A Dixmier trace formula for the density of states

Ed McDonald
Joint with N. Azamov, E. Hekkelman F. Sukochev and D. Zanin.

Penn State University

May 31, 2023

Introduction

This talk is about a connection between the density of states and Dixmier traces, covered in the two papers

- N. Azamov, E. M., F. Sukochev. and D. Zanin: *A Dixmier Trace Formula for the Density of States* Comm. Math. Phys. 377 (2020), no. 3, 2597–2628. `arXiv:1910.12380`.
- N. Azamov, E. Hekkelman, E.M., F. Sukochev and D. Zanin. *An application of singular traces to crystals and percolation.* J. Geom. Phys. 179 (2022), Paper No. 104608, 22 pp. `arXiv:2202.03676`

and the recent preprint

- E. Hekkelman and E. M. *A general Dixmier trace formula for the density of states on open manifolds* (2023) `arXiv:2304.13272`

Introduction

Dixmier traces are probably best known due to their use by Connes to define the integration functional in noncommutative geometry. In particular, the Hochschild class of the Chern character is

The basic idea

If H is a lower-bounded self-adjoint operator (on a Hilbert space) with discrete spectrum (i.e. the spectrum consists only of eigenvalues of finite multiplicity), then we can understand the spectrum through the spectral counting function

$$\begin{aligned} N(t,H) &= \mathrm{Tr}(\chi_{(-\infty,t]}(H)) \\ &= \text{ Dimension of the span of the eigenvectors} \\ &\text{corresponding to eigenvalues } \leq t. \end{aligned}$$

This is less useful when H has some essential spectrum. What is a good replacement?

Physical setting

Initially we concentrate on Schrödinger operators.
Let $d > 1$ and $R > 0$. Let $B(0, R)$ be the open ball in $\mathbb{R}^d$ of radius R,

$$B(0, R) = \{x \in \mathbb{R}^d \ : \ |x| < R\}.$$

Physical setting

Initially we concentrate on Schrödinger operators.
Let $d > 1$ and $R > 0$. Let $B(0,R)$ be the open ball in $\mathbb{R}^d$ of radius R,

$$B(0,R) = \{x \in \mathbb{R}^d \;:\; |x| < R\}.$$

On $L_2(B(0,R))$, we can define the Dirichlet Laplace operator with Dirichlet boundary conditions, Δ_R.

Physical setting

Initially we concentrate on Schrödinger operators.
Let $d > 1$ and $R > 0$. Let $B(0, R)$ be the open ball in $\mathbb{R}^d$ of radius R,

$$B(0, R) = \{x \in \mathbb{R}^d \ : \ |x| < R\}.$$

On $L_2(B(0, R))$, we can define the Dirichlet Laplace operator with Dirichlet boundary conditions, Δ_R.
The operator Δ_R is negative semidefinite and has purely discrete spectrum.

Schrödinger operators

Given $V \in L_\infty(B(0,R))$, denote by M_V the operator of pointwise multiplication by V. That is, $(M_V\xi)(t) = V(t)\xi(t)$.

Schrödinger operators

Given $V \in L_\infty(B(0,R))$, denote by M_V the operator of pointwise multiplication by V. That is, $(M_V\xi)(t) = V(t)\xi(t)$.
For the purposes of this talk a *Schrödinger operator* on $B(0,R)$ is a linear operator

$$H = -\Delta_R + M_V$$

where V is real-valued. Since we only consider bounded V, the operator H is self-adjoint with domain equal to that of Δ_R.

Schrödinger operators

Given $V \in L_\infty(B(0,R))$, denote by M_V the operator of pointwise multiplication by V. That is, $(M_V\xi)(t) = V(t)\xi(t)$.

For the purposes of this talk a *Schrödinger operator* on $B(0,R)$ is a linear operator

$$H = -\Delta_R + M_V$$

where V is real-valued. Since we only consider bounded V, the operator H is self-adjoint with domain equal to that of Δ_R.

Since H is a relatively compact perturbation of $-\Delta_R$, the spectrum of H is discrete and consists only of eigenvalues of finite multiplicity.

Spectral counting function

Let $H = -\Delta_L + M_V$ be a Schrödinger operator on $B(0, R)$.

