ANOMALOUS TRANSPORT AND QUASICRYSTALS

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ABSTRACT

We give an account of the existing rigorous results recently available concerning the description of anomalous quantum diffusion. We also propose a mathematically well-defined model describing dissipation and giving rise to the so-called "relaxation-time approximation". This model permits to prove rigorously the Greenwood-Kubo formula. In addition we can define properly a family of fractal exponents arising in the transport properties. We give various rigorous relations between them. This framework should be useful in view of the transport properties of quasicrystals.

1. Introduction

In the recent years many quantum systems have been found exhibiting anomalous transport properties. The oldest example is provided by the Fibonacci and Harper equations[1,2]. Anomalous diffusion was also found for the 2D octagonal quasicrystal in the metallic regime [3,4]. Actually, the series of experiments performed on stable quasicrystals alloys, like $AlFeCu$ or $AlPdRh$, show that the low temperature conductivity of quasicrystals is probably dominated by a quantum subdiffusive regime[5]. This is the main reason why it is necessary to know more about anomalous quantum diffusion.

By anomalous diffusion, we mean that the mean square displacement behaves like

$$\int_0^T \frac{dt}{T} \; < |X(t) - X|^2 > \sim \; T^{2\sigma} \; , \qquad \text{as} \qquad T \rightarrow \infty \; , \tag{1}$$

where $0 < \sigma < 1$. σ is called the *diffusion exponent*. Localization corresponds to $\sigma = 0$ whereas ballistic motion corresponds to $\sigma = 1$ and regular quantum diffusion to $\sigma = 1/2$. We will say that the anomalous quantum motion is *subdiffusive* if $0 < \sigma < 1/2$ and *overdiffusive* if $1/2 < \sigma < 1$.

Anomalous diffusion implies that the Hamiltonian describing the quantum motion has singular continuous or pure-point spectrum at least in 1D (see Guarneri's bound below). In particular, the local density of state (LDOS), namely the spectral measure, is expected to be multifractal. Note, however, that this does not necessarily imply the existence of gaps in the spectrum, as can be seen on the 2D octagonal quasicrystal[3].

Very few rigorous results concerning anomalous diffusion and its relation with spectral and transport properties are known by now. The oldest result in that respect is the Guarneri bound giving a relation between the fractal properties of the LDOS and the diffusion properties[6,7]. More is known about one-particle Hamiltonians with singular continuous spectrum[8,9,10,11]. A more systematic study of such Hamiltonians with is now available [12,13].

The purpose of this short note is to provide a mathematical background for the study of anomalous quantum transport and to give a few properties that may be useful for future investigations. Part of it can be found in a previous work of the authors concerning the quantum Hall effect[14] and in[15]. The other original results will be written in a forthcoming paper[16].

2. The Greenwood-Kubo Formula

For simplicity we will consider the electron fluid in a quasicrystal of physical dimension D and assume that it can be represented as a gas of independent fermions on the quasilattice defined by the equilibrium positions of the ions. We will always assume that the sample, denoted by Λ, is large enough to consider its volume $|\Lambda|$ as infinite. We will denote by H the one-particle Hamiltonian and by $\vec{X} = (X_1, \ldots, X_D)$ the position operators. The current operator is then $\vec{J} = e[\vec{X}, H]/(\imath\hbar)$. If the system is prepared in an equilibrium state at inverse temperature β with a chemical potential μ, the thermal averaged density of an homogeneous observable A is given by

$$< A >_{\beta,\mu} = \lim_{|\Lambda|\to\infty} \frac{1}{|\Lambda|} \mathrm{Tr}_\Lambda(f_{\beta,\mu}(H)\, A) \;, \tag{2}$$

where $f_{\beta,\mu}(E)$ is the Fermi distribution function. Clearly, at equilibrium, the average current vanishes. To get a non-zero current we need to switch on an external electric field $\vec{\mathcal{E}}$. For simplicity, we assume that this field is uniform in space and periodic in time with pulsation ω. We let therefore the time evolution of observables for $t \geq 0$ be governed by the Hamiltonian $H_{\vec{\mathcal{E}}}(t) = H + e\vec{\mathcal{E}}(t)\vec{X}$. The actual current density at frequency ω is the time average $\vec{j} = \lim_{T\to\infty} \int_0^T dt/T < \vec{J}(t) >_{\beta,\mu} e^{-\imath\omega t}$. We have proved in[14] for $\omega = 0$ the following result, valid for any frequency:

