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Adiabatic charge transport and topological invariants for electrons in a quasi-periodic potential and a magnetic field

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Abstract

An analysis is made of charge transport induced by adiabatic variations of the phases appearing in a quasi-periodic potential acting on non-interacting electrons. It is proved that this charge transport is quantised, when the chemical potential lies in a gap. The corresponding integers are topological invariants (first or higher Chern numbers), which label the gaps. Similar results are obtained for the Hall conductivity and charge transport of electrons in a periodic potential, under the influence of an irrational magnetic field.

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1. INTRODUCTION

Unexpected topological aspects of quantum theory have been discovered in recent years.

On one hand, Berry [1] showed that the wave function of a quantum system, acquires an additional geometric phase, when an adiabatic loop is made in the parameter space, if the corresponding eigenvalue is separated by a gap from the rest of the spectrum, during the adiabatic process. The topological meaning of this phase was clarified by Simon [2].

On the other hand, Thouless et al [3] (TKNN) considering a system of non-interacting electrons in a periodic potential and a rational magnetic field, proved that the Hall conductivity is quantised, when theelectronic chemical potential is in a gap. Avron et al [4] soon proved that the TKNN integers associated to the Hall conductivity had a topological interpretation. In fact, the topological aspect of such type of problems was discovered a bit earlier by Dubrovin and Novikov [5] and Novikov [6] who were discussing mostly the case of a periodic magnetic field.

The fact that such different looking problems are intimately related, was clearly demonstrated by Thouless [7]. He considered a one-dimensional electronic system acted on by a periodic potential, which varies adiabatically and periodically in time and discovered that the charge transport induced by such a varying potential is quantized, when the chemical potential of the electrons lies in a gap.

Later on, Niu and Thouless [8] and Avron and Seiler [9] looked at the integer quantum Hall effect, in the case of many-body interactions, using such an approach. More recently, Niu [23] proposed a way to realise experimentally the phenomenon of quantised adiabatic particle transport, induced by a slow and cyclic potential variation.

In this paper, we will also consider the problem of adiabatic charge transport, but for independent electrons under the influence of a quasi-periodic potential in one, two and three dimensions. We will prove that whereas charge transport is strictly quantised in one dimension, it is only given by a linear combination of integers in two or three dimensions. These integers are topological invariants. They correspond to first Chern numbers in one dimension and two and third Chern numbers in two and three dimensions respectively. Moreover, these integers label the gaps, in the sense that a linear combination of them gives the electronic density (integrated density of states), in the gap considered. Such a decomposition of the integrated density of states, when the chemical potential lies in a gap, has been called a gap-labelling theorem. It has already been proved in the one-dimensional case by Johnson and Moser [10] and in the multidimensional one by Bellissard, Lima and Testard [11].

In contrast to these proofs, a notable feature of ours is that it allows an identification of each integer appearing in the decomposition of the density of states.

We then consider the case of independent electrons, in a periodic potential and a constant magnetic field, whose flux through the unit cell is irrational in appropriate units. (The case of a rational flux was already considered by TKNN). This problem in two dimensions has many features in common with the one-dimensional problem of electrons in a quasi-periodic potential with two incommensurable frequencies. We prove that the quantum Hall conductivity and charge transport induced by an adiabatic variation of a phase in the potential are quantised. The corresponding integers are first Chern numbers of a certain vector bundle. The integrated density of states in the considered gap, is given by a linear combination of these two integers.

This last result was already proved by Avron, Dana and Zak [12], although no physical interpretation of one of the integers appearing in the decomposition was given.

The paper is organized as follows :

In § 2, we derive an adiabatic theorem for the density matrix, valid to second order in the adiabatic parameter, in a form suitable for our subsequent analysis.

In § 3, we apply this theorem, to get general formulas for the charge transport and the conductivity tensor, in a class of models of non-interacting electrons.

In § 4-7, we discuss quasi-periodic potentials.

We prove that certain quantities are topological invariants, in fact, Chern numbers of certain vector bundles. The basic strategy of the proof is to approximate the potential by a periodic one, of very large periods. For periodic hamiltonians, however, the corresponding quantities can be shown to Chern numbers of a suitable vector bundles. We may note that we have therefore constructed examples of topological invariants associated to an infinite dimensional geometry. In this sense, there should exist a connection between our work and the C^*-algebra approach used in [11], related to the non commutative geometry of A. Connes.

Finally, the relationship between the topological invariants introduced and the charge transport, or the density of states is established by purely algebraic means.

In § 8, we consider the case of electrons in a magnetic field and a periodic potential. Putting the problem in a form which closely resembles the quasi-periodical problem in one dimension, we prove the quantisation of the Hall conductivity and charge transport and establish the relationship between these quantities and the electronic density.

2. Adiabatic evolution of the density matrix

Consider a quantum system, whose dynamics is governed by a time dependent hamiltonian $H\left(\frac{t}{T}\right)$ during the time interval $[0, T]$. When the time scale T is large, the hamiltonian changes slowly with time. In this adiabatic limit, we will be interested by the evolution of the state of the system, described by its density matrix $\rho(t)$, when the family of hamiltonians $H\left(\frac{t}{T}\right)$ possess a common spectral gap. Initially, the system is in a state $\rho(0)$, given by a spectral projector associated to this gap.

Such problems have a long history briefly summarized by Avron, Seiler, Yaffe [13]. These authors have obtained an asymptotic expansion of the density matrix, valid to arbitrary order in T^{-1}, if the hamiltonian $H(t)$ is smooth enough in t. The presence of oscillating phase factors in their expansion prevents however its use in the case we are interested in. We will therefore derive another expansion valid to order T^{-2}.

We will make the following assumptions on the hamiltonian :

1) $\{H(s)\}$, $s \in I = [0, 1]$ is a family of self-adjoint operators on a Hilbert space $\mathcal{H}$, with a common dense domain D. H(s) is uniformly bounded from below, i.e. $H(s) \geq c\,1$, $\forall\, s \in I$.

2) For each $\psi \in D$, $H(s)\psi$ is strongly C^3 on I.

3) There exist a bounded real open set Δ, belonging to the resolvent set of H(s), for all $s \in I$.

Under such circumstances, a classical theorem [14] shows that there exist a unique unitary operator $\tau(t)$ mapping D into D, strongly continuous on D, and such that the following equation holds on D :

$$i\hbar\tau'(t) = H\left(\frac{t}{T}\right)\tau(t) \qquad 2.1$$

$$\tau(0) = 1$$

To any number $\mu \in \Delta$, we can associate the spectral projector

$$P(s) = E_{H(s)}(-\infty, \mu) \qquad 2.2$$

This projector is three times norm differentiable on I. One can see this by using the representation :

$$P(s) = \oint_{\Gamma} \frac{dz}{2\pi i} G_z(s) \qquad 2.3$$

where

$$G_z(s) = (z - H(s))^{-1} \qquad 2.4$$

and Γ is a s-independent circle in the complex plane, oriented counterclockwise and encircling the segment $[c, \mu]$ on the real axis.

Consider the unormalised density matrix

$$\rho(t) = \tau(t)\,P(0)\,\tau^{+}(t) \qquad 2.5$$

It is a bounded self-adjoint operator, mapping $\mathcal{H}$ into D, continuously differentiable on D and satisfies on D, Von-Neumann's equation :

$$i\hbar\rho'(t) = [H\left(\frac{t}{T}\right), \rho(t)] \tag{2.6}$$

Furthermore, this is the unique solution of 2.6. with these properties.

Let us call

$$V(s) = \tau(Ts) \quad s \in I \tag{2.7}$$

If we define

$$B(s) = P(0) - V^+(s)\, P(s)\, V(s) \tag{2.8}$$

then we see that we can write

$$\rho(Ts) = P(s) + V(s)\, B(s)\, V^+(s) \tag{2.9}$$

Furthermore, using the differential equation

$$i\hbar V'(s) = T\; H(s)\, V(s) \tag{2.10}$$

we see that on D :

$$B' = \frac{T}{i\hbar} V' [H, P]\, V - V^+ P' V = - V^+ P' V \tag{2.11}$$

Let us now define a bounded operator $A_1(s) \in C^2(I)$, by

$$A_1(s) = \oint_\Gamma \frac{dz}{2\pi i} \quad G_z'(s)\; G_z(s) \tag{2.12}$$

Using the relationship

$$G_z' = G_z H' G_z \tag{2.13}$$

and

$$\oint_\Gamma \frac{dz}{2\pi i} \quad G_z^2 = 0 \tag{2.14}$$

we see that on D we have

$$P'(s) = [G(s), A_1(s)] \tag{2.15}$$

and therefore on D :

$$B' = V^+ [H, A_1] V = \frac{i\hbar}{T} (V^{+'} A_1 V + V^+ A_1 V')$$

or

$$B' = \frac{i\hbar}{T} (V^+ A_1 V)' - \frac{i\hbar}{T} (V^+ A_1' V) \tag{2.16}$$

which shows that B' is of order T^{-1}. We now repeat the process.

Since we also have, from 2.14

$$A_1 = \frac{1}{2} \oint_\Gamma \frac{dz}{2\pi i} \quad [G_z', G_z] \tag{2.17}$$

then

$$A_1' = \frac{1}{2} \oint \frac{dz}{2\pi i} \quad [G_z'', G_z] \tag{2.18}$$

Therefore, if we define the bounded operator $A_2(s) \in C^1(I)$ by

$$A_2(s) = -\frac{1}{2} \oint_{\Gamma} \frac{dz}{2\pi i} G_z(s)\, G_z''(s)\, G_z(s) \qquad 2.19$$

we see that on D :

$$A_1'(s) = [H(s), A_2(s)] \qquad 2.20$$

from which follows that

$$B' = \frac{i\hbar}{T} (V^+ A_1 V)' + \left(\frac{i\hbar}{T}\right)^2 (V^+ A_2 V)' - \left(\frac{i\hbar}{T}\right)^2 (V^+ A_2' V) \qquad 2.21$$

Integrating this equation, it follows from the definition 2.9, that

$$\rho(Ts) = P(s) + \frac{i\hbar}{T} [A_1(s) - V(s) A_1(0) V^+(s)]$$

$$+ \left(\frac{i\hbar}{T}\right)^2 [A_2(s) - V(s) A_2(0) V^+(s)]$$

$$- \left(\frac{i\hbar}{T}\right)^2 \int_0^s ds' V(s) (V^+ A_2' V)(s') V^+(s) \qquad 2.22$$

an equation which holds on the full Hilbert space $\mathcal{H}$, all operators being bounded and D being dense in $\mathcal{H}$

We now see that in order to have an expansion in T^{-1}, we need some condition on $A_1(o)$. We choose $H'(0) = 0$ which gives $A_1(0) = 0$. We have therefore proven an adiabatic theorem.

Theorem 1

If the time dependent hamiltonian H(t) satisfies conditions 1), 2), 3) and H'(o) = o, then the density matrix $\rho(t)$ is given by :

$$\rho(Ts) = P(s) + \left(\frac{i\hbar}{T}\right) A_1(s) + \left(\frac{i\hbar}{T}\right)^2 A_{2,T}(s) \qquad 2.23$$

where

$$A_1(s) = \oint_\Gamma \frac{dz}{2\pi i} \quad G_z'(s)\ G_z(s) \qquad 2.24$$

and

$$\sup_{T;\, s\,\in\, I} \quad \| A_{2,T}(s) \| < \infty$$

where

$$A_{2,T}(s) = A_2(s) - V(s)\, A_2(0)\, V^+(s)$$

$$- \int_0^s ds'\ V(s)\ V^+(s')\ \ A_2'(s')\ V(s')\ V^+(s)$$

and

$$A_2(s) = -\frac{1}{2} \oint_\Gamma \frac{dz}{2\pi i} \quad G_z(s)\ G_z''(s)\ G_z(s)$$

3. Adiabatic charge transport

We would like now to apply the adiabatic theorem we have established, to the average value, in the statistical mechanical sense of some observable B, which could itself be slowly time dependent, i.e. a function of the rescaled time $\frac{t}{T}$. If the system was confined to a box of volume V, this would be given by :

$$<B>(t) = \frac{1}{V} \mathrm{tr}\ B\left(\frac{t}{T}\right) \rho(t) \tag{3.1}$$

We will in fact be interested by the infinite volume limit for which we can expect that for suitable operators A

$$M(A) = \lim_{V \to \infty} \frac{1}{V} \mathrm{tr}\ A \tag{3.2}$$

makes sense. Such a mean should have all the properties of a trace and in particular the cyclicity :

$$M(AB) = M(BA) \tag{3.3.}$$

For the sake of clarity, we will first give a formal derivation of the corresponding adiabatic theorem, we are interested in, by assuming simply that the property 3.3 holds for some "good" operators, and then give a precise theorem for a certain class of hamiltonians and operators.

We want to compute

$$\lim_{T \to \infty} \int_0^T dt\ \{<B>(t) - <B>(0)\} = \lim_{T \to \infty} T \int_0^1 ds\ \{M(B(s)\, \rho(Ts)) - M(B(0)P(0))\}$$

If we assume that

$$M(B(0)) = \int_0^1 M(B(s)\ P(s))\ ds$$

then the adiabatic theorem 1 gives

$$\lim_{T \to \infty} \int_0^T dt\ \{<B>(t) - <B>(0)\} = i\hbar \int_0^1 ds\ \{M(B(s)\ A_1(s))$$

Now A_1 has the following property :

$$A_1 = A_1\, P + P\, A_1 \tag{3.4}$$

In order to see this, let Γ' be a circle in the complex plane encircling the circle Γ, in the resolvent set of H(s).
Then

$$G_{z'} P = \oint_{\Gamma} \frac{dz}{2\pi i} \frac{G_z}{z'-z} \qquad \text{if } z' \in \Gamma' \tag{3.5}$$

and

$$(1-P)\ G_z = \oint_{\Gamma'} \frac{dz'}{2\pi i} \frac{G_{z'}}{z'-z} \qquad \text{if } z \in \Gamma \tag{3.6}$$

Therefore

$$A_1 P = \oint_{\Gamma'} \frac{dz'}{2\pi i} (G_{z'})' \, G_{z'} P = \oint_{\Gamma} \frac{dz}{2\pi i} \left[\oint_{\Gamma'} \frac{dz'}{2\pi i} \frac{G_{z'}}{z'-z} \right]' G_z$$

$$= (1-P) \oint_{\Gamma} \frac{dz}{2\pi i} G_z' \ G_z = (1-P)\, A_1$$

Hence, we can write, using 3.3 and 3.4

$$M\,(B(s)\, A_1\,(s)) = M\,(PBA_1\, P) + M\,(PA_1\, BP) =$$

$$= \oint_{\Gamma} \frac{dz}{2\pi i} \{M\,(PB\, G_z' \, G_z\, P) - M\,(P\, G_z\, G_z'\, BP)$$

$$= M\left(P\left\{\oint_{\Gamma} \frac{dz}{2\pi i}\,(G_z\, B\, G_z^{'} - G_z^{'}\; B\; G_z)\right\} P\right)$$

Let us define

$$\hat{B}(s) = \oint_{\Gamma} \frac{dz}{2\pi i}\, G_z(s)\;\; B(s)\;\; G_z(s) \qquad 3.7$$

then we have

$$P\,P'\,\hat{B} = \oint_{\Gamma'} \frac{dz'}{2\pi i} \oint_{\Gamma} \frac{dz}{2\pi i}\; \frac{P}{z'-z}\;\; [G_{z'}\,H'\,G_z\,B\,G_z - G_{z'}\,H'\,G_{z'}\,B\,G_z]$$

$$= -P \oint_{\Gamma} \frac{dz}{2\pi i}\; G_z^{'}\;\; B\,G_z\,P$$

Similarly

$$\hat{B}\;\; P'\,P \;=\; -P \oint_{\Gamma} \frac{dz}{2\pi i}\; G_z\,B\,G_z^{'}\;\; P$$

therefore

$$M\,(B(s)\;A_1(s)) \;=\; M(\,[P', \hat{B}]\,P) \qquad 3.8$$

and we have the following

<u>Quasi-theorem</u>

If $H'(o) = o$

and $$\int_0^1 M(B\,(s)\;\; P(s)) \;=\; M(B(0)\,P(0))$$

then

$$\lim_{T\to\infty} \int_0^T dt \left\{ M\left(B(\tfrac{t}{T})\, \rho(t) \right) - M\left(B(0)\, \rho(0) \right) \right\} = i\hbar \int_0^1 ds\, M([(P'(s), \hat{B}(s)]\ P(s)) \qquad 3.9$$

where $\hat{B}(s) = \oint_\Gamma \frac{dz}{2\pi i} G_z(s)\, B(s)\, G_z(s)$

In what follows, the operators and in particular the hamiltonian will depend on parameters φ which span an m-dimensional torus T_m, given by the product of m circles, identified in the usual way with the segment [0, 1]. The Hilbert space will be $\mathcal{H} = L^2(\mathbb{R}^d, dx)$.

