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Index Theorems in Quantum Mechanics

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Abstract In this article, extensions of the ideas about index theorems for Fredholm operators to pairs of unbounded (self-adjoint) operators and to pairs of projections in a Hilbert space are introduced, leading to applications in Quantum mechanical problems.

1 Introduction

Here two sets of circumstances in Quantum Mechanics will be discussed where index theorems occur naturally. In both situations, may be not so surprisingly, Krein's shift function makes it's appearance. The first one is about Witten index for a pair of Hamiltonians in Quantum Mechanics which is a generalisation of the Fredholm index for Fredholm operators, which these Hamiltonians are not. It is also shown that like the Fredholm index, the Witten index is invariant under "small" perturbations, the physicist's interpretation of which is to say that the number of bound states of a Hamiltonian is invariant under "weak coupling", since Witten index turns out to be negative of the number of bound states (a kind of Levinson's theorem). This result is next put in a perspective in the background of K-theory. The second story is about the Fredholm index for a pair of projections and application to Quantum Hall effect, the Krein's shift function for the pair equalling the index.

2 Schrodinger operator in quantum mechanics and mathematical theory of Scattering (a brief survey)

The physical states of a particle in Quantum Mechanics are given by vectors in a (separable) Hilbert space (more specifically, for our case) $h = L^2(\mathbb{R}^d)$ ($d =$ the dimension of the Euclidean space on which the particle lives). The Hamiltonian operator to describe the dynamics of the particle is given by $H = -\Delta + V$, where Δ is the Laplacian in $\mathbb{R}^d$ and V is a real-valued measurable function (called potential by physicists). Here we have set all physical constants like $h, 2m$ etc. equal to 1 so as to delineate only the mathematical ideas.

2.1 The self-adjointness problem

Since in Quantum Mechanics, we would like to have the time-evolution of the states to be described by one-parameter (strongly continuous) unitary group in h, their

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infinitesimal generator should be self-adjoint, leading to the question of self-adjointness of H.

Set $H_0 = -\Delta$, defined suitably i.e.,

$$D(H_0) = \left\{ f \in L^2(\mathbb{R}^d) \Big/ \int |k^2 \hat{f}(k)|^2 dk < \infty \right\}$$

(where $\hat{f}$ is the Fourier Transform of f in $L^2(\mathbb{R}^d)$) is clearly a self-adjoint operator. It is also known [1,2] that for a large class of functions V (e.g. if $V = V_1 + V_2$ with $V_1 \in L^p(\mathbb{R}^d), p = 2$ for $d \leq 3$ and $p > d/2$ for $d \geq 4$ and V_2 bounded and vanishing at infinity), H is self-adjoint with $D(H) = D(H_0)$.

2.2 Scattering and spectral problem

The operator H_0 being unitarily equivalent to a multiplication operator by the function $\mathbb{R}^2 \ni x \mapsto |x|^2 \in \mathbb{R}_+$ is spectrally positive and absolutely continuous. But what about H? For that it is convenient to introduce the *wave operators* $\Omega_\pm$ as

$$\Omega_\pm = s - \lim_{t \to \pm\infty} e^{iHt} e^{-iHot},$$

if they exist.

In fact, it is also known that for the class of potentials given in (i) with $V_2 = 0, \Omega_\pm$ exist and are isometries. A simple calculation shows that $H\Omega_\pm = \Omega_\pm H_0$ or equivalently

$$\Omega_\pm^* H|_{R(\Omega_\pm)} \Omega_\pm = H_0$$

i.e., the ranges $R(\Omega_\pm)$ of the isometries $\Omega_\pm$ (which is a closed subspaces of h) reduce H and the restrictions of H to $R(\Omega_\pm)$ are unitarily equivalent to H_0 and hence are positive and absolutely continuous, so that

$$R(\Omega_\pm) \subseteq h_{ac}(H).$$

That these two subspaces are indeed equal in many situations is the so called *completeness problem* and has indeed been proven for a large class of V's ([1,2]), i.e.,

$$R(\Omega_\pm) = h_{ac}(H).$$

If we, now assume that the (physically 'nasty' and 'untenable') singularly continuous subspace with respect to H is trivial, then we have that

$$R(\Omega_\pm)^\perp = Ph,$$

where P is the projection onto the eigenspaces (or the set of bound states) of H.

