Rotation Numbers, Boundary Forces and Gap Labelling

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Abstract

We review the Johnson-Moser rotation number and the K_0-theoretical gap labelling of Bellissard for one-dimensional Schrödinger operators. We compare them with two further gap-labels, one being related to the motion of Dirichlet eigenvalues, the other being a K_1-theoretical gap label. We argue that the latter provides a natural generalisation of the Johnson-Moser rotation number to higher dimensions.

1 Introduction

It is an interesting and very well known fact that the boundary of a domain plays a prominent role both in mathematics and in physics. A case that comes immediately into mind is the theory of differential equations where the boundary conditions determine quite a lot of the whole solution. Another class of prominent examples in physics are topological quantum field theories. In topological applications there are some even stronger statements which claim that what happens in the boundary determines the behaviour of the system in the bulk completely. Perhaps the most famous such statement is the holography principle in quantum gravity.

Similar ideas are manifested in [KS04a, KS04b] where a correspondance between bulk and boundary topological invariants for certain physical systems arising in solid state physics was found. This suggestion was mathematically based on K-theoretic and cyclic cohomological properties of the Wiener-Hopf extension of the C^*-algebra of observables. In most applications we have in mind in condensed matter physics this C^*-algebra of observables is obtained by considering the Schrödinger operator and its translates describing the 1-particle approximation of the solid.

Here we consider a simple example, a Schrödinger operator on the real line. The K_0-theory gap labels introduced by Bellissard et al. [BLT85, Be92] are bulk invariants. It is known that these are equal to the Johnson-Moser rotation numbers [JM82] the existing proof being essentially a corollary of the Sturm-Liouville theorem by which they are identified with the integrated density of states on the gaps. Here we give a direct identification of the Johnson-Moser rotation number (for energies in gaps) with a boundary invariant, namely a Dirichlet rotation number. This number has an operator algebraic and physical interpretation, namely as boundary force per unit energy, and a K_1-theoretical interpretation. The equality between the even and the odd K-theoretic gap labels is an application of the above-mentioned correspondence between bulk and boundary invariants.

We organise this article as follows: after recalling some well-known facts for one-dimensional systems we discuss the Johnson-Moser rotation number in Section 3.1. In Section 3.2 we introduce the Dirichlet rotation number of a gap and show that it coincides with the Johnson-Moser rotation number for energies in that gap. We interprete the Dirchlet rotation number in Section 3.3 as an odd K gap-label and in Section 3.4 as boundary force per unit energy. All of Section 3 is based on a single operator, although its translates play a fundamental role. In Section 4 we place this into the framework of ergodic theorems and prepare the ground for the discussion of the underlying non-commutative topology which is carried in Section 5. This section is held quite briefly, since it is mainly based on [Kel].

2 Preliminaries

In this article we consider as in [Jo86] a one-dimensional Schrödinger operator $H = -\partial^2 + V$ with (real) bounded potential which we assume (stricter as in [Jo86]) to be bounded differentiable. We also consider its translates $H_\xi := -\partial^2 + V_\xi$, $V_\xi(x) = V(x+\xi)$, and lateron its hull. The differential equation $H\Psi = E\Psi$ for complex valued functions Ψ over $\mathbb{R}$ has for all E two linear independent solutions but not all E belong to the spectrum $\sigma(H)$ of H as an operator acting on $L^2(\mathbb{R})$. In this situation the following property of solutions holds [CL55].

Theorem 1 *If $E \notin \sigma(H)$ there exist two real solutions Ψ_+ and Ψ_- of $(H-E)\Psi = 0$ which vanish at ∞ and $-\infty$, resp.. These solutions are linear independent and unique up to multiplication by a factor.*

We mention as an aside that Johnson proves even exponential dichotomy for such energies [Jo86]. Clearly $\sigma(H_\xi) = \sigma(H)$ for all ξ.

We consider also the action of H_ξ on $L^2(\mathbb{R}^{\leq 0})$ with Dirichlet boundary conditions at the boundary. If we need to emphazise this we will also write $\hat{H}_\xi$ for the half-sided operator. The spectrum is then no longer the same. Whereas the essential part of the spectrum of $\hat{H}_\xi$ is contained in that of H_ξ [Jo86] the half sided operator may have isolated eigenvalues in the gaps in $\sigma(H_\xi)$. Here a gap is a connected component of the complement of the spectrum, hence in particular an open set. E is an eigenvalue of $\hat{H}_\xi$ if $(\hat{H}_\xi - E)\Psi = \Psi$ for $\Psi \in L^2(\mathbb{R}^{\leq 0})$ which for E in a gap of $\sigma(H_\xi)$ amounts to saying that the solution Ψ_- of $(H_\xi - E)\Psi_- = 0$ from Theorem 1 satisfies in addition $\Psi_-(0) = 0$.

