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 generalization of the Johnson–Moser rotation number to higher dimensions.

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1. Introduction

It is an interesting and well-known observation that the boundary of a domain plays a prominent role both in mathematics and in physics. A case that comes immediately to mind is the theory of differential equations where the boundary conditions determine quite a lot of the whole solution. In a purely topological context the boundary may even determine the behaviour of the system in the bulk completely. A case like this was studied in [KS04a, KS04b] where a correspondence between bulk and boundary topological invariants for certain physical systems arising in solid state physics was found. This 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, this C^*-algebra is obtained by considering the Schrödinger operator and its translates describing the one-particle approximation of the solid.

In this paper we consider a simple example, a Schrödinger operator on the real line, where such a correspondence can be established more directly with the help of the Sturm–Liouville theorem. The K_0-theory gap labels (below referred to also as even K-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. In the first part of the paper (sections 2, 3) we provide a direct identification of the

Johnson–Moser rotation number (for energies in gaps) with a boundary invariant, here called the Dirichlet rotation number. This boundary invariant has a physical interpretation, namely as boundary force per unit energy. Moreover, it can be interpreted as a K_1-theory gap label (or odd K-gap label).

In the second part (sections 4, 5) we indicate how the equality between the K_0 and the K_1-theory gap labels also follows from the above-mentioned non-commutative topology of the Wiener–Hopf extension. The advantage of this approach is that, unlike the definition of the geometrical rotation numbers and the Sturm–Liouville theorem, it is not restricted in dimension. We tend to think of the K_1-theory gap label, which is naturally defined in any dimension, as the operator algebraic formulation of the Johnson–Moser rotation number.

Whereas the first part is based on a single operator, although its translates play a fundamental role, we consider in the second part covariant families of operators indexed by the hull of the potential. This is the right framework for the use of ergodic theorems and non-commutative topology. The last section is mainly based on [Kel] and therefore held briefly.

2. Preliminaries

In this paper 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 later on 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 $(H - E)\Psi = 0$, Ψ_+ vanishing at ∞ and Ψ_- vanishing at $-\infty$. 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 also consider the action of H_ξ on $L^2(\mathbb{R}^{\leq 0})$ with Dirichlet boundary conditions at the boundary. If we need to emphasize 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 $n - 1$ zeros 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

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

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

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

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 $\Psi' + \mathrm{i}\Psi : \mathbb{R} \to \mathbb{C}$ is nowhere vanishing and

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

(Our normalization 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 zeros of the above solution Ψ in $[a, b]$ then $\alpha_\Lambda(H, E)$ is the Λ-mean of the density of zeros 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

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

provided the limit exists. Here $|\Lambda_n| = b_n - a_n$ is the volume of Λ_n, H_{Λ_n} is 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 $\mathrm{Tr}\big(P_E(H_{\Lambda_n})\big)$ is the number of eigenfunctions of H_{Λ_n} to eigenvalue smaller or equal E theorem 2 implies

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

In particular, like the integrated density of states $\alpha_\Lambda(H, E)$ is monotonically 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 one-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.

We choose a gap Δ in $\sigma(H)$ for this section and define the set of right Dirichlet values in Δ

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

With respect to this choice of gap define

$$S(\mu) := \{\eta \mid \mu \in D_\eta(\Delta)\}.$$

Suppose $\mu \in D_\xi(\Delta)$ for some ξ (in particular, $D_\xi(\Delta) \neq \emptyset$). Then there exists a non-zero solution $(H_\xi - \mu)\Psi = 0$ satisfying $\Psi(0) = \Psi(-\infty) = 0$. Let

$$Z(\mu, \xi) := \{x \mid \Psi(x - \xi) = 0\}.$$

This set depends actually only on μ, since Ψ is unique up to a multiplicative factor and we have

Lemma 1. Let $\xi \in \mathbb{R}$ such that $D_\xi(\Delta) \neq \emptyset$ and $\mu \in D_\xi(\Delta)$. Then $S(\mu) = Z(\mu, \xi)$.

Proof. Let Ψ be a non-zero solution $(H_\xi - \mu)\Psi = 0$ satisfying $\Psi(0) = \Psi(-\infty) = 0$ and define $\Psi_\eta(x) = \Psi(x + (\eta - \xi))$. Then $(H_\eta - \mu)\Psi_\eta = 0$ and $\Psi_\eta(-\infty) = 0$ for all η. Hence $Z(\mu, \xi) = \{\eta \mid \Psi(\eta - \xi) = 0\} = \{\eta \mid \Psi_\eta(0) = 0\} \subset S(\mu)$.

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 $\eta \in Z(\mu, \xi)$, thus $S(\mu) \subseteq Z(\mu, \xi)$. $\qquad\square$

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:

$$\frac{\mathrm{d}\mu(\xi)}{\mathrm{d}\xi} = \int_{-\infty}^0 \mathrm{d}x |\Psi_\xi(x)|^2 V_\xi' = -|\Psi_\xi'(0)|^2 < 0.$$

Here Ψ_ξ is a normalized 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 $\hat{H}_\xi$ is norm continuous in ξ in the generalized sense, its spectrum $\sigma(\hat{H}_\xi)$ is lower semi-continuous [K] in ξ 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

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

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*

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

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 similarly define locally curves $\mu^*(\xi)$ whose first derivative is now strictly positive. They cannot 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 value s. 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. $\square$

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. $\alpha_\Lambda(H, E) = \beta_\Lambda(H, \Delta)$.

