The topological meaning of Levinson's theorem, half-bound states included

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We propose to interpret Levinson's theorem as an index theorem. This exhibits its topological nature. It furthermore leads to a more coherent explanation of the corrections due to resonances at thresholds.

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I. INTRODUCTION

Levinson's theorem is a relation between the number of bound states of a system and an expression related to the scattering part of that system. The latter expression can be written either in terms of an integral over the time delay, or as an evaluation of the spectral shift function (see the review papers [1, 2]). In the simplest situations, the relation is an equality, but that is not always the case. Depending on the space dimension and on the existence of resonances at thresholds, also called half-bound states, corrections to the former equality have to be taken into account.

We propose here a topological approach to this theorem by interpreting it as an index theorem. This does not only shed new light on it, but it provides also a more coherent and natural way to take the corrections into account. It is inspired by Bellissard's approach to topological phenomena in solid states physics [3] and was first proposed for simpler models in [4]. The proof relies on the use of boundary maps between the topological invariants of the bound part and of the continuous part of the system. It puts emphasis on the wave operators.

The content of this Letter is the following: First we recall a common form of Levinson's theorem written in terms of the time delay. In Sections III and IV, we expose our topological approach and introduce the framework suitable for Schrödinger operators on $\mathbb{R}^n$. In the last section, we illustrate our ideas with systems on $\mathbb{R}$.

II. A COMMON FORM OF LEVINSON'S THEOREM

We consider a quantum mechanical system described by a Hamiltonian H in a Hilbert space $\mathcal{H}$. The spectrum $\sigma(H)$ of H is composed of eigenvalues and of a continuous part. The eigenfunctions of H span a subspace $\mathcal{H}_p$ of $\mathcal{H}$, and the projection onto $\mathcal{H}_p$ is denoted by P_p.

The continuous part of the system can generally be described by scattering theory, that is, by comparison of the dynamics generated by H with the dynamics gener-

ated by a simpler Hamiltonian H_0. The latter operator is assumed to be absolutely continuous. We also assume that the following strong limits exist:

$$\Omega_\pm = \mathrm{s}-\lim_{t\to\pm\infty} e^{itH}e^{-itH_0}\ ,$$

and that the so-defined wave operators are asymptotically complete. It follows that the scattering operator $S = \Omega_+^*\Omega_-$ is unitary and that the isometry $\Omega := \Omega_-$ has support and range projections

$$\Omega^*\Omega = 1, \qquad \Omega\Omega^* = 1 - P_p\ . \tag{1}$$

Furthermore, since S commutes with H_0, it is unitarily equivalent to an operator-valued function $\sigma(H_0) \ni \lambda \mapsto S(\lambda) \in \mathcal{B}(\mathcal{H}_\lambda)$ resulting from the direct integral decomposition of $\mathcal{H} = \int_{\sigma(H_0)} \mathcal{H}_\lambda \mathrm{d}\lambda$ with respect to H_0. The operator $S(\lambda)$ is referred to as the S-matrix at energy λ, and $iS^*(\lambda)S'(\lambda)$ as the time delay operator at energy λ. Then, a common form of Levinson's theorem is:

$$\frac{1}{2\pi}\int_{\sigma(H_0)} \left(\mathrm{tr}_\lambda[iS^*(\lambda)S'(\lambda)]-c(\lambda)\right)\mathrm{d}\lambda = \mathrm{Tr}(P_p)+\nu\ . \tag{2}$$

Here tr_λ is the operator trace on $\mathcal{H}_\lambda$ and Tr is the operator trace on $\mathcal{H}$. In particular $\mathrm{Tr}(P_p)$ counts the number of bound states. The regularizing term $c(\lambda)$ is necessary if the map $\lambda \mapsto \mathrm{tr}_\lambda[iS^*(\lambda)S'(\lambda)]$ is not integrable. The correction term ν arises from the existence of resonances at thresholds in the spectrum of H. The explanation for the presence of ν in (2) is sometimes quite ad hoc.

For example, for Schrödinger operators on $\mathbb{R}^n$, the correction depends on the existence of 0-energy resonances and on the dimension n. 0-energy resonances are solutions of the equation $H\Psi = 0$ with Ψ not in $L^2(\mathbb{R}^n)$ but in some suitable larger space. If $n = 3$ and if such a 0-energy resonance exists, the correction ν is equal to $1/2$. In other dimensions the picture is different.

