A Dixmier trace formula for the density of states and Roe's index theorem

Wollongong OANCG Seminar

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Aims of this talk

1. Explain the concept of the density of states
2. Connect this concept to noncommutative geometry
3. Highlight a link with Roe's index theorem

This talk is based on

- unpublished progress with Ed McDonald;
- the paper 'An application of singular traces to crystals and percolation', by Azamov, H., McDonald, Sukochev and Zanin, Journal of Geometry and Physics, Volume 179, 2022.

Part 1: The density of states

Quantum physics

Physicists describe physical systems with a **Schrödinger operator** H on a Hilbert space $\mathcal{H}$. We will focus on describing electrons in a material in this manner.

Electrons can only be in very specific 'states', with associated discrete energy levels.

The allowed energy levels are usually the **eigenvalues** of H, and the corresponding states are the **eigenvectors**.

More generally, the entire spectrum of H is interpreted as the admitted energy levels, even though there might not be corresponding eigenvectors.

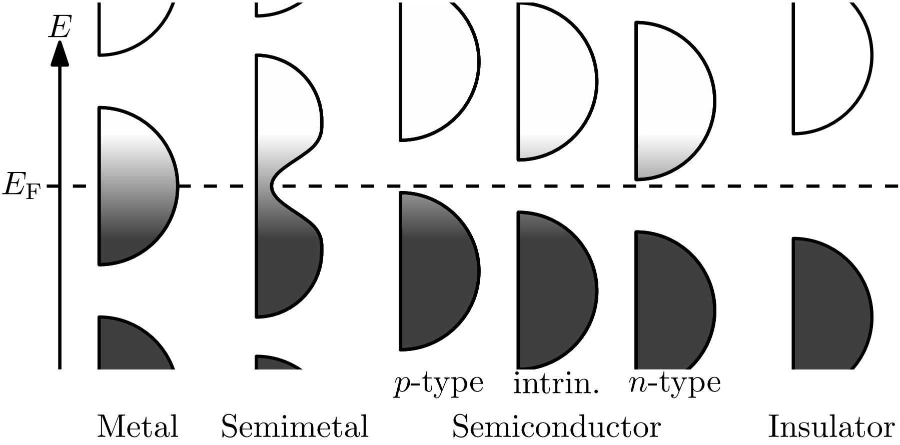
The density of states

In solid-state physics, the **density of states (DOS)** describes (usually) how many electrons can have a certain energy level, per unit volume of some material.

It is derived from the Schrödinger operator of the system.

The DOS gives rise to the electronic band structure of a material.

Electronic band structure



Getting more concrete

Suppose we model a material as some space X with a **Schrödinger operator** H on the Hilbert space $L_2(X)$. The density of states in its simplest form gives for each eigenvalue λ of H the dimension of the corresponding eigenspace divided by the volume of X.

We have to be more clever when the volume of X is infinite, and H does not have eigenvalues. **Idea:** restrict H to a ball, look at the DOS on there, and blow the ball up.

Conventions and notation

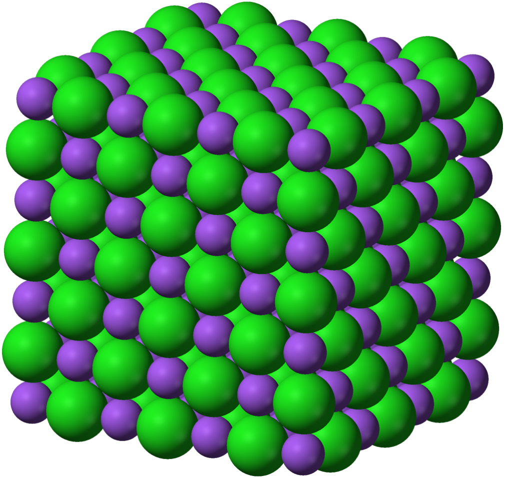
Let us stick to the following:

- Spaces X are assumed to be metric spaces with a Borel measure;
- A ball $B(x_0, R) \subset X$ is defined as

$$B(x_0, R) = \{x \in X : d(x, x_0) \leq R\};$$

- The measure of a set $B \subset X$ is denoted by $|B|$;
- We assume $0 < |B(x_0, R)| < \infty$ for all $x_0, R > 0$.

Typical crystal



From physics to math

Useful fact: if H is a self-adjoint operator with eigenvalue λ, the projection onto the eigenspace corresponding to λ is $\chi_{\{\lambda\}}(H)$. Hence $\mathrm{Tr}(\chi_{\{\lambda\}}(H))$ is the dimension of this eigenspace.

