TRACE FORMULAS

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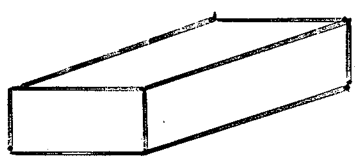
Overview

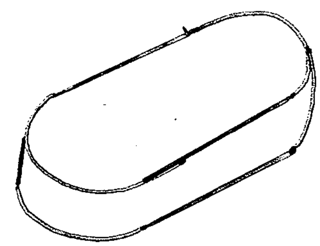
Goal: obtain detailed spectral information on certain PDOs from geometry / dynamics

Two major classes of examples:

(1) Electromagnetic fields in cavities



cube



"stadium"

inside cavity $(C \subset \mathbb{R}^3)$: em fields, no charges/currents
surface (∂C) : ideal conductor

wave eqn. for electric field (units with $c = 1$):

$$\left(\frac{\partial^2}{\partial t^2} - \Delta\right) E(t,x) = 0 \quad , \qquad E_t\big|_{\partial C} = 0$$

$$E(t,\cdot) : C \to \mathbb{R}^3$$

$E_t\big|_{\partial C}$: component tangent to ∂C

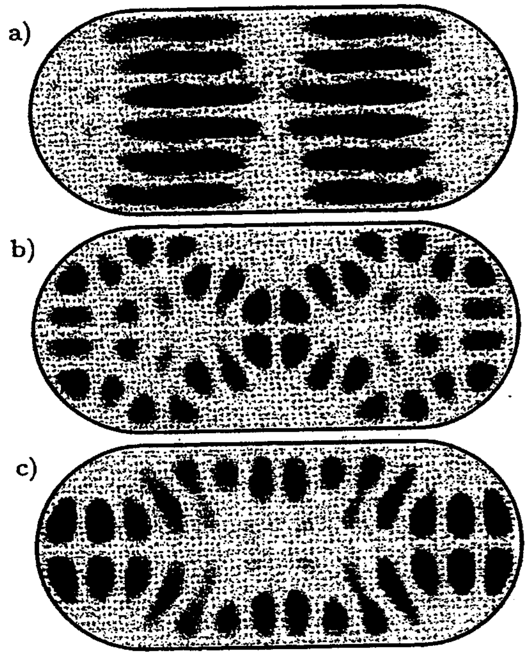


Figure 2.13. Experimental eigenfunctions in a microwave resonator of the shape of a stadium billiard ($l = 18$ cm, $r = 13.5$ cm) at three frequencies 3.384 GHz (a), 3.865 GHz (b), and 4.056 GHz (c). For the display of the wave functions the stadium has been completed by a twofold reflection. All wave functions show strong scarring close to classical periodic orbits [Ste92].

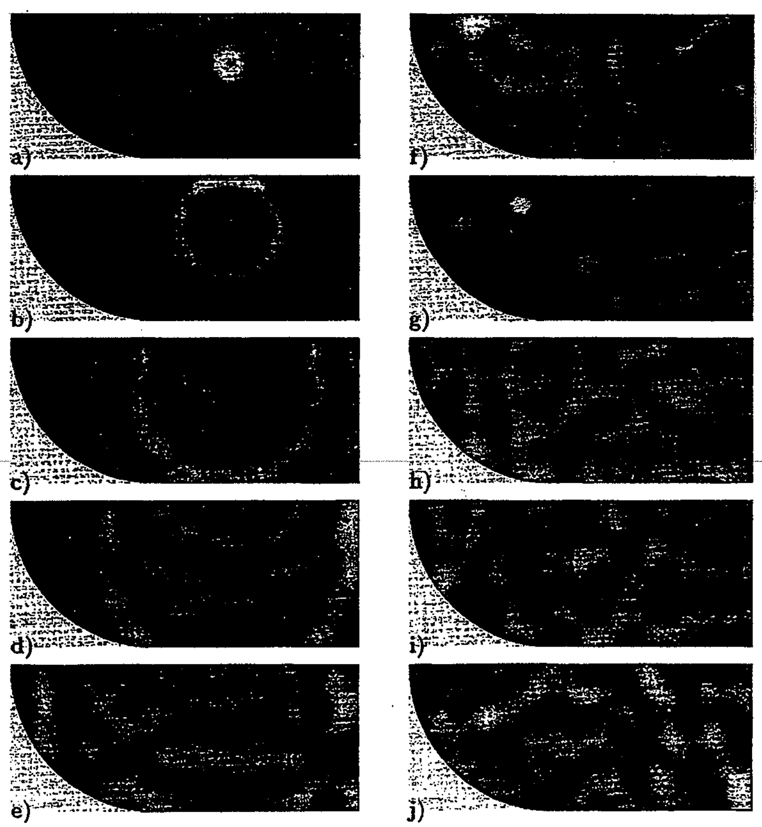


Figure 1.1. Propagation of a microwave pulse in a microwave cavity in the shape of a quarter stadium (length of the straight part $l = 18$ cm, radius $r = 13.5$ cm, height $h = 0.8$ cm) for different times $t/10^{-10}$ s: 0.36 (a), 1.60 (b), 2.90 (c), 3.80 (d), 5.63 (e), 9.01 (f), 10.21 (g), 12.0 (h), 14.18 (i), 19.09 (j) [Ste95] (Copyright 1995 by the American Physical Society)

cylindrical geometry:

$$E_3(t,x) = \sum_j e^{i\omega_j t}\, e_j(x_1,x_2) \sum_{n=0}^{\infty} \alpha_n \cos\left(\frac{n\pi}{d}\, x_3\right)$$

with: $\left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} - \left(\frac{n\pi}{d}\right)^2 + \omega_j^2\right) e_j(x_1,x_2) = 0 \quad , \quad e_j\Big|_{\partial C} = 0$

spectral data (ω_j^2, e_j) $\qquad\qquad$ geometry of cavity

$\updownarrow$ $\qquad\qquad\qquad\qquad\qquad\qquad$ $\updownarrow$

wave optics (light waves) $\xrightarrow[\text{short wavelengths } (\omega_j^2 \to \infty)]{}$ geometrical optics (light rays)

"Weyl's law":

$$\#\{\omega_j^2 \leq \lambda\} \underset{\lambda\to\infty}{\sim} \text{const.}\ \mathrm{vol}(C)\ \lambda^{3/2}$$

geometry

further geometric data $\overset{??}{\Longrightarrow}$ finer details of spectrum

M. Kac: "Can one hear the shape of a drum?"

Gordon - Webb - Wolpert: No! (but ...)

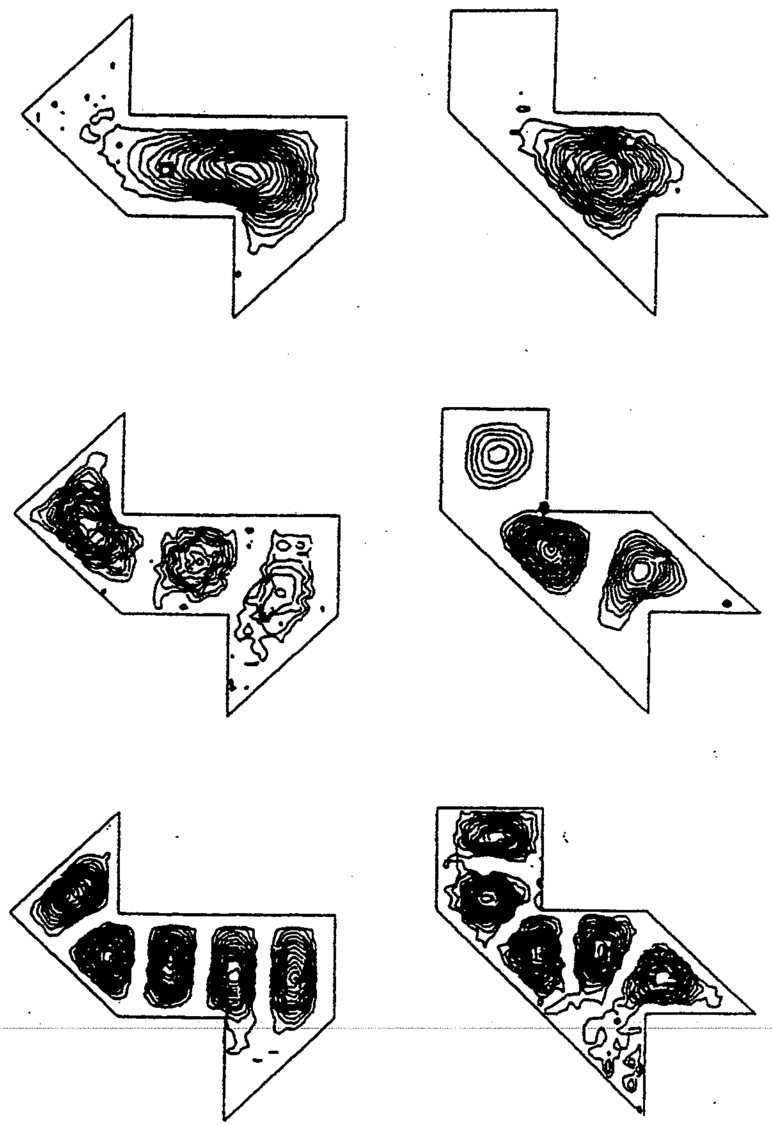
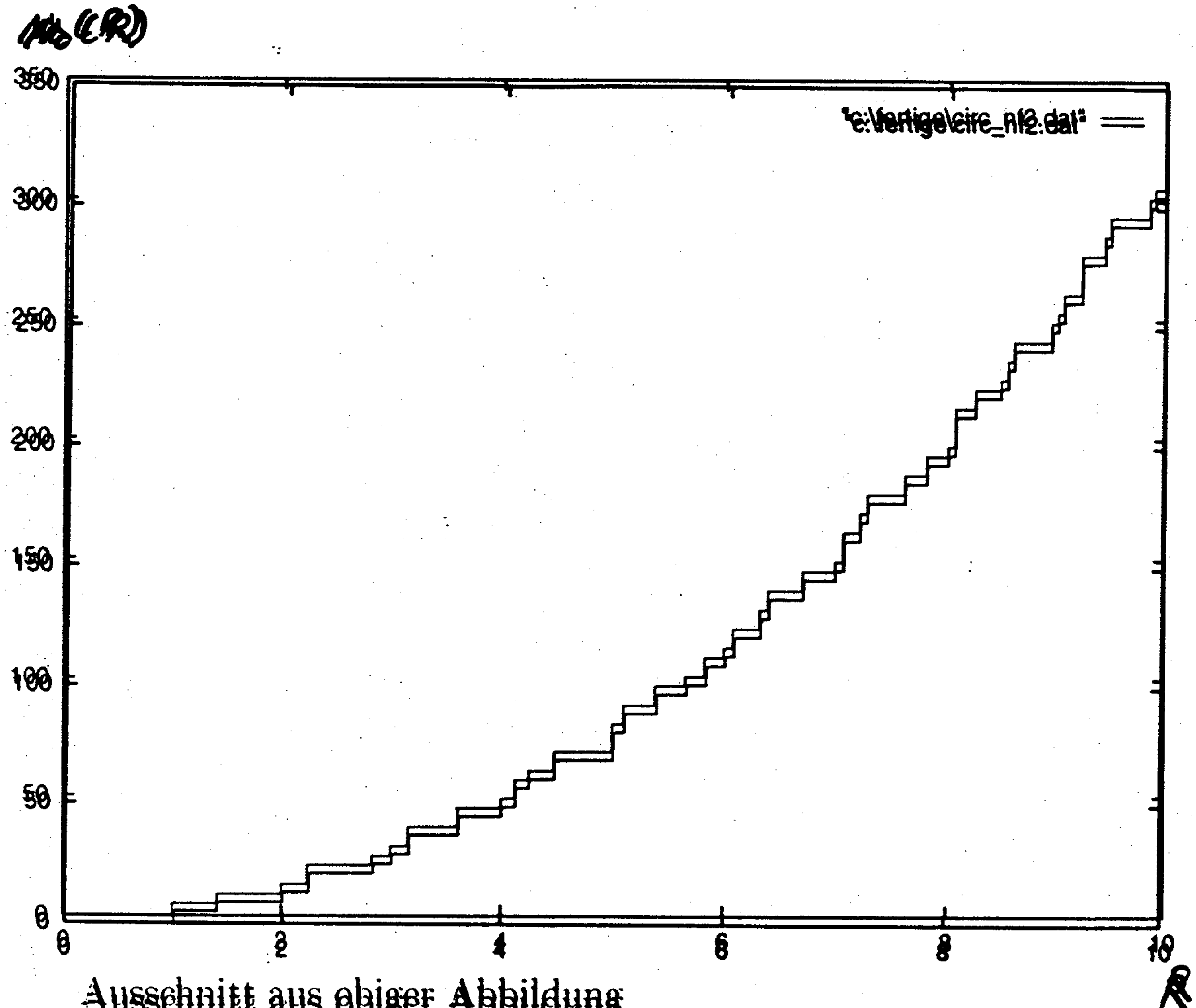


Figure 2.14. Three pairs of eigenfunctions for two isospectral microwave billiards. The cavities have a unit length of 7.6 cm. The eigenfrequencies in GHz are 1.9907, 1.9908 (top), 2.8413, 2.8418 (middle), 3.7964, 3.7924 (bottom) [Sri94] (Copyright 1994 by the American Physical Society).



