Course Spring Term 2012: Quantum mechanics: Tight-binding models of solid state systems

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Contents

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1 Formalism, models and problems of quantum mechanics

In this introductory chapter the mathematical axiomatics of quantum mechanics is presented. This is kept very short and thus cannot replace a detailed physics course on the matter. On the other hand, it allows a student of mathematics rather rapidly to get to mathematically interesting and physically relevant questions. After a short overview of these questions and a few results on specific quantum mechanical systems, we then sketch what topics are going to be covered in this course, namely questions linked to the motion of electrons in solid state systems of various nature.

Let us begin by recalling the classical mechanics of a system with N degrees of freedom, typically d per particle in d-dimensional space. Here the state space (also called phase space) is $\mathbb{R}^{2N}$ or, more generally, a $2N$ dimensional symplectic manifold. Each point $(x,p) \in \mathbb{R}^{2N}$ given by the positions x and momenta p of the particles completely determines the system and thus allows to calculate any observable quantity. The time evolution $(x(t),p(t))$ of the classical system is governed by the Hamilton equations

$$\partial_t x \;=\; \partial_p H \;, \qquad \partial_t p \;=\; -\,\partial_x H \;,$$

where $H : \mathbb{R}^{2N} \to \mathbb{R}$ is the Hamiltonian giving the energy of the system. In a typical situation it is of the form $H(x,p) = \frac{p^2}{2} + V(x)$ where V is the potential energy (and, a bit more generally, the kinetic term $\frac{p^2}{2}$ can also invoke various different masses of the particles). The Hamilton equation is an ordinary differential equation associated to a (Hamiltonian) vector field on phase space generated by the Hamiltonian H:

$$\partial_t \begin{pmatrix} x \\ p \end{pmatrix} \;=\; \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} \partial_x H \\ \partial_p H \end{pmatrix} \;.$$

Here is a very rough framework for the quantum mechanics of a single particle.

Axioms of one-particle quantum mechanics: *The state space for a single particle is a complex separable Hilbert space $\mathcal{H}$. The Hamiltonian H of the particle is a self-adjoint operator on $\mathcal{H}$. Then the time-evolution of a state $\psi \in \mathcal{H}$ is given by the Schrödinger equation*

$$\imath\,\hbar\,\partial_t \psi \;=\; H\psi \;, \tag{1.1}$$

where $\hbar = 1.05 \times 10^{-34} Js$ is Planck's constant, in Joule seconds. An observable is a self-adjoint operator A on $\mathcal{H}$. If the particle is in the state ψ, the expected value $\langle A \rangle_\psi \in \mathbb{R}$ of a measurement of A is given by

$$\langle A \rangle_\psi \;=\; \frac{\langle \psi | A | \psi \rangle}{\|\psi\|^2} \;. \tag{1.2}$$

Here $\langle \psi | A | \psi \rangle$ is the Dirac notation for the scalar product in $\mathcal{H}$ of the states ψ and $A\psi$. It will be used throughout. As in most mathematical and theoretical literature the units will from now on be chosen such that $\hbar = 1$ (an exception is, of course, semiclassics). In most interesting situations (see the examples below) the Hilbert space $\mathcal{H}$ is of infinite dimension. Hence the Schrödinger equation actually is a linear ordinary differential equation for infinitely many numbers. This is to be confronted with the situation in classical mechanics where the Hamilton equation only governs finitely many numbers. Now follows a number of important comments of elementary nature.

1.1 Remark The Schrödinger equation (1.1) is strictly speaking not well-defined unless the Hamiltonian H is bounded and therefore everywhere defined. If H is unbounded, one needs ψ to be in the domain $\mathcal{D}(H)$

of H. On the other hand, by Stone's theorem the one-parameter unitary group $e^{-\imath tH}$ is well-defined for the self-adjoint operator H and therefore the time-evolution of every state ψ is given by $\psi(t) = e^{-\imath tH}\psi$, which is formally a solution of the Schrödinger equation with initial condition $\psi(0) = \psi$. Because the evolution is unitary, one has $\|\psi(t)\| = \|\psi\|$. This is crucial for the probabilistic interpretation of quantum mechanics, see below. It also means that if the initial condition is normalized $\|\psi\| = 1$, then so is $\psi(t)$ and therefore one can calculate the expectation value of an observable by $\langle\psi(t)|A|\psi(t)\rangle$ instead of using (1.2). $\diamond$

1.2 Remark Suppose that the observable $A = A^*$ takes a discrete set of values $\{a_n \in \mathbb{R} \,|\, n \in \mathbb{N}\}$. If P_n is the spectral projection of A on a_n, then $A = \sum_{n\geq 1} a_n P_n$. Furthermore, $\sum_{n\geq 1} P_n$. For a normalized ψ, one can then set $p_n = \langle\psi|P_n|\psi\rangle$ and this is a classical probability distribution, namely $\sum_{n\geq 1} p_n = 1$. The expectation (1.2) is then the expectation of classical probability theory w.r.t. this distribution:

$$\langle A\rangle_\psi \;=\; \sum_{n\geq 1} a_n \,\langle\psi|P_n|\psi\rangle \;.$$

This is the probabilistic interpretation of quantum mechanics. In a measurement of A, one observes a_n with probability p_n. If A does not have discrete spectrum, one can work with spectral projections of A on spectral subsets. $\diamond$

1.3 Remark In a given measurement of A, one can only observe one value a_n. It is part of the axiomatics of quantum mechanics, that the measurement process modifies the state of the system from ψ to its projection on the span of P_n:

$$\psi \;\mapsto\; \frac{P_n\psi}{\|P_n\psi\|} \;.$$

There is a lot of literature debating this measurement process, but this will not be a point we focus in these lecture notes. $\diamond$

1.4 Remark It may happen that the initial state of a system is not precisely known, but only that it is in a normalized state ψ_k with probability q_k (then $\sum_{k\geq 1} q_k = 1$). In other words, only a statistical mixture of states is known. Then the expectation of an observable A is naturally given by $\sum_{k\geq 1} q_k\langle A\rangle_{\psi_k}$. For its calculation it is useful to set

$$\rho \;=\; \sum_{k\geq 1} q_k \,|\psi_k\rangle\langle\psi_k| \;. \tag{1.3}$$

This operator ρ is a so-called density matrix, namely it is positive $\rho \geq 0$ and traceclass with normalized trace $\mathrm{Tr}(\rho) = 1$. Now one readily checks that

$$\mathrm{Tr}(\rho\, A) \;=\; \sum_{k\geq 1} q_k\langle A\rangle_{\psi_k} \;.$$

One natural choice for the density matrix is the Boltzmann-Gibbs distribution associated to the inverse temperature $\beta > 0$:

$$\rho \;=\; \frac{1}{Z(\beta)}\, e^{-\beta H} \;, \qquad Z(\beta) \;=\; \mathrm{Tr}(e^{-\beta H}) \;,$$

which is well-defined if $e^{-\beta H}$ is traceclass. Other choices are the Fermi-Dirac and Bose-Einstein distribution at chemical potential μ:

$$\rho \;=\; (1 + e^{\beta(H-\mu)})^{-1} \;, \qquad \rho \;=\; (e^{\beta(H-\mu)} - 1)^{-1} \;.$$

Their trace is not 1 and they may even not be traceclass, but are nevertheless physically reasonable as will be discussed below (and have trace per unit volume equal to the particle density). $\diamond$

1.5 Remark Now suppose that a statistical mixture of initial states $\rho(0)$ in the form of (1.3) is given. According to the Schrödinger equation, the time evolution is then given by

$$\rho(t) \;=\; e^{-\imath tH}\,\rho(0)\,e^{\imath tH}\;.$$

This means that ρ satisfies the Liouville equation

$$\partial_t\rho \;=\; \mathcal{L}_H(\rho)\;,$$

where the Liouvillian is defined using the commutator with H:

$$\mathcal{L}_H(\rho) \;=\; \imath[\rho,H]\;.$$

Due to the cyclicity of the trace, the expectation value of an observable A then evolves as

$$\text{Tr}(\rho(t)A) \;=\; \text{Tr}(\rho(0)A(t))\;,$$

where the time evolution of the observable is given by

$$A(t) \;=\; e^{\imath tH}\,A\,e^{-\imath tH}\;,$$

and thus satisfies the Heisenberg equation

$$\partial_t A \;=\; -\,\mathcal{L}_H(A)\;.$$

When working with the time evolution of density matrices (which includes that of state in $\mathcal{H}$, also called pure states), one speaks of the Schrödinger picture of quantum mechanics, while working with the time evolution of observables (operators) is refered to as the Heisenberg picture or also matrix mechanics. $\diamond$

1.6 Remark In many situations it is useful and elegant to work with a smaller algebra of operators than with with the algebra $\mathcal{B}(\mathcal{H})$ of all bounded operators on the Hilbert space. For example, in a space homogeneous system it is better to work only with space homogeneous operators (details later in the course), or in quantum field theory with the CAR or CCR algebras generated by fermionic or bosonic creation and anhilation operators instead of all operators on Fock space (again details below). Often a good choice turns out to be a C^*-algebra $\mathcal{A}$. The time evolution on such an algebra is then given by an automorphism group and the physical state is a state on the algebra (a positive linear functional). This leads to an algebraic formulation of quantum mechanics. $\diamond$

Next let us provide a few first examples.

1.7 Example In the most simple situation the Hilbert space is finite dimensinal $\mathcal{H}=\mathbb{C}^L$ and the Hamiltonian a $L\times L$ self-adjoint matrix. This desribes, for example, a spin of spin $\frac{L-1}{2}$. If $L=2$ and the spin is thus $\frac{1}{2}$, the most general Hamiltonian is

$$H \;=\; B_0\,\mathbf{1} \;+\; \vec{B}\cdot\vec{\sigma} \tag{1.4}$$

where $B_0\in\mathbb{R}$, $\vec{B}=(B_1,B_2,B_3)^t\in\mathbb{R}^3$ is a magnetic field and $\vec{\sigma}=(\sigma^1,\sigma^2,\sigma^3)^t$ are the Pauli matrices

$$\sigma^1 \;=\; \frac{1}{2}\left(\begin{pmatrix}0&1\\1&0\end{pmatrix}\right)\;,\qquad \sigma^2 \;=\; \frac{1}{2}\left(\begin{pmatrix}0&-\imath\\\imath&0\end{pmatrix}\right)\;,\qquad \sigma^3 \;=\; \frac{1}{2}\left(\begin{pmatrix}1&0\\0&-1\end{pmatrix}\right)\;.$$

$\diamond$

1.8 Example Now let us consider a particle in d-dimensional euclidean space $\mathbb{R}^d$. Then the Hilbert space is $L^2(\mathbb{R}^d)$. A free particle is now described by the Laplacian

$$H_0 \;=\; -\,\Delta \;=\; -\,\sum_{j=1}^{d} \partial_j^2 \;.$$

This is a selfadjoint operator with domain given by the Sobolev space $H^2 = W^{2,2}$. Fourier transform shows that the operator H_0 has only absolutely continuous spectrum on $\mathbb{R}_{\geq 0}$. The harmonic oscillator is then obtained by confining the particle by a quadratic potential:

$$H \;=\; -\,\Delta \;+\; x^2 \;,$$

where x^2 is understood as a multiplication operator. Again the domain is H^2. If $d = 1$ and φ_n denote the Hermite functions, then $H\varphi_n = (2n+1)\varphi_n$ and one can check that the full spectrum is indeed given by $\{2n+1 \,|\, n \in \mathbb{N}\}$. These two operators are obtained by the so-called canonical quantization of the correpsonding classical Hamiltonian. This means that one replaces the classical Hamiltonian function $H(x,p)$ by the Hamiltonian operator $H(X,P)$ where X and P are the position and momentum operator on suitable subspaces of $L^2(\mathbb{R}^d)$ defined by $(X\psi)(x) = x\psi(x)$ and $(P\psi)(x) = \imath(\partial_x\psi)(x)$. For example, the harmonic oscillators simply is $H = P^2 + X^2$. As the two operators P and X don't commute, it may be necessary to symmetrize the Hamiltonian function in order to get a symmetric operator, albeit this is not necessary if $H(x,p) = p^2 + V(x)$. Another example of the latter is the hydrogen atom (more precisely, the electron in a hydrogen atom of an infinitely heavy nucleus, or alternatively the relative motion of the two) described by a Coulomb potential:

$$H \;=\; -\,\Delta \;-\; \frac{e^2\,Z}{|X|} \;,$$

where $-e$ is the charge of the electron and eZ that of the nucleus. This is the quantization of a classical Kepler Hamiltonian. Even though this formula is formally symmetric on $L^2(\mathbb{R}^d)$, one is now confronted with the problem to show that it allows to define a self-adjoint operator. Indeed, it is the sum of two unbounded operators of different sign and therefore no Friedrich's extension is available. So what should the adequate domain be? It turns out that the Kato-Rellich theorem [RS, X.12] is the right tool to prove that it is indeed selfadjoint on H^2 in dimension $d = 3$. This would be wrong for a potential of the form $\frac{1}{|X|^2}$! Proving self-adjointness of the Hamiltonian is often the first unavoidable task of a mathematician when confronted with models with singular potentials or interactions. It should also be pointed out that thee are alternatives to canonical quantization (*e.g.* Weyl and Husumi quantization using pseudodifferential operators) and all can have some unpleasent features in particular situations. Sometimes the best point of view is to accept quantum mechanics as he most most fundamental theory and see classical mechanics as a limiting case (however, it may not be clear what this quantum mechanics actually is in some cases). $\diamond$

1.9 Example Next let us consider the Hilbert space $\mathcal{H} = \ell^2(\mathbb{Z}^d)$ over a discrete physical space. If $|n\rangle \in \mathcal{H}$ denotes the state completely localized at the site $n \in \mathbb{Z}^d$, a typical one-particle Hamiltonian can be of the form

$$H \;=\; \sum_{n\neq m\in\mathbb{Z}^d} t_{n,m}\;|n\rangle\langle m| \;+\; \sum_{n\in\mathbb{Z}^d} v_n\;|n\rangle\langle n| \;. \qquad (1.5)$$

where $t_{n,m} = t^*_{m,n}$ is non-vanishing only for $|n-m| \leq r$ for some positive r and $v_n \in \mathbb{R}$. If the $t_{n,m}$ and v_n are uniformly bounded, then H is a bounded self-adjoint operator, namely there are no technical issues related to self-adjointness. A Hamiltonian such as (1.5) is called a tight-binding Hamiltonian. The points n represent positions of atoms in a solid, at each of which the electron can go into a given orbital state with energy v_n, then there are so-called hopping terms to neighboring sites at distances at most r (which is called the range). In the physics community this is widely excepted to be the most simple model for an electron in a solid capturing most of the interesting low energy physics (in particular, if adds spin as done below). Often one considers only the special case of translation invariant next neighbor hopping (also called discrete Laplacian), namely

$$H \;=\; t \sum_{|n-m|=1} |n\rangle\langle m| \;+\; \sum_{n\in\mathbb{Z}^d} v_n \,|n\rangle\langle n| \;.$$

Then the potential $(v_n)_{n\in\mathbb{Z}}$ can, moreover, be chosen to be periodic (perfect periodic crystal), quasiperiodic (quasicrystal) or random (Anderson model of a disordered alloy). Let us also note that a simple model as (1.5) can be deduced from a Schrödinger operator $H = -\Delta + V$ with a periodic potential as an effective model for the low energy physics (by the so-called Wannier transform). Most of these lectures are concerned with these models. The main mathematical questions concern the spectral theory of these operators and whether and, if so, how a particle spreads out in physical space $\mathbb{Z}^d$. This is linked to conduction properties of the solid if the particles are electrons, and heat conduction if they are phonons. $\diamond$

Next let us couple quantum systems.

Axioms for coupled systems in quantum mechanics: *The state space of two distinguishable particles separately described by Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$ is the Hilbert space tensor product $\mathcal{H}_1 \otimes \mathcal{H}_2$ (recall that this is the closure of the algebraic tensor product by the natural scalar product). The Hamiltonian of the two non-interacting systems is $H_1 \otimes \mathbf{1} + \mathbf{1} \otimes H_2$ where H_1 and H_2 are the one-particle Hamiltonians. An interaction is a supplementary summand to the Hamiltonian which is not of the non-interacting form. This naturally extends to a situation where $N \in \mathbb{N} \cup \{\infty\}$ distinguishable systems are coupled.*

1.10 Example The most basic example of a coupled system is to consider two spins, described by 2×2 matrices H_1 and H_2 of the form (1.4) with Pauli matrices $\vec{\sigma}_1$ and $\vec{\sigma}_2$. Then an interacting Hamiltonian is of the form

$$H \;=\; H_1 \otimes \mathbf{1} \;+\; \mathbf{1} \otimes H_2 \;+\; \vec{\sigma}_1 \cdot J\,\vec{\sigma}_2 \;,$$

where $J = (J_{i,j})_{i,j=1,2,3}$ is a 3×3 matrix and the interaction term is, more explicitly,

$$\vec{\sigma}_1 \cdot J\,\vec{\sigma}_2 \;=\; \sum_{i,j=1}^{3} J_{i,j}\; \sigma_1^i \otimes \sigma_2^j \;.$$

Now let us consider a d-dimensional lattice of spins so that the Hilbert space is $(\mathbb{C}^2)^{\otimes\mathbb{Z}^d} = \ell^2(\mathbb{Z}^d) \otimes \mathbb{C}^2$. Then an interesting Hamiltonian is of the form

$$H \;=\; -\sum_{|n-m|=1} \vec{\sigma}_n \cdot J_{n,m}\,\vec{\sigma}_m \;-\; \vec{B} \cdot \sum_{n\in\mathbb{Z}^d} \vec{\sigma}_n \;, \tag{1.6}$$

where $J_{n,m}$ is an 3×3 matrix and $\vec{B} \in \mathbb{R}^3$ is an external magnetic field. Often one first studies finite volume approximations of these operators and then takes the thermodynamic limit of expectations of physically interesting observables. Most of the time, one choses $\vec{B} = (0,0,1)^t$ and a diagonal matrix $J_{n,m} = \text{diag}(J_1, J_2, J_3)$ to be independent of n and m. In dimension $d = 1$ one speaks of spin chains, while in general such systems are called Heisenberg models. If $J_j = J$, one speaks of the isotropic Heisenberg model, while for $J_1 = J_2 \neq J_3$ of the Heisenberg XXY-model. For the isotropic model and in dimensions $d = 2$ and $d = 3$, for positive J the ground state is always ferromagnetic (alined spins), while for negative J the ground state is antiferromagnetic (Kennedy, Lieb, Shastry 1988) and there is a phase transition at finite temperature (Dyson, Lieb, Simon 1976, Fröhlich, Lieb 1977). In dimension $d = 1$ it is possible to construct all eigenfunctions using the Bethe Ansatz (Babbit, Thomas 1977). Concerning the spectral and scattering theory there is the interesting open problem of asymptotic completeness of the Heisenberg model which is even open in the finite magnon (spin wave) case (except for 2 magnons, see Graf, Schenker 1997 and Yafaev 2000). $\diamond$

1.11 Example Let us expand a bit on the one-particle Hamiltonian (1.5). In many situtions, it is physically necessary (and interesting) to add $L \in \mathbb{N}$ extra degrees of freedom at each lattice site. This could be either the electron spin or another atomic orbital which is relevant for the low energy physics. Thus the Hilbert space becomes $\ell^2(\mathbb{Z}^d) \otimes \mathbb{C}^L$. States are then denoted by $|n, l\rangle$ with $n \in \mathbb{Z}^d$ and $l \in \{1, \ldots, L\}$. Then a Hamiltonian generalizing (1.5) is of the form

$$H \;=\; \sum_{l,k=1}^{L} \sum_{n \neq m \in \mathbb{Z}^d} t_{n,m,l,k}\, |n,l\rangle\langle m,k| \;+\; \sum_{l,k=1}^{L} \sum_{n \in \mathbb{Z}^d} v_{n,l,k}\, |n,l\rangle\langle n,k| \;, \qquad (1.7)$$

where the coefficients are such that $H = H^*$. As already pointed out, this type of models captures many phenomena of solid state physics. One can see (1.6) as a special case of (1.7). $\diamond$

Next let us extend the axioms of quantum mechanics to many particle systems.

Axioms of many-particle quantum mechanics: *Indistinguishable quantum particles come in two classes: fermions (particles with odd half-integer spin) and bosons (particles with even half-integer spin). For N fermions the state space is the antisymmetric tensor product $\mathcal{F}_-^N = \Pi_- \mathcal{H}^{\otimes N}$, while for N bosons it is the symmetric tensor product $\mathcal{F}_+^N = \Pi_+ \mathcal{H}^{\otimes N}$ (recall that the projections Π_- and Π_+ are defined using a sum over the symmetric group with and without the signature respectively, combined with a normalization factor $(N!)^{-1}$). For arbitrarily many particles one works on the full bosonic and fermionic Fock spaces $\mathcal{F}_\pm(\mathcal{H}) = \oplus_{N \geq 0} \mathcal{F}_\pm^N$ where $\mathcal{F}_\pm^0 = \mathbb{C}$ is the span of the vacuum state. Hamiltonian, Schrödinger equation and expectation values are then defined as in the single particle case.*

One important part of these axioms is the Pauli principle which states that there cannot be two fermions in the same state ψ. An identity expressing this fact is

$$\Pi_- \; \psi \otimes \psi \otimes \psi_3 \otimes \ldots \otimes \psi_N \;=\; 0 \;.$$

There is also a full unsymmetrized Fock space $\mathcal{F}(\mathcal{H}) = \oplus_{N \geq 0} \mathcal{H}^{\otimes N}$, but this does not play such an important role. On $\mathcal{H}^{\otimes N}$, one defines annihilation and creation operators associated to $\psi \in \mathcal{H}$ by

$$\begin{aligned} a(\psi)\; \psi_1 \otimes \ldots \otimes \psi_N &= N^{\frac{1}{2}}\; \langle \psi | \psi_1 \rangle\; \psi_2 \otimes \ldots \otimes \psi_N \\ a^*(\psi)\; \psi_1 \otimes \ldots \otimes \psi_N &= (N+1)^{\frac{1}{2}}\; \psi \otimes \psi_1 \otimes \ldots \otimes \psi_N \;, \end{aligned}$$

which are then extended by linearity to all $\mathcal{F}(\mathcal{H})$. Combining with the projections $\Pi_\pm$ this defines corresponding operators on $\mathcal{F}_\pm(\mathcal{H})$ by

$$a_\pm(\psi) \;=\; \Pi_\pm\, a(\psi) \;, \qquad a_\pm^*(\psi) \;=\; \Pi_\pm\, a^*(\psi) \;.$$

Now the CAR algebra is the C^*-algebra generated by $\mathbf{1}$ and $a_-(\psi)$ with ψ running through $\mathcal{H}$, and similarly the CCR algebra the algebra generated by $\mathbf{1}$ and $a_+(\psi)$ with $\psi \in \mathcal{H}$. Then one can check the following commutation relations

$$[a_\pm(\psi), a_\pm(\phi)]_\mp \;=\; 0 \;, \qquad [a_\pm(\psi), a_\pm^*(\phi)]_\mp \;=\; \langle \psi | \phi \rangle\; \mathbf{1} \;,$$

where $[A, B]_\pm = AB \mp BA$ denote commutator and anti-commutator. Note that the Pauli principle implies that $a_-^*(\psi) a_-^*(\psi) = 0$. Most of the time, the index $\pm$ on $a_\pm(\psi)$ is dropped in the literature. More on the CAR and CCR algebras can be found in the classic book [BR].

1.12 Remark The most simple many body system is one of non-interacting particles. As the particles are indistinguishable, this means that each particle is described by the same one-particle Hamiltonian H on $\mathcal{H}$, which for simplicity is assumed to be bounded. Then the many body Hamiltonian is given by the second quantization $d\Gamma(H)$ of H acting on $\mathcal{F}_\pm(\mathcal{H})$:

$$d\Gamma(H) \;=\; 0 \oplus_{N\geq 1} \sum_{n=1}^{N} \mathbf{1}\otimes\cdots\otimes H\otimes\cdots\otimes\mathbf{1}\;,$$

where H stands in the nth component and again there is a closure involved on the r.h.s.. If one calculates the time-evolution, it is given by

$$e^{\imath d\Gamma(H)t} \;=\; \Gamma(e^{\imath Ht})\;, \tag{1.8}$$

where

$$\Gamma(U) \;=\; \mathbf{1} \oplus_{N\geq 1} U\otimes\cdots\otimes U\;.$$

It is a good exercise to check that this definition indeed leads to the identity (1.8). The passage from a one-particle operator H to the many particle operator $d\Gamma(H)$ is often called *second quantization*. $\diamond$

1.13 Remark The next aim is to briefly explain where the Fermi-Dirac distribution at inverse temperature β and chemical potential μ comes from (this will be relevant later on in the course). Let us consider a bounded one-particle Hamiltonian H on $\mathcal{H}$ and suppose that $e^{-\beta(H-\mu)}$ is a traceclass operator on $\mathcal{H}$. This typically only holds in finite volume which in the case of tight-binding models even means that the Hilbert space $\mathcal{H}$ is finite dimensional. Then the identity (exercise)

$$\mathrm{Tr}(e^{-\beta d\Gamma(H-\mu)}) \;=\; \exp\big(\mathrm{Tr}(e^{-\beta(H-\mu)})\big)\;,$$

shows that also $e^{-\beta d\Gamma(H-\mu)}$ is a traceclass operator on $\mathcal{F}_\pm(\mathcal{H})$. Next let us consider the Boltzmann-Gibbs state $\omega_{\beta,\mu}$ on $\mathcal{F}_-(\mathcal{H})$, namely, given an operator A on $\mathcal{F}_-(\mathcal{H})$,

$$\omega_{\beta,\mu}(A) \;=\; \frac{1}{Z_{\beta,\mu}}\,\mathrm{Tr}(e^{-\beta d\Gamma(H-\mu)}A)\;, \qquad Z_{\beta,\mu} \;=\; \mathrm{Tr}(e^{-\beta d\Gamma(H-\mu)})\;.$$

Using the identity

$$e^{-\beta d\Gamma(H-\mu)}a^*(\psi) \;=\; a^*(e^{-\beta(H-\mu)}\psi)\,e^{-\beta d\Gamma(H-\mu)}\;,$$

a short calculation (exercise) shows that

$$\omega_{\beta,\mu}(a^*(\psi)a(\phi)) \;=\; \langle\psi|(\mathbf{1}+e^{\beta(H-\mu)})^{-1}|\phi\rangle\;. \tag{1.9}$$

This shows why the Fermi-Dirac distribution

$$f_{\beta,\mu}(H) \;=\; (\mathbf{1}+e^{\beta(H-\mu)})^{-1}\;,$$

plays an important role when calculating thermodynamic expectation values in systems of independent fermions. If one takes the zero temperature limit $\beta\to\infty$, then the Fermi-Dirac distribution becomes the Fermi projection $P_\mu = \chi(H\leq\mu)$, which is just the spectral projection of H on all states below the chemical potential μ, also called the Fermi level. Finally let us note that also the expectation w.r.t. $\omega_{\beta,\mu}$ of higher polynomials in annihilation and creation operators can readily be calculated. It turns out that they can all be epressed in terms of the so-called two point functions of the type (1.9). This is also called Wick's theorem. States on the CAR algebra which have this property are called quasifree. For more details also on the calculation above, see again [BR]. $\diamond$

1.14 Example As a first example let us calculate the the second quantization of (1.5), hence acting on $\mathcal{F}_\pm(\ell^2(\mathbb{Z}^d))$. For that purpose, it is convenient to use the notation $a(n) = a(|n\rangle)$ for the annihilation operator of a particle at site $n \in \mathbb{Z}^d$. Then, if H is given by (1.5),

$$d\Gamma(H) \;=\; \sum_{n\neq m\in\mathbb{Z}^d} t_{n,m}\, a^*(n)\, a(m) \;+\; \sum_{n\in\mathbb{Z}^d} v_n\, a^*(n)\, a(n)\;. \tag{1.10}$$

This operator is quadratic in the annihilation and creation operators. Interactions terms between particles are not quadratic and typically of fourth order (because third order does not conserve the particle number). As an example, let us present the Hubbard model. Here one also includes a spin degree of freedom, so that the one-particle Hilbert space is $\mathcal{H} = \ell^2(\mathbb{Z}^d) \otimes \mathbb{C}^2$. Then the Hubbard Hamiltonian on $\mathcal{F}_-(\mathcal{H})$ with an on-site interaction U is

$$H \;=\; t\sum_{l=1,2}\;\sum_{|n-m|=1} a^*(n,l)\, a(m,l) \;+\; U\sum_{n\in\mathbb{Z}^d} a^*(n,1)\, a(n,1) a^*(n,2)\, a(n,2)\;.$$

Little is known mathematically about such models. In dimension $d = 1$, there is again a Bethe Ansatz for the solutions (Lieb, Wu 1968 and 2002). In the limit $U \to \infty$ an effective description is given in terms of a Heisenberg model (in all dimensions). This insight combined with second order perturbation theory allows to analyze the magnetic properties of the model (Lieb 1989). There are many questions which are of interest in connection with high-temperature superconductors (see the review of Lieb 1995) $\diamond$

This concludes the list of somewhat detailed examples. All except for Example 1.8 are models in discrete physical space. In most examples with continuous physical space one has to deal with partial differential operators and therefore unbounded Hamiltonians for which self-adjointness has to be checked. In this course, we will focus not focus on such models, but rather on the somewhat simpler discrete ones. As a word of justification be said that they do capture a lot of the physical phenomena, in particular, when it comes to solid state physics. In particular, we will focus on the following:

- Structural results on discrete Schrödinger operators of the type (1.5)
- Discrete operators (1.5) with random potential (Anderson model of localization)
- Transport theory for the above models (RAGE theorem, Guarneri bounds, Kubo formula)
- Magnetic operators of type (1.5) (Quantum Hall effect, boundary currents)
- Topological insulators

Of course, models with continuous physical space have their mathematical charm as well and there are lots of rigorous results on one-particle, few particle and many particle systems. I am unable to give an extensive list, but here are some fields that have drawn quite some interest of mathematical physicists:

- Semiclassical limits ($\hbar \downarrow 0$ or energy $\to \infty$) for a wide class of models. Here the interplay with classical mechanics is particularly interesting. Quantum chaos is a closely related field.
- Molecules composed of K nuclei and N electrons interacting by Coulomb potentials (generalizing the hydrogen atom). This relevant for quantum chemistry. Here one of the question which has drawn a lot of mathematical interest is *stability of matter*, namely if groundstate energy can be bounded below by $-C(N + K)$ for some constant C. A description of the state of the art is the recent book by Lieb and Seiringer (2009).