The scattering operator $S \equiv \Omega_+^* \Omega_-$ (well-defined and unitary since $R(\Omega_+) = R(\Omega_-)$) commutes with H_0 and hence can be "diagonalized" simultanously with H_0 as follows:

$$h \simeq \int_0^\infty \oplus L^2(S^{d-1}) d\mu(\lambda)$$

with $H_0 \simeq$ multiplication by λ and $S \simeq \{S_\lambda\}$ in this representation; where μ is a measure on $\mathbb{R}_+$, absolutely continuous with respect to the Lebesgue measure, S^{d-1} is the unit sphere in $\mathbb{R}^d$ and for almost all λ, S_λ is unitary on $L^2(S^{d-1})$.

One can now introduce a self-adjoint operator Δ_λ (called *phase-shift* operator at energy λ) such that $S_\lambda = \exp(2i\Delta\lambda)$. Under suitable conditions on V e.g. $V \in L^1 \cap L^2(\mathbb{R}^d)(d=3)$, it is known [2] that $S_\lambda - I_\lambda$ and hence, consequently Δ_λ are trace-class operators in $L^2(S^2)$ and we set $\xi(H, H_0; \lambda) \equiv \xi(\lambda) = \pi^{-1}\mathrm{Tr}\,(\Delta_\lambda)$ for almost all λ. This function ξ is called Krein's shift function ([3–5]).

There are very interesting results on the nature of Krein's shift function ([3–5]) of which we reproduce two without proof.

Theorem 2.1. *Let, H and H_0 be two self-adjoint operators (not necessarily bounded) in a Hilbert space h such that $V \equiv H - H_0$ is trace-class. Then there exists a unique real-valued $L^1(\mathbb{R})$-function ξ with support in the union of the spectra of H and H_0 with the properties:*

(i)

$$\int |\xi(\lambda)|d\lambda \le \|V\|_1, \quad \int \xi(\lambda)d\lambda = \mathrm{Tr}\,V,$$

(ii)

$$\textit{for} \quad \varphi : \mathbb{R} \longrightarrow \mathbb{C} \quad \textit{with} \quad \varphi(\lambda) = \int (it)^{-1}(e^{it\lambda} - 1)d\nu(t) + \textit{constant},$$

where ν is a complex measure, one has that $[\varphi(H) - \varphi(H_0)]$ is trace-class, and

$$\mathrm{Tr}\,[\varphi(H) - \varphi(H_0)] = \int \varphi'(\lambda)\xi(\lambda)d\lambda.$$

(iii) *If we define the perturbation determinant*

$$\Delta(z) \equiv \det\,[I + V(H_0 - z)^{-1}] \quad \textit{for} \quad \mathrm{Im}\,z > 0, \quad \textit{then}$$

$$\xi(\lambda) = \pi^{-1} \lim_{\varepsilon \downarrow 0} \mathrm{Im}\,\log \Delta(\lambda + i\varepsilon).$$

Theorem 2.2. *Let H and H_0 be two self-adjoint operators in h such that for some z with $\mathrm{Im}\,z > 0, [(H - z)^{-1} - (H_0 - z)^{-1}]$ is trace-class. Then there exists a function ξ on $\mathbb{R}$, unique upto an additive constant such that*

(i)

$$\int (1 + \lambda^2)^{-1}|\xi(\lambda)|d\lambda < \infty,$$

(ii)

$$\mathrm{Tr}\,[(H - z)^{-1} - (H_0 - z)^{-1}] = -\int \frac{\xi(\lambda)}{(\lambda - z)^2}dx, \quad \textit{and}$$

(iii) *For $\varphi \in \mathcal{S}(\mathbb{R})$, the class of smooth functions of rapid decrease, $[\varphi(H) - \varphi(H_0)]$ is trace-class and*

$$\mathrm{Tr}\,[\varphi(H) - \varphi(H_0)] = \int \varphi'(\lambda)\xi(\lambda)d\lambda.$$