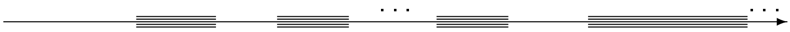
Schrödinger operators on $\mathbb{R}^d$

So far we have only discussed operators on bounded domains. What about unbounded domains? Let $\Delta = \sum_{j=1}^d \partial_{x_j}^2$ be the Laplace operator on $L_2(\mathbb{R}^d)$. This operator is self-adjoint, has spectrum $(-\infty, 0]$ and has no eigenvalues. We consider the Hamiltonian

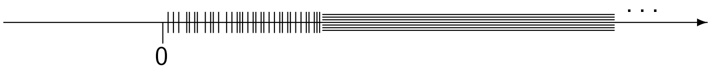
$$H = -\Delta + M_V$$

where $V \in L_\infty(\mathbb{R}^d)$ is real-valued.
What does the spectrum of H look like?

Suppose that V is periodic. The celebrated Bloch-Floquet theory asserts that the spectrum of a periodic Schrödinger operator is purely absolutely continuous and consists of a union of bands:



For Schrödinger operators with appropriately defined random potentials, the celebrated Anderson localisation theory asserts that the spectrum of a random Schrödinger operator has almost surely a pure point bottom part:



(thanks to Nurulla Azamov for these pictures).

The density of states

The spectral counting function usually does not make sense for Schrödinger operators on $\mathbb{R}^d$, since the spectrum can be continuous. What is a good replacement?

The density of states

The spectral counting function usually does not make sense for Schrödinger operators on $\mathbb{R}^d$, since the spectrum can be continuous. What is a good replacement?

Idea: (From solid-state physics.) Let $R > 0$, and "restrict" H to $B(0,R)$:

$$H_R := -\Delta_R + M_V$$

on $L_2(B(0,R))$. The *density of states* of H is a measure ν_H on $\mathbb{R}$ defined as

$$\nu_H((-\infty, t]) := \lim_{R\to\infty} \frac{N(t, H_R)}{\mathrm{Vol}(B(0,R))}, \quad t \in \mathbb{R}.$$

Optimistically, this limit exists and indeed defines a measure.

Problems with the density of states

There are many analytical issues with the "measure" ν_H.

- Does the limit as $R \to \infty$ really exist and does it define a measure?

Problems with the density of states

There are many analytical issues with the "measure" ν_H.

- Does the limit as $R \to \infty$ really exist and does it define a measure? Answer: Not always, but sometimes it does.

Problems with the density of states

There are many analytical issues with the "measure" ν_H.

- Does the limit as $R \to \infty$ really exist and does it define a measure? Answer: Not always, but sometimes it does.
- If it exists, what is the support of ν_H?

Problems with the density of states

There are many analytical issues with the "measure" ν_H.

- Does the limit as $R \to \infty$ really exist and does it define a measure? Answer: Not always, but sometimes it does.
- If it exists, what is the support of ν_H? Answer: the essential spectrum of H.

Problems with the density of states

There are many analytical issues with the “measure” ν_H.

- Does the limit as $R \to \infty$ really exist and does it define a measure? Answer: Not always, but sometimes it does.
- If it exists, what is the support of ν_H? Answer: the essential spectrum of H.
- Does ν_H depend on the choice of boundary conditions for H_R?

Problems with the density of states

There are many analytical issues with the "measure" ν_H.

- Does the limit as $R \to \infty$ really exist and does it define a measure? Answer: Not always, but sometimes it does.
- If it exists, what is the support of ν_H? Answer: the essential spectrum of H.
- Does ν_H depend on the choice of boundary conditions for H_R? Answer: No.

Problems with the density of states

There are many analytical issues with the "measure" ν_H.

- Does the limit as $R \to \infty$ really exist and does it define a measure? Answer: Not always, but sometimes it does.
- If it exists, what is the support of ν_H? Answer: the essential spectrum of H.
- Does ν_H depend on the choice of boundary conditions for H_R? Answer: No.
- Does it matter that we "restricted" H to balls $B(0, R)$? What about cubes or other domains?

Problems with the density of states

There are many analytical issues with the "measure" ν_H.

- Does the limit as $R \to \infty$ really exist and does it define a measure? Answer: Not always, but sometimes it does.
- If it exists, what is the support of ν_H? Answer: the essential spectrum of H.
- Does ν_H depend on the choice of boundary conditions for H_R? Answer: No.
- Does it matter that we "restricted" H to balls $B(0, R)$? What about cubes or other domains? Answer: For many classes of potentials (random, almost periodic), the choice of domain is irrelevant. For arbitrary potentials, the domain matters.