In order to give a precise meaning to the quasi-theorem, it is useful to introduce the following definitions :

An operator B_φ will be called <u>ergodic</u> if :

1) Its domain is independent of φ and left invariant by the unitary translation operator $U_a = e^{i\vec{a}\cdot\vec{p}}$ 3.10a

2) $$U_a\ B_\varphi\ U_a^{-1} = B_{\varphi(a)} \qquad (3.10b)$$

and $\varphi(a)$ defines an ergodic flow on the torus T_m. The $\varphi(a)$ we will consider are of the form

$$\varphi_j(a) = \varphi_j + \sum_{h=1}^{d} \Omega_{jh}\, a_h \qquad j = 1 \dots m \qquad (3.11)$$

the matrix Ω being such that $\Omega^T n = 0$ implies $n = 0$ if $n \in \mathbb{Z}^m$.

Note that the product of two ergodic operators is ergodic. We will assume that the hamiltonians $H_\varphi(t)$ are ergodic. From this follows that the density matrix $\rho_\varphi(t)$ is also ergodic. Another example of an ergodic operator is the momentum $\vec{p}$. An operator B_φ will be called <u>averageable</u> $B \in \mathcal{M}$ if :

1) B_φ is ergodic

2) B_φ is bounded and has a kernel $B_\varphi(r, r')$ continuous in (r, r') on $R^d \times R^d$

3) $\sup_\varphi |B_\varphi(0, 0)| < \infty$.

For such operators, we can define an average

$$M(B) = \int_{T^m} d\varphi\ B_\varphi(0,0) = \int_{T^m} d\varphi\ B_\varphi(r, r) \qquad 3.12$$

The kernel of such ergodic operators satisfies

$$B_{\varphi(a)}(r, r') = B_\varphi(r + a, r' + a) \qquad 3.13$$

And therefore, the usual ergodic theorem allows us to conclude that for such operators :

$$\lim_{\Lambda \uparrow R^d} \frac{1}{|\Lambda|} \int_\Lambda dr\ B_\varphi(r, r) = M(B) \qquad 3.14$$

for almost all φ, Λ is an increasing sequence of parallepipeds covering R^d.

It is useful to find criteria for an operator to be averageable. With this purpose in mind, we introduce the following class C of operators : $B_\varphi \in C$ if

1) B_φ is ergodic

2) B_φ is bounded and possesses a measurable kernel $B_\varphi(r, r')$ such that

$$|B| = \sup_{\varphi;\, r} \left(\int |B_\varphi(r, r')|^2 dr' \right)^{\frac{1}{2}} < \infty \qquad 3.15$$

3) $\lim_{r \to s} \ |B_\varphi|\ r, s = 0$

$$\text{where } |B_\varphi|\ r,s = \left(\int |B_\varphi(r,t) - B_\varphi(s,t)|^2\, dt\right)^{\frac{1}{2}} \qquad 3.16$$

These operators are essentially operators of Carleman type, except for the supplementary continuity property 3). We recall [15], that an operator T is Carleman if $\forall\, f \in D(T),\ \exists\, k(r)$ such that

$$|(Tf)(r)| \leq \|f\|\ k(r) \text{ a.e.}$$

This is equivalent [15] to the fact that T possesses a measurable kernel T(r, r') such that

$$|T|(r) = \left(\int |T(r,r')|^2\right)^{\frac{1}{2}} \qquad 3.17$$

Moreover, if B is bounded, TB is Carleman and

$$|TB|(r) \leq \|B\| \times |T|(r) \qquad 3.18$$

Let us call $\mathcal{B}$, the class of ergodic, bounded operators, B_φ such that

$$\|B\| = \sup_\varphi \|B_\varphi\| < \infty.$$

then we have

<u>Proposition 1</u>
If $A \in \mathcal{C}$, $B \in \mathcal{B}$, then $AB \in \mathcal{C}$.

It is clear that properties 1) and 2) are satisfied for A B, since

$$|AB| \leq |A|\ \ \|B\| \qquad 3.19$$

On the other hand

$$|AB|^2_{rs} = \sup_{f:\, \|f\| = 1} \left|\int [A(r,t) - A(s,t)]\ (Bf^*)(t)\, dt\right|$$

hence $|AB|_{r,s} \leq |A|_{r,s}\ \|B\|$ 3.20

The following property shows the usefulness of the introduction of the class $\mathcal{C}$ of operators.

Proposition 2

If $A \in \mathcal{C}$, and $B^+ \in \mathcal{C}$ then $AB \in \mathcal{M}$ and $|M(AB)| \leq |A|\ |B^+|$. The result follows simply from the fact that B has also a measurable kernel and Schwartz inequality which gives

$$|AB| \leq |A|\ |B^+| \tag{3.21}$$

and

$$|(AB)(r,s) - (AB)(r',s')| \leq |A|_{r,r'}\ |B^+| + |B^+|_{s,s'}\ |A|$$

Finally, we note that the operation M(B) has all the properties of a trace. Indeed :

1)	$M^*(A) = M(A^+)$	if	$A, A^+ \in \mathcal{M}$	
2)	$M(AA^+) \geq 0$	if	$A \in \mathcal{C}$	
3)	$\lvert M(AB)\rvert \leq M^{1/2}(AA^+)\, M^{1/2}(B^+B)$		if	$(A, B^+) \in \mathcal{C}$
4)	$M(AB) = M(BA)$	if	$(A, A^+, B, B^+) \in \mathcal{C}$	

The only non obvious result is 4).

We have

$$M(AB) = \int_{Tm} d\varphi \int dr\ A_\varphi(o,r)\ B_\varphi(r,o)$$

but

$$\int dr\ |A_\varphi(o,r)|\ \ |B_\varphi(r,o)| \leq |A|\ |B^+|$$

hence by Fubini

$$M(AB) = \int dr \int d\varphi\, A_\varphi(o,r)\ B_\varphi(r,o) = \int dr \int d\varphi\ A_\varphi(r,o)\ B_\varphi(o,r)$$

from the ergodicity of A and B. Since

$$\int dr\ |A_\varphi(r,o)|\ |B_\varphi(o,r)| \leq |A^+|\ |B|$$

we can apply Fubini's theorem again to conclude.

We can now give the precise conditions under which equation 3.9 of the quasi-theorem holds.

Theorem 2

Suppose that the time dependent hamiltonian $H_\varphi(t)$ is ergodic and satisfies the conditions

1) $\{H_\varphi(t)\}$ $t \in I = [0,1]$, $\varphi \in T_m$ is a family of self-adjoint operators with a common dense domain D. $H_\varphi(t)$ is uniformly bounded from below on I x T_m.

2) For each $\psi \in D$, $\frac{d^k}{dt^k} H_\varphi(t)\,\psi$ is strongly continuous on I x T_m, for each $k = 0, 1, 2, 3$.

3) There exist a bounded real open set Δ, belonging to the resolvent set of $H_\varphi(t)$, for all $(t, \varphi) \in I \times T_m$.

4) The resolvent $G_{z,\varphi}(t)$ of $H_\varphi(t)$ is such that $G_{i,\varphi}(t) \in \mathcal{C}$ and $\sup\limits_{\varphi;t} |G_{i,\varphi}(t)| < \infty$.

5) $H'_\varphi(t)\, G_{i,\varphi}(t)$ maps D into D.

Let $B_\varphi(t)$ be an ergodic closed operator, with a domain containing D, $\forall\ (t,\varphi) \in I \times T_m$, such that $B_\varphi(t)\,\psi$ is continuous on I x T_m, for each $\psi \in D$. Assume furthermore that

6) $B_\varphi(t)\ G^2_{i;\varphi}(t) \in \mathcal{C}$ and $\sup\limits_{\varphi;t} |B_\varphi(t)\ G^2_{i;\varphi}(t)| < \infty$.

Then, if $H'_\varphi(0) = 0$ and $M(B(0)\,P(0)) = \int_0^1 ds\, M(B(s)\,P(s))$ 3.22

in the adiabatic limit

$$\lim_{T\to\infty} \int_0^T dt\, \{M(B(\tfrac{t}{T})\, \rho(t)) - M(B(0)\, \rho(0)\} = i\hbar \int_0^1 ds\, M([P'(s), \hat{B}(s)]\, P(s)) \quad 3.23$$

where $P_\varphi(s) = E\, H_\varphi(s)\, (-\infty, \mu)$ with $\mu \in \Delta$ 3.24

and $$\hat{B}(s) = \oint_\Gamma \frac{dz}{2\pi i}\, G_{z,\varphi}(s)\, B_\varphi(s)\, G_{z,\varphi}(s) \quad 3.25$$

Proof

In the sequel we will use repeatedly the following property, which is a simple consequence of the closed graph and uniform boundedness theorems.

Proposition 4

Let $C_{z,\varphi}(t)$ be a bounded operator strongly continuous in (t, φ, z) on $I \times T_m \times \Gamma$, of range contained in D. If $A_{z,\varphi}(t)$ is a closed operator of domain containing D and strongly continuous in (t, φ, z), on D, then

$$\sup_{(t\,\varphi\,z) \in I \times T_m \times \Gamma} \| A_{z,\varphi}(t)\, C_{z,\varphi}(t) \| < \infty.$$

Consider now the first term in the adiabatic expansion : B(s) P(s). We can write $B(s)\, P(s) = B(s) G_i^2(s)\, (i-H(s))^2\, P(s)$.

From proposition 4, $\sup_{(s;\,\varphi)} \| (i-H_\varphi(s))^2\, P_\varphi(s) \| < \infty$.

It follows therefore from assumption 6) on B and proposition 1, that $B(s)\, P(s) \in \mathcal{C}$ and

$$\sup_{(s;\,\varphi)} | B_\varphi(s)\, P_\varphi(s) | < \infty \quad 3.26$$

Now, the second resolvent equation and proposition 1 shows that properties 4) and 5) of $G_{i,\varphi}(s)$ are valid for $G_{z,\varphi}$ if $z \in \Gamma$. Therefore, $P_\varphi(s) \in \mathcal{C}$ and $\sup_{(s;\,\varphi)} | P_\varphi(s) | < \infty$. Since $P^2(s) = P(s) = P^+(s)$ we conclude from proposition 2 that M (B(s) P(s)) is well defined.

Let us now look at the second term in the adiabatic expansion : $B(s)\ A_1(s)$. We have seen that in fact $A_1 = A_1 P + PA_1$. On the other hand, we have

$$(BA_1)(s) = -\oint_{\Gamma} \frac{dz}{2\pi i} (B G_z^2)(s)(H' G_z)(s)$$

The second resolvent equation, combined with assumption 6) on B shows that

$$\sup_{(\varphi;\ z;\ s)} \| B_\varphi(s)\ G_{z;\varphi}^2(s) \| < \infty \qquad 3.27$$

Using assumption 2) on the hamiltonian, we can conclude from proposition 4 that

$$\sup_{\substack{s;\varphi;z \\ 3 \geq k \geq 0}} \| H_\varphi^{(k)}(s)\ G_{z,\varphi}(s) \| < \infty \qquad 3.28$$

Proposition 1 allows us to deduce from these properties that

$$\sup_{(\varphi;s)} \| B_\varphi(s)\ A_{1,\varphi}(s) \| < \infty$$

and therefore $M(BA_1\ P)$ is well defined, from proposition 2. Since $(BA_1\ P)^+ \in \mathcal{C}$, we see by writing $BA_1\ P = (BA_1\ P)\ P$ that $M(BA_1\ P) = M(PBA_1\ P)$, by proposition 3. The result 3.28 shows that $A_{1,\varphi}(s)$ given by

$$A_{1,\varphi}(s) = -\oint_{\Gamma} \frac{dz}{2\pi i}\ G_{z,\varphi}(s)\ G_{z;\varphi}'(s) \in \mathcal{C}$$

and $\sup_{(\varphi;s)} \| A_{1,\varphi}(s) \| < \infty$. Using the fact that $BP \in \mathcal{C}$ and 3.26, we conclude that $M(BPA_1)$ is well defined. Writing $BPA_1 = (BP)\ (PA_1)$, and using the fact that $(BP)^+ = P\ (BP)^+$ and $A_1^+ = -A_1$, we can apply proposition 3 to write $M(BPA_1) = M(PA_1BP)$. We have therefore proved the formally established result

$$M(BA_1) = M(PA_1\ BP) + M(P\ BA_1\ P)$$

The remaining steps leading to the final formula 3.23, for this expression, can be justified in a similar way by noting that $\sup_{(s;\varphi;z)} \| B_\varphi(s)\, G_{z,\varphi}(s) \| < \infty$ as a consequence of proposition 4.

It remains to prove that all terms of order T^{-2} can be neglected in the adiabatic limit.

Let $$\alpha_{z;\varphi;T}(s\ s') = (z-H(s))_j \ \tau_{\varphi;T}(s\ s')\ G_{z,\varphi}(s') \qquad 3.29$$

where $$\tau_\varphi(s, s') = V_{\varphi,T}(s) \quad V^{+}_{\varphi;T}(s') \qquad 3.30$$

we will prove that $$\sup_{\substack{z \in \Gamma \\ \varphi \in Tm \\ 0 \le s' \le s \le 1;\, T>0}} \| \alpha_{z,\varphi,T}(s,s') \| < \infty \qquad 3.31$$

and that $\alpha_{z,\varphi,T}(s,s')$ maps D into D.

