcal{E}}\cdot\vec{\nabla}$. Therefore the Liouville operator defines a genuine $*$-derivation on the C^*-algebra leading to a well defined evolution. Thus, by duality, the evolution of the state is given by

$$\rho(t) \;=\; e^{-(t-t_{n-1})\mathcal{L}_{H_{\vec{\mathcal{E}}}}}\,\rho_{\beta,\mu}\,, \qquad\qquad t_{n-1}<t<t_n\,.$$

To compute the electric current, assuming, as before that only electrons contribute, it is enough to consider the current operator $\vec{J} = -(e/\hbar)\vec{\nabla}H$. Its average value will then be given by

$$\vec{j}_{el} \;=\; \int_0^\infty \frac{d\tau}{\tau_{coll}}\, e^{-\tau/\tau_{coll}}\,\mathcal{T}_{\mathbb{P}}\left(\rho(t_{n-1}+\tau)\,\vec{J}\right)\,.$$

Simple algebra gives, in the limit $\vec{\mathcal{E}}\downarrow 0$, the conductivity tensor in the form

$$\vec{j}_{el} \;=\; \sigma\,\vec{\mathcal{E}}\,, \qquad \sigma_{ij} \;=\; \frac{e^2}{\hbar}\,\mathcal{T}_{\mathbb{P}}\left(\partial_j\rho_{\beta,\mu}\,\frac{1}{\hbar/\tau_{coll} - \hbar\mathcal{L}_H}\,\partial_i H\right)\,, \qquad \textbf{(Kubo's formula)} \tag{62}$$

Using the current-current measure (see eq. 55), the Kubo formula becomes

$$\sigma_{ij} \;=\; \frac{e^2}{\hbar}\int_{\mathbb{R}^2} dm(E,E')\,\frac{f_{\beta,\mu}(E)-f_{\beta,\mu}(E')}{E'-E}\,\frac{1}{\hbar/\tau_{coll} - \imath(E'-E)}\,, \tag{63}$$

where $f_{\beta,\mu}$ is the Fermi-Dirac distribution of energy. As the temperature T goes to zero, the collision time τ_{coll} is likely to diverge, so that $\hbar/\tau_{coll}$ decreases to zero, leading to testing more and more of the current-current measure near the diagonal.

If the external electric field is AC with frequency $\tilde{\omega}$, a very similar approach can be performed to compute the linear response cœfficient. It requires, however, some extra technicality, namely the notion of Floquet theory. The treatment can be found in [44] and the result is the following

Lemma 8 *Within the relaxation time approximation the AC (or optical) conductivity is given by the Kubo formula*

$$\sigma_{ij}(\tilde{\omega}) \;=\; \frac{e^2}{\hbar}\,\mathcal{T}_{\mathbb{P}}\left(\partial_j\rho_{\beta,\mu}\,\frac{1}{\hbar/\tau_{coll} - \hbar\mathcal{L}_H - \imath\tilde{\omega}}\,\partial_i H\right)\,, \qquad \textbf{(Kubo's formula)} \tag{64}$$

This approach is actually too simplist. This is because as already noticed in Remark 1, the definition of current should be *mesoscopic*. Here the current was defined microscopically for the electrons. This is possible because electric charges are supported by individual particles. However, this current does not take into account the phonon drag ! This is because the latter cannot be defined microscopically. In addition it is not possible either to define the energy current microscopically for the same reason, because the notion of temperature is meaningless microscopically. This will be investigated in Section 7.2.

6.3 The anomalous Drude formula

Thanks to eq.(63) it is now possible to investigate the scaling behaviour of the conductivity at low temperature. For indeed, as $T \downarrow 0$, collisions with phonons become unlikely, because it is more difficult to produce phonons. Thus the relaxation time τ_{coll} should diverge. There are two types of law for the way τ_{coll} scales with T. On the one hand, the Landau theory of Fermi liquid predicts $\tau_{coll} \sim T^{-2}$, due to electron-electron interactions. Actually, this electron-electron interaction is not due to direct Coulomb forces, as explained in [32]. For indeed, the direct Coulomb potential is much too small to explain the values of the low temperature conductivities in metals. Instead electrons interacts through phonons, the same force that leads to the BCS instability. This contribution is much bigger (at least 100 times bigger). On the other hand the Bloch theory for electron-phonon interaction gives $\tau_{coll} \sim T^{-5}$ [59]. The dominant contribution for metal is provided by the shortest time so that the Bloch term can never be seen. As will be seen below, for materials exhibiting subdiffusive coherent transport, the Bloch law will dominate at low temperature.

Using the Lemma 3 and eq.(63), the behaviour of the DC conductivity as $\tau_{coll} \uparrow \infty$ will be given by the

Proposition 7 ([33]) *Within the relaxation time approximation, as the temperature decreases to zero, the DC conductivity behaves like*

$$\sigma \overset{\tau_{coll}\uparrow\infty}{\sim} \tau_{coll}^{2\beta_F - 1}, \qquad \textbf{(anomalous Drude formula)}$$

if $\beta_F = \overline{\beta}_2^{-}(E_F)$ *is the diffusion exponent computed at the Fermi energy* E_F*.*

This formula was proposed on the basis of theoretical arguments by D. Mayou (see a review in [17]) and later supplemented by Sire (see [159]). The rigorous proof was proposed for the first time in [160]. This formula leads to the following discussion

1. For ballistic transport (at Fermi level), $\beta_F = 1$ and the conductivity behaves like in the Drude formula. In presence of several collision times $\tau_{coll}^{(1)}, \cdots, \tau_{coll}^{(n)}$, the resulting Poisson law correspond to a relaxation time given by the *Mathiessen rule* $1/\tau_{rel} = \sum 1/\tau_{coll}^{(i)}$, so that the shortest time dominates.