Example

An example where the DOS is easily computed is the "free" Hamiltonian, corresponding to $V = 0$. We have

$$d\nu_{-\Delta}(t) = \frac{\mathrm{Vol}(S^{d-1})}{2(2\pi)^d} \max\{t, 0\}^{\frac{d}{2}-1}\, dt.$$

Example

Another example allowing explicit computation is when V is radially homogeneous (i.e., $V(r\xi) = V(\xi)$ for all $r > 0$). In this case, the DOS exists and

$$d\nu_{-\Delta+M_V}(t) = \frac{\mathrm{Vol}(S^{d-1})}{2(2\pi)^d} \cdot \frac{1}{|S^{d-1}|}\int_{S^{d-1}} \max\{t - V(\theta), 0\}^{\frac{d}{2}-1}\,d\theta\,dt.$$

See N. Azamov, E. M., F. Sukochev and D. Zanin *The density of states depends on the domain* `arXiv:2107.09828`.

Traces

Let $\mathcal{H}$ be a Hilbert space. An eigenvalue sequence of a compact operator $A \in B(\mathcal{H})$ is a sequence $\{\lambda(k, A)\}_{k\in\mathbb{N}}$ of the eigenvalues of A listed with multiplicity, such that $\{|\lambda(k, A)|\}_{k\in\mathbb{N}}$ is non-increasing.

The usual operator trace Tr can be characterised for trace class operators $A \in \mathcal{L}_1 \subset B(\mathcal{H})$ as

$$\mathrm{Tr}(A) = \lim_{n\to\infty} \sum_{k=1}^{n} \lambda(k, A).$$

The Dixmier trace is defined on so-called weak trace class operators $A \in \mathcal{L}_{1,\infty} \subset B(\mathcal{H})$ by

$$\mathrm{Tr}_\omega(A) = \omega\text{-}\lim_{n\to\infty} \frac{1}{\log(2+n)} \sum_{k=1}^{n} \lambda(k, A),$$

where $\omega \in \ell_\infty(\mathbb{N})^*$ is an extended limit. Note that $\mathcal{L}_1 \subset \mathcal{L}_{1,\infty}$, but if $A \in \mathcal{L}_1$, $\mathrm{Tr}_\omega(A) = 0$.

Connes' integral formula

A property of Dixmier traces (and all traces on $\mathcal{L}_{1,\infty}$) is that they vanish on finite rank operators. Dixmier thought that this would make them useless, and uncomputable.

Connes' integral formula

A property of Dixmier traces (and all traces on $\mathcal{L}_{1,\infty}$) is that they vanish on finite rank operators. Dixmier thought that this would make them useless, and uncomputable. His student Alain Connes realized that this is what makes them useful and computable. (One version of) Connes' integral formula states that if $f \in C_c^\infty(\mathbb{R}^d)$ then

$$\mathrm{Tr}_\omega(M_f(1-\Delta)^{-\frac{d}{2}}) = \frac{\mathrm{Vol}(S^{d-1})}{d(2\pi)^d}\int_{\mathbb{R}^d} f(t)\,dt.$$

This is taking place on the Hilbert space $\mathcal{H} = L_2(\mathbb{R}^d)$, and relies on the fact that $M_f(1-\Delta)^{-\frac{d}{2}} \in \mathcal{L}_{1,\infty}$.

Connes' integral formula reconsidered

Restrict attention to a function $f \in C_c^\infty(\mathbb{R}^d)$ which is radial. There exists $g \in C_0([0,\infty))$ such that $f(t) = g(|t|^2)$. Then Connes' integral formula implies Switch to the Fourier side (recall that Tr_ω is unitarily invariant!) and we get

$$\mathrm{Tr}_\omega(g(-\Delta)(1+M_{|x|}^2)^{-\frac{d}{2}}) = \frac{\mathrm{Vol}(S^{d-1})}{d}\int_0^\infty g(r)\,d\mu(r)$$

where μ is the measure $d\mu(r) = \frac{\mathrm{Vol}(S^{d-1})}{2(2\pi)^d} r^{\frac{d}{2}-1}\,dr$.

