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LETTER TO THE EDITOR

Topological quantization of boundary forces and the integrated density of states

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Abstract

For quantum systems described by Schrödinger operators on the half-space $\mathbb{R}^{d-1} \times \mathbb{R}^{\leqslant 0}$ the boundary force per unit area and unit energy is topologically quantized provided the Fermi energy lies in a gap of the bulk spectrum. Under this condition it is also equal to the integrated density of states at the Fermi energy.

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1. Introduction

Consider a quantum system on the half-space $\mathbb{R}^{d-1} \times \mathbb{R}^{\leqslant 0}$. One distinguishes between its behaviour for $x_d \ll 0$ and x_d near 0 considering the bulk behaviour in the first, and the edge (or boundary) behaviour of the system in the second case. Bulk and edge behaviour are not independent but topologically quantized observables in the bulk are related to topologically quantized observables at the edge. A famous example of this type is the quantum Hall effect in which the Hall conductivity can either be related to a current–current correlation in the bulk or is simply the conductance of the edge current [Pr90, F94, SKR00, KRS02, EG02, KS03b]. In this letter, we present another example relating the value of the integrated density of states on a gap (i.e. at energies lying in the gap) of the bulk spectrum to a force the boundary exhibits on the edge states.

We discuss in the next section the underlying model and provide a proof of our claims in the case of one-dimensional periodic systems. The proof for the general case will be given elsewhere.

2. The model

In line with recent descriptions of aperiodic systems [Pa80, B86, B93, KS03a] we describe the bulk behaviour of the system in the one-particle approximation by a covariant family of

Schrödinger operators $\{H_\omega\}_{\omega\in\Omega}$,

$$H_\omega = -\frac{\hbar^2}{2m}\sum_{j=1}^{d}\partial_j^2 + V_\omega$$

all acting on $L^2(\mathbb{R}^d)$, where Ω is a space of disorder configurations or of configurations which cannot be macroscopically distinguished. The second case is interesting for ordered systems, such as quasi-crystals, in which Ω can be the hull of a single point pattern describing the set of average positions of the atoms and possibly decorated with information to distinguish between the kinds of atoms. Ω carries three structures. First, a metric topology in which it is compact, namely two configurations are deemed ϵ-close if they agree up to an error of order ϵ on a $\frac{1}{\epsilon}$-neighbourhood around the origin $0 \in \mathbb{R}^d$ (see [FHK02] for a precise formulation). Second, an action of the group of translations which we denote by $\omega \mapsto x\cdot\omega$ where $x\cdot\omega$ is the translate of the configuration $\omega\in\Omega$ by 0 to x. Then a family of potentials $\{V_\omega\}_{\omega\in\Omega}$ is called covariant if $V_\omega(x-y) = V_{y\cdot\omega}(x)$ which implies the required covariance of the corresponding family of Schrödinger operators $\{H_\omega\}_{\omega\in\Omega}$. Third, Ω comes with a translation invariant Borel-probability measure $\mathbf{P}$ and all measurable quantities are averaged over Ω with respect to this measure. This average has the meaning of a disorder average but should also be carried out if the configurations in Ω describe ordered systems, because they are supposed to be macroscopically indistinguishable. The union $\bigcup_{\omega\in\Omega}\sigma(H_\omega)$ of all spectra $\sigma(H_\omega)$ is called the bulk spectrum.

2.1. Integrated density of states on gaps

The integrated density of states at energy E of a single operator H_ω from the family can be defined as the trace per unit volume τ of the spectral projection $P_E(H_\omega)$ of H_ω onto the states up to energy E. If the probability measure $\mathbf{P}$ is ergodic then the trace per unit volume of $P_E(H_\omega)$ is $\mathbf{P}$-a.s. constant over Ω and

$$\mathrm{IDS}(E) = \int_\Omega \mathrm{d}\mathbf{P}(\omega)\tau(P_E(H_\omega)). \tag{1}$$