- Derivation of approximate theories for molecules (density functional theory, Born-Oppenheimer approximation, Thomas-Fermi and Hartree-Fock theory).
- Asymptotic completeness of scattering on molecules (in particular, absense of singular continuous spectrum).
- Molecules interacting with a quantized electromagnetic field (light, QED) with ultraviolet cut-off (again stability of matter, Fermi's golden rule)
- Bose-Einstein condensation
- Derivation of limiting theory in scaling limits (effective few particle theories for many body physics, typically non-linear, examples are the Gross-Pitaevski equation for Bose-Einstein condensates and the BCS and Landau-Ginzburg equation for superconductivity). Study of these equation, such as non-linear Schrödinger equation (solitons).
- Fermi-liquid theory and Luttinger liquids
- Rigorous construction of quantum chromodynamics (QCD). This is one of the Clay foundations millennium problems (worth 1 million dollars!).
- Quantization of classical theories, in particular, construction of a theory of quantum gravity.

2 Framework for independent particles in homogeneous media

The aim is to model independent particles submitted to an enviroment that is homogeneous in space. This enviroment can, for example, be given by a periodic, quasiperiodic or random potential and as such describe perfect metals, quasicrystals or alloys and doped semiconductors. The independent particles could be either electrons or holes (both fermionic quasiparticles) or phonons (bosonic quasiparticles). We restrict ourselves to tight-binding Hamiltonians, but allow the particles to have $L \in \mathbb{N}$ internal degrees of freedom such as a spin or a sublattice variable. Therefore the one-particle Hilbert space will be throughout $\mathcal{H} = \ell^2(\mathbb{Z}^d) \otimes \mathbb{C}^L$. The main focus will be on dimensions $d = 2$ and $d = 3$.

2.1 Magnetic translations

In order to describe space homogenuity, it will be necessary to shift the system in space so that local environments can be compared. Therefore we need a strongly continuous unitary representation $a \in \mathbb{Z}^d \mapsto U_a \in \mathcal{B}(\mathcal{H})$ of the translation group $\mathbb{Z}^d$ on $\mathcal{H}$, namely each U_a is unitary and one has $U_a U_b = U_{a+b}$ for all $a, b \in \mathbb{Z}^d$. If there is no magnetic field, such a representation is simply given by the shifts

$$(U_a\psi)_n \;=\; \psi_{n-a}$$

If, however, there is a constant magnetic field described by an antisymmetric real matrix $\mathbf{B} = (B_{i,j})_{i,j=1...d}$, namely $B_{i,j} = -B_{j,i}$, one has to use the magnetic translations

$$(U_a\psi)_n \;=\; e^{\frac{\imath}{2} a\cdot \mathbf{B} n}\, \psi_{n-a}\;. \tag{2.1}$$

Here the notation $a \cdot \mathbf{B}n = \sum_{i,j} a_i B_{i,j} n_j$ is used. For dimension $d = 2$ and $d = 3$, the magnetic field is (as usual) parametrized as follows

$$\mathbf{B} \;=\; \begin{pmatrix} 0 & B_3 \\ -B_3 & 0 \end{pmatrix}\,, \qquad \mathbf{B} \;=\; \begin{pmatrix} 0 & B_3 & -B_2 \\ -B_3 & 0 & B_1 \\ B_2 & -B_1 & 0 \end{pmatrix}\;. \tag{2.2}$$

In dimension $d = 2$, the magnetic flux trough a unit cell is B_3, and, for $d = 3$, it is B_1, B_2 and B_3 in the directions 1, 2 and 3 respectively. As the magnetic field $\mathbf{B}$ only enters through the exponential factor in the magnetic translations, it is parametrized by values in the torus $\Xi = [-\pi, \pi)^{\frac{1}{2}d(d-1)}$. The magnetic translation are now only a projective unitary representation of the *translation group* $\mathbb{Z}^d$ on $\mathcal{H}$. Indeed, U_a and U_b do not commute (which would follow from $U_a U_b = U_{a+b}$), but one rather has

$$U_a\,U_b \;=\; e^{\imath\,a\cdot\mathbf{B}b}\,U_b\,U_a\;, \tag{2.3}$$

which follows from (easy exercise)

$$U_a\,U_b \;=\; e^{\frac{\imath}{2}\,a\cdot\mathbf{B}b}\,U_{a+b}\;. \tag{2.4}$$

The latter also implies that one still has $(U_a)^{-1} = U_{-a}$. Physically (2.3) means that during a walk $U_{-a}U_{-b}U_aU_b$ around a rectangle of side lengths b and a a particle collects a phase factor $e^{\imath\,a\cdot\mathbf{B}b}$.

There is another projective unitary representation $a \in \mathbb{Z}^d \mapsto \widetilde{U}_a$ obtained by a sign change

$$(\widetilde{U}_a\psi)_n \;=\; e^{-\frac{\imath}{2}a\cdot\mathbf{B}n}\psi_{n-a}\;. \tag{2.5}$$

One now checks that for all $a, b \in \mathbb{Z}^d$

$$U_a\,\widetilde{U}_b\,U_{-a} \;=\; \widetilde{U}_b\;, \tag{2.6}$$

namely the $\widetilde{U}_b$ are invariant under the magnetic translations.[1]

2.2 Homogeneous Hamiltonians

Homogeneous Hamiltonians will be families $(H_\omega)_{\omega\in\Omega}$ of operators on $\mathcal{H}$ indexed by a parameter $\omega \in \Omega$ which satisfy certain properties. The set Ω is called the set of crystalline configurations. It is supposed to be compact. On it is given a group action T of the group $\mathbb{Z}^d$, namely T_a is a homeomorphism of Ω for each $a \in \mathbb{Z}^d$ and $T_aT_b = T_{a+b}$. This action is naturally interpreted as the translation of the crystalline configuration. As further data will typically be given an invariant and ergodic probability measure $\mathbb{P}$ on the compact dynamical system $(\Omega, T, \mathbb{Z}^d)$. Invariance means by definition that for any Borel set $A \subset \Omega$ one has $\mathbb{P}(T_aA) = \mathbb{P}(A)$ for all $a \in \mathbb{Z}^d$, while ergodicity means that for any T-invariant set (satisfying $A = T_aA$ for all $a \in \mathbb{Z}^d$), one has either $\mathbb{P}(A) = 0$ or $\mathbb{P}(A) = 1$. Expectation values w.r.t. $\mathbb{P}$ are denoted by $\mathbf{E}_\mathbb{P}$.

2.1 Definition *Let $(\Omega, T, \mathbb{Z}^d, \mathbb{P})$ be a compact space furnished with a group action T of $\mathbb{Z}^d$ as well as a T-invariant and ergodic probability measure $\mathbb{P}$. A family $(H_\omega)_{\omega\in\Omega}$ of self-adjoint operators on $\mathcal{H} = \ell^2(\mathbb{Z}^d) \otimes \mathbb{C}^L$ is called homogeneous at magnetic field $\mathbf{B}$ if and only if $\omega \mapsto H_\omega$ is strongly continuous and the covariance relation*

$$U_a\,H_\omega\,U_a^{-1} \;=\; H_{T_a\omega}\;, \qquad a \in \mathbb{Z}^d\;, \tag{2.7}$$

holds.

Many other terms are frequently used instead of homogeneous operators, *e.g.* stochastic operators, ergodic operators, covariant operators, metric operators.

Next follow the main examples considered in this course. The Hamiltonian is the sum of a (magnetic) translation invariant kinetic operator H_0 and a potential energy V_ω of the form

$$H_\omega \;=\; H_0 + V_\omega\;, \qquad H_0 \;=\; \sum_{m\in\mathbb{Z}^d} T_m\,\widetilde{U}_m\;, \qquad V_\omega \;=\; \sum_{n\in\mathbb{Z}^d} |n\rangle\;V_{\omega,n}\;\langle n|\;. \tag{2.8}$$

[1]There is an analogous relation for generators of magnetic translations in the continuum.

Here the sum over m has only finitely many terms (or at least the coefficients are summable) and the coefficient matrices $T_m \in \mathrm{Mat}(L, \mathbb{C})$ satisfy $(T_m)^* = T_{-m}$. Furthermore, the matrices $V_{\omega,n} \in \mathrm{Mat}(L, \mathbb{C})$ depend continuously on ω and lie in the set $\mathrm{Her}(L, \mathbb{C})$of self-adjoint (hermitian) matrices. If $L = 1$ this simply means that $V_{\omega,n}$ is real. We also used the bra-ket notations to denote by $|n\rangle$ the partial isometry in $\mathcal{H}$ onto L-dimensional state space supported by $n \in \mathbb{Z}^d$. Then, if the $V_{\omega,n}$ are drawn from a compact set $K \subset \mathrm{Her}(L, \mathbb{C})$, the set Ω is simply the Tychonov space $K^{\times \mathbb{Z}^d}$ furnished with the shift action T. As the kinetic part H_0 is translation invariant by (2.6), the covariance relation (2.7) is guaranteed because $U_a V_\omega U_a^{-1} = V_{T_a \omega}$. Up to now there is little information on the model. Actually the most important data is now that of the invariant and ergodic measure $\mathbb{P}$. Here are the main examples of operators on the form (2.8).

2.2 Example The most simple example is a translation invariant operator. Here $V_{\omega,n} = V$ is a constant matrix and therefore $\mathbb{P}$ is a Dirac measure on a single point $\omega = (V)_{n \in \mathbb{Z}^d}$. The next more simple class is given by periodic operators with periods p_j, $j = 1, \ldots, d$. Those are characterized by the $P = p_1 \cdots p_d$ potentials V_n, where $n_j = 1, \ldots, p_j$ and $j = 1, \ldots, d$. Then a point $\omega_0 \in \Omega$ is given by periodizing this potential. If this ω_0 is translated by less than the periods one obtains different points in $\Omega = K^{\times \mathbb{Z}^d}$ (unless the periods are not chosen minimal). Alternatively, one can consider Ω to consist only of these P points. Now the only invariant measure on these P points is the equidistribution, namely

$$\mathbb{P} \;=\; \frac{1}{P} \sum_{1 \leq n_j \leq p_j} \delta_{T_n \omega_0} \;.$$

The spectral analysis of these operators is carried out in Section 2.5. $\diamond$

2.3 Example Let $\mathbb{T}^d = \mathbb{R}^d / (2\pi\mathbb{Z})^d \cong (-\pi, \pi]^d$ be the d dimensional torus and $V : \mathbb{T}^d \to \mathrm{Her}(L, \mathbb{C})$ be a continuous function. Given matrix $\alpha \in \mathrm{Mat}(d, \mathbb{R})$ one can then consider

$$V_{\omega,n} \;=\; V(\alpha n + \omega) \;, \qquad \omega \in \mathbb{T}^d \;. \tag{2.9}$$

Let us restrict to the case where $\alpha = \mathrm{diag}(\alpha_1, \ldots, \alpha_d)$ is a diagonal matrix. If $\alpha_1, \ldots, \alpha_d$ are rational multiples of 2π, then the potential is periodic and this is a special case of the example above. If, on the other hand, the $\alpha_1, \ldots, \alpha_d$ are irrational multiples of 2π, the potential is not periodic. If, moreover, the $\alpha_1, \ldots, \alpha_d$ and 2π are not rationally related (which is, in particular, given in dimension $d = 1$), then the sequences $(V_{\omega,n})_{n \in \mathbb{Z}^d}$ are different for different values of ω (exercise). As above can then identify $\mathbb{T}^d$ with a subset of $\Omega = K^{\times \mathbb{Z}^d}$ where $K \subset \mathrm{Her}(L, \mathbb{C})$, by setting $\omega = (V_{\omega,n})_{n \in \mathbb{Z}^d}$. Now the natural shift action T on $\Omega = K^{\times \mathbb{Z}^d}$ corresponds to the irrational rotation on the torus $\mathbb{T}^d$:

$$T_a \omega \;=\; \omega + \alpha a \;, \qquad \omega \in \mathbb{T}^d \;.$$

The unique invariant measure $\mathbb{P}$ on $\Omega \cong \mathbb{T}^d$ is the normalized Haar measure $\mathbb{T}^d$ (because the entries of α and 2π are irrational and not rationally related). It can be shown that this measure is ergodic (exercise, or see Katok-Hasselblatt, p. 146). Potentials of the type (2.9) are called quasiperiodic (there are also more general quasiperiodic potentials). The most prominent and most studied examples are in dimension $d = 1$ and with real analytic functions V with $L = 1$. In particular, the prototypical model is given by

$$V_{\omega,n} \;=\; 2\,\lambda\,\cos(\alpha n + \omega) \;.$$

It $H_0 = U_1 + U_{-1}$ with $\mathbf{B} = 0$ is the discrete Laplacian, then $H_\omega = U_1 + U_{-1} + V_\omega$ is called the Harper model. It has a large number of interesting properties, a lot of which are mathematically well-understood [Jit], but many important questions in the so-called critital case $\lambda = 1$ remain open.

When modelling potentials obtained by substitution rules (such as the Fibonacci sequence) one also uses discontinuous functions V in (2.9). Then there is standard construction of the so-called hull leading to a concrete form for Ω and $\mathbb{P}$ as well. $\diamond$

2.4 Example This example concerns random operators in the more restricted meaning, namely the $V_{\omega,n}$ are supposed to be independent and identically distributed random variables. If $\mathbf{p}$ is the probability distribution of each $V_{\omega,n}$ (for fixed n), then $\mathbb{P} = \mathbf{p}^{\times\mathbb{Z}^d}$. By a standard argument reproduced in Proposition 2.5, this measure is ergodic w.r.t. to the shift action T. In the case where H_0 is the disrete Laplacian at vanishing magnetic field $\mathbf{B} = 0$ and $L = 1$, one speaks of the (discrete) Anderson model of localization in dimension d. If $d = 2$ and $L = 1$, but $\mathbf{B} \neq 0$, one deals with the disordered Harper model. $\diamond$

2.5 Proposition *Let* $\mathbf{p}$ *be a probability on a compact space* K*, then* $\mathbb{P} = \mathbf{p}^{\times\mathbb{Z}^d}$ *is invariant and ergodic on* $\Omega = K^{\times\mathbb{Z}^d}$ *w.r.t. the shift action of* $\mathbb{Z}^d$*.*

Proof. Let $A \subset \Omega$ be a T-invariant Borel set, that is $A = T_a A$ for all $a \in \mathbb{Z}^d$. Let $\epsilon > 0$. By the definition of the product measure there exist a finite number $C_1, \ldots, C_N$ of disjoint cylinders such that

$$\mathbb{P}(A\Delta C) < \epsilon\,, \qquad C = \bigcup_{n=1}^{N} C_n\,.$$

Choose a sufficiently large such that $T_a C$ and C depend on different entries so that

$$\mathbb{P}(T_a C \cap C) \;=\; \mathbb{P}(T_a C)\,\mathbb{P}(C) \;=\; \mathbb{P}(C)^2\,,$$

where in the second inequality the invariance of $\mathbb{P}$ was used. Moreover,

$$\mathbb{P}(T_a C\Delta A) \;=\; \mathbb{P}(T_a C\Delta T_a A) \;=\; \mathbb{P}(T_a(C\Delta A)) \;=\; \mathbb{P}(C\Delta A) \;<\; \epsilon\,.$$

As $A\Delta(C\cap T_a C) \subset (A\Delta C) \cup (A\Delta T_a C)$, one thus has

$$\mathbb{P}(A\Delta(C\cap T_a C)) \;\leq\; \mathbb{P}(A\Delta C) + \mathbb{P}(A\Delta T_a C) \;<\; 2\,\epsilon\,,$$

so that

$$|\mathbb{P}(A) - \mathbb{P}(C\cap T_a C)| \;<\; 2\,\epsilon\,.$$

Combined with the above,

$$\begin{aligned}
|\mathbb{P}(A) - \mathbb{P}(A)^2| \;&\leq\; |\mathbb{P}(A) - \mathbb{P}(C\cap T_a C)| + \big|\mathbb{P}(A)^2 - \mathbb{P}(C\cap T_a C)\big| \\
&<\; 2\,\epsilon \;+\; \big|\mathbb{P}(A)^2 - \mathbb{P}(C)^2\big| \;=\; 2\,\epsilon \;+\; |\mathbb{P}(A) - \mathbb{P}(C)|\;(\mathbb{P}(A) + \mathbb{P}(C)) \\
&<\; 2\,\epsilon \;+\; \epsilon\,(\mathbb{P}(A) + \mathbb{P}(C)) \;\leq\; 4\,\epsilon\,.
\end{aligned}$$

As ϵ is arbitrary, it follows that $\mathbb{P}(A) = \mathbb{P}(A)^2$ and therefore $\mathbb{P}(A) \in \{0,1\}$. $\Box$

2.3 The almost sure spectrum

Let $\sigma(H)$ denote the spectrum of an operator H.

2.6 Theorem [Pastur 1974] *Let* $(H_\omega)_{\omega\in\Omega}$ *be a homogeneous family of Hamiltonian with ergodic probability* $\mathbb{P}$*. Then there is a closed set* $\Sigma \subset \mathbb{R}$ *such that* $\mathbb{P}$*-almost surely* $\sigma(H_\omega) = \Sigma$*.*

Proof. For any given interval $I \subset \mathbb{R}$, let us consider the following function

$$\omega \in \Omega \;\mapsto\; f_I(\omega) \;=\; \mathrm{Tr}(\chi_I(H_\omega)) \;.$$

The first claim is that this is function is measurable. Indeed, H_ω is strongly continuous and the characteristic function χ_I is measurable, thus $\omega \mapsto \chi_I(H_\omega)$ is measurable (exercise: weak, strong and norm measurability are equivalent as $\mathcal{H}$ is separable) which implies that f_I is measurable. Now by the covariance relation (2.7) and Lemma 2.8 below implies that

$$\chi_I(H_{T_a\omega}) \;=\; U_a\, \chi_I(H_\omega)\, U_a^* \;.$$

Therefore it follows from the cyclicity of the trace that f_I is T-invariant. Hence ergodicity implies by Lemma 2.7 that there is a set Ω_I of full measure on which f_I is constant, to a constant denoted by $c_I \in \mathbb{N} \cap \{\infty\}$. Now let us set

$$\widetilde{\Omega} \;=\; \bigcap_{a,b\in\mathbb{Q},\, a<b} \Omega_{[a,b]} \;.$$

Because this is a countable intersection of full measure sets one also has $\mathbb{P}(\widetilde{\Omega}) = 1$. Now the claim follows from the fact that $E \in \sigma(H_\omega)$ if and only if for all $a < E < b$ one has $\mathrm{Tr}(\chi_{(a,b)}(H_\omega)) > 0$. Therefore the set

$$\Sigma \;=\; \left\{ E \in \mathbb{R} \,\middle|\, c_{(a,b)} > 0 \;\text{ for all } a, b \in \mathbb{Q} \text{ with } a < E < b \right\} \;,$$

is exactly the spectrum of all operators in $\widetilde{\Omega}$. $\Box$

The following two lemmata were used in the proof.

2.7 Lemma *Let $\mathbb{P}$ be an invariant probability measure on the compact dynamical system $(\Omega, T, \mathbb{Z}^d)$. Then $\mathbb{P}$ is ergodic if and only if for every random variable $f : \Omega \to \mathbb{R} \cup \{\infty\}$ (a measurable function) satisfying the T-invariance $f \circ T = f$, one has that f is almost surely constant.*

Proof. Given the T-invariant function f, consider the sets $\Omega_{\leq c} = \{f \leq c\}$ and $\Omega_{<c} = \{f < c\}$ for $c \in \mathbb{R} \cup \{\infty\}$. These sets are T-invariant and thus have $\mathbb{P}$-measure either 0 or 1. Moreover, they are increasing in c. Thus one can set $C = \inf\{c \,|\, \mathbb{P}(\Omega_{\leq c}) = 1\}$. As $\Omega_{\leq C} = \bigcap_{n\in\mathbb{N}} \Omega_{\leq C+\frac{1}{n}}$ and all the sets on the right have full measure, one has $\mathbb{P}(\Omega_{\leq C}) = 1$. On the other hand, $\Omega_{<C} = \bigcup_{n\in\mathbb{N}} \Omega_{<C-\frac{1}{n}}$ so that $\mathbb{P}(\Omega_{<C}) = 0$. In conclusion, $\Omega_{\leq C} \setminus \Omega_{<C} = \{f = C\}$ has full measure. The converse is obvious. $\Box$

2.8 Lemma *Let H be a bounded selfadjoint operator on a Hilbert space and U a unitary. Then for any bounded Borel measurable function $f : \mathbb{R} \to \mathbb{R}$ one has*

$$f(UHU^*) \;=\; U\, f(H)\, U^* \;.$$

Proof. It is obviously true for any polynomial and by the theorem of Stone-Weierstraß therefore for all continuous functions (if H is not bounded one obtains the same conclusion by working with the resolvents). From this one deduces that the spectral measures $\mu_{\phi,\psi}$ and $\mu_{U^*\phi,U^*\psi}$ are equal for all $\phi, \psi \in \mathcal{H}$. By definition of measurable spectral calculus this implies the lemma. $\Box$

As a first property of the almost sure spectrum, one can exclude that it has isolated eigenvalues of finite multiplicity. Isolated eigenvalues of infinite multiplicity are not excluded in general and may indeed exist (so-called flat band of periodic systems are one example, Landau levels another).

2.9 Proposition *$\mathbb{P}$-almost surely the spectrum $\sigma(H_\omega)$ has no isolated eigenvalues of finite multiplicity, namely the discrete spectrum $\sigma_{\text{dis}}(H_\omega)$ is empty.*

Proof. Let I be an interval containing only at most one point of the $\mathbb{P}$-almost sure spectrum Σ. Let Ω_I be defined as above as the full measure set where $\mathrm{Tr}(\chi_I(H_\omega))$ is constant. Then for $\omega \in \Omega_I$ and any $N \in \mathbb{N}$,

$$\begin{aligned}\mathrm{Tr}(\chi_I(H_\omega)) &= \mathbf{E}_{\mathbb{P}}\,\mathrm{Tr}(\chi_I(H_\omega)) \;\geq\; \sum_{|n|\leq N} \mathbf{E}_{\mathbb{P}}\,\langle n|\chi_I(H_\omega)|n\rangle \\ &= \sum_{|n|\leq N} \mathbf{E}_{\mathbb{P}}\,\langle 0|\chi_I(H_\omega)|0\rangle \;=\; (2N+1)^d\,\mathbf{E}_{\mathbb{P}}\,\langle 0|\chi_I(H_\omega)|0\rangle\;,\end{aligned}$$

where again Lemma 2.8 and the translation invarinve of $\mathbb{P}$ was used to pass to the second line. Now, if $\mathbf{E}_{\mathbb{P}}\,\langle 0|\chi_I(H_\omega)|0\rangle > 0$, then $\mathrm{Tr}(\chi_I(H_\omega)) = \infty$, while if it vanishes there is no spectrum in I. □

In some situations it is possible to calculate the almost sure spectrum explicitly. Here is an easy example.

2.10 Proposition *Let $H_\omega = H_0 + \sum_{n\in\mathbb{Z}^d} v_n\,|n\rangle\langle n|$ be the Anderson model on $\ell^2(\mathbb{Z}^d)$ with a translation invariant operator H_0 of finite range and independent potential values v_n which are identically distributed according to a probability $\mathbf{p}$ on $\mathbb{R}$. Then the almost sure spectrum is given by $\Sigma = \sigma(H_0) + \mathrm{supp}(\mathbf{p})$.*

Sketch of proof. Let $E \in \sigma(H_0)$. Then there exists a Weyl sequence $(\psi_n)_{n\in\mathbb{Z}^d}$ for H_0 at E with each ψ_n compactly supported. On the other hand, for any value $v \in \mathrm{supp}(\mathbf{p})$, N and ϵ, there is a non-vanishing probability $p_{\epsilon,N}$ such that $|v_n - v| < \epsilon$ for all $|n| \leq N$. These facts allow to construct approximate Weyl sequences. □

Theorem 2.6 can be considerably refined by showing that each spectral component of the Lebesgue decomposition is almost surely constant. Some preparations of general nature are needed. Recall that the Lebesgue decomposition theorem states every measure μ on the real line can be uniquely decomposed into an absolutely continuous part w.r.t. the Lebesgue measure on $\mathbb{R}$ (this means that sets of zero Lebesgue measure also have zero μ_{ac}-measure, by the theorem of Radon-Nikodym this is equivalent to having a L^1-density f such that $\mu_{\mathrm{ac}}(dE) = f(E)dE$ holds), a pure-point part μ_{pp} (consisting of countable set of Dirac peaks with summable weights) and a remainder called the singular continuous part μ_{sc}:

$$\mu \;=\; \mu_{\mathrm{ac}} + \mu_{\mathrm{pp}} + \mu_{\mathrm{sc}}\;.$$

Moreover, the three measures on the r.h.s. are mutually singular, namely one is supported on a zero measure set of the others. Let us point out that μ_{pp} is readily defined using all atoms of μ. If one then sets $\mu_{\mathrm{c}} = \mu - \mu_{\mathrm{pp}}$, the main claim of the Lebesgue decomposition is that $\mu_{\mathrm{c}} = \mu_{\mathrm{ac}} + \mu_{\mathrm{sc}}$. But μ_{ac} is just obtained as the Radon-Nikodym derivative of μ_{c} w.r.t. $\mu_{\mathrm{c}} + \mu_{\mathrm{Leb}}$ (for details see any book on measure theory), and then μ_{sc} is simply the remainder. Furthermore, the mutual singularity implies

$$L^2(\mu) \;=\; L^2(\mu_{\mathrm{ac}}) \oplus L^2(\mu_{\mathrm{pp}}) \oplus L^2(\mu_{\mathrm{sc}})\;.$$

Now given a self-adjoint operator H on a Hilbert space $\mathcal{H}$, one introduces the pure point subspace $\mathcal{H}_{\mathrm{pp}} \subset \mathcal{H}$ as the closure of the span of all eigenvectors of H. Then $\mathcal{H}_{\mathrm{c}} = (\mathcal{H}_{\mathrm{pp}})^\perp$ is the continuous subspace. Then the absolutely continuous subspace is defined as

$$\mathcal{H}_{\mathrm{ac}} \;=\; \{\phi \in \mathcal{H}_{\mathrm{c}}\,|\,\mu_\phi \text{ is purely absolutely continuous}\}\;,$$

and finally $\mathcal{H}_{\mathrm{sc}} = \mathcal{H}_{\mathrm{c}} \ominus \mathcal{H}_{\mathrm{ac}}$.

2.11 Proposition *The subspaces $\mathcal{H}_{\mathrm{ac}}$, $\mathcal{H}_{\mathrm{pp}}$ and $\mathcal{H}_{\mathrm{sc}}$ associated to a bounded selfadjoint operator H are closed, mutually orthogonal, invariant under H and*

$$\mathcal{H} \;=\; \mathcal{H}_{\mathrm{ac}} \oplus \mathcal{H}_{\mathrm{pp}} \oplus \mathcal{H}_{\mathrm{sc}}\;. \tag{2.10}$$

Proof. It just remains to show that $\mathcal{H}_{\text{ac}}$ is closed. Let $(\psi_n)_{n\geq 1}$ be a sequence in $\mathcal{H}_{\text{ac}}$ converging to ψ. Then $\mu_{\psi_n} \to \mu_\psi$ weakly. If now $N \subset \mathbb{R}$ is a set of zero Lebesgue measure, then $\mu_\psi(N) = \lim_n \mu_{\psi_n}(N) = 0$ so that $\psi \in \mathcal{H}_{\text{ac}}$. $\square$

Now one sets $H_{\text{ac}} = H|_{\mathcal{H}_{\text{ac}}}$ and $\sigma_{\text{ac}}(H) = \sigma(H_{\text{ac}})$, and similarly $\sigma_{\text{pp}}(H)$ and $\sigma_{\text{sc}}(H)$ are defined. Obviously one has

$$\sigma(H) \;=\; \sigma_{\text{ac}}(H) \cup \sigma_{\text{pp}}(H) \cup \sigma_{\text{sc}}(H) \;,$$

but this decomposition is in general not disjoint. Also note that if $\sigma_{\text{p}}(H)$ denotes the set of eigenvalues of H (which is hence a countable set because $\mathcal{H}$ is separable), then $\sigma_{\text{pp}}(H) = \overline{\sigma_{\text{p}}(H)}$ as the spectrum of an operator such as $H_{\text{pp}} = H|_{\mathcal{H}_{\text{pp}}}$ is always closed.