3 Index theorem in Scattering theory

Let H and H_0, as introduced above, be such that $[(H-z)^{-1}-(H_0-z)^{-1}]$ is trace-class for some non real complex z (e.g. for $d=3$, the potential function $V \in L^1 \cap L^2(\mathbb{R}^3)$ will imply this). The Witten index of the pair, $\delta(H, H_0)$ is defined as

$$\delta(H, H_0) \equiv \lim_{\substack{z \to 0 \\ |\mathrm{Re}\, z| \leq C|\mathrm{Im}\, z|}} \{(-z)\mathrm{Tr}\,[(H-z)^{-1} - (H_0 - z^{-1})]\}, \quad \text{if it exists.}$$

A bounded linear operator A in h is said to be Fredholm if its range is closed with finite codimension (the dimension of the orthogonal complement) and if its null space is finite dimensional, and in such a case the (Fredholm) index of A is defined as:

$$\mathrm{ind}\,(A) = \dim(\text{Null space of } A)\text{-codim}(\text{Range of } A),$$

which is an integer. The following sets of results [6,7] show the importance of this concept:

(i) If A is Fredholm and B a compact operator in h, then

$$\mathrm{ind}\,(A+B) = \mathrm{ind}\,(A).$$

Also if A and B are bounded operators in h and A is Fredholm, then there exists $\alpha_0 > 0$ such that

$$\mathrm{ind}\,(A + \alpha B) = \mathrm{ind}\,(A)$$

for all α with $|\alpha| < \alpha_0$.

(ii) Let A be a densely defined closed operator and set

$$H_1 = A^*A, H_2 = AA^*$$

such that

$$(H_1 - z)^{-1} - (H_2 - z)^{-1}$$

is trace-class for $z \in \not{C}\setminus[0,\infty)$. If furthermore, A is Fredholm, then the Witten index equals Fredholm index, i.e.,

$$\delta(H_1, H_2) = \mathrm{ind}\,(A).$$

(iii) If the shift function $\xi(H_1, H_2; \lambda)$ is piecewise continuous on $[0, \infty)$ and bounded, then

$$\delta(H_1, H_2) = -\xi(H_1, H_2; 0+).$$

Unlike $\mathrm{ind}\,(A), \delta(\cdot,\cdot)$ makes sense for a much larger class of (self-adjoint) operators, but at the same time enjoys certain invariance property under "small perturbations" like that of Fredholm index as mentioned in (ii) in the paragraph above. Furthermore, the Witten index (which can be thought of as a generalization of Fredholm index) has a nice relation with the Krein's shift function ξ. The following theorem (whose proof can be bound in [8]) sums up these results.

Theorem 3.1. *Let $H_0 = -\Delta$ in $L^2(\mathbb{R}^3)$ and let $V_j \in L^1 \cap L^2(\mathbb{R}^3)$ $(j = 1, 2)$ be two potentials. Assume furthermore that $\{0\}$ is not an eigenvalue for either of the self-adjoint operators $H_j = H_0 + V_j$. Then*

(i) *There exists $\alpha_0 > 0$ such that for all α with*

$$|\alpha| < \alpha_0, \quad \delta(H_0 + V_1 + \alpha V_2, H_0 + \alpha V_2) = \delta(H_0 + V_1, H_0).$$

(ii) *Assume that $\xi(\lambda) \equiv \xi(H, H_0; \lambda)$ is locally bounded and piecewice continuous, then*

$$\xi(H_0 + \alpha V_2, H_0; 0-) = 0$$

and

$$\xi(H_0 + V_1 + \alpha V_2, H_0 + \alpha V_2; 0+) = \xi(H_0 + V, H_0; 0+) \text{ for } |\alpha| < \alpha_0.$$

(iii)

$$\begin{aligned} \delta(H_0 + V_1 + \alpha V_2, H_0 + \alpha V_2) &= \xi(H_0 + V_1 + \alpha V_2, H_0 + \alpha V_2; 0-) \\ -\xi(H_0 + V_1 + \alpha V_2, H_0 + \alpha V_2; 0+) &= -\xi(H_0 + V_1 + \alpha V_2, H_0 + \alpha V_2; 0+) \\ -\xi(H_0 + V_1, H_0; 0+) &= -n = -\operatorname{Tr} P, \end{aligned}$$

where P was the projection onto the bound states of the Hamiltonian H.