We will also prove that the operator

$$\beta_{z,\varphi,T}(s,s') = (z-H_\varphi(s))\, \alpha_{z,\varphi,T}(s,s')\, G_{z,\varphi}(s') = (z-H_\varphi(s))^2\, \tau_{\varphi,T}(s,s')\ G^2_{z;\varphi}(s') \qquad 3.32$$

is bounded and satisfies

$$\sup_{\substack{z \in \Gamma \\ \varphi \in Tm \\ 0 \le s' \le s \le 1;\, T>0}} \| \beta_{z,\varphi,T}(s,s') \| < \infty \qquad 3.33$$

On the other hand, let $K_{z,\varphi}(s) = (z-H_\varphi(s)) \ G''_{z\,\varphi}(s)$

$$K_{z,\varphi}(s) = 2\,(H'\,G_z)^2_\varphi\,(s) + H''_\varphi\,(s)\, G_{z,\varphi}\,(s) \qquad 3.34$$

It follows from 3.28 that

$$\sup_{(z;\varphi;s)} \{ \| K_{z,\varphi}(s) \| , \ \| K'_{z,\varphi}(s) \| \} < \infty \tag{3.35}$$

Since we can write

$$B(s)\, A_2(s) \ = \ -\frac{1}{2} \oint_{\Gamma} \frac{dz}{2\pi i} \ \{(B\ G_z^2)(s)\, K_z(s)\} \ \{G_{z^*}(s)\}^+$$

we see that $M(B(s)\ A_2(s))$ is well defined

and $\lim\limits_{T \to \infty} \frac{1}{T} \int_0^1 ds\ M(B(s)\ A_2(s)) \ = \ 0$

Writing

$$B(s)\ V(s)\ A_2(s)\ V^+(s) = \frac{-1}{2} \oint_{\Gamma} \frac{dz}{2\pi i} \ \{(BG_z^2)(s)\ \beta_z(s, 0)\ K_z(0)\ \} \ \{G_{z^*}(s)\ \alpha_{z^*}(s, 0)\ \}^+$$

it follows from 3.31, 3.33, 3.35, by proposition 1 and 2 that $M(B(s)\ V(s)\ A_2(s)\ V^+(s))$ is well defined and $\lim\limits_{T \to \infty} \frac{1}{T} \int_0^1 ds\ M(B(s)\ V_T(s)\ A_2(0)\ V_T^+(s)) \ = \ 0.$

Finally, a simple computation shows that

$$B(s)\ \tau(s, s')\ A_2'(s')\ \tau^+(s, s') \ = -\frac{1}{2} \oint_{\Gamma} \frac{dz}{2\pi i} \ \Lambda_z(s, s')$$

where

$$\Lambda_Z(s,s') = \{(BG_z^2)(s)\,\beta_Z(s,s')\,[(H'\,G_Z)\,K_Z + K_z' + (z-H)\,H'\,G_z^2]\,(s')\}$$

$$\times\ \{\,G_{Z^*}(s)\,\alpha_{Z^*}(s,s')\}^+$$

$$+\ \{(BG_z^2)(s)\,\beta_Z(s,s')\,K_Z(s')\}\ \{\,G_{Z^*}(s)\,\alpha_{Z^*}(s,s')\,H'(s')\,G_{Z^*}(s')\}^+$$

From hypothesis 5) of the theorem and proposition 4, follows that

$$\sup_{(z;\varphi;s)} \| (z-H_\varphi(s'))\ H_\varphi'(s)\ G_{z;\varphi}^2(s) \| < \infty \tag{3.36}$$

This result, combined with 3.31, 3.33, 3.35 again, proves that $M(B(s)\,\tau(s,s')\,A_2'(s')\,\tau^+(s,s'))$

is well defined and $\lim\limits_{T\to\infty} \frac{1}{T}\int_0^1 ds \int_0^s ds'\ M(B(s)\,\tau_T(s,s')\ A_2'(s')\ \tau_T^+(s,s')) = 0.$

To summarize, we have proven that

$$\lim_{T\to\infty} \frac{1}{T}\int_0^1 ds\ M(B(s)\,A_{2,T}(s)) = 0$$

and therefore theorem 2.

It remains to prove however the announced properties of $\alpha_Z(s,s')$ and $\beta_Z(s,s')$. First of all, note that by proposition 4, for any T : $\sup\limits_{(z;\varphi;s)} \| (\alpha_{Z,\varphi}(s,s') \| < \infty$.

On the other hand, the evolution equation for $V(s)$ shows that $\alpha_Z(s,s')$ satisfies the integral equation

$$\alpha_Z(s,s') = \tau(s,s') + \int_{s'}^{s} dt\ \alpha_Z(s,t)\ R_Z(t,s') \tag{3.37}$$

where $R_Z(t,s') = -\,H'(t)\,G_Z(t)\,\tau(t,s')$ (3.38)

We have $r = \sup_{\substack{(z;\varphi) \\ 0 \le s' \le s \le 1 \\ T}} \| (R_{z,\varphi}(s, s') \| < \infty$

Therefore, the operator given by the convergent series

$$\alpha_z (s, s') = \tau(s, s') + \sum_{n=1}^{\infty} dt_1 \dots dt_n \ \tau(s, t_n) \ R_z(t_n, t_{n-1}) \ \dots \ R(t, s')$$

$$s' \le t_1 \le \dots \le t_n \le s \qquad 3.39$$

is the unique solution of 3.37, such that $\sup_{0 \le s' \le s \le 1} \| (\alpha_z (s, s') \| < \infty$. It coincides therefore with the operator defined by 3.29.

3.39 shows that $\| \alpha (s, s') \| \le \exp \ r$ 3.40

Since $\tau(s, s')$ and $R_{z,\varphi} (t, s)$ maps D into D, the series 3.28 shows that $\alpha_z(s, s')$ maps D into D. We have proved therefore the stated properties of α. We can prove similarly that $\beta_z(s, s')$ obeys the equation

$$\beta_{z,\varphi} (s, s') = \alpha_{z,\varphi}(s, s') + \int_{s'}^{s} \beta_{z,\varphi} (s, t) \, Q_{z,\varphi} (t, s') \ dt \qquad 3.41$$

where

$$Q_{z,\varphi} (t, s') = -(z - H_\varphi(t)) \ H_\varphi'(t) \ G_z^2(t) \ \alpha_{z,\varphi}(t, s') \qquad 3.42$$

The result 3.36 and 3.40 allows to prove that

$$\sup_{\substack{(z;\varphi) \\ 0 \le s' \le t \le 1 \\ T}} \| Q_{z,\varphi} (t, s') \| = q < \infty,$$

and proceeding as for α to conclude that

$$\sup_{\substack{(z;\varphi) \\ 0 \le s' \le s \le 1 \\ T}} \| \beta_{z,\varphi} (s, s') \| \le \exp \ r + q$$

This ends the proof of the theorem.

In the applications we will consider the following situation. Our system will be made of independent electrons interacting with ions by means of quasi-periodic potentials, depending on some phases φ and in the possible presence of a magnetic field.

The electrons will be at zero temperature. The parameter μ is their chemical potential, assumed to be in a gap of the one-electron hamiltonian H_φ. Initially, these electrons are in their ground state, described by the Fermi projector $P(0) = E_{H(0)}(-\infty, \mu)$.

The first situation to be considered is that where only one of the phases, let us say φ_j, changes by 1 in the adiabatic process :

$$\varphi_j(s) = \varphi_j(0) + \psi(s) \qquad 3.43$$

with $\psi'(0) = 0$ and $\psi(0) = 0$ $\psi(1) = 1$ and $\psi(s) \in C^3(I)$

The other phases are supposed not to change.

We note that in such an adiabatic process, the system follows a loop in the parameter space, so that interesting topological effects can be expected if we choose for B an observable sensible to the phase of the wave functions. Such operators exist; they are simply momentum or velocity operators associated to currents. We will look therefore at the adiabatic charge transport in the space direction α generated by this process. This is defined by the quantitiy

$$Q(j\alpha) = \lim_{T \to \infty} e \int_0^T dt\, [M(v_\alpha \rho(t)) - M(v_\alpha \rho(0))] \qquad 3.44$$

where $\vec{v} = \frac{1}{m} (\vec{p} - e\vec{A}(r))$ 3.45

is the velocity operator.

To call such a quantity charge transport is justified by the fact that the charge going througe a surface element $d\vec{\sigma}$ pointing in the direction k, at the point r, during the time interval (t, t + dt) is given by

$$e\,(\vec{v}\,.\,d\vec{\sigma}\,\rho(t))\,(r,r)\ dt$$

so that $Q(j\alpha)$ measures the space average charge transported through such a surface element during the adiabatic process. It has the dimension : charge/(length)$^{d-1}$.

If we now apply formula 3.23 of theorem 2, we get :

$$-\,Q(j\alpha) = Q(\alpha j) = i\hbar e\, M(P[V_\alpha, P_j]) \tag{3.46}$$

where

$$V_\alpha = \oint_\Gamma \frac{dz}{2\pi i}\, G_z\, v_\alpha\, G_z \tag{3.47}$$

$$P_j = \oint_\Gamma \frac{dz}{2\pi i}\, G_z\, \partial_{\varphi_j}\, H_\varphi\, G_z = \frac{\partial P}{\partial_{\varphi_j}} \tag{3.48}$$

In doing this, we made the change of variables $\varphi(s)$ to φ (of jacobian 1), φ being the variables appearing in the mean. Because of this, condition 3.22 of theorem 2 is automatically satisfied and there is no more any time dependence of the operators appearing in 3.46.

The second case we will consider is that of an electric field E_l applied in the direction l on our system and adiabatically switched :

$$E_l(t) = \frac{1}{T}\, g\, \left(\frac{t}{T}\right) \tag{3.49}$$

with $\quad g\,(0) = 0 \qquad\qquad g\,(s) \in C^3(I)$

Choosing to represent it by a gauge potential - $\alpha(\frac{t}{T})$ in the direction l, given by

$$\alpha(s) = \int_0^s ds' \; g(s') \qquad 3.50$$

the average current generated in the direction k will be given by

$$j_k(t) = e\, M\left((v_k + e\frac{\delta k;l}{m}\; \alpha(\tfrac{t}{T}))\; \rho(t)\right) \qquad 3.51$$

The time dependent hamiltonian in this case is of the form

$$H(t) = \frac{1}{2} m \sum_{k=1}^{d} (v_k + e\frac{\delta k;l}{m}\; \alpha(t))^2 + V \qquad 3.52$$

Introducing the unitary operator $S_{\alpha(t)} = e^{ie\alpha(t)\, x_l}$ we see that

$$H(t) = S^*_{\alpha(t)}\, H(0)\; S_{\alpha(t)} \qquad 3.53$$

and the same unitary equivalence holds for $P(s)$, $G_z(s)$.

Since $M\left((v_k + e\,\frac{\delta k;l}{m}\; \alpha(s))\; P(s)\right) = M\left(\; S^*_{\alpha(s)} v_k\, P(0)\;\; P(0)\, S_{\alpha(s)}\right)$, if v_k satisfies the conditions of the operator B of theorem 2, we can use the cyclicity of M (proposition 3) to conclude that

$$\int_0^1 ds\, M\left((v_k + e\frac{\delta_{k;l}}{m}\; \alpha(s))\; P(s)\right) = M\left(v_k\, P(0)\right) \qquad (3.54)$$

Therefore, if there is no current initially, theorem 2 tells us that :

$$\lim_{T\to\infty} \int_0^T j_k(t)\;\; dt \;=\; -\, i\, \hbar e^2\, \alpha(1)\;\; M(P\, [V_k, V_l]) \qquad 3.55$$

the time dependence of the right-hand side of the equation being eliminated by the same argument that lead to 3.54.

Now note that we can write :

$$\int_0^T \frac{j_k(t)\,dt}{\alpha(1)} = \frac{\frac{1}{T}\int_0^T j_k(t)\,dt}{\frac{1}{T}\int_0^T E_l(t)\,dt} \tag{3.56}$$

We are therefore naturally lead to interpret

$$\sigma_{kl} = -i\hbar\, M\,(P[V_k, V_l])$$

as the conductivity tensor, when the chemical potential μ is in a gap.

It might look surprising at first sight that this expression does'nt contain a correction non linear in the electric field, but with the form choosen for the electric field, it remains always infinitesimally small, during the adiabatic process.

In any case, this expression can be derived from a Kubo formula, which is a perturbative computation of the conductivity (See [16], for a computation in the case of a random hamiltonian, for which an average like M(.) can be defined).

The two quantities we have introduced, i.e. the adiabatic charge transport and the conductivity tensor will be the only one for which the result of theorem 2 could be interpreted in physical terms. During the analysis of the adiabatic charge transport for multi-dimensionnal quasi-periodic potentials, we have been lead to introduce other quantities which appear to be topological invariants. The relationship of these quantities to an adiabatic process remains mysterious, but we suspect that they are related to higher order terms in the adiabatic expansion.

Finally, we can note that there is a mean like M(.) which appears in the study of other ergodic hamiltonians, namely random hamiltonians and all the analysis presented here can be extended to such systems (See [16], for a study of the quantum Hall effect).

4. Quasi-periodic potentials

We consider a system of independent electrons, at zero temperature, in interaction with a quasi-periodic potential in d dimensions. We choose as unit of length a, a typical length scale associated to the variation of the potential and as unit of energy $\frac{\hbar^2}{ma^2}$

The potential $V_\varphi(x)$ will be assumed to satisfy the conditions

1)

$$V_\varphi(x) = \sum_{n \in Z_m} a(n) \exp 2\pi i (n, \Omega x) + 2\pi i (n, \varphi) \qquad 4.1$$

where Ω is an m x d matrix, defining the basic frequencies of the potential. In order to define a quasi-periodic potential, Ω will be assumed to be such that $\Omega^T n=0$ implies $n = 0$, for all $n \in Z_m$. The phases $\varphi \in T_m$, the m-dimensional torus

2) $a^*(n) = a(-n)$, so that $V_\varphi(x)$ is real

and

$$\sum_{n \in Z_m} |a(n)| \left(\sup_{1 \le i \le m} |n_i| \right)^3 < \infty \qquad 4.2$$

Under this condition $V_\varphi(x)$ defines a bounded multiplication operator on $\mathcal{H} = L^2(R^d, dx)$, which is in norm $C^3(T_m)$.

The associated one electron hamiltonian will be given in these units by :

$$H_\varphi = -\frac{1}{2}\Delta + V_\varphi(x) \qquad 4.3$$

which is a self-adjoint operator on the dense domain

$$D = \{ \psi \in L^2 \mid \int k^4 |\hat{\psi}(k)|^2 d^d h < \infty \} \quad 4.4$$

which is simply the domain of the laplacian.
This domain is left invariant by the unitary translation operator $U_a = \exp i \vec{a} \cdot \vec{p}$ and we have

$$U_a H_\varphi U_a^{-1} = H_{\varphi(a)} \quad 4.5$$

where $\varphi(a) = \varphi + \Omega a$ 4.6

The condition imposed on Ω guarantees that $\varphi(a)$ defines an ergodic flow on the torus T_m. We see therefore that the hamiltonian H_φ is ergodic.

We also have (a known result, see for example [17])

Lemma 1
$\rho(H_\varphi)$, the resolvent set of H_φ is independent of φ.

Proof
Consider the functions $F_z(\varphi) = \begin{cases} 1 & \text{if } z \in \rho(H_\varphi) \\ 0 & \text{if } z \notin \rho(H_\varphi) \end{cases}$

4.5 shows that $F_z(\varphi) = F_z(\varphi + \Omega a)$

The ergodic theorem then implies that $F_z(\varphi)$ is almost surely constant in φ. On the other hand, the norm continuity in φ of H_φ, implies that $\rho(H_\varphi)$ is continuous in φ. This shows that $F_z(\varphi)$ is continuous in φ. Indeed, $|F_z(\varphi) - F_z(\varphi')| = 1$ if $z \in \rho(H_\varphi)$, $z \notin \rho(H_{\varphi'})$, or $z \in \rho(H_{\varphi'})$, $z \notin \rho(H_\varphi)$. But if $z \in \rho(H_\varphi)$, $\exists\, \delta(z, \varphi)$, such that if $|\varphi' - \varphi| > \delta$, $z \in \rho(H_{\varphi'})$, hence $|F_z(\varphi) - F_z(\varphi')| = 0$ if $|\varphi' - \varphi| < \delta$.

Consequently, $F_z(\varphi)$ is constant, which proves the lemma.