Ausschnitt aus obiger Abbildung
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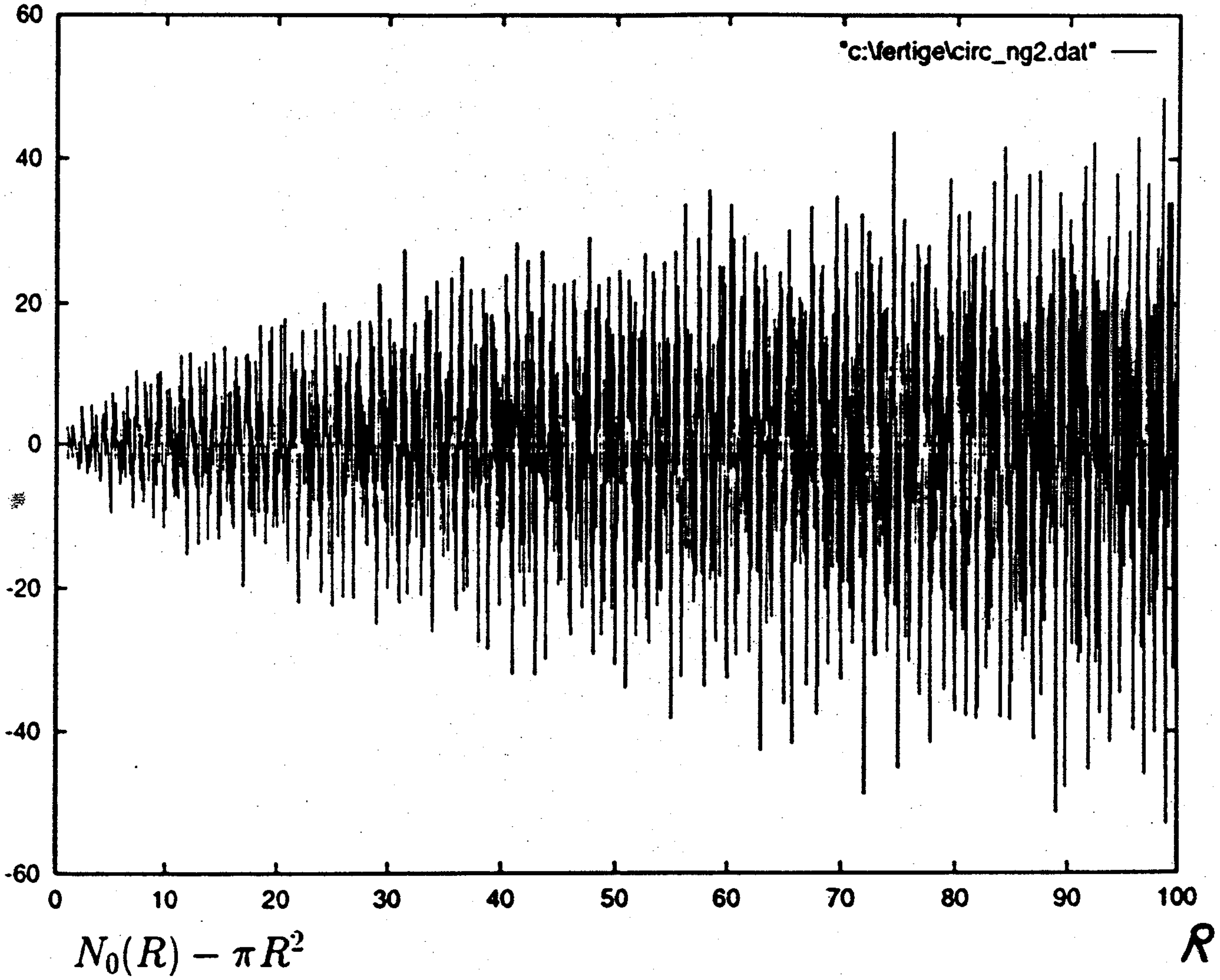
2d - Torus ($E = R^2 \rightsquigarrow p = R$)

$N_{fl}(R) = N_0(R) - \pi R^2$



$N_0(R) - \pi R^2$

circ_ng2.dat

② Quantum mechanics:

Schrödinger eqn (units with $m = 1$)

$$i\hbar \frac{\partial}{\partial t} \Psi(t,x) = \left(-\frac{\hbar^2}{2}\Delta + V(x)\right)\Psi(t,x)$$

with: – Δ: Laplacian on $\mathbb{R}^d$, $V \in C^\infty(\mathbb{R}^d)$ s.t. $\lim_{|x|\to\infty} V(x) = +\infty$

– $\left(-\frac{\hbar^2}{2}\Delta + V(x)\right)\psi_n(x) = E_n \psi_n(x)$

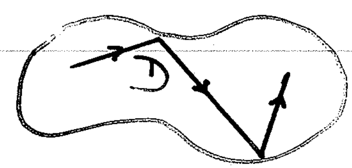
Then (in $L^2(\mathbb{R}^d)$):

$$\Psi(t,x) = \sum_n c_n \psi_n(x)\, e^{-\frac{i}{\hbar} t E_n}$$

Here "short-wavelength" asymptotics should provide a transition: quantum mechanics ("wave fcts") $\rightarrow$ classical mechani[cs] (particle traj.)

<u>Examples:</u>

i) Billiards



classical: trajectories + reflections

quantum:

$$\left.\begin{aligned} -\frac{\hbar^2}{2}\Delta\psi_n &= E_n\psi_n \\ \psi_n\big|_{\partial D} &= 0 \end{aligned}\right\} \text{ on } L^2(D)$$

transition:
- $E_n \to \infty$
- $\hbar \to 0$

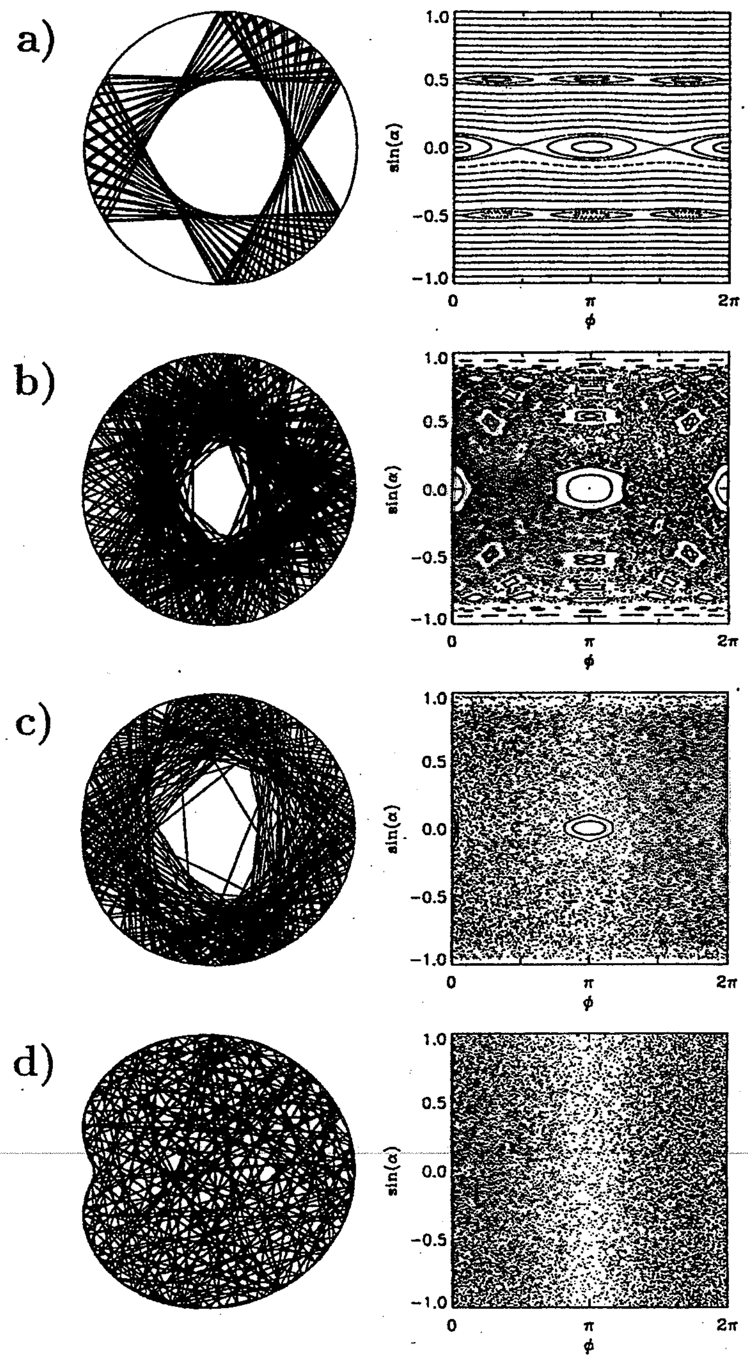
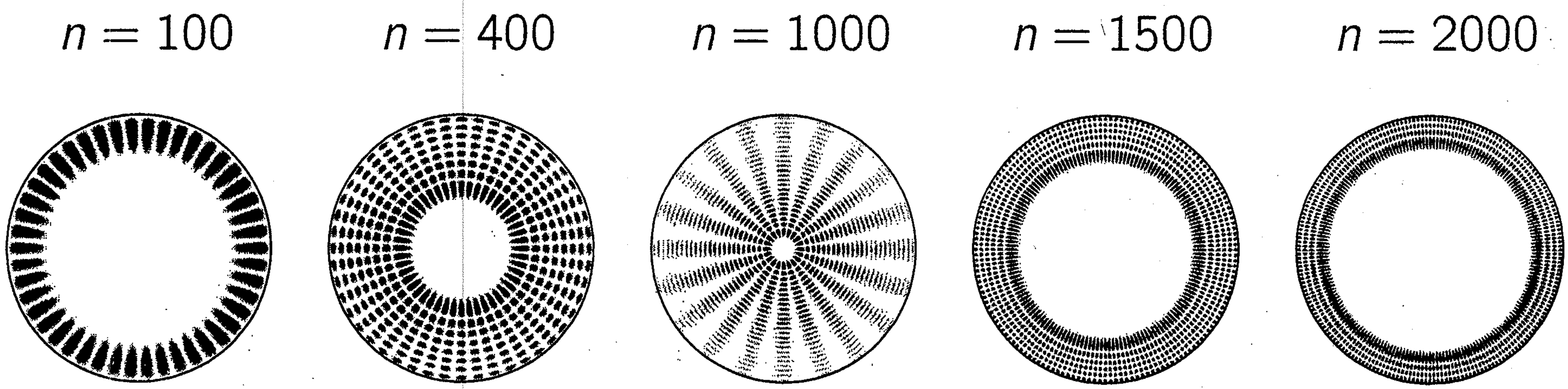
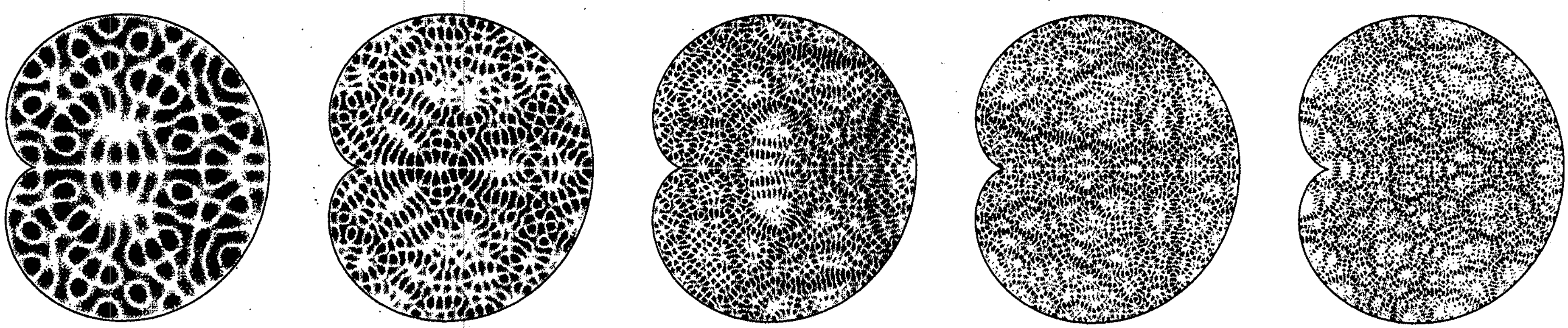