Idea: we can try to construct a measure ν_H such that for $E_1, E_2 \in \mathbb{R}$,

$$\nu_H((E_1, E_2)) = \lim_{R\to\infty} \frac{1}{|B(x_0, R)|} \mathrm{Tr}(\chi_{(E_1,E_2)}(H) M_{\chi_{B(x_0,R)}}),$$

where M_f is the multiplication operator $g \mapsto fg$ on $L_2(X)$.

Definition of the DOS (1/2)

Definition (DOS)

Let H be a self-adjoint, not necessarily bounded operator on $L_2(X)$. This operator is said to have a *density of states* with respect to a fixed base-point $x_0 \in X$ if for all functions $f \in C_c(\mathbb{R})$ the following limit exists:

$$\lim_{R\to\infty} \frac{1}{|B(x_0, R)|} \mathrm{Tr}(f(H) M_{\chi_{B(x_0,R)}}).$$

Definition of the DOS (2/2)

Definition (DOS, cont.)

If this limit indeed exists for all $f \in C_c(\mathbb{R})$, then

$$f \mapsto \lim_{R\to\infty} \frac{1}{|B(x_0, R)|} \mathrm{Tr}(f(H)M_{\chi_{B(x_0,R)}})$$

defines a positive linear functional on $C_c(\mathbb{R})$ and hence by the Riesz–Markov–Kakutani theorem there is a Borel measure ν_H on $\mathbb{R}$ such that

$$\lim_{R\to\infty} \frac{1}{|B(x_0, R)|} \mathrm{Tr}(f(H)M_{\chi_{B(x_0,R)}}) = \int_{\mathbb{R}} f d\nu_H$$

for all $f \in C_c(\mathbb{R})$. The measure ν_H is called the *density of states*.

Sanity check

This definition agrees with our intuition:

Proposition

If the function $\mathbb{R} \ni E \mapsto \nu_H((-\infty, E))$ exists and is continuous at E_1 and E_2, then

$$\nu_H((E_1, E_2)) = \lim_{R\to\infty} \frac{1}{|B(x_0, R)|} \mathrm{Tr}(\chi_{(E_1,E_2)}(H) M_{\chi_{B(x_0,R)}}).$$

See for example Proposition C.7.1 in B. Simon's *Schrödinger Semigroups*, Bull. Am. Math. Soc. 1982.

Part 2: Connecting the density of states to noncommutative geometry

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 $A \in \mathcal{L}_1$, $\mathrm{Tr}_\omega(A) = 0$.

Noncommutative geometry

The Dixmier trace is interpreted as a 'noncommutative integral' in Connes' noncommutative geometry. This is illustrated by results like Connes' trace formula on $\mathbb{R}^d$: for $f \in C_c(\mathbb{R}^d)$, we have for all Dixmier traces Tr_ω

$$\mathrm{Tr}_\omega(M_f(1-\Delta)^{-d/2}) = C_d \int_{\mathbb{R}^d} f(t)dt,$$

where Δ is the Laplacian on $\mathbb{R}^d$.

Hence, the Dixmier trace recovers integration with the Lebesgue measure. The core message of this talk is that integration with respect to the DOS measure can be achieved via the Dixmier trace.

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 $w \in L_\infty(X)$, there exists a constant $c > 0$ such that for all extended limits 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 non-compact manifold of bounded geometry plus some geometrical conditions, H a self-adjoint, lower bounded, elliptical second-order differential operator, $w(x) = \frac{1}{1+|B(x_0,d_X(x_0,x))|}$.

Explicit result

H., McDonald (WIP, 2023?)

Let (X, g) be a non-compact Riemannian manifold of bounded geometry with *Property (D)*. Let $P \in EBD^2(X)$ be self-adjoint and lower-bounded, and let w be the function on X defined by

$$w(x) = (1 + |B(x_0, d_X(x, x_0))|)^{-1}, \quad x \in X.$$

Then $f(P)M_w$ is an element of $\mathcal{L}_{1,\infty}$ for all compactly supported functions $f \in C_c(\mathbb{R})$. If P admits a density of states ν_P, we have for all extended limits ω

$$\mathrm{Tr}_\omega(f(P)M_w) = \int_{\mathbb{R}} f(\lambda) d\nu_P(\lambda), \quad f \in C_c(\mathbb{R}).$$

Part 3: Index theory

Atiyah–Singer's index theorem

Atiyah–Singer's index theorem concerns compact Riemannian manifolds, and famously connects analysis with topology.

Atiyah–Singer

Let X be a compact Riemannian manifold with vector bundles $E \to X$ and $F \to X$, and let $D : \Gamma(E) \to \Gamma(F)$ be a linear elliptical differential operator. Then

$$\mathrm{Ind}(D) = \int_X \mathbf{I}(D),$$

where $\mathrm{Ind}(D)$ is the Fredholm index of D and $\mathbf{I}(D)$ is topological in nature.