Definition 1 *We call $E \in \mathbb{R}$ a right Dirichlet value of H_ξ if it is an eigenvalue of $\hat{H}_\xi$.*

We recall the important Sturm-Liouville theorem.

Theorem 2 *Consider $H := -\partial^2 + V$ with (real) bounded continuous potential acting on $L^2([a,b])$ with Dirichlet boundary conditions. The spectrum is discrete and bounded from below. A real eigenfunction to the nth eigenvalue (counted from below) has exactly $n-1$ zeroes in the interior (a,b) of $[a,b]$.*

3 Rotation numbers

The winding number of a continuous function $f : \mathbb{R}/\mathbb{Z} \to \mathbb{R}/\mathbb{Z}$ is intuitively speaking the number of times its graph wraps around the circle $\mathbb{R}/\mathbb{Z}$. This is counted relative to the orientations induced by the order on $\mathbb{R}$. Let $\Lambda = \{\Lambda_n\}_n$ be an increasing chain of compact intervals $\Lambda_n = [a_n, b_n] \subset \Lambda_{n+1} \subset \mathbb{R}$ whose union covers $\mathbb{R}$. The quantity

$$\Lambda(f) := \lim_{n\to\infty} \frac{1}{b_n - a_n} \int_{a_n}^{b_n} f(x)dx$$

is called the Λ-mean of the function $f : \mathbb{R} \to \mathbb{R}$, existence of the limit assumed. Now let $f : \mathbb{R} \to \mathbb{R}/\mathbb{Z}$ be continuous and choose a continuous extension $\tilde{f} : \mathbb{R} \to \mathbb{R}$. To define the rotation number of f we consider the expression

$$\mathrm{rot}_\Lambda(f) = \lim_{n\to\infty} \frac{\tilde{f}(b_n) - \tilde{f}(a_n)}{b_n - a_n}$$

which becomes the winding number of f if f is periodic of period 1. The limit does not exist in general but if it does it is independent of the extension $\tilde{f}$. If f is piecewise differentiable then $\mathrm{rot}_\Lambda(f) = \Lambda(f')$. Moreover, if $U : \mathbb{R} \to \mathbb{C}$ is a nowhere vanishing continuous piecewise differentiable function then we can consider the rotation number of its argument function which becomes

$$\mathrm{rot}_\Lambda(\frac{\arg(U)}{2\pi}) = \lim_{n\to\infty} \frac{1}{2\pi i(b_n - a_n)} \int_{a_n}^{b_n} \frac{\overline{U}}{|U|} \left(\frac{U}{|U|}\right)' dx \qquad (1)$$

3.1 The Johnson-Moser rotation number

Johnson and Moser in [JM82] have defined rotation numbers for the Schrödinger operator $H = -\partial^2 + V$ on the real line where V is a real almost periodic potential. They are defined as follows: Let $\Psi(x)$ be the nonzero real solution of $(H-E)\Psi = 0$ which vanishes at $-\infty$, then $\Psi' + i\Psi : \mathbb{R} \to \mathbb{C}$ is nowhere vanishing and

$$\alpha_\Lambda(H,E) := 2\,\mathrm{rot}_\Lambda(\frac{\arg(\Psi' + i\Psi)}{2\pi}). \qquad (2)$$

(Our normalisation differs from that in [JM82] for later convenience.) For the class of potentials considered here the limit is indeed defined and even independent on the choice of Λ, we will come back to that in Section 4.

Note that $\alpha_\Lambda(H,E)$ has the following interpretations. If $N(a,b;E)$ denotes the number of zeroes of the above solution Ψ in $[a,b]$ then $\alpha_\Lambda(H,E)$ is the Λ-mean of the density of zeroes of Ψ, namely one has

$$\alpha_\Lambda(H,E) = \lim_{n\to\infty} \frac{N(a_n,b_n;E)}{b_n - a_n}.$$

The integrated density of states of H at E is

$$\mathrm{IDS}_\Lambda(H,E) = \lim_{n\to\infty} \frac{1}{|\Lambda_n|}\mathrm{Tr}(P_E(H_{\Lambda_n})) \tag{3}$$

provided the limit exists. Here $|\Lambda_n| = b_n - a_n$ is the volume of Λ_n, H_{Λ_n} the restriction of H to Λ_n with Dirichlet boundary conditions and, for self-adjoint A, $P_E(A)$ is the spectral projection onto the spectral subspace of spectral values smaller or equal to E. It will be important that $P(A)$ is a continuous function of A if E is not in the spectrum of A. Since $\mathrm{Tr}(P_E(H_{\Lambda_n}))$ is the number of eigenfunctions of H_{Λ_n} to eigenvalue smaller or equal E Theorem 2 implies

Corollary 1 $\alpha_\Lambda(H,E) = \mathrm{IDS}_\Lambda(H,E)$.

