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

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Abstract

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.

1 Introduction

Levinson’s theorem is a relation between the number of bound states of a quantum mechanical system and an expression related to the scattering part of that system. The latter 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 [3, 7, 11] and references therein). 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. Different explanations for these corrections can be found in the literature, but they often have the flavor of a case by case study. It has not been realized that Levinson’s theorem is a topological theorem, and this includes the corrections. We propose here a topological explanation 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 [2] and was first proposed for systems without resonances in [10]. The proof relies on evaluating the index of the wave operator by the winding number of an expression involving not only the scattering operator, but also new operators which describe the system at zero energy and at large energy.

The content of this Note is the following: First we recall one of the forms in which Levinson’s theorem can be commonly found in the literature. Then, we expose our topological approach and introduce the framework for potential scattering on $\mathbb{R}^n$. Finally, we illustrate our ideas with one dimensional scattering systems.
2 Levinson’s theorem

We consider a quantum mechanical system described by a Hamiltonian $H$ in a Hilbert space $\mathcal{H}$. The spectrum of $H$ is composed of a discrete part, the bound state energies, and of a continuous part. The projection onto the subspace spanned by the bound states is denoted by $P_p$. The continuous part of the system is commonly described by scattering theory. For example, in stationary scattering theory a system of generalized eigenfunctions of $H$ is constructed by solving the Lippmann-Schwinger equation for outgoing spherical wave asymptotics [12]. The wave operators $\Omega_{\pm}$ can then be defined as the linear operators which map the generalized eigenfunction of $H_0$ to a certain wave-vector to the generalized eigenfunction of $H$ to the same wave-vector. In time-dependent scattering theory, which seems more adapted to our approach, the wave operators are defined by the strong limits

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

and satisfy

$$\Omega_{\pm}^* \Omega_{\pm} = 1, \quad \Omega_{\pm} \Omega_{\pm}^* = 1 - P_p .$$

The scattering operator is given by $S = \Omega_+^* \Omega_-$, which can also be written as $\Omega := \Omega_-$ evolved to time $+\infty$: $S = s - \lim_{t \to +\infty} e^{itH_0} e^{-itH_0}$. Since $S$ commutes with $H_0$, it is unitarily equivalent to an operator-valued function $\lambda \mapsto S(\lambda)$ where $\lambda$ ranges over all values of the spectrum $\sigma(H_0)$ of $H_0$. $S(\lambda)$ is referred to as the $S$-matrix at energy $\lambda$ and $iS^*(\lambda)S'(\lambda)$ as the time delay operator at energy $\lambda$. Levinson’s theorem can then be expressed as

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

Here $S'$ denotes the derivative of $S$ w.r.t. energy, $\text{tr}_\lambda$ is the trace on the generalized eigenspace of $H_0$ to energy $\lambda$, and $\text{Tr}$ is the trace on $\mathcal{H}$. In particular $\text{Tr}(P_p)$ is the number of bound states. The regularizing term $c(\lambda)$ is necessary if the map $\lambda \mapsto \text{tr}_\lambda[iS^*(\lambda)S'(\lambda)]$ is not integrable. The correction term $\nu$ is related to resonances at thresholds in the spectrum of $H$. For example, for $H_0 = -\Delta$, the Laplacian on $\mathbb{R}^n$, and $H = -\Delta + V$, a perturbation by a rapidly vanishing potential, 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 $\Psi$ 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 $\nu$ is equal to $1/2$. In other dimensions the picture is different.