2. If states near the Fermi level are strongly localized, $\beta_F = 0$ and the previous formula predicts that $\sigma \sim 1/\tau_{coll}$. Such a behaviour can be called *anti-Drude*. This is not observed in practice, because such a formula indicates that the dominant contribution is given by the longest collision time (inverse Mathiessen rule [17]). But because of the Mott hopping transport (see Section 2.3) there is a spectrum of relaxation times with various weights modifying qualitatively this behaviour.

3. For quantum diffusion near E_F, $\beta_F = 1/2$ leading to a *residual conductivity*. This is actually the case for materials for which the Random Matrix Theory applies. This is also the result of the perturbation theory for the Anderson model in the weak localization regime [11]. In particular, if, in quasicrystals, the numerical calculations by [155] suggest that RMT applies to quasicrystals explaining why most of such material exhibit a residual conductivity at low temperature.

4. For subballistic but overdiffusive coherent transport near the Fermi level, the conductivity increases as the temperature decreases leading to a metallic behaviour. It is probably difficult to discriminate between such a behaviour and a normal metal. No example of such material is known.

5. For subdiffusive coherent transport, on the contrary, the conductivity decreases with the temperature, leading to an insulating state. Then Mathiessen rules are inverted [17]: the longest relaxation time dominates. It gives a chance for the Bloch law to show up in such systems.

6.4 Quantum Diffusion and Residual Conductivity

The case of quantum diffusion deserves a special treatment. The main result discussed in this section is the following

Theorem 11 *Let $H = H^*$ be a Hamiltonian affiliated to $\mathcal{A}$ such that its current-current correlation function is absolutely continuous in a neighbourhood $\mathcal{U}$ of the diagonal point (E_F, E_F) where E_F denotes the Fermi level. In addition it is assumed that this density is continuous in $\mathcal{U}$ and denoted by*

$$dm_{i,j}(E,E') \;=\; \rho^{(2)}_{i,j}(E,E')\,dE\,dE'\,, \qquad\qquad \rho^{(2)}(E,E') \;=\; \sum_{i=1}^{d} \rho^{(2)}_{i,j}(E,E')\,.$$

Then, whenever Δ is contained in a sufficiently small neighbourhood of E_F
(i) The diffusion exponents $\overline{\beta}_2^{\pm}(\Delta)$ are both equal to $1/2$.
(ii) The diffusion cœfficient $D(\Delta) = \lim_{t\uparrow\infty} L_{\Delta,2}(t)^2/t$ is finite and given by

$$D(\Delta) \;=\; \pi \int_{\Delta} dE\,\rho^{(2)}(E,E)\,.$$

(ii) If the relaxation time τ_{coll} tends to zero with the temperature, the diagonal part of the AC conductivity tensor admits a finite non zero limit at $T = 0$ given by

$$\sigma_{i,i}(\tilde\omega)\restriction_{T\downarrow 0} = \frac{e^2}{\hbar}\,\frac{\pi}{\tilde\omega}\int_{E_F-\tilde\omega}^{E_F} dE\,\rho^{(2)}_{i,i}(E,E+\tilde\omega) + O(\tilde\omega) \;\xrightarrow{\tilde\omega\downarrow 0}\; \frac{\pi\,e^2}{\hbar}\,\rho^{(2)}_{i,i}(E_F,E_F)\,.$$

In particular the corresponding material admits a residual conductivity at zero temperature.

Remark 10 The definitions given in this section do not take units into account correctly. Since the trace per unit volume has the unit of L^{-d}, the expression giving $L_{\Delta,q}(t)$ has the unit of $L^{1-d/q}$. To get a length, one possibility is to multiply the expression (54) by the charge carrier density n_e. In much the same way, the definition of the current-current correlation measure (55) gives units $L^{2-d}E^2$ if E is an energy. Consequently the formulæ given in Theorem 11 are not expressed in the correct unit system. □

Sketch of the proof: this result is actually well known from the experts [33]. However it is not clearly published in the literature.
The claim (i) is an elementary consequence of proposition 6.