This measure μ is precisely the density of states measure for the "free" Hamiltonian $H = -\Delta$. This is not a coincidence!

Idea of the formula

Idea: Replace $-\Delta$ with $H = -\Delta + M_V$. An argument using the Riesz representation theorem implies that there exists a measure μ_H on $\mathbb{R}$ such that

$$\mathrm{Tr}_\omega(f(H)(1+M_{|x|}^2)^{-\frac{d}{2}}) = \frac{\mathrm{Vol}(S^{d-1})}{d}\int_{\mathbb{R}} f\, d\mu_H$$

for all $f \in C_c(\mathbb{R})$.

Theorem

$\nu_H = \mu_H$.

That is, if the density of states measure ν_H exists, then it is given by the formula

$$\mathrm{Tr}_\omega(f(H)(1+M_{|x|}^2)^{-\frac{d}{2}}) = \frac{\mathrm{Vol}(S^{d-1})}{d}\int_{\mathbb{R}} f\, d\nu_H, \quad f \in C_c(\mathbb{R}).$$

Advantages of the Dixmier trace formula for DOS

1. Simplifies proofs of some properties of DOS, such as insensitivity to localised perturbations.
2. Makes some computations very easy. For example, the formula for radially homogeneous potentials stated above was first derived using the Dixmier trace formula.

Trace formulas

General form

Let (X, d_X) be a certain kind of metric space. Let H be a certain kind of self-adjoint operator on $L_2(X)$ for which the DOS exists with respect to $x_0 \in X$. Then for a certain (fixed) function $w \in L_\infty(X)$, for all Dixmier traces Tr_ω and for all $f \in C_c(\mathbb{R})$ we have

$$\mathrm{Tr}_\omega(f(H)M_w) = c \int_{\mathbb{R}} f \, d\nu_H.$$

Flavours

Different flavours of this theorem have been proven.

Azamov, McDonald, Sukochev, Zanin (2020)

$X = \mathbb{R}^d$, $H = \Delta + M_V$, $w(x) = (1 + |x|^2)^{\frac{-d}{2}}$.

Azamov, H., McDonald, Sukochev, Zanin (2022)

X a discrete metric space with some geometrical conditions, H a general self-adjoint operator, $w(x) = \frac{1}{1+|B(x_0, d_X(x_0, x))|}$.

H., McDonald (WIP, 2023?)

X a manifold of bounded geometry plus some geometrical conditions, H a self-adjoint, lower bounded, elliptical second-order differential operator, $w(x) = \frac{1}{1+|B(x_0, d_X(x_0, x))|}$.

The local index theorem

Let M be a (possibly non-compact) Riemannian d-manifold with a spinor bundle $S \to M$. Assume that S has a grading $\gamma \in \Gamma(\mathrm{End}(S))$, and associated Dirac operator D. With respect to the grading, write

$$D = \begin{pmatrix} 0 & D_+ \\ D_- & 0 \end{pmatrix}.$$

The local index theorem

Let M be a (possibly non-compact) Riemannian d-manifold with a spinor bundle $S \to M$. Assume that S has a grading $\gamma \in \Gamma(\mathrm{End}(S))$, and associated Dirac operator D. With respect to the grading, write

$$D = \begin{pmatrix} 0 & D_+ \\ D_- & 0 \end{pmatrix}.$$

Theorem (Patodi, Gilkey)

For all $x \in M$, we have

$$\lim_{t \to 0} \mathrm{Tr}_x(\gamma_x e^{-tD^2}(x,x))|dx| = \widehat{A}(R)(x)^{(d)}.$$

The integrated local index theorem

Write the local index theorem in a slightly different way. For all $f \in C_c(M)$, we have

$$\lim_{t\to 0} \mathrm{Tr}(\gamma e^{-tD^2} M_f) = \int_M \widehat{A}(R) f.$$

The "lim" on the left hand side is necessary.