3 Topological approach

In this section, we show how to rewrite (2) as an index theorem. Our approach is based on the construction of a norm-closed algebra $\mathcal{E}$ which sits in between the algebra of compact operators $\mathcal{K}(\mathcal{H})$ and that of bounded operators $\mathcal{B}(\mathcal{H})$ on $\mathcal{H}$: $\mathcal{K}(\mathcal{H}) \subset \mathcal{E} \subset \mathcal{B}(\mathcal{H})$. $\mathcal{K}(\mathcal{H})$ is the norm-closed algebra generated by operators with finite dimensional image. It forms an ideal in $\mathcal{B}(\mathcal{H})$. $F \in \mathcal{B}(\mathcal{H})$ is a Fredholm operator if its kernel and cokernel are finite dimensional. This is the case whenever it is invertible modulo a compact operator, that is, its image $q(F)$ in the quotient algebra $\mathcal{B}(\mathcal{H})/\mathcal{K}(\mathcal{H})$ is invertible. The difference of the dimensions of kernel and cokernel is its index. The index is a topological (even homotopy) invariant, namely it is stable against
perturbations of $F$ along continuous paths of Fredholm operators. By (1) the wave operator $\Omega$ is a Fredholm operator of index $-\text{Tr}(P_p)$.

Suppose $F$ belongs to $\mathcal{E}$ and that $\mathcal{E}/K(\mathcal{H})$ is isomorphic to $C\left(S, K(\mathcal{H}')\right)^\sim$, where $C\left(S, K(\mathcal{H}')\right)$ is the algebra of continuous functions over the circle with values in $K(\mathcal{H}')$, and $\sim$ means that a unit has been added. Here $\mathcal{H}'$ is some possibly finite dimensional separable Hilbert space. Then, viewing $q(F)$ as such a function we can take pointwise its determinant (if needed regularized) to obtain a non-vanishing function over the circle. The winding number of that latter function results in

$$w\left(q(\Omega)\right) = -\text{Tr}(P_p),$$

and we shall see below how the winding number $w\left(q(\Omega)\right)$ is related to the time delay.

We note that (3) can be refined: if $P$ is a projection which commutes with $\Omega$, then restricting the analysis to the Hilbert space $PH$ results in $w\left(q(\Omega P)\right) = -\text{Tr}(P_pP)$. For example, choosing for $P$ a projection on an angular momentum sector leads to a Levinson’s theorem for that sector.

3.1 Potential scattering on $\mathbb{R}^n$

When $H_0 = -\Delta$ in $\mathcal{H} := L^2(\mathbb{R}^n)$, we construct $\mathcal{E}$ with the help of $H_0$ and with the generator $A = -\frac{1}{2}(\nabla \cdot X + X \cdot \nabla)$ of dilations. The crucial property is that $A$ and $B := \frac{1}{2}\ln(H_0)$ satisfy the canonical commutation relation $[A, B] = i$ so that $A$ generates translations in $B$ and vice versa, $e^{itB}Ae^{-itB} = A + t, \quad e^{isA}Be^{-isA} = B - s$. (4)

The spectrum of $H_0$ is $\mathbb{R}_+$ and that of $A$ is $\mathbb{R}$.

Let $\mathcal{E}'$ be the closure in $B(\mathcal{H})$ of the algebra generated by elements of the form $\eta(A)\psi(H_0)$, where $\eta$ is a continuous function on $\mathbb{R}$ which converges at $\pm \infty$, and $\psi$ is a continuous function $\mathbb{R}_+$ which converges at 0 and at $+\infty$. Stated differently, $\eta \in C(\mathbb{R})$, where $\mathbb{R} = [-\infty, +\infty]$, and $\psi \in C(\mathbb{R}_+)$ with $\mathbb{R}_+ = [0, +\infty]$. Let $\mathcal{J}'$ be the norm closed algebra generated by $\eta(A)\psi(H_0)$ with functions $\eta$ and $\psi$ for which the above limits vanish. $\mathcal{J}'$ can be identified with $K(L^2(\mathbb{R}_+))$. It is an ideal of $\mathcal{E}'$.