Figure 3.11. Robnik billiard for $\lambda = 0.05$ (a), 0.15 (b), 0.2 (c), 0.375 (d). The right column shows the corresponding Poincaré sections. The abscissa corresponds to the polar angle determining the position of the collision point on the boundary, the ordinate corresponds to the sine of the reflection angle.

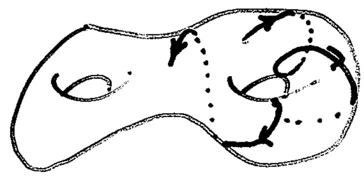
Eigenstates circular billiard



Eigenstates cardioid billiard



ii) Riemannian manifold (M, g) (compact) :



classical : geodesic flow on TM / T^*M

quantum:

$$-\frac{\hbar^2}{2} \Delta_g \psi_n = E_n \psi_n \quad ; \quad \Delta_g : \text{Laplace-Beltrami operator}$$

transition :
- $E_n \to \infty$
- $\hbar \to 0$

iii) Homogenous potential : $V(\lambda x) = \lambda^{\kappa} V(x)$

classical : Hamiltonian flow on $T^*\mathbb{R}^d$, generated by $H(q,p) = \frac{1}{2} p^2 + V(q)$: ϕ_H^t

preserves "energy shell" $\Omega_E := \{ (q,p) \in T^*\mathbb{R}^d ; \; H(q,p) = E \}$

scaling property : $H(\lambda^{\frac{1}{\kappa}} q, \lambda^{\frac{1}{2}} p) = \lambda \, H(q,p)$

transition :
- $E \to \infty$
- $\hbar \to 0$

iv) General :

transition : $\hbar \to 0$

Distribution of eigenvalues:

analogue of Weyl's law

$$\# \{ E_n ; \ E - \hbar\omega \leq E_n \leq E + \hbar\omega \} \sim 2\hbar\omega \ \frac{\mathrm{vol}\, \Omega_E}{(2\pi\hbar)^d}$$

("one quantum state per Planck cell")

here:

- energy shell $\Omega = \{ (q,p) \in T^*M \, ; \ H(q,p) = E \}$
- Liouville measure $\mathrm{vol}\, \Omega_E = \iint\limits_{T^*M} \delta(H(q,p) - E) \, dq \, dp$

again:

$$\left. \begin{array}{l} \text{further dynamical data} \\ \text{(Hamiltonian flow)} \end{array} \right\} \overset{??}{\Rightarrow} \text{finer details of spectrum}$$

Technical tool: trace formulas

① Wave eqn.:

Propagation of soln. of $\left(\frac{\partial^2}{\partial t^2} - \Delta\right) u(t,x)$

with initial data $u(0,x)$, $\frac{\partial u}{\partial t}(0,x)$:

$$\begin{pmatrix} u(t,x) \\ \frac{\partial u}{\partial t}(t,x) \end{pmatrix} = e^{itG} \begin{pmatrix} u(0,x) \\ \frac{\partial u}{\partial t}(0,x) \end{pmatrix}$$

$$\Rightarrow \quad G = \begin{pmatrix} 0 & -i \\ -i\Delta & 0 \end{pmatrix}$$

Then: $\quad \mathrm{Tr}\, e^{itG} = \mathrm{Tr} \cos\left(t\sqrt{-\Delta}\right) = \sum_j \cos \omega_j t$

Fourier trsfn $\Rightarrow$ spectral density of $P = \sqrt{-\Delta}$

$$\sigma(\omega) = \sum_j \delta(\omega - \omega_j)$$

Balian - Bloch (1970-74):

$$\sum_j \delta(\omega - \omega_j) \underset{\omega \to \infty}{\sim} \text{"Weyl-term"} + \sum_\gamma A_\gamma e^{i\omega l_\gamma}$$

γ: periodic light rays

l_γ: length of γ

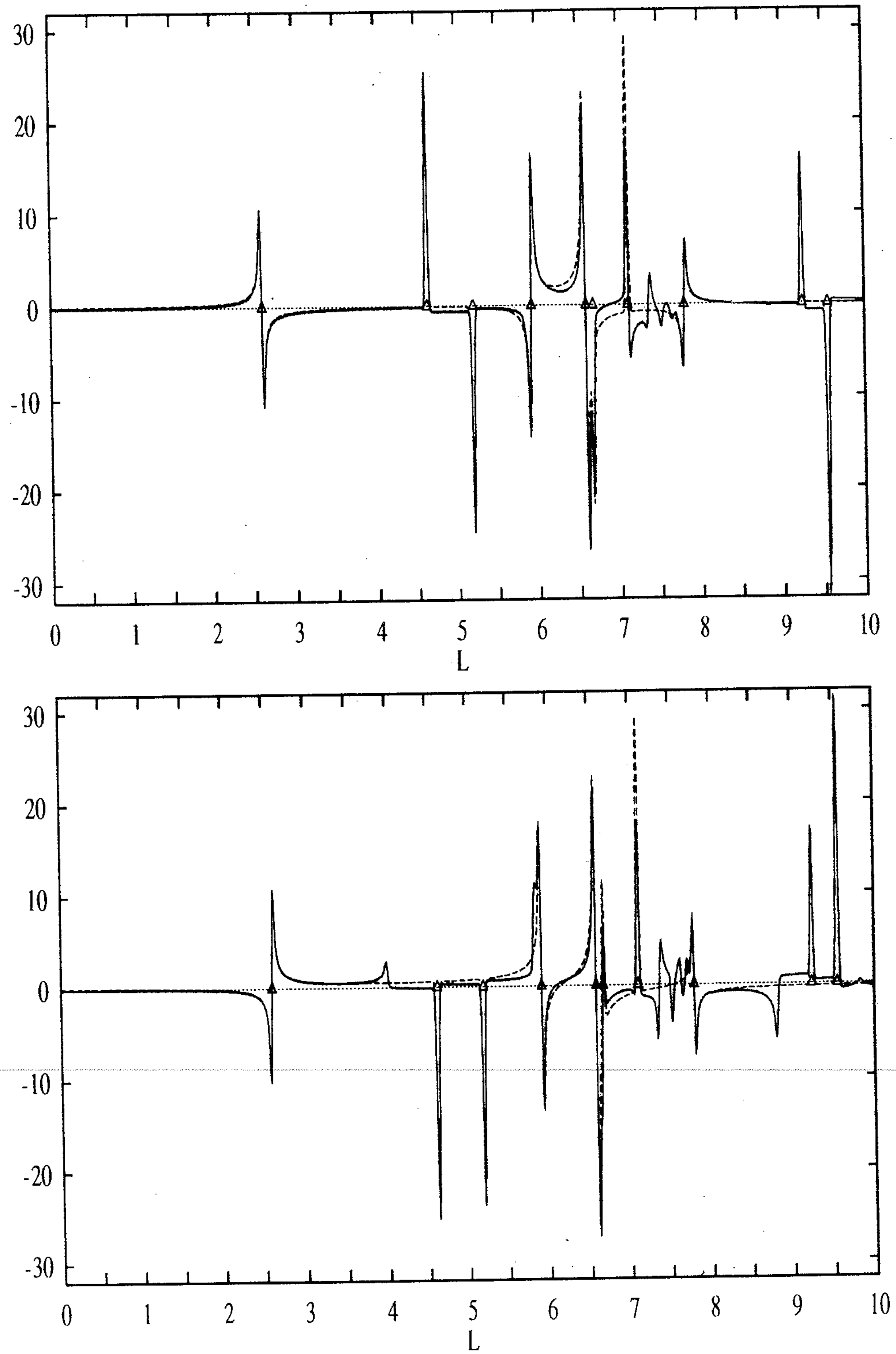


Abbildung 43: Spur des Kosinus-modulierten Heat-Kernels mit $t_\gamma = 0.0001$. Durchgezogene Linie: linke Seite der Spurformel (62), unterbrochene Linie: rechte Seite der Spurformel (62). Oben ungerade und unten gerade Symmetrie. Die Dreiecke auf der L-Achse markieren die Längen der primitiven periodischen Orbits mit $L \leq 10$ und deren Mehrfachumläufe.

② quantum mechanics:

Hamiltonian $H = -\frac{\hbar^2}{2}\Delta + V(x)$

with discrete spectrum $E_1 \leq E_2 \leq E_3 \leq \dots$

Propagation of soln of $i\hbar \frac{\partial \psi}{\partial t} = H\psi$

with initial data $\psi(0) = \psi_0$.

$$\psi(t) = e^{-\frac{i}{\hbar}tH}\psi_0$$

Then: $\operatorname{Tr} e^{-\frac{i}{\hbar}tH} = \sum_n e^{-\frac{i}{\hbar}tE_n}$

Fourier trsfm $\Rightarrow$ spectral density $d(E) = \sum_n \delta(E-E_n)$

Gutzwiller (1967-71):

$$\sum_n \delta(E-E_n) \underset{\hbar\to 0}{\sim} \text{"Weyl-term"} + \sum_\gamma A_\gamma e^{\frac{i}{\hbar}S_\gamma}$$

γ: periodic orbit of ϕ_H^t

$S_\gamma = \int_\gamma p\cdot dq$ (action)

Mathematical proofs in various steps:

Colin de Verdière 1973, Chazarain 1974/80,

Duistermaat-Guillemin 1975, Brummelhuis-Uribe 1991,

Meinrenken 1992, Paul-Uribe 1991/95,

Combescure-Ralston-Robert 1998

Further variations:

(A) Quantum maps

(discrete-time) classical dynamics

$$A : \mathbb{T}^2 \to \mathbb{T}^2$$

(CAT-map, baker-map, ...)

quantisation:

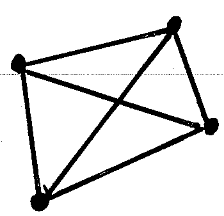
$$U_N(A) : \mathbb{C}^N \to \mathbb{C}^N \qquad \text{unitary}$$

$$\cong$$

$$e^{-\frac{i}{\hbar} tH} \qquad \text{with} \quad \hbar = \frac{1}{2\pi N} \to 0$$

$$\operatorname{Tr}_{\mathbb{C}^N} U_N(A) \underset{N\to\infty}{\sim} \text{"Weyl-term"} + \sum_\gamma A_\gamma e^{2\pi i N S_\gamma}$$

(B) Quantum graphs



V vertices

B bonds (lengths L_b)

operator: $$\left(i\frac{d}{dx} + A\right)^2 \quad \text{on} \quad \bigoplus_{b=1}^{B} L^2([0, L_b])$$

Trace formula: Roth 1983, Kottos-Smilansky 1997

(C) Non-scalar operators (Pauli, Dirac, ...)