2.12 Theorem [Kirsch-Martinelli 1982] *Let $(H_\omega)_{\omega\in\Omega}$ be a homogeneous family of Hamiltonians with ergodic probability $\mathbb{P}$. Then $\sigma_{\text{ac}}(H_\omega)$, $\sigma_{\text{pp}}(H_\omega)$ and $\sigma_{\text{sc}}(H_\omega)$ are $\mathbb{P}$-almost surely constant.*

Proof. The proof is basically the same as that of Theorem 2.6, modulo the important technical point to check that the projections $P_{\omega,\text{ac}}$, $P_{\omega,\text{pp}}$ and $P_{\omega,\text{sc}}$ on the absolutely continuous, pure point and singular subspace of H_ω are measurable in ω. Actually it is sufficient to show this for two of these projections, due to (2.10). Once this is checked (a detailed proof of this fact can be found in [CL]), one considers the measurable function $\omega \mapsto \text{Tr}(P_{\omega,\text{ac}}\chi_I(H_\omega))$ and proceeds as above. $\square$

2.4 The density of states

The density of states $\frac{d\mathcal{N}}{dE}(E)$ at energy E is, roughly stated, the number of eigenvalues of H_ω per volume of physical space and lying in the interval $[E, E + dE]$. One way to make sense of this is to restrict the operator H_ω to a cube Λ of finite volume (*e.g.* with Dirichlet boundary conditions), count the number of its eigenvalues below E, divide by the volume and then take the thermodynamic limit $|\Lambda| \to \infty$. This gives a Stieltjes function in E (increasing and right-continuous) and the assoicated measure is then the density of states. Of course, one has to assure that the thermodynamic limit exists and also analyze its dependence on ω. All this is possible and will be done below, but there is a more direct way to introduce the density of states that will be presented first.

2.13 Definition *Let $(H_\omega)_{\omega\in\Omega}$ be a homogeneous family of Hamiltonians on $\ell^2(\mathbb{Z}^d) \otimes \mathbb{C}^L$ with ergodic probability $\mathbb{P}$. Its density of states $\mathcal{N}$* (DOS) *is the probability measure weakly defined* (*using the Riesz-Markov theorem*) *by*

$$\int \mathcal{N}(dE)\; f(E) \;=\; \mathbf{E}_{\mathbb{P}}\, \frac{1}{L}\, \text{Tr}_L\big(\langle 0|f(H_\omega)|0\rangle\big) \;, \qquad f \in C_0(\mathbb{R}) \;.$$

The associated Stieltjes distribution function

$$\mathcal{N}(E) \;=\; \mathcal{N}((-\infty, E]) \;,$$

is called the integrated density of states (IDOS).

The density of states measure $\mathcal{N}$ is again the Stieljes measure associated to the Stieltjes function $\mathcal{N}$ which explains also the choice of notations. Let us point out that the DOS is a non-random object. Another immediate consequence is that $\mathcal{N}$ is supported by the non-random spectrum Σ given in Theorem 2.6. Indeed, if f is a function supported outside of Σ, one has $f(H_\omega) = 0$ $\mathbb{P}$-almost surely and therefore $\int \mathcal{N}(dE)\; f(E) = 0$. It follows that $\mathcal{N}(I) = 0$ for any set $I \subset \mathbb{R}$ with $I \cap \Sigma = \emptyset$. The following theorem is the first result that makes connection to the intuitive definition stated above.

2.14 Theorem *Let $(H_\omega)_{\omega\in\Omega}$ be a homogeneous family of Hamiltonians with ergodic probability $\mathbb{P}$. Further let $\Lambda_N = \mathbb{Z}^d \cap [-N,N]^d$ be the centered cube with volume $|\Lambda_N| = (2N+1)^d$ and χ_{Λ_N} be the indicator function on Λ_N which will be seen as a trace-class multiplication operator on $\ell^2(\mathbb{Z}^d)\otimes\mathbb{C}^L$. Then $\mathbb{P}$-almost surely one has*

$$\int \mathcal{N}(dE)\, f(E) \;=\; \lim_{N\to\infty} \frac{1}{|\Lambda_N|}\,\frac{1}{L}\,\mathrm{Tr}\big(\chi_{\Lambda_N}\, f(H_\omega)\,\chi_{\Lambda_N}\big)\;, \qquad \forall\; f\in C_0(\mathbb{R})\;, \tag{2.11}$$

where the trace is on $\ell^2(\mathbb{Z}^d)\otimes\mathbb{C}^L$.

Proof. Given a fixed funciton $f\in C_0(\mathbb{R})$, let us calculate the r.h.s. using the covariance relation:

$$\begin{aligned}\frac{1}{|\Lambda_N|}\,\frac{1}{L}\,\mathrm{Tr}\big(\chi_{\Lambda_N}\, f(H_\omega)\,\chi_{\Lambda_N}\big) \;&=\; \frac{1}{|\Lambda_N|}\,\frac{1}{L}\sum_{n\in\Lambda_N}\mathrm{Tr}_L\big(\langle n|f(H_\omega)|n\rangle\big) \\ &=\; \frac{1}{|\Lambda_N|}\sum_{n\in\Lambda_N}\frac{1}{L}\,\mathrm{Tr}_L\big(\langle 0|f(H_{T_n\omega})|0\rangle\big)\;.\end{aligned} \tag{2.12}$$

This is the Birkhoff sum of the continuous function $\omega\in\Omega\mapsto\frac{1}{L}\mathrm{Tr}_L(\langle 0|f(H_\omega)|0\rangle)$. In particular, this function is integrable and therefore the Birkhoff ergodic theorem for the ergodic dynamical system $(\Omega,T,\mathbb{Z}^d,\mathbb{P})$ implies that there is a full measure set Ω_f such that for all $\omega\in\Omega_f$

$$\lim_{N\to\infty}\frac{1}{|\Lambda_N|}\,\frac{1}{L}\,\mathrm{Tr}\big(\chi_{\Lambda_N}\, f(H_\omega)\,\chi_{\Lambda_N}\big) \;=\; \mathbf{E}_{\mathbb{P}}\,\frac{1}{L}\,\mathrm{Tr}_L\big(\langle 0|f(H_{\omega'})|0\rangle\big)\;.$$

Comparing the r.h.s. with the definition of the DOS shows that (2.11) holds $\mathbb{P}$-almost surely for a given function $f\in C_0(\mathbb{R})$. It remains to show that it holds $\mathbb{P}$-almost surely simultaneously for all continous functions. First of all, it is sufficient to work with continuous functions f supported by an interval I containing the almost sure spectrum Σ (on a full measure set, on has $f(H_\omega)=0$ for all functions supported outside of Σ). In $C(I)$ the Stone-Weierstrass theorem furnishes us with a dense set $\mathcal{D}\subset C(I)$ (w.r.t. the $\|\,.\|_\infty$ norm; alternatively, one can directly work with a dense countable set $\mathcal{D}\subset C_0(\mathbb{R})$ if one is ready to accept the fact that $C_0(\mathbb{R})$ is separable). Then set

$$\widetilde{\Omega} \;=\; \bigcap_{f\in\mathcal{D}}\Omega_f\;.$$

Then $\widetilde{\Omega}$ has full $\mathbb{P}$-measure. It remains to show by a 3ϵ-approximation argument that (2.11) holds for all $\omega\in\widetilde{\Omega}$ and all $f\in C_0(I)$. Let $\mathcal{N}_{\omega,N}(f)$ denote the expression (2.12) and $\mathcal{N}(f)=\int\mathcal{N}(dE)\,f(E)$. Given $f\in C_0(I)$, choose a sequence $(f_k)_{k\in\mathbb{N}}$ in $\mathcal{D}$. Then

$$|\mathcal{N}(f)-\mathcal{N}_{\omega,N}(f)| \;\leq\; |\mathcal{N}(f-f_k)| + |\mathcal{N}(f_k)-\mathcal{N}_{\omega,N}(f_k)| + |\mathcal{N}_{\omega,N}(f_k-f)|\;.$$

The first and last terms are each bounded by $\|f-f_k\|_\infty$ and are thus arbitrarily small for k large, while the middle term goes to 0 as $N\to\infty$ because $\omega\in\widetilde{\Omega}$. □

2.15 Proposition *Let $(H_\omega)_{\omega\in\Omega}$ be a homogeneous family of Hamiltonians with ergodic probability $\mathbb{P}$. Furthermore suppose that the hopping is given by the discrete Laplacian, that is, $\langle n|H_\omega|m\rangle = \delta_{|n-m|=1}$. Then the* DOS *has no atoms, namely $\mathcal{N}(\{E\})=0$ for all $E\in\mathbb{R}$.*

Sketch of the proof. By Theorem 2.14

$$\mathcal{N}(\{E\}) \;=\; \lim_{N\to\infty} \frac{1}{|\Lambda_N|}\,\frac{1}{L}\,\mathrm{Tr}\big(\chi_{\Lambda_N}\,\chi_{\{E\}}(H_\omega)\,\chi_{\Lambda_N}\big)\;.$$

We will show that the span of $\chi_{\Lambda_N}\,\chi_{\{E\}}(H_\omega)$ has a dimension bounded above by $C\,N^{d-1}$ for some constant C, which then immediately implies the result as $|\Lambda_N| = \mathcal{O}(N^d)$. Now $\chi_{\{E\}}(H_\omega)$ is the span of all eigenvectors ψ at energy E, satisfying the Schrödinger equation $H_\omega\psi = E\psi$. Once such an eigenfunction ψ is known on 1-neighborhood of the boundary $\partial\Lambda_N$ of Λ_N, it can be calculated in all of Λ_N (this is a property of the discrete Laplacian that may be checked more carefully as an exercise). As there are only $\mathcal{O}(N^{d-1})$ directions associated to this 1-neighborhood of $\partial\Lambda_N$, the range of $\chi_{\Lambda_N}\,\chi_{\{E\}}(H_\omega)$ can at most be of dimension $\mathcal{O}(N^{d-1})$. □

Let us point out that there exist kinetic operators H_0 other than the discrete Laplacian that may lead to Dirac peaks in the DOS. These so-called *flat bands* result from compactly supported eigenfunctions.

Finally let us come to the definition of the density of states described in the introduction to this section. Given $\Lambda \subset \mathbb{Z}^d$, let H_Λ denote the restriction of a Hamiltonian on H on $\ell^2(\mathbb{Z}^d)\otimes\mathbb{C}^L$ to $\ell^2(\Lambda)\otimes\mathbb{C}^L$, namely

$$\langle n|H_\Lambda|m\rangle \;=\; \langle n|H|m\rangle\;, \qquad n,m\in\Lambda\;.$$

Then let us introduce a discrete measure $\widetilde{\mathcal{N}}_{\omega,N}$ by

$$\int \widetilde{\mathcal{N}}_{\omega,N}(dE)\;f(E) \;=\; \frac{1}{|\Lambda_N|}\,\frac{1}{L}\,\mathrm{Tr}_{\ell^2(\Lambda)\otimes\mathbb{C}^L}(f(H_{\omega,N}))\;, \qquad f\in C_0(\mathbb{R})\;.$$

If $E_{\omega,N,n}$, $n = 1,\ldots,L|\Lambda_N|$, denote the eigenvalues of $H_{\omega,N}$, then

$$\int \widetilde{\mathcal{N}}_{\omega,N}(dE)\;f(E) \;=\; \frac{1}{|\Lambda_N|}\,\frac{1}{L}\,\sum_{n=1}^{L|\Lambda_N|} f(E_{\omega,N,n})\;.$$

2.16 Theorem *Let $(H_\omega)_{\omega\in\Omega}$ be a homogeneous family of Hamiltonians with ergodic probability $\mathbb{P}$. Further furthermore suppose that the hopping is only finite range, that is, $\langle n|H_\omega|m\rangle = 0$ for $|n-m| > r$ where $r\in\mathbb{N}$ is the range. Then $\widetilde{\mathcal{N}}_{\omega,N}$ converges vaguely to the* DOS *$\mathcal{N}$ $\mathbb{P}$-almost surely:*

$$\int \mathcal{N}(dE)\;f(E) \;=\; \lim_{N\to\infty}\frac{1}{|\Lambda_N|}\,\frac{1}{L}\,\mathrm{Tr}\big(f(H_{\omega,\Lambda_N})\big)\;, \qquad f\in C_0(\mathbb{R})\;. \tag{2.13}$$

Moreover, the IDOS *is given by*

$$\mathcal{N}(E) \;=\; \lim_{N\to\infty}\frac{1}{|\Lambda_N|}\,\frac{1}{L}\,\#\{\text{eigenvalues of } H_{\omega,\Lambda_N} \;\leq\; E\}\;,$$

where the convergence on the r.h.s. is again $\mathbb{P}$-almost sure.

Proof. The functions $E\in\mathbb{R}\mapsto(E-z)^{-1}$, $z\in\mathbb{C}\setminus\mathbb{R}$, are dense in $C_0(\mathbb{R})$ (exercise). As $\mathcal{N}_{\omega,N}$ defined by (2.12) converges to $\mathcal{N}$ by Theorem 2.14, it is sufficient to check that the difference between

$$\int \mathcal{N}_{\omega,N}(dE)\;(E-z)^{-1} \;=\; \frac{1}{|\Lambda_N|}\,\frac{1}{|L|}\,\sum_{n\in\Lambda_N}\langle n|(H_\omega - z)^{-1}|n\rangle\;,$$

and

$$\int \widetilde{\mathcal{N}}_{\omega,N}(dE)\;(E-z)^{-1} \;=\; \frac{1}{|\Lambda_N|}\,\frac{1}{|L|}\,\sum_{n\in\Lambda_N}\langle n|(H_{\omega,\Lambda_N}-z)^{-1}|n\rangle\;,$$

vanishes in the limit $N\to\infty$. As this will turn out to be true deterministically, let us drop the index. Also set $\Lambda=\Lambda_N$ for now and $\Lambda^c=\mathbb{Z}^d\setminus\Lambda$. Also let us set

$$\Gamma \;=\; H\;-\;H_\Lambda\;-\;H_{\Lambda^c}\;. \tag{2.14}$$

The operator Γ consists of all matrix elements of H from Λ to Λ^c. As H has finite range, there are of order $|\partial\Lambda|$ non-vanishing entries, if $\partial\Lambda$ denote the boundary of Λ. In the case of Λ_N, one has $|\partial\Lambda_N|=\mathcal{O}(N^{d-1})$. Therefore, one says that Γ is a surface term. Finally let us also note that $H_\Lambda+H_{\Lambda^c}=H_\Lambda\oplus H_{\Lambda^c}$ is diagonal in the orthogonal decomposition $\ell^2(\mathbb{Z}^d)=\ell^2(\Lambda)\oplus\ell^2(\Lambda^c)$, and that the resolvent identity associated to (2.14) reads

$$\begin{aligned}(H-z)^{-1} \;&=\; (H_\Lambda\oplus H_{\Lambda^c}-z)^{-1}\;-\;(H_\Lambda\oplus H_{\Lambda^c}-z)^{-1}\,\Gamma\,(H-z)^{-1}\\ &=\;(H_\Lambda-z)^{-1}\oplus(H_{\Lambda^c}-z)^{-1}\;-\;(H_\Lambda-z)^{-1}\oplus(H_{\Lambda^c}-z)^{-1}\,\Gamma\,(H-z)^{-1}\;.\end{aligned}$$

Therefore

$$\langle n|(H-z)^{-1}|n\rangle-\langle n|(H_\Lambda-z)^{-1}|n\rangle \;=\; \sum_{m\in\Lambda,\,k\in\Lambda^c}\langle n|(H_\Lambda-z)^{-1}|m\rangle\,\langle m|\Gamma|k\rangle\,\langle k|(H-z)^{-1}|n\rangle\;.$$

Next let us use the rough uniform norm estimate $|\langle m|\Gamma|k\rangle|\leq C$, as well as the Cauchy-Schwarz inequality:

$$\begin{aligned}&\sum_{n\in\Lambda}\big(\langle n|(H-z)^{-1}|n\rangle-\langle n|(H_\Lambda-z)^{-1}|n\rangle\big)\\ &\leq\; C\sum_{m\in\Lambda,\,|m-\partial\Lambda|\leq r}\;\sum_{k\in\Lambda^c,\,|k-m|\leq r}\left(\sum_{n\in\Lambda}|\langle n|(H_\Lambda-z)^{-1}|m\rangle|^2\right)^{\frac12}\left(\sum_{n\in\Lambda}|\langle k|(H-z)^{-1}|n\rangle|^2\right)^{\frac12}\\ &=\; C\sum_{m\in\Lambda,\,|m-\partial\Lambda|\leq r}\;\sum_{k\in\Lambda^c,\,|k-m|\leq r}\|(H_\Lambda-z)^{-1}|m\rangle\|\;\|(H-z)^{-1}|k\rangle\|\\ &\leq\; C'\,|\partial\Lambda|\,(\Im m(z))^{-2}\;.\end{aligned}$$

Applying this to $\Lambda=\Lambda_N$,

$$\left|\int\mathcal{N}_{\omega,N}(dE)\;(E-z)^{-1}-\int\widetilde{\mathcal{N}}_{\omega,N}(dE)\;(E-z)^{-1}\right|\;\leq\;C''\,\frac{|\partial\Lambda_N|}{|\Lambda_N|}\,(\Im m(z))^{-2}\;,$$

which converges to 0 as $N\to\infty$. □

As a first physical application, let us consider the specific heat $C_{\beta,\mu}$ at inverse temperature β and chemical potential μ of a system of independent fermions (*e.g.* electrons) described by a homogeneous family of Hamiltonians $(H_\omega)_{\omega\in\Omega}$. The specific heat is defined as the derivative w.r.t. β of the grand-canoninical energy density given by

$$u_{\beta,\mu}\;=\;\lim_{N\to\infty}\frac{1}{|\Lambda_N|}\,\frac{1}{L}\,\mathrm{Tr}_{\ell^2(\Lambda_N)\otimes\mathbb{C}^L}\big(H_{\omega,\Lambda_N}(1+e^{\beta(H_{\omega,\Lambda_N}-\mu)})^{-1})\big)\;.$$

This can also be written out in a grand-canonical manner using the formulas of Remark 1.13, in particular (1.9) for the matrix elements used in the calculation of the trace:

$$u_{\beta,\mu}\;=\;\lim_{N\to\infty}\frac{1}{|\Lambda_N|}\,\frac{1}{L}\,\frac{1}{Z_{\beta,\mu,\omega}}\mathrm{Tr}\big(d\Gamma(H_{\omega,\Lambda_N})\,e^{-\beta d\Gamma(H_{\omega,\Lambda_N}-\mu)}\big)\;,$$

where the trace is over the Fock space of $\ell^2(\Lambda_N)\otimes\mathbb{C}^L$ and

$$Z_{\beta,\mu,\omega} \;=\; \mathrm{Tr}\big(e^{-\beta d\Gamma(H_{\omega,\Lambda_N}-\mu)}\big)\;.$$

By Theorem 2.16, one now knows that the limit defining $u_{\beta,\mu}$ exists almost surely and is almost surely equal to

$$u_{\beta,\mu} \;=\; \int \mathcal{N}(dE)\;\frac{E}{1+e^{\beta(E-\mu)}}\;.$$

The specific heat is now by definition the derivative of of $u_{\beta,\mu}$ w.r.t. the temperature $T=\frac{1}{\beta}$:

$$c_{\beta,\mu} \;=\; \partial_T\, u_{\beta,\mu} \;=\; -\,\frac{1}{\beta^2}\,\partial_\beta\, u_{\beta,\mu}\;.$$

Due to the above, one thus finds

$$c_{\beta,\mu} \;=\; \frac{1}{\beta^2}\int \mathcal{N}(dE)\;\frac{E(E-\mu)}{(1+e^{\beta(E-\mu)})^2}\;.$$

2.5 Periodic operators and the Bloch-Floquet decomposition

The aim of this section is to analyze basic spectral properties of periodic operators as introduced in Example 2.2, namely there are d periods $p_1,\ldots,p_d$ of the potential (actually one could also consider a periodic kinetic operator by the same formulas). Let us set $\mathbf{P}=\mathrm{diag}(p_1,\ldots,p_d)$, then the $\mathbf{P}$-periodicity of the potential means that

$$V_{n+\mathbf{P}a} \;=\; V_n\;,\qquad \forall\;\; a\in\mathbb{Z}^d\;.$$

Such a periodic potential is completely specified by its $P=p_1\cdots p_d$ values on a periodicity cell $\mathbb{Z}^d_{\mathbf{P}}=\mathbb{Z}^d \bmod \mathbf{P}$. The corresponding $\mathbf{P}$-periodic operators can be partially diagonalized by an extension of the Fourier transformation called the Bloch-Floquet transform. It is a unitary operator

$$\mathcal{F}:\ell^2(\mathbb{Z}^d)\otimes\mathbb{C}^L\to L^2(\mathbb{T}^d_{\mathbf{P}})\otimes\mathbb{C}^P\otimes\mathbb{C}^L\;,$$

where $P=p_1\cdots p_d$ is as above the product of the periods so that $\mathbb{C}^P=\ell^2(\mathbb{Z}^d_{\mathbf{P}})=\mathbb{C}^{p_1}\otimes\ldots\otimes\mathbb{C}^{p_d}$, and further $\mathbb{T}^d_{\mathbf{P}}=\mathbb{R}^d \bmod 2\pi\,\mathbf{P}=\prod_{j=1}^d\mathbb{T}_{p_j}$ is d-dimensional torus with side lengths given by $\mathbb{T}_p=(-\frac{\pi}{p},\frac{\pi}{p}]$. If a dot $\cdot$ denotes the scalar product of vectors, then the formula for $\mathcal{F}$ is

$$(\mathcal{F}\phi)_n(k) \;=\; \frac{1}{|\mathbb{T}^d_{\mathbf{P}}|^{\frac{1}{2}}}\sum_{m\in\mathbb{Z}^d}\phi_{n+\mathbf{P}m}\;e^{\imath(n+\mathbf{P}m)\cdot k}\;,\qquad n\in\mathbb{Z}^d_{\mathbf{P}}\;,\;\;k\in\mathbb{T}^d_{\mathbf{P}}\;,$$

and

$$(\mathcal{F}^*\phi)_n \;=\; \frac{1}{|\mathbb{T}^d_{\mathbf{P}}|^{\frac{1}{2}}}\int_{\mathbb{T}^d_{\mathbf{P}}} dk\;\phi_{n \bmod \mathbf{P}}(k)\;e^{-\imath k\cdot n}\;,$$

where $n \bmod \mathbf{P}\in\mathbb{Z}^d_{\mathbf{P}}$ is understood componentwise.

2.17 Proposition *$\mathcal{F}$ is unitary with inverse $\mathcal{F}^*$ given by the formula above.*

Proof. Let us start by checking the unitarity

$$\begin{aligned}\langle\mathcal{F}\phi|\mathcal{F}\psi\rangle \;&=\; \int_{\mathbb{T}^d_{\mathbf{P}}} dk\sum_{n\in\mathbb{Z}^d_{\mathbf{P}}}\frac{1}{|\mathbb{T}^d_{\mathbf{P}}|}\sum_{m,m'\in\mathbb{Z}^d}\overline{\phi_{n+\mathbf{P}m}}\;e^{-\imath k\cdot(n+\mathbf{P}m)}\psi_{n+\mathbf{P}m'}\;e^{\imath k\cdot(n+\mathbf{P}m')}\\ &=\; \sum_{m\in\mathbb{Z}^d}\sum_{n\in\mathbb{Z}^d_{\mathbf{P}}}\overline{\phi_{n+\mathbf{P}m}}\;\psi_{n+\mathbf{P}m} \;=\; \langle\phi|\psi\rangle\;.\end{aligned}$$

Furthermore, with the above formula for $\mathcal{F}^*$ one has

$$
\begin{aligned}
(\mathcal{F}^*\mathcal{F}\phi)_n &= \frac{1}{|\mathbb{T}^d_{\mathbf{P}}|^{\frac{1}{2}}} \int_{\mathbb{T}^d_{\mathbf{P}}} dk \; (\mathcal{F}\phi)_{n \,\mathrm{mod}\, \mathbf{P}}(k) \; e^{-\imath k\cdot n} \\
&= \frac{1}{|\mathbb{T}^d_{\mathbf{P}}|} \int_{\mathbb{T}^d_{\mathbf{P}}} dk \sum_{m\in\mathbb{Z}^d} \phi_{n \,\mathrm{mod}\, \mathbf{P}+m} \; e^{\imath(n \,\mathrm{mod}\, \mathbf{P}+m)\cdot k} \; e^{-\imath k\cdot n} \\
&= \sum_{m\in\mathbb{Z}^d} \phi_{n \,\mathrm{mod}\, \mathbf{P}+m} \; \delta_{n,n \,\mathrm{mod}\, \mathbf{P}+m} \;=\; \phi_n \;.
\end{aligned}
$$

This implies indeed $\mathcal{F}^*\mathcal{F} = \mathbf{1}$. □

The following explains the use of the Bloch-Floquet transformation.

2.18 Proposition *Let A be a bounded $\mathbf{P}$-periodic operator on $\ell^2(\mathbb{Z}^d)\otimes\mathbb{C}^L$, namely its (matrix-valued) matrix elements satisfy*

$$
\langle n+\mathbf{P}a|A|m+\mathbf{P}a\rangle \;=\; \langle n|A|m\rangle \;, \qquad \forall \;\; a\in\mathbb{Z}^d \;. \tag{2.15}
$$

Suppose that the sum

$$
\langle n|A(k)|l\rangle \;=\; \sum_{a\in\mathbb{Z}^d} \langle n|A|l+\mathbf{P}a\rangle \; e^{\imath k\cdot(n-l-\mathbf{P}a)} \;, \qquad n,l\in\mathbb{Z}^d_{\mathbf{P}} \;, \tag{2.16}
$$

converges absolutely and thus defines a $PL\times PL$ matrix $A(k)$ acting on $\mathbb{C}^P = \ell^2(\mathbb{Z}^d_{\mathbf{P}})\otimes\mathbb{C}^L$. Then one has

$$
(\mathcal{F}\,A\,\mathcal{F}^*\phi)(k) \;=\; (A(k)\,\phi)(k) \;, \qquad k\in\mathbb{T}^d_{\mathbf{P}} \;. \tag{2.17}
$$

Proof. The is merely a calculation, but for sake of completeness let us give it anyway:

$$
\begin{aligned}
(\mathcal{F}\,A\,\mathcal{F}^*\phi)_n(k) &= \frac{1}{|\mathbb{T}^d_{\mathbf{P}}|^{\frac{1}{2}}} \sum_{m\in\mathbb{Z}^d} (A\,\mathcal{F}^*\phi)_{n+\mathbf{P}m} \; e^{\imath(n+\mathbf{P}m)\cdot k} \\
&= \frac{1}{|\mathbb{T}^d_{\mathbf{P}}|^{\frac{1}{2}}} \sum_{m\in\mathbb{Z}^d} \sum_{l\in\mathbb{Z}^d_{\mathbf{P}}} \sum_{a\in\mathbb{Z}^d} \langle n+\mathbf{P}m|A|l+\mathbf{P}a\rangle (\mathcal{F}^*\phi)_{l+\mathbf{P}a} \; e^{\imath(n+\mathbf{P}m)\cdot k} \\
&= \frac{1}{|\mathbb{T}^d_{\mathbf{P}}|} \sum_{m\in\mathbb{Z}^d} \sum_{l\in\mathbb{Z}^d_{\mathbf{P}}} \sum_{a\in\mathbb{Z}^d} \langle n|A|l+\mathbf{P}(a-m)\rangle \int_{\mathbb{T}^d_{\mathbf{P}}} dk' \; \phi_l(k') \; e^{-\imath(l+\mathbf{P}a)\cdot k'} \; e^{\imath(n+\mathbf{P}m)\cdot k} \\
&= \frac{1}{|\mathbb{T}^d_{\mathbf{P}}|} \sum_{l\in\mathbb{Z}^d_{\mathbf{P}}} \sum_{a\in\mathbb{Z}^d} \langle n|A|l+\mathbf{P}a\rangle \int_{\mathbb{T}^d_{\mathbf{P}}} dk' \; \phi_l(k') \; e^{-\imath(l+\mathbf{P}a)\cdot k'} \; e^{\imath n\cdot k} \; (2\pi)^d \, \delta\big(\mathbf{P}(k-k')\big) \\
&= \sum_{l\in\mathbb{Z}^d_{\mathbf{P}}} \sum_{a\in\mathbb{Z}^d} \langle n|A|l+\mathbf{P}a\rangle \; e^{\imath(n-l-\mathbf{P}a)\cdot k} \; \phi_l(k) \;.
\end{aligned}
$$

This is precisely the claim. □

The equation (2.17) shows that the Bloch-Floquet transformation of the periodic operator (and in particular, a periodic potential) is a so-called fibered operator, namely an operator A of the form

$$
\mathcal{F}\,A\,\mathcal{F}^* \;=\; \int^{\oplus}_{\mathbb{T}^d_{\mathbf{P}}} dk \; A(k) \;,
$$

where $A(k)$ is a $PL \times PL$ matrix. One says that the operator A is partially diagonalized by $\mathcal{F}$ because one merely has to diagonalize the matrices $A(k)$ in order to calculate the spectrum of A:

$$\sigma(A) \;=\; \bigcup_{k\in\mathbb{T}^d_{\mathbf{P}}} \sigma(A(k)) \;.$$

Moreover, in the case of the periodic potential indicates that $V(k)$ is independent of k and diagonal in the space variables in $\mathbb{Z}^d_{\mathbf{P}}$ (but not yet in the L internal degrees of freedom because each V_n is up to now an arbitrary self-adjoint $L \times L$ matrix). On the other hand, one can check that the Fourier transform of the magnetic translation $\widetilde{U}_a$ is not a fibered operator unless a supplementary assumption is made assuring that $\widetilde{U}_a$ is $\mathbf{P}$-periodic (otherwise the Fourier transform shifts fibers!).