As we mentioned before the time dependent hamiltonian associated to the adiabatic process in this case will be $H(t) = H_{\varphi(t)}$

where $\varphi_k(t) = \varphi_k + \delta_{k,j}\, \psi(t)$ 4.7

with $\psi(0) = 0$ $\psi(1) = 1$ $\psi'(0) = 0$ and $\psi(t) \in C^3(I)$

We see that conditions 1) and 2) on the hamiltonian in theorem 2 are satisfied as a consequence of property 4.2 of the potential and the definition of $\varphi(t)$. Lemma 1 shows that condition 3) is also satisfied. The remaining conditions will force us to consider only the case where the space dimensionality d = 1, 2, 3.

Proposition 5

If $1 \leq d \leq 3$ $\qquad G_{i,\varphi_t} \in C \quad$ and $\quad \sup_{\varphi;\, t} |G_{i,\varphi_t}| < \infty$

Indeed, the first resolvent equation $\quad G_{i,\varphi} = G_i^0 + G_i^0 \, V_\varphi \, G_{i,\varphi} \quad$ with

$$G_i^0 = (i + \tfrac{1}{2}\Delta)^{-1} \tag{4.8}$$

and the fact that $\sup_\varphi \|V_\varphi\| < \infty$ will give the result, by proposition 1, if we prove it for G_i^0.

G_i^0 has a kernel given by :

$$G_i^0(r, r') = \int \frac{d^d k}{(2\pi)^d} \frac{1}{i - \frac{k^2}{2}} \exp i k (r - r')$$

therefore $|G_i^0|^2 = \int |G_i^0(r, r')|^2 \, dr' = \int \frac{d^d k}{(2\pi)^d} \frac{1}{1 + \frac{k^4}{4}} < \infty$ if $d \leq 3$

and

$$|G_i^0|^2_{s;r} = \int \frac{d^d k}{(2\pi)^d} \frac{|1 - e^{ik(s-r)}|^2}{1 + \frac{k^4}{4}}$$

tends to zero, if $d \leq 3$, when $r \to s$. Therefore, $G_i^0 \in C$.

We also have

Proposition 6

$H'_{\varphi}(t)\, G_{i,\varphi}(t)$ maps D into D.

We have to prove that $(\partial_{\varphi_j} V_\varphi)\, G_{i,\varphi}$ maps D into D.

But

$$[\vec{p}^{\,2}\,(\partial_{\varphi_j} V_\varphi)\, G^0_{i;\varphi}\,\psi](r) = (-\Delta\, \partial_{\varphi_j} V_\varphi)(r)\;(G^0_i\,\psi)(r)$$

$$+\, 2\,i\,(\vec{\nabla}\partial_{\varphi_j} V_\varphi)(r)\;(\vec{p}\, G^0_i\,\psi)(r)$$

$$+\, (\partial_{\varphi_j} V_\varphi)(r)\;(\vec{p}^{\,2}\, G^0_i\,\psi)(r)$$

Since $\| -\Delta\,\partial_{\varphi_j} V_\varphi \|_\infty < \infty$ and $\| \vec{\nabla}\partial_{\varphi_j} V_\varphi \|_\infty < \infty$ from condition 4.2 on the potential, and $(\vec{p}\, G^0_i\,\psi) \in L^2$ as well as $(\vec{p}^{\,2}\, G^0_i\,\psi) \in L^2$ for any $\psi \in L^2$, we see that $\partial_{\varphi_j} V_\varphi\, G^0_i\,\psi \in D$ for any $\psi \in L^2$. The result follows by using the first resolvent equation.

We now look at the conditions for the operator B(t) that we take as $B(t) = p_k$.

It is clear that it is an ergodic operator, closed with a domain containing D.
We have moreover

Proposition 7

If $d \le 3$, $p_k\; G^2_{i;\varphi_t} \in \mathcal{C}$ and $\sup_{\varphi;\,t} |p_k\, G^2_{i;\varphi_t}| < \infty$

The first resolvent equation gives

$$p_k\; G^2_{i;\varphi} = p_k (G^0_i)^2\,[1 + V_\varphi\, G_{i,\varphi}] + G^0_i\;\; p_k\, V_\varphi\, G^2_{i;\varphi}$$

$p_k (G^0_i)^2$ is bounded. Since $p_k\, V_\varphi\, G_{i,\varphi} = (p_k\, V_\varphi)\; G_{i,\varphi} + V_\varphi\; (p_k\; G_{i,\varphi})$ and $\sup_\varphi \| p_k\;\; V_\varphi \|_\infty < \infty$ from 4.2, and $\| p_k\, G^0_i \| < \infty$, we have from the first resolvent equation $\sup_{\varphi} \| p_k V_\varphi G^2_{i;\varphi} \| < \infty$. From proposition 1 follows therefore that $\sup_{\varphi} | p_k G^2_{i;\varphi} | < \infty$ if $| p_k (G^0_i)^2 | < \infty$ but

$$| p_k (G^0_i)^2 |^2 = \int \frac{d^d p}{(2\pi)^d} \frac{p_k^2}{(1 + \frac{p^2}{4})^2} < \infty \quad \text{if} \quad d \leq 5.$$

We can therefore conclude that theorem 2 is valid in the case considered. We summarize the results in the

Theorem 3 Let H_φ be the hamiltonian

$$H_\varphi = -\frac{1}{2} \Delta + V_\varphi (x)$$

If the quasi-periodic potential satisfies the conditions 1) and 2), the adiabatic charge transport corresponding to the adiabatic change of φ_j from 0 to 1 is given in units of $\frac{e}{a^{d-1}}$ by the expression $-\ Q(\alpha j)$, with

$$Q(\alpha j) = i \ M \ (P [V_\alpha , \partial_{\varphi_j} P])$$

where $V_\alpha = \oint_\Gamma \frac{dz}{2\pi i} G_z \, p_\alpha G_z$

if the space dimensionality d = 1, 2, 3.

We will not consider in this case, the conductivity tensor, since it will be zero in most cases, because we have not applied a magnetic field on the system.

5. The topological invariants and the periodic approximation

We will see that in one dimension, charge transport is quantized, because it is a topological invariant. In analyzing the multi-dimensional situation, we were led to introduce other quantities, whose physical interpretation remains elusive, but which are also topological invariants. They are defined in the following way. If we denote the generalized velocity operator V_α of § 4 by P_α and $\frac{\partial P}{\partial \varphi_j}$ by P_j, then charge transport $Q(\alpha\ j)$ is given by the expression

$$Q(\alpha\, j) = i \sum_{\pi} (-1)^{\pi} M\left(P\ P_{\pi(\alpha)}\ P_{\pi(j)}\right) \qquad 5.1$$

where π is a permutation of α and j. It is antisymmetric in α and j. We then define the two quantities

$$Q\,(\alpha\, j\, \beta k) = \frac{i^2}{2!} \sum_{\pi} (-1)^{\pi} M\left(P\ P_{\pi(\alpha)}\ P_{\pi(j)}\ P_{\pi(\beta)}\ P_{\pi(k)}\right) \qquad 5.2$$

and

$$Q\,(\alpha\, j\, \beta k\, \gamma\, l) = \frac{i^3}{3\,!} \sum_{\pi} (-1)^{\pi} M\left(P\ P_{\pi(\alpha)}\ P_{\pi(j)}\ P_{\pi(\beta)}\ P_{\pi(k)}\ P_{\pi(\gamma)}\ P_{\pi(l)}\right) \qquad 5.3$$

Π being a permutation of the indices appearing in the sum. The Greek letters designate velocities, whereas the Latin ones correspond to phases. These expressions are fully antisymmetric in all their indices. They make sense, since we proved in § 4 that $P_\alpha = P_\alpha^+$, $P_j = P_j^\dagger$ belong to $\mathcal{C}$. The operator P_α can also be regarded as the derivative of the projector P with respect to some variable. This can be seen as follows.

Let $$S_\lambda = \exp i \sum_{\alpha=1}^{d} \lambda_\alpha x_\alpha \qquad 5.4.$$

If A is an averageable operator $(A \in \mathcal{M})$, we define

$$A(\lambda) = S_\alpha^{-1} A S_\lambda \qquad 5.5$$

which is such that

$$M\,(A(\lambda)) = M\,(A) \qquad 5.6$$

On D the unitary operator S_λ transforms the hamiltonian H in the hamiltonian $H(\lambda)$:

$$H(\lambda) = S_\lambda^{-1} H S_\lambda = \frac{1}{2} \sum_{\alpha=1}^{d} (p_\alpha + \lambda_\alpha)^2 + V \qquad 5.7$$

and since

$$\frac{\partial H}{\partial \lambda_\alpha} = p_\alpha + \lambda_\alpha \qquad 5.8$$

the operator V_α is transformed into $V_\alpha(\lambda)$:

$$V_\alpha(\lambda) = \oint_\Gamma \frac{dz}{z\pi i} G_z(\lambda)(p_\alpha + \lambda_\alpha) G_z(\lambda) = \frac{\partial}{\partial \lambda_\alpha} P(\lambda) \qquad 5.9$$

Property 5.6 shows then that $Q(\alpha\, j)$, $Q(\alpha\, j\, \beta\, k)$, $Q(\alpha\, j\, \beta\, k\, \gamma\, l)$ can be written in the form 5.1, 5.2, 5.3 in which $P_\alpha \equiv \frac{\partial P}{\partial \lambda_\alpha}$ and the expression for these quantities is independent of λ. This fact will appear useful later on.

We are now going to prove that these expressions are topological invariants. More precisely, in one dimension $Q(\alpha\, j)$ is an integer, whereas in two dimensions this is the case for $Q(\alpha\, j\, \beta\, k)$ and in three dimensions for $Q(\alpha j\, \beta\, k\gamma\, l)$.The general strategy of the proof is simple, but perhaps obscured by the technical details. We will approximate the quasi-periodic potential by a periodic one. The approximation will be such that the gap is preserved and the quantities like $Q(\alpha\, j)$, $Q(\alpha\, j\, \beta\, k)$... are given as the limit of the corresponding ones for the periodic potentials. Finally, for the periodic potentials, they will appear as Chern numbers of certain unitary vector bundles. This will prove their quantization in the quasi-periodic case.

We approximate the potential V_φ by a periodic potential V_φ^L, of period L, in the following way. If we call Λ_L the d-dimensional cube $[0, L]^d$, then we take $V_\varphi^L(x) = V_\varphi(x)$ when $x \in \Lambda_L$, and extend it periodically, i.e. $V_\varphi^L(x + n\, L) = V_\varphi^L(x)$ for all $n \in \mathbb{Z}^d$. Note that V_φ^L is uniformly bounded, so that

$$\| V \| = \sup_{\varphi;x} (|V_\varphi(x)|, (|V_\varphi^L(x)|) < \infty \qquad 5.10$$

The corresponding periodic hamiltonian H_φ^L is defined as

$$H_\varphi^L = -\frac{1}{2}\Delta + V_\varphi^L \qquad 5.11$$

One easily sees that H_φ is the strong limit of H^L_φ, but this property doesn't guarantee that a gap of H_φ corresponds to a gap of H^L_φ, when L is large enough. This will be the result of the following lemma, in which $\rho(H)$ designates the resolvent set of a hamiltonian.

<u>Lemma</u> Let Δ be a compact subset of $\rho(H_\varphi) \cap \mathbb{R}$, then there exist a $L_o(\Delta)$ such that $\Delta \subset \rho(H^L_\varphi) \cap \mathbb{R}$, for all φ.

<u>Proof</u> If A_φ is a bounded operator of kernel $A_\varphi(x, x')$, we will call

$$|A|_1 = \sup_{x;\varphi} \int |A_\varphi(x, x')| \, dx' \tag{5.12}$$

then we have the inequality

$$|AB|_1 \leq |A|_1 \, |B|_1 \tag{5.13}$$

In order to prove that for all $z \in \rho(H\varphi)$ we have $|G_z|_1 < \infty$, we note that it follows from Schwartz inequality that :

$$|G_z|_1^2 \leq c(\epsilon) \sup_{|a| \leq \epsilon} \|G_z(a)\| \tag{5.14}$$

where

$$G_z(a) = \exp(a, x) \; G_z \exp -(a, x) \tag{5.15}$$

On the other hand, one can show that

$$\sup_{|a| \leq \epsilon} \|G_z(a)\| \leq \frac{b}{1 - \epsilon(d+1)b} \tag{5.16}$$

where

$$b = \sup_{1 \leq j \leq d} (\|G_z p_j\|, \|G_z\|)$$

Let us now assume that there exist an energy $e \in \Delta$ in the spectrum of H^L_φ. By Bloch theorem, there exist a solution of the equation $H^L_\varphi \psi^L = e\, \psi^L$, such that $\sup_x(|\psi^L(x)|, \ |\nabla \psi^L(n)|) < \infty$. This function ψ^L is also a solution of the equation

$$\psi^L(x) = \int G_z(x, x') \ (V^L - V) \ (x') \ \psi(x') \, d x' \qquad 5.17$$

Indeed let $\varphi_n(x) = \psi^L(x) f_n(x)$, where $f_n(x) = \exp \frac{-x^2}{n}$ and $\varepsilon_n = (e - H^L) \varphi_n$ Since $\varepsilon_n(x) = \frac{1}{2}(\Delta f_n)(x) \ \psi(x) + \nabla f_n \, . \, (\nabla \psi^L)(x)$, we see that $\varepsilon_n \in L_2 \cap L_\infty$ and $\lim_{n \to \infty} \varepsilon_n(x) = 0$. As $\varphi_n \in L_2 \cap L_\infty$ the equation $\varepsilon_n = (e - H) \varphi_n - (V^L - V) \varphi_n$ can be solved in L_2.

$$\varphi_n(x) = \int G_e(x, x') \ \varepsilon_n(x') \, dx' + \int G_e(x, x') \, (V^L - V)(x') \ \varphi_n(x') \, dx'$$

As $|G_e|_1 < \infty$, this equation holds pointwise. Taking the limit n going to infinity gives 5.17.

On the other hand from 5.17, follows that

$$\|\psi^L\|_\infty \leq 2 \|V\| \ f(e, L) \ \|\psi^L\|_\infty \qquad 5.18$$

$$\text{where } f(e, L) = \sup_{x;\varphi} \int_{R^d \setminus \Lambda_L} dx' \ |G_e(x, x')| \qquad 5.19$$

If we can show that there exist an $L_o(\Delta)$ such that if $L > L_o(\Delta)$, then $f(e, L) < \frac{1}{2\|V\|_\infty}$, $\forall e \in \Delta$, (5.20), then $\|\psi^L\|_\infty = 0$, which would contradict the assumption and therefore prove the lemma.

The second resolvent equation gives

$$|f(e, L) - f(e', L)| \leq |e' - e| \ |G_e|_1 \ |G_{e'}|_1$$

There exist therefore for all ε, a $\delta(\varepsilon)$ independent of L such that $|f(e, L) - f(e', L)| \leq \varepsilon$ if $|e' - e| \leq \delta$.

On the other hand, there exist a finite covering of Δ by balls of center e_j and radius δ, such that for every e_j, there is a L_j such that $f(e_j\ L_j) \leq \varepsilon$. Since 5.19 shows that $f(e, L)$ is decreasing in L, we have

$$f(e_j, L) \leq \varepsilon$$

if $\quad L \geq \sup_j L_j \quad$, and therefore $\quad 0 \leq f(e, L) \leq 2\varepsilon$

which proves 5.20 and ends the proof of the lemma.