Thus the integrated density of states should be thought of as an expectation value of the whole family of operators. The integrated density of states is constant on gaps in the bulk spectrum. It has been shown that equation (1) has a C^*-algebraic interpretation if E lies outside the bulk spectrum. In particular, the family $\{P_E(H_\omega)\}_{\omega\in\Omega}$ can be viewed as a projection in the natural C^*-algebra associated with the configuration space Ω and the lhs of (1) depends only on the homotopy class of P_E in this C^*-algebra [B93]. This formulation makes clear that the value of the integrated density of states on a gap is topologically quantized, namely, first, it is stable under perturbations of the Schrödinger operator by covariant operators which do not lead to a closing of the gap, and second, it lies in a countable subgroup of $\mathbb{R}$, the gap-labelling group, which depends only on the topology of Ω, its measure $\mathbf{P}$ and the translation action, but not on the specific form of the potentials. In specific cases this group can be determined, e.g. for hulls of Delone sets of finite local complexity this group is the sub-group generated by the relative frequencies of the patterns appearing in the Delone set [BBG, BO, KP].

2.2. Boundary force per unit area and unit energy in gaps

To describe the behaviour near the edge we consider the same family of operators but restrict them to $L^2(\mathbb{R}^{d-1}\times\mathbb{R}^{\leqslant s})$ demanding Dirichlet boundary conditions at the boundary $\mathbb{R}^{d-1}\times\{s\}$. We define the total boundary force to be minus the variation of the energy under a variation

of the position s of the boundary. To describe this in one and the same Hilbert space, say the one corresponding to $s = 0$, we vary instead the position of the configuration in the opposite direction. The boundary force exhibited per unit area on the states in some energy interval Δ is therefore

$$\int_\Omega \mathrm{d}\mathbf{P}(\omega)\hat{\tau}(P_\Delta(\hat{H}_\omega)\delta(\hat{H}_\omega)) \qquad \delta(\hat{H}_\omega) := \lim_{x_d\to 0}\frac{\hat{H}_{x_d e_d\cdot\omega}}{x_d} = \frac{\partial V_\omega}{\partial x_d}$$

where $\hat{\tau}$ is the trace per unit area parallel to the boundary and we have for clarity denoted the restriction of H_ω to $L^2(\mathbb{R}^{d-1}\times\mathbb{R}^{\leqslant 0})$ with Dirichlet boundary conditions with a hat. Note that we include the $\mathbf{P}$-average directly into the definition of the boundary force. This is crucial for its topological quantization and it is not true that $\hat{\tau}(P_\Delta(\hat{H}_\omega)\delta(\hat{H}_\omega))$ is $\mathbf{P}$-a.s. constant over Ω for ergodic measures. The boundary force per unit area and energy at energy E is then

$$F_b(E) = \lim_{\Delta\to\{E\}}\frac{1}{|\Delta|}\int_\Omega \mathrm{d}\mathbf{P}(\omega)\hat{\tau}\left(P_\Delta(\hat{H}_\omega)\frac{\partial V_\omega}{\partial x_d}\right). \tag{2}$$

$|\Delta|$ is the length of the interval which tends to 0 in that limit. The limit exists if E lies in a gap of the bulk spectrum. Moreover, if E lies in a gap then $F_b(E)$ is a topological quantity. In fact, it can be shown that

$$\frac{1}{|\Delta|}\int_\Omega \mathrm{d}\mathbf{P}(\omega)\hat{\tau}(P_\Delta(\hat{H}_\omega)\delta(\hat{H}_\omega)) = 2\pi\hat{\tau}((\mathcal{U}_\omega^*(\Delta)-1)\delta(\mathcal{U}_\omega(\Delta))) \tag{3}$$

where

$$\mathcal{U}_\omega(\Delta) - 1 = (\mathrm{e}^{2\pi\mathrm{i}t(\hat{H}_\omega - E_0)} - 1)P_\Delta(\hat{H}_\omega) \qquad t = \frac{1}{|\Delta|} \quad E_0 = \min\Delta.$$