2.19 Proposition *Suppose $H_\omega = H_0 + V_\omega = \sum_{b\in\mathbb{Z}^d} T_b\,\widetilde{U}_b + V_\omega$ is of the form (2.8) with translation invariant kinetic part H_0 given by an absolutely summable sequence T_b and a periodic potential V_ω with periods $p_1,\ldots,p_d$. Furthermore, suppose that the magnetic field is rational in the sense that $\frac{1}{4\pi}\,\mathbf{P}\,\mathbf{B}$ is a matrix with integer entries (this holds trivially in the case $\mathbf{B}=0$). Then*

$$\mathcal{F}\,H_\omega\,\mathcal{F}^* \;=\; \int^{\oplus}_{\mathbb{T}^d_{\mathbf{P}}} dk\; H(k)\;,$$

where the matrix $H(k) = H_0(k) + V$ acting on $\mathbb{C}^P \otimes \mathbb{C}^L$ is given by the diagonal matrix V and

$$H_0(k) \;=\; \sum_{n,l\in\mathbb{Z}^d_{\mathbf{P}}} \left(\sum_{a\in\mathbb{Z}^d} T_{n-l-\mathbf{P}a}\; e^{-\frac{\imath}{2}\,l\cdot\mathbf{B}n}\; e^{\imath k\cdot(n-l-\mathbf{P}a)} \right) |n\rangle\langle l| \;. \tag{2.18}$$

Proof. The diagonal $\mathbf{P}$-periodic operator V is dealt with immediatly by Proposition 2.18 because (2.16) only the terms with $a = 0$ and $n = l$ remain. Due to (2.5) the matrix elements of the magnetic translations $\widetilde{U}_b$ are given by

$$\langle n|\widetilde{U}_b|m\rangle \;=\; e^{-\frac{\imath}{2}b\cdot\mathbf{B}n}\,\delta_{n,m-b}\;.$$

Thus

$$\langle n+\mathbf{P}a|\widetilde{U}_b|m+\mathbf{P}a\rangle \;=\; e^{-\frac{\imath}{2}b\cdot\mathbf{B}\mathbf{P}a}\,\langle n|\widetilde{U}_b|m\rangle \;=\; e^{\frac{\imath}{2}a\cdot\mathbf{P}\mathbf{B}b}\,\langle n|\widetilde{U}_b|m\rangle\;,$$

so that the invariance property (2.15) is indeed verified if $\frac{1}{4\pi}\mathbf{P}\mathbf{B}$ is integer-valued. Therefore one can now apply Proposition 2.18, namely for $n,l \in \mathbb{Z}^d_{\mathbf{P}}$:

$$\begin{aligned}
\langle n|\mathcal{F}\,H_0\,\mathcal{F}^*(k)|l\rangle \;&=\; \sum_{m\in\mathbb{Z}^d} T_m\,\langle n|\mathcal{F}\,\widetilde{U}_m\,\mathcal{F}^*(k)|l\rangle\\
&=\; \sum_{m\in\mathbb{Z}^d} T_m \sum_{a\in\mathbb{Z}^d} \langle n|\widetilde{U}_m|l+\mathbf{P}a\rangle\; e^{\imath k\cdot(n-l-\mathbf{P}a)}\\
&=\; \sum_{m\in\mathbb{Z}^d} T_m \sum_{a\in\mathbb{Z}^d} e^{-\frac{\imath}{2}\,m\cdot\mathbf{B}n}\delta_{n,l+\mathbf{P}a-m}\; e^{\imath k\cdot(n-l-\mathbf{P}a)}\\
&=\; \sum_{a\in\mathbb{Z}^d} T_{n-l-\mathbf{P}a}\; e^{-\frac{\imath}{2}\,l\cdot\mathbf{B}n}\; e^{\imath k\cdot(n-l-\mathbf{P}a)}\;,
\end{aligned}$$

which gives the formula. □

2.20 Remark Let us recall that the sum in (2.18) is supposed to be either finite (then H_0 has finite range) or at least to be absolutely summable. As an example, let us consider the case of vanishing magnetic field. Then (2.18) becomes

$$H_0(k) \;=\; \sum_{n,m\in\mathbb{Z}^d_{\mathbf{P}}} \left(\sum_{a\in\mathbb{Z}^d} T_{m-\mathbf{P}a}\, e^{\imath k\cdot(m-\mathbf{P}a)}\right)\; |n\rangle\langle n-m|\;.$$

If one introduces the cyclic shift S_m, $m\in\mathbb{Z}^d_{\mathbf{P}}$, on $\ell^2(\mathbb{Z}^d_{\mathbf{P}})=\mathbb{C}^{p_1}\otimes\ldots\otimes\mathbb{C}^{p_d}$ by

$$S_m \;=\; \sum_{n\in\mathbb{Z}^d_{\mathbf{P}}} |n\rangle\langle n-m|\;,$$

then

$$H_0(k) \;=\; \sum_{m\in\mathbb{Z}^d_{\mathbf{P}}} \left(\sum_{a\in\mathbb{Z}^d} T_{m-\mathbf{P}a}\, e^{\imath k\cdot(m-\mathbf{P}a)}\right)\; S_m\;.$$

To simplify even further, let us consider the case of the discrete Laplacian where $T_m=\delta_{|m|=1}\,\mathbf{1}$. Then

$$H_0(k) \;=\; \sum_{m\in\mathbb{Z}^d_{\mathbf{P}},|m|=1} e^{\imath k\cdot m}\, S_m\;.$$

For sake of concreteness, let us consider the case $d=1$ with one-dimensional fiber $L=1$. If $H_0=U_1+U_{-1}$ is the discrete Laplacian and the p-periodic potential is given by a sequence $v_1,\ldots,v_p$ of real numbers, then

$$H(k) \;=\; \begin{pmatrix} v_1 & e^{\imath k} & & & & e^{-\imath k} \\ e^{-\imath k} & v_2 & e^{\imath k} & & & \\ & \ddots & \ddots & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ & & & e^{-\imath k} & v_{p-1} & e^{\imath k} \\ e^{\imath k} & & & & e^{-\imath k} & v_p \end{pmatrix}\;.$$

Techniques to study the spectrum of such Jacobi matrices are discussed later on. ⋄

One sees that the function $k\in\mathbb{T}^d_{\mathbf{P}}\mapsto H(k)\in\mathrm{Her}(PL,\mathbb{C})$ is real analytic and has an extension to a complex neighborhood of the torus $\mathbb{T}^d_{\mathbf{P}}$ in $\mathbb{C}^d$ (recall that the coefficient matrices T_m either have finite range so that they vanish for $|m|$ sufficiently large or are at least supposed to be summable in m). A lot is known about the eigenvalues and eigenvectors of such analytic families (this is called analytic perturbation theory). The best reference is definitely Kato's book [Kat], but the essentials can also be found in [RS, Sec. XII]. The most important result is the following:

2.21 Theorem [Rellich's Theorem] *Let $H(k)$ be a matrix-valued analytic function in a region $D\subset\mathbb{C}$ containing a real interval $I\subset\mathbb{R}\subset\mathbb{C}$ and suppose that $H(k)$ is self-adjoint on $D\cap\mathbb{R}$. Then the eigenvalues are analytic functions of k provided their enumeration at level crossings are chosen adequately.*

Sketch of the proof. The eigenvalues satisfy the characteristic equation $\det(H(k)-\lambda)=0$ which is polynomial in λ with analytical coefficients in k. From this one checks that simple zeros (eigenvalues) are locally analytic. At degeneries, the eigenvalues are in general only given by a Puiseux expansion in k (a Taylor series in fractional power $(k-k_0)^{\frac{1}{p}}$ where p is the multiplicity at k_0). For self-adjoint matrices, one can prove that the coefficients of fractional powers vanish. Details in [Kat] or [RS]. □

2.22 Corollary *Let $d = 1$. Suppose that the assumptions of* Proposition 2.19 *hold. Then there are PL real-valued real analytic functions $E_j(k)$, $j = 1, \ldots, PL$, giving the eigenvalues of $H(k)$. These functions are called the Bloch bands.*

In dimension $d \geq 2$, non-degenerate eigenvalues are still real analytic as function of several complex variables, but there may be degeneracies with singularities at which it is not possible to choose analytic branches. An example is a conic singularity in dimension $d = 2$ (a so-called Dirac point). The Bloch bands can, in general, have so-called band overlaps ($E_j(k) = E_{j'}(k')$ for $j \neq j'$ and $k \neq k'$) and even band touching ($E_j(k) = E_{j'}(k)$ for $j \neq j'$). Band touching corresponds to degenerecies in the spectrum of $H(k)$. It is also possible to have a constant function E_j in which case one speaks of a *flat band*. Next let us come to the density of states (DOS) as defined in Section 2.4.

2.23 Proposition *Suppose that the assumptions of* Proposition 2.19 *hold. Then the* DOS *is given by*

$$\int \mathcal{N}(dE)\, f(E) \;=\; \frac{1}{|\mathbb{T}^d_{\mathbf{P}}|}\,\frac{1}{PL}\int_{\mathbb{T}^d_{\mathbf{P}}} dk\;\mathrm{Tr}(f(H(k)))\;.$$

Proof. Let us start from the formula in Definition 2.13. Because of the explicit form of $\mathbb{P}$ in Example 2.2, one has

$$\int \mathcal{N}(dE)\, f(E) \;=\; \frac{1}{PL}\sum_{n\in\mathbb{Z}^d_{\mathbf{P}}} \mathrm{Tr}_L\big(\langle n|f(H_\omega)|n\rangle\big)\;.$$

Now let us insert the Fourier transform twice:

$$\int \mathcal{N}(dE)\, f(E) \;=\; \frac{1}{PL}\sum_{n\in\mathbb{Z}^d_{\mathbf{P}}} \mathrm{Tr}_L\big(\langle n|\mathcal{F}^*\mathcal{F}f(H_\omega)\mathcal{F}^*\mathcal{F}|n\rangle\big)\;.$$

By Proposition 2.19 and functional calculus the operator $\mathcal{F}f(H_\omega)\mathcal{F}^*$ is fibered. Furthermore $\mathcal{F}|n\rangle$ can be calculated explicitly:

$$(\mathcal{F}\,|n\rangle)(k) \;=\; \frac{1}{|\mathbb{T}^d_{\mathbf{P}}|^{\frac{1}{2}}}\; e^{\imath n\cdot k}\;.$$

Writing out the scalar product shows

$$\int \mathcal{N}(dE)\, f(E) \;=\; \frac{1}{PL}\sum_{n\in\mathbb{Z}^d_{\mathbf{P}}} \frac{1}{|\mathbb{T}^d_{\mathbf{P}}|}\int_{\mathbb{T}^d_{\mathbf{P}}} dk\;\mathrm{Tr}_L\big(\langle n|f(H(k))|n\rangle\big)\;.$$

This is precisely the claimed formula. □

In particular, it follows from Proposition 2.23 that the integrated density of states $\mathcal{N}$ (IDOS) is given by

$$\mathcal{N}(E) \;=\; \frac{1}{|\mathbb{T}^d_{\mathbf{P}}|}\,\frac{1}{PL}\int_{\mathbb{T}^d_{\mathbf{P}}} dk\;\mathrm{Tr}(\chi(H(k)\leq E))\;.$$

It is possible to further calculate the IDOS and DOS under the hypothesis that there are no flat bands (which would lead to Dirac peaks in the DOS). In fact, using the eigenbasis of $H(k)$ shows

$$\begin{aligned}\mathcal{N}(E) \;&=\; \frac{1}{|\mathbb{T}^d_{\mathbf{P}}|}\,\frac{1}{PL}\sum_{j=1}^{PL}\int_{\mathbb{T}^d_{\mathbf{P}}} dk\;\chi(E_j(k)\leq E)\\ &=\; \frac{1}{|\mathbb{T}^d_{\mathbf{P}}|}\,\frac{1}{PL}\sum_{j=1}^{PL}\int_{-\infty}^{E} de\int_{\Sigma_{j,e}} \nu_{j,e}(d\sigma)\,\frac{1}{\|\nabla E_j(\sigma)\|}\;.\end{aligned} \qquad (2.19)$$

Here the second equality follows from the coarea formula associated to the function $k \in \mathbb{T}^d_{\mathbf{P}} \mapsto E_j(k)$ stating that the integral over $\mathbb{T}^d_{\mathbf{P}}$ can be decomposed into an integral over energies combined with an integral over the constant energy surfaces $\Sigma_{j,e} = \{k \in \mathbb{T}^d_{\mathbf{P}} \,|\, E_j(k) = e\}$ with respect to the induced Riemannian volume measure $\nu_{j,e}$ on $\Sigma_{j,e}$:

$$\int_{\mathbb{T}^d_{\mathbf{P}}} dk\; f(k) \;=\; \int de \int_{\Sigma_{j,e}} \nu_{j,e}(d\sigma)\; \frac{1}{\|\nabla E_j(\sigma)\|}\; f(\sigma)\;, \qquad f \in L^1(\mathbb{T}^d_{\mathbf{P}})\;.$$

A proof can be found in books on geometric measure theory or differential geometry, *e.g.* [Sak]. Generically $\Sigma_{j,e}$ is of dimension $d-1$ so that, in particular, in dimension $d = 1$ the integral in (2.19) is just counting the number of points on the constant energy surface. It follows from (2.19) that the density of states is given by

$$\frac{d\mathcal{N}}{dE}(E) \;=\; \frac{1}{|\mathbb{T}^d_{\mathbf{P}}|}\;\frac{1}{PL}\sum_{j=1}^{PL}\int_{\Sigma_{j,E}} \nu_{j,E}(d\sigma)\;\frac{1}{\|\nabla E_j(\sigma)\|}\;.$$

As the energy bands are real analytic, it follows the density of states is also real analytic, except at the critical values of the energy bands (which are those energies E for which there exist $k \in \mathbb{T}^d_{\mathbf{P}}$ and j such that $\nabla E_j(k) = 0$ and $E_j(k) = E$. The band edges are always critical energies, but in dimension $d \geq 2$ there are other critical points at which the Hessian $\nabla^2 E_j(k)$ has indefinite signature (by Morse theory, the number of critical points with signature p is bounded below by the Betti numbers $\beta_p = \binom{d}{p}$ of the d-dimensional torus). At all critical values, the density of states is not analytic. These values are called van Hove singularities.

As an example, let us consider the bottom of the spectrum E_0 which is supposed to correspond to a single regular critical point k_0 (quadratic) of a single band E_j. Then $\|\nabla E_j(k_0 + \delta k)\| \sim \|\delta k\| \sim (E_j(k_0 + \delta k) - E_0)^{\frac{1}{2}} \sim \epsilon^{\frac{1}{2}}$ if we use ϵ as the energy difference to E_0. As the volume of the constant energy surfaces varies as $\nu_{j,E}(\Sigma_{j,E_0+\epsilon}) \sim \epsilon^{\frac{d-1}{2}}$ (because it is like a $d-1$ dimensional sphere of radius $|\delta k| \sim \epsilon^{\frac{1}{2}}$), it follows from (2.19) that

$$\frac{d\mathcal{N}}{dE}(E_0 + \epsilon) \;\sim\; \epsilon^{\frac{d-1}{2}}\,\epsilon^{-\frac{1}{2}} \;=\; \epsilon^{\frac{d-2}{2}}\;.$$

The leading order coefficient can also be calculated and involves the product of the eigenvalues of the Hessian (these eigenvalues m_j are also called *effective masses* and the leading order coefficient is proportional to $(m_1 \cdots m_d)^{-\frac{1}{d}}$). The errors can be rigorously estimated using a Morse lemma which brings the energy band locally at k_0 into a quadratic normal form. Using the Morse lemma, one can also calculate the behavior at the other van Hove singularities. For details, see [BSB]

The range of the Fourier transform contains the Hilbert space $L^2(\mathbb{T}^d_{\mathbf{P}})$ on which there is a natural unbounded self-adjoint operator $\frac{1}{\imath}\partial_k$ with core given by the smooth functions. Here $\partial_k = (\partial_{k_1}, \ldots, \partial_{k_d})$ denotes the gradient for which often the notation nabla is used, but this is reserved for another object later on. Oft course, $\imath\partial_k$ is not a fibered operator, quite the contrary, the differential quotient used for the definition compares different fibers. Nevertheless, there is a natural way to construct a new fibered operator by deriving the fibered operator (if the latter is differentiable). The following proposition makes this more precise.

2.24 Proposition *Let the (unbounded selfadjoint) position operator $X = (X_1, \ldots, X_d)$ on $\ell^2(\mathbb{Z}^d) \otimes \mathbb{C}^L$ be densely defined by*

$$(X_j\,\psi)_n \;=\; n_j\,\psi_n\;, \qquad \psi \in \ell^2(\mathbb{Z}^d) \otimes \mathbb{C}^L\;,$$

when ever the r.h.s. is again a vector in $\ell^2(\mathbb{Z}^d) \otimes \mathbb{C}^L$. Then

$$\mathcal{F}\,X\,\mathcal{F}^* \;=\; \frac{1}{\imath}\,\partial_k\;.$$

Furthermore, if A is a $\mathbf{P}$-periodic bounded operator on $\ell^2(\mathbb{Z}^d) \otimes \mathbb{C}^L$ such that also $\imath[X, A]$ is bounded, then the Fourier transform of $\imath[X, A]$ is also a fibered operator given by

$$\mathcal{F}\,\imath[X, A]\,\mathcal{F}^* \;=\; \int_{\mathbb{T}^d_{\mathbf{P}}}^{\oplus} dk\;\partial_k A(k)\;. \tag{2.20}$$

Proof. Let us begin by writing out the definition of the Fourier transform:

$$\begin{aligned}(\mathcal{F}^*\,\partial_k\,\mathcal{F}\,\phi)_n \;&=\; \frac{1}{|\mathbb{T}^d_{\mathbf{P}}|^{\frac{1}{2}}}\int_{\mathbb{T}^d_{\mathbf{P}}} dk\;(\partial_k\,\mathcal{F}\,\phi)_{n \,\mathrm{mod}\,\mathbf{P}}(k)\;e^{-\imath k\cdot n}\\ &=\; \frac{1}{|\mathbb{T}^d_{\mathbf{P}}|^{\frac{1}{2}}}\int_{\mathbb{T}^d_{\mathbf{P}}} dk\;\partial_k\,(\mathcal{F}\,\phi)_{n \,\mathrm{mod}\,\mathbf{P}}(k)\;e^{-\imath k\cdot n}\;.\end{aligned}$$

Now follows a partial integration on the manifold $\mathbb{T}^d_{\mathbf{P}}$ without boundary:

$$(\mathcal{F}^*\,\partial_k\,\mathcal{F}\,\phi)_n \;=\; \frac{1}{|\mathbb{T}^d_{\mathbf{P}}|^{\frac{1}{2}}}\int_{\mathbb{T}^d_{\mathbf{P}}} dk\;(\mathcal{F}\,\phi)_{n \,\mathrm{mod}\,\mathbf{P}}(k)\;\imath\,n\,e^{-\imath k\cdot n}\;=\;\imath\,n\,\phi_n\;=\;\imath\,(X\,\phi)_n\;,$$

which shows the first claim. The second follows by writing out the commutator. □

Now let us rapidly resume some of the results of this section in a structural manner which is then allows to generalize these concepts in the next section. Let us set

$$\mathcal{B} \;=\; \big\{\text{bounded } \mathbf{P}\text{-periodic operators on } \ell^2(\mathbb{Z}^d)\otimes\mathbb{C}^L\big\}\;.$$

As linear combinations, products and adjoints of bounded $\mathbf{P}$-periodic operators are again bounded $\mathbf{P}$-periodic operators, the set $\mathcal{B}$ has the structure of a $*$-algebra. After Bloch-Floquet transformation, this algebra becomes the algebra of fibered, matrix-valued bounded operators on $L^2(\mathbb{T}^d_{\mathbf{P}})\otimes\mathbb{C}^{PL}$. Within this algebra let us consider the subalgebra $\mathcal{A}\subset\mathcal{B}$ of operators the continuous fibers:

$$\mathcal{A} \;=\; \left\{A\in\mathcal{B}\;\middle|\;\mathcal{F}A\mathcal{F}^* = \int_{\mathbb{T}^d_{\mathbf{P}}}^{\oplus} dk\,A(k)\text{ with }k\mapsto A(k)\text{ continuous}\right\}\;. \tag{2.21}$$

This algebra is a C*-algebra when furnished with the operator norm. It contains yet another subalgebra

$$C^n(\mathcal{A}) \;=\; \left\{A\in\mathcal{A}\;\middle|\;\mathcal{F}A\mathcal{F}^* = \int_{\mathbb{T}^d_{\mathbf{P}}}^{\oplus} dk\,A(k)\text{ with }k\mapsto A(k)\;\;n\text{ times continuously differentiable}\right\}\;.$$

This algebra is not a C*-algbra though, but only a Banach algebra. The set $C^1(\mathcal{A})$ is precisely the domain of the derivation (2.20), that is the set of those elements of $\mathcal{A}$ for which (2.20) is well-defined as a $\mathbf{P}$-periodic bounded operator with continuous fibers. This furnishes $\mathcal{A}$ with a differentiable structure. Furthermore, an integral of operators in $\mathcal{A}$ is given by

$$\int_{\mathbb{T}^d_{\mathbf{P}}}\frac{dk}{|\mathbb{T}^d_{\mathbf{P}}|}\,\frac{1}{P\,L}\,\mathrm{Tr}_{PL}(A(k)) \;=\; \lim_{N\to\infty}\frac{1}{|\Lambda_N|}\,\frac{1}{L}\,\mathrm{Tr}(\chi_{\Lambda_N}A\chi_{\Lambda_N})\;,$$

where the equality follows from the same calculation as in the proof of Proposition 2.23. The r.h.s. of this equation shows that the integral is given by the trace per unit volume. It is the aim of the next section to carry over this differential and integral structure to general homogeneous operators which are not necessarily periodic.

Reminder A $*$-Banach algebra is a normed complete vector space furnished with an algebraic structure structure and an involution $*$ such that $\|AB\| \leq \|A\| \, \|B\|$. It is a C*-algebra if, moreover, the C*-equation $\|A^*A\| = \|A\|^2$ holds. Due to the GNS-construction one can always think of an abstract C*-algebra as a norm-closed subalgebra of bounded operators on some Hilbert space (called the GNS-Hilbert space, there is one for each positive linear functional on the algebra). A W*-algebra or von Neumann algebra is a weakly closed C*-algebra. A W*-algebra is invariant under measurable functional calculus, while a C*-algebra is only invariant under continuous functional calculus. For the analysis of topological quantities, one has to work in the C*-category.

2.6 The algebra of homogeneous operators

The object of this section is to construct an algebra of homogeneous operators which contains the homogenous Hamiltonian in the sense of Definition 2.1, but also all other homogeneous operators. Of physical relevance are, for example, commutators of the Hamiltonian with the position operator which are indeed again homogeneous operators. On this algebra there will be given again tools of non-commutative analysis, namely a tracial state as well as a derivations. We will first work with a C*-algebra simply because it already contains many interesting operators, but also because it still has topological content. Furthermore, it is possible to go on and construct a W*-algebra.

In order to motivate the constructions below, let us begin from a strongly continuous family $(A_\omega)_{\omega\in\Omega}$ of operators on $\ell^2(\mathbb{Z}^d)\otimes\mathbb{C}^L$ satisfying the covariance relation $U_n A_\omega U_{-n} = A_{T_n\omega}$ w.r.t. the magnetic translations. This implies that the (matrix-valued) matrix elements satisfy

$$\langle n|A_\omega|m\rangle \;=\; \langle 0|U_{-n}A_\omega|m\rangle \;=\; \langle 0|A_{T_{-n}\omega}U_{-n}|m\rangle \;=\; \langle 0|A_{T_{-n}\omega}|m-n\rangle\, e^{\frac{\imath}{2}\,m\cdot\mathbf{B}n}\;.$$

Therefore all matrix elements can be obtained from the function $(\omega,m)\mapsto A(\omega,m)=\langle 0|A_\omega|m\rangle$ which is continuous by hypothesis. This suggests that such functions may be the adequate objects to look at. When looking to define a $*$-algebra structure on these functions, one should be guided by the equation

$$\langle 0|A^*_\omega|m\rangle \;=\; \langle m|A_\omega|0\rangle^* \;=\; \langle 0|A_{T_{-m}\omega}|-m\rangle^*\;,$$

as well as, if $(B_\omega)_{\omega\in\Omega}$ is another family of homogeneous operators,

$$\langle 0|A_\omega B_\omega|m\rangle \;=\; \sum_{l\in\mathbb{Z}^d}\langle 0|A_\omega|l\rangle\,\langle l|B_\omega|m\rangle \;=\; \sum_{l\in\mathbb{Z}^d}\langle 0|A_\omega|l\rangle\,\langle 0|B_{T_{-l}\omega}|m-l\rangle\, e^{\frac{\imath}{2}\,m\cdot\mathbf{B}l}\;.$$

Now let us construct the operator algebra $\mathcal{A}$ at a fixed magnetic field $\mathbf{B}$. The basic object is the topological vector space $C_c(\Omega\times\mathbb{Z}^d,\mathrm{Mat}(L,\mathbb{C}))$ of continuous functions with compact support on $\Omega\times\mathbb{Z}^d$ and values in $\mathrm{Mat}(L,\mathbb{C})$. It is endowed with a $*$-algebra structure (inspired by the above equations):

$$AB(\omega,n) \;=\; \sum_{l\in\mathbb{Z}^d} A(\omega,l)\,B(T^{-l}\omega,n-l)\,e^{\frac{\imath}{2}n\cdot\mathbf{B}l}\;, \qquad A^*(\omega,n) \;=\; A(T^{-n}\omega,-n)^*\;, \tag{2.22}$$

where the last $*$ denotes the adjoint matrix. For $\omega\in\Omega$, let us define a map π_ω from this $*$-algebra into the bounded operators on the Hilbert space $\ell^2(\mathbb{Z}^d)\otimes\mathbb{C}^L$ by

$$\big(\pi_\omega(A)\psi\big)_n \;=\; \sum_{l\in\mathbb{Z}^d} A(T^{-n}\omega,l-n)\,e^{\frac{\imath}{2}l\cdot\mathbf{B}n}\,\psi_l\;, \qquad \psi\in\ell^2(\mathbb{Z}^d)\otimes\mathbb{C}^L\;. \tag{2.23}$$

2.25 Proposition *Each π_ω is representation of $C_c(\Omega\times\mathbb{Z}^d,\mathrm{Mat}(L,\mathbb{C}))$ on $\ell^2(\mathbb{Z}^d)\otimes\mathbb{C}^L$, namely*

$$\pi_\omega(A+\lambda B) \;=\; \pi_\omega(A)+\lambda\pi_\omega(B)\;, \qquad \pi_\omega(AB)\;=\;\pi_\omega(A)\pi_\omega(B)\;, \qquad \pi_\omega(A^*)\;=\;\pi_\omega(A)^*\;.$$

Moreover, π_ω is strongly continuous in ω and the covariance relation holds:

$$U_a\pi_\omega(A)U_a^{-1} \;=\; \pi_{T^a\omega}(A)\;, \qquad a\in\mathbb{Z}^d\;. \tag{2.24}$$

Now define the norm $\|A\|=\sup_{\omega\in\Omega}\|\pi_\omega(A)\|$ on $C_c(\Omega\times\mathbb{Z}^d,\mathrm{Mat}(L,\mathbb{C}))$ and let $\mathcal{A}=C(\Omega)\rtimes\mathbb{Z}^d\otimes\mathrm{Mat}(L,\mathbb{C})$ be the completion of $C_c(\Omega\times\mathbb{Z}^d,\mathrm{Mat}(L,\mathbb{C}))$ under this norm. The $*$-algebraic operations and representations π_ω can be extended by continuity to $\mathcal{A}$.

