Asymptotic distribution of eigenvalues of Laplace operator

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We will talk about:

- the number of eigenvalues of Laplace operator smaller than some $\lambda$ as a function of $\lambda$
- asymptotic behaviour of this function for $\lambda \to \infty$
- the use of all of this in statistical physics
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Still, this theorem is used in statistical physics without any proof, nor proper formulation. We just say that entropy is the same in all containers, depending only on their volume.

Let’s discover how and why this works!
Number of states of self-adjoint operator $A$ smaller than some $\lambda$ is number of eigenfunctions that have eigenvalues smaller than this $\lambda$. We denote it $N_A(\Omega, \lambda)$, where $\Omega$ is the domain of the functions in the domain of the operator $A$. 

Correct for operators with only point spectrum!
Number of states

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Correct for operators with only point spectrum!

**Definition**

Let $A$ be self-adjoint operator, defined on some dense subset of Hilbert space and bounded from below. Number of states of this operator is equal to:

$$N_A(\Omega, \lambda) = \dim \text{Im} P_{(-\infty, \lambda)}$$

where $P_{(-\infty, \lambda)}$ is projection-valued measure.

We just have to count the number of point of spectra smaller than $\lambda$ and if there is essential spectrum, than number of states is infinity.
Density of states is just the value of derivation of the number of states in some point. We use it to obtain entropy of ideal gas. The important point is that entropy is function of:

$$\ln \left( \frac{d}{d\lambda} N_D(\Omega, \lambda) \right)$$

where $N_D(\Omega, \lambda)$ stands for number of states of (minus) Laplace operator with Dirichlet boundary condition on the bounder of $\Omega$. We mark this operator $-\Delta^\Omega_D$. In 3 dimensions it looks like this:

$$-\Delta^\Omega_D = -\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} - \frac{\partial^2}{\partial z^2}$$
Density of states and statistical physics

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But that is Hamilton’s operator for a particle trapped inside a box. Shape and volume of the box is defined by $\Omega$, since $\Omega$ is the box.
Let’s consider scalar particle trapped inside a box. We want to find all possible states of this particle by solving Schroedinger’s equation. The potential in Hamilton’s operator looks like this:

\[
V(x, y, z) = \begin{cases} 0 & (x, y, z) \in \Omega \\ \infty & (x, y, z) \notin \Omega \end{cases}
\]

Since we require the wave function to vanish outside \(\Omega\), this is the same as solving eigenvector-eigenvalue problem for operator \(-\triangle_{D}^{\Omega}\). We will ignore some constants in Hamilton’s operator. The solution for \(\Omega\) shaped like a cube is known.

We want to find number of states (and density of states) to get entropy.
Theorem (Weyl)

Let $\Omega$ be bounded, open and contented (Jordan measurable) subset of $\mathbb{R}^3$. Let $N_D(\Omega, \lambda)$ denote number of states of operator $-\Delta^\Omega_D$, who’s eigenvalues are smaller than $\lambda$ and let $V$ denote Jordan measure of $\Omega$. Then it holds that:

$$\lim_{\lambda \to \infty} \frac{N_D(\Omega, \lambda)}{\lambda^\frac{3}{2}} = \frac{V}{6\pi^2}$$

If we prove this theorem, we can estimate the entropy of a particle of ideal gas.
Important parts of the proof

The proof is based on combining few ideas:

- Known estimates for the cube
- Inequality of operators
- Min-max principle
Known estimates for the cube

We denote by $-\triangle^\Omega_N$ Laplace’s operator defined on subset of functions who’s normal derivative vanishes on the border of $\Omega$.

Let $\square$ denote $\Omega$ shaped like a cube, that satisfy the requirements of Weyl’s theorem. It holds that:

\[
\left| N_D(\square, \lambda) - \frac{V\lambda^\frac{3}{2}}{6\pi^2} \right| \leq C \left( 1 + \frac{V}{3} \lambda \right)
\]

\[
\left| N_N(\square, \lambda) - \frac{V\lambda^\frac{3}{2}}{6\pi^2} \right| \leq C \left( 1 + \frac{V}{3} \lambda \right)
\]

where $V$ is the volume of the cube and $C$ is some constant.
Operators and quadratic forms