The integrated local index theorem

Write the local index theorem in a slightly different way. For all $f \in C_c(M)$, we have

$$\lim_{t\to 0} \mathrm{Tr}(\gamma e^{-tD^2} M_f) = \int_M \widehat{A}(R) f.$$

The "lim" on the left hand side is necessary.
Mysticism of index theory: if $f = 1$ (and M is of course compact) then no limit is needed! $\mathrm{Tr}(\gamma e^{-tD^2})$ is independent of t, and equal to $\mathrm{Index}(D_+)$. The conventional explanation for this is to expand $\mathrm{Tr}(\gamma e^{-tD^2})$ as

$$\mathrm{Tr}(\gamma e^{-tD^2}) = \sum_{k=0}^{\infty} e^{-t\lambda_k(D_+D_-)} - e^{-t\lambda_k(D_-D_+)} = \mathrm{Index}(D_+).$$

The integrated local index theorem

Write the local index theorem in a slightly different way. For all $f \in C_c(M)$, we have

$$\lim_{t\to 0} \mathrm{Tr}(\gamma e^{-tD^2} M_f) = \int_M \widehat{A}(R) f.$$

The "lim" on the left hand side is necessary.
Mysticism of index theory: if $f = 1$ (and M is of course compact) then no limit is needed! $\mathrm{Tr}(\gamma e^{-tD^2})$ is independent of t, and equal to $\mathrm{Index}(D_+)$. The conventional explanation for this is to expand $\mathrm{Tr}(\gamma e^{-tD^2})$ as

$$\mathrm{Tr}(\gamma e^{-tD^2}) = \sum_{k=0}^{\infty} e^{-t\lambda_k(D_+D_-)} - e^{-t\lambda_k(D_-D_+)} = \mathrm{Index}(D_+).$$

Another argument is to simply differentiate $\mathrm{Tr}(\gamma e^{-tD^2})$.

The integrated local index theorem (cont.)

If we consider f not necessarily constant, we get

$$\frac{d}{dt}\mathrm{Tr}(\gamma e^{-tD^2}M_f) = \frac{1}{2}\mathrm{Tr}(\gamma e^{-tD^2}D[D,M_f]).$$

If f is not constant on connected components of M, then $[D,M_f]$ remains stubbornly non-zero, and $\mathrm{Tr}(\gamma e^{-tD^2}M_f)$ will probably depend on t.

The Roe index theorem

Suppose that M has a *regular exhaustion*. That is, M is an increasing union of compact subsets $M = \bigcup_{n=0}^{\infty} M_n$, satisfying certain technical conditions. Given $f \in L_\infty(M)$, define

$$\phi_n(x) = \frac{1}{|M_n|} \int_{M_n} f.$$

By the Banach-Alaoglu theorem, there exists a weak*-limit point m of the sequence $\{\phi_n\}_{n=0}^{\infty}$. That is, m is a functional such that

$$m\{f\} = \lim_{n\to\infty} \frac{1}{|M_n|} \int_{M_n} f$$

whenever the limit exists, and extended to all bounded functions f.

The Roe index theorem (cont.)

The local index theorem implies that for every n,

$$\lim_{t\to 0} \frac{1}{|M_n|}\int_{M_n} \mathrm{Tr}_x(\gamma_x e^{-tD^2}(x,x))\,dx = \frac{1}{|M_n|}\int_{M_n} \widehat{A}(R)^{(d)}.$$

Roe proved that under suitable uniformity assumptions on the metric and the spinor bundle S you can take the “limit” as $n\to\infty$, and get

$$\lim_{t\to 0} m\{x\mapsto \mathrm{Tr}_x(\gamma_x e^{-tD^2}(x,x))\} = m\{\widehat{A}(R)\}.$$

The Roe index theorem (cont.)

The local index theorem implies that for every n,

$$\lim_{t\to 0} \frac{1}{|M_n|}\int_{M_n} \mathrm{Tr}_x(\gamma_x e^{-tD^2}(x,x))\,dx = \frac{1}{|M_n|}\int_{M_n} \widehat{A}(R)^{(d)}.$$

Roe proved that under suitable uniformity assumptions on the metric and the spinor bundle S you can take the "limit" as $n\to\infty$, and get

$$\lim_{t\to 0} m\{x \mapsto \mathrm{Tr}_x(\gamma_x e^{-tD^2}(x,x))\} = m\{\widehat{A}(R)\}.$$

Roe's mysticism: The limit on the left hand side is unnecessary, and we have

$$m\{x\mapsto P_{\ker(D_+)}(x,x) - P_{\ker(D_-)}(x,x)\} = m\{\widehat{A}(R)\}.$$

This is the Roe index theorem.