K-theory

Recall the cyclic six term exact sequence in K-theory,

$$\begin{array}{ccccc} K_0(J) & \longrightarrow & K_0(A) & \longrightarrow & K_0(A/J) \\ {\scriptstyle Ind}\uparrow & & & & \downarrow \\ K_1(A/J) & \longleftarrow & K_1(A) & \longleftarrow & K_1(J) \end{array}$$

where A is a C^*-algebra and $J \subset A$ an ideal.
For $A = B(\mathcal{H})$ and $J = K(\mathcal{H})$ the compact operators, the map *Ind* gives exactly the Fredholm index.

Non-compact manifolds

Now let X be a non-compact Riemannian manifold of bounded geometry, $S \to X$ a Clifford bundle, D an elliptic differential operator (of a suitable type) on $L_2(S)$. In general, D is not invertible modulo compact operators (Fredholm), so the Fredholm index is not defined.

However, Roe shows that D is invertible modulo so-called 'uniformly smoothing operators' $U_{-\infty}(X)$, which are operators with a particularly nice kernel k_A such that

$$Au(x) = \int_X k_A(x,y)u(y)\mathrm{vol}(y).$$

Analytical index

Hence, we can define an abstract index of D as an element of $K_0(U_{-\infty}(X))$.

Furthermore, if we can define some kind of trace $\tau : U_{-\infty}(X) \to \mathbb{R}$, this can be extended to a trace on $Mat(U_{-\infty}(X)^+)$ (the $^+$ denotes unitisation). The tracial property gives that this map then descends to a map called the dimension-homomorphism $\dim_\tau : K_0(U_{-\infty}(X)) \to \mathbb{R}$.

Therefore, a trace τ would give

$$\dim_\tau(\mathrm{Ind}(D)) \in \mathbb{R},$$

which is what Roe takes as the analytical index in his index theorem.

The details

Roe starts with taking a linear functional m on the Banach space of bounded d-forms $\Omega^d_\beta(X)$, such that

$$\liminf_{R\to\infty}\left| m(\alpha) - \frac{1}{|B(x_0,R)|}\int_{B(x_0,R)}\alpha\right| = 0.$$

One can always find such a functional, but to make it have desirable properties Roe puts a geometrical condition on X. It is implied by *Property (D)* used in our Dixmier trace formula for the DOS on manifolds.

Roe's trace

The trace τ on 'uniformly smoothing operators' $U_{-\infty}(X)$ is constructed using this functional m. Recall that uniformly smoothing operators A are given by a kernel k_A.

Since $\alpha_A : x \mapsto k_A(x,x)\mathrm{vol}(x)$ is a bounded d-form, we define

$$\tau(A) := m(\alpha_A), \quad A \in U_{-\infty}(X).$$

Note,

$$\begin{aligned}\tau(A) &= \lim_{R\to\infty} \frac{1}{|B(x_0,R)|} \int_{B(x_0,R)} k_A(x,x)\mathrm{vol}(x) \\ &= \lim_{R\to\infty} \frac{1}{|B(x_0,R)|} \mathrm{Tr}(AM_{\chi_{B(x_0,R)}})\end{aligned}$$

if the RHS converges.

Roe's index theorem

Roe's index theorem

Let X be a non-compact Riemannian manifold of bounded geometry (plus an extra geometric condition). Let $S^+ \oplus S^- = S \to X$ be a Clifford bundle with grading η, and let $D = \begin{pmatrix} 0 & D_- \\ D_+ & 0 \end{pmatrix}$ be a Dirac operator on S. Then

$$\dim_\tau(\mathrm{Ind}(D)) = m(\mathbf{I}(D)).$$

Essential step of the proof: for any Schwartz function f on $\mathbb{R}$ such that $f(0) = 1$, we have

$$\dim_\tau(\mathrm{Ind}(D)) = \tau(\eta f(D^2)).$$

'Dixmier-Roe' index theorem

Note that if D^2 admits a density of states, then (sketch):

$$\begin{aligned}\tau(f(D^2)) &= \lim_{R\to\infty} \frac{1}{|B(x_0,R)|}\mathrm{Tr}(f(D^2)M_{\chi_{B(x_0,R)}})\\ &= \int_{\mathbb{R}} f d\nu_{D^2}\\ &= \mathrm{Tr}_\omega(f(D^2)M_w).\end{aligned}$$

Therefore, (sparing you some technicalities),

$$\mathrm{Tr}_\omega(\eta f(D^2)M_w) = \dim_\tau(\mathrm{Ind}(D)) = m(\mathbf{I}(D)).$$

Thanks

Thank you for your attention!