Let $A$ be dense defined, semi-bounded and self-adjoint operator on some infinite dimensional Hilbert space $\mathcal{H}$, with eigenvectors $\psi_n$ and eigenvalues $\lambda_n$. If we pass to the spectral representation, image of some vector $\varphi \in \mathcal{H}$ is:

$$A\varphi = A \sum_{n=1}^{\infty} a_n \psi_n = \sum_{n=1}^{\infty} a_n \lambda_n \psi_n$$

which is true if and only if $\varphi$ is in operator domain $D(A)$. $\varphi \in D(A)$ if and only if:

$$(A\varphi, A\varphi) = \sum_{n=1}^{\infty} |a_n \lambda_n|^2 < \infty$$

Although some vector $\vartheta \in \mathcal{H}$ is in the domain of quadratic quadratic form assigned to $A$ if and only if:

$$(\vartheta, A\vartheta) = \sum_{n=1}^{\infty} |\lambda_n| |b_n|^2 < \infty$$
Definition

Let $\Omega$ be open region in $\mathbb{R}^n$. Dirichlet Laplace operator on $\Omega$, $-\triangle_D^\Omega$, is the only self-adjoint operator defined on $L^2(\Omega, d^m x)$, who’s quadratic form is the closure of the form:

$$q(f, g) = \int (\nabla f)^* \cdot \nabla g d^m x$$

with form domain $C_0^\infty(\Omega)$.

Definition

Let $\Omega$ be open region in $\mathbb{R}^n$. Neumann Laplace operator on $\Omega$, $-\triangle_N^\Omega$, is the only self-adjoint operator defined on $L^2(\Omega, d^m x)$, who’s quadratic form is:

$$q(f, g) = \int (\nabla f)^* \nabla g d^m x$$

with form domain $H^1(\Omega)$. 
Inequality of operators

Definition

Let operators $A, B$ have form domains $Q(A), Q(B)$ and let both be self-adjoint and positive. We say that:

$$0 \leq A \leq B$$

if and only if

$$Q(A) \supset Q(B)$$

$$\forall \psi \in Q(B) : (\psi, A\psi) \leq (\psi, B\psi)$$
Min-max principle

**Theorem**

Let $A$ denote bounded from below and self-adjoint operator. Let $\varphi_1 \ldots \varphi_{n-1}$ be any $n-1$ tuple of vectors. We define:

$$
\mu_n = \sup_{\varphi_1 \ldots \varphi_{n-1}} \left\{ \inf_{\chi \in Q(A), \|\chi\|=1, \chi \in [\varphi_1 \ldots \varphi_{n-1}]^\perp} (\chi, A\chi) \right\}
$$

The if we arrange the element of spectra of $A$ from the smallest up, counting even their multiplicity, then for a fix $n \in \mathbb{N}$ one of the following holds:

(a) $\mu_n$ is the $n^{th}$ eigenvalue of $A$.

(b) there is at most $n-1$ eigenvalues of $A$ smaller than $\mu_n$ and it holds that:

$$
\mu_n = \mu_{n+1} = \mu_{n+2} = \ldots
$$
Demonstration of min-max principle

Let’s demonstrate min-max principle on a well known quantum system: particle bound to a finite line.

The formula for $\mu_n$:

$$\mu_n = \sup_{\phi_1 \ldots \phi_{n-1}} \left\{ \inf_{\chi \in Q(H), \|\chi\|=1, \chi \in [\phi_1 \ldots \phi_{n-1}]^\perp} (\chi, H\chi) \right\}$$

According to the theorem $\mu_n$ is the $n^{th}$ eigenvalue of Hamilton’s operator. Let’s proceed from inside to outside. We have take all of the unit vectors $\chi$, which are orthogonal on some vectors $\phi_1 \ldots \phi_{n-1}$ and find the infimum of set containing elements $(\chi, H\chi)$. If we for example set $n = 3$, $\phi_1 \ldots \phi_{n-1}$ to be $\psi_{12}, \psi_{42}$, then the minimum is the first energy level $E_1$ and the $\chi$ for which the minimum happens is $\psi_1$.
Demonstration of min-max principle

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Now we have to do this for all tuples of vectors $\varphi_1 \ldots \varphi_{n-1}$ and find the supremum of this set. For the case of $n = 3$ we took $\psi_{12}, \psi_{42}$. But if we change one of them for $\psi_1$ then clearly mimicking the steps we did before the number we would get would be $E_2$, the second energy level. The ”correct” choice of vectors $\varphi_1 \ldots \varphi_{n-1}$ is to take $\psi_1, \psi_2$, which would give us $E_3$, the third eigenvalue of Hamilton’s operator.
Theorem

*If:*  

\[ 0 \leq A \leq B \]

*as defined before, then:*  

\[ N_A(\Omega, \lambda) \geq N_B(\Omega, \lambda) \]
Merging min-max principle and inequality of operators

**Theorem**

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**Proof.**

All we have to prove is that \( k \)th element of spectrum of operator \( A \) is smaller or equal the \( k \)th element of spectrum of operator \( B \). Since one of the requirements of definition of the inequality of operators is that:

\[ \forall \psi \in Q(B) : (\psi, A\psi) \leq (\psi, B\psi) \]

and because adding supremum and infimum preserves the inequality above, we get the expressions of elements of spectrum of both operators as in min-max principle.
Theorem