Thus $\mathcal{U}_\omega(\Delta)$ is essentially the time evolution of the states of energy in Δ by the time which is the inverse of the width of Δ. Equation (3) can be interpreted in a C^*-algebraic context and shown to depend only on the homotopy class of the unitary $\mathcal{U}_\omega(\Delta)$. Therefore, $F_b(E)$ is topologically quantized in the same way as the integrated density of states. In fact, we can show using the tools of non-commutative topology of C^*-algebras developed in [KS03b] that, for energies E in gaps and ergodic $\mathbf{P}$,

$$|F_b(E)| = \mathrm{IDS}(E). \tag{4}$$

The proof of this result in the general case will be given in a separate publication. In the next section we give an elementary proof of the above equality for periodic one-dimensional systems.

3. One-dimensional periodic systems

We consider in this section probably the simplest case, in which we have a one-dimensional periodic configuration ω_0, of period L, and Ω is the set of its translates. Then $\Omega = \{x\cdot\omega_0 | x\in\mathbb{R}\} \cong \mathbb{R}/L\mathbf{Z}$ with standard action of $\mathbb{R}$ by translation and Lebesgue measure. If we choose a differentiable periodic potential V then $V_{\xi\cdot\omega_0}(x) = V(x+\xi)$ defines a covariant family of potentials. For simplicity we write V_ξ in place of $V_{\xi\cdot\omega_0}$. We need to combine results about the spectral theory of the family $H_\xi := -\frac{\hbar^2}{2m}\partial^2 + V_\xi$, $\xi\in[0,L)$, on three different spaces, see e.g. [DS88, B93] for background information.

(1) On $L^2(\mathbb{R})$. Fixing $E\in\mathbb{R}$ and $\xi\in[0,L)$ one finds for each $a,b\in\mathbb{C}$ a unique solution of $(H_\xi - E)\Psi = 0$ with initial condition $\Psi(0) = a$, $\Psi'(0) = b$. Ψ is a function over $\mathbb{R}$ which is not normalizable. Since H_ξ is a linear operator these unique solutions define a linear map $\mathbb{C}^2\to\mathbb{C}^2$: $\binom{\Psi(0)}{\Psi'(0)} \mapsto \binom{\Psi(L)}{\Psi'(L)}$ whose associated matrix is called the

monodromy matrix, we denote it by $M(E, \xi)$. The spectrum of H_ξ on $L^2(\mathbb{R})$ is the set $\{E \in \mathbb{R} | -2 \leqslant M_{11}(E, \xi) + M_{22}(E, \xi) \leqslant 2\}$. It is independent of ξ and hence equal to the bulk spectrum. It is convenient to call the closures of the connected components of the open set $\{E \in \mathbb{R} | -2 < M_{11}(E, \xi) + M_{22}(E, \xi) < 2\}$ the bands. Then bands may touch.

(2) On $L^2([0, L])$ with Dirichlet boundary conditions at the boundary points. On that space the spectrum of H_ξ is a discrete countably infinite set $\{\mu_1(\xi), \mu_2(\xi), \ldots\}$ $(\mu_j(\xi) < \mu_{j+1}(\xi))$. We call these spectral values Dirichlet eigenvalues of H_ξ. They are determined by the equation $M_{12}(E, \xi) = 0$. Between $\mu_j(\xi)$ and $\mu_{j+1}(\xi)$ lies the $(j + 1)$th band of the bulk spectrum (counted from the lowest band). We call a Dirichlet eigenvalue $\mu_n(\xi)$ a left or right eigenvalue if its corresponding eigenfunction $\psi_{n,\xi}$ satisfies $|\psi'_{n,\xi}(L)| < |\psi'_{n,\xi}(0)|$ or $|\psi'_{n,\xi}(L)| > |\psi'_{n,\xi}(0)|$, respectively. The terminology comes from the exponential increase if the functions are considered over many periods which physically means that eigenfunctions of right eigenvalues are localized at the right edge. If two bands touch they touch at a Dirichlet eigenvalue which is neither a left nor a right eigenvalue.