Proposition: *If H is bounded, the component of the current j parallel to $\vec{\mathcal{E}}$ vanishes.*

This surprising result is actually due to the absence of dissipation mechanisms. To introduce some dissipation we have proposed to add to the Hamiltonian a term of the form

$$H_{coll} = \sum_{n\in\mathbf{Z}} \delta(t - t_n) W_n \;, \tag{3}$$

where the collision times t_n are random in such a way that the $\tau_n = t_n - t_{n-1}$ are independent random variables Poisson distributed with average τ_{coll}, and the collision operators W_n's are independent random operators. We have also assumed that the distribution of the collision operators is such that $\kappa(H) = H$ if $\kappa(A) = \mathbf{E}(e^{\imath W_n} A e^{-\imath W_n})$ and $\mathbf{E}$ represents the average over the collision operators. This last property is needed if we want the collisions to enforce the equilibrium.

Now the collision average of the current is not zero anymore. As $\vec{\mathcal{E}} \to 0$, the current is given by linear response theory, namely $\vec{j} = \hat{\sigma}\vec{\mathcal{E}}$ where $\hat{\sigma}$ is the conductivity tensor

Kubo's formula in relaxation time approximation[14]:

$$\hat{\sigma}_{a,b}(\omega) \;=\; -\frac{e^2}{\hbar} \lim_{|\Lambda|\to\infty} \frac{1}{|\Lambda|} \mathrm{Tr}_\Lambda \left(\partial_b f_{\beta,\mu}(H) \frac{1}{(1-\kappa)/\tau_{\mathrm{coll}} - \mathcal{L}_H - \imath\omega} \partial_a H \right) \;, \tag{4}$$

where we have set $\partial_a A = \imath[X_a, a]$ and $\mathcal{L}_H(A) = \imath[H, A]/\hbar$. In periodic media this formula yields the usual one[17].

3. Spectral and Transport Exponents

Let $f(\varepsilon)$ be a positive measurable function of the variable $\varepsilon \in [0,1]$. According to[6,15], we will say that $f(\varepsilon) \sim \varepsilon^{\alpha}$ as $\varepsilon \to 0$ if

$$\alpha \;=\; \sup\{\, \gamma \in \mathbf{R} \mid \exists\, 0 < a \leq 1 \text{ such that } \int_0^a \frac{d\varepsilon}{\varepsilon^{1+\gamma}} f(\varepsilon) \;<\; \infty \,\} \,. \tag{5}$$

A similar definition holds for $\varepsilon \to \infty$. Let now ν be a positive measure on the real line $\mathbf{R}$. We define its local exponent $\alpha_\nu(E)$ by $\int_{E-\varepsilon}^{E+\varepsilon} d\nu(E') \sim \varepsilon^{\alpha_\nu(E)}$ as $\varepsilon \to 0$.

Proposition: *The following results hold* [15,16]:

(i) The map $E \mapsto \alpha_\nu(E)$ is borelian and $0 \leq \alpha_\nu(E) \leq 1$ for ν-almost all E's.

(ii) If ν is pure-point, then $\alpha_\nu(E) = 0$ ν-almost surely. If ν is absolutely continuous then $\alpha_\nu(E) = 1$ ν-almost surely. In particular, if $0 < \alpha_\nu(E) < 1$ (ν-almost surely) then ν is singular continuous.

