The Dixmier trace and the Density of States

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Based on joint work with N. Azamov, E. Hekkelman F. Sukochev and D. Zanin.

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Introduction

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

- Azamov, M., Sukochev. and Zanin *A Dixmier Trace Formula for the Density of States* Comm. Math. Phys. 377 (2020), no. 3, 2597–2628. `arXiv:1910.12380`.
- Azamov, Hekkelman, M., Sukochev and 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

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

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But their use is not limited to NCG. Today I will talk about one Dixmier trace formula which is meaningful in mathematical physics.

This formula was conjectured and proved on the basis of developments in NCG.

Section 1: The density of states of Schrödinger operators

The fundamental problem

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

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

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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,

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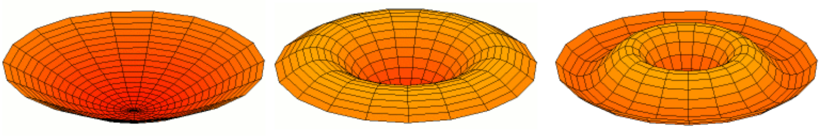
On $L_2(B(0, R))$, we can define the Dirichlet Laplace operator with Dirichlet boundary conditions, Δ_R.

Physical setting

The operator Δ_R is negative semidefinite and has purely discrete spectrum.



As $R \to \infty$, $N(t, -\Delta_R) \sim R^d$.

Schrödinger operators on bounded domains

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

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.

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What does the spectrum of H look like? The spectral counting function usually does not make sense for Schrödinger operators on $\mathbb{R}^d$, since the spectrum can be continuous.

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

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

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.

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- 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 V (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

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

Insensitivity to localised perturbations

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For example, if $V_1, V_0 \in L_\infty(\mathbb{R}^d)$ are such that $V_1 - V_0$ is compactly supported, then

$$\nu_{-\Delta+M_{V_1}} = \nu_{-\Delta+M_{V_0}}.$$

(assuming that both measures exist, of course.)

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 weak trace class

A compact operator T is said to be weak trace-class ($T \in \mathcal{L}_{1,\infty}$) if $\mu(k, T) = \mathcal{O}(k^{-1})$. Equivalently,

$$\|T\|_{1,\infty} := \sup_{k \geq 0} (1+k)\lambda(k, |T|) < \infty.$$

The class $\mathcal{L}_{1,\infty}$ is an an ideal.

Dixmier traces

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If $T \in \mathcal{L}_{1,\infty}$, then

$$\sum_{k=0}^{N} \lambda(k, T) = \mathcal{O}(\log(N)), \quad N \to \infty.$$

An extended limit is a linear functional $\omega \in \ell_\infty(\mathbb{N})^*$ which coincides with the "limit" functional on the subspace of convergent sequences.
If $T \geq 0$ is a positive element of $\mathcal{L}_{1,\infty}$, define $\mathrm{Tr}_\omega(T)$ as

$$\mathrm{Tr}_\omega(T) = \omega\left(\left\{\frac{1}{\log(2+N)}\sum_{k=0}^{N}\mu(k, T)\right\}_{N=0}^{\infty}\right).$$

Connes' integral formula

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

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A property of Dixmier traces (and all traces on $\mathcal{L}_{1,\infty}$) is that they vanish on finite rank operators. It was probably Connes whose realised that this property makes Dixmier traces computable in many situations. (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 described above.
2. Makes some computations very easy. For example, when V is radially homogeneous (i.e., $V(r\xi) = V(\xi)$ for all $r > 0$). In this case, the DOS exists and

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

See N. Azamov, E. M., F. Sukochev and D. Zanin *The density of states depends on the domain* Oper. Matrices **16**, No. 4 (2022), 1185–1189 `arXiv:2107.09828`.

Section 2: Recent developments

Trace formulas

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In particular:

1. The underlying space does not need to be Euclidean
2. The operator does not need to be Schrödinger operator.

A general theorem

If (X, d_X) is a measure space equipped with a Borel measure μ, and H is an operator on $L_2(X, \mu)$, we can define a density of states for H in a similar way to how it was defined for Schrödinger operators on $\mathbb{R}^d$.

General form

Let (X, d_X) be a metric space equipped with a measure μ *satisfying certain assumptions*. Let H be a self-adjoint operator on $L_2(X)$ *satisfying certain assumptions* for which the DOS ν_H exists *in some particular sense*. Then for a certain (fixed) function $w \in L_\infty(X)$ and for all Dixmier traces Tr_ω and for all $f \in C_c(\mathbb{R})$ we have

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

where c is a constant depending on w but not H or f.

We have proved this theorem in two different settings, using totally different methods.

Azamov–Hekkelman–M.–Sukochev–Zanin (2022)

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

Hekkelman–M. (2023)

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

In both cases, $x_0 \in X$ is some fixed base-point.

Section 3: The Roe index theorem

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

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

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Theorem (Patodi (1971), Gilkey (1973), Atiyah–Bott-Patodi (1973))

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 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 continuous 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

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

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Roe's non-compact McKean–Singer identity: 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. The left hand side is called $\mathrm{Ind}_\tau(D)$, the Roe index.

The process of “dividing by the volume and taking the limit” used in the formulation of the Roe index theorem is reminiscent of the density of states. Is there a Dixmier trace formmula for the Roe index?

A "Dixmier–McKean–Singer" formula

Theorem (Hekkelman-M. (2023))

Under (admittedly quite restrictive) technical assumptions, the Roe index is given by the Dixmier trace formula

$$\mathrm{Tr}_\omega(\gamma \exp(-tD^2)M_w) = \mathrm{Ind}_\tau(D).$$

Here, w is the function $w(x) = \frac{1}{1+|B(x_0,d_X(x_0,x))|}$.

Thank you for listening!