In particular, like the integrated density of states $\alpha_\Lambda(H,E)$ is monotomically increasing in E and constant on the gaps of the spectrum of H. It is moreover the same for all H_ξ.

3.2 The Dirichlet rotation number

We now consider the continuous 1-parameter family of operators $\{H_\xi\}_\xi$ with $\xi \in \mathbb{R}$ and $H_\xi = -\partial^2 + V_\xi$, where $V_\xi(x) = V(x+\xi)$. We shall prove that the Johnson-Moser rotation number is a rotation number which is defined by right Dirichlet values as a function of ξ.

Let Δ be a gap in $\sigma(H_\xi) = \sigma(H)$ and define the set of right Dirichlet values in Δ

$$D_\xi(\Delta) := \{\mu \in \Delta | \exists \Psi : \ (H_\xi - \mu)\Psi = 0 \text{ and } \Psi(0) = \Psi(-\infty) = 0\}\ .$$

Suppose $D_\xi(\Delta) \neq \emptyset$ for some ξ and let $\mu \in D_\xi(\Delta)$ and Ψ the corresponding solution $(H_\xi - \mu)\Psi = 0$ satisfying the required boundary conditions. Define the following two sets $S(\mu) := \{\eta | \mu \in D_\eta(\Delta)\}$ and $Z(\mu) := \{x | \Psi(x-\xi) = 0\}$.

Lemma 1 $S(\mu) = Z(\mu)$.

Proof: Define $\Psi_\eta(x) = \Psi(x + (\eta - \xi))$. Then $(H_\eta - \mu)\Psi_\eta = 0$ and $\Psi_\eta(-\infty) = 0$ for all η. Hence $Z(\mu) = \{\eta | \Psi(\eta - \xi) = 0\} = \{\eta | \Psi_\eta(0) = 0\} \subset S(\mu)$.

For the opposite inclusion if $\mu \in D_\eta(\Delta)$, then there exists Φ such that $(H_\eta - \mu)\Phi = 0$ with $\Phi(0) = \Phi(-\infty) = 0$. Define $\Phi_\xi(x + (\eta - \xi)) = \Phi(x)$. Then $(H_\xi - \mu)\Phi_\xi = 0$ with $\Phi_\xi(-\infty) = 0$. By Theorem 1, $\Psi = \lambda\Phi_\xi$ for some $\lambda \in \mathbb{C}^*$, which implies $\Psi(\eta - \xi) = \lambda\Phi(0) = 0$ and hence $\eta \in Z(\mu)$, thus $S(\mu) \subseteq Z(\mu)$. □

Let $\xi \in S(\mu)$, $\mu \in \Delta$. Since the spectrum of $\hat{H}_\xi$ in the gap Δ consists of isolated eigenvalues which are non-degenerate by Theorem 1 we can use perturbation theory to find a neighbourhood $(\xi - \epsilon, \xi + \epsilon)$ and a differentiable function $\xi \mapsto \mu(\xi)$ on this neighbourhood which is uniquely defined by the property that $\mu(\xi) \in D_\xi(\Delta)$. In fact, level-crossing of right Dirichlet values cannot occur in gaps, since it would lead to degeneracies. As in [Ke04] we see that its first derivative is strictly negative:

$$\frac{d\mu(\xi)}{d\xi} = \int_{-\infty}^0 dx |\Psi_\xi(x)|^2 V'_\xi = -|\Psi'_\xi(0)|^2 < 0.$$

Here Ψ_ξ is a normalised eigenfunction of $\hat{H}_\xi$. Thus around each value ξ for which we find a right Dirichlet value in Δ we have locally defined curves $\mu(\xi)$ which are strictly monotonically decreasing and non-intersecting. Since $\{H_\xi\}_\xi$ is a norm-continuous family, the spectra $\sigma(H_\xi)$ are continuous in ξ (w.r.t. Hausdorff topology) so that the curves $\mu(\xi)$ can be continued until they reach the boundary of Δ or their limit at $+\infty$ or $-\infty$, if it exists.

