A Dixmier trace formula for the density of states

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Introduction

This talk is about a surprising connection between the density of states and Dixmier traces, based on the paper

N. Azamov, E. McDonald, F. S. and D. Zanin: *A Dixmier Trace Formula for the Density of States* Commun. Math. Phys. (2020)

See also `arXiv:1910.12380 [math-ph]`.

Physical setting

Let $d > 1$ and $L > 0$. Let Ω_L be the open d-cube of side length $2L$. That is,

$$\Omega_L := (-L, L)^d.$$

The linear operator $\Delta = \sum_{j=1}^{d} \frac{\partial^2}{\partial x_j^2}$ is essentially self-adjoint on $C_c^\infty(\Omega_L) \subset L_2(\Omega_L)$. The closure is Δ_L, the Dirichlet Laplacian on Ω_L. That is, Δ_L is the Laplace operator on functions vanishing on the boundary of Ω_L.
The operator Δ_L is negative semidefinite, and the resolvent $(1 - \Delta_L)^{-1}$ is compact.
Given $V \in L_\infty(\Omega_L)$, denote by M_V the operator of pointwise multiplication by V. That is, $(M_V\xi)(t) = V(t)\xi(t)$.

Schrödinger operators

For the purposes of this talk a *Schrödinger operator* on Ω_L is a linear operator

$$H = -\Delta_L + M_V.$$

where V is real-valued. Since we only consider bounded V, the H is self-adjoint with domain equal to that of Δ_L. Since H is a relatively compact perturbation of $-\Delta_L$, the spectrum of H is discrete and consists only of eigenvalues of finite multiplicity. (In the language of spectral theory, H has no essential spectrum).

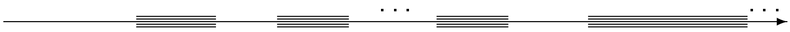
Schrödinger operators on $\mathbb{R}^d$

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

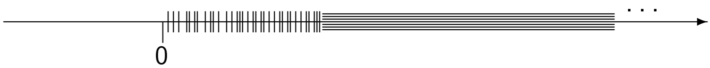
$$H = -\Delta + M_V$$

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:



Spectral counting function

Let $H = -\Delta_L + M_V$ be a Schrödinger operator on Ω_L. Since the spectrum of H consists of eigenvalues of finite multiplicity, we can define the *spectral counting function*:

$$N(t, H) = \mathrm{tr}(\chi_{(-\infty,t]}(H)), \quad t \in \mathbb{R}.$$

Equivalently, $N(t, H)$ is the dimension of the span of the eigenfunctions of H with corresponding eigenvalue $\leq t$. Since H is lower bounded and has no essential spectrum, we have $N(t, H) < \infty$ for all $t \in \mathbb{R}$.
If we replace Ω_L with $\mathbb{R}^d$, then the inequality $N(t, H) < \infty$ is also true for $t \leq 0$ (under certain conditions on V). These are famous Cwikel-Lieb-Rozenblum estimates.

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 physics.) Let $L > 0$, and "restrict" H to $(-L, L)^d$:

$$H_L := -\Delta_L + M_V$$

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

$$\nu_H((-\infty, t]) := \lim_{L\to\infty} \frac{N(t, H_L)}{(2L)^d}, \quad t \in \mathbb{R}.$$

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 $L \to \infty$ 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_L? Answer: No. If you use Dirichlet, Neumann or periodic boundary conditions on $(-L, L)^d$, it results in the same ν_H.
- Does it matter that we "restricted" H to cubes $(-L, L)^d$? Could we have used some other sequence $\{\Omega_L\}_{L>0}$ of domains approximating $\mathbb{R}^d$? Answer: We are not aware if this question has been studied in the literature. This could be open.

Example

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

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

Weak trace ideal

Now for something completely different. Let $\mathcal{H}$ be a Hilbert space. If T is a compact operator on H, the singular value sequence of T is defined as

$$\mu(k, T) := \inf\{\|T - R\|_{\mathrm{op}} \ : \ \mathrm{rank}(R) \leq k\}, \quad k \geq 0.$$

(Equivalently, $\mu(T) = \{\mu(k, T)\}_{k=0}^{\infty}$ is the sequence of eigenvalues of the absolute value $|T|$ arranged in non-increasing order with multiplicities.)
A compact operator T is said to be weak trace-class ($T \in \mathcal{L}_{1,\infty}$) if $\mu(k, T) = O(k^{-1})$. Equivalently,

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

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

Dixmier traces

The ideal $\mathcal{L}_{1,\infty}$ admits *traces*. That is, there exist nontrivial unitarily invariant linear functionals on $\mathcal{L}_{1,\infty}$.

An important class of examples are the famous Dixmier traces. 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

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

It is a theorem that tr_ω extends to a continuous linear unitarily invariant functional on $\mathcal{L}_{1,\infty}$.

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.

His student Alain Connes realized that this is what makes them useful.

(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

$$\begin{aligned}\mathrm{tr}_\omega(M_f(1-\Delta)^{-\frac{d}{2}}) &= \frac{\mathrm{Vol}(S^{d-1})}{d(2\pi)^d}\int_{\mathbb{R}^d} g(|t|^2)\,dt\\ &= \frac{\mathrm{Vol}(S^{d-1})^2}{2d(2\pi)^d}\int_0^\infty g(r)r^{\frac{d}{2}-1}\,dr.\end{aligned}$$

Switch to the Fourier side (recall that tr_ω is unitarily invariant!) and we get

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

where ν is the measure $d\nu(r) = \frac{\mathrm{Vol}(S^{d-1})}{2(2\pi)^d}r^{\frac{d}{2}-1}\,dr$.
This measure ν 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 ν_H on $\mathbb{R}$ such that

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

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

Theorem

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, if V is positively homogeneous (i.e. $V(\lambda t) = V(t)$ for all $\lambda > 0$) then

$$\nu_H((-\infty, t])) = \frac{1}{d(2\pi)^d} \int_{S^{d-1}} \max\{t - V(\xi), 0\}^{\frac{d}{2}}\, d\xi.$$

We think that the latter formula is new. Its proof follows from the Dixmier trace formula for DOS and some pre-existing work on Connes' Trace Theorem.

Lies and omissions in this talk

1. Technically we proved the result for the DOS defined on via approximation of $\mathbb{R}^d$ by balls, rather than cubes.
2. We did not use the "physicists" definition of DOS. Instead, we defined DOS by the following formula (taken from Simon)

$$\nu_H(I) = \lim_{R\to\infty} \frac{1}{\mathrm{Vol}(B(0,R))} \mathrm{Tr}(M_{\chi_{B(0,R)}} \chi_I(H) M_{\chi_{B(0,R)}}).$$

These definitions known to coincide for many important classes of potenetials, however, the general equivalence theorem remains open.

Thank you!