Some Mathematical and Physical Background

Linear partial differential operators

Let H be a second-order, elliptic, self-adjoint PDO, on scalar functions, in a d-dimensional region Ω.

Prototypical categories

- **Billiard:** $H = -\nabla^2$, $\Omega \subset \mathbf{R}^d$, boundary conditions (say Dirichlet, $u = 0$ on $\partial\Omega$). *Example:* Ω = rectangular parallelepiped in $\mathbf{R}^3$ ("brick"),

$$-H = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\,,$$

$$\begin{aligned} u(0,y,z) = u(L_1,y,z) = u(x,0,z) = u(x,L_2,z) \\ = u(x,y,0) = u(x,y,L_3) = 0. \end{aligned}$$

- **Laplace–Beltrami operator:** $\Omega = d$-dimensional Riemannian manifold (without boundary),

$$Hu = -\Delta_g u = -\sum_{j,k=1}^{d} \frac{1}{\sqrt{g}} \frac{\partial}{\partial x^j} \left[\sqrt{g}\, g^{jk} \frac{\partial u}{\partial x^k} \right].$$

  Example: $\Omega = 2$-sphere,

$$Hu = -\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial u}{\partial\theta} \right) - \frac{1}{\sin^2\theta} \frac{\partial^2 u}{\partial\phi^2}\,.$$

- **Schrödinger operator:** $\Omega = \mathbf{R}^d$ (say),

$$H = -\nabla^2 + V(\mathbf{x}).$$

  Example: Harmonic oscillator ($d = 1$),

$$H = -\frac{d^2}{dx^2} + x^2.$$

Ignoring: external magnetic potential
Neumann and Robin boundary conditions
fourth-order operators, etc.
pseudodifferential operators
vector field u (electromagnetism)
first-order elliptic system (Dirac field)

Spectral decomposition

All the examples so far have discrete spectrum.
Eigenvalues and normalized eigenvectors:

$$H\varphi_n = E_n\varphi_n\,, \qquad \|\varphi_n\|^2 = \int_\Omega |\varphi_n(x)|^2\,dx = 1.$$

$$u(x) = \sum_{n=1}^{\infty} c_n\varphi_n(x), \quad c_n = \langle\varphi_n, u\rangle = \int_\Omega \overline{\varphi_n(x)}u(x)\,dx.$$

$$f(H)u = \sum_{n=1}^{\infty} f(E_n)c_n\varphi_n\,.$$

In other words, H is diagonal in this basis.

Examples

- **Brick:** $\varphi_{mnp} = \sqrt{\dfrac{2^3}{L_1L_2L_3}}\sin\dfrac{m\pi x}{L_1}\sin\dfrac{n\pi y}{L_2}\sin\dfrac{p\pi z}{L_3}$,

  $$E_{mnp} = \left(\frac{m\pi}{L_1}\right)^2 + \left(\frac{n\pi}{L_2}\right)^2 + \left(\frac{p\pi}{L_3}\right)^2 \quad (m, n, p \in \mathbf{Z}^+).$$

- **Sphere:** $E_l = l(l+1)$, $l \in \mathbf{N}$, $m = -l, \ldots, l-1, l$.

  $$\varphi_{lm} = Y_l^m(\theta,\phi) = \left[\frac{2l+1}{4\pi}\,\frac{(l-m)!}{(l+m)!}\right]^{\frac{1}{2}} P_l^m(\cos\theta)e^{im\phi}$$

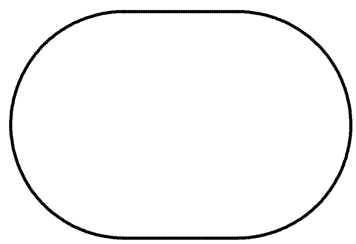
  (spherical harmonic).

- **Harmonic oscillator:** $E_n = 2n + 1 \quad (n \in \mathbf{N})$,

$$\varphi_n(x) = (\sqrt{\pi}\, 2^n n!)^{-\frac{1}{2}} e^{-\frac{1}{2}x^2} H_n(x)$$

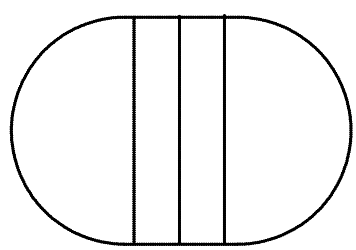
(Hermite function).