Thus for many Quantum Mechanical systems, the Witten index turns out to be the negative of the number of bound states of the associated Hamiltonian and furthermore, this integer is invariant under "small perturbations".

4 Non-commutative K-theory and Scattering

Here we shall deal with concrete, C^*-algebras as relevant to the Scattering theory, described earlier (see [9] and [10] for K-theory for C^*-algebras).

For our discussions, it is convenient to introduce the generator of the group of dilations in $\mathbb{R}^d$: for $\lambda \in \mathbb{R}$

$$(Y_\lambda f)(x) = \exp(-\lambda d/2) f(e^\lambda x).$$

It is easily seen that this describes a strongly continuous one-parameter group of unitaries in $L^2(\mathbb{R}^d)$, whose Stone-generator is $A = -i/2(x \cdot \nabla + \nabla \cdot x)$, where $x \in \mathbb{R}^d$ and ∇ is the gradient. If we set $B = 1/2 \ln H_0$ (where $H_0 = -\Delta$ in $L^2(\mathbb{R}^d)$), then A and B are self-adjoint operators in $L^2(\mathbb{R}^d)$ with whole real line as their (absolutely continuous) spectra and $[A, B] = -i$, just like the momentum P and position Q operators in Quantum Mechanics in one dimension. There is however, a major difference: while P and Q have *no spectral degeneracy*, A and B are infinitely degenerate (infact, for almost all points in $\mathbb{R}$, the space of degeneracy is $L^2(S^{d-1})$) because of their obvious rotational invariance.

Set $K = B_0(L^2(S^{d-1}))$, the C^*-algebra of compact operators on the degeneracy space, $\mathcal{A} = Span\{\varphi(A)\varphi(B)\}$ (for $\varphi, \psi \in C_0(\mathbb{R})$, continuous functions on $\mathbb{R}$, vanishing at ∞), $\mathcal{J} = \mathcal{A} \otimes \mathcal{K}, \tilde{\mathcal{A}} = (\mathcal{A} + \{\eta(B)\}) \otimes \mathcal{K}$ (with $\eta \in C_0(\mathbb{R})$ and $\{\eta(B)\}$ signifying the commutative C^*-algebra generate by B), and $\mathcal{C} = \{\eta(B)\} \otimes \mathcal{K}$. Note that all these C^*-algebra are without identity and also recalling the discussions on Scattering theory in section 2, we observe that $S - I \in \mathcal{C}$, since under the hypothesis there $S_\lambda - I_\lambda$ is trace-class and hence belongs to $\mathcal{K}$. Also note that $\mathcal{A} \subseteq B_0(L^2(\mathbb{R}))$ (since products of the type $\varphi(A)\psi(B)$ gives a compact operator ([1,2])) and $\mathcal{J} \subseteq B_0(L^2(\mathbb{R}^d))$. Thus we have the following short exact sequence ([10]):

$$O \to \mathcal{J} \xrightarrow{\chi} \tilde{\mathcal{A}} \xrightarrow{\pi} \tilde{\mathcal{A}}/\mathcal{J} \simeq \mathcal{C} \to 0,$$

where χ is the inclusion map and π is the projection map. Incidentally, it is worth noting that $\mathcal{J} \simeq C_0(\mathbb{R}; \mathcal{K}) \rtimes_\tau \mathbb{R}, \tilde{\mathcal{A}} \simeq C_0(\mathbb{R} \cup \{\infty\}; \mathcal{K}) \rtimes_\tau \mathbb{R}$ and $\mathcal{C} \simeq \mathcal{K} \rtimes_\alpha \mathbb{R}$, where action τ of the group $\mathbb{R}$ is that of translation and α is the trivial action and $\rtimes_\tau$ is the crossed product (see [9]).