To prove (ii), the eq. (54) and the DuHamel formula gives

$$L_{\Delta,2}(t)^2 \;=\; \int_{-t}^{+t} \frac{ds}{2t} \int_0^s du \int_0^s du' \, \mathcal{T}_{\mathbb{P}} \left(e^{\imath(u-u')H} \, \vec{\nabla} H \, e^{-\imath(u-u')H} \, \Pi_\Delta \, \vec{\nabla} H \right) ,$$

Using the current-current correlation measure, the integral over u, u' can be performed easily, leading to

$$= \int_{-t}^{+t} \frac{|s|ds}{2t} \int_\Delta dE_0 \int_{-\infty}^{+\infty} d\xi \, \rho^{(2)}(E_0 + \frac{\xi}{s}, E_0 - \frac{\xi}{s}) \left(\frac{\sin \xi}{\xi} \right)^2$$

dividing by t and letting $t \uparrow \infty$ gives the expression for $D(\Delta)$.
To prove (iii) the Kubo formula (63) and its AC version (64) will be used. It should be remarked that, as $T \downarrow 0$, then $\beta = 1/k_B T \uparrow \infty$, while the chemical potential converges to the Fermi energy E_F. In addition, the relaxation time $\tau_{coll} \uparrow \infty$. Using the symmetry $\rho^{(2)}_{i,i}(E, E') = \rho^{(2)}_{i,i}(E', E)$, this gives

$$\sigma_{i,i}(\tilde{\omega}) \restriction_{T \downarrow 0} = \frac{e^2}{\hbar} \int_{E<E_F<E'} dE dE' \, \frac{\rho^{(2)}_{i,i}(E, E')}{E' - E} \left(\frac{1}{0^+ + \imath(E' - E - \tilde{\omega})} - \frac{1}{0^+ + \imath(E - E' - \tilde{\omega})} \right)$$

The classical result

$$\frac{1}{x - \imath 0^+} \;=\; \mathrm{PP}\frac{1}{x} \,+\, \imath\pi\delta(x) \,,$$

where PP denotes the principal part, is the key point in getting the result. □

In [161, 44] one example of a model was shown to satisfy the previous properties. This is the so-called N-orbital Wegner model [162], which, in the limit $N \uparrow \infty$ coincides with the coherent phase approximation (CPA) of the Anderson model [163]. Let $\mathcal{L} = \mathbb{Z}^d$ be the regular cubic d-dimensional lattice in $\mathbb{R}^d$. Let H_0 a periodic Hamiltonain of the form

$$H \;=\; H_0 + V \,, \qquad (H_0 \, \psi)(x) \;=\; \sum_{y \in \mathbb{Z}^d \setminus \{x\}} h(y - x) \, \psi(y) \,, \qquad (V \, \psi)(x) \;=\; V_x \, \psi(x) \,,$$

where h is a sequence of complex numbers such that $\overline{h(x)} = h(-x)$ and $h(x) = O(|x|^{-d-1-\epsilon})$ for some $\epsilon > 0$. Here also the family $(V_x)_{x \in \mathbb{Z}^d}$ is a set of *free variables* with same distributions [164]. Free random variables are a noncommutative extension of independant random variables. A random variable V is a selfadjoint element of a C^*-algebra $\mathcal{A}$ together with a state Φ on $\mathcal{A}$. Its distribution is the probability measure μ_V defined by $\Phi(f(V)) = \int d\mu_V f$ for $f \in \mathcal{C}_0(\mathbb{R})$. A family $(V_x)_{x \in \mathcal{L}}$ of such random (non commuting) variables is *free* if $\Phi(P_1(V_{x(1)}) P_2(V_{x(2)}) \cdots P_m(V_{x(m)})) = 0$ for any set of indices (including repeated ones) such that $x(i) \neq x(i+1)$ and every set of polynomials P_i's such that $\Phi(P_i(V_{x(i)})) = 0$ for all $i \in [1, m]$. In Wegner's model, let the C^*-algebra generated by $f(V_x)$ ($f \in \mathcal{C}_0(\mathbb{R})$) be denoted by $\mathcal{B}_x$. Actually, $\mathcal{B}_x$ is isomorphic to $\mathcal{C}_0(\mathbb{R})$. Then if the V_x's are free, they generate a C^*-algebra $\mathcal{B}$ isomorphic to the infinite free product of the $\mathcal{B}_x$'s. For the Wegner model, $\mathcal{B}$ plays the rôle of the non-commutative Brillouin zone (namely the C^*-algebra of the transversal in the case of a uniform disctrete set). The shift $\mathrm{T}^a(V_x)_{x\in\mathbb{Z}^d} = (V_{x-a})_{x\in\mathbb{Z}^d}$ defines an action of $\mathbb{Z}^d$ by automorphisms. The existence of a common distribution μ to all V_x's defines a unique state Φ_μ on $\mathcal{B}$ such that the V_x's become free random variables [164]. The computation of the average Green function and of the average of a product of two Green functions can be done explicitly to show that such a model satisfies the hypothesis of Theorem 11.