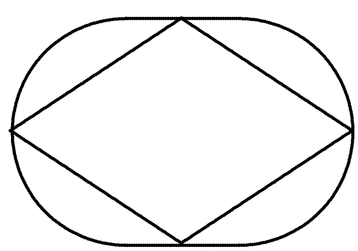
- **Stadium** (classically chaotic billiard)**:**

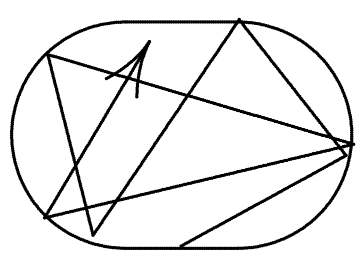


$$0 < E_0 < E_1 \le E_2 \le E_3 \le \cdots \le E_n \cdots \to +\infty.$$

Eigenfunctions φ_n have been computed numerically up to $n \gtrsim 10^3$.







Integral kernels (Green functions) and their traces

$$f(H)u = \sum_{n=1}^{\infty} f(E_n)\langle\varphi_n, u\rangle\varphi_n \,.$$

At least formally, $f(H)u(x) = \int_\Omega G(x,\tilde{x})u(\tilde{x})\,d\tilde{x}$,

$$G(x,y) = \sum_{n=1}^{\infty} f(E_n)\varphi_n(x)\overline{\varphi_n(y)}.$$

If f is sufficiently rapidly decreasing, this converges to a smooth function.

Trace: $\displaystyle\int_\Omega G(x,x)\,dx = \sum_{n=1}^{\infty} f(E_n)$.

Classic example: **Heat kernel**, $f_t(H) = e^{-tH}$.

$$u(t,x) = \int_\Omega K(t,x,y)u_0(y)\,dy \quad \text{solves}$$

$$\frac{\partial u}{\partial t} = -H_{(x)}u, \qquad u(0,x) = u_0(x).$$

$$K(t,x,y) = \sum_{n=1}^{\infty} e^{-tE_n}\varphi_n(x)\overline{\varphi_n(y)}.$$

Theorem 1: For compact manifolds and compact billiards, with $H = -\Delta_g + V(x)$ (and assuming all $E_n \geq 0$), there is an asymptotic expansion as $t \downarrow 0$,

$$\int_\Omega K(t,x,x)\,dx \sim (4\pi t)^{-d/2} \sum_{m=0}^{\infty} a_{m/2}\, t^{m/2},$$

where a_s is an integral of geometrical data over Ω or its boundary. (When s is half-integral (m odd), a_s comes entirely from the boundary.) In particular, for Dirichlet boundary conditions,

$$a_0 = |\Omega| = d\text{-dimensional volume of } \Omega,$$

$$a_{\frac{1}{2}} = -\frac{\sqrt{\pi}}{2} \times (\text{surface area, } |\partial\Omega|),$$

$$a_1 = \int_\Omega \left(\tfrac{1}{6}R - V\right) dx + \tfrac{1}{3}\int_{\partial\Omega} \kappa\, d\sigma$$

(R = Ricci scalar curvature, κ = extrinsic curvature (trace of second fundamental form)).

This theorem assumes all the geometrical functions are *smooth*. For the brick we will find directly instead the same a_0 and $a_{\frac{1}{2}}$ as above, but

$$a_1 = \pi(L_1 + L_2 + L_3), \quad a_{\frac{3}{2}} = -\pi^{3/2}.$$

Implications:

1. **Inverse problem:** From K (hence from $\{E_n\}$) we can deduce aspects of the geometry of Ω.
2. **Tauberian problem:** From K (hence from Ω and V) we can deduce aspects of the spectrum $\{E_n\}$ by taking the inverse Laplace transform.