Proof. By lemma 1 $\alpha_\Lambda(H, \mu)$ is the Λ-mean of the density of $S(\mu)$. Suppose the hypothesis of 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 $\alpha_\Lambda(H, \mu) = 0$. 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 2. An even nicer geometric picture arises 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 $\text{rot}_\Lambda \left(\frac{\arg \tilde{\mu}}{2\pi} \right)$ 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 $\beta_\Lambda(H, \Delta)$ 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

$$\mathcal{U}_\xi := P_\Delta \, \mathrm{e}^{2\mathrm{i}\pi \frac{\hat{H}_\xi - E_0}{|\Delta|}} + 1 - P_\Delta \tag{4}$$

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 localized near the edge and therefore the following expression is a boundary quantity.

Definition 3. *The odd K-gap label is*

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

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 $\mathcal{U}_\xi^* - 1 = P_\Delta\big(\mathrm{e}^{2\mathrm{i}\pi \frac{\hat{H}_\xi - E_0}{|\Delta|}} - 1\big)$ we can express the trace using the normalized eigenfunctions Ψ_ξ of $\hat{H}_\xi$ to $\mu(\xi)$, provided $|D_\xi(\Delta)| = 1$,

$$\mathrm{Tr}[(\mathcal{U}_\xi^* - 1)\partial_\xi \mathcal{U}_\xi] = \langle \Psi_\xi | \mathcal{U}_\xi^* - 1 | \Psi_\xi \rangle \langle \Psi_\xi | \partial_\xi \mathcal{U}_\xi | \Psi_\xi \rangle. \tag{5}$$

Substituting

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

in the previous expression we arrive at

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

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

$$\Pi_\Lambda(H, \Delta) = -\lim_{n \to \infty} \frac{1}{2\mathrm{i}\pi \, |b_n - a_n|} \int_{a_n}^{b_n} (\overline{\tilde{\mu}(\xi)} - 1)\tilde{\mu}'(\xi) \, \mathrm{d}\xi = -\frac{1}{2\mathrm{i}\pi} \Lambda(\overline{\tilde{\mu}} \tilde{\mu}') \tag{6}$$

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

If $|D_\xi| > 1$ one has to replace the rhs of (5) by a sum over eigenfunctions of $\hat{H}_\xi$ and the calculation will be similar. $\qquad \square$

3.4. Interpretation as boundary force per unit energy

We assume for simplicity $|D_\xi| \leqslant 1$. Then we obtain from (6)

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

The rhs 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 edge 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

So far we have worked with a single potential and its translates. When completed w.r.t. a natural metric topology this set of translates yields a topological space, called the hull of the potential. As it has become apparent in recent years, many topological invariants of the physical system depend mainly on the topology of this hull with its $\mathbb{R}$ action by translation of the potential. Besides, the use of invariant ergodic probability measures on the hull allows us to tackle the problem of existence of the Λ-means in a probabilistic sense. It is therefore most natural to interpret the results of the last section in the framework of $\mathbb{R}$-actions on hulls. This allows for a generalization to higher dimensional systems, to which the theorems of section 2 do not extend.

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 $V_\xi = V_{-\xi \cdot \omega_0}$. Also $V_{y \cdot \omega}(x) = V_\omega(x - y)$ and so 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, see [BHZ00] for considerations relating it to the Gibbs measure.

Theorem 5. *Suppose that $(\Omega, \mathbb{R})$ carries an invariant ergodic probability measure* **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* **P**-*average*

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

where $(\delta^\perp f)(\omega) = \frac{df(t \cdot \omega)}{dt}\big|_{t=0}$ and $\mathcal{U}_\omega$ is defined as in (4) with $\hat{H}_\omega$ in place of $\hat{H}_\xi$.

Proof. The crucial input is Birkhoff's ergodic theorem which allows us 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. $\qquad\square$

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 for constructing the hull directly from this set, cf [BHZ00, FHK02]. The detailed 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 algebra continuous observables which is 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 of $\{H_\omega\}_{\omega \in \Omega}$ so that in particular there exists a projection $\tilde{P}_E \in C(\Omega) \rtimes_\varphi \mathbb{R}$ such that $\pi_\omega(\tilde{P}_E) = P_E(H_\omega)$ is the projection onto the spectral subspace of H_ω to energies below the gap. Suppose that the potential which gave rise to the hull Ω is smooth. Then 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

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

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 (or K_0-theory gap label) of the gap. This is the K_0-theoretical gap labelling of [BLT85, Be92].

There is a similar identification of the odd K-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 $\mathbb{R}^{\leqslant s}$ with Dirichlet boundary conditions at s. Let $\mathcal{U} = \{\mathcal{U}_{\omega,s}\}$,

$$\mathcal{U}_{\omega,s} := P_\Delta \, e^{2i\pi \frac{H_{\omega,s} - E_0}{|\Delta|}} + 1 - P_\Delta, \tag{7}$$

similar to (4). 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 $\hat{T}(f) = \int_\Omega \int_\mathbb{R} d\mathbf{P} \, ds \, f(0)$.

Theorem 7 ([Kel]). *Let Δ be a gap in the bulk spectrum of $\{H_\omega\}_{\omega \in \Omega}$. The almost sure value of $\Pi(\Delta)$ is*

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

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 $U \mapsto \hat{T}((U^* - 1)\delta^\perp U)$ induces a functional on this group. It is therefore that we refer to $\frac{1}{2i\pi} \hat{T}(\widehat{\mathcal{U}^* - 1} \delta^\perp \widehat{\mathcal{U} - 1})$ as an odd K-gap label of the gap.

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

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

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 half sided 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 analogue of the Sturm–Liouville theorem. The advantage is that Π, IDS and theorem 8 generalize naturally to higher dimensions [Kel]. In fact, the expression for IDS is the same as in (3) if one uses Føllner 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 $\mathbb{R}^{d-1} \times \mathbb{R}^{\leqslant 0}$ with Dirichlet boundary conditions. Then

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

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

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

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