Sturm–Liouville theory gives us the important information that a real eigenfunction $\psi_{n,\xi}$ of H_ξ to $\mu_n(\xi)$ has exactly n zeroes on the half open interval $[0, L)$ (so the zero at L is not counted).

(3) On $L^2(\mathbb{R}^{\leqslant 0})$ with Dirichlet boundary condition at the boundary 0. The spectrum of H_ξ on that space is the union of the bulk spectrum with the right Dirichlet eigenvalues. In fact, E belongs to that spectrum iff the eigenvalues of $M(E, \xi)$ have modulus 1 or $\binom{0}{1}$ is an eigenvector of $M(E, \xi)$ to an eigenvalue ρ of modulus strictly larger than 1. In the first case E belongs to a band and in the second the corresponding eigenfunction satisfies $|\psi'_{n,\xi}(L)| = |\rho\psi'_{n,\xi}(0)| > |\psi'_{n,\xi}(0)|$.

We give an alternative description of left or right Dirichlet eigenvalues, namely $\mu_n(\xi)$ is a left or right eigenvalue iff $\mu'_n(\xi) > 0$ or $\mu'_n(\xi) < 0$, respectively. In fact, we calculate $\mu'_n(\xi)$ for right eigenvalues

$$\mu'_n(\xi) = \partial_\xi \int_{-\infty}^{0} \mathrm{d}x\, \overline{\hat{\psi}_{n,\xi}(x)} H_\xi \hat{\psi}_{n,\xi}(x) = \int_{-\infty}^{0} \mathrm{d}x |\hat{\psi}_{n,\xi}(x)|^2 V'_\xi(x) \tag{5}$$

where $\hat{\psi}_{n,\xi}$ is the *normalized* eigenfunction, $\int_{-\infty}^{0} \mathrm{d}x |\hat{\psi}_{n,\xi}(x)|^2 = 1$. Clearly, this normalization is only possible since $\mu_n(\xi)$ is a right eigenvalue. Using integration by parts and $\hat{\psi}_{n,\xi}(0) = \hat{\psi}_{n,\xi}(-\infty) = \hat{\psi}'_{n,\xi}(-\infty) = 0$ we find

$$\begin{aligned}
\int_{-\infty}^{0} \mathrm{d}x |\hat{\psi}_{n,\xi}(x)|^2 V'_\xi(x) &= -\int_{-\infty}^{0} \mathrm{d}x\, \overline{\hat{\psi}'_{n,\xi}(x)} \hat{\psi}_{n,\xi}(x) V_\xi(x) - \text{c.c.} \\
&= -\int_{-\infty}^{0} \mathrm{d}x\, \overline{\hat{\psi}'_{n_\xi}(x)} (E\hat{\psi}_{n,\xi}(x) + \frac{\hbar^2}{2m} \hat{\psi}''_{n,\xi}(x)) - \text{c.c.} \\
&= -\frac{\hbar^2}{2m} |\hat{\psi}'_{n,\xi}(0)|^2 < 0.
\end{aligned}$$

For left eigenvalues one proceeds similarly, but uses the space $L^2(\mathbb{R}^{\geqslant 0})$ instead. Since 0 is then the left boundary of the integral one obtains a relative minus sign in the calculation. The remaining case is that $\mu_n(\xi)$ is neither a left nor a right eigenvalue. Then it must be at a band edge and therefore an extremum of μ_n.

This has the following consequence which is crucial below: since a real eigenfunction to a right Dirichlet eigenvalue $\mu_n(\xi)$ has n zeroes on $[0, L)$ the equations $\mu_n(\xi) = \mu$, $\mu'_n(\xi) < 0$ have exactly n solutions on $\xi \in [0, L)$.

Using an approximation of the trace per unit volume by the trace per unit volume in the representations $L^2([-NL, NL])$ with Dirichlet boundary conditions one obtains from Sturm–Liouville theory in the limit $N \to \infty$

$$\mathrm{IDS}(\mu_n(\xi)) = \frac{n}{L} \tag{6}$$

independent of ξ.