Remark 11 The Anderson model (see eq. (59)) at small coupling λ, and Gaussian potentials, can be obtained as a special case of the N-orbital model. In such an equivalence, $\mathbb{Z}^d$ is decomposed into blocks of size $O(\lambda^{-2})$ and labelled by $x \in \mathbb{Z}^d$. The Hamiltonian H is restricted to each such box and to an energy interval of size $O(\lambda^2)$. Let V_x the resulting matrix for the box labelled by x. Then, as shown by Magnen *et al.* [151], it is an $N \times N$ Gaussian random matrices where $N = O(\lambda^{-2(d-1)})$ is its dimension. Then the effective Hamiltonian obtained from the Anderson model, in an energy interval of size $O(\lambda^2)$ around the Fermi level, has the form of an N-orbital Wegner model. In the limit $\lambda \downarrow 0$ the V_x's becomes free and it is likely that the results mentionned above apply. This phenomena is the reason why Random Matrix Theory can be used so efficiently in the weak localization regime for disordered systems. □

6.5 Application to quasicrystals

The main points concerning transport properties of quasicrystals have been given in Section 2.4. The previous discussion may indeed apply to quasicrystal. In a paper by Roche and Fujiwara [165] such discussion has been carried out quantitatively for realistic quasicrystals. Using the Bloch law for the behaviour of τ_{coll}, this gives

$$\sigma \sim T^{5(1-2\beta_F)} .$$

Using an LMTO calculation of the structure, it has been possible to get an estimate of the diffusion exponent for a decagonal $AlCuCo$, giving

$$\beta_F \approx .375 , \qquad \Rightarrow \qquad \sigma \sim T^{1.25} ,$$

giving a scaling law compatible with the experimental data (see Fig. 3). Thus this a mechanism liable to explain the occurence of the scaling laws.

However, this law is not observed all the way down to $T = 0$ in most material. For indeed there is a residual conductivity (see $AlPdMn$ sample in Fig. 3). Several mechanisms may be responsible for such a residual conductivity. For indeed, the DOS of all quasicrystals exhibits a pseudogap exactly at the Fermi energy. At the energy scale of the order of $1eV$ this pseudo gap is created through the Hume-Rothery mechanism namely due to the coincidence of the first (pseudo)-Brillouin zone and the Fermi sphere, the Fermi see decreases its total energy by creating a pseudogap at the Fermi level [17]. However looking at smaller energy scale of the order of $50meV$ instead, tunneling junction experiments [166] show the existence of a pseudogap of the form predict by Altshuler-Ahoronov [167] (see Fig. 7): due to the residual electron-electron Coulomb interaction, the DOS vanishes exactly at the Fermi level like $d\mathcal{N}/dE(E) \sim |E-E_F|^{1/2}$. Experiments show that the pseudogap is actually partially filled, depending on how clean the sample is. This suggests that, like in semiconductors, the low temperature conductivity is dominated by impurities. At very low level of impurities, however, the states in the pseudogap

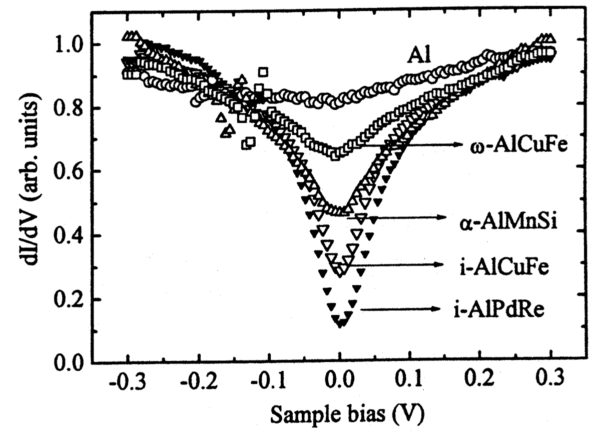

Figure 7: DOS of quasicrystals measured from tunneling experiments [166]

are likely to be localized, which should produce rather a Mott hopping conductivity. But even in very clean samples (with impurity concentration less than 10^{-5} [168]), a residual conductivity is observed.

It seems therefore that another mechanism should be at work. The existence of quantum chaos, seen in the level spacing distribution [155] suggests indeed that the Hamiltonian behaves like a Random Matrix of the Wigner ensemble. Therefore, according to the heuristic discussion in Section 6.3 and the results of Section 6.4, the diffusion exponent should be $\beta_F = 1/2$ at the Fermi level, leading, through the anomalous Drude formula, to a residual conductivity. This way a reasonning has, however, a drawback: as was remarked by Didier Mayou [169], the numerical computation of the level spacing distribution performed by [155] requires the use of a finite sample; it is legitimate to address the question of whether the Wigner-Dyson law is a finite size effect or not then. The answer to Mayou's objection is actually well known and was the purpose of Thouless approach to quantum chaos in mesoscopic systems [170]. In a finite size sample, there are indeed several energy or length scales:

1. At large temperature, namely on large energy scale, the effective Hamiltonian is simply the one-particle one and exhibits quantum diffusion with diffusion exponent β_F. However at low energy scale, the Hamiltonian looks like a random matrix.

2. If the sample size is L, the mean level spacing is given by $\delta E \sim L^{-d}$, since the Hilbert space has dimension $\sim L^d$. The time it takes for the quantum particle to realize that the spectrum is discrete, is the *Heisenberg time* $t_H = \hbar/\delta E \sim L^d$.

3. On the other hand, due to the anomalous quantum diffusion, the time it takes for the wave packet to reach the boundary of the sample, the so-called *Thouless time* t_{Th}, is given by $L \sim t_{Th}^{\beta_F}$, namely $t_{Th} \sim L^{1/\beta_F}$.