To describe the quotient $\mathcal{E}'/\mathcal{J}'$ we consider the square $\square := \mathbb{R}_+ \times \mathbb{R}$ whose boundary $\partial \square$ is the union of four parts: $\partial \square = B_1 \cup B_2 \cup B_3 \cup B_4$, with $B_1 = \{0\} \times \mathbb{R}, B_2 = \mathbb{R}_+ \times \{+\infty\}, B_3 = \{+\infty\} \times \mathbb{R}$ and $B_4 = \mathbb{R}_+ \times \{-\infty\}$. We can also view $C(\partial \square)$ as the subalgebra of $C(\mathbb{R}) \oplus C(\mathbb{R}_+) \oplus C(\mathbb{R}) \oplus C(\mathbb{R}_+)$ 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 $\mathcal{E}'/\mathcal{J}'$ is isomorphic to $C(\partial \square)$ and the image $q'(\eta(A)\psi(H_0))$ in $C(\mathbb{R}) \oplus C(\mathbb{R}_+) \oplus C(\mathbb{R}) \oplus C(\mathbb{R}_+)$ is given by $\Gamma_1(A) = \eta(A)\psi(0), \Gamma_2(H_0) = \eta(+\infty)\psi(H_0), \Gamma_3(A) = \eta(A)\psi(+\infty)$ and $\Gamma_4(H_0) = \eta(-\infty)\psi(H_0)$.

The generalized eigenspaces of $H_0$ can be naturally identified with $L^2(S^{n-1})$, the square-integrable functions on the sphere in momentum space, and $\mathcal{H}$ can be written as the tensor product $L^2(\mathbb{R}_+) \otimes L^2(S^{n-1})$. Thus $K(\mathcal{H}) = \mathcal{J}' \otimes K(L^2(S^{n-1}))$. We define $\mathcal{E}$ as the tensor product of $\mathcal{E}'$ with $K(L^2(S^{n-1}))$, and add a unit. As a result, $K(\mathcal{H})$ is an ideal of $\mathcal{E}$ and $\mathcal{E}/K(\mathcal{H}) \cong C(\partial \square, K(L^2(S^{n-1})))^\sim$. Thus, $\mathcal{E}$ is suitable for the index theorem of Krein and Gohberg, and
in fact $E'$ is the Toeplitz extension of $C(S)$. Let us furthermore observe that for any $F \in E$, it follows from (4) that $\Gamma_{2,4} \in C(\mathbb{R}, \mathcal{K}(L^2(S^{n-1})))$ are obtained by $s-\lim_{t \to \pm \infty} e^{itB} F e^{-itB}$.

Our basic assumption is that $\Omega$ belongs to $E$. We will verify it below for one-dimensional systems. From the above observation we get from the intertwining relation and from the invariance principle that $g(\Omega) = (\Gamma_1, \Gamma_2, \Gamma_3, \Gamma_4)$ with $\Gamma_2(H_0) = s-\lim_{t \to \pm \infty} e^{itB} \Omega e^{-itB} = S$ and similarly $\Gamma_4(H_0) = 1$. We will determine below $\Gamma_1(A)$ and $\Gamma_3(A)$.

The winding number $w(g(\Omega))$ is the sum of four terms, each side of the square contributing for one. In regular cases, the winding along $B_j$ contributes with $w_j = \frac{1}{2\pi i} \int_{B_j} \text{tr}[\Gamma_j^{-1} d\Gamma_j]$. Then

$$w_2 = \frac{1}{2\pi i} \int_{0}^{\infty} \text{tr}_\lambda [S^\ast(\lambda)S'(\lambda)] d\lambda$$

and $w_4 = 0$. Comparing (2) with (3) we see therefore that the correction term arises now on the l.h.s. of the equality from the possible contribution of $\Gamma_1$ and $\Gamma_3$ to the winding number.

We believe that the above construction is sufficient to describe scattering for perturbations of $-\Delta$ by a large class of potentials vanishing at infinity. But the algebraic framework is flexible enough to cover all kinds of situations. In fact, there is a very well developed index theory which is based on non-commutative topology and allows for situations in which not only $E$ can be an arbitrary Banach algebra but also $\mathcal{K}(H)$ can be replaced by any ideal of $E$. We expect that these generalisations will lead to new Levinson’s type identities.