Theorem 2 (Weyl's Law): Let $N(E)$ be the number of eigenvalues $\leq E$. Under conditions of Theorem 1, as $E \to \infty$

$$N(E) \sim \frac{(4\pi)^{-d/2}}{\Gamma(1+d/2)} E^{d/2} |\Omega|.$$

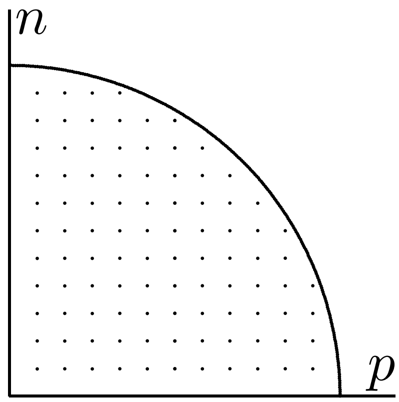
Formal check:

$$\begin{aligned}
\sum_{n=1}^{\infty} e^{-tE_n} &= \int_0^{\infty} e^{-tE} \, dN(E) \\
&\sim \int_0^{\infty} \frac{(4\pi)^{-d/2}}{\Gamma(1+d/2)} \frac{d}{2} e^{-tE} E^{\frac{d}{2}-1} \, dE \, |\Omega| \\
&= \Gamma\left(\frac{d}{2}\right) \frac{(4\pi)^{-d/2}}{\Gamma(1+d/2)} \frac{d}{2} \, |\Omega| \\
&= (4\pi)^{-d/2} |\Omega| \sim \int_{\Omega} K(t,x,x) \, dx.
\end{aligned}$$

Examples

$$N(E) \sim \frac{(4\pi)^{-d/2}}{\Gamma(1+d/2)}\, E^{d/2}|\Omega|.$$

- **Brick:** Theorem 2 predicts $N(E) \sim \frac{L_1 L_2 L_3}{6\pi^2}\, E^{3/2}$.



In fact, by counting lattice points (m, n, p) in octant of an ellipsoid (handling the coordinate planes by inclusion-exclusion principle) one approximates

$$N(E) \approx \frac{V}{6\pi^2}\, E^{3/2} - \frac{S}{16\pi}\, E + \frac{L}{16\pi}\, E^{1/2} - \frac{C}{64}\,,$$

where

$$V = \text{volume} = L_1 L_2 L_3\,,$$

$$S = \text{surface area} = 2(L_1 L_2 + L_1 L_3 + L_2 L_3),$$

$$L = \text{total edge length} = 4(L_1 + L_2 + L_3),$$

$$C = \text{number of corners} = 8.$$

Laplace transform agrees exactly with (promised) heat kernel expansion!

- **Sphere:** Theorem 2 predicts $N(E) \sim E$. Well,

$$N(E) = \sum_{l=0}^{L} (2l+1) \sim L^2, \text{ where } E = L(L+1) \sim L^2.$$

- **Harmonic oscillator:** Theorem 2 predicts $N(E) \propto E^{\frac{1}{2}}$, but the eigenvalues are equally spaced, so actually $N(E) \sim \frac{E}{2}$. The region is not compact, so Theorem 1 and the simplest version of Weyl's formula *do not apply*!

The inverse Laplace transform of the heat-kernel expansion *cannot be evaluated term-by-term* beyond the leading (Weyl) term. $N(E)$ is a step function (and $N'(E)$ a series of delta functions), so the expansion

$$N(E) \sim E^{d/2} \sum_{m=0}^{\infty} \frac{(4\pi)^{-d/2}}{\Gamma(1 + (d-m)/2)} E^{-m/2} a_{m/2}$$

must be literally false beyond order $m = d$ at best. However, it is correct in some **averaged** sense. (I tacitly averaged $N(E)$ for the brick by not counting lattice points carefully near the ellipsoidal surface.)

Some popular averaging methods

1. **Riesz means:** Integrate $N(E)$ p times , then divide by the volume of the p-simplex you integrated over.

   $$p = 2 : \qquad \frac{2!}{E^2} \int_0^E dE_1 \int_0^{E_1} dE_2\, N(E_2).$$

   (Related to **Cesàro summation** of series.)
   Then the first $p+1$ terms of the formal series in $1/\sqrt{E}$ (for this new object) are rigorously asymptotic.

2. **Lorentzian smoothing:** $(\rho = N')$

   $$\overline{\rho(E)} = \frac{\epsilon}{\pi} \int_{-\infty}^{\infty} \frac{\rho(E_1)\, dE_1}{(E-E_1)^2 + \epsilon^2} \,.$$

   (Equivalent to analytically continuing the *resolvent kernel* into the complex plane.)
   For sufficiently large ϵ, $\overline{\rho}$ has a valid asymptotic expansion in $1/\sqrt{E}$.

3. **Gaussian smoothing** (better in high dimensions).