III. TOPOLOGICAL APPROACH

In this section, we show how to rewrite (2) as an index theorem. Our approach is based on the following construction: Let $\mathcal{E}$ be a closed unital subalgebra of $\mathcal{B}(\mathcal{H})$

containing an ideal $\mathcal{J}$. Let us assume that (i) Ω belongs to $\mathcal{E}$, (ii) the image of Ω through the quotient map $q : \mathcal{E} \to \mathcal{E}/\mathcal{J}$ is a unitary operator incorporating S. We shall see that in the simplest situation, $q(\Omega) = S$, but that in the general case, $q(\Omega)$ incorporates besides S other components which account for the correction in (2).

Before explaining how to construct $\mathcal{E}$ we demonstrate how these assumptions lead to a topological version of Levinson's theorem. We think of $\mathcal{J}$ as the algebra related to the bound states system, and of $\mathcal{E}/\mathcal{J}$ as the one corresponding to the scattering system. By the general machinery of K-theory of C^*-algebras the map q gives rise to a topological boundary map, called the index map, $\mathrm{ind} : K_1(\mathcal{E}/\mathcal{J}) \to K_0(\mathcal{J})$ which can be described as follows: If $u \in \mathcal{E}/\mathcal{J}$ is a unitary representing an element $[u]_1$ in $K_1(\mathcal{E}/\mathcal{J})$ and having a preimage $\omega \in \mathcal{E}$ under q which is an isometry, then $\mathrm{ind}([u]_1) = [\omega\omega^*]_0 - [\omega^*\omega]_0$, the difference of the classes in $K_0(\mathcal{J})$ of the range and the support projections of ω. Thus if Ω belongs to $\mathcal{E}$, the relation (1) yields

$$\mathrm{ind}([q(\Omega)]_1) = -[P_p]_0 . \qquad (3)$$

This result is our abstract Levinson's theorem. In the simplest situation, this relation reads $\mathrm{ind}([S]_1) = -[P_p]_0$, but in the general case the corrections arise from the difference between $[q(\Omega)]_1$ and $[S]_1$. Concrete Levinson theorems as (2) arise if we apply functionals to the K-groups to obtain numbers.

For a large class of scattering systems including potential scattering we expect that $\mathcal{J} = \mathcal{K}(\mathcal{H})$, where $\mathcal{K}(\mathcal{H})$ is the algebra of compact operators on $\mathcal{H}$, and that $\mathcal{E}/\mathcal{J}$ is isomorphic to $C(S^1, \mathcal{K}(\mathcal{H}_\lambda))$, the continuous functions on the circle with values in $\mathcal{K}(\mathcal{H}_\lambda)$. In that case $K_0(\mathcal{J})$ and $K_1(\mathcal{E}/\mathcal{J})$ are both isomorphic to $\mathbb{Z}$ so that, up to a normalization, the only functional on $K_0(\mathcal{J})$ is given by the trace $\mathrm{Tr} : [p]_0 \mapsto \mathrm{Tr}(p)$, and the only functional on $K_1(\mathcal{E}/\mathcal{J})$ is given by $w : [u]_1 \mapsto w(u)$, the winding number of $t \mapsto \det\big((u(t))\big)$, the determinant possibly needing regularization. In particular (3) reduces to the index theorem of Krein-Gohberg

$$w(q(\Omega)) = \mathrm{index}(\Omega) = -\mathrm{Tr}(P_p) . \qquad (4)$$

This is our formulation of the concrete Levinson's theorem (2). Note that there is room for further, potentially unknown, identities of Levinson type by choosing other functionals in cases in which the K-groups are richer than the one considered above.

IV. CONSTRUCTING THE ALGEBRAS

We do not expect that there is a universal construction of the algebra $\mathcal{E}$ and its ideal $\mathcal{J}$, rather to the contrary, we believe that part of the richness of the theory lies in the flexibility of their choice. But for simple scattering systems, i.e. when H_0 is the free Laplacian $-\Delta$ on $\mathbb{R}^n$,

we construct $\mathcal{E}$ with the help of the conjugate operator to H_0, namely the generator A of dilations. In $\mathcal{H} = L^2(\mathbb{R}^n)$, the operators H_0 and A have a purely absolutely continuous spectrum equal to $\mathbb{R}_+$ and $\mathbb{R}$, respectively.