Let K be the circle of complex numbers of modulus 1. We define the function $\tilde{\mu} : \mathbb{R} \to K$ by

$$\tilde{\mu}(\xi) = \exp 2\pi i \sum_{\mu \in D_\xi} \frac{\mu - E_0}{|\Delta|}$$

where $E_0 = \inf \Delta$ and $|\Delta|$ is the width of Δ. Then $\tilde{\mu}$ is a continuous function which is differentiable at all points where none of the curves $\mu(\xi)$ touches the boundary.

Definition 2 *The Dirichlet rotation number is*

$$\beta_\Lambda(H, \Delta) := -\mathrm{rot}_\Lambda(\frac{\arg \tilde{\mu}}{2\pi}) \ .$$

Lemma 2 *If, for some $\mu \in \Delta$, $|S(\mu)| > 1$ then Δ contains at most one right Dirichlet value of H_ξ.*

Proof: We first remark that the same discussion can be performed for the left Dirichlet values of H_ξ, namely values E for which exist Ψ solving $(H_\xi - E)\Psi = 0$ with $\Psi(0) = \Psi(+\infty) = 0$. These similarily define locally curves $\mu^*(\xi)$ whose first derivative are now strictly positive. They can't intersect with any of the curves $\mu(\xi)$, because a right Dirichlet value which is at the same time a left Dirichlet value must be a true eigenvalue of H. Let $S^*(\mu)$ and $Z^*(\mu)$ be defined as $S(\mu)$ and $Z(\mu)$ but for left Dirichlet values. We claim that between two points of $S(\mu)$ lies one point of $S^*(\mu)$. This then implies the lemma, because if D_ξ contained two points an elementary geometric consideration would show that the curves defined by right Dirichlet values through these points necessarily have to intersect a curve defined by left Dirichlet values. To prove our claim we consider the analogous statement for $Z(\mu)$ and $Z^*(\mu)$ and let $\Psi_\pm$ be a real solution of $(H_0 - \mu)\Psi = 0$ with $\Psi_\pm(\pm\infty) = 0$. Since μ is not an eigenvalue the Wronskian $[\Psi_+, \Psi_-]$ which is always constant does not vanish. Furthermore, if $\Psi_+(x) = 0$ then $\Psi_-(x) = -[\Psi_+, \Psi_-]/\Psi'_+(x)$. This expression changes sign between two consecutive zeroes of Ψ_+ and hence Ψ_- must have a zero in between. □

Remark 1 Under the hypothesis of the lemma the sum in the definition of $\tilde{\mu}$ contains at most one element. We believe that the result of the lemma is true under all circumstances.

Theorem 3 *$\alpha(H, E) = \beta(H, \Delta)$.*

Proof: By Lemma 1 $\alpha(H, \mu)$ is the Λ-mean of the density of $S(\mu)$. Suppose the hypothesis of the Lemma 2 holds. Then $S(\mu)$ can be identified with the set of intersection points between the constant curve $\xi \mapsto \exp 2\pi i \frac{E - E_0}{|\Delta|}$ and $\tilde{\mu}(\xi)$. Since $\mu'(\xi) < 0$ the Λ-mean of the density of these intersection points is minus the rotation number of $\frac{\arg \tilde{\mu}}{2\pi}$.

Now suppose that $S(\mu)$ contains at most one element. Then $\alpha(H,\mu) = 0$. On the other hand, there can only be finitely many curves defined by right Dirichlet values. Since they intersect the constant curve $\xi \mapsto \exp 2\pi i \frac{\mu - E_0}{|\Delta|}$ only once $\beta_\Lambda(H,\Delta)$ must be 0. $\square$

Remark 1 An even nicer geometric picture arrises if we take into account also the left Dirichlet values of H_ξ for the definition of $\tilde{\mu}$. For this purpose redefine $\tilde{\mu} : \mathbb{R} \to K$ by

$$\tilde{\mu}(\xi) = \exp \pi i \left(\sum_{\mu \in D_\xi} \frac{\mu - E_0}{|\Delta|} - \sum_{\mu \in D_\xi^*} \frac{\mu - E_0}{|\Delta|} \right)$$

where $D_\xi(\Delta)^*$ is the set of left Dirichlet values of H_ξ in Δ. Then $\tilde{\mu}$ is as well a continuous piecewise differentiable function and $\mathrm{rot}_\Lambda(\frac{\arg \tilde{\mu}}{2\pi})$ is the same number as before except that it yields the Λ-mean of the winding per length of the Dirichlet values around a circle which is obtained from two copies of Δ by identification of their boundary points. For periodic systems, this circle can be identified with the homology cycle corresponding to a gap in the complex spectral curve of H [BBEIM] and so $\beta(H,\Delta)$ is the winding number of the Dirichlet values around it. This is similar to Hatsugai's interpretation of the edge Hall conductivity as a winding number (see [Ha93]). There the role of the parameter ξ is played by the magnetic flux.