Continuous spectrum

Example: **Half-line** $0 < x < \infty$ with Dirichlet BC. Here we have a *generalized eigenfunction expansion*, the **Fourier sine transform**:

$$u(x) = \int_0^\infty c_k \varphi_k(x)\,dk, \quad c_k = \int_0^\infty \overline{\varphi_k(x)} u(x)\,dx,$$

$$\varphi_k(x) = \sqrt{\frac{2}{\pi}}\,\sin(kx) \notin L^2(0,\infty).$$

For general operators it may be more convenient to start with the heat kernel (which exists by abstract PDE or operator theory) and consider its (exact) inverse Laplace transform, which will be the integral kernel of the spectral projection operator. That is, if

$$K(t,x,y) = \int_0^\infty e^{-tE}\,dP(E,x,y),$$

then $P(E,x,y)$ is the integral kernel of $P(E)$, the orthogonal projection onto the part of L^2 corresponding to spectrum $\le E$. (If you don't know Stieltjes integration, think of $dP(E)$ as $P'(E)\,dE$.) When the spectrum is discrete, we just have

$$P(E,x,y) = \sum_{n: E_n \le E} \varphi_n(x)\overline{\varphi_n(y)}.$$

In the half-line example,

$$P(E,x,y) = \int_0^{\sqrt{E}} \frac{2}{\pi} \sin(kx)\sin(ky)\,dk,$$

equivalent to

$$K(t,x,y) = (4\pi t)^{-1/2}\left[e^{-(x-y)^2/4t} - e^{-(x+y)^2/4t}\right].$$

$P(E,x,x)$ is a **local spectral density**. Analogs of Theorems 1 and 2 hold for it and $K(t,x,x)$, but *the expansions are nonuniform in x and can't be integrated up to the boundary to recover the integrated quantities a_s etc.*

For a billiard, at any interior point

$$K(t,x,x) \sim (4\pi t)^{-d/2} + O(t^\infty),$$

but we know the integral $\int_\Omega K\,dx$ contains a boundary term $O(t^{-(d-1)/2})$. For the half-line,

$$\int_0^L K(t,x,x)\,dx = (4\pi t)^{-1/2}\int_0^L \left[1 - e^{-x^2/t}\right]dx$$

$$\approx (4\pi t)^{-1/2}\left(L - \tfrac{1}{2}\sqrt{\pi t}\right).$$

So for the brick, we get $\displaystyle\prod_{j=1}^{3}(4\pi t)^{-1/2}\left(L_j - \sqrt{\pi t}\right) =$

$(4\pi t)^{-3/2}\left[V - \dfrac{S\sqrt{\pi t}}{2} + \dfrac{L\pi t}{4} - \dfrac{C(\pi t)^{3/2}}{8}\right]$, as claimed.

The main game

the operator: potentials
geometry
classical mechanics

$\Updownarrow$

integral kernels

$\Updownarrow$

spectral apparatus: eigenvalues
eigenfunctions
spectral projections
local spectral densities
vacuum energy

Old spectral asymptotics: *(this talk)*

gross geometry $\leftrightarrow$ heat trace at small t

$\leftrightarrow$ average eigenvalue density at high frequency

New spectral asymptotics: *(rest of workshop)*

classical mechanics $\leftrightarrow$ kernels $\leftrightarrow$ details of spectrum

A variety of kernels

Heat: $f_t(H) = e^{-tH}$;

$$\frac{\partial K}{\partial t} = -HK, \quad K(0,x,y) = \delta(x-y)$$

Quantum: $f_t(H) = e^{-itH}$; $\quad i\,\frac{\partial U}{\partial t} = HU$, $U(0) = \delta$
(analytic continuation of K)

Resolvent: $f_z(H) = \frac{1}{H-z}$; $\quad (H-z)G = \delta(x-y)$

$$N'(E) = \rho(E) = \frac{1}{\pi}\int_\Omega \operatorname{Im} G(E+i\epsilon,x,x)\,dx.$$

Zeta: $f_s(H) = H^{-s}$ $\quad$ (meromorphic function of s)

Wave:

- D'Alembert: $f_t(H) = \cos(t\sqrt{H})$;

$$\frac{\partial^2 D}{\partial t^2} = -HD, \quad D(0,x,y) = \delta(x-y), \quad \frac{\partial D}{\partial t}(0) = 0$$

- Wightman: $f_t(H) = \frac{e^{-it\sqrt{H}}}{2\sqrt{H}}$
  (*positive frequency* solution)

Cylinder: $f_t(H) = e^{-t\sqrt{H}}$;

$$\frac{\partial^2 T}{\partial t^2} = +HT, \quad T(0,x,y) = \delta, \quad T \to 0 \text{ as } t \to \infty$$

(related to wave kernels by analytic continuation)

Physical interpretations and physical quantities

(What happened to $\hbar$, m, c, and all that?)