4. If the Thouless time is much larger than the Heisenberg time, in the limit of large samples, namely if $\beta_F d > 1$, then the system will never see the anomalous diffusion and the Wigner-Dyson distribution will dominate, leading to a quantum diffusion at low temperature with

$\beta_F = 1/2$ and a residual conductivity. On the other hand if $\beta_F d < 1$, then the wave packet will never reach the boundary of the sample fast enough. Thus quantum diffusion dominates all the way to zero temperature.

Its is remarkable that the borderline between *Quantum Chaos* and *Quantum Diffusion* is exactly given by the identity

$$\beta_F d = 1 \qquad \Leftrightarrow \qquad \textbf{diffusion-chaos Thouless borderline}$$

For indeed, due to Guarneri's inequality (see Theorem 10), the quantum diffusion regime requires that the spectrum near the Fermi level, be *singular continuous* ! This leads to interpret the difference between the $AlPdMn$ and $AlPdRe$ samples shown in Fig. 3 as due to the fact that the effective Hamiltonian in the latter has singular continuous spectrum near the Fermi level. Such a claim should be checked. For instance, a numerical *ab initio* calculation to compute an effective Hamiltonian in both sample, may be the way to check that such singular spectrum may occur.

7 Beyond the Relaxation Time Approximation

As pointed out in the previous section, the RTA already gives a good account for many phenomenons concerning the electronic transports in aperiodic media. However, the RTA, especially in the version presented in Section 6, is too limited in many respects. The most important limitation comes from its inability to explain the Mott transport by variable range hopping. For instance, as shown by the discussion in [35] about the accuracy of the plateaus in the Integer Quantum Hall effect, the Mott transport controls the thickness of the plateaus and explains why the measurement of the Hall resistance is so accurate. Besides, the way the Kubo formula was derived in the last Section 6 neglects the mesoscopic part of the current coming from other contributions, such as the phonon drag. In this section an extension of the RTA is proposed along the line drawn by the Drude model. This extension is still phenomenological in that the dissipation is represented by an external noise with many adjustable parameters. But these parameters are actually computable perturbatively from a model of interacting particles. This last computation will not be presented here. The goal here is to derive a compact formula for the transport cœfficients that includes, in principle, all possible terms that can be observed in any materials. The price to be paid for such a generality is the implict character of the parameters entering in the description of the noise terms. The results presented here are taken from [88, 45, 46].

7.1 The quantum jump models

The Mott argument concerning the hopping conductivity of strongly localized charged particles induced by phonons suggests that instead of considering one type of relaxation time, a better model should include a family of relaxation times associated with various types of jumps. Let the Example 7 be considered again. Here $\mathcal{L}$ will be a uniformly discrete set in $\mathbb{R}^d$. Let H be a selfadjoint operator in the C^*-algebra $\mathcal{B}$ of the transversal. For simplicity H will be chosen in $\mathcal{B}_0$, so that for each $\omega \in X$, its representative $H_\omega = \pi_\omega(H)$ will have only a finite range: there is $R > 0$ such that $\langle x|H_\omega|y\rangle = 0$ for $|x-y| > R$ and all $\omega \in X$. Then $H_{\Lambda,\omega}$ denotes the restriction of H_ω to $\ell^2(\mathcal{L}_\omega \cap \Lambda)$. Let then J a finite set labelling an orthonormal basis of $\ell^2(\mathcal{L}_\omega \cap \Lambda)$ made of eigenvectors of $H_{\Lambda,\omega}$. For each pair (i,j) of elements of J, let $\Gamma_{i\to j}(\omega) \geq 0$ represents the rate of jumps from the state i to the state j. Then the Drude model will be extended as follows

1. Each jump processes occurs at random times $\cdots < t^{(n)}_{i\to j} < t^{(n+1)}_{i\to j} < \cdots$ that are Poisson distributed with an average time $\langle t^{(n+1)}_{i\to j} - t^{(n)}_{i\to j}\rangle = \Gamma_{i\to j}(\omega)^{-1}$.

2. The various jump processes are stochastically independent.

3. At each time $t^{(n)}_{i\to j}$ the collision experienced by the particle results in changing the wave function ψ, representing the instantaneous state of the particle before the collision, into $W_{i\to j}\psi$ (see the definition in Example 7).

4. Between two such collisions, the evolution of the state is provided by $H_{\Lambda,\omega}$.

As discussed in [45] such a model is not physical. For indeed this evolution is not unitary, which is normal, because the jump process being dissipative, cannot preserves the norm of the instantaneous state. But since this model is liable to represents the evolution of an electron (or hole) in the material, the average evolution should conserve the number of particles. Thus the square of the norm of the wave packet $\|\psi\|^2$ should have an average equal to one. This is possible only if the Hamiltonian $H_{\Lambda,\omega}$ is *renormalized* by adding an imaginary part $\imath K_{\Lambda,\omega}$ that will be fixed by demanding that

$$\langle \|\psi(t)\|^2\rangle \;=\; 1\,, \qquad\qquad \forall t\,.$$

It turns out that [45]

Theorem 12 *For the model defined above, the average evolution of the density matrix is given by the Lindbladian (50).*

The next problem is to figure out what happens in the infinite volume limit. This problem was also investigated in [45] in the special case of the variable range hopping (see Example 8). Then the set J is nothing but the set of sites in $\mathcal{L}_\omega \cap \Lambda$. In order to control the infinite volume limit it is necessary to impose some decay to large jumps. Typically such a decay should satisfy