Matrix-valued PDEs, e.g. Dirac eqn

$$i\hbar \frac{\partial \psi}{\partial t} = \left(\sum_{k=1}^{3} \alpha_k \left(\frac{\hbar}{i} \frac{\partial}{\partial x_k} - A_k(x) \right) + \beta + \phi(x) \mathbb{1} \right) \psi$$

$\beta, \alpha_1, \alpha_2, \alpha_3$ generate Clifford algebra:

$$\beta^2 = \mathbb{1}, \quad \alpha_k \alpha_\ell + \alpha_\ell \alpha_k = 2 \delta_{k\ell} \mathbb{1}, \quad \alpha_k \beta + \beta \alpha_k = 0$$

2 types of dynamics:

- scalar $\hat{=}$ Hamiltonian flow $\leftarrow$ particle motion
- matrix $\hat{=}$ driven dynamics $\leftarrow$ spin precession

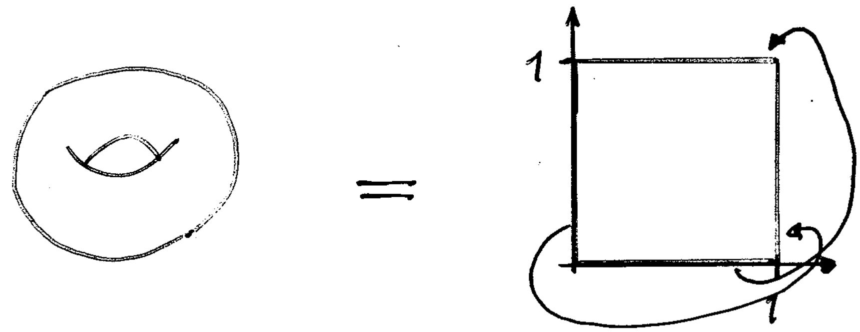
(J.B. - S. Keppeler '98/99)

(D) Periodic flows and spectral clustering

(E) Degenerate flows

$\vdots$

Wave eqn. and QM on a torus:



$\mathbb{T}^2 \qquad\qquad \mathbb{R}^2/\mathbb{Z}^2$

2 spectral problems on $L^2(\mathbb{R}^2/\mathbb{Z}^2)$:

① (wave eqn.) $\quad \sqrt{-\Delta}\, e^{2\pi i k\cdot x} = 2\pi |k|\, e^{2\pi i k\cdot x}$

② (QM) $\quad -\frac{\hbar^2}{2}\Delta\, e^{2\pi i k\cdot x} = 2\pi^2 \hbar^2 k^2\, e^{2\pi i k\cdot x}$

both cases: $\quad \{e^{2\pi i k\cdot x};\ k\in\mathbb{Z}^2\}$ is onb in $L^2(\mathbb{R}^2/\mathbb{Z}^2)$

Trace formula via Poisson summation:

f: "suitable" fct. on $\mathbb{R}^2$ $\quad$ (e.g. $f\in\mathcal{S}(\mathbb{R}^2)$)

Then: $\quad \displaystyle\sum_{k\in\mathbb{Z}^2} f(k) = \sum_{n\in\mathbb{Z}^2} \tilde{f}(n)$

$$\tilde{f}(\xi) = \int_{\mathbb{R}^2} e^{2\pi i \xi\cdot x} f(x)\, dx$$

Idea of proof: $\quad F(x) := \displaystyle\sum_{k\in\mathbb{Z}^2} f(x+k)$ is $\mathbb{Z}^2$-periodic

$\Rightarrow F(x) = \displaystyle\sum_{n\in\mathbb{Z}^2} a_n\, e^{-2\pi i x\cdot n}, \quad a_n = \tilde{f}(n)$

$\rightsquigarrow$ set $x=0$ $\quad\blacksquare$

① Wave eqn.:

choose $h \in \mathcal{S}(\mathbb{R})$ such that $f(x) = h(2\pi|x| - \omega)$

in Poisson summation,

$$\sum_{k \in \mathbb{Z}^2} h(2\pi|k| - \omega) = \sum_{n \in \mathbb{Z}^2} \int_{\mathbb{R}^2} e^{2\pi i n \cdot x} h(2\pi|x| - \omega)\, dx$$

$$= \sum_{n \in \mathbb{Z}^2} \frac{1}{2\pi} \int_0^\infty h(\mu - \omega)\, \mu\, J_0(\mu|n|)\, d\mu$$

→ l.h.s. = spectral side:

$$\sum_{k \in \mathbb{Z}^2} h(2\pi|k| - \omega) = \sum_j m_j\, h(\omega_j - \omega) = \operatorname{Tr} h(\sqrt{-\Delta} - \omega)$$

- $\omega_j = 2\pi|k|$ eigenvalue of $\sqrt{-\Delta}$
- m_j : multiplicity of ω_j

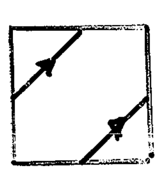
→ r.h.s. = geometric side:

i) $|n| = 0$ (⇝ "Weyl-term")

$$\frac{1}{2\pi} \int_0^\infty h(\mu - \omega)\, \mu\, d\mu = \frac{1}{2\pi} \int_{-\omega}^\infty h(\rho)(\omega + \rho)\, d\rho$$

$$\underset{\omega \to \infty}{\sim} \omega \tilde{h}(0) - i \tilde{h}'(0)$$

ii) $|n| > 0$ (⇝ length of closed geodesic)



closed geodesic $\gamma \mathrel{\hat{=}} n = (1,1)$

length $l_\gamma = |n| = \sqrt{2}$

Contribution of l_γ:

$$\frac{1}{(2\pi)^2} \int_{-\omega}^{\infty} h(\rho)\,(\omega+\rho) \int_0^{2\pi} e^{i(\omega+\rho) l_\gamma \cos\varphi}\, d\varphi\, d\rho$$

$$\underset{\omega\to\infty}{\sim} \frac{\omega}{(2\pi)^2} \int_0^{2\pi} e^{i\omega l_\gamma \cos\varphi} \underbrace{\left(\int_{-\infty}^{+\infty} h(\rho)\, e^{i\rho l_\gamma \cos\varphi} d\rho \right)}_{= 2\pi \tilde{h}(l_\gamma \cos\varphi)} d\varphi$$

Apply method of stationary phase to φ-integral,

isol. stationary points $\quad \varphi_+ = 0,\ \varphi_- = \pi$

$$\underset{\omega\to\infty}{\sim} \sqrt{\frac{\omega}{2\pi}} \left\{ e^{i\omega l_\gamma - i\pi/4} \sum_{j=0}^{\infty} D_j^+(\tilde{h})(l_\gamma)\, \omega^{-j} + e^{-i\omega l_\gamma + i\pi/4} \sum_{j=0}^{\infty} D_j^-(\tilde{h})(-l_\gamma) * \omega^{-j} \right\}$$

$D_j^\pm$: differential operators of order j,

$$D_0^+(\tilde{h})(l_\gamma) = l_\gamma^{-1/2}\, \tilde{h}(l_\gamma), \quad D_0^-(\tilde{h})(l_\gamma) = l_\gamma^{-1/2}\, \tilde{h}(-l_\gamma)$$

$\Rightarrow$ leading term when $\tilde{h}$ even: $\sqrt{\dfrac{2\omega}{\pi l_\gamma}} \cos\left(\omega l_\gamma - \frac{\pi}{4}\right) \tilde{h}(l_\gamma)$

<u>Trace Formula:</u>

$$\sum_j m_j\, h(\omega_j - \omega) \underset{\omega\to\infty}{\sim} \omega\, \tilde{h}(0) - i\, \tilde{h}'(0)$$
$$+ \sqrt{\frac{\omega}{2\pi}} \sum_{l_\gamma} \Big\{ e^{i\omega l_\gamma - i\frac{\pi}{4}} \sum_{j\geq 0} D_j^+(\tilde{h})(l_\gamma)\, \omega^{-j}$$
$$+ e^{-i\omega l_\gamma + i\frac{\pi}{4}} \sum_{j\geq 0} D_j^-(\tilde{h})(l_\gamma)\, \omega^{-j} \Big\}$$

Generalisation : $\sqrt{-\Delta}$ on compact Riemannian mfd.

$\to$ Duistermaat – Guillemin '75

Formal application:

choose $h(x) = \delta(x)$, then

$$\sigma(\omega) = \sum_j \delta(\omega_j - \omega) \underset{\omega\to\infty}{\sim} \frac{\omega}{2\pi} = \text{area}(\mathbb{T}^2)\,\frac{\omega}{2\pi}$$

$\Rightarrow$ Weyl's law:

$$N(\omega) := \#\{\omega_j\,;\ 0 \le \omega_j \le \omega\} = \int_0^\omega \sigma(\mu)\,d\mu$$

$$\underset{\omega\to\infty}{\sim} \frac{\text{area}(\mathbb{T}^2)}{4\pi}\,\omega^2$$

Thus: Sum over closed geodesics introduces corrections to Weyl's law $\rightsquigarrow$ details of eigenvalue distribution

But: Difficult to extract!

$$N(\omega) = \#\{k \in \mathbb{Z}^2\,;\ |k| \le \tfrac{\omega}{2\pi}\}$$

$\rightsquigarrow$ counting eigenvalues $\equiv$ circle problem

known results:

- $$\limsup_{\omega\to\infty} \frac{N(\omega) - \omega^2/4\pi}{\sqrt{\omega}} > 0$$
- $$\liminf_{\omega\to\infty} \frac{N(\omega) - \omega^2/4\pi}{\sqrt{\omega}\,(\log\omega)^{1/4}} < 0$$

} Hardy '16

- $$N(\omega) = \frac{\omega^2}{4\pi} + O\left(\omega^{\frac{46}{73}} (\log\omega)^{\frac{630}{146}}\right)$$ Huxley '92

② QM:

$$\text{operator } -\frac{\hbar^2}{2}\Delta \quad \text{instead of} \quad \sqrt{-\Delta}$$

$$\downarrow \qquad\qquad\qquad \downarrow$$

$$E_j = \frac{\hbar^2}{2}\omega_j^2 \qquad\qquad \omega_j$$

Goal: l.h.s. of Poisson summation = spectral side related to $\{E_j\}$

Choose $\varphi \in \mathcal{S}(\mathbb{R})$ such that $\varphi\left(\frac{2\pi^2\hbar^2 x^2 - E}{\hbar}\right) = f(x)$

in Poisson summation:

$$\text{l.h.s.} = \sum_{k\in\mathbb{Z}^2} \varphi\left(\frac{2\pi^2\hbar^2 k^2 - E}{\hbar}\right) = \sum_j m_j\, \varphi\left(\frac{E_j - E}{\hbar}\right)$$

For $E = \frac{\hbar^2}{2}\omega^2$ fixed, $\omega \to \infty$ is equiv. to $\hbar \to 0$

$\rightsquigarrow$ expect for r.h.s.:

$$\sum_j m_j\, \varphi\left(\frac{E_j - E}{\hbar}\right) \underset{\hbar\to 0}{\sim} \text{"Weyl-term"} + \sum_{l_\gamma} A_{l_\gamma}\, e^{\frac{i}{\hbar}\sqrt{2E}\, l_\gamma}$$

Dynamical interpretation:

$$H(q,p) = \tfrac{1}{2}p^2 \quad \text{on } T^*(\mathbb{R}^2/\mathbb{Z}^2) \quad \Rightarrow \begin{cases} \dot q(t) = p(t) \\ \dot p(t) = 0 \end{cases}$$

$$\Rightarrow \phi_H^t(q_0, p_0) = (p_0 t + q_0,\, p_0) \quad (\mathrm{mod}\ 1)$$

Hamiltonian flow = geodesic flow

action: $\int_\gamma p\, dq = \sqrt{2E}\, l_\gamma$

Trace Formulas : The Spectral Side

Consider the QM case:

Hamilton operator H, self-adjoint on a suitable domain $\mathcal{D}_H \subset L^2(\mathbb{R}^d)$, bounded from below.

