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Adiabatic charge transport and topological invariants for quasi-periodic hamiltonians

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During the last decade, it became increasingly clear that the topological or global aspects of a physical theory could have important consequences and was worth of a deep study. We can quote among others the problem of anomalies in field theory, the classification of defects in condensed matter physics, the quantum Hall effect and Berry's phase. These last items are in fact intimately related to the results I will present.

I will show that for a certain class of systems describing essentially non interacting electrons in the presence of an incommensurate potential (describing the effect of ions on the electronic motion in a quasi-crystal for example), with the possible presence of a magnetic field (a case of interest for the quantum Hall effect), there exist interesting topological invariants, characterizing the gaps in the excitation spectrum. These topological invariants correspond to quantized currents, associated to a charge transport induced by an adiabatic variation of a parameter in the hamiltonian. Laughlin [1], when discussing the integer quantum Hall effect was apparently the first to argue for quantization of adiabatic charge transport. The idea was developed in more precise terms in two seminal papers by Thouless [2] and Thouless and Niu [3].

The adiabatic process we consider has in common with that considered by Berry [4] that it corresponds to a loop in the parameter space. In the end of the process, the hamiltonian of the system is the same, but the physical state is not. Let us recall that Berry considers the following situation. An hamiltonian $H(t/T)$ is slowly time dependent (T large), through variation of some parameters during the time interval $0 \leq t \leq T$. At time T, the parameters recover their initial values : $H(0) = H(1)$. If an eigenvalue, supposed simple to simplify matters, is permanently separated by a gap from the rest of the spectrum during the adiabatic process, the final state $\psi(0)$ will differ, from the initial one $\psi(0)$, by a phase γ

$$\psi(1) = e^{i\gamma}\,\psi(0)$$

as a consequence of the adiabatic theorem. Berry shows that γ has a topological interpretation, i.e. it depends only on some global features of the path followed. For example in the case of a spin moving under the influence of a magnetic field, the phase will be given by the solid angle made by the magnetic field in the process.

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We will now consider a more general situation. Suppose that the state of our system is not pure, but described by a density matrix ρ. Berry's phase is invisible for ρ. We can however consider the average value $\bar{B}$ of some observable B and ask the question : do there exist some observables B (in some systems) for which some non-trivial topological effect can be seen on $\bar{B}$, when the parameter follow a loop during the adiabatic process. The answer will be positive. Natural candidates for the observable B, will be currents which are sensible to the phase of the wave function. But what is more surprising is that we will have to look for the first correction, of order T^{-1}, to the adiabatic evolution. We have derived the following generalization of the adiabatic theorem.

Assume that there exist a gap Δ in the spectrum of all hamiltonians H(s), when $s \in [0, 1]$. Let us call P(s) the projector on a subspace corresponding to an energy interval separated by Δ from the rest of the spectrum. Take initially the system in the state $\rho(0) = P(0)$. The average value of the observable B which can be considered itself slowly time dependent will be defined by

$$\bar{B}(t) = M\,(B(t/T)\,\rho(t)) \tag{1}$$

where $M(A) = 1/V\ \mathrm{tr}A$ for a bounded system in a volume V and some natural generalization for an infinite system.

If $H'(0) = 0$ and $\quad \int_0^1 ds\, M(B(s)P(s)) = M(B(0)\rho(0))$
then

$$\lim_{T\to\infty} \int_0^T dt\,[M(B(\tfrac{t}{T})\,\rho(t)) - M(B(0)\rho(0))] = i\hbar \int_0^1 ds\, M(P(s)[P'(s), \hat{B}(s)]) \tag{2}$$

where $$\hat{B}(s) = \oint_\Gamma \frac{dz}{2\pi i}\,(z-H(s))^{-1} B(s)\,(z-H(s))^{-1} \tag{3}$$

Γ being a contour in the complex plane cutting the real axis in Δ and at some large negative energy.

As a first example, we consider the following thought experiment. Imagine that during the adiabatic evolution, some charged particles contained in our system cross a surface element $d\sigma$ in the direction k at the point r.

The total amount of charge transported will be

$$Q_k = \frac{1}{V}\int_V dr \int_0^T dt\; e\,(v_k\, d\sigma\, \rho(t))(r, r) \tag{4}$$

v being the velocity operator.