Hypothesis 1 (Transition rates)
Γ.1)- *The transition rate is covariant:* $\Gamma_{x\to y}(\omega) = \Gamma_{x+a\to y+a}(\mathrm{T}^a\omega)$.
Γ.2)- *The map* $(\omega, x) \in \Gamma(X) \mapsto \Gamma_{0\to x}(\omega) \in \mathbb{R}_+$ *is continuous.*
Γ.3)- *The transition rate decays exponentially fast: there are constants* $r > 0$ *and* $C_\Gamma > 0$ *such that uniformly in* ω, $|\Gamma_{x\to y}(\omega)| \leq C_\Gamma \cdot e^{-r|x-y|}$. □

In much the same way, the jump operators should satisfy

Hypothesis 2 (Jump Operators)
W.1)- *The jump operators depend on* ω*. Moreover they are covariant in the following sense:* $T(a)W_{x\to y}(\omega)T(a)^{-1} = W_{x+a\to y+a}(\mathrm{T}^a\omega)$*.*
W.2)- *The maps* $(\omega, x) \in \Gamma(X) \mapsto \|W_{0\to x}(\omega) - \mathbf{1}\| \in \mathbb{R}_+$ *and* $(\omega, x, y, z) \mapsto \langle y|W_{0\to x}(\omega)|z\rangle \in \mathbb{C}$ *are continuous.*
W.3)- *The jump operators are localized exponentially near the jump from site* x *to site* y*, namely there is a constant* $C_W > 0$ *such that uniformly in* ω

$$|\langle y'|W_{x\to y}(\omega)|x'\rangle - (\delta_{x',y'}(1 - \delta_{x,x'}) + \delta_{x,x'}\delta_{y,y'})| \;\leq\; C_W \cdot e^{-r(|x-x'|+|y-y'|)}\,.$$

In particular the $(W_{x\to y}(\omega) - \mathbf{1})$*'s are compact.* □

Note that in condition W.2 above, (ω, x, y, z) belongs to the closed subset of $X \times \mathbb{R}^{d\times 3}$ such that x, y, z all belong to $\mathcal{L}_\omega$. Then under such conditions it was proved in [45] that the instantaneous infinite volume limit evolution exists. However it is not unitary, nor even bounded. Nevertheless the averaged evolution is driven by the following

Proposition 8 *The Lindblad operator defined for* $A \in \mathcal{B}$ *by*

$$\mathfrak{L}_\omega(A) \;=\; \sum_{x,y\in\mathcal{L}_\omega} \Gamma_{x\to y}(\omega) \left\{ W_{x\to y}(\omega)^*\, A_\omega\, W_{x\to y}(\omega) \;-\; \frac{1}{2}\{W_{x\to y}(\omega)^* W_{x\to y}(\omega), A_\omega\} \right\}\,, \qquad (65)$$

defines a completely dissipative bounded map $\mathfrak{L}$ *on* $\mathcal{B}$*. In particular it generates a Markov semigroup on* $\mathcal{B}$

Sketch of the proof: (i) using the Hypothesis 1 and Hypothesis 2, it is elementary to check that $\mathfrak{L}_\omega(A)$ is covariant and strongly continuous in ω as soon a the series is shown to be convergent. Thus only convergence matters.
(ii) To prove convergence, let $K_{x\to y}(\omega) = (W_{x\to y}(\omega) - \mathbf{1})$. It is a compact operator that decays exponentially fast away from (x, y). Then $\mathfrak{L}_\omega$ can be decomposed into a sum of four terms:

$$\mathfrak{L}_\omega(A) \;=\; C_\omega(A) + \frac{1}{2}\{K^{(2)}_\omega, A_\omega\} + \frac{1}{2}([K^*_\omega, A_\omega] + [A_\omega, K_\omega])\,,$$

where $K, K^{(2)}$ are given by

$$K_\omega \;=\; \sum_{x,y\in\mathcal{L}_\omega} \Gamma_{x\to y}(\omega) K_{x\to y}(\omega)\,, \qquad K^{(2)}_\omega \;=\; \sum_{x,y\in\mathcal{L}_\omega} \Gamma_{x\to y}(\omega) K_{x\to y}(\omega)^* K_{x\to y}(\omega)\,,$$

whereas C is defined by

$$C_\omega(A) \;=\; \sum_{x,y\in\mathcal{L}_\omega} \Gamma_{x\to y}(\omega) K_{x\to y}(\omega)^*\, A_\omega\, K_{x\to y}(\omega)\,.$$

(iii) Clearly C defines a completely positive map, which is completely bounded if and only if $C_\omega(\mathbf{1}) = K^{(2)}_\omega$ is bounded. By covariance, it is enough to show that $K^{(2)}$ defines an element of $\mathcal{B}$ to conclude that C defines a completely positive bounded map from $\mathcal{B}$ into itself.