It generates the unitary 1-parameter group $U(t) = e^{-\frac{i}{\hbar}tH}$

Suppose: spec(H) is pure point, eigenvalues

$$E_1 \leq E_2 \leq E_3 \leq \dots$$

Then (formally):

$$\operatorname{Tr} U(t) = \sum_n e^{-\frac{i}{\hbar}tE_n}$$

Fourier transform: $\left[(\mathcal{F}\rho)(\lambda) = \tilde{\rho}(\lambda) = \int \rho(t)\, e^{i\lambda t}\, dt \right]$

$$\frac{1}{2\pi\hbar}\, \mathcal{F}[\operatorname{Tr} U]\left(\frac{E}{\hbar}\right) = \sum_n \delta(E_n - E) =: d(E)$$

(spectral density of H)

Hence:

analyse $\operatorname{Tr} U(t) \Rightarrow$ determine $d(E)$

More specifically:

$\mathrm{Tr}\, \mathcal{U}(t)$ is a (tempered) distribution,

$$\mathcal{S}(\mathbb{R}) \ni \rho \longmapsto \int \rho(t)\, \mathrm{Tr}\, \mathcal{U}(t)\, dt$$

$$= \sum_n \tilde{\rho}\left(-\frac{E_n}{\hbar}\right),$$

if, e.g., $E_n = O(n^K)$ for some $K < \infty$.

Q: What are the singularities of this distribution?

① Singular support

$u \in \mathcal{S}'(\mathbb{R}^n)$, $\quad x_0 \in \text{sing supp } u \; :\Leftrightarrow$

$$\nexists\, U \ni x_0 \text{ s.t. on } U: \quad u = u^{(\infty)} \in C^\infty(U)$$

Paley-Wiener thm $\Rightarrow$

$x_0 \notin \text{sing supp } u \Leftrightarrow \exists\, \chi \in C_0^\infty(\mathbb{R}^n)$ with $\chi(x_0) \neq 0$ and

$$\widetilde{\chi u}(\xi) = O(|\xi|^{-\infty})$$

$$(\text{i.e., } \ldots = O(|\xi|^{-N}) \;\; \forall N > 0)$$

Here: $t_0 \notin \text{sing supp } \mathrm{Tr}\, \mathcal{U} \Leftrightarrow$

$\exists\, \rho \in C_0^\infty(\mathbb{R})$ with $\rho(t_0) \neq 0$ and

$$\widetilde{\rho \mathrm{Tr} \mathcal{U}}(\lambda) = \int \rho(t)\, \mathrm{Tr}\, \mathcal{U}(t)\, e^{i\lambda t}\, dt$$

$$= \sum_n \tilde{\rho}\left(\lambda - \frac{E_n}{\hbar}\right) \overset{!}{=} O(\lambda^{-\infty})$$

② Frequency set

u_h bounded family of (tempered) distributions, smoothly depending on $h \in (0, h_0)$. Introduce $FS(u_h) \subset T^*\mathbb{R}^d$ via:

$$(x_0, \xi_0) \notin FS(u_h) :\Leftrightarrow \exists\, V \times W \ni (x_0, \xi_0) \text{ s.t. } \forall\, \chi \in C_0^\infty(V) \text{ and } \forall\, \xi \in W,$$

$$\int \chi(x)\, u_h(x)\, e^{\frac{i}{h} x\cdot\xi}\, dx = O(h^\infty)$$

<u>Remark:</u> If $u \in \mathcal{S}'(\mathbb{R}^n)$ indep. of h, then

$$\int \chi(x)\, u(x)\, e^{\frac{i}{h} x\cdot\xi}\, dx = O(h^\infty)$$

$$\Leftrightarrow \quad \int \chi(x)\, u(x)\, e^{i x\cdot\xi}\, dx = \widetilde{\chi u}(\xi) = O(|\xi|^{-\infty})$$

Thus: $\quad$ sing supp $u \subset \mathbb{R}^n$

$\quad = \text{projection of } FS(u) \subset T^*\mathbb{R}^n \text{ to } \mathbb{R}^n$

$\leadsto$ $FS(u)$ contains locations and "directions" of the singularities

Example: $\quad u(x) = e^{-\frac{i}{\hbar} S(x)}, \quad S \in C^\infty(\mathbb{R}^n)$

Apply method of (non-) stationary phase to

$$\int \chi(x)\, e^{-\frac{i}{\hbar}(S(x) - x\cdot\xi)}\, dx \overset{!}{=} O(\hbar^\infty)$$

$$\Leftrightarrow \quad \operatorname{supp} \chi \cap \left\{ x \in \mathbb{R}^n;\ \frac{\partial S}{\partial x}(x) = \xi \right\} = \emptyset$$

Thus: $\quad FS\left(e^{-\frac{i}{\hbar}S}\right) = \left\{ \left(x, \frac{\partial S}{\partial x}(x)\right) \right\} = \text{graph } dS$

Here: $\quad (t_0, E_0) \notin FS(\operatorname{Tr} U) \quad \Leftrightarrow$

$\exists\ I \times J \ni (t_0, E_0)$ s.t. $\forall \rho \in C_0^\infty(I)$ and $\forall E \in J$

$$\int \rho(t)\, \operatorname{Tr} U(t)\, e^{\frac{i}{\hbar}Et}\, dt = \sum_n \tilde{\rho}\left(\frac{E - E_n}{\hbar}\right)$$

$$\overset{!}{=} O(\hbar^\infty)$$

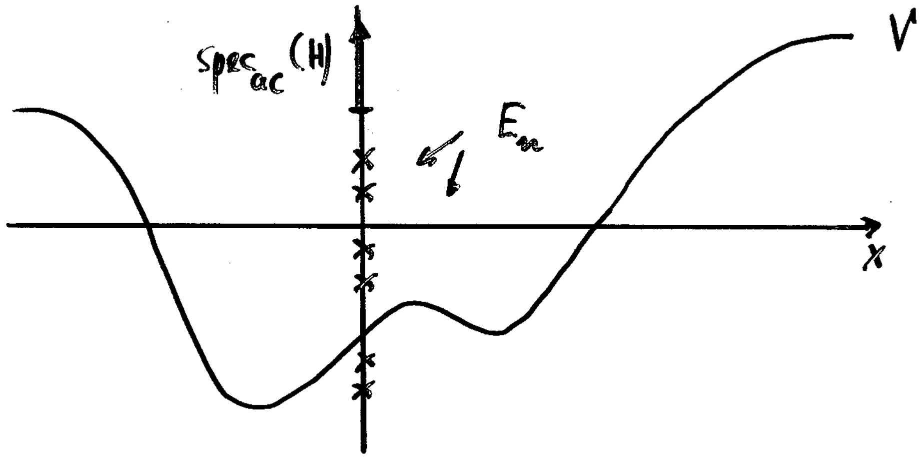
Remarks:

- $\operatorname{Tr} U(t)$ is not of the form $e^{\frac{i}{\hbar}S(t)}$, but introducing Schwartz-kernels and semiclassical representations leads to a refined version of this.

• Often spec(H) is not pure point, but there may be an interval I s.t.

$$\#\left(\operatorname{spec}(H) \cap I\right) < \infty$$

E.g., $H = -\frac{\hbar^2}{2}\Delta + V(x)$ with

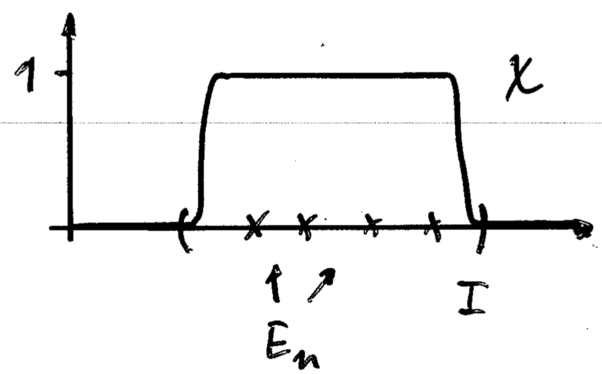


Then: "spectral localisation"

$\chi \in C_0^\infty(\mathbb{R})$, $\operatorname{supp}\chi \subset I$

$\Rightarrow$ $\operatorname{spec}(\chi(H))$ is pure point, eigenvalues $\chi(E_n)$

especially:



$\Rightarrow \chi(E_n) = 1$

Restricted unitary group:

$$U_\chi(t) = \chi(H)\, e^{-\frac{i}{\hbar}Ht}$$

$$\Rightarrow \operatorname{Tr} U_\chi(t) = \sum \chi(E_n)\, e^{-\frac{i}{\hbar}tE_n}$$

Interlude: Some semiclassical calculus (Weyl)

Aim: phase-space representation of the Hamilton operator $\hat{H}$

fct. $H(x,\xi)$ on $T^*\mathbb{R}^d$:

classical Hamiltonian, generates flow ϕ_H^t via Hamilton's eqns.

$$\downarrow$$

operator $\hat{H} = op^W[H]$ on $C_0^\infty(\mathbb{R}^d) \subset L^2(\mathbb{R}^d)$ via

$$\left(op^W[H]\psi\right)(x) := \frac{1}{(2\pi\hbar)^d} \iint H\left(\frac{x+y}{2}, \xi\right) e^{\frac{i}{\hbar}\xi\cdot(x-y)} \psi(y)\, d\xi\, dy$$

(oscillatory integral)

(Ex: $H(x,\xi) = \frac{1}{2}\xi^2 + V(x) \Rightarrow op^W[H] = -\frac{\hbar^2}{2}\Delta + V(x)$)

Restrict class of fcts. H ("symbols") to the following:

$H \in S(m)$, $m = (m_x, m_\xi) \in \mathbb{R}^2$:$\Leftrightarrow$

$H \in C^\infty(T^*\mathbb{R}^d)$ s.t. $\left|\partial_x^\alpha \partial_\xi^\beta H(x,\xi)\right| \leq C_{\alpha\beta} (1+x^2)^{\frac{m_x}{2}} (1+\xi^2)^{\frac{m_\xi}{2}}$

Thm. (Calderón - Vaillancourt '71)

$H \in S(0) \Rightarrow op^W[H]$ bounded operator on $L^2(\mathbb{R}^d)$

$\hbar$- dependent symbols:

$H \in S_{cl}(m) \quad :\Leftrightarrow$

$H(\cdot,\cdot;\hbar) \in S(m)$ uniformly in $\hbar \in (0,\hbar_0)$

and:

$$H(x,\xi;\hbar) \sim \sum_{j=0}^{\infty} \hbar^j \, H_j(x,\xi)$$

i.e. $\quad H - \sum_{j=0}^{N-1} \hbar^j H_j = O(\hbar^N)$ in $S(m) \quad \forall N$

$H_0(x,\xi)$: principal symbol

$H_1(x,\xi)$: subprincipal symbol

Some technicalities:

- $H_0(x,\xi)$ bounded below $\Rightarrow$ $op^W[H]$ bounded below (if $\hbar$ suff. small)
- Ellipticity:

$$|H_0(x,\xi) + i| \geq K \, (1+x^2)^{\frac{m_x}{2}} (1+\xi^2)^{\frac{m_\xi}{2}}$$

$\Rightarrow$ $op^W[H]$ essentially self-adjoint on $C_0^\infty(\mathbb{R}^d)$ (if $\hbar$ suff. small)

- E is regular value of $H_0(x,\xi)$, then the energy shell

$$\Omega_E = \{ (x,\xi) \in T^*\mathbb{R}^d \, ; \, H_0(x,\xi) = E \}$$

is a smooth $(2d-1)$-dim. submfd. of $T^*\mathbb{R}^d$

- Ω_E compact mfd. $\Rightarrow$ $\exists$ interval $J \ni E$ s.t.