2.26 Proposition *$\mathcal{A}$ is a C*-algebra when furnished with the norm $\|A\|$.*

2.27 Remark The C*-algebra $\mathcal{A}$ constructed above is a special case of a standard construction called the crossed product algebra associated to the action α of a discrete group G on a C*-algebra $\mathcal{B}$. Such an action is given by a automorphisms $\alpha_g:\mathcal{B}\to\mathcal{B}$ (namely $\alpha_g(AB)=\alpha_g(A)\alpha_g(B)$ and $\alpha_g(A^*)=\alpha_g(A)^*$) satisfying, moreover, that $\alpha_g\alpha_h=\alpha_{gh}$. One also calls $(\mathcal{A},G,\alpha)$ a C*-dynamical system. Now for compactly supported functions $m\in G\mapsto A_m\in\mathcal{B}$ and $m\in G\mapsto B_m\in\mathcal{B}$ which are for simplicity are also denoted by A and B, one defines

$$(AB)_m \;=\; \sum_{l\in G} A_l\,\alpha_l(B_{l^{-1}m})\;, \qquad (A^*)_m \;=\; \alpha_{-m}(B_{-m})^*\;.$$

Then one defines adequate representations on $\ell^2(G)$ and uses them to define a C*-closure of this $*$-algebra. The C*-algebra is then called the C*-crossed product $\mathcal{B}\rtimes_\alpha G$. A very detailed and good reference on crossed products are the corresponding chapters of Pedersen's book [Ped]. In the situation above, one has $G=\mathbb{Z}^d$, $\mathcal{B}=C(\Omega)$ and $\alpha_m(f)(\omega)=f(T_{-m}\omega)$. ⋄

2.28 Example Let us exhibit explicitly an element $H\in\mathcal{A}$ the representations $\pi_\omega(H)$ of which are equal to the operator H_ω given in (2.8). It is given by the following continuous function on $\Omega\times\mathbb{Z}^d$ which can also be called the symbol of H:

$$H(\omega,n) \;=\; T_n \,+\, \delta_{n,0}\,V_{\omega,0}\;. \tag{2.25}$$

As an exercise, one can write out the symbol for $\imath[X,H_\omega]$. ⋄

2.29 Example If one considers the $\mathbf{P}$-periodic operators as in Section 2.5, then $\mathcal{A}\cong C(\mathbb{T}^d_{\mathbf{P}})\otimes\mathrm{Mat}(PL,\mathbb{C})$ (check this claim as an exercise!). As in (2.21) this can be seen as the concrete algebra of fibered operators on $L^2(\mathbb{T}^d_{\mathbf{P}})\otimes\mathbb{C}^{PL}$. After Bloch-Floquet transformation these operators are the $\mathbf{P}$-periodic operators on $\ell^2(\mathbb{Z}^d)\otimes\mathbb{C}^L$. ⋄

The next objective is the construction of a differential structure on the C*-algebra $\mathcal{A}$. This will be given by unbounded operators on $\mathcal{A}$ (just as derivatives on continuous functions are densely defined, but not everywhere), so that one has to deal with domain questions. In general, an elegant way to circumvent this (which is, of course, not hard here) is to first write out the associated group of $*$-automorphisms and the define the generators with natural domain (as given by Stone's theorem, for example). Here there exists a d-parameter group $k\in\mathbb{T}^d\mapsto\rho_k$ of $*$-automorphisms defined by

$$(\eta_k A)(\omega,n) \;=\; e^{\imath k\cdot n}\,A(\omega,n)\;, \tag{2.26}$$

namely η_k is linear, satisfies $\eta_k(AB)=\eta_k(A)\eta_k(B)$, $\eta_k(A^*)=\eta_k(A)^*$ and the group property $\eta_k\eta_{k'}=\eta_{k+k'}$ (as an exercise, check all these claims). As every $*$-automorphism, ρ_k also conserves the C*-norm. Its generators $\nabla = (\nabla_1, \ldots, \nabla_d)$ are unbounded, but closed $*$-derivations with domain $C^1(\mathcal{A})$. The family of $*$-derivations satisfies the Leibniz rule (this follows immediately from $\eta_k(AB) = \eta_k(A)\eta_k(B)$)

$$\nabla(AB) \;=\; (\nabla A)B + A(\nabla B) \;, \qquad A, B \in C^1(\mathcal{A}) \;,$$

as well as

$$\nabla(A^*) \;=\; (\nabla A)^* \;, \qquad A \in C^1(\mathcal{A}) \;.$$

This shows, in particular, that $C^1(\mathcal{A})$ is a sub-*-algebra of $\mathcal{A}$. It becomes a Banach $*$-algebra when furnished with the norm $\|A\|_{C^1} = \|A\| + \sum_j \|\nabla_j A\|$. Indeed, from the Leibniz rule,

$$\|AB\|_{C^1} \leq \|AB\| + \sum_j (\|\nabla_j A\|\,\|B\| + \|A\|\,\|\nabla_j B\|) \;\leq \|A\|_{C^1}\|B\|_{C^1} \;.$$

Explicitly the generators are given by

$$\nabla_j A(\omega, n) \;=\; \imath\, n_j\, A(\omega, n) \;, \qquad A \in C^1(\mathcal{A}) \;. \tag{2.27}$$

Furthermore, the sub-algebra $C^1(\mathcal{A}) \subset \mathcal{A}$ is endowed with the graph norm $\|A\|_{C^1} = \|A\| + \sum_j \|\nabla_j A\|$ which makes it a Banach $*$-algebra. If the position operator $X = (X_1, \ldots, X_d)$ on $\mathcal{H}$ is defined as above, then

$$\pi_\omega(\nabla_j A) \;=\; \imath[\pi_\omega(A), X_j] \;. \tag{2.28}$$

2.30 Lemma *For $A \in C^1(\mathcal{A})$ and $z \in \mathbb{C}$, Duhamel's formula holds:*

$$\nabla\, e^{zA} \;=\; z \int_0^1 ds\, e^{(1-s)zA} \nabla A\, e^{szA} \;.$$

Proof. For $n \geq 1$,

$$\begin{aligned}
\nabla\, e^{zA} \;&=\; \nabla \left(e^{\frac{z}{n}A}\right)^n \\
&=\; \nabla\, e^{\frac{z}{n}A} \big(e^{\frac{z}{n}A}\big)^{n-1} + e^{\frac{z}{n}A}\, \nabla \big(e^{\frac{z}{n}A}\big)^{n-1} \\
&=\; \sum_{k=0}^{n-1} e^{\frac{n-k-1}{n}zA} \nabla\, e^{\frac{z}{n}A}\; e^{\frac{k}{n}zA} \;,
\end{aligned}$$

where the third identity follows from iterating the second one. Now, with norm convergence,

$$\lim_{n\to\infty} n\, \nabla\, e^{\frac{z}{n}A} \;=\; z\, \nabla A \;.$$

Therefore the norm convergent Riemann integrals lead to Duhamel's formula. □

2.31 Proposition *Let $H = H^*$ be an element of $C^1(\mathcal{A})$. Then for any compactly supported smooth function $f \in C_c^\infty(\mathbb{R})$, the operator $f(H)$ belongs to $C^1(\mathcal{A})$.*

Proof. Lemma 2.30 shows

$$\|\nabla\, e^{\imath t H}\| \;\leq\; C\, t \;. \tag{2.29}$$

Therefore also $\|e^{\imath t H}\|_{C^1} \leq 1 + C\, t$. Now one has

$$f(H) \;=\; \int dt\; \hat{f}(t)\; e^{\imath t H} \;, \qquad \hat{f}(t) \;=\; \int \frac{dE}{2\pi}\; e^{-\imath E t}\, f(E) \;, \tag{2.30}$$

where the integral is norm convergent in $\mathcal{A}$ because $\hat{f}$ is a Schwartz function. Therefore the above estimate show that $f(H)$ is in $C^1(\mathcal{A})$. $\square$

Exercise Strengthen the above proof so that less regularity of f is required.

Now we come to the non-commutative integration. Given a T-invariant probability measure $\mathbb{P}$ on Ω, a positive trace $\mathcal{T}$ on $\mathcal{A}$ is defined by

$$\mathcal{T}(A) \;=\; \int_\Omega \mathbb{P}(d\omega)\,\frac{1}{L}\,\mathrm{Tr}\big(A(\omega,0)\big)\,. \tag{2.31}$$

The following is readily verified.

2.32 Lemma *$\mathcal{T}$ is a linear functional defined on all of $\mathcal{A}$ and satisfies*
(i) (*normalization*) $\mathcal{T}(\mathbf{1}) = 1$
(ii) (*positivity*) $\mathcal{T}(A^*A) \geq 0$ *and* $\mathcal{T}(A^*) = \overline{\mathcal{T}(A)}$
(iii) (*cyclicity*) $\mathcal{T}(AB) = \mathcal{T}(BA)$
(iv) (*norm bound*) $\mathcal{T}(|AB|) \leq \|A\|\,\mathcal{T}(|B|)$ *where* $|B| = (B^*B)^{\frac{1}{2}}$
(v) (*invariance*) $\mathcal{T}(\nabla A) = 0$ *for* $A \in C^1(\mathcal{A})$
(vi) (*partial integration*) $\mathcal{T}(A\nabla B) = -\mathcal{T}(\nabla A\, B)$ *for* $A, B \in C^1(\mathcal{A})$

If $\mathbb{P}$ is in addition ergodic, then Birkhoff's ergodic theorem implies that for any increasing sequence $(\Lambda_N)_{N\in\mathbb{N}}$ of cubes centered at the origin

$$\mathcal{T}(A) \;=\; \int_\Omega \mathbb{P}(d\omega)\,\frac{1}{L}\,\mathrm{Tr}\big(\langle 0|\pi_\omega(A)|0\rangle\big) \;=\; \lim_{N\to\infty}\frac{1}{L\,|\Lambda_N|}\sum_{n\in\Lambda_N}\mathrm{Tr}\big(\langle n|\pi_\omega(A)|n\rangle\big)\,, \tag{2.32}$$

for $\mathbb{P}$-almost all $\omega \in \Omega$. This shows that $\mathcal{T}$ is the trace per unit volume. Furthermore, comparing with Theorem 2.16, the DOS is given in terms of the trace per unit volume by

$$\mathcal{T}\left(f(H)\right) \;=\; \int_\mathbb{R} \mathcal{N}(dE)\,f(E)\,, \qquad f \in C_0(\mathbb{R})\,. \tag{2.33}$$

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

$$\|A\|_{L^\infty} \;=\; \mathbb{P}\text{-}\operatorname*{ess\,inf}_{\omega\in\Omega}\,\|A_\omega\|_{\mathcal{B}(\mathcal{H})}\,.$$

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

3 Quantum transport

In this chapter, we begin by discussing basic approaches to the phenomena of quantum transport: escape probabilities and diffusion exponents. Then their connections to spectral properties are analyzed. It follows a derivation of the Kubo formula for the electrical conductivity in homogeneous media. This is done by linear response theory and in presence of a dissipation mechanism. What happens when this dissipation mechanism is removed is discussed in the final section. Again we restrict our discussion to tight-binding models.

3.1 The time-averaged transition and return probabilities

Let H be a selfadjoint Hamiltonian on the Hilbert space $\ell^2(\mathbb{Z}^d)$. Suppose the system is initially in a normalized state ψ, *e.g.* the state $|0\rangle$ localized at the origin. Then the probability to be in a normalized state ϕ at time t is $|\langle\phi|e^{-\imath tH}|\psi\rangle|^2$. Unfortunately it is difficult to analyze this quantity directly and one therefore usually considers the time-averaged probability to reach ϕ when starting from ψ:

$$p_T(\phi,\psi) \;=\; \int_0^T \frac{dt}{T}\; |\langle\phi|e^{-\imath tH}|\psi\rangle|^2 \;.$$

Then $p_T(\phi,\psi)$ is called the time-averaged transition probability from ψ to ϕ (under the dynamics generated by H) and $p_T(\psi,\psi)$ is often also called the time-averaged return probability to ψ. Clearly, if ψ is an eigenstate of H with energy E so that $e^{-\imath tH}\psi = e^{-\imath tE}\psi$, then $p_T(\psi,\psi)=1$. On the other hand, if initial state ψ lies in the continuous spectral subspace of H, that is, its spectral measure contains no atom, then the return probability $p_T(\psi,\psi)$ converges to 0 in the long time limit. This follows from the so-called RAGE theorem which can be tracked back to contributions by Ruelle, Amrein, Georgescu and Enss in 1970's.

3.1 Theorem (RAGE theorem) *Let H be a self-adjoint operator and K a compact operator on a separable Hilbert space $\mathcal{H}$. Then for any ψ in the continuous subspace $\mathcal{H}_{\rm c}\subset\mathcal{H}$ associated to H, one has*

$$\lim_{T\to\infty}\int_0^T \frac{dt}{T}\; \|K\,e^{-\imath Ht}\,\psi\|^2 \;=\; 0\;.$$

The main ingredient of the proof is following classical result of Wiener on the Fourier transform of a measure.

3.2 Theorem (Wiener) *Let ν be a complex measure on $\mathbb{R}$. Then*

$$\lim_{T\to\infty}\int_0^T \frac{dt}{T}\;\left|\int\nu(dE)\;e^{\imath tE}\right|^2 \;=\; \sum_{E\in\mathbb{R}}|\nu(\{E\})|^2\;.$$

Proof. Let us begin by evaluating the l.h.s. before the limit:

$$\begin{aligned}\int_0^T \frac{dt}{T}\;\left|\int\nu(dE)\;e^{\imath tE}\right|^2 \;&=\; \int_0^T\frac{dt}{T}\int\nu(dE)\int\overline{\nu(dE')}\;e^{\imath t(E-E')}\\ &=\;\int\nu(dE)\int\overline{\nu(dE')}\;\left(\frac{e^{\imath T(E-E')}-1}{\imath(E-E')T}\;\delta_{E\neq E'}+\delta_{E=E'}\right)\;,\end{aligned}$$

where the δ is of Kronecker and not Dirac type. Now the integrand is bounded by 1 and therefore the dominated convergence theorem allows to move the limit inside of the integral. Thus

$$\lim_{T\to\infty}\int_0^T\frac{dt}{T}\;\left|\int\nu(dE)\;e^{\imath tE}\right|^2 \;=\;\int\nu(dE)\int\overline{\nu(dE')}\;\delta_{E=E'}\;=\;\int\nu(dE)\;\overline{\nu(\{E\})}\;,$$

which implies the result. □

3.3 Lemma *Let H be a self-adjoint operator and ψ, ϕ normalized vectors in Hilbert space. Further let μ be the spectral (probability) measure of ψ and ν the spectral (complex) measure of ψ, ϕ correspondingly, namely*

$$\langle\psi|f(H)|\psi\rangle = \int \mu(dE)\, f(E)\ , \qquad \langle\phi|f(H)|\psi\rangle = \int \nu(dE)\, f(E)\ , \qquad f \in C_0(\mathbb{R})\ . \tag{3.1}$$

Then ν is absolutely continuous w.r.t. μ and the (complex) Radon-Nykodym derivative in $\nu(dE) = g(E)\mu(dE)$ satisfies $g \in L^2(\mu) \cap L^1(\mu)$.

Proof. If P_ψ denotes the orthogonal projection on the cyclic subspace of ψ which by the spectral theorem is isomorphic to $L^2(\mu)$, then $P_\psi|\phi\rangle$ is also in the cyclic subspace and isomorphic to an element $\overline{g} \in L^2(\mu)$. But as $L^2(\mu) \subset L^1(\mu)$ for any finite measure space, the result follows. Alternatively, for any Borel set $B \subset \mathbb{R}$, the Cauchy-Schwarz inequality implies

$$|\nu(B)| \;=\; |\langle\phi|\chi_B(H)|\psi\rangle| \;\leq\; |\langle\phi|\phi\rangle|^{\frac{1}{2}}|\langle\psi|\chi_B(H)|\psi\rangle|^{\frac{1}{2}} \;=\; \mu(B)^{\frac{1}{2}}\ ,$$

where it was used that $\chi_B(H)$ is a projection. Thus ν (more precisely, its real and imaginary parts separately) is absolutely continuous w.r.t. μ and there exists a density $g \in L^1(\mu)$. To prove that g is also in $L^2(\mu)$ requires again the above argument. □

Proof of Theorem 3.1. As the compact operators are norm limits of finite rank operator, it is sufficient to prove the result for finite rank operators. Furthermore, by the triangle inequality one then shows that it is even sufficient to prove the result for a rank one operator $K = |\phi\rangle\langle\phi|$ (it is an exercise to fill in the details). Thus we need to show

$$\lim_{T\to\infty} \int_0^T \frac{dt}{T}\ \left|\langle\phi|e^{-\imath Ht}|\psi\rangle\right|^2 \;=\; 0\ .$$

But using the spectral measure ν as in (3.1) this becomes

$$\lim_{T\to\infty} \int_0^T \frac{dt}{T}\ \left|\int \nu(dE)\ e^{-\imath Et}\right|^2 \;=\; 0\ .$$

As ν has no atoms, the Wiener theorem concludes the proof. □

There are two other ways to take time averages which are technically convenient later on. One uses a gaussian cut-off, the other is obtained by averaging with an exponential weight which effectively cuts of the integral at $\frac{1}{2}T$:

$$p^{\mathrm{g}}_T(\phi,\psi) \;=\; \frac{1}{(2\pi)^{\frac{1}{2}}T} \int_{\mathbb{R}} dt\ e^{-\frac{t^2}{T^2}}\ |\langle\phi|e^{-\imath tH}|\psi\rangle|^2\ , \qquad p^{\mathrm{e}}_T(\phi,\psi) \;=\; \frac{2}{T} \int_0^\infty dt\ e^{-\frac{2t}{T}}\ |\langle\phi|e^{-\imath tH}|\psi\rangle|^2\ .$$

Using the upper bound $\chi_{[0,T]}(t) \leq e\, e^{-\frac{t^2}{T^2}}$ and $(2\pi)^{-\frac{1}{2}}\, e^{-\frac{t^2}{T^2}} \leq 2e^{-\frac{t}{T}}$ for $t \geq 0$, one gets

$$p_T(\phi,\psi) \;\leq\; e\,(2\pi)^{\frac{1}{2}}\, p^{\mathrm{g}}_T(\phi,\psi) \;\leq\; 2\,e\,(2\pi)^{\frac{1}{2}}\, p^{\mathrm{e}}_T(\phi,\psi)\ .$$

We will see further below that so-called scaling exponent are independent of the choice of time-averaging. The following formula explains why it is convenient to introduce the factor $\frac{1}{2}$ in the exponential average and also why this variant is of the interest in the first place (it is possible to calculated $p^{\mathrm{e}}_T(\phi,\psi)$ from the resolvent of H):

3.4 Lemma *Let H be a self-adjoint operator on a separable Hilbert space $\mathcal{H}$. Then*

$$p^{\rm e}_T(\phi,\psi) \;=\; \frac{1}{\pi\, T}\,\int_{\mathbb{R}} dE\;\left|\langle\phi|(E+\imath\, T^{-1}-H)^{-1}|\psi\rangle\right|^2\;.$$

Proof. Let ν be the complex spectral measure of H associated to ϕ and ψ. Then

$$\begin{aligned} p^{\rm e}_T(\phi,\psi) &= \frac{2}{T}\int_0^\infty dt\; e^{-\frac{2t}{T}}\;\int\overline{\nu(dE')}\int\nu(dE'')\;e^{\imath t(E'-E'')} \\ &= \frac{2}{T}\int\overline{\nu(dE')}\int\nu(dE'')\;\frac{-1}{2\,T^{-1}-\imath(E'-E'')} \\ &= \frac{2\,\imath}{T}\int\overline{\nu(dE')}\int\nu(dE'')\;\frac{1}{(E''-\imath\,T^{-1})-(E'+\imath\,T^{-1})} \\ &= \frac{2\,\imath}{T}\int\overline{\nu(dE')}\int\nu(dE'')\;\int\frac{dE}{2\pi\imath}\;\frac{1}{E'+\imath\,T^{-1}-E}\;\frac{1}{E''-\imath\,T^{-1}-E}\;, \end{aligned}$$

where the last equation follows from a contour integration. Now again using Fubini's theorem and replacing the spectral theorem shows the claim. □

Again a RAGE theorem can be formulated for exponential time averages. Let us directly focus on the return probability in the following proposition.

3.5 Proposition *Let H be a self-adjoint operator on a separable Hilbert space $\mathcal{H}$. If ν denotes the spectral measure of H associated to ϕ and ψ, then one has*

$$\lim_{T\to\infty}\;p^{\rm e}_T(\phi,\psi)\;=\;\lim_{T\to\infty}\;p^{\rm g}_T(\phi,\psi)\;=\;\sum_{E\in\mathbb{R}}\;|\nu(\{E\})|^2\;.$$

In particular, if ψ is in the continuous subspace $\mathcal{H}_{\rm c}\subset\mathcal{H}$ associated to H, the time-averaged transition probability $p_T(\phi,\psi)$ vanishes as $T\to\infty$.

Proof. Due to the spectral theorem, one has

$$p^{\rm e}_T(\phi,\psi)\;=\;\frac{2}{T}\int_0^\infty dt\;e^{-\frac{2t}{T}}\;\int\overline{\nu(dE)}\int\nu(dE')\;e^{\imath t(E-E')}\;=\;\int\overline{\nu(dE)}\int\nu(dE')\;\frac{1}{1+\imath\,\frac{T}{2}\,(E-E')}\;.$$

The integrand is bounded above by 1 and therefore the limit $T\to\infty$ can again be taken into the integral and one can conclude as in the proof of Wiener's theorem. Similarly for the gaussian averages,

$$p^{\rm g}_T(\phi,\psi)\;=\;\frac{1}{(2\pi)^{\frac{1}{2}}T}\int_{\mathbb{R}}dt\;e^{-\frac{t^2}{T^2}}\;\int\overline{\nu(dE)}\int\nu(dE')\;e^{\imath t(E-E')}\;=\;\int\overline{\nu(dE)}\int\nu(dE')\;e^{-\frac{1}{4}T^2(E-E')^2}\;.$$

Again one can proceed as before. □

The next aim is to get more quantitative information on the decay of transition probabilities. Roughly, one wants to show that continuity properties of the spectral measures implies decay properties of the transition properties. Such continuity properties are typically associated to fractal dimensions of the spectral measure and there is a whole zoology of such dimensions: Hausdorff dimensions, packing dimensions, multifractal dimensions, box-counting dimensions, and so on. A very rough version is the following:

3.6 Definition *Let $\alpha\in\mathbb{R}$. A probability measure μ on $\mathbb{R}$ is said to be uniformly α-continuous if there is a constant C such that for all $E\in\mathbb{R}$ and $\epsilon>0$:*

$$\mu([E-\epsilon,E+\epsilon])\;\leq\;C\,\epsilon^\alpha\;.$$

A measure with Dirac peaks has the minimal regularity $\alpha = 0$, which an absolutely continuous measure with a smooth density has $\alpha = 1$. In between are the fractal measures. However, if one considers $\mu(dE) = (E^2-1)^{-\frac{1}{2}}\chi_{|E|\leq 1}dE$ (as van Hove singularities at the band edges in dimension 1), then the regularity is only $\alpha = \frac{1}{2}$ even though this results only from the two points $E = \pm 1$. Here is a more refined definition:

3.7 Definition *The local spectral exponents of a probability measure μ on $\mathbb{R}$ are defined by*

$$\alpha_\mu(E) \;=\; \liminf_{\epsilon\to 0}\; \frac{\log(\mu([E-\epsilon,E+\epsilon]))}{\log(\epsilon)}\;.$$

The Hausdorff dimension of μ is then

$$\dim_{\rm H}(\mu) \;=\; \mu\text{-}\operatorname*{ess\,inf}_{E\in\mathbb{R}}\; \alpha_\mu(E)\;.$$

Then one can show that to every absolutely continuous measure with an integrable density has Hausdorff dimension 1. In general, for every uniformly α-continuous measure μ one has $\dim_{\rm H}(\mu)\geq\alpha$. Actually the notion of uniform α-continuity is of limit practical use because typically fractal measures have a much larger Hausdorff dimension, but it does allow to derive simple quantitative decay estimates of the transition probability based on the following result from harmonic analysis.

3.8 Theorem (Strichartz 1990) *Let μ be a uniform α-continuous probability measure on $\mathbb{R}$ and let $f\in L^2(\mu)$. Then there is a constant C such that*

$$\int_0^T \frac{dt}{T}\left|\int\mu(dE)\;f(E)\,e^{\imath tE}\right|^2 \;\leq\; C\,T^{-\alpha}\;.$$

The same holds for a gaussian time average.

Proof. Let us begin from

$$\begin{aligned}\int_0^T \frac{dt}{T}\left|\int\mu(dE)\;f(E)\,e^{\imath tE}\right|^2 \;&\leq\; \frac{e}{T}\int_{\mathbb{R}}dt\;e^{-\frac{t^2}{T^2}}\int\mu(dE)\int\mu(dE')\;\overline{f(E)}\,f(E')\,e^{\imath t(E-E')}\\ &=\; e\,(2\pi)^{\frac{1}{2}}\int\mu(dE)\int\mu(dE')\;\overline{f(E)}\,f(E')\,e^{-\frac{1}{4}T^2(E-E')^2}\\ &\leq\; e\,(2\pi)^{\frac{1}{2}}\int\mu(dE)\,|f(E)|^2\int\mu(dE')\;e^{-\frac{1}{4}T^2(E-E')^2}\;,\end{aligned}$$

where in the last step the Cauchy-Schwarz inequality was used. Now using the hypothesis

$$\begin{aligned}\int\mu(dE')\;e^{-\frac{1}{4}T^2(E-E')^2} \;&=\; \sum_{n\geq 0}\int_{\frac{n}{T}\leq|E-E'|<\frac{n+1}{T}}\mu(dE')\;e^{-\frac{1}{4}T^2(E-E')^2}\\ &\leq\; \sum_{n\geq 0}\int_{\frac{n}{T}\leq|E-E'|<\frac{n+1}{T}}\mu(dE')\;e^{-\frac{1}{4}n^2}\\ &\leq\; \sum_{n\geq 0}2\,C\,T^{-\alpha}\;e^{-\frac{1}{4}n^2}\\ &=\; C'\,T^{-\alpha}\;,\end{aligned}$$

for some constant C'. Replacing this bound completes the proof. □

Now follows the quantitative version of the RAGE theorem.

3.9 Proposition *Let H be a self-adjoint operator on a separable Hilbert space $\mathcal{H}$. Suppose that the spectral measure μ of H associated to ψ is uniformly α-continuous. Then there is a constant C such that for any ϕ*

$$p_T^{\mathrm{g}}(\phi,\psi) \;\leq\; C\,T^{-\alpha}\;.$$

Proof. By Lemma 3.3,

$$p_T^{\mathrm{g}}(\phi,\psi) \;=\; \frac{1}{(2\pi)^{\frac{1}{2}}T}\int_{\mathbb{R}} dt\; e^{-\frac{t^2}{T^2}}\;\left|\int \mu(dE)\;g(E)\,e^{\imath tE}\right|^2\;,$$

with $g \in L^2(\mu)$. Thus the result follows immediately from Strichartz theorem. □

3.2 The diffusion exponents and their basic properties

The RAGE theorem tells us that the particle leaves its initial state when the spectrum is continuous, but it does not tell us where it goes or how far it gets. Of course, in order to address such issues one needs to use the spatial structure of the Hilbert space. Let us introduce the notations

$$p_T(n,m) \;=\; p_T(|n\rangle,|m\rangle)\;,$$

for the time-averaged probability to pass from site m to n. Note that $(p_T(n,m))_{n\in\mathbb{Z}^d}$ is for each time T and initial site $m \in \mathbb{Z}^d$ a classical probability distribution:

$$\sum_{n\in\mathbb{Z}^d} p_T(n,m) \;=\; \frac{2}{T}\int_0^\infty dt\; e^{-\frac{2t}{T}}\sum_{n\in\mathbb{Z}^d}\langle m|e^{\imath Ht}|n\rangle\langle n|e^{-\imath Ht}|m\rangle \;=\; 1\;.$$

As for every classical probability distribution, one can now calcuate the moments of these distributions. For sake of concreteness, let the initial state be localized at the origin:

$$M_q(T) \;=\; \sum_{n\in\mathbb{Z}^d}|n|^q\,p_T(n,0)\;,\qquad q>0\;,\tag{3.2}$$

Now $M_q(T)$ measures the spread of the distribution and it typically grows with a powerlaw in time and the exponent of the powerlaw behavior is then by definition the diffusion exponent. For larger q, the growth is faster so that one should extract a factor q, namely one defines the diffusion exponents β_q roughly by

$$M_q(T) \;\approx\; C_q\,T^{q\beta_q}\qquad \text{as } T\to\infty\;.$$

Some mathematical care is needed to give a precise meaning to the diffusion exponents. Most used in the literature are the upper and lower exponents defined by

$$\beta_{q,+} \;=\; \limsup_{T\to\infty}\frac{\log(M_q(T))}{\log(T^q)}\;,\qquad \beta_{q,-} \;=\; \liminf_{T\to\infty}\frac{\log(M_q(T))}{\log(T^q)}\;,$$

but sometimes it is also technically convenient to work with exponents defined via Mellin transform:

$$\beta_q \;=\; \frac{1}{q}\,\inf\left\{\gamma>0\;\middle|\;\int_1^\infty dT\,T^{-1-\gamma}\,M_q(T)<\infty\right\}\;,$$

and in this latter case we also write $M_q(T)\sim T^{q\beta_q}$. We shall shortly show that $\beta_q\in[0,1]$, which is why the factor $\frac{1}{q}$ is taken out. Then the following terminology is used:

- If $\beta_q = 1$, say for all q, one speaks of ballistic motion.
- If $\beta_q = \frac{1}{2}$, say again for all q, one speaks of diffusive motion.
- If $\beta_q < \frac{1}{2}$ one speaks of subdiffusive motion, for $\beta_q > \frac{1}{2}$ of superdiffusive motion.
- For $\beta_q = 0$, the system or Hamiltonian is called localized. As a vanishing diffusion exponent does allow for logarithmically divergent terms (in time), the term dynamical localization is reserved for the situation where

$$\sup_{T>0} M_q(T) \;\leq\; C \;<\; \infty \;, \qquad q > 0 \;.$$

  One then speaks of Anderson localization, namely localization of quantum wave packets due to destructive quantum interferences.
- For any other value of the diffusion exponents one speaks of anomalous diffusion (in the framework of classical mechanics also of Levy flights), and if there is, moreover a non-trivial dependence of β_q on q of quantum intermittency.