In the context of Scattering theory, the map π can be understood as follows:

$$\|1_{(A \geq t)}[T - \pi(T)]\| \to 0 \;\text{ for } T \in \tilde{\mathcal{A}}.$$

This happens because

$$T - \pi(T) \in \mathcal{A} \subseteq B_0(L^2(\mathbb{R}) \simeq B_0(L^2(sp(A))) \text{ and } 1_{(A \geq t)},$$

the family of characteristic functions converge strongly to 0 as $t \longrightarrow \infty$.

For some special operators one can complete $\pi(\cdot)$.

Theorem 4.1. *Assume that $\Omega_- - I \in \tilde{\mathcal{A}}$. Then*

(i) $\pi(\Omega_- - I) = S - I \in \mathcal{C}$,

(ii) *the projection operator point the bound state of $\mathcal{H}$ belong to $\mathcal{J}$ and one has at the level of K-theory*

$$\text{ind}\,[S]_1 = -[P]_0.$$

Here $[S]_1$ in the K_1-class of S and $[P]_0$ is the K_0-class of P_1 and ind *is the index map of Pimsner-Voiculescu from $K_1(\mathcal{C})$ into $K_0(\mathcal{J})$.*

For the proof of (i) the reader is referred to [11,12] and for (ii) [9]. This demonstrates how abstract K-theory can be used in a nice way to understand some of the results in Quantum Mechanics in a different perspective.

5 The story of a pair of projections

The story begins with an interesting article by Effros with an intriguing title "why the circle is connected" ([13]) in which the following result is stated and proved "." if P and Q are two orthogonal projections in a Hilbert space such that $P - Q$ is trace-class, then $\text{Tr}(P - Q) \in \mathbb{Z}$, the set of integers. In two papers [14,15] the authors revived an old geometric idea of Halmos [16] to prove the above result, relate the trace with the relative Fredholm index and Krein's shift function.

Theorem 5.1 ([13–16]).

(i) *Let P and Q be two orthogonal projections in h. Then setting \ = {{ ∈ |𝒫{ = {, 𝒬{ = \{}(, \ = ,), h decomposes as direct sum of five subspaces (all reducing both P and Q):*

$$h = h_{00} \oplus h_{01} \oplus h_{10} \oplus h_{11} \oplus h_g,$$

where h_g (called the subspace 'generic' with respect to the pair P, Q) consisting of vectors, none if which are eigenvectors of P or Q and with respect to this, P and Q decompose as

$$P = O \oplus O \oplus I \oplus I \oplus P_g$$

$$Q = O \oplus I \oplus O \oplus I \oplus Q_g.$$

(ii) *Furthermore, if P and Q is a generic pair of projections (i.e. like the P_g, Q_g in the above decomposition), then Ranges of $P, P^\perp, Q$ and $Q^\perp$ are all mutually unitarily isomorphic and with respect to the decomposition of the (generic) subspace $= R(P) \oplus R(P^\perp)$, P and Q assumes the canonical forms:*

$$P = \begin{bmatrix} I & O \\ O & O \end{bmatrix}, Q = \begin{bmatrix} C^2 & CS \\ CS & S^2 \end{bmatrix},$$

where C and S are two commuting positive contractions satisfying $C^2 + S^2 = I$.

From this theorem Effros result follows easily since $P - Q$ trace-class implies that $P_g - Q_g$ is trace-class, but on the other hand $P_g - Q_g$ takes the matrix form $\begin{bmatrix} S^2 & -CS \\ -CS & -S^2 \end{bmatrix}$, leading to the result that $\mathrm{Tr}\,[(P_g - Q_g)^p] = 0$ *if p is odd and therefore*

$$\mathrm{Tr}\,(P - Q)^p = \dim h_{10} - \dim h_{01} \in \mathbb{Z}$$

if p is odd (each of these dimensions are finite because each of the associated projections are trace-class).