We are now able to define the expressions corresponding to charge transport $Q(\alpha j)$ and the other quantities for the hamiltonian H^L. For any $z \in \Gamma$, we can define

$$G^L_{z;\varphi} = (\tau - H^L_\varphi)^{-1} \tag{5.21}$$

if $L \geq L_o$, and $\sup\limits_{\substack{z \in \Gamma \\ \varphi \in Tm \\ L \geq L_0}} \| G^L_{z;\varphi} \| < \infty$ 5.22

The projector P^L is defined by $\quad P^L = \oint_\Gamma \frac{dz}{2\pi i} G^L_z$ 5.23

and $$P^L_\alpha = \oint_\Gamma \frac{dz}{2\pi i} G^L_z\ P\alpha\ G^L_z \tag{5.24}$$

$$\partial_{\varphi_j} P^L \equiv P^L_j = \oint_\Gamma \frac{dz}{2\pi i} G^L_z\, \partial_{\varphi_j}\ V^L_\varphi\ G^L_z \tag{5.25}$$

The equation

$$G^L_z = G_z + G_z (V^L - V) G^L_z = G_z + G^L_z\ (V^L - V)\ G_z \tag{5.26}$$

and equations 5.22 allows us to deduce from the corresponding properties for the resolvent $G_{z,\varphi}$ that

$$a = \sup_{\substack{z \in \Gamma \\ \varphi \in Tm \\ L \geq L_0}} \{ \| G^L_{z;\varphi} \|, | G^L_{z;\varphi} |, | G^L_{z;\varphi} p_\alpha \|, | G^L_{z;\varphi} p_\alpha |, | G^L_{z;\varphi} \partial_{\varphi_j} V^L_\varphi \| \; G^L_{z\,\varphi} \partial_{\varphi_j} V^L_\varphi | \} \quad 5.27$$

is finite. And we conclude that if we call $P^L_0 \equiv P^L$, we have

$$P^L_s = (P^L_s)^+ \in \mathcal{C} \text{ for } s = 0, \alpha \text{ or } j. \quad 5.28$$

and

$$\sup_{\varphi; L \geq L_0} \| P^L_{s;\varphi} \| < \infty$$

5.29

We can therefore define the quantities

$$Q^L(\alpha\, j) = i \sum_\pi (-1)^\pi M\left(P^L \; P^L_{\pi(\alpha)} \; P^L_{\pi(j)}\right) \quad 5.30$$

$$Q^L(\alpha\, j\, \beta k) = \frac{i^2}{2\,!} \sum_\pi (-1)^\pi M\left(P^L \; P^L_{\pi(\alpha)} \; P^L_{\pi(j)} \; P^L_{\pi(\beta)} \; .P^L_{\pi(k)}\right) \quad 5.31$$

$$Q^L(\alpha\, j\, \beta k\, \gamma\, l) = \frac{i^3}{3\,!} \sum_\pi (-1)^\pi M\left(P^L \; P^L_{\pi(\alpha)} \; P^L_{\pi(j)} \; P^L_{\pi(\beta)} \; .P^L_{\pi(k)} \; P^L_{\pi(\gamma)} \; P^L_{\pi(l)}\right)$$

5.32

where now we understand by $M(A^L)$:

$$M(A^L) = \int_{\Lambda_L} \frac{dx}{|\Lambda_L|} \int_{T_m} d\varphi \;\; A^L_\varphi \;\; (x, x) \quad 5.33$$

Note that this definition for an operator A related to the quasi-periodic hamiltonian coincides with the old one.

We can now prove that these expression converge to those of the quasi-periodic hamiltonian, when $L \to \infty$.

Let us call $m(A) = M(AA^+)^{1/2}$ 5.34

We first prove $\lim\limits_{L\to\infty} m\left(P_s - P_s^L\right) = 0$ 5.35

for $s = 0, \alpha$ or j.

This will result from the following property

If $A_\varphi(z) \in 1$ and $\sup\limits_{\substack{z\in\Gamma\\ \varphi}} |A_\varphi(z)| < \infty$ 5.36

then $\lim\limits_{L\to\infty} \oint_\Gamma d|z|\ m(A(z)(V - V^L)) = 0$ 5.37

and $\lim\limits_{L\to\infty} \oint_\Gamma d|z|\ m[A(z)(\partial_{\varphi_j}(V_\varphi - V_\varphi^L)] = 0$ 5.38

Indeed

$$m^2[A(V - V^L)] = \int_{\Lambda_L} \frac{dx}{|\Lambda_L|} \int d\varphi \int dy\ |A_\varphi(x,y)|^2 (V - V^L)^2(y)$$

so that by the ergodicity of A_φ

$$m^2[A(V - V^L)] \le 4\|V\|^2 \int_{\Lambda_L} \frac{dx}{|\Lambda_L|} \int d\varphi \int_{R^d\setminus\Lambda_L} dy\ |A_\varphi(0, y-x)|^2$$

Let $g(x) = \int d\varphi \oint_\Gamma d|z|\ |A_\varphi^{(z)}(0,x)|^2$. From 5.36, we know that $g \in L_1$, therefore

$$\oint_\Gamma d|z|\ m[A(V - V^L)] \le |\Gamma|^{1/2} \left(\int_{\Lambda_L} \frac{dx}{|\Lambda_L|} \int_{R^d\setminus\Lambda_L} dy\ g(y-x)\right)^{1/2}$$

tends to zero, when L tends to infinity. The same proof goes for 5.38, since

$$\sup_\varphi \|\partial_{\varphi_j} V_\varphi^L\|_\infty < \infty.$$

Proposition 1 gives :

$$m\,(AB) \le m\,(A) \sup_{\varphi} \| B_{\varphi} \| \tag{5.39}$$

Using equation 5.26, we see therefore that

$$m(P - P^L) \le \oint_{\Gamma} d|z|\ m\,[G_z\,(V - V^L)] \sup_{\varphi; z; L} \| G^L_{z;\varphi} \|$$

which tends to zero by 5.37.

Since

$$P_j - P^L_j = \oint_{\Gamma} \frac{dz}{2\pi i} \{G_{z,j}(V_\varphi - V^L_\varphi)\ G^L_z + G_z\,(\partial_{\varphi_j}(V_\varphi - V^L_\varphi))\ G^L_z + G_z\,(V_\varphi - V^L_\varphi)\ G^L_{z\,j}\}$$

where $G_{z,j} = \partial_{\varphi_j} G_z = G_z\,\partial_{\varphi_j} V_\varphi G_z$

and the corresponding expression holds for $G^L_{z\ j}$

We get, using 5.39 :

$$m\,(P_j - P^L_j) \le a \oint_{\Gamma} d|z|\ \{m[G_{z,j}\,(V - V^L)] + m\,(G_z\,\partial_{\varphi_j}(V_\varphi - V^L_\varphi)\} +$$

$$+\ a^2 \oint_{\Gamma} d|z|\ m\,(G_z\,(V_\varphi - V^L_\varphi))$$

But since $G_{z,j}$ and G_z both satisfy condition 5.36, we see that $\lim_{L\to\infty} m\,(P_j - P^L_j) = 0$, by 5.37 and 5.38.

Finally, we note that

$$P_\alpha - P^L_\alpha = \oint_{\Gamma} \frac{dz}{2\pi i} \{G_{z,\alpha}(V_\varphi - V^L_\varphi)\ G^L_z + G_z\,(V_\varphi - V^L_\varphi)\ G^L_{z\ \alpha}\}$$

where $G_{z,\alpha} = G_z\,p_\alpha\,G_z$ and $G^L_{z\ \alpha} = G^L_z\ p_\alpha\,G^L_z$.

Since both $G_{z,\alpha}$ and G_z satisfy condition 5.36 and $\| G_{z\,\alpha}^2 \| \leq a^2$, we conclude that $\lim_{L \to \infty} m(P_\alpha - P^L_\alpha) = 0$

Consider now the difference between any of the quantities $Q(\alpha\, j \ldots)$ and $Q^L(\alpha\, j \ldots)$. It will be made of a sum of terms of the form

$$M(P^L_{s_1}\ P^L_{s_2}, \ldots\ P^L_{s_{k-1}}\ \delta\ P^L_{s_k}\ \ P_{s_{k+1}} \ldots P_{s_n})$$

$$= M\ (\delta\ P^L_{s_k} P_{s_{k+1}} \ldots P_{s_n} P^L_{s_1} \ldots\ P^L_{s_{k-1}})$$

where $\delta P^L_s = P_s - P^L_s$.

By proposition 3 $|M(AB)| \leq m(A)\, m(B^+)$ so that each term in the difference is bounded by

$$m(\delta\ P^L_{s_k})\ m(\ P^L_{s_{k-1}} \ldots\ P^L_{s_1}\ P_{s_k} \ldots\ P_{s_{k+1}})$$

which tends to zero, from 5.35, 5.29 and 5.39.

We have therefore proven that :

<u>Proposition 8</u>

1) $\lim_{L \to \infty} M(P^L) = M(P)$

2) $\lim_{L \to \infty} Q^L(\alpha j) = Q(\alpha j)$, $\lim_{L \to \infty} Q^L(\alpha j \beta\, k) = Q(\alpha j \beta k)$

$\lim_{L \to \infty} Q^L(\alpha j \beta\, k\, \gamma\, l) = Q(\alpha j \beta\, k\, \gamma\, l)$.

6. Chern numbers

The usefulness of the periodic approximation will appear by expressing the quantities related to adiabatic charge transport we have introduced, in a more transparent way.

The hamiltonian H^L commuting with the abelian group of translation $T(\underline{n}\ L)$, Bloch theorem tells us that it is unitarily equivalent to

$$\int_0^1 \prod_{\alpha=1}^{d} dk_\alpha \ H^L(k) \qquad 6.1$$

where $H^L(k)$ is the operator :

$$H^L(k) = \frac{1}{2} \sum_{\alpha=1}^{d} (p_\alpha + \frac{2\pi}{L} k_\alpha)^2 + V^L(r) \qquad 6.2$$

defined on $L^2(\Lambda_L)$, with periodic boundary conditions.

The quantities P^L, P^L_α, P^L_j commuting also with the translations, they admit the same integral decomposition, so that in the expression for the topological invariants 5.30, 5.31, 5.32, we can simply replace P^L by

$$P^L(k) = \oint_\Gamma \frac{dz}{2\pi i} G^L_z(k) \qquad 6.3$$

P^L_α by

$$P^L_\alpha(k) = \oint_\Gamma \frac{dz}{2\pi i} G^L_z(k)\ (p_\alpha + \frac{2\pi}{L} k_\alpha)\ G^L_z(k) \qquad 6.4$$

and finally $P^L_j(k)$ by $\frac{\partial P^L(k)}{\partial \varphi_j}$

The average $M(A^L)$ of such observables meaning now :

$$M(A^L) = \frac{1}{L^d} \int_0^1 \prod_{\alpha=1}^{d} dk_\alpha \int_{T_m} d\varphi \ \mathrm{Tr}\ A^L(k, \varphi) \qquad 6.5$$

This is possible, because $G^L(k)$ is compact and $P^L(k)$ is trace class, as is easily seen.

Now since

$$p_\alpha + \frac{2\pi}{L} k_\alpha = \frac{L}{2\pi} \partial_{k_\alpha} H^L(k) \qquad 6.6$$

and G_z^L is C^2 in k, we can write 6.4 more simply as :

$$P_\alpha^L(k) = \frac{L}{2\pi} \partial_{k_\alpha} P^L(k) \qquad 6.7$$

This allows us to get a more compact expression for the invariants using the language of differential forms. Considering $P^L(k, \varphi)$, as a 0-form, let $dP^L(j\ \alpha\ k\ \beta ...)$ be the exterior derivative of P^L with respect to the variables $(\varphi_j, k_\alpha, \varphi_k, k_\beta, ...)$.

For example

$$dP^L(j\ \alpha\ k\ \beta) = \partial_{\varphi_j} P^L d\varphi^j + \partial_{k_\alpha} P^L dk^\alpha + \partial_{\varphi_k} P^L d\varphi^k + \partial_{k_\beta} P^L dk^\beta \qquad 6.8$$

Let $\Omega(j\ \alpha\ k\ \beta)$ be the associated 2-form

$$\Omega\ (j\ \alpha\ k\ \beta ...) = P^L dP^L (j\ \alpha\ k\ \beta ...) \wedge dP^L\ (j\ \alpha\ k\ \beta ...) \qquad 6.9$$

Since P^L is a projector we have

$$P^L dP^L = dP^L\ (1 - P^L) \qquad 6.10$$

Using these quantities we can write the invariants as

$$Q^L\ (j\ \alpha) = \frac{i}{2\pi} \int \bar{d}k\ \bar{d}\varphi\ \mathrm{Tr}\ \Omega^L\ (j\ \alpha) \qquad 6.11$$

$$Q^L\ (j\ \alpha\ k\ \beta) = \frac{i^2}{2!(2\pi)^2} \int \bar{d}k\ \bar{d}\varphi\ \mathrm{Tr}\ (\wedge\ \Omega^L\ (j\ \alpha\ k\ \beta\ )^2 \qquad 6.12$$

$$Q^L\ (j\ \alpha\ k\ \beta\ l\ \gamma) = \frac{i^3}{3!(2\pi)^3} \int \bar{d}k\ \bar{d}\varphi\ \mathrm{Tr}\ (\wedge\ \Omega^L\ (j\ \alpha\ k\ \beta\ l\ \gamma)^3 \qquad 6.13$$

The symbols $\bar{d}k$, $\bar{d}\varphi$ meaning all the differentials which are not included in the form Ω^L.

At this stage however, the variables k and φ are not quite on the same footing, because the projector P^L is periodic in the φ variables but not in the k variables. The projector $P^L(k)$ is however unitarily equivalent to a projector $F^L(k)$ periodic in the k variables. Indeed, let $\hat{H}^L(k)$ be the hamiltonian

$$\hat{H}^L(k) = -\frac{1}{2}\Delta + V^L \qquad 6.14$$

defined on $L^2(\Lambda_L)$ with the k-dependent boundary conditions

$$\psi(\ldots \underset{\alpha'}{L}, \ldots) = e^{i2\pi k_\alpha}\psi(\ldots \underset{\alpha'}{0}, \ldots)$$

$$\text{grad}\,\psi(\ldots \underset{\alpha'}{L}, \ldots) = e^{i2\pi k_\alpha}\,\text{grad}\;\psi(\ldots \underset{\alpha'}{0}, \ldots) \qquad 6.15$$

This hamiltonian is periodic in k.

If $F^L(k)$ is the projector, defined by

$$F^L(k) = \oint_\Gamma \frac{dz}{2\pi i}\,(z - \hat{H}^L(k)^{-1} \qquad 6.16$$

It is related to the old one $P^L(k)$ by the unitary transformation

$$P^L(k) = \exp\; -i\frac{2\pi}{L}\,k\,.\,r\;\; F^L(k)\;\; \exp\; +i\frac{2\pi}{L}\,k\,.\,r \qquad 6.17$$

Considered as a function of the variables k and φ, $F^L(k, \varphi)$ can be seen as defined on the d + m torus $[0, 1]^{d+m}$. We are now going to prove that the invariants given by equations 6.11, 6.12, 6.13 take the same value if we replace $P^L(k)$ by $F^L(k)$ in the corresponding expressions. This fact already points to their topological nature.

Let $\beta(k) = -i\frac{2\pi}{L}k\,.\,r$ and consider the family of projectors

$$P_t = e^{t\beta}\,F^L(k)\;e^{-t\beta} \qquad 6.18$$

where $t \in [0, 1]$.