4 One dimensional scattering

We illustrate our approach with one-dimensional systems, first for so-called point interactions, and second for ordinary potential scattering. In both cases, the decomposition of $\mathcal{H} = L^2(\mathbb{R})$ into even and odd functions leads to $\mathcal{H}' = \mathbb{C}^2$ and $E/\mathcal{K}(\mathcal{H}) \cong C(\partial\mathbb{C}, M_2(\mathbb{C}))$. Our aim is to obtain a formula for $\Omega$ which shows that it belongs to $E$, to determine each $\Gamma_j$ and to show how they contribute to $w(g(\Omega))$. For that purpose, the following observation taken from [9] is essential: Let $g$ be a smooth rapidly vanishing function on $\mathbb{R}$ and $T$ be the operator defined by $[Tg](r\omega) = \frac{1}{2\pi i} \int_{\partial \mathbb{C}} e^{ix\xi} g(x) dx$, with $r \geq 0$, $\omega \in \{-1, 1\}$ and $\hat{g}$ the Fourier transform of $g$. Then $T = \frac{1}{2}(1 - R)$ with

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

where $P_e$ and $P_o$ are the projections onto the even (symmetric) and odd functions, respectively, and

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

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

4.1 One dimensional point interactions

Here we consider two families of point interactions, the so-called $\delta$-interactions at 0 and the $\delta'$-interactions at 0. They can be described by boundary conditions at 0 for solutions of the free Schrödinger equation on $\mathbb{R}\backslash\{0\}$.

A $\delta$-interaction at 0 can be formally interpreted as arising from a potential $V = \alpha \delta$ ($\delta$-function at 0). The solutions of the Schrödinger equation for a $\delta$-interaction of strength $\alpha \in \mathbb{R}$ at energy $\lambda$ are continuous functions $\Psi$ satisfying $-\Psi'' = \lambda \Psi$ on $\mathbb{R}\backslash\{0\}$ and the boundary condition $\Psi'(0^+) - \Psi'(0^-) = \alpha \Psi(0)$ (this is to be interpreted as $\Psi(0) = 0$ if $\alpha = \infty$). In particular $\alpha = 0$ corresponds to the free Laplacian and $\alpha = \infty$ to the Laplacian on $\mathbb{R}\backslash\{0\}$ with Dirichlet boundary
In this section, we consider $H = -\Delta + V$ with a sufficiently regular potential $V$ given by a multiplication operator. The wave operator $\Omega$ can be expressed with the help of the solutions $\Psi_k$ of the Lippmann-Schwinger equation for all wave vectors $k \in \mathbb{R}$:

$$\left[\Omega g\right](x) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \Psi_k(x) \hat{g}(k) \, dk,$$

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

### 4.2 One dimensional potential scattering

In this section, we consider $H = -\Delta + V$ with a sufficiently regular potential $V$ given by a multiplication operator. The wave operator $\Omega$ can be expressed with the help of the solutions $\Psi_k$ of the Lippmann-Schwinger equation for all wave vectors $k \in \mathbb{R}$:
with \( g \) as above. They have asymptotic behaviour

\[
\Psi_k(x) \xrightarrow{|x| \to \infty} e^{ikx} + e^{i|k||x|} f(k^2, \omega_k, \omega_x),
\]

where \( f \) is the scattering amplitude, \( x = r\omega_x, \ k = |k|\omega_k \) with \( \omega_x, \omega_k \in \{-1, 1\} \). Consider the integral operator

\[
[\hat{\Omega}g](x) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{i|k|r} f(k^2, \omega_k, \omega_x) \tilde{g}(k) \, dk
\]

\[
= \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}^+} e^{i\kappa r} \left[ \sum_{\omega_k = \pm 1} f(k^2, \omega_k, \omega_x) \tilde{g}(\kappa \omega_k) \right] \, d\kappa
\]

\[
= \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}^+} e^{i\kappa r} \left[ (S(\kappa^2) - 1) \tilde{g}(\kappa \omega_x) \right] \, d\kappa
\]

\[
= \left[ \frac{1}{2}(1 - R)(S - 1) \tilde{g} \right](x).
\]