Schrödinger equation: $$i\hbar\,\frac{\partial u}{\partial t} = -\,\frac{\hbar^2}{2m}\,\nabla^2 u + \lambda V(\mathbf{x})u$$

Klein–Gordon equation: $$\frac{1}{c^2}\frac{\partial^2 u}{\partial t^2} = \nabla^2 u - \left(\frac{mc}{\hbar}\right)^2 u$$

(Nonrelativistic and relativistic meanings of m are different!) Wave equation is case $m = 0$; instead, could generalize to $\left(\frac{mc}{\hbar}\right)^2 V(\mathbf{x})u$.

Can choose time unit and redefine constants so

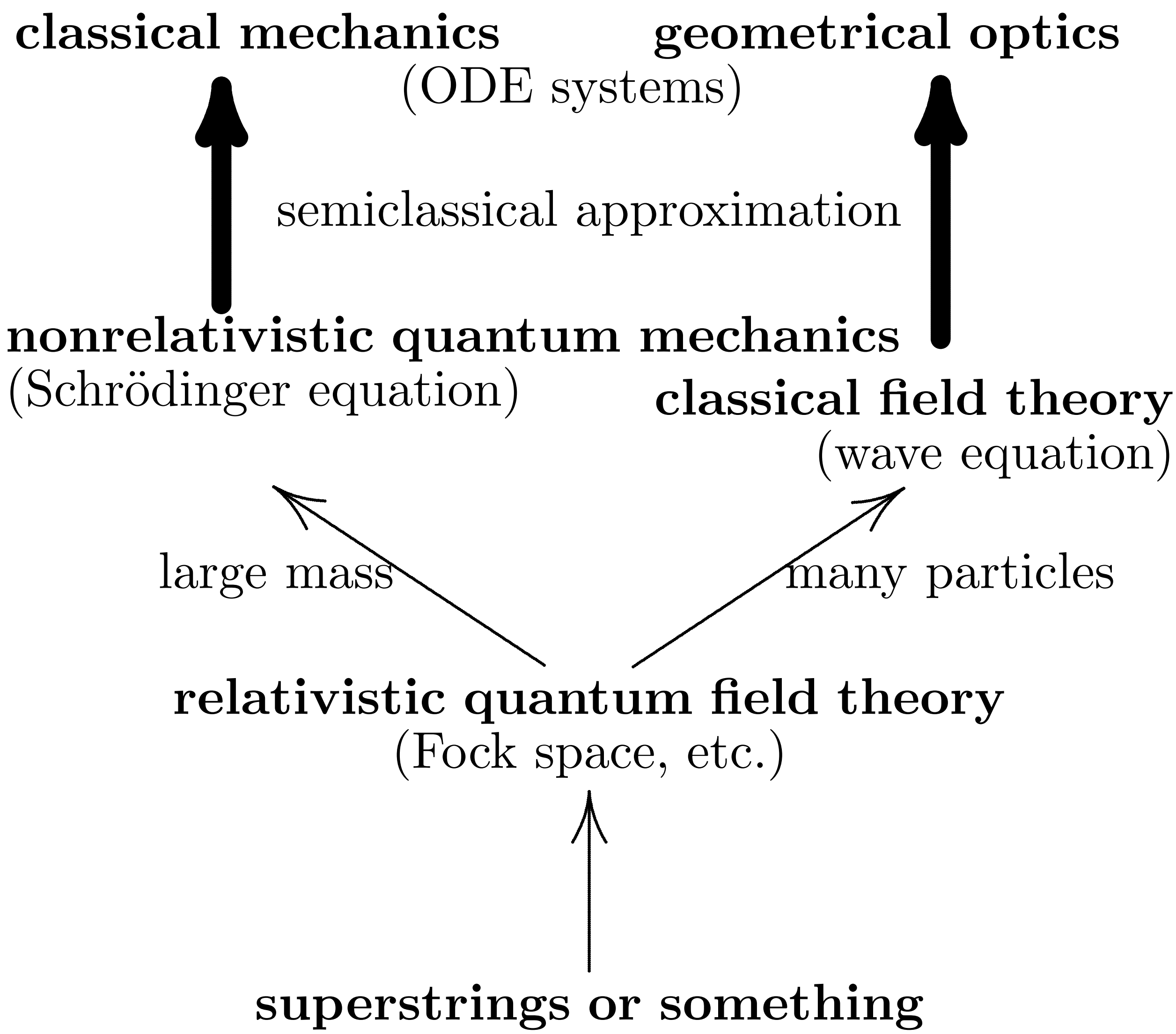
$$i\,\frac{\partial u}{\partial t} = -\nabla^2 u + \lambda V u \equiv Hu, \quad -\frac{\partial^2 u}{\partial t^2} = -\nabla^2 u + \lambda V u.$$