A Dixmier trace perspective on Roe's index theorem

I claim that if $0 \leq W \in L_{1,\infty}(M)$, then

$$\lim_{t\to 0} \mathrm{Tr}_\omega(\gamma e^{-tD^2} M_W) = \mathrm{Tr}_\omega(\widehat{A}(R)W).$$

This is, if you like, a "Dixmier local index theorem".

A Dixmier trace perspective on Roe's index theorem

I claim that if $0 \leq W \in L_{1,\infty}(M)$, then

$$\lim_{t\to 0} \mathrm{Tr}_\omega(\gamma e^{-tD^2} M_W) = \mathrm{Tr}_\omega(\widehat{A}(R)W).$$

This is, if you like, a "Dixmier local index theorem".

"Proof": We have

$$\begin{aligned}
\lim_{t\to 0} \mathrm{Tr}_\omega(\gamma e^{-tD^2} M_W) &= \lim_{t\to 0}\lim_{s\to 1}(s-1)\mathrm{Tr}(\gamma e^{-tD^2} M_W^s) \\
&= \lim_{s\to 1}\lim_{t\to 0}(s-1)\mathrm{Tr}(\gamma e^{-tD^2} M_W^s) \\
&= \lim_{s\to 1}(s-1)\int_M \widehat{A}(R)W^s \\
&= \mathrm{Tr}_\omega(\widehat{A}(R)W).
\end{aligned}$$

Regular exhaustions and $L_{1,\infty}(M)$

I also claim that associated to every regular exhaustion $M = \bigcup_{n=0}^{\infty} M_n$, there is a function $W \in L_{1,\infty}(M)$ such that $dW \in L_1(M)$.
Roughly speaking, W should be

$$W(x) = \frac{1}{|M_n|} \text{ where } n = \min\{k \geq 0 \ : \ x \in M_k\}$$

except smooth.

Regular exhaustions and $L_{1,\infty}(M)$

I also claim that associated to every regular exhaustion $M = \bigcup_{n=0}^{\infty} M_n$, there is a function $W \in L_{1,\infty}(M)$ such that $dW \in L_1(M)$.
Roughly speaking, W should be

$$W(x) = \frac{1}{|M_n|} \text{ where } n = \min\{k \geq 0 \ : \ x \in M_k\}$$

except smooth. We have,

$$\frac{d}{dt}\mathrm{Tr}_\omega(\gamma e^{-tD^2} M_W) = \frac{1}{2}\mathrm{Tr}_\omega(\gamma e^{-tD^2} D[D, M_W]).$$

But since $dW \in L_1(M)$... this is (probably) just zero!

Regular exhaustions and $L_{1,\infty}(M)$

I also claim that associated to every regular exhaustion $M = \bigcup_{n=0}^{\infty} M_n$, there is a function $W \in L_{1,\infty}(M)$ such that $dW \in L_1(M)$.
Roughly speaking, W should be

$$W(x) = \frac{1}{|M_n|} \text{ where } n = \min\{k \geq 0 \ : \ x \in M_k\}$$

except smooth. We have,

$$\frac{d}{dt}\mathrm{Tr}_\omega(\gamma e^{-tD^2} M_W) = \frac{1}{2}\mathrm{Tr}_\omega(\gamma e^{-tD^2} D[D, M_W]).$$

But since $dW \in L_1(M)$... this is (probably) just zero!
Mysticism: When W is chosen correctly, $\mathrm{Tr}_\omega(\gamma e^{-tD^2} M_W)$ is independent of t, and we have

$$\mathrm{Tr}_\omega(\gamma e^{-tD^2} M_W) = \mathrm{Tr}_\omega(\widehat{A}(R) W).$$

A "Dixmier-Roe index theorem"

Optimistically, we can take the limit as $t \to \infty$ to arrive at

$$\mathrm{Tr}_\omega((P_{\ker(D_+)} - P_{\ker(D_-)})M_W) = \mathrm{Tr}_\omega(\widehat{A}(R)W).$$

A "Dixmier-Roe index theorem"

Optimistically, we can take the limit as $t \to \infty$ to arrive at

$$\mathrm{Tr}_\omega((P_{\mathrm{ker}(D_+)} - P_{\mathrm{ker}(D_-)})M_W) = \mathrm{Tr}_\omega(\widehat{A}(R)W).$$

Even if this can all be made into proper mathematics, this is not a new index theorem, but simply a restatement of Roe's index theorem.

Thank you for listening!