We determine the boundary force (2). If Δ is an interval in the nth gap of the bulk spectrum then H_ξ has exactly one non-degenerate eigenvalue (a right Dirichlet eigenvalue) provided $\mu(\xi) \in \Delta$ and $\mu_n'(\xi) < 0$, otherwise it has none. Hence the integral kernel $\langle x|P_\Delta(\hat{H}_\xi)|y\rangle$ of $P_\Delta(\hat{H}_\xi)$ is $\hat{\psi}_{n,\xi}(x)\overline{\hat{\psi}_{n,\xi}(y)}\chi_\Delta(\mu_n(\xi))\Theta(-\mu_n'(\xi))$ where χ_Δ is the characteristic function on the interval Δ and Θ the Heaviside function. In one dimension $\hat{\tau}$ is the operator trace and therefore

$$\hat{\tau}(P_\Delta(\hat{H}_\xi)V_\xi') = \int_{-\infty}^{0} \mathrm{d}x|\hat{\psi}_{n,\xi}(x)|^2\chi_\Delta(\mu_n(\xi))\Theta(-\mu_n'(\xi))V_\xi'(x).$$

By (5) and the fact that $\mu_n(\xi) = \mu$, $\mu_n'(\xi) < 0$ has exactly n solutions on $\xi \in [0, L)$

$$\begin{aligned}\int_0^L \mathrm{d}\xi \int_{-\infty}^{0} \mathrm{d}x|\hat{\psi}_{n,\xi}(x)|^2\chi_\Delta(\mu_n(\xi))\Theta(-\mu_n'(\xi))V_\xi' &= \int_0^L \mathrm{d}\xi\, \mu_n'(\xi)\chi_\Delta(\mu_n(\xi))\Theta(-\mu_n'(\xi)) \\ &= -n\int_\Delta \mathrm{d}\mu = -n|\Delta|.\end{aligned}$$

As it should be, this expression is negative and so the force points into the sample. We conclude that

$$|F_b(E)| = \frac{n}{L}$$

and so the strength of the boundary force per unit area and unit energy is equal to the integrated density of states for an energy E which lies in a gap of the bulk spectrum. We end this section with some remarks.

1. The integer n appearing in the above expression may also be interpreted as a winding number of the Dirichlet eigenvalue on the complex spectral curve of H_ξ. This is similar but not identical to the phenomenon observed in [H93].
2. The above also yields, for an arbitrary interval Δ in the nth gap,
$$\begin{aligned}&\frac{\hbar^2}{2m|\Delta|}\int_0^L \mathrm{d}\xi|\hat{\psi}_{n,\xi}'(0)|^2\chi_\Delta(\mu_n(\xi))\Theta(\pm\mu_n'(\xi)) \\ &\qquad = \frac{\hbar^2}{2mw_n}\int_0^L \mathrm{d}\xi|\hat{\psi}_{n,\xi}'(0)|^2\Theta(\pm\mu_n'(\xi)) = n.\end{aligned}$$
Here w_n is the width of the nth gap and, for the + sign ($-$ sign), $\hat{\psi}_{n,\xi}$ is a normalized eigenfunction to the left (right) Dirichlet eigenvalue. These two equations seem interesting in their own right for one-dimensional periodic operators.
3. Since, by the boundary conditions,
$$|\hat{\psi}_{n,\xi}'(0)|^2 = \left.\frac{\partial_x^2|\hat{\psi}_{n,\xi}(x)|^2}{2}\right|_{x=0}$$
we see that the boundary force per unit area and unit energy is determined by the **P**-average of the first non-vanishing coefficient in the Taylor expansion of the density of the particles at the edge.
4. We note again that the **P**-average is crucial for the topological quantization. In fact, $\hat{\psi}_{n,\xi}'(0)$ tends to 0 if ξ tends to the extrema of the function $\mu_n(\xi)$.

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