(iv) That K and $K^{(2)}$ defines elements of $\mathcal{B}$ is proved by proving following estimates

$$\|K\|_{L^{1,\infty}}^{\tilde{}} \;=\; \sup_{\omega\in X} \sum_{x'\in\mathcal{L}_\omega} |\langle 0|K_\omega|x'\rangle| \;<\; \infty$$

By the same argument it will then follow that $\|K^*\|_{L^{1,\infty}}^{\tilde{}} < \infty$ showing that $\langle 0|K_\omega|x\rangle$ defines an element of $\mathcal{B}$ since $\|A\|_{\mathcal{B}} \leq \max\{\|A\|_{L^{1,\infty}}^{\tilde{}}, \|A^*\|_{L^{1,\infty}}^{\tilde{}}\}$. A similar estimates holds for $K^{(2)}$. Then, using the Hypothesis 1 and 2 it follows that

$$\|K\|_{L^{1,\infty}}^{\tilde{}} \;\leq\; C_\Gamma \cdot C_W \sum_{x,y,x'\in\mathcal{L}_\omega} e^{-r(|x-y|+|y|+|x-x'|)} \;<\; \infty\,,$$

since $\mathcal{L}_\omega$ is uniformly discrete. □

Example 9 In the case of the Mott hopping conductivity (see Example 8)) the following model is relevant:
(i) Let $\mathcal{L}_0$ be a (periodic) lattice in $\mathbb{R}^d$ (for the case of semiconductors, $d = 3$ and $\mathcal{L}_0$ is the diamond lattice).
(ii) Considering a finite alphabet $\mathfrak{A}$ containing the letter 0 and at least another letter, let Ξ be the infinite product $\mathfrak{A}^{\mathcal{L}_0}$. This is a compact completely discontinuous space on which $\mathbb{Z}^d$ acts by the shift. In the case of Silicon say, 0 denotes the silicon sites,whereas the other letters denote the various impurities.
(iii) The probability $\mathbb{P}_\Xi$ is the product measure on Ξ obtained by assigning to each site the letter 0 with probability $(1-c)$ and the letter $a \in \mathfrak{A}\setminus\{0\}$ the probability $c_a > 0$ such that $\sum_{a\neq 0} c_a = c \ll 1$.
(iv) The set of atomic sites is given by $\mathcal{L}_\xi = \{x\in\mathcal{L}_0; \xi_x \neq 0\}$ if $\xi \in X$.
(v) To each site $x \in \mathcal{L}_\xi$ is assigned a number (the occupation number) $n_x \in \{0,1\}$ that says whether the impurity located at x is ionized or not. Then the transversal X is given by the set of pairs $(\xi, \underline{n})$ where $\underline{n} \in \{0,1\}^{\mathcal{L}_\xi}$ with $\xi \in \Xi$. There is also an obvious action of $\mathbb{Z}^d$. Any $\omega \in X$ has a unique projection ξ on Ξ. So that $\mathcal{L}_\xi$ can actually be denoted by $\mathcal{L}_\omega$ without ambiguity.
(vi) The Hamiltonian describing electrons or holes in the limit of extreme localizations is given by a site potential $V_\omega(x)$ that satisfies the covariance condition. It will be assumed that X is endowed with a probability measure that factorizes through $\mathbb{P}_\Xi$ and makes the $V_\omega(x)$'s independent identically distributed random variables. It is also possible to add hopping terms of the form $\langle x|H_0|y\rangle = t(y-x) = t_0 O(e^{-r|x-y|})$ with t_0 small or r large enough to make this term a small perturbation of the potential term. It is important to remark that the current operator $\vec{J}$ is entirely coming from H_0, since the position operator commutes with the potential term. In particular there is no coherent transport if $H_0 = 0$. Then the transport will come entirely from the jump processes.
(vii) The jump rates will be given by the Mott argument as

$$\Gamma_{x\to y}(\omega) \;=\; \gamma \cdot e^{-(V_\omega(x)-V_\omega(y))/k_B T - |x-y|/\ell}\, n_x(1-n_y)\,,$$

where ℓ is the localization length of the electrons near the impurities and T the temperature. The term $n_x(1-n_y)$ means that x must contain a particle while the site y must be empty, otherwise, by Pauli's principle, the jump is impossible. If an external electric field is added the local potentials $V_\omega(x)$ are modified into $V_\omega(x) \pm e\vec{\mathcal{E}}\cdot\vec{x}$, depending upon the charge carriers are holes or electrons. □

7.2 Kubo's formula

If there is a family of jump processes leading to the construction of a Lindbladian $\mathfrak{L}$ acting on the algebra $\mathcal{B}$ (or on $\mathcal{A}$) of the Brillouin zone, it is possible to compute the transport cœfficients through the following steps. First of all, the Lindbladian represents the evolution over a mesoscopic scale of time, since it is the result of an averaging over the noise. Then the various currents involve a velocity namely a derivative of the position in time. However, this derivative must be considered as mesoscopic. Therefore the velocity that should be taken into account is given by the following operator called *adiabatic current* [171]

$$\vec{J}_{ad} \;=\; \frac{d}{dt}\Phi_t(\vec{X}) \;=\; \frac{\imath}{\hbar}[H,\vec{X}] + \mathfrak{L}(\vec{X})\,. \tag{66}$$

In the previous expression, the index ω has been droped. This current is a sum of two terms. The first one $\vec{J}_{coh} = (\imath/\hbar)[H,\vec{X}]$ is the *coherent* part, the one that is defined microscopically and produces interference effects for the wave packet. The other $\vec{J}_{diss} = \mathfrak{L}(\vec{X})$ is the *dissipative* part and represents the part of the current induced by the jump processes. The phonon drag is contained into this dissipative part. The *electric current* corresponds to $\vec{J}_{el} = e\vec{J}_{ad}$ while the *energy current* will be given by $\vec{J}_U = 1/2\{\vec{J}_{ad}, H\}$.