3.3 Odd K-gap labels and Dirichlet rotation numbers

We define another type of gap label which is formulated using operators traces and derivations instead of curves on topological spaces. It has its origin in an odd pairing between K-theory and cyclic cohomology.

We fix a gap Δ in the spectrum of H of length $|\Delta|$ and set $E_0 = \inf(\Delta)$. Let $P_\Delta = P_\Delta(\hat{H}_\xi)$ be the spectral projection of $\hat{H}_\xi$ onto the energy interval Δ. Then

$$\mathcal{U}_\xi := P_\Delta e^{2i\pi \frac{\hat{H}_\xi - E_0}{|\Delta|}} + 1 - P_\Delta$$

acts essentially as the unitary of time evolution by time $\frac{1}{|\Delta|}$ on the eigenfunctions of $\hat{H}_\xi$ in Δ. These eigenfunctions are all localised near the edge and therefore is the following expression a boundary quantity.

Definition 3 *The odd K-gap label is*

$$\Pi_\Lambda(H,\Delta) = -\lim_{n\to\infty} \frac{1}{2i\pi|b_n - a_n|} \int_{a_n}^{b_n} \mathrm{Tr}[(\mathcal{U}_\xi^* - 1)\partial_\xi \mathcal{U}_\xi] d\xi$$

Where Tr *is the standard operator trace on $L^2(\mathbb{R})$.*

Theorem 4 $\Pi_\Lambda(H,\Delta) = \beta_\Lambda(H,\Delta)$.

Proof: Note that the rank of P_Δ is equal to $|D_\xi(\Delta)|$, the number of elements in $D_\xi(\Delta)$. Let us first suppose that this is either 1 or 0 which would be implied under the conditions of Lemma 2. Since $\mathcal{U}_\xi^* - 1 = P_\Delta(e^{2i\pi\frac{\hat{H}_\xi - E_0}{|\Delta|}} - 1)$ we can express the trace using the normalised eigenfunctions Ψ_ξ of $\hat{H}_\xi$ to $\mu(\xi)$, provided $|D_\xi(\Delta)| = 1$,

$$\mathrm{Tr}[(\mathcal{U}_\xi^* - 1)\partial_\xi \mathcal{U}_\xi] = \langle \Psi_\xi | \mathcal{U}_\xi^* - 1 | \Psi_\xi \rangle \langle \Psi_\xi | \partial_\xi \mathcal{U}_\xi | \Psi_\xi \rangle. \tag{4}$$

Substituting

$$\langle \Psi_\xi | \partial_\xi \mathcal{U}_\xi | \Psi_\xi \rangle = \partial_\xi \langle \Psi_\xi | \mathcal{U}_\xi | \Psi_\xi \rangle = \partial_\xi e^{2i\pi\frac{\mu(\xi)-E_0}{|\Delta|}}$$

in the previous expression we arrive at

$$\mathrm{Tr}[(\mathcal{U}_\xi^* - 1)\partial_\xi \mathcal{U}_\xi] = (e^{-2i\pi\frac{\mu(\xi)-E_0}{|\Delta|}} - 1)\partial_\xi e^{2i\pi\frac{\mu(\xi)-E_0}{|\Delta|}}.$$

Since $\mathcal{U}_\xi^* - 1 = 0$ if $D_\xi(\Delta) = \emptyset$ we have

$$\Pi_\Lambda(H,\Delta) = -\lim_{n\to\infty} \frac{1}{2i\pi|b_n - a_n|} \int_{a_n}^{b_n} (\overline{\tilde{\mu}(\xi)} - 1)\tilde{\mu}'(\xi)d\xi = -\frac{1}{2i\pi}\Lambda(\overline{\tilde{\mu}}\tilde{\mu}') \tag{5}$$

which is the expression for $\beta_\Lambda(H,\Delta)$.

If $|D_\xi| > 1$ one has to replace the r.h.s. of (4) by a sum over eigenfunctions of $\hat{H}_\xi$ and the calculation will be similar. □

3.4 Interpretation as boundary force per unit energy

We assume for simplicity $|D_\xi| \le 1$. Then we obtain from (5)

$$\Pi_\Lambda(H,\Delta) = -\lim_{n\to\infty} \frac{1}{|b_n - a_n|} \int_{a_n}^{b_n} \mu'(\xi)\frac{|D_\xi(\Delta)|}{|\Delta|}d\xi\ .$$

The r.h.s. is $\frac{1}{|\Delta|}$ times the Λ-mean of the expectation value of the gradient force w.r.t. the density matrix associated with the egde states in the gap. Since translating $\hat{H}_\xi$ in ξ is unitarily equivalent to translating the position of the boundary, Π can be seen as the force per unit energy the edge states in the gap of the system exhibit on the boundary [Kel].