We call Q_k the adiabatic charge transport in the direction k, in the thermodynamic limit.

From formula 2 and 3, it is given by

$$Q_h = i \hbar\, e\, M(P[P', V_k]) \tag{5}$$

where
$$V_k = \oint_\Gamma \frac{dz}{2\pi i} (z-H)^{-1} v_k (z-H)^{-1} \tag{6}$$

all quantities being taken at time 0, for example.

As a second example, we can consider the effect of an electric field $E_l(t)$ adiabatically switched in the direction l in the form $E_l(t) = 1/T\, g\,(t/T)$.

If we then consider the conductivity tensor defined by

$$\sigma_{kl} = \lim_{T\to\infty} \frac{-\frac{1}{T}\int_0^T j_k(t)\,dt}{\frac{1}{T}\int_0^T E_l(t)\,dt} \tag{7}$$

$j_k(t)$ being the average current in the direction k. Taking for the observable B : $B(t) = v_k - \int_0^t g(s)\,ds$, our formula 2 and 3 give

$$\sigma_{kl} = i\, e^2 \hbar\, M(P[V_l, V_k]) \tag{8}$$

What we will prove is that for electrons in incommensurate potentials, or in periodic potentials and magnetic fields, these quantities are quantized, namely they are given by a linear combination of integers, when the Fermi energy is in a gap.

The integers are topological invariants (in fact, Chern numbers of certain vector bundles). The initial condition $\rho(0) = P(0)$ will simply mean that we are at zero temperature, $P(0)$ projects on all energies below the Fermi energy μ, assumed to be in a gap Δ. We will also find that the electronic density is given by a combination of these integers.

Quasi-periodic potentials

Choosing as unit of length a, a typical length scale associated with the potential V_φ and as unit of energy $\hbar^2/ma$, the one electron hamiltonian is given by

$$H_\varphi = -1/2\, \Delta + V_\varphi\,(x) \tag{9}$$

where the potential can be written as $V_\varphi = \sum_{n\in Z_m} a(n) \exp 2\pi i (n, \Omega x) + 2\pi i (n, \varphi)$

where Ω is an m x d matrix defining the basic frequencies of the potential. d is the space dimensionality. The potential is quasi-periodic if $\Omega^T n = 0$ implies $n = 0$, when $n \in Z^m$. The coefficients a(n) are such that the potential is real and three times differentiable in x. The phases φ define naturally an m-dimensional torus. Imagine now that we adiabatically vary the phase φ_j from 0 to 1. This will induce a charge transport of electrons, in the direction α given by

$$Q(\alpha j) = i\, M(P[P_\alpha, P_j]) \tag{10}$$

where $P_\alpha \equiv V_\alpha$ and $P_j = \frac{\partial P}{\partial \varphi_j}$, P being the Fermi projector

$$P = \begin{cases} 1 & \text{if } H \leqslant \mu \\ 0 & \text{if } H > \mu \end{cases} \tag{11}$$

the mean $M(A_\varphi)$ of translation invariant observable being given for such systems by

$$M(A) = \int_0^1 \prod_j d\varphi_j \ \langle 0 | A_\varphi | 0 \rangle \tag{12}$$

In the analysis of $Q(\alpha j)$, certain other quantities appeared naturally. Let us define them (Greek letters designate space variables, Latin letters phase variables)

$$Q(\alpha j \beta k) = \frac{i^2}{2!} \sum_\Pi sg(\Pi)\, M(P\, P_{\Pi(\alpha)}\, P_{\Pi(j)}\, P_{\Pi(\beta)}\, P_{\Pi(k)}) \tag{13}$$

$$Q(\alpha j \beta k \gamma e) = \frac{i^3}{3!} \sum_\Pi sg(\Pi)\, M(P\, P_{\Pi(\alpha)}\, P_{\Pi(j)}\, P_{\Pi(\beta)}\, P_{\Pi(k)}\, P_{\Pi(\gamma)}\, P_{\Pi(e)}) \tag{14}$$

Π is a permutation, and $sg(\Pi)$ its signature. Our results can be summarized in the following :