Since $\vec{X}$ is neither bounded nor covariant it is not obvious that the right hand side defines an element of $\mathcal{B}$ or, at least, a selfadjoint operator affiliated to $\mathcal{B}$ (or to $\mathcal{A}$). This has to be checked. However by translation $\vec{X}$ transform into $\vec{X} + \vec{a}\mathbf{1}$. Since any Lindbladian $\mathfrak{L}$ satisfies $\mathfrak{L}(\mathbf{1}) = 0$, it follows that the lack of covariance of $\vec{X}$ is harmless, so that $\vec{J}_{ad}$ itself is covariant. In general, however, proving that $\vec{J}_{ad}$ is affiliated to the algebra will require more details about the model. In the case investigated in Section 7.1 the result is the following

Proposition 9 *Let $\mathfrak{L}$ be defined by (65) where the transition rates and the jump operators obeys to Hypothesis 1 and 2. Let $H = H^*$ be an element of $\mathcal{B}$ such that $\vec{\nabla} H \in \mathcal{B}$. Then, all components of the adiabatic current $\vec{J}_{ad}$ are selfadjoint elements of $\mathcal{B}$.*

Proof: By inspection. The coherent part is given by $\vec{J}_{coh} = \imath[H,\vec{X}] = \vec{\nabla} H$ and defines an element of $\mathcal{B}$ by hypothesis. The dissipative part must be estimated as in the proof of Proposition 8. The effect of $\vec{X}$ is to add terms of the form $|x-y|, |x|, |y|$ or $|x'|$ in front of the exponentials so that the convergences holds anyway. □

The current that is measured in experiment is obtained as follows: the mesoscopic evolution is provided by the Lindbladian in which some external force has been added, such as a (mesoscopic) gradient of the electric potential or of the temperature, in order to force the system out of equilibrium. Here, only the case of time independent external forces is considered. To first order in these external forces, the Lindbladian is given by $\mathfrak{L}_{eq} + \delta\mathfrak{L}$ in which the Hamiltonian part is included. The evolution equation for the density matrix $\rho = \rho_{\beta,\mu} + \delta\rho$ is then given by

$$\frac{d\delta\rho}{dt} \;=\; (\mathfrak{L}_{eq}^{\dagger} + \delta\mathfrak{L}^{\dagger})(\rho_{\beta,\mu} + \delta\rho)\,,$$

where $\mathfrak{L}^{\dagger}$ is the dual of $\mathfrak{L}$, namely the action on states instead of observables. A stationnary state is establish if, to first order in the external forces,

$$\delta\rho \;=\; -\mathfrak{L}_{eq}^{\dagger\,-1}\delta\mathfrak{L}^{\dagger}(\rho_{\beta,\mu})\,.$$

The thermal average of the current is given by

$$\vec{j}(t) \;=\; \mathcal{T}_{\mathbb{P}}\left(\rho(t)\vec{J}_{ad}\right)\,.$$

The equilibrium current should vanish and this is possible whenever $\mathfrak{L}_{eq}^{\dagger}\rho_{\beta,\mu} = 0$. Thus ρ can be replaced by $\delta\rho$. In addition the adiabatic current itself admits a part depending on the external forces, namely $\delta\vec{J} = \delta\mathfrak{L}(\vec{X})$. Moreover, the measurement is made when a stationary state has been reached, so that

$$\vec{j} \;=\; \mathcal{T}_{\mathbb{P}}\left(\delta\mathfrak{L}(\rho_{\beta,\mu})\,\frac{1}{\mathfrak{L}_{eq}}\,\vec{J}_{ad}\right) + \mathcal{T}_{\mathbb{P}}\left(\rho_{\beta,\mu}\,\delta\mathfrak{L}(\vec{X})\right)\,.$$

Developing, this formula exhibit five different terms as follows

$$\vec{j} \;=\; \mathcal{T}_{\mathbb{P}}\left((\mathcal{L}_{\delta H} + \delta\mathfrak{L}_0)(\rho_{\beta,\mu})\,\frac{1}{\mathcal{L}_H + \mathfrak{L}_0}\,(\vec{\nabla}H + \mathfrak{L}_0(\vec{X}))\right) + \mathcal{T}_{\mathbb{P}}\left(\rho_{\beta,\mu}\,\delta\mathfrak{L}_0(\vec{X})\right) \qquad \textbf{(Kubo)}\,, \tag{67}$$

where H is the one-particle Hamiltonian, $\mathfrak{L}_0$ is the dissipative part of the Lindbladian at equilibrium. while δH and $\delta\mathfrak{L}_0$ are the linear contributions of the external forces to H and $\mathfrak{L}$.

Since this part of the work has not been completely discussed in the literature yet, no additional comment will be made here, leaving details for future research.

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