Let $\mathcal{E}'$ be the closure in $\mathcal{B}(\mathcal{H})$ of the algebra generated by elements of the form $\eta(A)\psi(H_0)$, where η is a continuous function on $\mathbb{R}$ which converges at $\pm\infty$, and ψ is a continuous function $\mathbb{R}_+$ which converges at 0 and at $+\infty$. Stated differently, $\eta \in C(\overline{\mathbb{R}})$, where $\overline{\mathbb{R}} = [-\infty, +\infty]$ is the two point compactification of $\mathbb{R}$, and by analogy $\psi \in C(\overline{\mathbb{R}_+})$. Let $\mathcal{J}'$ be the norm closed algebra generated by $\eta(A)\psi(H_0)$ with $\eta \in C_0(\mathbb{R})$ and $\psi \in C_0(\mathbb{R}_+)$ i.e. all limits vanish. $\mathcal{J}'$ is clearly an ideal of $\mathcal{E}'$.

To describe the quotient $\mathcal{E}'/\mathcal{J}'$ we consider the square $\square := \overline{\mathbb{R}_+} \times \overline{\mathbb{R}}$ whose boundary $\partial(\square)$ is the union of four parts: $\partial(\square) = B_1 \cup B_2 \cup B_3 \cup B_4$, with $B_1 = \{0\} \times \overline{\mathbb{R}}$, $B_2 = \overline{\mathbb{R}_+} \times \{+\infty\}$, $B_3 = \{+\infty\} \times \overline{\mathbb{R}}$ and $B_4 = \overline{\mathbb{R}_+} \times \{-\infty\}$. We can also identify $C(\partial(\square))$ with the subalgebra of $C(\overline{\mathbb{R}}) \oplus C(\overline{\mathbb{R}_+}) \oplus C(\overline{\mathbb{R}}) \oplus C(\overline{\mathbb{R}_+})$ given by elements $(\Gamma_1, \Gamma_2, \Gamma_3, \Gamma_4)$ which coincide at the corresponding end points, that is, for instance, $\Gamma_1(+\infty) = \Gamma_2(0)$. Then, the quotient map $q' : \mathcal{E}' \to \mathcal{E}'/\mathcal{J}' \cong C(\partial(\square))$, evaluated on elements generating $\mathcal{E}'$, is given by $q'(\eta(A)\psi(H_0)) = (\Gamma_1(A), \Gamma_2(H_0), \Gamma_3(A), \Gamma_4(H_0))$, where $\Gamma_1(A) = \eta(A)\psi(0)$, $\Gamma_2(H_0) = \eta(+\infty)\psi(H_0)$, $\Gamma_3(A) = \eta(A)\psi(+\infty)$ and $\Gamma_4(B) = \eta(-\infty)\psi(H_0)$. Observe that $\mathrm{s}-\lim_{t\to\pm\infty} e^{itB}\eta(A)\psi(H_0)e^{-itB}$, with $B = \frac{1}{2}\ln(H_0)$, are equal to $\Gamma_2(H_0)$ and $\Gamma_4(H_0)$, respectively.

Finally, $\mathcal{E}$ and $\mathcal{J}$ are obtained by adding to the generators of $\mathcal{E}'$ and $\mathcal{J}'$ all compact operators in angular momentum. The unit 1 is also added to $\mathcal{E}$. Since H_0 and A are rotation invariant, such modifications do not perturb the above picture. In particular, $\mathcal{J} = \mathcal{K}(\mathcal{H})$ and $\mathcal{E}/\mathcal{J} \cong C(\partial(\square), \mathbb{C} + \mathcal{K}[L^2(\mathbb{S}^{n-1})])$.