It is also possible to define local (in energy) diffusion exponents $\beta_q(\Delta)$ by inserting spectral projections $P_\Delta = \chi_\Delta(H)$ on intervals $\Delta \subset \mathbb{R}$:

$$\sum_{n\in\mathbb{Z}^d} \int_0^T \frac{dt}{T}\; |\langle n|e^{-\imath tH}|0\rangle|^2 \;\sim\; T^{q\beta_q(\Delta)} \;.$$

This will not be developed in detail below. We will now first prove a series of general results on diffusion exponents and then come to examples towards the end of this section.

3.10 Proposition *Suppose that $|0\rangle$ is not an eigenvector of H and the matrix elements of H satisfy*

$$|\langle n|H|m\rangle| \;\leq\; C\, e^{-\eta|n-m|} \;,$$

for some positive constants η and C. Then the diffusion exponents satisfy

$$0 \;\leq\; \beta_{q,-} \;\leq\; \beta_q \;\leq\; \beta_{q,+} \;\leq\; 1 \;.$$

The functions $q \in (0,\infty) \mapsto \beta_{q,*}$ are increasing.

Proof. First let us prove $0 \leq \beta_{q,-}$. Using $n^q \geq 1$ for $n \neq 0$, one obtains

$$M_q(T) \;\geq\; \sum_{n\neq 0} p_T(n,0) \;=\; 1 - p_T(0,0) \;.$$

But $p_T(0)$ converges to some number strictly less than 1 by Proposition 3.5 and the hypothesis that $|0\rangle$ is not an eigenvector (note that this does not exclude other point spectrum). Thus $M_q(T)$ is larger than some positive constant and thus $\beta_{q,-} \geq 0$. The proofs for the inequalities $\beta_{q,-} \leq \beta_q \leq \beta_{q,+}$ are elementary and left as an exercise, so let us now focus on the bound $\beta_{q,+} \leq 1$ (this is called a ballistic upper bound). For each $\alpha > 0$ let us define $B_\alpha \subset \ell^2(\mathbb{Z}^d)$ as the set of vectors having finite norm $\|\psi\|_\alpha = \sup_{k\in\mathbb{Z}^d} e^{\alpha|k|}|\langle k|\psi\rangle| < \infty$.

Furnished with this norm B_α is actually a Banach space. Let us next show that H is a bounded operator on B_α as long as $\alpha \leq \frac{\eta}{2}$:

$$
\begin{aligned}
\|H\psi\|_\alpha &= \sup_{k\in\mathbb{Z}^d} e^{\alpha|k|}|\langle k|H|\psi\rangle| \\
&\leq \sup_{k\in\mathbb{Z}^d} e^{\alpha|k|} \sum_{n\in\mathbb{Z}^d} |\langle k|H|n\rangle|\,|\langle n|\psi\rangle| \\
&\leq \sup_{k\in\mathbb{Z}^d} e^{\alpha|k|} \sum_{n\in\mathbb{Z}^d} C\, e^{-\eta|k-n|}\,\|\psi\|_\alpha\, e^{-\alpha|n|} \\
&\leq \|\psi\|_\alpha\, C \sup_{k\in\mathbb{Z}^d} e^{\alpha|k|} \sum_{n\in\mathbb{Z}^d} e^{-2\alpha|k-n|}\, e^{-\alpha|n|} \\
&\leq \|\psi\|_\alpha\, C \sup_{k\in\mathbb{Z}^d} \sum_{n\in\mathbb{Z}^d} e^{-\alpha|k-n|}
\end{aligned}
$$

where in the last step the triangle inequality $|k-n|-|n|+|k|\geq 0$ was used. The sum over n is now finite and thus $\|H\|_\alpha < \infty$. This implies that

$$
|\langle n|e^{-\imath Ht}|0\rangle| \;\leq\; e^{-|n|\,\alpha+t\,\|H\|_\alpha}\;.
$$

Thus, for any $\epsilon > 0$,

$$
\begin{aligned}
\sum_{n\in\mathbb{Z}^d} |n|^q\,|\langle n|e^{-\imath Ht}|0\rangle|^2 &\leq t^{q(1+\epsilon)} \sum_{|n|\leq t^{1+\epsilon}} |\langle n|e^{-\imath Ht}|0\rangle|^2 + \sum_{|n|>t^{1+\epsilon}} |n|^q\, e^{-2\,|n|\,\alpha+2\,t\,\|H\|_\alpha} \\
&\leq t^{q(1+\epsilon)} + \sum_{|n|>t^{1+\epsilon}} |n|^q\, e^{-2\,|n|\,\alpha+2\,t\,\|H\|_\alpha}\;.
\end{aligned}
$$

Now the second summand vanishes in the limit $t\to\infty$. Furthermore, the inequality remains true with exponential time average so that $M_q(T)\leq T^{q(1+\epsilon)}+o(1)$ which implies $\beta_q\leq 1+\epsilon$. As ϵ is arbitrary, the inequality follows.

Now let us come to the fact that the diffusion exponents are increasing in q. Actually, the moments $M_q(T)^{\frac{1}{q}}$ are increasing in q. Indeed, as already pointed out, $p_T = (p_T(n,0))_{n\in\mathbb{Z}^d}$ is a probability measure on $\mathbb{Z}^d$ and $M_q(T) = \mathbf{E}_{p_T}(X^q)$ where X is the position operator on $\mathbb{Z}^d$. Therefore the Hölder inequality implies

$$
M_q(T) \;=\; \mathbf{E}_{p_T}(X^q\,1) \;\leq\; \mathbf{E}_{p_T}(X^p)^{\frac{q}{p}}\,\mathbf{E}_{p_T}(1)^{1-\frac{q}{p}} \;=\; M_p(T)^{\frac{q}{p}}\;,
$$

so that the claim follows. □

The a priori ballistic upper bound proved above combined with the following lemma shows that one can also use the exponential and gaussian averaged transition probabilities in (3.2) if one is only interested in calculating the diffusion exponents.

3.11 Lemma *Let f be a non-negative measurable function satisfying $f(t)\leq Ct^n$ for some $C>0$ and $n\geq 0$. Then*

$$
\liminf_{T\to\infty} \frac{\log\left(\int_0^T dt\, f(t)\right)}{\log(T)} \;=\; \liminf_{T\to\infty} \frac{\log\left(\int_0^\infty dt\, e^{-t^2/4T^2} f(t)\right)}{\log(T)}\;.
$$

Similar equalities hold for $\limsup$ *and other growth exponents, as well as an exponential mean instead of gaussian mean.*

Proof: Let α and β denote the exponents on the left and right hand side respectively. The inequality

$$\int_0^T dt\, f(t) \;\leq\; e^4 \int_0^\infty dt\, e^{-\frac{t^2}{4T^2}} f(t)$$

implies that $\alpha \leq \beta$. On the other hand, we have

$$\begin{aligned}\int_0^\infty dt\, e^{-\frac{t^2}{4T^2}} f(t) \;&\leq\; \int_0^{T^{1+\epsilon}} dt f(t) \,+\, C \int_{T^{1+\epsilon}}^\infty dt\, e^{-\frac{t^2}{4T^2}} t^n \\ &\leq\; \int_0^{T^{1+\epsilon}} dt f(t) \,+\, C' e^{-\frac{T^\epsilon}{4}} T^n \,.\end{aligned}$$

This implies that $\beta \leq (1+\epsilon)\alpha$ for any $\epsilon > 0$. The other claims are left as an exercise. □

The following so-called Guarneri bound is the main general (in the sense of model independent) connection there is between diffusion exponents and spectral properties of the Hamiltonian.

3.12 Theorem (Guarneri 1989) *Let H be a Hamiltonian on $\ell^2(\mathbb{Z}^d)$. Suppose that the spectral measure of $|0\rangle$ is uniformly α-continuous. Then*

$$\beta_{q,-} \;\geq\; \frac{\alpha}{d} \,.$$

Proof. Let us work with the gaussian time averages. Then the basic estimates are, for arbitrary N,

$$M_q^{\rm g}(T) \;\geq\; N^q \sum_{|n|>N} p_T^{\rm g}(n,0) \;\geq\; N^q \left(1 - \sum_{|n|\leq N} p_T^{\rm g}(n,0)\right) \;\geq\; N^q \left(1 - (2N+1)^d \sup_{|n|\leq N} p_T^{\rm g}(n,0)\right) \,.$$

Now using the hypothesis and Proposition 3.9 one finds

$$M_q^{\rm g}(T) \;\geq\; N^q \left(1 - C\, N^d\, T^{-\alpha}\right) \;=\; \frac{1}{2}\, (2C)^{-\frac{q}{d}}\, T^{q\,\frac{\alpha}{d}} \,,$$

where in the second inequality we chose $N = (\frac{1}{2C}\, T^\alpha)^{\frac{1}{d}}$. This completes the proof. □

3.13 Remark Theorem 3.12 can be significantly improved to

$$\beta_{q,-} \;\geq \frac{1}{d}\, \dim_{\rm H}(\mu) \,.$$

Actually this is the bound proved by Guarneri. If furthermore the so-called multifractal dimensions D_q of the spectral measure μ of H associated to $|0\rangle$ are used, another generalization is:

$$\beta_{q,-} \;\geq \frac{1}{d}\, D_{\frac{1}{1+q}} \,, \qquad q > 0 \,.$$

Also lower bounds on the upper diffusion exponents $\beta_{q,+}$ can be given in terms of packing dimensions. For a list of references, see [SB]. ◇

3.14 Remark The main message of all variants of the Guarneri bound is that continuity properties of the spectral measures (namely, α-continuity) imply diffusion properties of the wave packet spreading, and this in a quantitative way. The bounds imply, in particular:

- In dimension $d = 1$ absolutely continuous spectral measures imply ballistic transport.
- In dimension $d = 2$ it is possible to have absolutely continuous measures and nevertheless a diffusion motion.
- In dimension $d \geq 3$ one can have a (slow) subdiffusive motion even though the spectral measures are absolutely continuous.
- The Guarneri bound does not exclude non-trivial transport (positive β_q) if the spectral measures are pure point so that the Hausdorff dimension vanishes.

Now let us cite some examples. Each of them needs quite extensive analysis which can be found in the literature, except for the first one which will be studied below:

- For periodic systems (Bloch electrons) the transport is always ballistic.
- There are numerous one-dimensional quasi-periodic and almost periodic models for which one can prove that the transport is anomalous (by proving lower bounds on the Hausdorff dimension of the spectral measures and corresponding upper bounds on the transport).
- There are examples of models with $\lim_{q\to 0} \beta_q = \frac{1}{d}$ and absolutely continuous spectral measures. This means that the Guarneri bound cannot be improved (except with supplementary assumptions).
- There are several models with pure-point spectrum (so that the Hausdorff dimension of the spectral measures vanishes), but $\lim_{q\to\infty} \beta_q = 1$. In these models the Hilbert space is spanned by eigenfunctions of H, but many of these eigenfunctions are very extended.

Finally let us conclude with one of most prominent conjectures in the field Schrödinger operators: in dimension $d \geq 3$ the motion in the Anderson model (Laplacian plus random potential) is expected to be diffusion, namely $\beta_q = \frac{1}{2}$. ◇

3.3 The diffusion exponents for homogeneous Hamiltonians

Now let us come back to homogeneous operators. Then it is natural (and more simple) to consider $\mathbb{P}$-averaged moments of the position operator. Furthermore another modification of the definition of the moments is necessary. In fact, the time evolution $X_\omega(t) = e^{\imath t H_\omega} X e^{-\imath t H_\omega}$ of the position operator X is not a homogeneous operator. Actually, already the position operator itself is not a homogeneous operator. However, the difference $X_\omega(t) - X$ is again a homogeneous operator because

$$X_\omega(t) - X \;=\; \imath\, e^{\imath t H_\omega}\, \imath\, [e^{-\imath t H_\omega}, X] \;=\; \imath\, \pi_\omega \left(e^{\imath t H}\, \nabla\, e^{-\imath t H} \right) \;,$$

where H is the element of the observable algebra representing the Hamiltonian. Now one defines the averaged moments by

$$\widetilde{M}_q(T) \;=\; \int_0^T \frac{dt}{T} \int \mathbb{P}(d\omega)\, \langle 0|\, |X_\omega(t) - X|^q \,|0\rangle \;=\; \int_0^T \frac{dt}{T}\, \mathcal{T}\left(|\nabla e^{-\imath t H}|^q \right) \;.$$

Now one can go on and define diffusion exponents $\widetilde{\beta}_{q,*}$ as above, also using exponential or gaussian averages if this is technically convenient. It is worth mentioning that (2.29) following from Duhamel's formula allows to derive immediately ballistic upper bound bounds under the condition that $H \in C^1(\mathcal{A})$, in some sense in a less painless manner than before. Let us point out that in general one does not have equality between $\widetilde{M}_q(T)$ and $\mathbf{E}_{\mathbb{P}}\, M_q(T)$, but one can derive inequalities between these quantities. Moreover, the main focus will in this section be on the second moment $q = 2$ for which $X|0\rangle = 0$ leads to

$$\widetilde{M}_2(T) \;=\; \mathbf{E}_{\mathbb{P}}\, M_2(T)\;.$$

The main reason why the second moment is of great importance is that it can be calculated from the current-current correlation measure which also intervenes in the Kubo formula for the conductivity. Let us first introduce this measure and then establish the link.

3.15 Definition *Let $H \in C^1(\mathcal{A})$. The associated current-current correlation measure m on $\mathbb{R}^2$ is defined by*

$$\mathcal{T}\left(f(H)\nabla H g(H)\cdot \nabla H\right) \;=\; \int_{\mathbb{R}\times\mathbb{R}} m(dE,dE')\; f(E)\, g(E')\;, \qquad f,g\in C_0(\mathbb{R})\;,$$

where the dot denotes the scalar product $\nabla H g(H)\cdot\nabla H = \sum_{j=1}^d \nabla_j H g(H)\,\nabla_j H$.

Therefore m is a positive measure on $\mathbb{R}^2$ with finite mass $\mathcal{T}(\nabla H\cdot\nabla H)$. Now by Cauchy-Schwarz

$$|\mathcal{T}\left(f(H)\nabla_i H g(H)\,\nabla_j H\right)|^2 \;\leq\; \mathcal{T}\left(|f|^2(H)\,\nabla_i H\,|g|^2(H)\,\nabla_i H\right)\,\mathcal{T}\left(\nabla_j H\,\nabla_j H\right)$$

and thus, by the Radon-Nykodym theorem, there exist functions $D_{i,j}\in L^1(\mathbb{R}^2,m)$ such that

$$\mathcal{T}\left(f(H)\nabla_i H g(H)\,\nabla_j H\right) \;=\; \int_{\mathbb{R}\times\mathbb{R}} m(dE,dE')\, D_{i,j}(E,E')\; f(E)\, g(E')\;.$$

Let us set $m_{i,j} = D_{i,j} m$. Only the diagonal measures $m_{j,j}$ are positive, but the matrix-valued measure $(m_{i,j})_{i,j=1,\ldots,d}$ is again positive. Furthermore, if $\Delta\times\Delta'$ is a rectangle and $P_\Delta = \chi_\Delta(H)$ denotes the spectral projection on Δ, then again by Cauchy-Schwarz

$$m(\Delta\times\Delta') \;\leq\; \left(\mathcal{T}\big((P_\Delta\nabla H)^* P_\Delta\nabla H\big)\,\mathcal{T}\big((P_{\Delta'}\nabla H)^* P_{\Delta'}\nabla H\big)\right)^{\frac{1}{2}} \;\leq\; \left(\mathcal{T}(P_\Delta)\,\mathcal{T}(P_{\Delta'})\right)^{\frac{1}{2}}\;\|\nabla H\|^2\;.$$

Therefore, recalling that the density of states measure $\mathcal{N}$ is given by (2.33), one has

$$m(\Delta\times\Delta') \;\leq\; C\;\left(\mathcal{N}(\Delta)\,\mathcal{N}(\Delta')\right)^{\frac{1}{2}}\;.$$

3.16 Proposition *Let $H = H^*\in C^1(\mathcal{A})$. Then the diffusion exponent $\widetilde{\beta}_2$, calculated via Mellin transform, is given by*

$$2(1-\widetilde{\beta}_2) \;=\; \sup\left\{\gamma\in\mathbb{R}\;\middle|\;\int m(dE,dE')\;|E-E'|^{-\gamma}\;<\;\infty\right\}\;. \tag{3.3}$$

Proof. Using Duhamel's formula and the cyclicity of the trace, one gets

$$\begin{aligned}
\mathcal{T}(|\nabla(e^{-\imath Ht})|^2) \;&=\; \int_0^1 ds\int_0^1 ds'\; t^2\;\mathcal{T}\Big(e^{\imath(s-s')tH}\,\nabla H\, e^{\imath(s'-s)tH}\cdot\nabla H\Big)\\
&=\; \int_0^1 ds\int_0^1 ds'\; t^2 \int m(dE,dE')\; e^{\imath(s-s')tE}\; e^{\imath(s'-s)tE'}\\
&=\; \int m(dE,dE')\;\frac{2-2\cos((E-E')t)}{(E-E')^2}\;.
\end{aligned}$$

Hence the exponential average can be calculated:

$$\int_0^\infty \frac{dt}{T}\, e^{-\frac{t}{T}}\, \mathcal{T}(|\nabla(e^{-\imath Ht})|^2) \;=\; \int m(dE,dE')\, \frac{2\,T^2}{1+T^2(E-E')^2}\;.$$

Let now $\gamma\in\mathbb{R}$ be such that $2-\gamma>2\widetilde{\beta}_2$, that is $\gamma<2(1-\widetilde{\beta}_2)$. Fubini's theorem then leads to

$$\int_1^\infty \frac{dT}{T^{1+(2-\gamma)}} \int_0^\infty \frac{dt}{T}\, e^{-\frac{t}{T}}\, \mathcal{T}(|\nabla(e^{-\imath Ht})|^2) \;=\; \int \frac{m(dE,dE')}{|E-E'|^\gamma} \int_{|E-E'|}^\infty \frac{ds}{s^{1-\gamma}}\,\frac{2}{1+s^2}$$

The integral over s is bounded for $\gamma\in(0,2)$. From this the result follows (note that the case $\widetilde{\beta}_2=1$ is trivial). □

3.4 Kubo formula for the electrical conductivity

The aim of this section is to derive the Kubo formula for the electrical conductivity (Hall and direct) for independent electrons described by a homogeneous Hamiltonian operator H in the observable algebra $\mathcal{A}$. The way to derive this formula can be roughly summarized as follows:

- Determine the current operator J as the relevant observable for electrical conduction. The current density in a state described by a density matrix ρ is then $\mathcal{T}(J\,\rho)$.
- Consider the dynamics of ρ as given by the Liouville equation, however, with a supplementary term resulting from an external electric field $\mathcal{E}$.
- As the time averaged current still vanishes (a phenomena termed Bloch oscillations), add a dissipative collision term similar as in the Boltzmann equation.
- Calculate the current in the stationary state and linearize in the external electric field. The coefficient of the linear terms is then the conductivity.

This procedure is actually not restricted to the electrical conductivity, but is of general nature and called linear response theory. As the quantum mechanical version of it was pioneered by Kubo in the 1950's one calls the resulting formulas for the linear reponse coefficients Kubo formulas. In our derivation below, we will set all physical constants equal to 1, in particular, the Planck constant $\hbar=1$, the charge of the electron $e=1$ and the mass of the electron $m_e=1$.

Let us now begin with the current operator J. As in classical mechanics, the current is calculated from the velocity of the particles and the velocity is the time derivative of the position of the particle. The position operator is X as before, and the time derivative is due to Heisenberg's equation given by the commutator with the Hamiltonian:

$$J \;=\; \dot{X} \;=\; \imath\,[H,X] \;=\; \nabla H\;.$$

Of course, we will require $H\in C^1(\mathcal{A})$ such that $J=\nabla H$ is again a homogeneous observable. Let us also point out that $J=(J_1,\ldots,J_d)$ is vector-valued just as the position observable. Now if the system of electrons be in the Fermi-Dirac state $f_{\beta,\mu}(H)=(\mathbf{1}+e^{\beta(H-\mu)})^{-1}$ at thermodynamic equilibrium. Then the current density is given by

$$j_{\beta,\mu} \;=\; \mathcal{T}(f_{\beta,\mu}(H)\,J)\;.$$

First of all let us note that this is well-defined because $f_{\beta,\mu}(H)$ and J are homogeneous observables and therefore so is their product, and the trace per unit volume is defined for all homogeneous observables (elements of the algebra $\mathcal{A}$). On the other hand, the following proposition shows that the current density vanishes as it should on physical grounds.

3.17 Proposition *Let $H = H^*$ be an element of $C^1(\mathcal{A})$ and $f \in C_0(\mathbb{R})$. Then $\mathcal{T}(f(H)\nabla H) = 0$.*

Proof. As the trace $\mathcal{T}$ is invariant under ∇, Leibniz rule implies $0 = \mathcal{T}(\nabla H^n) = n\mathcal{T}_{\mathbf{B}}(H^{n-1}\nabla H)$ for all $n \geq 1$. Thus by density $\mathcal{T}(f(H)\nabla H) = 0$ for any continuous function. $\Box$

Next let us change the dynamics by adding a constant external electric field $\mathcal{E} \in \mathbb{R}^d$. The potential energy at X is then $\mathcal{E} \cdot X$ and thus the new Hamiltonian is $H_{\mathcal{E}} = H + \mathcal{E} \cdot X$. This operator is clearly neither bounded nor homogeneous and thus not in $\mathcal{A}$. On the other hand, all we need is the associated time evolution remains in the algebra $\mathcal{A}$. In the Schrödinger picture it is governed by the Liouville equation:

$$\partial_t \rho \;=\; -\imath\,[H_{\mathcal{E}}, \rho] \;=\; -\imath\,[H + \mathcal{E} \cdot X, \rho] \;=\; -\mathcal{L}_H(\rho) \;+\; \mathcal{E} \cdot \nabla(\rho)\,. \tag{3.4}$$

At this point, it is necessary to guarantee the existence of solutions of this equation. Indeed, on the r.h.s. appears the sum of two generators, one of which is unbounded. A Dyson series argument is one of the standard procedures to deal with this type of a situation.

3.18 Proposition *$\pm\mathcal{L}_H + \mathcal{E} \cdot \nabla$ are generators of automorphism groups in $\mathcal{A}$.*

Proof. For sake of concreteness we restrict ourselves to the sign $+$ and then denote $\mathcal{L}_{H_{\mathcal{E}}} = \mathcal{L}_H + \mathcal{E} \cdot \nabla$. Let us also set $\eta_t = e^{t\mathcal{E}\cdot\nabla}$ for the automorphism group defined in (2.26). The idea is now to use the formal identity

$$e^{t\mathcal{L}_{H_{\mathcal{E}}}} \;=\; e^{t\mathcal{E}\cdot\nabla} \;+\; \int_0^t ds\; e^{(t-s)\mathcal{E}\cdot\nabla}\mathcal{L}_H e^{s\mathcal{L}_{H_{\mathcal{E}}}}\;, \tag{3.5}$$

which follows from integrating

$$\partial_s\, e^{(t-s)\mathcal{E}\cdot\nabla}\, e^{s\mathcal{L}_{H_{\mathcal{E}}}} \;=\; e^{(t-s)\mathcal{E}\cdot\nabla}\mathcal{L}_H e^{s\mathcal{L}_{H_{\mathcal{E}}}}\;.$$

However, this is formal because $e^{s\mathcal{L}_{H_{\mathcal{E}}}}$ is to be constructed and appears both on the left and right hand side of 3.5. But one can next iterate (3.5):

$$\begin{aligned} e^{t\mathcal{L}_{H_{\mathcal{E}}}} \;&=\; e^{t\mathcal{E}\cdot\nabla} \;+\; \int_0^t ds\; e^{(t-s)\mathcal{E}\cdot\nabla}\mathcal{L}_H e^{s\mathcal{E}\cdot\nabla} \;+\; \int_0^t ds \int_0^s ds'\; e^{(t-s)\mathcal{E}\cdot\nabla}\mathcal{L}_H e^{(s-s')\mathcal{E}\cdot\nabla}\mathcal{L}_H e^{s'\mathcal{L}_{H_{\mathcal{E}}}} \\ &=\; e^{t\mathcal{E}\cdot\nabla} \;+\; \sum_{n\geq 1}\int_0^t ds_1 \int_0^{s_1} ds_2 \cdots \int_0^{s_{n-1}} ds_n\; e^{(t-s_1)\mathcal{E}\cdot\nabla}\mathcal{L}_H e^{(s_1-s_2)\mathcal{E}\cdot\nabla}\cdots\mathcal{L}_H e^{s_n\mathcal{E}\cdot\nabla}\;. \end{aligned}$$

Now all terms on the r.h.s. are well-defined and, moreover, the sum over n is weakly convergent because $e^{s\mathcal{E}\cdot\nabla}$ is a (norm-conserving) automorphism and $\|\mathcal{L}_H(A)\| \leq 2\|H\|\,\|A\|$ for $A \in \mathcal{A}$, so that

$$\|e^{t\mathcal{L}_{H_{\mathcal{E}}}}(A)\| \;\leq\; \|A\| + \sum_{n\geq 1}\int_0^t ds_1 \int_0^{s_1} ds_2 \cdots \int_0^{s_{n-1}} ds_n\; (2\|H\|)^{n-1}\|A\| \;=\; \left(1 + \sum_{n\geq 1}\frac{(2t\|H\|)^n}{2\|H\|n!}\right)\|A\|\,.$$

Thus the Dyson series converges and can be used to define $A(t) = e^{t\mathcal{L}_{H_{\mathcal{E}}}}(A)$. Deriving shows

$$\partial_t A(t) \;=\; \mathcal{E} \cdot \nabla(A(t)) \;+\; \mathcal{L}_H(A(t)) \;=\; \mathcal{L}_{H_{\mathcal{E}}}(A(t))\;.$$

Thus (3.4) holds (up to the sign because we considered observables and not density matrices). $\Box$

3.19 Remark A modification of the procedure combine with Stone's theorem allows to show that $H_{\mathcal{E}} = H + \mathcal{E} \cdot X$ is a self-adjoint operator (with adequate domain). More generally, if H_0 is self-adjoint and V is bounded, then also $H_0 + V$ is self-adjoint (note that in the above $\mathcal{E} \cdot X$ is the unbounded part). $\diamond$

Next let us consider the time-averaged current under the dynamics with presence of a magnetic field. It is defined by

$$j_{\beta,\mu,\mathcal{E}} \;=\; \lim_{T\to\infty} \frac{1}{T}\int_0^T dt\; \mathcal{T}\big(f_{\beta,\mu}(H)\; e^{t\mathcal{L}_{H_{\mathcal{E}}}}(J)\big)\;. \tag{3.6}$$

Because the trace $\mathcal{T}$ is invariant under both ∇ and $\mathcal{L}_H$, the Dyson series shows that

$$j_{\beta,\mu,\mathcal{E}} \;=\; \lim_{T\to\infty} \frac{1}{T}\int_0^T dt\; \mathcal{T}\big(J\, e^{-t\mathcal{L}_{H_{\mathcal{E}}}}(f_{\beta,\mu}(H))\big)\;. \tag{3.7}$$

The equality of (3.6) and (3.7) is only a manifestation of the fact that one can either calculate in the Schrödinger picture (evolution of density matrices) or in the Heisenberg picture (evolution of observables). Let us also point out that one may replace the time average by an exponential or gaussian time average without changing the value of $j_{\beta,\mu,\mathcal{E}}$. Now one has:

3.20 Proposition *The time-averaged current $j_{\beta,\mu,\mathcal{E}}$ along the direction of the electric field $\mathcal{E}$ vanishes.*

Proof. Let us compute $\mathcal{E}\cdot J(t)$ where $J(t) = e^{t\mathcal{L}_{H_{\mathcal{E}}}}(J)$. Using the Heisenberg equation it is easy to see that

$$\mathcal{E}\cdot J(t) \;=\; e^{t\mathcal{L}_{H_{\mathcal{E}}}}(\mathcal{E}\cdot\nabla(H)) \;=\; e^{t\mathcal{L}_{H_{\mathcal{E}}}}(\mathcal{L}_{H_{\mathcal{E}}}(H)) \;=\; \frac{dH(t)}{dt}\;,$$

if $H(t) = e^{t\mathcal{L}_{H_{\mathcal{E}}}}(H)$. Taking the time average gives us

$$\frac{1}{T}\int_0^T dt\; \mathcal{E}\cdot J(t) = \frac{H(T)-H}{T}$$

Since H is bounded in norm and $\|H(t)\| = \|H\|$, the r.h.s. vanishes as $T\to\infty$. □