In [14], the authors introduced the notion that two projections P and Q are said to be Fredholm pair when

$$G \equiv QP : \mathrm{Range}\,(P) \longrightarrow \mathrm{Range}\,(Q)$$

is Fredholm, and in such a case the relative Fredholm index of the pair, ind (P, Q) is defined to be the Fredholm index of the operator G. Then it follows easily ([15]) from the Theorem 5.1 that (P, Q) is a Fredholm pair if and only if $\dim h_{10}$ and $\dim h_{01}$ are both finite and the pair (P_g, Q_g) is a Fredholm pair. Furthermore, ind $(P_g, Q_g) = 0$ so that

$$\mathrm{ind}\,(P, Q) = \dim h_{10} - \dim h_{01} \in \mathbb{Z}.$$

How does the two sets of results compare with each other? For this one needs to observe ([15]) that if $P - Q$ is a compact operator in h, then (P, Q) is a Fredholm pair and therefore, in the light of the earlier observations, one can say that if $P - Q$ is a trace-class, then ind $(P, Q) = \mathrm{Tr}(P - Q)$. One can also think of P and Q as "Hamiltonians" such that the perturbation $P - Q$ is trace-class and as discussed in section 2, consider the Krein's shift function $\xi(\lambda) = \xi(P, Q; \lambda)$ and find that when $P - Q$ is trace-class, $\xi(\lambda) = \dim h_{10} - \dim h_{01}$, for $\lambda \in [0, 1]$ and $= 0$ for $\lambda \notin [0, 1]$.

One nice application of these ideas was given in [17] in the context of the Landau model of paramangnetism and considering an idealized model of Quantum Hall effect by introducing a "quantized flux tube" through the origin.

Consider an electron in uniform, constant magnetic field B perpendicular to the x-y plane, the associated Landau Hamiltonian (after factoring out the free motion in the z-direction) in $\mathbb{R}^2$ is given as:

$$H = (2m)^{-1}(p_x^2 + p_y^2) + \frac{e^2 B^2}{8}(x^2 + y^2) - \frac{eB}{2} L,$$

where e and m are the electric charge and mass of an electron respectively, p_x and p_y are the momentum operators in x and y directions and $L \equiv xp_y - yp_x$ is the z-component of the angular momentum operator. We introduce a convenient (unbounded) operator D as $D = \frac{\partial}{\partial \bar{z}} + \frac{1}{2}z$, where z is the complex variable $z = x + iy$ and the relevant Hilbert space $h = L^2(\mathbb{R}^2)$ gets unitarily transformed by the change of variable to h (by an abuse of notation) made up of (the equivalance classes of) complex-valued measurable functions of z and $\bar{z}$, square-integrable with respect to the planar Lebesgue measure. Then the Hamiltonian looks like

$$H = 2(D^* D + I)$$

(where we have set for convenience $m = \hbar = 1$ and $eB = 2$). Then the (simultaneous) eigenstates of H and L are:

$$\psi_{n,0}(z) = (\pi n!)^{-1/2} z^n \exp(-1/2|z|^2)$$
$$L\psi_{n,0} = n\psi_{n,0}; \quad H\psi_{n,0} = \psi_{n,0}; \quad \text{and}$$

if we set

$$\psi_{n,m}(z) \equiv (m!)^{-1/2}(D^{*m}\psi_{n,0})(z),$$

then

$$L\psi_{n,m} = (n-m)\psi_{n,m} \quad \text{and} \quad H\psi_{n,m} = (2m+1)\psi_{n,m},$$

with $n, m \in \mathbb{N} \cup \{0\}$. Next, let P_m be the (infinite-dimensional) projection onto the mth (energy) eigenstate of H and let $Q_M = UP_mU^*$ be another projection where U is the unitary multiplication operator in h by the function $U(z) = z/|z|$ for $z \in \mathbb{C} \setminus [0, \infty); = 1$ for $z \in [0, \infty)$. Then we have

Theorem 5.2 ([15,17,18]).

(i) *For every* $m \in \mathbb{N}U\{0\}, (P_m, Q_m)$ *is a Fredholm pair of projections and* $\operatorname{ind}(P_m, Q_m) = +1$.
(ii) *In particular,* $P_0 - Q_0$ *is not compact even though the pair* (P_0, Q_0) *is Fredholm showing that compactness of the difference of projections is a sufficient, but not a necessary condition for the pair to be Fredholm.*

The operator U is supposed to represent the introduction of an (idealized) thin fluxtube along the Z-direction through the origin and the index $(P_m, Q_m) = +1$ is interpreted as the charge transport of the system by one unit of electronic charge (Quantum Hall effect).

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