Our basic assumption is that Ω belongs to $\mathcal{E}$. From the above observation, the intertwining relation and the invariance principle, it follows that $\Gamma_2(H_0) = S$ and $\Gamma_4(H_0) = 1$. The winding number $w(q(\Omega))$ is the sum of four terms, each side of the square contributing for one. In regular cases, the winding along B_j contributes with $w_j = \frac{1}{2\pi i} \int_{B_j} \mathrm{tr}[\Gamma_j^* \, \mathrm{d}\Gamma_j]$. Then $w_2 = \frac{1}{2\pi i} \int_0^\infty \mathrm{tr}_\lambda[S^*(\lambda)S'(\lambda)]\mathrm{d}\lambda$ and $w_4 = 0$. Comparing (2) with (4) we see therefore that the correction term arises now on the l.h.s. of the equality from the possible contribution of Γ_1 and Γ_3 to the winding number. If $c(\lambda) \neq 0$ the above formulas have to be regularized.

We finally note that (4) can be refined: if P is a projection in $\mathcal{J}$ which commutes with Ω then $\mathrm{ind}[q(\Omega P)]_1 = -[P_p P]_0$ leading to $w(q(\Omega P)) = \mathrm{index}(\Omega P)$. For example, choosing for P a projection on an angular momentum sector leads to a Levinson's theorem for that sector.

V. ONE DIMENSIONAL SCATTERING

We illustrate our approach with one-dimensional systems described by Schrödinger operators on $\mathcal{H} = L^2(\mathbb{R})$, first with $-\Delta$ perturbed by a one point interaction, and

second with $-\Delta$ perturbed by multiplication operators. In both cases, $\mathcal{H}_\lambda = \mathbb{C}^2$ and $\mathcal{E}/\mathcal{J} \cong C\big(\partial(\square), M_2(\mathbb{C})\big)$. Our aim is to obtain a formula for Ω which shows that it belongs to $\mathcal{E}$, to determine each Γ_j and to show how they contribute to $w(q(\Omega))$. For that purpose, the following observation taken from [5] is essential: Let g be a smooth rapidly decreasing function on $\mathbb{R}$ and T be the operator defined by $[Tg](r\omega) = \frac{1}{\sqrt{2\pi}} \int_0^\infty e^{i\kappa r}\hat{g}(\kappa\omega)\mathrm{d}\kappa$, with $r \geq 0$, $\omega \in \{+1, -1\}$ and $\hat{g}$ the Fourier transform of g. Then T extends to the operator $\frac{1}{2}\big(1 - R\big)$ with

$$R := R(A) = r_e(A)P_e + r_o(A)P_o ,$$

where P_e, P_o are the projections onto the even (symmetric), odd functions of $\mathcal{H}$, respectively, and

$$r_e(x) := -\tanh(\pi x) - i[\cosh(\pi x)]^{-1} , \quad r_o := \overline{r_e} .$$

Clearly, r_e and r_o belong to $C(\overline{\mathbb{R}})$.

A. One dimensional point interactions

Schrödinger operators with one point interaction at the origin can be defined as the family of self-adjoint extensions of the restriction of the Laplacian on a suitable subset of $L^2(\mathbb{R})$ [6]. Different point interactions arise from different extensions and we concentrate here on the two families of point interaction called δ-interaction and δ'-interaction. In these cases the wave operator has the form [5]:

$$\Omega = 1 + \tfrac{1}{2}(1 - R)(S - 1) .$$

Let us stress that the first factor is universal and does not depend on the choice of any self-adjoint extension, only the S-term depends on such a particular choice. We shall see later that a similar form holds for the wave operator in the case of potential scattering. Nevertheless, the contributions to the winding number corresponding to Γ_1 and Γ_3 clearly depend on the different behaviour of the matrix $S(\lambda)$ for $\lambda = 0$ or $\lambda = +\infty$. For example if $S(0) = 1$, then $\Gamma_1 = 1$. More interesting phenomena arise if $P_e S(0) \neq P_e$ or $P_o S(0) \neq P_o$, as exhibited in the following situations.

The family of extensions called δ-interaction is parameterized by $\alpha \in \mathbb{R} \cup \{\infty\}$. The parameter describes the boundary condition of the wave function $\Psi'(0_+) - \Psi'(0_-) = \alpha\Psi(0)$ which can be formally interpreted as arising from a potential $V = \alpha\delta$ where δ is the Dirac δ-function at 0. The extension for $\alpha = 0$ is equal to H_0 and the extension for $\alpha = \infty$ is the Laplacian with a Dirichlet boundary conditions at the origin. These extensions have a single eigenvalue if $\alpha < 0$ and no eigenvalue if $\alpha \in [0, \infty]$. The scattering operator is given by $S = s^\alpha(H_0)P_e + P_o$ with $s^\alpha(\lambda) = \frac{2\sqrt{\lambda} - i\alpha}{2\sqrt{\lambda} + i\alpha}$. Note that $s^\alpha \in C(\overline{\mathbb{R}_+})$ with values at 0 and $+\infty$ depending on α.