(iii) For a complex number z, let $G(z) = \int_{\mathbf{R}} d\nu(E')(z-E')^{-1}$ be the Green function associated to ν. Then the spectral exponent can be calculated by be the exponent defined by $\Im m G(E+\imath\varepsilon) \sim \varepsilon^{\alpha_\nu(E)-1}$ as $\varepsilon \to 0$.

We now consider the Hamiltonian H describing the one-particle motion of the electron fluid. By our hypothesis, its matrix elements $<x|H|y>$ are indexed by the lattice sites of the quasicrystal. We let P_Δ be the projection onto the eigenspace corresponding to energies in an interval $\Delta \subset \mathbf{R}$. The diffusion exponent $\sigma_x(\Delta)$ will be defined as

$$\frac{1}{2} \inf\,\{\, \gamma \in \mathbf{R} \mid \int_1^\infty \frac{dT}{T^{1+\gamma}} \int_0^T \frac{dt}{T} <x|P_\Delta(\vec{X}(t) - \vec{X})^2 P_\Delta|x> \;< \infty \,\} \,. \tag{6}$$

The diffusion exponent $\sigma_x(E)$ is the infimum of the $\sigma_x(\Delta)$'s over all intervals containing E.

On the other hand, given x in the lattice, the spectral measure relative to x is defined by ρ_x defined by $\int_{\mathbf{R}} d\rho_x(E) f(E) =< x|f(H)|x >$ for a continuous function f. If $\alpha_{\rho_x}(E)$ is the corresponding exponent, for Δ a Borel subset of the real line, let $\alpha_x(\Delta)$ denote the essential infimum of the $\alpha_{\rho_x}(E)$'s ($E \in \Delta$) obtained after cutting out from Δ a subset of zero ρ_x–measure if necessary. If D is the dimension of physical space, we have

Guarneri's inequality[6,7]: $\qquad \alpha_x(\Delta) \;\leq\; D\,\sigma_x(\Delta)$.

Note that this result gives interesting consequences. In 1D, anomalous diffusion produces automatically a singular spectrum. However if $D > 1$, we may have coexistence of anomalous diffusion and absolutely continuous spectrum. For indeed, absolutely continuous spectrum implies $\alpha_x(\Delta) = 1$, whereas Guarneri's bound permits $\sigma_x(\Delta) \geq 1/D$. In 3D we may have subdiffusive behavior with an absolutely continuous spectrum provided $\sigma_x(\Delta) \geq 1/3$.

An averaged diffusion exponent $\sigma(E)$ can be defined in much the same way by taking in (6) the space average over x and letting Δ shrink to E[16].

Let us now consider the conductivity given by the Kubo formula (4) in the limit for which the operator $(1-\kappa)$ can be viewed as a real number. Then we define the relaxation time by $\tau_{\text{rel}} = \tau_{\text{coll}}/(1-\kappa)$. For a normal metal, Drude's formula implies that $\hat{\sigma}_{a,a} \sim \tau_{\text{rel}}$ as $\tau_{\text{rel}} \to \infty$. Here, if E_F is the Fermi level, we get in the limit of very low temperature

Anomalous Drude formula: $\qquad \hat{\sigma}_{a,a} \;\sim\; \tau_{\text{rel}}^{2\sigma(E_F)-1} \,, \qquad \text{as } \tau_{\text{rel}} \to \infty$.

This result shows that if the diffusion is ballistic, the Drude formula holds, if the system is localized, then the conductivity vanishes as the dissipation disappears. If the quantum diffusion is normal, namely if $\sigma(E_F) = 1/2$, the conductivity is finite in the limit of vanishing dissipation.

These last results are actually compatible with the experiments performed on quasicrystals provided we accept that in a 3D quasicrystal the quantum motion is subdiffusive. In this case the larger the relaxation time, the smaller is the conductivity. This mechanism has been proposed by Mayou[5] and Sire[4] to explain why the conductivity decreases to zero at very low temperatures and why the inverse Mathiessen rule holds. More details will be given in[16].

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