Defining as before the exterior derivative dP_t and the 2-form $\Omega_t = P_t\, dP_t \wedge dP_t$, let

$$C_k(t) = \mathrm{Tr}\, (\wedge\, \Omega_t)^k \qquad 6.19$$

we have

$$\overset{o}{C}_k = k\, \mathrm{Tr}\, \overset{o}{\Omega} \wedge (\wedge\, \Omega)^{k-1} \qquad 6.20$$

but $$\overset{o}{\Omega} = P\,[dP, d\beta]\; P + [\beta, \Omega] \qquad 6.21$$

therefore

$$\overset{o}{C}_k = k\, \mathrm{Tr}\, d\,(P\, d\, \beta \wedge \Omega^{k-1}) + k\, \mathrm{Tr}\, P d\beta \wedge \{d\Omega^{k-1} + [\Omega^{k-1}, dP]\} \qquad 6.22$$

Using the fact that $d\Omega^{k-1} = (\wedge dP)^{2k-1}$, we see that $d\Omega^{k-1}\, P + [\Omega^{k-1}, dP]\, P = 0$ and we can conclude that

$$C_k(1) - C_k(0) = d\, \mu \qquad 6.23$$

where

$$\mu = \int_0^1 dt\, \mathrm{Tr}\, P\, d\, \beta \wedge\; \Omega_t^{k-1} \qquad 6.24$$

Since $$d\beta = -\, i\, \frac{2\pi}{L} \sum_{\alpha} x_\alpha\, dk^\alpha \qquad 6.25$$

and $$dP = e^{t\beta}\, \{\, t\, [d\beta, F] + dF\}\; e^{-t\beta} \qquad 6.26$$

we see that μ is periodic in k and φ, therefore when we integrate 6.23, on a 2k torus, we get, using Stokes theorem

$$\int_{T_{2k}} C_k(1) = \int_{T_{2k}} C_k(0) \qquad 6.27$$

The case k = 1, 2, 3 corresponds to the invariants 6.11, 6.12, 6.13 and we can replace in these expressions the form Ω^L by that defined on a 2k torus

$$\bar{\Omega}^L(j\,\alpha\,k\,\beta\ldots) = F^L\, dF^L(j\,\alpha\,k\,\beta\ldots) \wedge dF^L(j\,\alpha\,k\,\beta\ldots) \qquad 6.28$$

We are now going to show that the quantities appearing in the expression 6.11, 6.12, 6.13 for the invariants are characteristic Chern classes of a vector bundle.

Consider the following situation. Let P(x) be a family of projectors of dimension N in a Hilbert space, $\mathcal{H}$, x being a point of a manifold M. Assume that $P \in C^2(M)$. If 0_α is a coordinate neighborhood of M, a theorem of Kato [18] ensures that there exist an orthonormal set of N vectors in $\mathcal{H}$, $\{\psi_j^\alpha(x)\}_{j=1}^N$, which span the subspace corresponding to P, when $x \in 0_\alpha$, and which are C^2 in x. Let $g_{\alpha\beta}(x)$ be the N x N matrix whose elements are given by :

$$g_{\alpha\beta}^{ij}(x) = (\psi_i^\alpha(x), \psi_j^\beta(x)) \qquad 6.29$$

when $x \in 0_\alpha \cap 0_\beta$. It is easily seen that

$$g_{\alpha\beta}(x) \in U(N) \qquad 6.30$$

and

$$g_{\alpha\beta}(x) \quad g_{\beta\gamma}(x) = g_{\alpha\gamma}(x) \qquad 6.31$$

when $x \in 0_\alpha \cap 0_\beta \cap 0_\gamma$, the $g_{\alpha\beta}(x)$ being C^2. We thus see that the set of $g_{\alpha\beta}$ constitute a system of coordinate transformations with values in the group U(N), in the sense of [19]. A theorem [19] ensures that there exist a vector bundle $E(M, C_N, U(N))$, with base space M, fiber C_N and group U(N) and coordinate transformations $g_{\alpha\beta}$.

Let us define now the matrix valued one-form A^α in 0_α, of matrix elements :

$$A^\alpha(i\,j) = (\psi_i^\alpha, d\psi_j^\alpha) \qquad 6.32$$

d being the exterior derivative with respect to the local coordinates x in O_α. It follows immediately from 6.32 that A^α belongs to u(N), the algebra of U(N).

Using the definition 6.29 for $g_{\alpha\beta}$, we see that

$$A^\alpha(x) = g_{\alpha\beta}(x)\ A^\beta g_{\alpha\beta}(x)^{-1} + g_{\alpha\beta}(x)\, d\ g_{\alpha\beta}(x)^{-1} \qquad 6.33$$

when $x \in 0_\alpha \cap 0_\beta$

A theorem [20] ensures from these properties that there is a unique connection form A on E, corresponding to the locally defined A^α.

The associated curvature two-form F is locally defined by

$$F^\alpha = dA^\alpha + A^\alpha \wedge A^\alpha \qquad 6.34$$

we have the following representation for F^α

$$F^\alpha\ (i\,j) = \left(\psi_i^\alpha\, ,\ [dP \wedge dP]\, \psi_j^\alpha\right) \qquad 6.35$$

Consider now the following quantity

$$c_k = \frac{i^k}{k!\,(2\pi)^k}\ \operatorname{tr}\ (\wedge\,\Omega)^k \qquad 6.36$$

where $\Omega = P\ dP \wedge dP$ 6.37

From the representation 6.35, it follows easily that we have :

$$c_k = \frac{i^k}{k!\,(2\pi)^k}\ \operatorname{tr}\ (\wedge\, F)^k \qquad 6.38$$

the trace being now in c_k.

Equation 6.38 shows that c_k is the k-th characteristic Chern class of the bundle E. A beautiful theorem [20] tells us that $\int_M c_k$ is an integer, the k^{th} Chern number of the bundle, when M has dimension 2k and is without boundary. Thus we have proven that

$$\frac{i^k}{k!\,(2\pi)^k} \int_{M_{2k}} \mathrm{Tr}\,(\wedge\,\Omega^L)^k = a_k \in \mathbb{Z} \qquad 6.39$$

In order to apply this result to our situation, note that we have a projector $F^L(x)$, defined on a T_{m+d} torus, C^2 on this torus, where x denotes the d Bloch vectors k and the m phases φ. Consider the invariant $Q^L(j\,\alpha)$ for example. In the expression (6.11) appears $\Omega^L(j\,\alpha) = F^L(\varphi_j, k_\alpha)\, dF^L(\varphi_j, k_\alpha) \wedge dF^L(\varphi_j, k_\alpha)$. In one dimension, we look at the projector$F^L((\varphi_j, k_\alpha)$ as defined on a 2-torus(φ_j, k_α). (6.39) then tells us that

$$\frac{i}{2\pi} \int_{T_2} \mathrm{Tr}\,\Omega^L(\varphi_j, k_1) = n_\alpha \in \mathbb{Z} \qquad 6.40$$

is the 1st Chern number of the associated bundle. Since 6.40 is continuous in the other phases φ, we see that $Q^L(j1) = n_1$, is the 1st Chern number of the bundle. Similarly, in 2 dimensions, $Q^L(j\,\alpha\,k\,\beta)$ is the second Chern number of a bundle with basis a 4-torus, and $Q^L(j\,\alpha\,k\,\beta\,l\,\gamma)$ is the 3rd Chern number of a bundle, with basis a 6-torus, in three dimensions. And of course, since these integers have a limit as L tends to infinity as we have shown, we have the

<u>Theorem 4</u>

a) In one dimension, the adiabatic charge transport Q(j1) is an integer. Q(j1) is the 1st Chern number of a unitary vector bundle with basis a 2-torus.

b) In two dimensions, $Q(j\,\alpha\,k\,\beta)$ is an integer, the 2nd Chern number of a unitary vector bundle with basis a 4-torus

c) In three dimensions, $Q(j\,\alpha\,k\,\beta\,l\,\gamma)$ is an integer, the 3rd Chern number of a unitary vector bundle with basis a 6-torus.

7. The relationship between charge transport, density of states and the topological invariants

We are now going to prove that there exist some algebraic relationship between the topological invariants that we have introduced, the adiabatic charge transport and the density of states.

<u>Lemma</u> The following relationships holds between the topological invariants :

1) $$M(P) = \sum_j \Omega(j\,\alpha)\, Q(\alpha\, j)$$

2) $$Q(k\,\beta) = \sum_j \Omega(j\,\alpha)\, Q(\alpha\, j\, k\,\beta)$$

3) $$Q(k\,\beta\, l\,\gamma) = \sum_j \Omega(j\,\alpha)\, Q(\alpha\, j\, k\,\beta\, l\,\gamma)$$

<u>Proof</u> Let us introduce the following forms :

$$\sigma(j\,\alpha) = i\, M(P\,[\wedge\, dP(j\,\alpha)]^{2)} \qquad 7.1$$

$$\sigma(j\,\alpha\, k\,\beta) = \frac{i^2}{2\,!}\, M(P\,[\wedge\, dP(j\,\alpha\, k\,\beta)]^{4)} \qquad 7.2$$

$$\sigma(j\,\alpha\, k\,\beta\, l\,\gamma) = \frac{i^3}{3\,!}\, M(P\,[\wedge\, dP(j\,\alpha\, k\,\beta\, l\,\gamma)]^{6)} \qquad 7.3$$

where

$$dP(j\,\alpha) = P_j e^1 + P_\alpha e^2 \qquad 7.4$$

$$dP(j\,\alpha\, k\,\beta) = P_j e^1 + P_\alpha e^2 + P_k e^3 + P_\beta e^4 \qquad 7.5$$

$$dP(j\,\alpha\, k\,\beta\; l\,\gamma) = P_j e^1 + P_\alpha e^2 + P_k e^3 + P_\beta e^4 + P_l e^5 + P_\gamma e^6 \qquad 7.6$$

The notation dP is intended to mean that d acts like an exterior derivative on forms so that $d^2 P = 0$ for example. These forms are naturally related to the quantities we have introduced, namely :

$$\sigma(j\,\alpha) = Q(j\,\alpha)\; e^1 \wedge e^2 \qquad 7.7$$

$$\sigma(j\,\alpha\,k\,\beta) = Q(j\,\alpha\,k\,\beta)\, e^1 \wedge e^2 \wedge e^3 \wedge e^4 \qquad 7.8$$

$$\sigma(j\,\alpha\,k\,\beta\,l\,\gamma) = Q(j\,\alpha\,k\,\beta\,l\,\gamma)\, e^1 \wedge e^2 \wedge e^3 \wedge e^4 \wedge e^5 \wedge e^6 \qquad 7.9$$

We now note the relationship

$$\sum_j \Omega\,(j\,\mu)\frac{\partial V}{\partial \varphi_j} = \frac{\partial V}{\partial x_\mu} = i\,[p_\mu, H] \qquad 7.10$$

on the dense domain D. Hence

$$\sum_j \Omega\,(j\,\mu)\,P_j = i\,[p_\mu, H] \equiv C_\mu \qquad 7.11$$

On the other hand, it follows easily from proposition 7 that

$$p_\mu P = (P p_\mu)^+ \in \mathcal{C} \qquad 7.12$$

so that we can write :

$$\sum_j \Omega(j\,\alpha)\;\sigma(j\,\alpha) = i\,M(P[\wedge(C_\alpha e^1 + P_\alpha e^2)]^2) \qquad 7.13$$

$$\sum_j \Omega(j\,\alpha\,)\;\sigma(j\,\alpha\,k\,\beta) = \frac{i^2}{2\,!}M(P[\wedge(C_\alpha e^1 + dP(\alpha\,k\,\beta))]^4) \qquad 7.14$$

$$\sum_j \Omega(j\,\alpha\,)\;\sigma(j\,\alpha\,k\,\beta\,l\,\gamma) = \frac{i^3}{3\,!}M(P[\wedge(C_\alpha e^1 + dP(\alpha\,k\,\beta\,l\,\gamma))]^6) \qquad 7.15$$

Consider first the expression 7.13

$$M(P(C_\alpha e^1 + P_\alpha e^2)^2) = M(P[C_\alpha, P_\alpha]P)\;\; e^1 \wedge e^2 \qquad 7.16$$

But

$$M(PC_\alpha P_\alpha P) = -\,i\,M\,(P\,p_\alpha P_\alpha P) = -\,i\,M(P\,p_\alpha P_\alpha)$$

Since $P\, p_\alpha\, P = 0$, and the cyclic permutation in the average M(.) is justified by property 7.12 of $P\, p_\alpha$, and the similar one for P_α.

Consequently,

$$M(P[C_\alpha, P_\alpha]P) = i\, M\,(P\, p_\alpha P_\alpha + P_\alpha\, p_\alpha P) = -\, i\, M\,(\partial_\alpha\,(P\, p_\alpha\, P)) \qquad 7.17$$

If we define

$$R_\alpha\,(\lambda) = P\,(\lambda)\,(p_\alpha + \lambda_\alpha)\, P\,(\lambda) = S_\lambda^{-1}\, R_\alpha\,(0)\, S_\lambda \qquad 7.18$$

then we see that

$$\sum_j \Omega(j\,\alpha)\;\sigma(j\,\alpha) = M(\partial_\alpha\, R_\alpha) - M(\partial_\alpha\,(\lambda_\alpha P)) \qquad 7.19$$

since the left hand side of this equation is independent of λ, we can integrate both sides on λ_α. Since $(R_\alpha, \partial_\alpha\, R_\alpha) \in \mathcal{M}$ we have

$$\int_0^1 d\lambda_\alpha\, M(\partial_\alpha R_\alpha) = M(R_\alpha\,(\lambda_\alpha = 1)) - M(R_\alpha(\lambda_\alpha = 0)) = 0 \qquad 7.20$$

and

$$\int_0^1 d\lambda_\alpha\, M(\partial_\alpha(\lambda_\alpha\, P)) = M(P) \qquad 7.21$$

so that equation 7.19 becomes

$$\sum_j \Omega(j\,\alpha)\;\sigma(j\,\alpha) = -\, M(P)\, e^1 \wedge e^2 \qquad 7.22$$

which proves the first part of the lemma.

Consider now the expression 7.14. If we call

$$dg \equiv dP\,(\alpha\, k\, \beta) = \sum_{\nu=2}^{4} P_\nu\, e^\nu \tag{7.23}$$

we have

$$M(P[\wedge(C_\alpha e^1 + dg)]^4) = \sum_\nu M(P\{[C_\alpha P_\nu]\, dg \wedge dg + dg \wedge dg[C_\alpha, P_\nu]\})\, e^1 \wedge e^\nu \tag{7.24}$$

But

$$Pdg = dg(1\text{-}P) \tag{7.25}$$

and consequently

$$Pdg \wedge dg = dg \wedge dg\, P \tag{7.26}$$

Using the cyclicity of M, we get therefore

$$M(P[\wedge(C_\alpha e^1 + dg\,)]^4) = 2\sum_\nu M(P[C_\alpha, P_\nu]P\, dg \wedge dg)\, e^1 \wedge e^\nu \tag{7.27}$$

But $$P[C_\alpha, P_\nu]P = -\, i\, P\,(p_\alpha P_\nu + P_\nu\, p_\alpha)\, P \tag{7.28}$$

Using again the cyclicity of M and 7.26, equation 7.27 becomes

$$\begin{aligned} M[P[\wedge(C_\alpha e^1 + dg)]^4) &= -\,2i \sum_\nu M(\partial_\nu(Pp_\alpha P)\, dg \wedge dg)\, e^1 \wedge e^\nu \\ &= 2i\, M(d(R_\alpha - \lambda_\alpha P) \wedge dg \wedge dg) \wedge e^1 \\ &= 2i\, M(d[(R_\alpha - \lambda_\alpha P)\;\; dg \wedge dg]) \wedge e^1 \end{aligned}$$

since $d^2 g = 0$.