4 Hulls and ergodic theorems

We have seen that, under the assumption that the limits exist, $\alpha_\Lambda = \mathrm{IDS}_\Lambda$ and $\alpha_\Lambda(H,E) = \Pi_\Lambda(H,\Delta)$ for $E \in \Delta$, a gap in the spectrum of H. In this section we present some known results which guarantee the existence of the limit and show its independence of the sequence Λ. This is achieved by viewing the potential as an element of the topological space underlying a $\mathbb{R}$-dynamical system with invariant ergodic probability measure so that the result follows from an ergodic theorem. A second aim of the construction is perhaps more important. It allows for a K-theoretic description of the odd and even K-gap labels (justifying the terminology) and is the natural framework to prove their equality in any dimension.

Given a potential V consider its hull

$$\Omega = \overline{\{V_\xi | \xi \in \mathbb{R}\}} ,$$

which is a compactification of the set of translates of V in the sense of [Jo86, Be92]. The action of $\mathbb{R}$ by translation of the potential extends to an action on Ω by homeomorphisms which we denote by $\omega \mapsto x \cdot \omega$. The elements of Ω may be identified with those real functions (potentials) which may be obtained as limits of sequences of translates of V. We will write V_ω for the potential corresponding to $\omega \in \Omega$. If ω_0 is the point of Ω corresponding to V then $V_\xi = V_{-\xi \cdot \omega_0}$. Then $V_{y\cdot\omega}(x) = V_\omega(x-y)$ and the family of Hamiltonians $H_\omega = -\partial^2 + V_\omega$ is covariant in the sense that $H_{x\cdot\omega} = U(x) H_\omega U^*(x)$ were $U(x)$ is the operator of translation by x. The bulk spectrum is by definition the union of their spectra.

The assumption of the following theorem, namely that Ω carries an $\mathbb{R}$-invariant ergodic probability measure, can be verified for many situations and related to thermodynamical considerations [BHZ00].

Theorem 5 *Suppose that* $(\Omega, \mathbb{R})$ *carries an invariant ergodic probability measure* $\mathbf{P}$. *Let* Δ *be a gap in the bulk spectrum and* $E \in \Delta$. *Then almost surely (w.r.t. this measure) the limits to define* $\alpha_\Lambda(H_\omega, E)$ *and* $\Pi_\Lambda(H_\omega, \Delta)$ *exist and are independent of* Λ *and* $\omega \in \Omega$. *The almost sure value of* Π_Λ *is the* $\mathbf{P}$*-average*

$$\Pi(\Delta) = \frac{1}{2i\pi} \int_\Omega d\mathbf{P}(\omega) \mathrm{Tr}((U_\omega^* - 1)\delta^\perp U_\omega)$$

where $(\delta^\perp f)(\omega) = \left.\frac{df(t\cdot\omega)}{dt}\right|_{t=0}$.

Proof: The crucial input is Birkhoff's ergodic theorem which allows to replace

$$\lim_{n\to\infty} \frac{1}{|\Lambda_n|} \int_{\Lambda_n} F(x\cdot\omega) dx = \int_\Omega d\mathbf{P} F(\omega)$$

for almost all ω and any $F \in L^1(\Omega, \mathbf{P})$. The corresponding construction for the rotation number α has been carried out in [JM82] for almost periodic potentials and for the more general set up in [Jo86, Be92]. For Π_Λ the relevant function is $F(\omega) = \mathrm{Tr}((\mathcal{U}_\omega^* - 1)\delta^\perp \mathcal{U}_\omega)$ which leads to the expression of the almost sure value of Π_Λ. □

5 K-theoretic interpretation

The dynamical system $(\Omega, \mathbb{R})$ does not depend on the details of V, but only on its spatial structure (or what may be called its long range order). In fact, for systems whose atomic positions are described by Delone sets there are methods to construct the hull directly from this set, c.f. [BHZ00, FHK02]. The detailled form of the potential is rather encoded in a continuous function $v : \Omega \to \mathbb{R}$ so that $V_\omega(x) = v(-x \cdot \omega)$ is the potential corresponding to ω. $C(\Omega)$ is thus the algebra of continuous potentials for a given spatial structure.