The family of extensions referred to as δ'-interaction is parameterized by $\beta \in \mathbb{R} \cup \{\infty\}$, the parameter describing the boundary condition of the wave function $\Psi(0_+) - \Psi(0_-) = \beta\Psi'(0)$. This can be formally interpreted as arising from a potential $V = \beta\delta'$. The extension for $\beta = 0$ is equal to H_0 and the extension $\beta = \infty$ is the Laplacian on $\mathbb{R}$ with Neumann boundary conditions at the origin. These extensions possess a single eigenvalue if $\beta < 0$ and no eigenvalue if $\beta \in [0, \infty]$. The scattering operator is $S = P_e + s^\beta(H_0)P_o$ with $s^\beta(\lambda) = \frac{2 + i\beta\sqrt{\lambda}}{2 - i\beta\sqrt{\lambda}}$. Again $s^\beta \in C(\overline{\mathbb{R}_+})$ with values at 0 and $+\infty$ depending on β.

In all these examples, the wave operator Ω clearly belongs to the algebra $\mathcal{E}$ introduced above. Since Ω commutes with P_e and P_o we obtain a Levinson's theorem for each sector separately. But for δ-interactions $\Omega_o := \Omega P_o = P_o$ and hence the odd sector theorem is trivial. Likewise the even sector theorem is trivial for a δ'-interaction. We present the non-trivial results in the two tables below with the notations $\Gamma_i^{o/e} := \Gamma_i P_{o/e}$ and $w_i^{o/e} := w(\Gamma_i^{o/e})$.

δ-interaction	Γ_1^e	Γ_2^e	Γ_3^e	Γ_4^e	w_1^e	w_2^e	w_3^e	w_4^e	$w(q(\Omega_e))$
$\alpha < 0$	r_e	s^α	1	1	$-\frac{1}{2}$	$-\frac{1}{2}$	0	0	-1
$\alpha = 0$	1	1	1	1	0	0	0	0	0
$\alpha > 0$	r_e	s^α	1	1	$-\frac{1}{2}$	$\frac{1}{2}$	0	0	0
$\alpha = \infty$	r_e	-1	r_e	1	$-\frac{1}{2}$	0	$\frac{1}{2}$	0	0

δ'-interaction	Γ_1^o	Γ_2^o	Γ_3^o	Γ_4^o	w_1^o	w_2^o	w_3^o	w_4^o	$w(q(\Omega_o))$
$\beta < 0$	1	s^β	r_o	1	0	$-\frac{1}{2}$	$-\frac{1}{2}$	0	-1
$\beta = 0$	1	1	1	1	0	0	0	0	0
$\beta > 0$	1	s^β	r_o	1	0	$\frac{1}{2}$	$-\frac{1}{2}$	0	0
$\beta = \infty$	r_o	-1	r_o	1	$\frac{1}{2}$	0	$-\frac{1}{2}$	0	0

We thus see that both, w_1 and w_3 contribute to the correction term ν in (2).

B. One dimensional potential scattering

In this section, we consider Schrödinger operators of the form $H = H_0 + V$, with potential V given by a multiplication operator. If the potential is regular enough and vanishes sufficiently rapidly at infinity, the wave operator Ω can be expressed with the help of the solution Ψ of the Lippmann-Schwinger equation:

$$[\Omega g](x) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \Psi(k, x)\hat{g}(k)\,\mathrm{d}k ,$$

with g as above. The solution has asymptotic behaviour

$$\Psi(k, x) \overset{|x| \to \infty}{\sim} e^{ik \cdot x} + e^{i\kappa r}f(\kappa^2, \omega_k, \omega_x) , \qquad (5)$$

where $k = \kappa\omega_k$, $x = r\omega_x$, and f is the scattering amplitude. Furthermore, the coefficients of the scattering matrix $S(\lambda)$ at energy $\lambda = \kappa^2$ in the momentum representation are given by $1 + f(\kappa^2, \pm 1, \pm 1)$.