The left hand side of this equation is independent of λ so that we can integrate both sides on λ_α and λ_β. Now, if $A(\lambda) = S_\lambda^{-1}\, A(0)\, S_\lambda \in \mathcal{M}$ and $\partial_\alpha\, A(\lambda) \in \mathcal{M}$

$$\int_0^1 d\lambda_\alpha\, M(\partial_\alpha A(\lambda)) = 0 \tag{7.30}$$

and

$$\int_0^1 d\lambda_\alpha \, M(\partial_\alpha(\lambda_\alpha A)) = M(A) \tag{7.31}$$

On the other hand, if $A_\varphi \in \mathcal{M}$ and $\partial_{\varphi_j} A_\varphi \in \mathcal{M}$ we have

$$M(\partial_{\varphi_j} A_\varphi) = 0 \tag{7.32}$$

Indeed

$$M(\partial_{\varphi_j} A_\varphi) = \int_0^1 d\varphi_j \, M(\partial_{\varphi_j} A_\varphi) = \lim_{\Lambda \uparrow R^d} \frac{1}{|\Lambda|} \int_\Lambda dr \, (A_{\varphi_j=1}(r, r) - A_{\varphi_j=0}(r, r)] = 0$$

Since $(R_\alpha \, dg \wedge dg)(\lambda) = S_\lambda^{-1} (R_\alpha \, dg \wedge dg)(0) S_\lambda$, all these properties allow us to write equation 7.29 in the form

$$M[P[\wedge(C_\alpha e^1 + dg)]^4) = +2i \, M(P \, dg \wedge dg) \wedge e^1 \wedge e^2$$

or

$$M[P[\wedge(C_\alpha e^1 + dg)]^4) = 2i \, M(P \, [\wedge \, dP(k_\beta)]^2) \wedge e^1 \wedge e^2 \tag{7.33}$$

which gives for equation 7.19

$$\sum_j \Omega(j \, \alpha) \, \sigma(j \, \alpha \, k \, \beta) = - e^1 \wedge e^2 \wedge \sigma \, (k\beta) \tag{7.34}$$

which proves the second part of the lemma.

Finally, if we call $df \equiv dP \, (\alpha \, k \, \beta \, l \, \gamma)$, then

$$[\wedge(C_\alpha e^1 + df)]^6 = \sum_{\nu=2}^{6} \{[C_\alpha, P_\nu] \, [\wedge \, df]^4 + [\wedge \, df]^4 \, [C_\alpha, P_\nu]$$

$$+ [\wedge df]^2 \, [C_\alpha, P_\nu] \, [\wedge \, df]^2\} \wedge e^1 \wedge e^\nu$$

Using the relation P df $\wedge$ df = df $\wedge$ df P and the cyclicity of M, we see that

$$M[P[\wedge(C_\alpha e^1 + df)]^6) = 3\sum_\nu M[P[C_\alpha, P_\nu]P(\wedge df)^4) \; e^1 \wedge e^\nu \qquad 7.35$$

From 7.28 and cyclicity of M, we can rewrite this expression as

$$M[P[\wedge(C_\alpha e^1 + df)]^6) = 3i\sum_\nu M(\partial_\nu(Pp_\alpha P)\, e^\nu \wedge (df)^4)) \wedge e^1$$

$$= 3i\, M\,(d\,[(R_\alpha - \lambda_\alpha P)\,(\wedge\, df)^4]) \wedge e^1$$

Proceeding as before, using 7. 30, 7.31, 7.32, we get

$$M[P[\wedge(C_\alpha e^1 + df)]^6) = 3i\, e^1 \wedge e^2\, M[P\,[\wedge\, dP\,(k\,\beta\,1\,\gamma)]^4)$$

so that equation 7.15 becomes

$$\sum_j \Omega(j\,\alpha)\,\sigma(j\,\alpha\,k\,\beta\,1\,\gamma) = -\,e^1 \wedge e^2 \wedge \sigma\,(k\,\beta\,1\,\gamma)$$

which proves the third part of the lemma.

We can now combine all the results we have derived, for the electronic density (or integrated density of states) ρ = M(P), the adiabatic charge transport Q(α j) and the topological invariants Q(α j β k), Q(α j β k γ l), in various space dimensions d. We summarize them in the following theorem, which is our main result.

Theorem 5 If the quasi-periodic potential V_φ defined by

$$V_\varphi(x) = \sum_{n\in \mathbb{Z}_m} a(n) \exp 2\pi i\,(n, \Omega x) + 2\pi i\,(n, \varphi)$$

satisfies the two conditions :

1) The m x d frequency matrix Ω is such that $\Omega^T\, n = 0$ implies $n = 0, \forall\, n \in \mathbb{Z}_m$

2) $a^*(n) = a(-n)$ and

$$\sum_{n \in \mathbb{Z}_m} |a(n)| \left(\sup_{1 \leq i \leq m} |n_i| \right)^3 < \infty$$

then, the following properties hold, when the chemical potential μ is in a gap.

a) In one dimension, the adiabatic charge transport $Q(1\ j)$ is quantized, i.e. $Q(1\ j) \in \mathbb{Z}$ and is the 1st Chern number of a vector bundle. The integrated density of states ρ is given by

$$\rho = \sum_j \Omega(j\ 1)\, Q\,(1\ j)$$

b) In two dimensions, the adiabatic charge transport $Q(\alpha\ j)$ is weakly quantized, i.e. it is given by

$$Q(\alpha\ j) = \sum_k \Omega(k\ \beta)\, Q\,(\beta\ k\ \alpha\ j)$$

where $Q\,(\beta\ k\ \alpha\ j) \in \mathbb{Z}$ and is the 2nd Chern number of a vector bundle. The integrated density of states can be expressed as

$$\rho = \sum_{k\,j} \Omega(j\ \alpha)\, \Omega(k\ \beta)\, Q(\beta\ k\ \alpha\ j)$$

c) In three dimensions, the adiabatic charge transport is again weakly quantized, i.e. it is given by

$$Q\,(\alpha\ j) = \sum_{k\,l} \Omega(k\ \beta)\, \Omega(l\ \gamma)\, Q(\gamma\ l\ k\ \beta\ \alpha\ j))$$

where $Q\,(\gamma\ l\ k\ \beta\ \alpha\ j) \in \mathbb{Z}$ and is the 3rd Chern number of a vector bundle.

The integrated density of states is given by :

$$\rho = \sum_{j\,k\,l} \Omega(j\ \alpha)\, \Omega(k\ \beta)\, \Omega(l\gamma)\, Q(\gamma\ l\ k\ \beta\ \alpha\ j))$$

In one dimension, our theorem gives a new proof (with more restrictive conditions on the potential) of a theorem of Johnson and Moser [10]. They showed that the integrated density of states ρ as a linear combination of integers, when the energy (or our chemical potential μ) is in a gap

$$\rho = \sum_j \Omega(j\,1)\, n_j \qquad \text{with} \qquad n_j \in \mathbb{Z}$$

In their approach, however, they could not identify, individually, each of the integers n_j appearing in the decomposition. A clear advantage of our approach is to allow the identification of each of the integers with the charge transport Q(1j).

The decomposition of the density of states in a linear combination of integers, in the multidimensional case, was proven by Bellissard, Lima and Testard, using C^*-algebra techniques. Once more, no identification of the integers was made, although there should be some connection between this approach and ours.

Finally, we may note a useful consequence of the density of states when it is non vanishing, at least one of the topological number is non zero, so that the associated bundle is not trivial.

8. Periodic potentials and magnetic field : the Hall conductivity

The discovery of the quantum Hall effect in some two dimensional electronic systems has stimulated a renewed interest in the old problem of non interacting electrons moving in a periodic potential in the presence of a magnetic field. The Hall conductivity has been analyzed in [3] when the flux of the magnetic field through a unit cell is rational. Our approach will be used to discuss this problem in the case where the magnetic flux through a unit cell is irrational.

We will mainly be concerned by the two-dimensional situation, electrons moving in the (x, y) plane and the magnetic field being applied in the z-direction. We choose as units of energy $\hbar \frac{eB}{m}$, and of length of $l = \sqrt{\frac{\hbar}{eB}}$. The one electron hamiltonian is given by

$$H_\varphi = \frac{1}{2} v_x^2 + \frac{1}{2} v_y^2 + V_\varphi(x, y) \qquad 8.1$$

where the velocity operators $v_{\substack{x\\y}}$ are defined by

$$v_x = p_x + y \qquad \qquad 8.3$$

$$v_y = p_y$$

in the Landau gauge.

As a periodic potential we take

$$V_\varphi(x, y) = \sum_{n_1 n_2} c(n_1, n_2) \exp 2\pi i \left[\frac{n_1 x}{a_x} + \frac{n_2 x}{a_y} + n_2 \varphi\right] \qquad 8.3$$

and impose the technical condition

$$\sum_{n\ n_2} |e(n, n_2)| \ (|n_1| + |(n_2|)^3 < \infty \qquad 8.4$$

making the potential three time differentiable.

The usefulness of the introduction of the phase φ will appear later on. The domain D of the hamiltonian will be that of the non interacting one

$$H_o = \frac{1}{2} v_x^2 + \frac{1}{2} v_y^2 \qquad 8.5$$

The hamiltonian commutes with the magnetic translations operators

$$T(n\ a) = \exp i [n_y a_y x] \ \exp i [n_x a_x p_x + n_y a_y p_y] \qquad 8.6$$

If we make successive translations along a loop we get however a non trivial result :

$$T(n_x a_x 0) \ T(0, n_y a_y) \ T(n_x a_x, 0)^{-1} \ T(0, n_y a_y)^{-1} = \exp i 2\pi \varnothing n_x n_y \qquad 8.7$$

where

$$\varnothing = \frac{a_x a_y}{2\pi} \qquad 8.8$$

is the flux (in our units) of the magnetic field through a unit cell. If this flux is a rational number $\varnothing = \frac{p}{q}$, the group generated by $T(a_x, 0)$ and $T(0, qa_y)$ is abelian and commutes with the hamiltonian. It is then possible to apply Bloch theorem. This is the situation considered first by Thouless et al [3] where they could prove quantization of the Hall conductivity in a gap. We will however discuss here the other case, $\varnothing$ is an irrational number. In this case we are still left with an abelian group $\{T(n_x a_x, 0)\}$ commuting with the hamiltonian. We can therefore apply Bloch theorem in the x direction, to reduce the problem to that in a band.

There exist a unitary map U of $L^2(R^2)$ onto

$$\int_{[0;1]}^{\oplus} d\theta \; L^2([0, a_x] \times R]) \tag{8.9}$$

such that

$$U H_\varphi U = \int_{[0;1]}^{\oplus} d\theta \; H_{\varphi,\theta} \tag{8.10}$$

where $H_{\varphi,\theta}$ is the hamiltonian restricted to $\mathcal{H} = L^2([0, a_x] \times R)$

$$H_{\varphi,\theta} = \frac{1}{2} v_x^2(\theta) + \frac{1}{2} v_y^2 + V_\varphi(x, y) \tag{8.11}$$

where

$$v_x(\theta) = p_x(\theta) + y \tag{8.12}$$

$p_{x(\theta)}$ being the operator $\frac{1}{2} \frac{\partial}{\partial_x}$ on the domain

$$\begin{aligned} \psi(a_x, y) &= e^{i2\pi\theta} \psi(0, y) \\ \psi_x(a_x, y) &= e^{i2\pi\theta} \psi_x(0, y) \end{aligned} \tag{8.13}$$

This hamiltonian is an operator valued function on the 2-torus $(\varphi. \theta)$, since $H_{\varphi+1,\theta} = H_{\varphi,\theta+1} = H_{\varphi,\theta}$.

On the other hand, let $\tau_t = \exp i\, t\, (p_y + a)$, $t \in \mathbb{R}$. This is also a magnetic translation operator in the y direction, which is such that

$$\tau_t \; H_{\varphi,\theta} \; \tau_t^{-1} = H_{\varphi_t,\theta_t} \tag{8.14}$$

where

$$\varphi_t = \varphi + \frac{t}{a_y}$$

$$\theta_t = \theta + \frac{a_x}{2\pi}\, t \tag{8.15}$$

We now see that if the magnetic flux $\varnothing = \frac{a_x\, a_y}{2\pi}$ is irrational, magnetic translations in the y direction induce an <u>ergodic</u> flow on the 2-torus.

We are now essentially in the same situation as in the one of quasi-periodic potentials, in fact in the case where two frequencies are incommensurable. As in this case, the ergodic theorem tells us that the resolvent set of $H_{\varphi,\theta}$ is almost surely independent of φ and θ. An adaptation of the proof we gave in the quasi-periodic case shows that the resolvent set of H_φ is independent of φ (this follows essentially from the norm continuity of H_φ with respect to φ). In physical terms, the gaps of H_φ do not depend on φ.

We are now in position to adopt the same strategy as before. We will be interested by self-adjoint operators A_φ, commuting with $T(n_x\; a_x\; 0)$, so that we can apply Bloch theorem in the x direction. We will also require that the corresponding operators $A_{\varphi,\theta}$ satisfy

$$\tau_t \; A_{\varphi,\theta} \; \tau_t^{-1} = A_{\varphi_t,\theta_t} \tag{8.16}$$

and we introduce the corresponding notions of averageable operators $A_{\varphi,\theta} \in \mathcal{M}$.

The average being given by

$$M(A_\varphi) = \frac{1}{a_x} \int_0^{a_x} dx \int_0^1 d\theta \int_0^1 d\varphi \;\; A_{\varphi,\theta}\,(x\,0 \mid x\,0) \tag{8.17}$$

There are two quantities of interest for us in such a system. The Hall conductivity, measuring the current in the x direction resulting from an adiabatically switched electric field in the y direction. In the units of $\frac{e^2}{n}$, it is given by

$$\sigma_H = -i\, M\,(P\,[V_x, V_y]) \tag{8.18}$$

with

$$V_{\substack{x\\y}} = \oint_\Gamma \frac{dz}{2\pi i} G_z\ v_{\substack{x\\y}}\ G_z \tag{8.19}$$

The charge transport in the direction y resulting from an adiabatic increase of φ by one, is given in units of $\frac{e}{l}$, by:

$$\sigma_\varphi = Q(\varphi\, y) = -i\, M\,(P[V_y, P_\varphi]) \tag{8.20}$$

with

$$P_\varphi = \frac{\partial P}{\partial \varphi} \tag{8.21}$$

Before analyzing such quantities, it remains to see that they make mathematical sense and to check that their derivation from the adiabatic theorem is justified. These technical conditions will now be verified.

Consider the hamiltonian

$$H_o(\theta) = \frac{1}{2} v_x^2(\theta) + \frac{1}{2} v_y^2 \tag{8.22}$$

Defining the creation and annihilation operators

$$a = \frac{1}{\sqrt{2}}(v_x(\theta) + i\, v_y) \tag{8.23}$$

$$a^+ = \frac{1}{\sqrt{2}}(v_x(\theta) - i\, v_y) \tag{8.24}$$

satisfying the commutation relation

$$[a, a^+] = 1 \tag{8.25}$$

We see that

$$H_o(\theta) = a^+ a + \frac{1}{2} \tag{8.26}$$

so that the spectrum of $H_o(\theta)$, $\sigma(H_o(\theta))$ is that of an harmonic oscillator

$$\theta(H_o(\theta)) = \{ n + \frac{1}{2} , n = 0, 1, 2, \dots \} \tag{8.27}$$

The corresponding spectral projectors P_n are given by operators of kernel

$$P_n(x\, y; x'y') = \frac{1}{a_x} \sum_{j \in \mathbb{Z}} \exp i \frac{2\pi}{a_x} (j+\theta)(x-x')\, \varphi_n\left(y + \frac{2\pi}{a_x}(j+\theta)\right) \varphi_n\left(y' + \frac{2\pi}{a_x}(j+\theta)\right) \tag{8.28}$$

where

$$\varphi_n(y) = [\sqrt{\pi}\ 2^n\ n!\,]^{-\frac{1}{2}}\ H_n(y) \exp - \frac{y^2}{2} \tag{8.29}$$

$H_n(y)$ being the Hermite polynomial of order n. With the help of this representation, we can prove the following properties.