If one combines this algebra with the Weyl-algebra of rapidly decreasing functions of momentum operators one obtains the observable algebra which is in the continuous category the C^*-crossed product $C(\Omega) \rtimes_\varphi \mathbb{R}$. It is the C^*-closure of the convolution algebra of functions $f : \mathbb{R} \to C(\Omega)$ with product $f_1 f_2(x) = \int_\mathbb{R} dy f_1(y) \varphi_y f_2(x-y)$ and involution $f^*(x) = \varphi_x \overline{f(-x)}$, where $\varphi_y(f)(\omega) = f(y \cdot \omega)$. It has a faithful family of representations $\{\pi_\omega\}_{\omega \in \Omega}$ on $L^2(\mathbb{R})$ by integral operators,

$$\langle x|\pi_\omega(f)|y\rangle = f(y-x)(-x \cdot \omega).$$

It has the following important property. For each continuous function $F : \mathbb{R} \to \mathbb{C}$ vanishing at 0 and ∞ there exists an element $\tilde{F} \in C(\Omega) \rtimes_\varphi \mathbb{R}$ such that $F(H_\omega) = \pi_\omega(\tilde{F})$. Some of the topological properties of the family of Schrödinger operators $\{H_\omega\}_{\omega\in\Omega}$ are therefore captured by the topology of the C^*-algebra. The invariant measure $\mathbf{P}$ over Ω gives rise to a trace $\mathcal{T} : C(\Omega) \rtimes_\varphi \mathbb{R} \to \mathbb{C}$, $\mathcal{T}(f) = \int_\Omega d\mathbf{P} f(0)$.

Theorem 6 ([Be92]) *Let E be in a gap of the bulk spectrum and suppose that the potential is smooth. The almost sure value of* $\mathrm{IDS}_\Lambda(H,E)$ *is* $\mathrm{IDS}(E) := \mathcal{T}(\tilde{P}_E)$.

We mention that this result is more subtle then just an application of Birkhoff's theorem and interpretating the result in C^*-algebraic terms as it needs a Shubin type argument which holds for smooth potentials, namely

$$\lim_{n\to\infty} \frac{1}{|\Lambda_n|}(\mathrm{Tr}(P_E(H_{\Lambda_n}) - \mathrm{Tr}(\chi_{\Lambda_n} P_E(H))) = 0.$$

The element $\tilde{P}_E$ is a projection. As any trace on a C^*-algebra, $\mathcal{T}$ depends only on the homotopy class of $\tilde{P}_E$ in the set of projections of $C(\Omega) \rtimes_\varphi \mathbb{R}$. The even K-group $K_0(C(\Omega \rtimes_\varphi \mathbb{R})$ is constructed from homotopy classes of projections and the map on projections $P \mapsto \mathcal{T}(P)$ induces a functional on this group, or stated differently, the elements of the K_0-group pair with $\mathcal{T}$. It is therefore that we refer to $\mathcal{T}(\tilde{P}_E)$ as an even K-gap label of the gap.

There is a similar identification of the odd gap label as the result of a functional applied to the odd K-group of a C^*-algebra. This C^*-algebra is the C^*-algebra of observables on the half space near 0, the position of the boundary. It turns out convenient to consider also the cases in which the boundary is at $s \neq 0$. We therefore consider the space $\Omega \times \mathbb{R}$ with product topology. This topological space, whose second component denotes the position of the boundary, carries an action of $\mathbb{R}$ by translation of the potential and the boundary (so that their relative position remains the same). The relevant C^*-algebra is then the crossed product (constructed as above) $C_0(\Omega\times\mathbb{R}) \rtimes_{\tilde{\varphi}} \mathbb{R}$ with $\tilde{\varphi}_y(f)(\omega, s) = f(y\cdot\omega, s+y)$. It has a family of representations $\{\pi_{\omega,s}\}_{\omega\in\Omega, s\in\mathbb{R}}$ on $L^2(\mathbb{R})$ by integral operators,

$$\langle x|\pi_{\omega,s}(f)|y\rangle = f(y-x)(-x \cdot \omega, s-x).$$

It has the following important property. For each continuous function $F : \mathbb{R} \to \mathbb{C}$ vanishing at 0 and ∞ and such that $F(H_\omega) = 0$ for all ω there exists an element $\hat{F} \in C_0(\Omega \times \mathbb{R}) \rtimes_{\tilde{\varphi}} \mathbb{R}$ such that $F(H_{\omega,s}) = \pi_{\omega,s}(\hat{F})$ where $H_{\omega,s}$ is the restriction of H_ω to $\mathbb{R}^{\leq s}$ with Dirichlet boundary conditions at s.