Separation of variables (respectively, $u = \varphi e^{-iEt/\hbar}$, or $u = \varphi e^{-i\omega t/\hbar}$ with $E = \omega^2$), leads always to

$$H\varphi_n = E_n\varphi_n\,.$$

There are two independent constants, λ and E. But it is customary and convenient to reintroduce $\hbar$, as we'll see.

The hierarchy of physical theories



Semiclassical and high-frequency limits

Let's set Schrödinger $m = \frac{1}{2}$ and Klein–Gordon $c = 1$, but leave $\hbar$ visible. In either case,

$$-\hbar^2\nabla^2\varphi + \lambda V\varphi = E\varphi.$$

There are two similar limits:

- **High frequency:** $E \to +\infty$, $\hbar$ and λ fixed.
- **Semiclassical:** $\hbar \downarrow 0$ — equivalent to $E \to \infty$ and $\lambda \to \infty$ simultaneously.

In a billiard ($V = 0$) these are the same!

Underlying classical system: $\mathbf{p} \leftrightarrow -i\nabla$, so

$$H = \mathbf{p}^2 + \lambda V(\mathbf{x}).$$

$$\frac{d\mathbf{x}}{dt} = \frac{\partial H}{\partial \mathbf{p}} = 2\mathbf{p}\,, \quad \frac{d\mathbf{p}}{dt} = -\frac{\partial H}{\partial \mathbf{x}} = -\lambda\nabla V(\mathbf{x}).$$

Thus, *Newton's law of motion*:

$$\frac{d^2\mathbf{x}}{dt^2} = -2\lambda\nabla V(\mathbf{x}) = \frac{F}{m} \qquad (\text{recall } m = \tfrac{1}{2}).$$

Semiclassical approximation is built on the classical trajectories.
High-frequency approximation is built on force-free classical trajectories (straight rays).

Field quantization and vacuum energy

Consider the wave equation in a billiard,

$$\frac{\partial^2 u}{\partial t^2} = \nabla^2 u, \quad u = 0 \text{ on } \nabla\Omega.$$

Expand in the normal modes:

$$u(t, \mathbf{x}) = \sum_{n=1}^{\infty} c_n(t)\varphi_n(\mathbf{x}), \qquad H\varphi_n = {\omega_n}^2 \varphi_n\,.$$

Now treat each mode amplitude c_n as a quantum system. It behaves as a harmonic oscillator: $\exists$ state $|N_n\rangle$ with N_n quanta ($N_n = 0, 1, \ldots$) whose energy is $(N_n + \frac{1}{2})\hbar\omega_n$.
Vacuum state is $N_n = 0\ \forall n$.

Set $\hbar = 1$. Total energy $E = \dfrac{1}{2}\displaystyle\sum_{m=1}^{\infty} \omega_n = \infty$?

$$Z(s) = \sum_{n=1}^{\infty} ({\omega_n}^2)^{-s},$$

$E = \frac{1}{2} Z\bigl(-\frac{1}{2}\bigr)$, defined by analytic continuation.

One-dimensional billiard yields *Riemann zeta function*: $\omega_n = \frac{n\pi}{L}$,

$$Z\left(-\tfrac{1}{2}\right) = \frac{\pi}{L}\sum_{n=1}^{\infty} n = -\frac{\pi}{12L} = 2E.$$

L dependence $\Rightarrow$ $\dfrac{dE}{dL} = \dfrac{\pi}{24L^2} > 0$, attractive force.