<u>Proposition 9</u>

$$G_{i,\theta,\varphi} \in C \qquad \text{and} \qquad \sup_{\theta;\varphi} \quad |G_{i,\theta,\varphi}| < \infty$$

The first resolvent equation and the fact that the potential V_φ satisfies $\sup_\varphi \|V_\varphi\| < \infty$, shows that it is enough to prove these properties when $V = 0$. And in the latter case, the second resolvent equation allows us to reduce the proof to the case where we take $z = 0$, instead of $z = i$.

The identity

$$\sum_{n=0}^{\infty} e^{-\lambda(n+\frac{1}{2})} \varphi_n^2(y) = (2\pi \operatorname{sh}\lambda)^{-\frac{1}{2}} \exp -y^2 \operatorname{th}\frac{\lambda}{2} \tag{8.30}$$

and the spectral decomposition give the following identity for

$$K_\lambda = e^{-\lambda H_o} \tag{8.31}$$

$$K_\lambda(xy\,;xy) = (2\pi a_x \,\mathrm{sh}\lambda)^{-\frac{1}{2}} \sum_{j \in \mathbb{Z}} \exp -\left(y + \frac{2\pi}{a_x}(j+\theta)\right)^2 \mathrm{th}\frac{\lambda}{2} \tag{8.32}$$

From this representation, we can get the bound

$$K_\lambda(r,r) \le \frac{c}{\mathrm{sh}\lambda} \tag{8.33}$$

where c is some constant.

Using the identity

$$H_0^{-2} = \int_0^\infty d\lambda \ \lambda \ K_\lambda \tag{8.34}$$

we can conclude that $\sup_\theta \ |G^0_{0\,\theta}|^2 < \infty$

since

$$|G^0_0|^2 = \sup_r \int dr' \ |H_0^{-1}(r,r')|^2 = \sup_r H_0^{-2}(r,r') \tag{8.35}$$

On the other hand, we have

$$|G^0_0|^2_{r,s} = H_0^{-2}(r,r) + H_0^{-2}(s,s) - H_0^{-2}(s,r) - H_0^{-2}(r,s) \tag{8.36}$$

Using the identity 8.34, this gives

$$|G^0_0|^2_{r,s} = \int_0^\infty d\lambda \ \lambda \ [K_\lambda(r,r) + K_\lambda(s,s) - K_\lambda(s,r) - K_\lambda(r,s)] \tag{8.37}$$

But Schwartz inequality applied to the expression for $K_\lambda(r, s)$ obtained by using the spectral representation of H_o gives

$$|K_\lambda(r,s)| \le [K_\lambda(r,r)]^{1/2}\ [K_\lambda(s,s)]^{1/2} \tag{8.38}$$

Combined with 8.33, this inequality shows that the integrand in 8.37, is bounded by a function $g(\lambda)$ uniformly in r and s, with $\int_0^\infty \lambda\, g(\lambda)\, d\lambda < \infty$. We can therefore apply the dominated convergence theorem, to conclude that $\lim_{r \to s} |G_0^0|_{r,s} = 0$.

Proposition 10

$v_{\substack{x\\y}}\ G_{i,\theta,\varphi}$ and $\partial_\varphi V_\varphi\ G_{i,\theta,\varphi}$ map D into D.

First of all, we note that the following properties of P_N

$$\begin{aligned} a P_N &= P_{N-1} a \\ a^+ P_N &= P_{N+1} a^+ \end{aligned} \tag{8.39}$$

imply the identities

$$aG_i^0 = (i-\tfrac{1}{2})^{-1} [(i-\tfrac{1}{2})\ G_{i-1}^0 - G_{-1/2}^0] a \tag{8.40}$$

$$a^+G_i^0 = [\ G_{i+1}^0 - \frac{1}{i+1/2} P_o] a^+ \tag{8.41}$$

This shows that a G_i^0 and $a^+G_i^0$ map D into D. On the other hand, the first resolvent equation gives

$$a\, G_i = aG_i^0 + aG_i^0\ V\ G_i \tag{8.42}$$

Using the identity 8.40 and the fact that aV G_i maps D into D, from the assumed properties of V, we conclude that a G_i (and similarly $a^+ G_i$) maps D into D.

One can prove similarly that $\partial_\varphi V_\varphi G_i$ maps D into D.

Proposition 11

$$\underset{y}{v_x} \; G^2_{i;\theta;\varphi} \in \mathcal{C} \qquad \text{and} \quad \sup_{\theta;\varphi} \mid \underset{y}{v_x} \; G^2_{i;\theta;\varphi} \mid < \infty$$

First of all note that $aG^0_{i;\theta} \in \mathcal{B}$ and $a^+G^0_{i;\theta} \in \mathcal{B}$

indeed

$$\| \, aG^0_{i;\theta} \, \|^2 = \| \, aG^0_{i;0} \, \|^2 = \sup_{\varphi:\|\varphi\|=1} \sum_{n=1}^{\infty} \frac{n}{1+(n+1/2)^2} \, (\varphi \, , P_n \, (0) \, \varphi) < \infty \qquad 8.43$$

$$\| \, a^+G^0_{i;\theta} \, \|^2 = \| \, a^+G^0_{i;0} \, \|^2 = \sup_{\varphi:\|\varphi\|=1} \sum_{n=0}^{\infty} \frac{n+1}{1+(n+1/2)^2} \, (\varphi \, , P_n \, (0) \, \varphi) < \infty \qquad 8.44$$

It follows therefore from the identities 8.40, 8.41 that

$$\underset{y}{v_x} \; [G^0_{i;\theta;\varphi}]^2 \in \mathcal{C}$$

The result follows now from the equation

$$\underset{y}{v_x} \; G^2_i = \underset{y}{v_x} \; [G^0_i]^2 \; [1 + V \, G_i] \; + \underset{y}{v_x} \; G^0_i \; V \, G_i \qquad 8.45$$

using again the identities 8.40, 8.41 and the fact that $\underset{y}{v_x} \; V \, G_i \in \mathcal{B}$.

We can now check that all the conditions of theorem 2 are satisfied for the operators considered and that the expected formula hold. We can now adopt the strategy followed in the case of quasi-periodic potentials. We approximate the potential V_φ by a periodic potential V^L_φ in the y direction of period L chosen in such a way that the flux through a unit cell $\emptyset = \frac{a_x \, L}{2\pi}$ is integer for example. We can prove that σ^L_H and σ^L_φ converge when L tends to infinity to σ_H and σ_φ respectively. The needed technical estimates are given basically in propositions 9 and 11. In the periodic case with integer flux we can apply Bloch theorem and repeat the computations made before. The Hall conductivity is given by

$$\sigma^L_H = \frac{-i}{(2\pi)^2} \int_0^1 d\theta \int_0^1 d\theta' \, \mathrm{Tr} \, [\partial_\theta \, F^L, \partial_\theta \, F^L)] \qquad 8.46$$

and the charge transport

$$\sigma_\varphi^L = \frac{-i}{(2\pi)^2} \int_0^1 d\theta \int_0^1 d\varphi \int_0^1 d\theta' \,\mathrm{Tr}\, F^L \,[\partial_\theta F^L, \partial_\varphi F^L)] \qquad 8.47$$

The angle θ' corresponds to the Bloch momentum $\frac{2\pi\,\theta}{L}$ in the y direction. F^L is a projector periodic in $(\theta, \theta', \varphi)$.

From this follows, as before, that :

$$\sigma_H^L = \frac{1}{2\pi}\, n_H \qquad 8.48$$

and

$$\sigma_\varphi^L = \frac{1}{2\pi}\, n_\varphi \qquad 8.49$$

where the integer n_H, is the first Chern number attached to the 2-torus (θ, θ'), whereas n_φ is the first Chern number attached to the 2-torus (θ', φ).

As in the case of quasi-periodic potentials, there exist an algebraic relationship between the electronic density $\rho = M(P)$ and the two topological invariants found. We now derive it.

The result will be basically a consequence of the following relationship

$$i\,[p_y, H] = v_x + \frac{1}{a_y}\, \partial_\varphi V_\varphi \qquad 8.50$$

valid on the dense domain D. We used in the derivation of 8.49 the equality $a_y\, \partial_y V_\varphi = \partial_\varphi V_\varphi$.

From 8.50 follows that

$$C_y = i\,[p_y, P] = v_x + \frac{1}{a_y}\, P_\varphi \qquad 8.51$$

But

$$p_y P = (P\, p_y)^+ \in C \qquad 8.52$$

as an easy consequence of proposition 11, so that we can write

$$\frac{1}{a_y} Q(y\varphi) + \sigma_H = i\, M(P[V_y C_y] P) \qquad 8.53$$

Using the fact that

$$P V_y P = 0 \qquad 8.54$$

we get

$$M(P[V_y , C_y] P) = i\, M(V_y p_y P + P V_y p_y) \qquad 8.55$$

Note that in deriving 8.55, we could use the cyclicity property of M, because of 8.52 and the fact that $V_y = V_y^+ \in C$.

If we now introduce the operator

$$S_\lambda = \exp i \lambda y \qquad 8.56$$

which is such that if

$$A(\lambda) = S_\lambda^{-1} A S_\lambda \qquad 8.57$$

then $M(A(\lambda)) = M(A)$, for all λ, when $A \in \mathcal{M}$.

Since $p_y(\lambda)$ and $V_y(\lambda) = \frac{\partial P}{\partial \lambda}$ we can rewrite equation 8.55 in the form

$$M(P[V_y, C_y]P) = i\, M(\partial_\lambda (P p_y P)) \qquad 8.58$$

If we define

$$R(\lambda) = P(\lambda) (p_y + \lambda) P(\lambda) = S_\lambda^{-1} R(0) S_\lambda \qquad 8.59$$

we can rewrite 8.58 as

$$M(P[V_y, C_y]P) = i\, M(\partial_\lambda R(\lambda)) - i\, M(\partial_\lambda (\lambda P)) \qquad 8.60$$

Since the left hand side of the equation is independent of λ, we can integrate both sides on λ. Since $(R(\lambda), \partial_\lambda R(\lambda)) \in \mathcal{M}$ we have

$$\int_0^1 d\lambda\, M(\partial_\lambda R(\lambda)) = 0 \tag{8.61}$$

$$\int_0^1 d\lambda\, M(\partial_\lambda (\lambda P)) = M(P) \tag{8.62}$$

Combining equations 8.61, 8.62 with 8.53, we see that we have proven the desired result

$$\frac{1}{a_y} Q(y\,\varphi) + \sigma_H = M(P) = \rho \tag{8.63}$$

A priori, we should also look at charge transport in the x direction

$$Q(\varphi x) = -i\, M(P[V_x, P_\varphi])$$

but this vanishes identically, as could be expected physically.

Indeed, from 8.51 follows that

$$\frac{1}{a_y} Q(\varphi x) = -i\, M(P[V_x, C_y]P)$$

But proceeding as before, we can see that

$$M(P[V_x, C_y]P) = i \int_0^\lambda d\lambda\, M(\partial_\lambda (P\, p_y P)) = 0$$

where now

$$(P\, p_y P)(\lambda) = \exp - i\, \lambda\, x\, (P\, p_y\, P) \,\exp i\, \lambda\, x.$$

We can now summarize the results obtained in a theorem.

Theorem 6

Let H be the hamiltonian of an electron moving in the plane (x, y), submitted to a constant magnetic field in the z direction, in the presence of a periodic potential $V_\varphi(x, y)$.

$$H = \frac{1}{2}(p_x + y)^2 + \frac{1}{2} p_y^2 + V_\varphi(x, y) \qquad 8.64$$

If the potential $V_\varphi(x, y)$, defined by

$$V_\varphi(x, y) = \sum_{h \in Z^2} a(n) \exp 2\pi i \left[\frac{n_1 x}{a_x} + \frac{n_2 y}{a_y} + n_2 \varphi\right] \qquad 8.65$$

satisfies the two conditions

1) $\frac{a_x a_y}{2\pi} \notin \mathbb{Q}$, i.e. the magnetic flux through a unit cell is irrational

2) $a^*(n) = a(-n)$

and

$$\sum_{h \in Z^2} |a(n)| \left(\sup_{1 \le i \le 2} |n_i|\right)^3 < \infty \qquad 8.66$$

Then when the chemical potential μ is in a gap, the following properties hold :

a) The Hall conductivity is quantized, i.e.

$$\sigma_H = \sigma_{xy} = -\sigma_{yx} = \frac{1}{2\pi} n_H \qquad n_H \in \mathbb{Z} \qquad 8.67$$

The integer n_H is the first Chern number of a vector bundle.

b) The charge transport in the y direction induced by an adiabatic change of φ by one unit is quantized, i.e.

$$\sigma_\varphi = Q(\varphi y) = \frac{1}{a_x} n_\varphi \qquad n_\varphi \in \mathbb{Z} \qquad 8.68$$

The integer n_φ is the first Chern number of a vector bundle.

c) Charge transport in the x direction vanishes

d) The electronic density ρ (integrated density of states) is given by

$$\rho = -\frac{1}{a_x}\sigma_\varphi + \sigma_H \qquad 8.69$$

Dana, Avron and Zak [12] had already proven that the density ρ in a gap should be given by a linear combination of two integers, when the chemical potential is in a gap

$$\rho = \frac{1}{a_x a_y} n_\varphi + \frac{1}{2\pi} n_H$$

Whereas the integer n_H was shown to be the one expressing the quantized Hall conductivity, the physical interpretation of the second one, was left undecided.

Recently, Tesanovic, Axel and Halperin [21] have computed the integers n_H and n_φ in some two-dimensional model.

The three dimensional situation has been considered by Halperin [22], who showed that the conductivity tensor is quantized.

In fact, it is not difficult to treat this case with our method. If we keep the magnetic field in the z direction, and take a periodic potential of the form

$$V_\varphi(x, y, z) = \sum_{h\in Z^3} a(n) \exp 2\pi i \left[\frac{n_1}{a_x} x + \frac{n_2}{a_y} y + \frac{n_3}{a_z} z + n_2 y\right]$$

Then the Hall conductivity is given by

$$\sigma_{yx} = \frac{1}{2\pi a_z} n_{yx} \quad , \qquad \sigma_{yz} = \frac{1}{2\pi a_x} n_{yz} \quad ,$$

when the integers n_{yx} and n_{yz} are first Chern number. The charge transport along the y direction $Q(y, \varphi)$ is again quantized, i.e. $Q(y\,\varphi) = \frac{1}{a_x a_z} n_\varphi$, the integer n_φ being again a first Chern number. The electronic density is again given by

$$\rho = \frac{1}{a_y} Q(y\,\varphi) + \sigma_{xy}.$$

Conclusion

This work could be continued in various directions. On the mathematical side, the results could be extended to more general quasi-periodic elliptic operators, lattice models and hamiltonians describing a particle in a quasi-periodic potential, submitted to a constant magnetic field.

On the physical side, it would be quite interesting to find a direct physical interpretation of the higher topological invariants (the second and third Chern numbers appearing in two and three space dimension). And of course, it would be very helpful to find two or three dimensional models with quasi-periodic potentials, of interest for describing electronic motion in quasi-crystals, and to show that there exist gaps in the energy spectrum for which the corresponding topological invariants could be computed.

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