  $\mathrm{spec}(\mathrm{op}^W[H]) \cap J$ is pure point

  (if $\hbar$ suff. small)

Moreover ("Weyl's law"):

$$\#\{E_n \in J\} = \frac{1}{(2\pi\hbar)^d} \iint_{\{H_0(x,\xi) \in J\}} dx\, d\xi + O(\hbar^{1-d})$$

- $\chi \in C_0^\infty(\mathbb{R})$, $H \in S_{cl}(m)$ $\Rightarrow$

  $\chi(H) \in S_{cl}(m)$ with principal symbol

  $\chi(H)_0 = \chi(H_0)$

Spectral calculations

Suppose $\operatorname{spec}(H)$ is pure point

$$H \psi_n = E_n \psi_n \qquad (n \in \mathbb{N})$$

then $\{\psi_n ; n \in \mathbb{N}\} \subset L^2(\mathbb{R}^d)$ is an onb.

Construct a bounded operator on $L^2(\mathbb{R}^d)$, $\rho \in \mathcal{S}(\mathbb{R})$,

$$U_\rho := \int \rho(t)\, U(t)\, dt$$

with Schwartz kernel

$$K_\rho(x,y) = \sum_n \psi_n(x) \overline{\psi_n(y)}\, \tilde{\rho}\left(-\frac{E_n}{\hbar}\right)$$

(L^2-convergence)

Then:

$$\int \rho(t)\, \operatorname{Tr} U(t)\, dt = \int K_\rho(x,x)\, dx = \sum_n \tilde{\rho}\left(-\frac{E_n}{\hbar}\right)$$

Formally: $U(t)$ has Schwartz-kernel

$$K(t,x,y) = \sum_n \psi_n(x) \overline{\psi_n(y)}\, e^{-\frac{i}{\hbar} E_n t}$$

(distributional convergence)

Properties:

$$i\hbar \frac{\partial}{\partial t} U(t) = H\, U(t) \quad , \quad U(0) = id$$

$$\Rightarrow \begin{cases} i\hbar \frac{\partial}{\partial t} K(t,x,y) = H_x K(t,x,y) \\ K(0,x,y) = \delta(x-y) \end{cases}$$

If spec(H) is not pure point, but spec$(H) \cap J$ is

$\rightsquigarrow$ spectral localisation with $\chi \in C_0^\infty(\mathbb{R})$; supp $\chi \subset J$

Replace $U(t)$ with $U_\chi(t) = \chi(H)\, e^{-\frac{i}{\hbar} t H}$,

- $K_\rho^\chi(x,y) = \sum_n \chi(E_n)\, \psi_n(x) \overline{\psi_n(y)}\, \tilde{\rho}\left(-\frac{E_n}{\hbar}\right)$
- $K^\chi(t,x,y) = \sum_n \chi(E_n)\, \psi_n(x) \overline{\psi_n(y)}\, e^{-\frac{i}{\hbar} t E_n}$

Finally (with $\varphi \in \mathcal{S}(\mathbb{R})$ s.t. $\varphi(E) := \tilde{\rho}(-E)$)

$$\sum_n \chi(E_n)\, \varphi\left(\frac{E_n - E}{\hbar}\right) = \frac{1}{2\pi} \int_{\mathbb{R}_t} \tilde{\varphi}(t)\, \mathrm{Tr}\, U_\chi(t)\, e^{\frac{i}{\hbar} E t}\, dt$$

$$= \frac{1}{2\pi} \int_{\mathbb{R}_t} \int_{\mathbb{R}^d_x} \tilde{\varphi}(t)\, \underbrace{K^\chi(t,x,x)}_{\uparrow}\, e^{\frac{i}{\hbar} E t}\, dt\, dx$$

requires semiclassical representation, ...

finally: dynamical side

Extension

symbol $B \in S_{cl}(0)$ s.t. $op^W[B]$ is a bounded and self-adjoint operator on $L^2(\mathbb{R}^d)$,

replace $\mathrm{Tr}\, U_\chi(t)$ with $\mathrm{Tr}\left(op^W[B]\, U_\chi(t)\right)$

Formally:

- $$\mathrm{Tr}\left(op^W[B]\, U_\chi(t)\right) = \sum_n \langle \psi_n, op^W[B]\psi_n\rangle\, e^{-\frac{i}{\hbar}E_n t}$$

- kernels:

$$\left(op^W[B]\, U_\chi(t)\, \psi\right)(x) = \frac{1}{(2\pi\hbar)^d}\iint B\left(\tfrac{x+y}{2},\xi\right) e^{\frac{i}{\hbar}\xi\cdot(x-y)} \left(U_\chi(t)\psi\right)(y)\, d\xi\, dy$$

$$= \frac{1}{(2\pi\hbar)^d}\iiint B\left(\tfrac{x+y}{2},\xi\right) e^{\frac{i}{\hbar}\xi\cdot(x-y)}\, K^\chi(t,y,z)\,\psi(z)\, d\xi\, dy\, dz$$

- trace:

$$\mathrm{Tr}\left(op^W[B]\, U_\chi(t)\right)$$

$$= \frac{1}{(2\pi\hbar)^d}\iiint B\left(\tfrac{x+y}{2},\xi\right) e^{\frac{i}{\hbar}\xi\cdot(x-y)}\, K^\chi(t,y,x)\, d\xi\, dy\, dx$$

Hence:

$$\sum_n \chi(E_n)\,\langle \psi_n, op^W[B]\psi_n\rangle\, \varphi\left(\frac{E_n-E}{\hbar}\right)$$

$$= \frac{1}{2\pi}\frac{1}{(2\pi\hbar)^d}\int\cdots\int \tilde{\varphi}(t)\, e^{\frac{i}{\hbar}(Et+\xi\cdot(x-y))} B\left(\tfrac{x+y}{2},\xi\right) K^\chi(t,y,x)\, dt\, d\xi\, dy\, dx$$

Trace Formulas: The Dynamical Side

- Find semiclassical representation for the Schwartz-kernel of $U(t)$.
- Calculate trace.

$$\psi(t,x) = (U(t)\psi_0)(x) \quad \text{with} \quad \psi(0,x) = \psi_0(x)$$

is solution of Schrödinger eq.

$$i\hbar \frac{\partial}{\partial t}\psi(t,x) = H\psi(t,x)$$

(I) Special initial conditions allow WKB-method:

$$\psi_0(x) = A_0(x)\, e^{\frac{i}{\hbar}\xi_0 \cdot x}$$

$$\left(\text{recall: } FS(\psi_0) = \{(x,\xi_0);\, x \in \operatorname{supp} A_0\}\right)$$

WKB-Ansatz:

$$\psi(t,x) = \sum_{k=0}^{N} \left(\frac{\hbar}{i}\right)^k a_k(t,x)\, e^{\frac{i}{\hbar}S(t,x)} + O(\hbar^{N+1})$$

$$\left(\Rightarrow \quad FS(\psi_t) \subseteq \left\{\left(x, \frac{\partial S_t}{\partial x}\right);\, x \in \mathbb{R}^d\right\} = \operatorname{graph} dS_t\right)$$

Then (with $H = -\frac{\hbar^2}{2}\Delta + V(x)$):

$$\left(H - i\hbar\frac{\partial}{\partial t}\right) \sum_k \left(\frac{\hbar}{i}\right)^k a_k \, e^{\frac{i}{\hbar}S}$$

$$= \left[\frac{1}{2}\left(\frac{\partial S}{\partial x}\right)^2 + V + \frac{\partial S}{\partial t}\right] a_0$$

$$+ \frac{\hbar}{i}\left[\left(\frac{1}{2}\left(\frac{\partial S}{\partial x}\right)^2 + V + \frac{\partial S}{\partial t}\right) a_1 + \left(\frac{\partial}{\partial t} + \frac{\partial S}{\partial x}\cdot\frac{\partial}{\partial x} + \frac{1}{2}\Delta S\right) a_0\right]$$

$$+ \sum_{k\geq 2}\left(\frac{\hbar}{i}\right)^k \left[\left(\frac{1}{2}\left(\frac{\partial S}{\partial x}\right)^2 + V + \frac{\partial S}{\partial t}\right) a_k + \left(\frac{\partial}{\partial t} + \frac{\partial S}{\partial x}\cdot\frac{\partial}{\partial x} + \frac{1}{2}\Delta S\right) a_{k-1} - \frac{1}{2}\Delta a_{k-2}\right]$$

Conditions for vanishing to all orders in $\hbar$:

① In $O(\hbar^0)$:

$$H\left(x, \frac{\partial S}{\partial x}\right) + \frac{\partial S}{\partial t} = 0 \qquad \text{with} \qquad S(0,x) = \xi_0 \cdot x$$

(Hamilton-Jacobi eqn, HJE)

call solution $S(t, x; \xi_0)$ or $S_t(x;\xi_0)$

② In $O(\hbar^k)$, $k \geq 1$:

$$\left(\frac{\partial}{\partial t} + \frac{\partial S}{\partial x}\cdot\frac{\partial}{\partial x} + \frac{1}{2}\Delta S\right) a_{k-1} = \begin{cases} 0, & k = 1 \\ \frac{1}{2}\Delta a_{k-2}, & k \geq 2 \end{cases}$$

$$\text{with} \qquad a_{k-1}(0,x) = \begin{cases} A(x), & k = 1 \\ 0, & k \geq 2 \end{cases}$$

(transport eqns, (in)homogeneous)

Solutions:

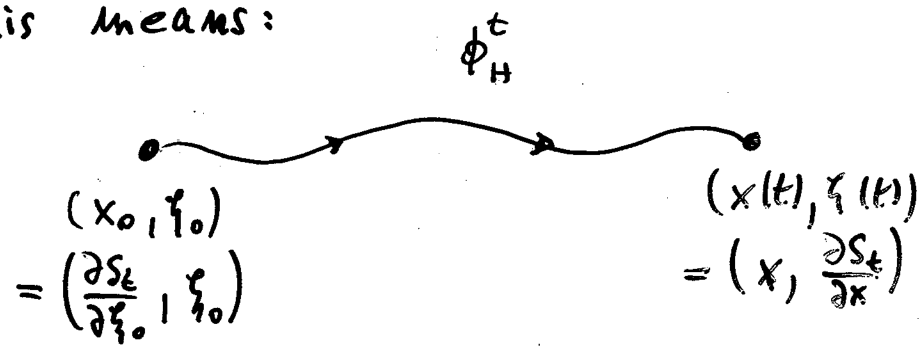
① There exists a connection between solns. of HJE and solns. of the eqns. of motion (Hamiltonian flow).