Then, it follows that

\[
\Omega = 1 + \frac{1}{2}(1 - R)(S - 1) + K
\]

with \([Kg](x) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \rho(k, x) \tilde{g}(k) \, dk\) where \( \rho(k, x) \) is the difference between the l.h.s. and the r.h.s. in (5). In particular \( \Omega \) belongs to \( \mathcal{E} \) provided the map \( \lambda \mapsto S(\lambda) \) is continuous and has limits at 0 and \( +\infty \), and \( K \) is a compact operator. Both conditions require assumptions on the potential which go beyond the ones implicitly assumed for the validity of the above approach. Without aiming at the most general case here, we can say that \( \rho \) is square integrable and hence \( K \) compact provided \(|V(x)| \leq C(1 + |x|)^{-\frac{7}{2} - \epsilon} \) for some \( \epsilon > 0 \) and \( C > 0 \). This condition is sufficient to conclude that \( \Omega \) belongs to \( \mathcal{E} \).

We finally explain how the correction term \( \nu \) of (2) arises in our approach. For that purpose we use a basis for \( M_2(\mathbb{C}) \) in which \( R = \begin{pmatrix} r_e & 0 \\ 0 & r_o \end{pmatrix} \). It corresponds to the decomposition of \( L^2(\mathbb{R}) \) into even and odd sectors. The form of \( S(0) \) falls into two cases, characterized by the value of \( \det(S(0)) \). One finds accordingly [1]

\[
S(0) = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \quad \text{or} \quad \frac{1}{\gamma + 1} \begin{pmatrix} 2\gamma & 1 - \gamma^2 \\ \gamma^2 - 1 & 2\gamma \end{pmatrix}
\]

with \( \gamma \in \mathbb{R} \setminus \{0\} \). The first case occurs if \( H \) does not admit a resonance at energy zero, it is referred to as the generic case (g.c.) The second, so-called exceptional case (e.c.), occurs when such a zero energy resonance exists. The contribution to the winding number coming from \( \Gamma_1 \) can be determined: \( w(\Gamma_1) = -\frac{1}{2} \) in the generic case, and \( w(\Gamma_1) = 0 \) in the exceptional one. Thus, taking into account that \( \hat{\Gamma}_3 = \hat{\Gamma}_4 = 1 \) (the former because \( S(\infty) = 1 \)) one obtains from (3)

\[
\frac{1}{2\pi} \int_{\mathbb{R}^+} \text{tr}_\lambda [iS^*(\lambda)S'(\lambda)] \, d\lambda = \begin{cases} \frac{N}{2}, & \text{g.c.} \\ \frac{N}{2}, & \text{e.c.} \end{cases}
\]

where \( N = \text{Tr}(P_p) \) is the number of bound states of \( H \). In particular, the correction term \( \nu \) corresponds to \( w_1 \). This result is in accordance with the literature [4, 5, 8, 13].

If the potential is symmetric, a Levinson’s theorem holds for each sector. In that situation, the exceptional case \( \gamma = 1 \) in (6) corresponds to an even zero energy resonance, and \( \gamma = -1 \) corresponds to an odd zero energy resonance. The results for the even and odd sector are summarized in the following two tables.
Summing up the results of both sectors one obtains (7) as there is never an even and an odd zero energy resonance at the same time.

5 Conclusion

Levinson’s theorem is an index theorem. We have elaborated the general framework supporting this statement, and corroborated it with one-dimensional scattering systems with point interaction or rapidly vanishing potentials. Our formulation reveals its topological nature and explains the corrections in a coherent and natural way. The proof is based on a new formula for the wave operator involving up to a compact operator the scattering operator and a universal function of the dilation operator. This formula is of independent interest and might be of use in other contexts as well.

References