The product measure of $\mathbf{P}$ with the Lebesgue measure is an $\mathbb{R}$-invariant measure on $\Omega \times \mathbb{R}$ and defines a trace $\hat{\mathcal{T}}(f) = \int_\Omega \int_\mathbb{R} d\mathbf{P} ds f(0)$.

Theorem 7 ([Kel]) *The almost sure value of* $\Pi(\Delta)$ *is*

$$\Pi_\Lambda(H,\Delta) = \Pi(\Delta) := \frac{1}{2i\pi}\hat{\mathcal{T}}(\widehat{\mathcal{U}^* - 1}\delta^\perp \widehat{\mathcal{U} - 1}).$$

The expression of the theorem depends only on the homotopy class of $\widehat{\mathcal{U} - 1} + 1$ in the set of unitaries of (the unitization of) $C_0(\Omega \times \mathbb{R}) \rtimes_{\tilde{\varphi}} \mathbb{R}$. The odd K-group $K_1(C_0(\Omega \times \mathbb{R}) \rtimes_{\tilde{\varphi}} \mathbb{R})$ is constructed from homotopy classes of unitaries and the map on unitaries $U \mapsto \hat{\mathcal{T}}((U^* - 1)\delta^\perp U)$ induces a functional on this group. It is therefore that we refer to $\frac{1}{2i\pi}\hat{\mathcal{T}}(\widehat{\mathcal{U}^* - 1}\delta^\perp \widehat{\mathcal{U} - 1})$ as an odd gap label of the gap.

The proof of the following theorem is based on the topology of the above C^*-algebras.

Theorem 8 ([Kel]) $\mathcal{T}(\tilde{P}_E) = \frac{1}{2i\pi}\hat{\mathcal{T}}(\widehat{\mathcal{U}^* - 1}\delta^\perp \widehat{\mathcal{U} - 1})$. *In other words,* $\mathrm{IDS}(E) = \Pi(\Delta)$.

6 Conclusion and final remarks

We have discussed four quantities which serve as gap-labels for one-dimensional Schrödinger operators. They are all equal but their definition relies on different concepts. The Johnson-Moser rotation number α measures the mean oscillation of a single solution. The Dirichlet rotation number β counts the mean winding of the eigenvalues of the halfsided operators around a circle compactification of the gap. Π and IDS are operator algebraic expressions with concrete physical interpretations, the boundary force per energy and the integrated density of states. Whereas the identities $\alpha = \beta = \Pi$ are rather elementary, their identity with IDS is based on a fundamental theorem, the Sturm-Liouville theorem. We tend to think therefore of Π as the natural operator algebraic formulation of the Johnson-Moser rotation number and of Theorem 8 as an operator analog of the Sturm-Liouville theorem. The advantage is that Π, IDS and Theorem 8 generalise naturally to higher dimensions [Kel]. In fact, the expression for IDS is the same as in (3) if one uses Følner sequences $\{\Lambda_n\}_n$ for $\mathbb{R}^d$. The expression of Π_Λ in $\mathbb{R}^d$ requires a choice of a $d-1$-dimensional subspace, the boundary, and so $\hat{H}_\xi$ is the restriction of the Schrödinger operator $H_\xi = -\Sigma_j \partial_j^2 + V_\xi$, $V_\xi(x) = V(x + \xi e_d)$, to the half space $\mathbb{R}^{d-1} \times \mathbb{R}^{\leq 0}$ with Dirichlet boundary conditions. Then, for a single operator

$$\Pi_\Lambda = -\lim_{n\to\infty} \frac{1}{|\Sigma_n|(b_n - a_n)} \int_{a_n}^{b_n} \mathrm{Tr}((\mathcal{U}^*_{\xi,\Sigma_n} - 1)\partial_\xi \mathcal{U}_{\xi,\Sigma_n}) d\xi \ ,$$

$$\mathcal{U}_{\xi,\Sigma_n} = P_\Delta(\hat{H}_{\xi,\Sigma_n}) e^{2\pi i \frac{\hat{H}_{\xi,\Sigma_n} - E_0}{|\Delta|}} + 1 - P_\Delta(\hat{H}_{\xi,\Sigma_n}) \ ,$$

Here Σ_n is a Følner sequence for the boundary and $\hat{H}_{\xi,\Sigma_n}$ is the restriction of H_ξ to $\Sigma_n \times \mathbb{R}^{\leq 0}$ with Dirichlet boundary conditions. We do not know of a direct link between this expression and the generalisation proposed by Johnson [Jo91] for odd-dimensional systems.

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