<u>Prop.:</u>

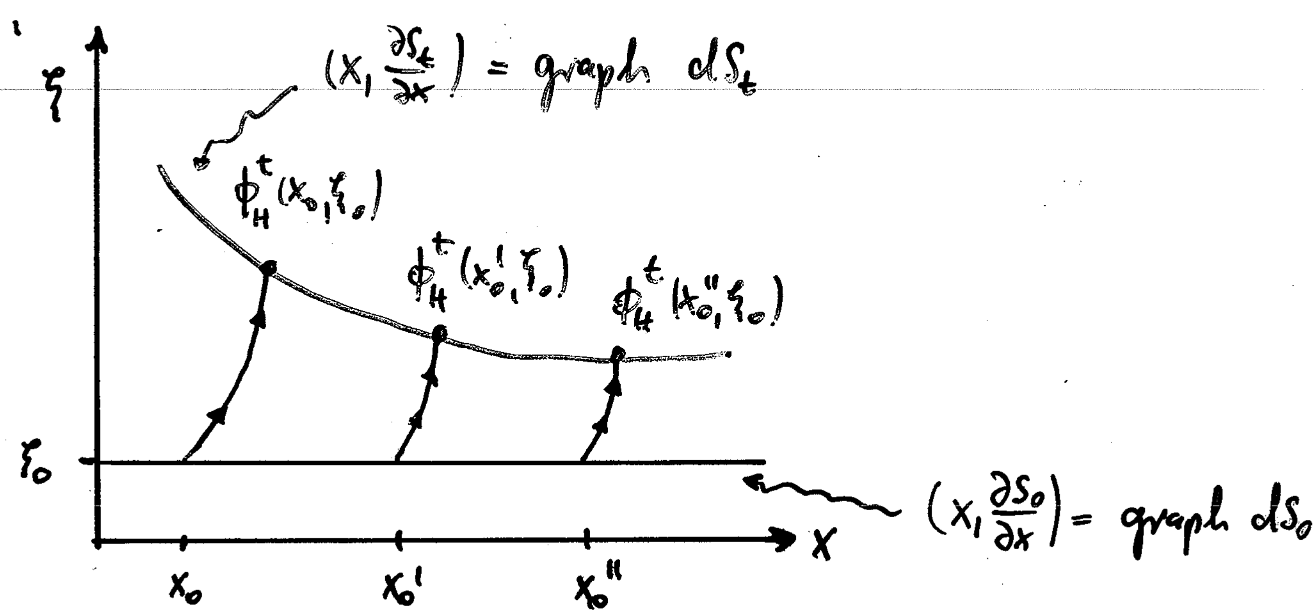
$\exists\, T>0$ s.t. for $|t|<T$ ex. unique solution $S \in C^\infty\big((-T,T)\times\mathbb{R}^d\times\mathbb{R}^d\big)$ of HJE. Moreover:

$$\Big(x, \frac{\partial S}{\partial x}(t,x;\xi_0)\Big) = \phi_H^t\Big(\frac{\partial S}{\partial \xi}(t,x;\xi_0), \xi_0\Big).$$

This means:



or:

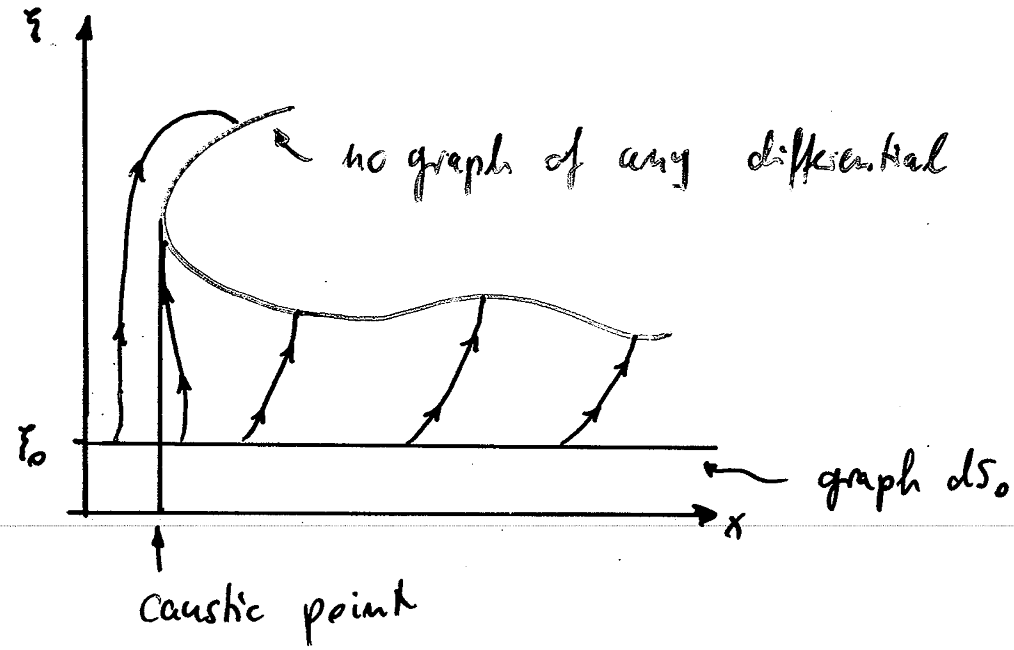


For all $|t| < T$ graph $dS_t \subset T^*\mathbb{R}^d$ is a Lagrangian submfd.

- $\omega := \sum_{k=1}^{d} dx_k \wedge d\xi_k = 0$ on graph dS_t
- $\dim \operatorname{graph} dS_t = d = \frac{1}{2} \dim T^*\mathbb{R}^d$

<u>Thus:</u> HJE is evolution eq. for the Lagrangean mfd $FS(\psi_{WKB})$!

<u>Remark:</u> Unique sol. $S(t,x)$ of HJE exists for suff. small t $(t<T)$. Beyond $(t>T)$:



T: time of occurrence of first caustic (caustic time)

beyond caustic time $(t>T)$:

- local pieces of Lagrangean mfd : graph $dS_t(x)$ or graph $d\tilde{S}_t(\xi)$
- away from caustics : parametr. by branches $S^{(j)}(t,x)$

② Transport eqn (hom. case):

- $\frac{\partial S_t}{\partial x} = \xi(t) = \dot{x}(t)$,

- $\frac{d}{dt}\frac{\partial x(t)}{\partial x_0} = \frac{\partial^2 S_t}{\partial x \partial x}\frac{\partial x(t)}{\partial x_0} \Rightarrow \frac{d}{dt}\log\det\left(\frac{\partial x}{\partial x_0}\right) = \mathrm{tr}\frac{\partial^2 S_t}{\partial x \partial x}$
$= \Delta S_t$

Hence:

$$\left(\frac{\partial}{\partial t} + \dot{x}\cdot\frac{\partial}{\partial x} + \frac{1}{2}\frac{d}{dt}\log\det\frac{\partial x}{\partial x_0}\right) a_0(t,x) = 0 \quad , \quad a_0\big|_{t=0} = A_0,$$

$$\Rightarrow \quad a_0(t,x) = \left(\det\frac{\partial x}{\partial x_0}\right)^{-1/2} A_0(x)$$

Before caustic time $(t<T)$:

invert $x(t, x_0, \xi_0) \rightsquigarrow x_0(t,x,\xi_0) \quad = \frac{\partial S}{\partial \xi}(t,x;\xi_0)$

$$\Rightarrow \quad a_0(t,x) = \left(\det\left(\frac{\partial^2 S_t}{\partial x \partial \xi}\right)\right)^{+1/2} A_0(x)$$

Remark: Failure at T since $\frac{\partial^2 S_t}{\partial x \partial \xi}$ singular!

WKB-solution before (first) caustic time:

$$\Psi_{WKB}(t,x) = \sqrt{\det\left(\frac{\partial^2 S_t}{\partial x \partial \xi}\right)}\; e^{\frac{i}{\hbar}S(t,x)} + O(\hbar),$$

and for $t>T$ (not at some caustic time and away from caustic points):

$$\Psi_{WKB}(t,x) = \sum_j \sqrt{\det\left(\frac{\partial^2 S_t^{(j)}}{\partial x \partial \xi}\right)}\; e^{\frac{i}{\hbar}S^{(j)}(t,x)} + O(\hbar)$$

$\left.\begin{matrix}\text{sum over pieces of} \\ \text{Lagr. mfd. at time } t\end{matrix}\right\} \hat{=} \left\{\begin{matrix}\text{sum over trajectories from } (x_0^{(j)},\xi_0) \\ \text{to } (x^{(j)}(t),\xi^{(j)}(t)) \text{ with } x^{(j)}(t) = x\end{matrix}\right.$

II General initial condition

$$\psi(0,x) = \psi_0(x)$$

then: $$\psi(t,x) = \int K(t,x,y)\,\psi_0(y)\,dy$$

Introduce WKB-type ansatz for the kernel,

(*) $$K(t,x,y) = \frac{1}{(2\pi\hbar)^d}\int \sum_{k=0}^{N}\left(\frac{\hbar}{i}\right)^k a_k(t,x,y;\xi)\, e^{\frac{i}{\hbar}\left(S(t,x;\xi)-y\cdot\xi\right)}d\xi + O(\hbar^{N+1})$$

Recall:

(**) $$i\hbar\frac{\partial}{\partial t}K(t,x,y) = H_x K(t,x,y), \qquad K(0,x,y) = \delta(x-y)$$

Conditions on (*) to fulfill (**):

α) $t=0$:

$$a_k(0,x,y;\xi) = \begin{cases} 1, & k=0 \\ 0, & k\geq 1 \end{cases}, \qquad S(0,x;\xi) = x\cdot\xi$$

β) Schrödinger eq.

In $O(\hbar^0)$: HJE

$$H\left(x,\frac{\partial S}{\partial x}\right) + \frac{\partial S}{\partial t} = 0$$

In $O(\hbar^k)$, $k\geq 1$: transport eqs.

$$\left(\frac{\partial}{\partial t} + \frac{\partial S}{\partial x}\cdot\frac{\partial}{\partial x} + \frac{1}{2}\Delta S\right) a_{k-1} = \begin{cases} 0, & k=1 \\ \frac{1}{2}\Delta a_{k-2}, & k\geq 2 \end{cases}$$

Frequency set of $\operatorname{Tr} U(t)$

$(t_0, E_0) \notin FS(\operatorname{Tr} U) \iff$

$\exists\ I \times J \ni (t_0, E_0)$ s.t. $\forall \varphi \in \mathcal{S}(\mathbb{R})$ with $\tilde{\varphi} \in C_0^\infty(I)$

and $\forall\ E \in J$

$$\sum_n \varphi\left(\frac{E_n - E}{\hbar}\right) = \underbrace{\frac{1}{2\pi} \int \tilde{\varphi}(t) \operatorname{Tr} U(t)\, e^{\frac{i}{\hbar} E t}\, dt}_{\parallel \ (\mathrm{mod}\ O(\hbar^\infty))} \overset{!}{=} O(\hbar^\infty)$$

$$\frac{1}{2\pi} \frac{1}{(2\pi\hbar)^d} \int_{\mathbb{R}_t} \int_{\mathbb{R}^d_x} \int_{\mathbb{R}^d_\xi} \tilde{\varphi}(t) \sum_{k \geq 0} \left(\frac{\hbar}{i}\right)^k a_k(t, x, x; \xi)\ e^{\frac{i}{\hbar}\left(S(t,x;\xi) - x\cdot\xi + Et\right)} d\xi\, dx\, dt$$

Apply method of (non-) stationary phase:

$(t_0, E_0) \notin FS(\operatorname{Tr} U) \iff$

$\forall E \in J$: $I \times \mathbb{R}^d_x \times \mathbb{R}^d_\xi$ contains no stationary point of the phase $\Phi_E(t, x, \xi) := S(t, x; \xi) - x\cdot\xi + Et$

stationary points are solutions of

$$\left.\begin{aligned} &i)\ \frac{\partial S}{\partial x}(t, x; \xi) \overset{!}{=} \xi \\ &ii)\ \frac{\partial S}{\partial \xi}(t, x; \xi) \overset{!}{=} x \end{aligned}\right\} \iff$$

(x, ξ) is point on a periodic traject. of Hamilt. flow with period t

iii) $\frac{\partial S}{\partial t}(t, x; \xi) \overset{!}{=} -E \implies (x, \xi)$ is point on a trajectory with energy E

<u>Thus:</u> (Poisson relation; Chazarain '74 / '80)

$$\mathrm{FS}\,(\mathrm{Tr}\,U) \subseteq \left\{ (t,E)\,;\ \exists\ (x,\xi)\in\Omega_E \text{ s.t. } \phi_H^t(x,\xi) = (x,\xi) \right\}$$

Consequences for the Trace Formula:

- relevant contributions $\left(\neq O(\hbar^\infty)\right)$ are determined by stationary points of $S(t,x;\xi) - x\cdot\xi + Et$, i.e., by periodic trajectories ("periodic orbits") of energy E.
- calculate contribution of each singularity with method of stationary phase.

