The density of states and Roe's index theorem

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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This talk is based on unpublished progress, and the paper 'An application of singular traces to crystals and percolation', by Azamov, H., McDonald, Sukochev and Zanin, Journal of Geometry and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

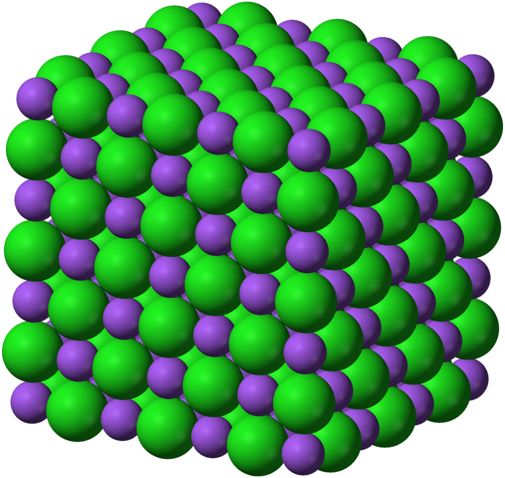
Crash course solid-state physics

A fundamental object in the study of materials is the **density of states (DOS)**. It (usually) describes how many electrons can have a certain energy, per unit volume of the material.

We can model a material as some space X, with a **Schrödinger operator** H on the Hilbert space $L_2(X)$ encoding the laws of physics. 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.

Typical crystal



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.

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 $\ell_2(X)$.

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 $w \in L_\infty(X)$, 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, $w(x) = \frac{1}{1+|B(x_0, d_X(x_0,x))|}$.

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.

Non-compact manifolds

In the non-compact case, neither $\mathrm{Ind}(D)$ nor $\int_X \mathbf{I}(D)$ is well-defined.

John Roe modified both sides to produce an index theorem for non-compact Riemannian manifolds of bounded geometry (plus an extra geometric condition).

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

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

Roe's trace

The functional m defines a trace on 'uniformly smoothing operators' $U_{-\infty}(X)$, which are operators with a particularly nice kernel k_A such that

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

Namely, 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

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

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!