The fact proved in Proposition 3.20 is known in the physics community under the name of Bloch oscillations. In the so-called semiclassical picture [AM] the Bloch electrons are described as classical particles moving along the constant energy surfaces given by the Bloch bands. As these are typically given by compact manifold (such as circles or spheres), this motion comes (arbitrarily close) back to its initial condition so that time averages along the orbit vanish. The main conclusion drawn from it is that adding a dissipative term to the time evolution is a necessity. One way to do this is to add a collision term as in the Boltzmann equation of classical mechanics. Let us first consider the situation without external field, namely $\mathcal{E} = 0$. Then the quantum Boltzmann equation is

$$\partial_t\,\rho + \mathcal{L}_H(\rho) \;=\; -\,\Gamma(\rho)\;. \tag{3.8}$$

Here Γ is the collision operator sending homogeneous density matrices to homogeneous density matrices (Γ is a positivity and trace preserving superoperator on $\mathcal{A}$). It can be quadratic in ρ if binary collisions between electrons are described, or even of fourth order in ρ if also Pauli blocking is modelled. If only collisions with an external bath (of phonons) are taken into account, then Γ is linear in ρ and we restrict ourselves to this case because then existence of solutions of (3.8) is guaranteed. It is possible to make more concrete physical models for Γ by using the underlying scattering processes, but this will not be done here as these details will not be essential for the derivation of the Kubo formula. Now (3.8) should describe the thermalization of the electron system with the bath, namely the solution $\rho(t)$ of (3.8) should satisfy

$$\rho(t) \;\to\; f_{\beta,\mu}(H)\;, \qquad \text{as }\; t\to\infty\;,$$

where μ is such that $\mathcal{T}(f_{\beta,\mu}(H)) = \mathcal{T}(\rho(0))$ and β is specified by Γ (which depends beneath other things on temperature of the bath). In particular, $f_{\beta,\mu}(H)$ should be a fixed point of the dynamics and this is equivalent to

$$\Gamma(f_{\beta,\mu}(H)) \;=\; 0\;. \tag{3.9}$$

We will not dwell further on these thermalization properties, but rather consider the situation where again an electric field is added. Then the time evolution of the density matrix is given by

$$\partial_t\,\rho + \mathcal{L}_H(\rho) - \mathcal{E}\cdot\nabla(\rho) \;=\; -\,\Gamma(\rho)\;. \tag{3.10}$$

Again the argument from Proposition 3.18 shows that the solution exists. It will be denoted again by

$$\rho(t) \;=\; e^{-t(\mathcal{L}_H-\mathcal{E}\cdot\nabla+\Gamma)}(\rho(0))\;.$$

The initial state is chosen to be the thermal equilibrium state $\rho(0) = f_{\beta,\mu}(H)$, the physical input being that the system is at thermal equilibrium at time $t = 0$ when the electric field is turned on. The time-averaged current density given as in (3.7) but with an exponential average becomes

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

Thanks to Proposition 3.17, the current carried by the equilibrium state vanishes and therefore we can subtract

$$0 \;=\; \delta\,\mathcal{T}\left(J\,\frac{1}{\delta}\;f_{\beta,\mu}(H)\right) \;=\; \delta\,\mathcal{T}\left(J\,\frac{1}{\delta+\mathcal{L}_H+\Gamma}\,(f_{\beta,\mu}(H))\right)\;,$$

where we used (3.9) to conclude that $(\mathcal{L}_H+\Gamma)(f_{\beta,\mu}(H)) = 0$. Combined with the resolvent identity this leads to:

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

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

$$j_{\beta,\mu,\mathcal{E}} \;=\; \lim_{\delta\to 0}\;\sum_{j=1}^d \mathcal{E}_j\;\;\mathcal{T}\left(J\;\frac{1}{\delta+\Gamma+\mathcal{L}_H-\mathcal{E}\cdot\nabla}(\nabla_j f_{\beta,\mu}(H))\right)\;. \tag{3.11}$$

If now $\nabla f_{\beta,\mu}(H)$ is in the domain of the inverse of $\Gamma+\mathcal{L}_H-\mathcal{E}\cdot\nabla$, the limit $\delta\to 0$ can be taken. One obtains a closed and mathematically sound formula for the current, with all non-linear terms in the electric field $\mathcal{E}$. Most of the time, one is interested in small electric field and therefore wants to extract only the linear behavior in $\mathcal{E}$. The linear coefficients $\sigma_{i,j}(\beta,\mu)$, $i,j = 1\ldots d$, of $(j_{\beta,\mu,\mathcal{E}})_i$ with respect to the electric field, define the conductivity tensor. We therefore have proved the following result:

3.21 Theorem *Suppose the time-evolution of density matrices is given by* (3.10) *with initial condition* $\rho(0) = f_{\beta,\mu}(H)$ *and with a linear collision operator* Γ *on* $\mathcal{A}$ *satisfying* (3.9). *If the inverse of* $\Gamma+\mathcal{L}_H$ *contains* $\nabla f_{\beta,\mu}(H)$ *in its domain, the conductivity tensor is given by the following Kubo formula:*

$$\sigma_{i,j}(\beta,\mu) \;=\; \mathcal{T}\left(\nabla_i H\;\frac{1}{\Gamma+\mathcal{L}_H}(\nabla_j f_{\beta,\mu}(H))\right)\;. \tag{3.12}$$

The Kubo formula still contains, apart from the homogeneous Hamiltonian H, the collision operator Γ as supplementary input. As already pointed out, detailed physical modeling of Γ is possible, but here we restrict ourself to a very rough model, namely the so-called relaxation time approximation in which Γ is simply replaced by a number $\frac{1}{\tau}$ multiplied with the identity operator:

$$\sigma_{i,j}(\beta,\mu,\tau) \;=\; \mathcal{T}\left(\nabla_i H\,\frac{1}{\frac{1}{\tau}+\mathcal{L}_H}(\nabla_j f_{\beta,\mu}(H))\right)\,. \tag{3.13}$$

Let us point out that the inverse of $\frac{1}{\tau}+\mathcal{L}_H$ indeed exists because $\mathcal{L}_H$ is an anti-self-adjoint operator on the Hilbert space $L^2(\mathcal{A},\mathcal{T})$ and therefore has its spectrum lying on the imaginary axis so that the real part $\frac{1}{\tau}$ allows to define the inverse by spectral calculus. Of course, problems may arise in the limit $\tau\to\infty$ where this real part vanishes. The number τ is called the relaxation time. This simple approximation of the collision operator is well-known [AM] for the classical Boltzmann equation where τ is then interpreted as the mean time between collisions with scatterers (in solids typically the phonons). Some more details can be found in [BES].

The Hall conductivity is the (anti-symmetric!) off-diagonal part of the conductivity tensor. It will be analyzed in detail later, here let us rather focus on the direction-averaged direct conductivity $\sigma(\beta,\mu,\tau)$ given by the average of the diagonal entries of the conductivity tensor:

$$\sigma(\beta,\mu,\tau) \;=\; \frac{1}{d}\sum_{j=1}^{d}\sigma_{j,j}(\beta,\mu,\tau)\,.$$

By the following result it can conveniently be calculated from the conductivity measure m introduced in Definition 3.15.

3.22 Proposition *In the relaxation time approximation, the direction-averaged direct conductivity is given by*

$$\sigma(\beta,\mu,\tau) \;=\; \frac{1}{d\,\tau}\int m(dE,dE')\,\frac{f_{\beta,\mu}(E')-f_{\beta,\mu}(E)}{E-E'}\,\frac{1}{\frac{1}{\tau^2}+(E-E')^2}\,. \tag{3.14}$$

Proof. Let us start from (3.13). In order to use the current-current correlation measure we need to express $\nabla f_{\beta,\mu}(H)$ in terms of ∇H:

$$\nabla f_{\beta,\mu}(H) \;=\; -\,f_{\beta,\mu}(H)\,\nabla e^{\beta(H-\mu)}\,f_{\beta,\mu}(H) \;=\; -\,f_{\beta,\mu}(H)\,e^{-\beta\mu}\int_0^\beta ds\;e^{sH}\,\nabla H\,e^{(\beta-s)H}\,f_{\beta,\mu}(H)\,.$$

As for continuous functions f,F,g,

$$\mathcal{T}\big(f(H)\,\nabla H\cdot F(\mathcal{L}_H)\big(g(H)\nabla H\big)\big) \;=\; \int m(dE,dE')\,f(E)\,F(\imath(E'-E))\,g(E')\,,$$

on thus has (using Fubini's theorem) that

$$\begin{aligned}
\sigma(\beta,\mu,\tau) \;&=\; -\frac{1}{d}\int_0^\beta ds\;e^{-\beta\mu}\int m(dE,dE')\,f_{\beta,\mu}(E)\,\frac{1}{\frac{1}{\tau}+\imath(E'-E)}\,e^{sE}\,e^{(\beta-s)E'}\,f_{\beta,\mu}(E')\\
&=\; \frac{1}{d}\int m(dE,dE')\,\frac{1}{\frac{1}{\tau}+\imath(E'-E)}\,f_{\beta,\mu}(E)\,f_{\beta,\mu}(E')\,\frac{e^{\beta(E-\mu)}-e^{\beta(E'-\mu)}}{E'-E}\\
&=\; \frac{1}{d}\int m(dE,dE')\,\frac{1}{\frac{1}{\tau}+\imath(E'-E)}\,\frac{f_{\beta,\mu}(E)-f_{\beta,\mu}(E')}{E'-E}\,.
\end{aligned}$$

Now the cyclicity of the trace implies that

$$\int m(dE, dE')\, f(E, E') \;=\; \frac{1}{2} \int m(dE, dE')\, \big(f(E, E') + f(E', E)\big)\,. \tag{3.15}$$

From this one readily deduces the result. □

Now let us study the behavior of the direct conductivity in limit of large relaxation time, that is, small dissipation. The result has important physical consequences discussed below.

3.23 Theorem [SBB] *If $\beta < \infty$, the direct conductivity given in* (3.14) *satisfies*

$$\sigma(\beta, \mu, \tau) \underset{\tau\uparrow\infty}{\sim} \tau^{-1+2\widetilde{\beta}_2}\,, \tag{3.16}$$

where the exponent is defined via Mellin transform.

Proof. The integrand in (3.14) is positive (because the Fermi-Dirac function has a negative slope) such that we may apply Fubini's theorem. After a change of variables we obtain

$$\int_1^\infty \frac{d\tau}{\tau^{1+\gamma}}\, \sigma(\beta, \mu, \tau) \;=\; \frac{1}{d} \int dm(E, E')\, \frac{f_{\beta,\mu}(E') - f_{\beta,\mu}(E)}{E - E'}\, (E - E')^{\gamma - 1} \int_{E-E'}^\infty ds\, \frac{s^{-\gamma}}{s^2 + 1}\,.$$

The integral over s is bounded for $-1 < \gamma < 1$. For $\beta < \infty$, the only singularity in the integrand of m comes from the factor $(E - E')^{\gamma-1}$. The result now follows from Proposition 3.16 □

Let us highlight some special cases:

- If transport is ballistic, namely $\widetilde{\beta}_2 = 1$ as for Bloch electrons, then $\sigma(\beta, \mu, \tau) \sim \tau$. This is the same behavior as in the Drude formula derived from a stochastically scattered motion of a classical free particle in 1900 [AM]. Therefore 3.16 is called the anomalous Drude formula.

- If the motion is superdiffusive, namely $\widetilde{\beta}_2 > \frac{1}{2}$, then the conductivity diverges in the zero dissipation limit. This means that dissipation is needed in order to have a well-defined finite conductivity.

- If the motion is subdiffusive, namely $\widetilde{\beta}_2 < \frac{1}{2}$, then the conductivity vanishes in the zero dissipation limit. This means again that dissipation is needed in order to have a well-defined finite conductivity.

- Only if $\widetilde{\beta}_2 = \frac{1}{2}$ so that one has a quantum diffusive motion, the conductivity can be finite at zero dissipation. This reflects the Einstein relation that the conductivity is up to a constant equal to the diffusion constant (namely the prefactor D in $X^2(t) \cong Dt$).

This does not mean that the relaxation time approximation is viable in all situations. For example, in the case of a system in the Anderson localizaed phase, it is not and a different approach is needed.

4 Integer quantum Hall effect

4.1 Brief introduction to the physics of the quantum Hall effect

At the interface between two differently doped semiconductors there is a potential well. At low temperatures (say below 1 Kelvin) all particles are in the fundamental of the well. Thus one effectively has a two-dimensional electron gas. The sample size is at least a few microns wide, which corresponds to about

10000 atoms. By varying a so-called gate voltage it is possible to modidify the number of electrons in the two-dimensional system, that is, change its chemical potential. Moreover, due to the doping the electron gas is submitted to a disordered potential. Now suppose that such a sample is a placed in a strong perpendicular constant magnetic field B (typically more than 1 Tesla). Then one measures the Hall conductance of the sample, namely the quotient of the current I through the sample (forced by some battery) and the measured tension U transverse to I. This Hall conductance is a macroscopic quantity of a solid state system. The suprising experimental finding is that it is nevertheless equal to an integer multiple of $\frac{e^2}{h}$ (here e is the electron charge, and h the Planck constant) for a wide range of magnetic fields B and chemical potentials μ. This so-called quantization of the Hall conductance is completely different nature than the quantization of atomic levels. As we shall see in this section, it results from an interplay of two phenomena:

- topological invariants associated to quantum mechanical phases
- Anderson dynamical localization

The basic explanation of the effect uses the so-called Landau Hamiltonian with core $C_0^\infty(\mathbb{R}^2)$:

$$H_L \;=\; \frac{1}{2}\,(\imath\partial - A)^2\;,$$

where $\partial = (\partial_1, \partial_2)$ are the partial derivatives and $A = (A_1, A_2)$ a vector potential (vector-valued function on $\mathbb{R}^2$) satisfying

$$\partial_1 A_2 - \partial_2 A_1 = B\;.$$

There are two standard choices for the gauge, the symmetric gauge $A(r,\theta) = (-\frac{B}{2}r\sin(\theta), \frac{B}{2}r\cos(\theta))$ (expressed in polar coordinates) and the Landau gauge $A(x_1, x_2) = (-Bx_2, 0)$. For sake of concreteness, let us work with the Landau gauge here and introduce the following operators (all with common core $C_0^\infty(\mathbb{R}^2)$)

$$D_1 \;=\; \imath\partial_1 + BX_2\;,\qquad D_2 \;=\; \imath\partial_2\;,\qquad K_1 \;=\; \imath\partial_1\;,\qquad K_2 \;=\; \imath\partial_2 + BX_1\;.$$

Then the Landau operator can be written as $H_L = \frac{1}{2}(D_1^2 + D_2^2)$. As $[D_1, D_2] = \imath B$, this shows that the Landau operator is actually a harmonic oscillator and its spectrum is given by

$$E_n = B\left(n + \frac{1}{2}\right)\;,\qquad n \in \mathbb{N}\;.$$

However, one readily verifies that both $K_{1,2}$ commute with both $D_{1,2}$. Hence the Landau operator has a large symmetry group and each of its eigenvalues is infinitely degenerated. Moreover, it can be shown that these eigenfunctions span the whole Hilbert space so that there is no other spectrum. One calls the energies E_n the Landau bands or Landau levels. It is possible (with rigorous proofs) to show that, as long as the chemical potential lies between two Landau levels and the temperature is 0, the Hall conductivity as calculated by the Kubo formula is quantized. Furthermore, one can show stability w.r.t. to perturbations by a random potential. Instead of this theory in continuous space, we will here rather focus on tight-binding models on discrete physical space. Thus a typical Hamiltonian on $\ell^2(\mathbb{Z}^2)$ is given by

$$H_\omega \;=\; U_1 + U_1^* + U_2 + U_2^* + V_\omega\;,$$

where U_1 and U_2 are the magnetic translations associated to the magnetic field B as defined in (2.1) and $V_\omega = \sum_{n\in\mathbb{Z}^2} v_{\omega,n}\;|n\rangle\langle n|$ is a random potential. However, the explicit form of the operator will not be relevant below and all that is really needed is that $(H_\omega)_{\omega\in\Omega}$ is a homogeneous family of operators on $\ell^2(\mathbb{Z}^2)$. We will investigate the Kubo formula for the Hall conductivity below.

Before that we will investigate another phenomena present in quantum Hall systems, namely edge currents. That such currents are present can already be understood for charged particles described by classical mechanics. Indeed, when submitted to a magnetic field these particles move on cyclotron orbits. In presence of a hard wall boundary, they are reflected but continue to rotate in the same orientation. This leads to edge currents along the boundary, also called chiral currents. In the next section, we will study these currents in a quantum mechanical model and prove a quantization result for them. The connection to the Kubo formula is then analyzed below.

4.2 Edge currents and their quantization

Let $(H_\omega)_{\omega\in\Omega}$ is a homogeneous family of operators on $\ell^2(\mathbb{Z}^2)$ which for sake of simplicity is assumed to be of finite range throughout this section. The restriction of each operator to the half-space $\ell^2(\mathbb{Z}\times\mathbb{N})$ is denoted by $\widehat{H}_\omega$. Actually, all operators on the half-space will carry a hat from now on. By restriction, we mean that simply all matrix elements from and to sites not in $\mathbb{Z}\times\mathbb{N}$ are set to 0. The family $(\widehat{H}_\omega)_{\omega\in\Omega}$ is still covariant in the 1-direction, but not the 2-direction. The observable for edge currents along the boundary is the 1-component $\widehat{J}_1$ of the current operator. Let $\widehat{\rho} = g(\widehat{H})$ be a density matrix defined by spectral calculus from a real valued smooth function g on $\mathbb{R}$ with $\int dE\, g(E) = 1$. Now the edge current $j^{\mathrm{e}}(g)$ is defined by

$$j^{\mathrm{e}}(g) \;=\; \widehat{\mathcal{T}}\big(\widehat{J}_1\, g(\widehat{H})\big)\;, \tag{4.1}$$

where $\widehat{\mathcal{T}} = \mathcal{T}_1\,\mathrm{Tr}_2$ is the trace per unit volume in the 1-direction along the boundary and Tr_2 the usual trace in the 2-direction perpendicular to the boundary. For any operator family $\widehat{A} = (\widehat{A}_\omega)_{\omega\in\Omega}$ on $\ell^2(\mathbb{Z}\times\mathbb{N})$ which is homogeneous in the 1-direction, it is more formally defined by

$$\widehat{\mathcal{T}}(\widehat{A}) \;=\; \mathbf{E}_{\mathbb{P}} \sum_{n_2\geq 0} \langle 0, n_2|\widehat{A}_\omega|0,n_2\rangle\;. \tag{4.2}$$

As is obvious from this definition, not all operators $\widehat{A}$ are traceclass w.r.t. $\widehat{\mathcal{T}}$ due to the sum over n_2. Thus one has to prove that (4.1) actually makes sense for adequate functions g. This is part of the result below.

4.1 Theorem [KRS] *Let Δ be a gap of the (almost sure) spectrum of $H \in C^1(\mathcal{A})$. Then for any function g with $\mathrm{supp}(g)\subset\Delta$ and $\int dE\, g(E) = 1$, the operator $g(\widehat{H})$ is $\widehat{\mathcal{T}}$-traceclass and one has*

$$j^{\mathrm{e}}(g) \;=\; \mathrm{Ind}\;, \tag{4.3}$$

where Ind *is the Winding number of*

$$\widehat{U}_\omega(g) \;=\; \exp\big(2\,\pi\,\imath\, G(\widehat{H}_\omega)\big)\;,$$

where $G(E) = \int_{-\infty}^{E} dE'\, g(E')$. This winding number is also equal to the $\mathbb{P}$-almost sure index of the Fredholm operator $\Pi_1^*\widehat{U}_\omega(g)\Pi_1$ where Π_1 is the embedding of the quarter plane Hilbert space $\ell^2(\mathbb{N}\times\mathbb{N})$ into $\ell^2(\mathbb{Z}\times\mathbb{N})$.

Before going into the proof let us discuss briefly the physics behind the definition (4.1) and Theorem 4.1. First of all, the trace $\widehat{\mathcal{T}}$ is used in (4.1) because the current flows everywhere along the boundary (*cf.* the classical picture of reflected cyclotron orbits), but the quantum states carrying these boundary currents do not have a support restricted to a finite strip along the boundary. Therefore one has to trace out the full 2-direction in (4.1) in order to calculate the full boundary current. As to the interpretation of (4.3), let us first claim without proof that this equation holds (under a continuity assumption on the density of boundary states) also for the non-continuous function $g = \frac{1}{|\Delta'|}\,\chi_{\Delta'}$ where $\Delta' \subset \Delta$ is a given subinterval. Then (4.3) can be written as

$$\widehat{\mathcal{T}}\big(\widehat{J}_1\,\chi_{\Delta'}(\widehat{H})\big) \;=\; |\Delta'|\;\mathrm{Ind}\;, \tag{4.4}$$

which holds for all $\Delta' \subset \Delta$. Now Δ' is interpreted as the difference of chemical potentials on the two opposite boundaries of a (infinitely long) sample. This difference of chemical potentials in turn can be interpreted as the Hall tension measured. Furthermore, the edge currents on the opposite boundaries have a different orientation and if the two boundaries are sufficiently far apart so that they are independent, then modeling them by separate half-space geometries seems adequate (tunnel effects from one boundary to the other decay exponentially in the distance and this gives correction terms). Therefore, the net current through the boundary states is given by the current carried by the surplus of states on one of the boundaries, namely those states lying in Δ'. Resuming, (4.4) provides a theoretical explanation of the quantum Hall effect based on edge currents only.

The first point of the proof is that (4.3) is well-defined. Let $\Pi : \ell^2(\mathbb{Z}^2) \to \ell^2(\mathbb{Z}\times\mathbb{N})$ denote the partial isometry from $\ell^2(\mathbb{Z}^2)$ onto $\ell^2(\mathbb{Z}\times\mathbb{N})$, namely $\Pi\Pi^*$ is the identity on $\ell^2(\mathbb{Z}\times\mathbb{N})$ and $\Pi^*\Pi$ is the projection on $\ell^2(\mathbb{Z}\times\mathbb{N})$ seen as subspace of $\ell^2(\mathbb{Z}^2)$. Then one has $\widehat{H} = \Pi H \Pi^*$.

4.2 Proposition *For any smooth non-negative function g of compact support lying in a gap of the spectrum of H, then the operator $g(\widehat{H})$ is $\widehat{\mathcal{T}}$-traceclass.*

For the proof, we will use a tool which is of independent interest.

4.3 Proposition *Let $g : \mathbb{R} \to \mathbb{C}$ be a smooth function of compact support and $\chi : \mathbb{R} \to [0,1]$ also smooth, even, compactly supported, and equal to 1 on $[-\delta,\delta]$. For a given $N \geq 1$, let us then introduce a so-called quasi-analytic extension $\widetilde{g} : \mathbb{C} \to \mathbb{C}$ of g by*

$$\widetilde{g}(x,y) \;=\; \sum_{n=0}^{N} g^{(n)}(x)\,\frac{(\imath y)^n}{n!}\,\chi(y)\;, \qquad z = x + \imath y\;.$$

If furthermore $\partial_{\overline{z}} = \partial_x + \imath\partial_2$ as usual, then for any bounded self-adjoint operator H the functional calculus can be done by the Helffer-Sjöstrand formula:

$$g(H) \;=\; \frac{-1}{2\pi}\int_{\mathbb{R}^2} dx\,dy\;\partial_{\overline{z}}\widetilde{g}(x,y)\;(z-H)^{-1}\;, \qquad z = x+\imath y\;, \tag{4.5}$$

where the integral is defined as norm-convergent Riemann sum. In particular, the r.h.s. is independent of the choice of N and χ.

Proof. Let $\mathrm{supp}(\chi) \subset [-1,1]$. Then $\widetilde{g}$ is smooth and compactly supported on a rectangle given by $\{(x,y)\,|\,x\in I,\ |y|\leq 1\}$ where I is an inteval containing the support of g. The crucial identity is

$$\begin{aligned}\partial_{\overline{z}}\widetilde{g}(x,y) \;&=\; \sum_{n=0}^{N} g^{(n+1)}(x)\,\frac{(\imath y)^n}{n!}\,\chi(y) \;-\; \sum_{n=1}^{N} g^{(n)}(x)\,\frac{(\imath y)^{n-1}}{(n-1)!}\,\chi(y) \;+\; \imath\sum_{n=0}^{N} g^{(n)}(x)\,\frac{(\imath y)^n}{n!}\,\chi'(y)\\ &=\; g^{(N+1)}(x)\,\frac{(\imath y)^N}{N!}\,\chi(y) \;+\; \imath\sum_{n=0}^{N} g^{(n)}(x)\,\frac{(\imath y)^n}{n!}\,\chi'(y)\;.\end{aligned}$$

In particular, uniformly in x, y,

$$|\partial_{\overline{z}}\widetilde{g}(x,y)| \;\leq\; C\,|y|^N\;. \tag{4.6}$$

Note that this also shows that $\partial_{\overline{z}}\widetilde{g}(x,0)=0$. As furthermore by self-adjointness

$$\|(z-H)^{-1}\| \;\leq\; \frac{1}{|y|}\;,$$

the integral on the r.h.s. of (4.5) converges in the norm sense (indeed, as $N\geq 1$, the integrand remains bounded and the size of a rectangle around the real axis goes to 0 with its width vanishing). It is thus sufficient to show that for every $E\in\mathbb{R}$ the numbers

$$g_\epsilon(E) \;=\; \frac{-1}{2\pi}\int_{|y|\geq\epsilon} dx\,dy\;\partial_{\overline{z}}\widetilde{g}(x,y)\;\frac{1}{z-E}\;,$$

converge to $g(E)$ in the limit $\epsilon\downarrow 0$, and this independent of N and χ. By partial integration in x and y separately, one finds

$$g_\epsilon(E) \;=\; \int_{|y|\geq\epsilon}\frac{dx\,dy}{2\pi}\;\widetilde{g}(x,y)\;\partial_{\overline{z}}\;\frac{1}{z-E}\;+\;\int_{\mathbb{R}}\frac{dx}{2\pi}\;\left(\frac{\widetilde{g}(x,\epsilon)}{x+\imath\epsilon-E}-\frac{\widetilde{g}(x,-\epsilon)}{x-\imath\epsilon-E}\right)$$

The first summand vanishes because $(z-E)^{-1}$ is analytic away from the real axis. In the second summand we replace the definition of $\widetilde{g}$:

$$\begin{aligned} g_\epsilon(E) \;&=\; \sum_{n=0}^{N}\int_{\mathbb{R}}\frac{dx}{2\pi}\;\frac{g^{(n)}(x)}{n!}\left(\frac{(\imath\epsilon)^n}{x+\imath\epsilon-E}-\frac{(-\imath\epsilon)^n}{x-\imath\epsilon-E}\right)\\ &=\;\int_{\mathbb{R}}\frac{dx}{\pi}\;g(x)\;\frac{\epsilon}{(x-E)^2+\epsilon^2}\;+\;\int_{\mathbb{R}}\frac{dx}{\pi}\;g'(x)\;\frac{\imath\,\epsilon\,(x-E)}{(x-E)^2+\epsilon^2}\;+\;\mathcal{O}(\epsilon)\;.\end{aligned}$$

The first summand converges indeed to $g(E)$. In the second summand, the integrand is bounded above by $\|g'\|<\infty$ and converges pointwise to 0 in the limit $\epsilon\downarrow 0$ except if $x=E$. Therefore the second integral vanishes in the limit $\epsilon\downarrow 0$. □

Proof of Proposition 4.2. In the Helffer-Sjöstrand formula for $g(\widehat{H})$ we replace the geometric resolvent identity

$$\frac{1}{z-\widehat{H}} \;=\; \Pi\,\frac{1}{z-H}\,\Pi^*+\frac{1}{z-\widehat{H}}\,(\widehat{H}\,\Pi^*-\Pi\,H)\,\frac{1}{z-H}\,\Pi^*\;, \tag{4.7}$$

where in $(z-H)^{-1}$ there is the identity on $\ell^2(\mathbb{Z}^2)$ as factor of z (for a proof, see the argument after (2.14)). Then one obtains

$$g(\widehat{H}) \;=\; \Pi\,g(H)\,\Pi^*\;+\;\widehat{K}\;, \tag{4.8}$$

where

$$\widehat{K} \;=\; \frac{-1}{2\pi}\int_{\mathbb{R}^2} dx\,dy\;\partial_{\overline{z}}\widetilde{g}(x,y)\;\frac{1}{z-\widehat{H}}\;(\widehat{H}\,\Pi^*-\Pi\,H)\;\frac{1}{z-H}\,\Pi^*\;. \tag{4.9}$$

Under the hypothesis of the proposition, $g(H)=0$ and $\widehat{K}=g(\widehat{H})$. Now the resolvents have a fall-off of their matrix elements off the diagonal. Indeed, for a given $k\in\mathbb{N}$ and $j=1,2$ (and, more generally, $j=1,\ldots,d$),

$$(n_j-m_j)^k\langle n|(z-H)^{-1}|m\rangle \;=\; \imath^k\;\langle n|\nabla_j^k(z-H)^{-1}|m\rangle\;. \tag{4.10}$$

Now $\nabla^k(z-H)^{-1}$ can be expanded by the Leibniz rule for ∇. As $\|\nabla^k H\|\leq C$ and $\|(z-H)^{-1}\|\leq|y|^{-1}$, one concludes

$$|\langle n|(z-H)^{-1}|m\rangle| \;\leq\; \frac{1}{|y|^{k+1}}\;\frac{C_k}{1+|n_j-m_j|^k}\;.$$

The same bound holds for the resolvent of $\widehat{H}$. (It is a good exercise to show that the decay is under adequate hypothesis actually $|y|^{-1}e^{-\eta\,|y|\,|n-m|}$, a fact that is often called a Combes-Thomas estimate). Now let us go back to (4.9). By the finite range assumption, $\widehat{H}\Pi^* - \Pi H$ has matrix elements only on the boundary. Then

$$\begin{aligned} |\langle 0,n_2|\widehat{K}|0,n_2\rangle| \;&\leq\; \sum_{m\in\mathbb{Z}\times\mathbb{N}}\sum_{k\in\mathbb{Z}^2}\frac{1}{2\pi}\int_{\mathbb{R}^2}dx\,dy\,|\partial_{\overline{z}}\widetilde{g}(x,y)|\;|\langle 0,n_2|(z-H)^{-1}|m\rangle| \\ &\qquad\qquad |\langle m|\widehat{H}\,\Pi^*-\Pi\,H|k\rangle|\;|\langle k|(z-H)^{-1}|0,n_2\rangle| \\ &\leq\; C\sum_{m_1\geq 0}\int_{\mathbb{R}^2}dx\,dy\,|\partial_{\overline{z}}\widetilde{g}(x,y)|\;\frac{1}{|y|^{2k+2}}\;\frac{1}{1+|n_2|^{2k}}\;\frac{1}{1+|m_1|^{2k}}\;. \end{aligned}$$

Now just remains to use (4.6) for $N\geq 2k+2$, the fact that the integral is over a bounded region, and then to carry out the sum in order to deduce

$$|\langle 0,n_2|\widehat{K}|0,n_2\rangle|\;\leq\;\frac{C}{1+|n_2|^{2k}}\;.$$

But this implies the desired $\widehat{\mathcal{T}}$-traceclass estimate, compare the definition (4.2). □

4.4 Remark The above proof is deterministic and actually shows that for each H_ω the quantity

$$\sum_{n_2\geq 0}\langle 0,n_2|g(\widehat{H}_\omega)|0,n_2\rangle$$

is finite if the support of g lies in a gap of the spectrum of H_ω. ◇

4.5 Remark Let us provide a re-interpretation of the definition of $\widehat{\mathcal{T}}$ and the results above. Denote by $\mathcal{E}$ the algebra of operator families $\widehat{A}=(\widehat{A}_\omega)_{\omega\in\Omega}$ on $\ell^2(\mathbb{Z}\times\mathbb{N})$ which are covariant in the 1-direction. Then $\mathcal{T}_1:\mathcal{E}\to\mathcal{B}(\ell^2(\mathbb{N}))$ defined by

$$\langle n_2|\mathcal{T}_1(\widehat{A})|m_2\rangle\;=\;\mathbf{E}_{\mathbb{P}}(\langle 0,n_2|\widehat{A}_\omega|0,m_2\rangle\;,$$

is an partial trace (in particular, completely positive and trace preserving). Now a positive operator $\widehat{A}\in\mathcal{E}$ is $\widehat{\mathcal{T}}$-traceclass if and only if $\mathcal{T}_1(\widehat{A})$ is traceclass on $\ell^2(\mathbb{N})$ in the conventional sense. ◇

4.6 Definition *Let $\mathcal{D}$ be the set of families $\widehat{A}=(\widehat{A}_\omega)_{\omega\in\Omega}$ of a operators on the half-space $\ell^2(\mathbb{Z}\times\mathbb{N})$ that are covariant w.r.t. the 1-direction and satisfy the bound*

$$|\langle n_1,n_2|\widehat{A}_\omega|m_1,m_2\rangle|\;\leq\;C\;\frac{1}{1+|n_2|^2}\;\frac{1}{1+|m_2|^2}\;\frac{1}{1+|n_1-m_1|^2}\;,$$

for some constant C.