<u>Theorem</u> If the Fermi energy μ is in a gap

1) In one dimension, the adiabatic charge transport is quantized, i.e. $Q(1j)$ is an integer, which is the first Chern number of a vector bundle. The electronic density ρ is given by

$$\rho = \sum_j \Omega(j1)\, Q(1j) \tag{15}$$

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

$$Q(\alpha j) = \sum_k \Omega(k\beta)\, Q(\beta k \alpha j) \tag{16}$$

where $Q(\beta k\alpha j)$ is an integer, the 2[nd] Chern number of a vector bundle. The electronic density can be expressed as

$$\rho = \sum_{jk} \Omega(j\alpha)\,\Omega(k\beta)\; Q(\beta k \alpha j) \qquad (17)$$

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

$$Q(\alpha j) = \sum_{kl} \Omega(k\beta)\,\Omega(l\gamma)\; Q(\gamma l k\beta \alpha j) \qquad (18)$$

where $Q(\gamma l k\beta \alpha j)$ is an integer, and the 3[th] Chern number of a vector bundle. The electronic density ρ is given by

$$\rho = \sum_{jkl} \Omega(j\alpha)\,\Omega(k\beta)\,\Omega(l\gamma)\; Q(\gamma l k\beta \alpha j) \qquad (19)$$

The fact that the electronic density in a gap is a linear combination of integers was first proved by Johnson and Moser in the one-dimensional case [5] and by Bellissard, Lima, Testard [6] in the multi-dimensional one. None of these authors however provided an interpretation of the integers appearing in the decomposition. It would be quite interesting to give a physical interpretation of the higher topological invariants $Q(\alpha j \beta k \gamma l)$ we have introduced. We conjecture that they are related to terms of higher order in T^{-1} in the adiabatic expansion.

Periodic potentials and magnetic fields

Similar ideas can be applied to the old problem of electronic motion in periodic potentials and magnetic fields. In units of length $\left(\frac{\hbar c}{eB}\right)^{\frac{1}{2}}$ and energy $\frac{\hbar eB}{mc}$ the one electron hamiltonian reads in two dimensions

$$H = \frac{1}{2} v_x^2 + \frac{1}{2} v_y^2 + V_\phi(x,y) \qquad (20)$$

where

$$v_x = \frac{1}{i}\partial_x + y \qquad (21)$$

$$v_y = \frac{1}{i}\partial_y$$

and

$$V_\phi(x,y) = \sum_{n_1,n_2} a(n_1,n_2)\exp 2\pi i\left[\frac{n_1 x}{a} + \frac{n_2 y}{b} + n_2\phi\right] \qquad (22)$$

is a periodic potential.

If the flux through a unit cell $\frac{ab}{2\pi}$ is rational, it was proved by Thouless et al. [7] that the Hall conductivity is quantized, when the Fermi energy is in a gap. We consider now the case where the flux is irrational. The situation resembles that of an incommensurate potential. We consider two quantities :

The Hall conductivity

$$\sigma(x, y) = i\,M\,(P[V_x, V_y]) \qquad (23)$$

where $$V_{\substack{x\\y}} = \oint_{\Gamma} \frac{dz}{2\pi i} (z-H)^{-1} v_{\substack{x\\y}} (z-H)^{-1} \qquad (24)$$

and the adiabatic transport Q(y, ϕ) in the direction μ induced by an adiabatic change of the phase ϕ from 0 to 1.

$$Q(y\,\phi) = i\,\mathrm{Tr}\left(P\left[V_y, \frac{\partial P}{\partial \phi}\right]\right) \qquad (25)$$

Our result is the following :

<u>Theorem</u> In two dimensions, if the flux is irrational and the Fermi energy is in a gap, the Hall conductivity is quantized, i.e. 2π . Q (x, y) is an integer (the 1st Chern number of a vector bundel), the charge transport Q(y, ϕ) is quantized, i.e. Q(y, ϕ) is an integer (the 1st Chern number of a vector bundle), and the electronic density is given by

$$\rho = \sigma(x, y) - \frac{1}{a_3} Q(y\,\phi) \qquad (26)$$

Recently, Halperin [8] has generalized the result on the Hall conductivity to the three dimensional situation, showing that in a gap it should be given by a linear combination of vectors of the reciprocal lattice.

To conclude, it appears to me that some rather interesting topological structure exist in these problems of condensed matter physics and it would certainly be very exciting to find an experimental indication of their existence, in quasi-crystals for example.

A brief summary of some results presented here has already appeared [9] and all the details of the derivation will be given in a forthcoming article.

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