Let $\Omega_1$ and $\Omega_2$ be disjoint open subsets of open set $\Omega$. Let
\[(\Omega_1 \cup \Omega_2)^{int} = \Omega\] and let $\Omega \setminus (\Omega_1 \cup \Omega_2)$ have measure of 0. Then:

\[0 \leq -\Delta_D \Omega \leq -\Delta_D \Omega_1 \cup \Omega_2 \]
\[0 \leq -\Delta_N \Omega_1 \cup \Omega_2 \leq -\Delta_N \Omega \]
One more inequality theorem

**Theorem**

*For any $\Omega$ it holds that:*

\[
0 \leq -\Delta_{\Omega}^N \leq -\Delta_{\Omega}^D
\]

**Theorem**

*Let $\Omega \subset \Omega_0$, then it holds that:*

\[
0 \leq -\Delta_{\Omega}^{\Omega_0} \leq -\Delta_{\Omega}^D
\]
The proof

Let $\Omega$ be a contented set. We will call inner cubes all cubes of the same size that fit inside $\Omega$ without crossing the bounder of $\Omega$ and we will denote them $\Omega^-_n$. We will call outer cubes all cubes of the same size that cover all of $\Omega$ and denote them $\Omega^+_n$. We get inequalities in given order:

\[
0 \leq -\triangle\Omega^+_n \leq -\triangle\Omega^+_D
\]
\[
0 \leq -\triangle\Omega^-_n \leq -\triangle\Omega^-_D
\]
\[
0 \leq \oplus_{\alpha=1}^{A^+(n)} - \triangle C^+_{n,\alpha} \leq -\triangle\Omega^+_n
\]

which sums up to:

\[
0 \leq \oplus_{\alpha=1}^{A^+(n)} - \triangle C^+_{n,\alpha} \leq -\triangle\Omega_D
\]

That means:

\[
N_D(\Omega, \lambda) \leq \sum_{\alpha=1}^{A^+(n)} N_N(C^+_{n,\alpha}, \lambda)
\]
The proof

Similarly we get:

\[ 0 \leq -\Delta_D \leq \bigoplus_{\alpha=1}^{A^- (n)} - \triangle_{C_{n,\alpha}} \]

which leads us to:

\[
\sum_{\alpha=1}^{A^- (n)} N_D (C_{n,\alpha}, \lambda) \leq N_D (\Omega, \lambda)
\]

Now we have to put together both inequalities of numbers of states:

\[
\sum_{\alpha=1}^{A^- (n)} N_D (C_{n,\alpha}, \lambda) \leq N_D (\Omega, \lambda) \leq \sum_{\alpha=1}^{A^+ (n)} N_N (C_{n,\alpha}, \lambda)
\]

which after dividing by \( \lambda^{\frac{3}{2}} \) and passing to limits as \( \lambda \to \infty \) and \( n \to \infty \) we get:

\[
\frac{V}{6\pi^2} \leq \liminf_{\lambda \to \infty} N_D (\Omega, \lambda) \lambda^{-\frac{3}{2}} \leq \limsup_{\lambda \to \infty} N_D (\Omega, \lambda) \lambda^{-\frac{3}{2}} \leq \frac{V}{6\pi^2}
\]

which proves Weyl’s theorem.
The use in statistical physics

We have proven that:

\[ N_D(\Omega, \lambda) = \frac{V}{6\pi^2} \lambda^\frac{3}{2} + o(\lambda^\frac{3}{2}) \]
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Let's suppose that:

\[ N_D(\Omega, \lambda) = \frac{V}{6\pi^2} \lambda^{\frac{3}{2}} + C_1 \lambda + C_2 \lambda^{\frac{1}{2}} \]

as in the case of a cube. This, when used in the formula for entropy, gives us:

\[
\ln \left( \frac{d}{d\lambda} N_D(\Omega, \lambda) \right) = \ln \left( \frac{V}{4\pi^2} \lambda^{\frac{1}{2}} \right) + \ln \left( 1 + \frac{4\pi^2 C_1}{V} \lambda^{-\frac{1}{2}} + \frac{4\pi^2 C_2}{V} \lambda^{-1} \right)
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\]

If we consider one electron in box shaped like a cube with the volume of 1\(m^3\) at temperature 300\(K\), then:

\[ \lambda \approx 10^{18} m^{-2} \]
Numerical simulation

Asymptotic distribution of eigenvalues of Laplace operator
Thank you for your attention.