The choice of the power 2 in all the denominators is rather arbitrary. It is sufficient to assure summability, and, moreover, that $\mathcal{D}$ is an algebra w.r.t. the usual operator product because

$$\sum_{k_1\in\mathbb{Z}}\frac{1}{1+|n_1-k_1|^2}\;\frac{1}{1+|k_1-m_1|^2}\;\leq\;\frac{C}{1+|n_1-m_1|^2}\;,$$

which follows by discretizing the identity

$$\int_{\mathbb{R}}dy\;\frac{1}{1+y^2}\;\frac{1}{1+(x-y)^2}\;=\;\frac{2\,\pi}{4+x^2}\;.$$

By the same argument, if $\widehat{B}$ satisfies

$$|\langle n_1,n_2|\widehat{B}_\omega|m_1,m_2\rangle| \;\leq\; C\;\frac{1}{1+|n_2-m_2|^2}\,\frac{1}{1+|n_1-m_1|^2}\;,$$

then also $\widehat{A}\widehat{B}\in\mathcal{D}$ and $\widehat{B}\widehat{A}\in\mathcal{D}$. The following follows immediately from the definitions.

4.7 Corollary *Any $\widehat{\mathcal{A}}\in\mathcal{D}$ is $\widehat{\mathcal{T}}$-traceclass.*

Now a slight modification of the proof of Proposition 4.2 shows the following.

4.8 Corollary *For any smooth non-negative function g of compact support lying in a gap of the spectrum of H, one has $g(\widehat{H})\in\mathcal{D}$.*

As an analytical preparation for the algebraic calculations below, we need the next result.

4.9 Proposition *Let the sign-operator of the first component be defined by*

$$\Sigma_1\,|n_1,n_2\rangle \;=\; \left\{\begin{array}{rl} |n_1,n_2\rangle\;, & n_1\geq 0\;,\\ -|n_1,n_2\rangle\;, & n_1<0\;,\end{array}\right. \qquad (n_1,n_2)\in\mathbb{Z}\times\mathbb{N}\;.$$

For any $\widehat{A}\in\mathcal{D}$, the operators $[\Sigma_1,\widehat{A}_\omega]$ are Hilbert-Schmidt operator on $\ell^2(\mathbb{Z}\times\mathbb{N})$.

Proof. First let us write out explicitly

$$\begin{aligned}\mathrm{Tr}_{\ell^2(\mathbb{Z}\times\mathbb{N})}\left(\left|\left[\Sigma_1,\widehat{A}_\omega\right]\right|^2\right) \;&=\; \sum_{n,m\in\mathbb{Z}\times\mathbb{N}}(\mathrm{sgn}(m_1)-\mathrm{sgn}(n_1))^2\,|\langle n|\widehat{A}_\omega|m\rangle|^2\\ &=\;4\left(\sum_{n_1\geq 0>m_1}+\sum_{n_1<0\leq m_1}\right)\sum_{m_2,n_2\geq 0}|\langle n|\widehat{A}_\omega|m\rangle|^2\;.\end{aligned}$$

Now the decay properties in $\mathcal{D}$ allow to conclude. □

Now follows a longer calculation which generalizes the proof of the Gohberg-Krein index theorem (showing that winding numbers of invertible functions on the unit circle are given by a Fredholm index). Let $\widehat{A}$, $\widehat{B}$ and $\widehat{C}$ all be covariant family of operators on the half-space lying in $\mathcal{D}$. Set

$$\xi_1(\widehat{A},\widehat{B}) \;=\; \imath\,\widehat{\mathcal{T}}(\widehat{A}\,\nabla_1\widehat{B})\;. \tag{4.11}$$

Note that $\nabla_1\widehat{B}$ is not necessarily in $\mathcal{D}$ if $\widehat{B}\in\mathcal{D}$. Nevertheless, ξ_1 is well-defined because $\widehat{A}\,\nabla_1\widehat{B}$ is $\widehat{\mathcal{T}}$-traceclass.

4.10 Lemma *ξ_1 is a cyclic 1-cocycle on $\mathcal{D}$, notably it is cyclic and closed under the Hochschild boundary operator b:*

(i) $\xi_1(\widehat{A},\widehat{B})=-\xi_1(\widehat{B},\widehat{A})$

(ii) $0=b\xi_1(\widehat{A},\widehat{B},\widehat{C})=\xi_1(\widehat{A}\widehat{B},\widehat{C})-\xi_1(\widehat{A},\widehat{B}\widehat{C})+\xi_1(\widehat{C}\widehat{A},\widehat{B})$

Proof. Both algebraic identities can be verified using the product rule for the derivation ∇_1 and the invariance of the trace $\widehat{\mathcal{T}}$ under ∇_1. □

Next we introduce another 1-cocycle on $\mathcal{D}$ by setting

$$\zeta_1(\widehat{A},\widehat{B}) \;=\; \int \mathbb{P}(d\omega)\;\zeta_1^\omega(\widehat{A},\widehat{B})\;,$$

where

$$\zeta_1^\omega(\widehat{A},\widehat{B}) \;=\; \frac{1}{4}\,\mathrm{Tr}_{\ell^2(\mathbb{Z}\times\mathbb{N})}\left(\Sigma_1\left[\Sigma_1,\widehat{A}_\omega\right]\left[\Sigma_1,\widehat{B}_\omega\right]\right)\;. \tag{4.12}$$

Note that this is well-defined by Proposition 4.9.

4.11 Proposition *On $\mathcal{D}$, one has $\zeta_1=\xi_1$.*

Proof. Writing out the definition shows that

$$\zeta_1(\widehat{A},\widehat{B}) \;=\; -\frac{1}{4}\int \mathbb{P}(d\omega)\sum_{m\in\mathbb{Z}\times\mathbb{N}}\sum_{l\in\mathbb{Z}\times\mathbb{N}}\mathrm{sgn}(m_1)(\mathrm{sgn}(m_1)-\mathrm{sgn}(l_1))^2\langle m|\widehat{A}_\omega|l\rangle\,\langle l|\widehat{B}_\omega|m\rangle\;.$$

By the traceclass property, the sum can be exchanged with the integral over $\mathbb{P}$. Then we make the change of variables $n_1=l_1-m_1$ and use the covariance relation (2.7) in order to obtain:

$$\begin{aligned}\zeta_1(\widehat{A},\widehat{B}) \;&=\; -\frac{1}{4}\sum_{m_1\in\mathbb{Z}}\int \mathbb{P}(d\omega)\sum_{m_2,l_2\in\mathbb{N}}\sum_{n_1\in\mathbb{Z}}\mathrm{sgn}(m_1)\;(\mathrm{sgn}(m_1)-\mathrm{sgn}(m_1+n_1))^2\;\cdot\\ &\qquad\cdot\;\langle 0,m_2|\widehat{A}_{T_{(-m_1,0)}\omega}|n_1,l_2\rangle\;\langle n_1,l_2|\widehat{B}_{T_{(-m_1,0)}\omega}|0,m_2\rangle\;.\end{aligned}$$

Next, by invariance of the measure $\mathbb{P}$, one can replace $T_{(-m_1,0)}\omega$ by ω. Then let us change the sum over m_1 and the integral over $\mathbb{P}$ again and use the identity

$$\sum_{m_1\in\mathbb{Z}}\mathrm{sgn}(m_1)\;(\mathrm{sgn}(m_1)-\mathrm{sgn}(m_1+n_1))^2 \;=\; -\,4\,n_1\;.$$

By definition of ∇_1, one therefore has

$$\zeta_1(\widehat{A},\widehat{B}) \;=\; \imath\int \mathbb{P}(d\omega)\sum_{m_2\in\mathbb{N}}\langle 0,m_2|\widehat{A}_\omega\nabla_1\widehat{B}|0,m_2\rangle\;,$$

which is precisely $\xi_1(\widehat{A},\widehat{B})$. □

Finally let us introduce a further 1-cocyle using the projection operator $\Pi_1=\frac{1}{2}\,(1+\Sigma_1)$ on the quarter space Hilbert space $\ell^2(\mathbb{N}\times\mathbb{N})$:

$$\eta_1(\widehat{A},\widehat{B}) \;=\; \int \mathbb{P}(d\omega)\;\eta_1^\omega(\widehat{A},\widehat{B})\;,$$

where

$$\eta_1^\omega(\widehat{A},\widehat{B}) \;=\; \mathrm{Tr}_{\ell^2(\mathbb{Z}\times\mathbb{N})}(\Pi_1\widehat{B}_\omega\widehat{A}_\omega\Pi_1-\Pi_1\widehat{B}_\omega\Pi_1\widehat{A}_\omega\Pi_1)\;-\;\mathrm{Tr}_{\ell^2(\mathbb{Z}\times\mathbb{N})}(\Pi_1\widehat{A}_\omega\widehat{B}_\omega\Pi_1-\Pi_1\widehat{A}_\omega\Pi_1\widehat{B}_\omega\Pi_1)\;. \tag{4.13}$$

4.12 Proposition *On $\mathcal{D}$, both expressions in* (4.13) *are finite and one has $\eta_1^\omega=\zeta_1^\omega$ for all $\omega\in\Omega$.*

Proof. Some algebra shows

$$\Pi_1 \widehat{A}_\omega \widehat{B}_\omega \Pi_1 - \Pi_1 \widehat{A}_\omega \Pi_1 \widehat{B}_\omega \Pi_1 \;=\; -\frac{1}{4}\,\Pi_1 \left[\Sigma_1, \widehat{A}_\omega\right] \left[\Sigma_1, \widehat{B}_\omega\right] . \tag{4.14}$$

As $\left[\Sigma_1, \widehat{A}_\omega\right] \left[\Sigma_1, \widehat{B}_\omega\right]$ is trace-class, so is the left-hand side. Hence using the same identity with $\widehat{A}$ and $\widehat{B}$ exchanged, we obtain:

$$\begin{aligned} \eta_1^\omega(\widehat{A}, \widehat{B}) \;&=\; \frac{1}{4}\,\mathbf{Tr}_{\ell^2(\mathbb{Z}\times\mathbb{N})} \left(\Pi_1 \left[\Sigma_1, \widehat{A}_\omega\right] \left[\Sigma_1, \widehat{B}_\omega\right] - \Pi_1 \left[\Sigma_1, \widehat{B}_\omega\right] \left[\Sigma_1, \widehat{A}_\omega\right]\right) \\ &=\; \frac{1}{8}\,\mathbf{Tr}_{\ell^2(\mathbb{Z}\times\mathbb{N})} \left(\Sigma_1 \left[\Sigma_1, \widehat{A}_\omega\right] \left[\Sigma_1, \widehat{B}_\omega\right] - \Sigma_1 \left[\Sigma_1, \widehat{B}_\omega\right] \left[\Sigma_1, \widehat{A}_\omega\right]\right) . \end{aligned}$$

Note here that the second equality holds because both $\left[\Sigma_1, \widehat{A}_\omega\right]$ and $\left[\Sigma_1, \widehat{B}_\omega\right]$ are Hilbert-Schmidt. From (4.12) it follows that

$$\eta_1^\omega(\widehat{A}, \widehat{B}) \;=\; \frac{1}{2}\left(\zeta_1^\omega(\widehat{A}, \widehat{B}) - \zeta_1^\omega(\widehat{B}, \widehat{A})\right) ,$$

and the cyclicity property of ζ_1^ω allows to conclude. □

4.13 Corollary *On $\mathcal{D}$, one has $\xi_1 = \zeta_1 = \eta_1$.*

4.14 Proposition *Suppose (only for the purpose of this proposition) that $\mathbb{P}$ is ergodic w.r.t. the $\mathbb{Z}$-action T_1. Let $\widehat{A}$ be a unitary such that $\widehat{A} - \mathbf{1} \in \mathcal{D}$. Then $\Pi_1 \widehat{A}_\omega \Pi_1$ is $\mathbb{P}$-almost surely a Fredholm operator on $\ell^2(\mathbb{N}\times\mathbb{N})$ the index of which is $\mathbb{P}$-almost surely independent of $\omega \in \Omega$. Its common value is equal to $\xi_1(\widehat{A} - \mathbf{1}, \widehat{A}^* - \mathbf{1})$.*

Proof. By (4.14) with $\widehat{B}_\omega = \widehat{A}_\omega^{-1} = \widehat{A}_\omega^*$,

$$\Pi_1 - \Pi_1 \widehat{A}_\omega \Pi_1 \Pi_1 \widehat{A}_\omega^* \Pi_1 \;=\; \frac{1}{4}\,\Pi_1 \left[\Sigma_1, \widehat{A}_\omega\right] \left[\Sigma_1, \widehat{A}_\omega\right]^* \;=\; \frac{1}{4}\,\Pi_1 \left[\Sigma_1, \widehat{A}_\omega - \mathbf{1}\right] \left[\Sigma_1, \widehat{A}_\omega - \mathbf{1}\right]^* ,$$

The r.h.s. is traceclass by hypothesis and Proposition 4.9. Therefore $\Pi_1 \widehat{A}_\omega \Pi_1$ is a Fredholm operator on $\Pi_1 \ell^2(\mathbb{Z}\times\mathbb{N}) = \ell^2(\mathbb{N}\times\mathbb{N})$ with pseudo-inverse $\Pi_1 \widehat{A}_\omega^* \Pi_1$. Moreover, by the Fedosov formula and (4.13), its index is equal to $\eta_1^\omega(\widehat{A}, \widehat{A}^*)$. Because

$$\Pi_1 \widehat{A}_{T_{(a,0)}\omega} \Pi_1 \mid_{\ell^2(\mathbb{N}\times\mathbb{N})} = \; \Pi_1 \widehat{A}_\omega \Pi_1 + K \mid_{U(a,0)\ell^2(\mathbb{N}\times\mathbb{N}) \cong \ell^2(\mathbb{N}\times\mathbb{N})} \;\;,$$

where K is a compact operator on $\ell^2(\mathbb{N}\times\mathbb{N})$ and the Fredholm index is invariant under compact perturbations, we see that the index is T_1-translation invariant in $\omega \in \Omega$. Hence it is $\mathbb{P}$-almost surely constant by the ergodicity of $\mathbb{P}$ with respect to T_1. □

In our context, the measure $\mathbb{P}$ is only ergodic w.r.t. the $\mathbb{Z}^2$-action T. However, this is sufficient to give an almost sure index for certain elements in $\mathcal{D}$, notably those in the image of the exponential map.

4.15 Proposition *Let $\widehat{H}$ satisfy the hypothesis of* Proposition 4.2 *and let G be a real C^4 function with values in $[0, 1]$, equal to 0 or 1 outside of Δ. Set $\widehat{U} = \exp(2\pi\imath\, G(\widehat{H}))$. Then $\Pi_1 \widehat{U}_\omega \Pi_1$ is $\mathbb{P}$-almost surely a Fredholm operator on $\ell^2(\mathbb{N}\times\mathbb{N})$ the index of which is $\mathbb{P}$-almost surely independent of $\omega \in \Omega$. The almost sure value is equal to $\xi_1(\widehat{U} - \mathbf{1}, \widehat{U}^{-1} - \mathbf{1})$.*

Proof. First of all, there is a smooth positive function $\chi : \mathbb{R} \to [0, 1]$ which is equal to 0 outside of Δ and equal to 1 on the subset of Δ on which G is not equal to 0 or 1. Then $\chi(\widehat{H}) \in \mathcal{D}$ by Corollary 4.8 (which follows from the proof of Proposition 4.2). Thus the ideal property of $\mathcal{D}$ and

$$\widehat{U} - \mathbf{1} \;=\; \chi(\widehat{H})\,(\widehat{U} - \mathbf{1}) \;,$$

shows that $\widehat{U} - \mathbf{1} \in \mathcal{D}$. Thus from the proof of Proposition 4.14 follows that $\Pi_1 \widehat{U}_\omega \Pi_1$ is $\mathbb{P}$-almost surely a Fredholm operator and that its index is T_1-invariant. To conclude, we have to show its T_2-invariance. By the covariance relation $U(0, a)H_{T_{(0,a)}\omega}U(0, a)^* = H_\omega$ and the finite range condition on H_ω, one has

$$\widehat{H}_\omega \;=\; U(0, a)\widehat{H}_{T_{(0,a)}\omega}U(0, a)^* + \widehat{R}_\omega \;,$$

where $\widehat{R}_\omega$ is an operator family, covariant in the 1-direction and finite range from the boundary in the 2-direction. Hence

$$\widehat{U}_\omega(\lambda) \;=\; \exp(2\pi\imath\, G(U(0, a)\widehat{H}_{T_{(0,a)}\omega}U(0, a)^* + \lambda\widehat{R}_\omega)) \;,$$

is $\mathbb{P}$-almost surely a norm-continuous family (in λ) of Fredholm operators because the finite range perturbation $\lambda\widehat{R}$ does not alter the argument that $G(\widehat{H} + \lambda\widehat{R}) \in \mathcal{D}$ so that again $\widehat{U}(\lambda) \in \mathcal{D}$. Clearly $\widehat{U}_\omega(1) = \widehat{U}_\omega$ and $\widehat{U}_\omega(0) = U(0, a)\widehat{U}_{T_{(0,a)}\omega}U(0, a)^*$. Therefore the homotopy invariance of the Fredholm index implies:

$$\text{Ind}(\Pi_1\widehat{U}_\omega\Pi_1) \;=\; \text{Ind}(\Pi_1 U(0, a)\widehat{U}_{T_{(0,a)}\omega}U(0, a)^*\Pi_1) \;=\; \text{Ind}(\Pi_1\widehat{U}_{T_{(0,a)}\omega}\Pi_1) \;,$$

which concludes the proof. □

The following is the last preparation for the proof of Theorem 4.1, which is a non-commutative analog of the additivity of winding numbers.

4.16 Proposition *Let $\widehat{U}$ and $\widehat{V}$ be two unitaries with $\widehat{U} - \mathbf{1} \in \mathcal{D}$ and $\widehat{V} - \mathbf{1} \in \mathcal{D}$ so that* $\text{Ind}(\widehat{U}) = \xi_1(\widehat{U} - \mathbf{1}, \widehat{U}^* - \mathbf{1})$ *and* $\text{Ind}(\widehat{V}) = \xi_1(\widehat{V} - \mathbf{1}, \widehat{V}^* - \mathbf{1})$ *are well-defined. Then the unitary $\widehat{U}\widehat{V}$ is such that $\widehat{U}\widehat{V} - \mathbf{1}$ is $\widehat{\mathcal{T}}$ and the index satisfies*

$$\text{Ind}(\widehat{U}\,\widehat{V}) \;=\; \text{Ind}(\widehat{U}) \,+\, \text{Ind}(\widehat{V}) \;.$$

Proof. The first claim follows from $\widehat{U}\widehat{V} - \mathbf{1} = (\widehat{U} - \mathbf{1})\widehat{V} + (\widehat{V} - \mathbf{1})$ and the ideal property of the $\widehat{\mathcal{T}}$-traceclass operators w.r.t. products with covariant operators (note that alternatively, one can use that $\mathcal{D}$ is also an ideal). Now by the Leibniz rule and cyclicity

$$\begin{aligned}
\text{Ind}(\widehat{U}\,\widehat{V}) \;&=\; \imath\,\widehat{\mathcal{T}}\big((\widehat{U}\,\widehat{V} - \mathbf{1})^*(\nabla_1\widehat{U}\,\widehat{V} + \widehat{U}\,\nabla_1\widehat{V})\big) \\
&=\; \text{Ind}(\widehat{U}) \,+\, \text{Ind}(\widehat{V}) \,+\, \imath\,\widehat{\mathcal{T}}\big((\mathbf{1} - \widehat{V})\nabla_1\widehat{U} \;+\; (\mathbf{1} - \widehat{U})\nabla_1\widehat{V}\big) \;.
\end{aligned}$$

But an integration by parts shows that the sum of the last two summands vanishes. □

Proof of Theorem 4.1. According to the Proposition 4.14,

$$\text{Ind} \;=\; \imath\,\widehat{\mathcal{T}}\big((\widehat{U}^* - \mathbf{1})\nabla_1\widehat{U}\big) \;.$$

Let us express $\widehat{U}$ as exponential series and use the Leibniz rule:

$$\widehat{\mathcal{T}}((\widehat{U}^* - 1)\,\nabla_1\widehat{U}) \;=\; \imath\sum_{m=0}^{\infty}\frac{(2\pi\imath)^m}{m!}\sum_{l=0}^{m-1}\widehat{\mathcal{T}}\left((\widehat{U}^* - \mathbf{1})\,G(\widehat{H})^l\,\nabla_1 G(\widehat{H})\,G(\widehat{H})^{m-l-1}\right) \;,$$

where the trace and the infinite sum could be exchanged because of the traceclass properties of $\widehat{U}-\mathbf{1}$. Due to cyclicity and the fact that $[\widehat{U}, G(\widehat{H})] = 0$, each summand is now equal to $\widehat{\mathcal{T}}((\widehat{U}^* - 1)\, G(\widehat{H})^{m-1}\, \nabla_1 G(\widehat{H}))$. Exchanging again sum and trace and summing the exponential up again, one gets

$$\text{Ind} \;=\; -2\pi\, \widehat{\mathcal{T}}\left((\mathbf{1} - \widehat{U})\, \nabla_1 G(\widehat{H})\right)\,.$$

Now let us invoke Proposition 4.16 and then repeat the same argument for $\widehat{U}^k = \exp(-2\pi\imath\, k\, G(\widehat{H}))$ for $k \neq 0$,

$$\text{Ind} \;=\; \frac{\imath}{k}\, \widehat{\mathcal{T}}\big((\widehat{U}^k - \mathbf{1})^* \nabla_1 \widehat{U}^k\big) \;=\; -\,2\pi\, \widehat{\mathcal{T}}\left((\mathbf{1} - \widehat{U}^k)\, \nabla_1 G(\widehat{H})\right)\,.$$

Writing $G(E) = \int dt\, \tilde{G}(t)\, e^{-E(1+\imath t)}$ with adequate $\tilde{G}$, the DuHamel formula gives

$$\text{Ind} \;=\; 2\pi \int dt\, \tilde{G}(t)\, (1+\imath t) \int_0^1 dq\, \widehat{\mathcal{T}}\left((\widehat{U}^k - \mathbf{1})\, e^{-(1-q)(1+\imath t)\widehat{H}}(\nabla_1 \widehat{H}) e^{-q(1+\imath t)\widehat{H}}\right)\,.$$

One therefore finds using $G'(E) = -\int dt\, (1+\imath t)\, \tilde{G}(t)\, e^{-E(1+\imath t)}$, for $k \neq 0$,

$$\text{Ind} \;=\; 2\pi\, \widehat{\mathcal{T}}\left((\widehat{U}^k - \mathbf{1})\, G'(\widehat{H})\, \nabla_1 \widehat{H}\right)\,.$$

For $k = 0$, the r.h.s. vanishes.

To conclude, let $\phi : [0,1] \to \mathbb{R}$ be a differentiable function vanishing at the boundary points 0 and 1. Let its Fourier coefficients be denoted by $a_k = \int_0^1 dx\, e^{-2\pi\imath k x}\phi(x)$. Then $\sum_k a_k e^{2\pi\imath k x} = \phi(x)$ and, in particular, $\sum_k a_k = 0$. Hence

$$\begin{aligned}
a_0\, \text{Ind} \;&=\; -\sum_{k\neq 0} a_k\, \text{Ind} \\
&=\; 2\pi \sum_k a_k\, \widehat{\mathcal{T}}\left((\mathbf{1} - \widehat{U}^k)\, G'(\widehat{H})\, \nabla_1 \widehat{H}\right) \\
&=\; 2\pi\, \widehat{\mathcal{T}}\big((0 - \phi(G(\widehat{H})))\, G'(\widehat{H})\, \nabla_1 \widehat{H}\big)\,.
\end{aligned}$$

Let now ϕ converge to the indicator function of $[0,1]$. Then $a_0 \to 1$, while $\phi(G(\widehat{H}))G'(\widehat{H}) \to G'(\widehat{H})$ on the other side (the Gibbs phenomenon is damped). As $J_1 = \nabla_1 \widehat{H}$, this concludes the proof. □

4.3 Hall conductivity

4.17 Theorem (IQHE-Kubo Formula) *If the Fermi level is not a discontinuity point of the DOS of H, in the zero temperature and infinite relaxation time limit and provided the Fermi projection $P = \chi(H \leq \mu)$ satisfies $\nabla P \in L^2(\mathcal{A}, \mathcal{T})$, the conductivity tensor is given by*

$$\sigma_{i,j}(\infty,\infty) \;=\; 2\imath\pi\, \mathcal{T}\left(P[\nabla_i P, \nabla_j P]\right)\,.$$

In particular the direct conductivity vanishes and the Hall conductivity is given by a non-commutative Chern character.

4.18 Theorem *Under the same conditions as in the previous theorem, there is a Fredholm operator with index* Ind *such that the Hall conductivity satisfies*

$$\sigma_{1,2}(\infty,\infty) \;=\; \text{Ind}\,.$$

4.19 Theorem *If H has a gap and P is the Fermi projection under this gap, then its Chern character is equal to the Fredholm index calculated from the edge currents.*

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