<u>Remark:</u> The above discussion is only correct if $|t|<T$, i.e., if $\operatorname{supp}\tilde{\varphi} \subset (-T,T)$.

Beyond caustic times:

local representation of Lagrangean mfd. in terms of pieses of graph $dS_t^{(j)}$ $\Rightarrow$ ... (stationary phase) ... $\Rightarrow$ line bundle with transition fcts.

$$\exp\Big[\frac{i\pi}{4}\underbrace{\Big(\operatorname{sgn}\frac{\partial^2 S^{(k)}}{\partial x\,\partial\xi} - \operatorname{sgn}\frac{\partial^2 S^{(l)}}{\partial x\,\partial\xi}\Big)}_{\in 2\mathbb{Z}}\Big]$$

(Maslov-bundle $\rightsquigarrow$ Maslov-phase)

Now: apply method of stationary phase to

$$\iiint \tilde{\varphi}(t) \sum_{k \geq 0} \left(\frac{\hbar}{i}\right)^k a_k(t,x,x;\xi)\, e^{\frac{i}{\hbar}\left(S(t,x;\xi) - x\cdot\xi + Et\right)}\, d\xi\, dx\, dt$$

Remarks:

- for leading order in $\hbar$ use
$$a_0 = \sqrt{\det \frac{\partial^2 S}{\partial x \partial \xi}}$$

- value of the phase at a stationary point:
  - Lagrangean fct. $L(x,\dot{x}) = \dot{x}\cdot\xi - H(x,\xi)$
  - $\displaystyle\int_0^t L(x(s), \dot{x}(s))\, ds = S(t,x;\xi) - x\cdot\xi$
  - action of periodic orbit γ:
$$S_\gamma := \int_\gamma \xi\cdot dx = \int_0^t L\, ds + Et = S(t,x;\xi) - x\cdot\xi + Et$$

- no stationary point is isolated:

  (x,ξ,t) stationary point $\Leftrightarrow$ (x,ξ) on periodic orbit of period t

  i.e., (x,ξ) isolated $\Leftrightarrow$ (x,ξ) fixed point of flow

  but: E non-critical for $H \Rightarrow \left(\frac{\partial H}{\partial x}, \frac{\partial H}{\partial \xi}\right) \neq 0$ on Ω_E

  $\Rightarrow$ no fixed points

Thus: stationary-phase thm. for non-isolated stationary points required!

Consider: $$I(\hbar) = \int_{\mathbb{R}^n} a(x)\, e^{\frac{i}{\hbar}\varphi(x)}\, dx$$

with $a \in C_0^\infty(\mathbb{R}^n)$, $\varphi \in C^\infty(\mathbb{R}^n)$ s.t.

- $M := \left\{ x \in \mathbb{R}^n ;\ \frac{\partial \varphi}{\partial x}(x) = 0 \right\} \subset \mathbb{R}^n$ smooth submfd., $\dim M = m$
- $\operatorname{rank} \frac{\partial^2 \varphi}{\partial x \partial x}(x) = n-m \quad \forall x \in M$

Then:

- local diffeom. $\mathbb{R}^n \supset W \ni x \mapsto (u,v) \in U \times V \subset \mathbb{R}^m \times \mathbb{R}^{n-m}$ s.t. (locally) M is given by points $(u,0)$
- $\tilde{\varphi}(u(x), v(x)) = \varphi(x) \Rightarrow \tilde{\varphi}(u,0) = \varphi|_M = \text{const}$
- $u \in U$ fixed: $v \mapsto \tilde{\varphi}(u,v)$ has isolated stationary point at $v=0$

$$I(\hbar) = \int_M \underbrace{\left\{ \int J(u,v)\, \tilde{a}(u,v)\, e^{\frac{i}{\hbar}\tilde{\varphi}(u,v)}\, dv \right\}}_{\text{isol. stat. point } v=0} du$$

$$= (2\pi\hbar)^{\frac{n-m}{2}}\, e^{\frac{i}{\hbar}\varphi_M + i\frac{\pi}{4}\operatorname{sgn}\frac{\partial^2\tilde{\varphi}}{\partial v \partial v}} \int_M A(u)\, du + O(\hbar^{\frac{n-m}{2}+1})$$

Contribution of one mfd. M of stationary points to the Trace Formula:

$$\hbar^{\frac{1-\dim M}{2}} A_M \, e^{i/\hbar \, S_M} \quad , \quad A_M \sim \sum_{k \geq 0} \hbar^k A_{M,k}$$

- M with max. dimension $\Rightarrow$ leading contribution:

  $M_0 = \{0\} \times \Omega_E$ has dimension $2d-1$

  $\updownarrow$

  $(x,\xi) \in \Omega_E \Rightarrow \Phi_H^{t=0}(x,\xi) = (x,\xi) \Rightarrow (0,x,\xi)$ stat. point

  order of contribution: $\hbar^{\frac{1-\dim M_0}{2}} = \hbar^{1-d}$

- M with min. dimension: $\dim M = 1$

  γ: isolated periodic orbit $\rightsquigarrow M_\gamma = \{T_\gamma\} \times \gamma$,

  $\dim M_\gamma = 1$

  order of contribution: $\hbar^{\frac{1-\dim M_\gamma}{2}} = \hbar^0$

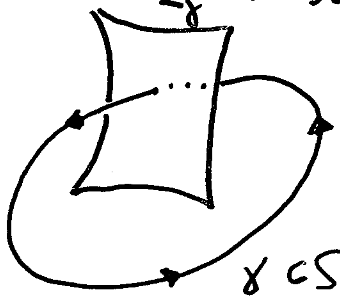
Additional requirement:

- non-degeneracy of phase transversal to mfd. M

M_0: E non-critical for $H(x,\xi)$ suffices

- M_γ requires additional condition:

Σ_γ : surface of section,



$\gamma \subset \Omega_E$

$\Sigma_\gamma \subset \Omega_E$ smooth submfd., $\dim \Sigma_\gamma = 2d-2$,

s.t. $X_H = \frac{\partial H}{\partial \xi}\cdot\frac{\partial}{\partial x} - \frac{\partial H}{\partial x}\cdot\frac{\partial}{\partial \xi}$ not tangent to Σ_γ

Poincaré recurrence map $R_\gamma : \Sigma_\gamma \to \Sigma_\gamma$ ($\leadsto$ flow)

Poincaré map: $P_\gamma := dR_\gamma$

γ non-degenerate $:\Leftrightarrow$ P_γ has no eigenvalue 1

phase non-deg. transversal to M_γ $\Leftrightarrow$ γ non-deg.

<u>Suppose from now on:</u>

Hamiltonian flow Φ_H^t on Ω_E has only isolated and non-degenerate periodic orbits γ

Calculate leading $\hbar$-orders of stat. mfds. M:

i) M_0 : $\dfrac{\mathrm{vol}\,\Omega_E}{(2\pi\hbar)^{d-1}}\;\dfrac{\tilde\varphi(0)}{2\pi}$

ii) M_γ : $\dfrac{\tilde\varphi(T_\gamma)}{2\pi}\;\dfrac{T_\gamma^\# \, e^{\frac{i}{\hbar}S_\gamma - i\frac{\pi}{4}\mu_\gamma}}{|\det(\mathbb{1}-P_\gamma)|^{1/2}}$

$T_\gamma^\#$: primitive (min.) period of γ

μ_γ : Maslov index

Trace Formula:

Suppose:
- $\hat{H} = op^W[H]$, $H \in S_{cl}(m)$, self-adjoint
- E regular value for $H_0(x,\xi)$, Ω_E compact
- M_j $(j = 0,1,2,..)$ connected mfds of periodic

points of $\phi^t_{H_0}$ on Ω_E of periods T_j are all non-degenerate, $S_{M_j} = \int_{\gamma \subset M_j} \xi \cdot dx$

Then:

$$\sum_n \chi(E_n)\,\varphi\left(\frac{E_n - E}{\hbar}\right) \underset{\hbar\to 0}{\sim} \sum_j A_{M_j}\, e^{\frac{i}{\hbar} S_{M_j}},$$

$$A_{M_j} \sim \sum_{k \geq 0} \hbar^{k + \frac{1 - \dim M_j}{2}} A_{M_j,k}$$

holds for all $\varphi \in \mathcal{S}(\mathbb{R})$ with $\tilde{\varphi} \in C_0^\infty(\mathbb{R})$.

In particular,

$$A_{M_0,0} = \frac{\mathrm{vol}\,\Omega_E}{(2\pi\hbar)^{d-1}}\;\frac{\tilde{\varphi}(0)}{2\pi}$$

$$A_{M_\gamma,0} = \frac{\tilde{\varphi}(T_\gamma)}{2\pi}\;\frac{T_\gamma^{\#}\, e^{\frac{i}{\hbar}S_\gamma - i\frac{\pi}{4}\mu_\gamma}}{|\det(\mathbb{1} - P_\gamma)|^{1/2}}$$

Remarks:

- $\phi^t_{H_0}$ has only isolated, non-deg. periodic orbits:

$$\sum_n \chi(E_n)\varphi\left(\frac{E_n-E}{\hbar}\right) \sim \frac{\mathrm{vol}\,\Omega_E}{(2\pi\hbar)^{d-1}}\frac{\tilde\varphi(0)}{2\pi} + O(\hbar^{2-d})$$

$$+\sum_\gamma \frac{\tilde\varphi(T_\gamma)}{2\pi} T_\gamma^{\#} \frac{e^{\frac{i}{\hbar}S_\gamma - i\frac{\pi}{4}\mu_\gamma}}{|\det(\mathbb{1}-P_\gamma)|^{1/2}} + O(\hbar)$$

- supp $\tilde\varphi$ compact $\Rightarrow$ long p.o.'s are cut-off

$\Rightarrow$ limited resolution on l.h.s.

Q: Is it possible to relax support condition on $\tilde\varphi$?

E.g., one would like to allow

$$\varphi_\varepsilon(\lambda) = \frac{1}{\varepsilon\sqrt\pi}e^{-\lambda^2/\varepsilon^2} \xrightarrow[\varepsilon\to0]{} \delta(\lambda)$$

$$\updownarrow$$

$$\tilde\varphi_\varepsilon(t) = e^{-\varepsilon^2t^2/4} \xrightarrow[\varepsilon\to0]{} \underset{\text{Gutzwiller}}{\underset{\uparrow}{1}}$$

one obstacle: convergence of $\sum_\gamma \tilde\varphi(T_\gamma)T_\gamma^{\#}|\det(P_\gamma-\mathbb{1})|^{-1/2}$?

- classical dynamics on Ω_E hyperbolic $\Rightarrow \exists\,\delta>0$ s.t.

$\varphi(\lambda)$ holom. in strip $|\mathrm{Im}\,\lambda|\le\delta$ ensures convergence

(δ computable from p.o.'s)