General quantum resurgence surmised with Gutzwiller's trace formula

André Voros
Institut de physique théorique, Université Paris-Saclay, CEA, CNRS
F-91191 Gif-sur-Yvette Cedex (France)
E-mail: andre.voros@ipht.fr

Conference on Resurgence, KITP, Nov. 1, 2017

Short title: Resurgent Θ-functions

Quantum resurgence

$$\hat{H}\psi \;=\; E\psi \qquad\qquad \hat{H} : \text{quantum Hamiltonian}$$

$$\hat{H} \;\stackrel{\text{def}}{=}\; -\hbar^2\Delta_q + V(q) \qquad (\text{Schrödinger operator}).$$

We focus on *spectral functions* $F\{E_k\}$, and on their dependence upon $1/\hbar \stackrel{\text{def}}{=} x$ as asymptotic (large) parameter.

Some spectral functions F known / expected to be *resurgent in* x:

$$F(x) \;\sim\; \Big(\sum_m f_m x^{-m}\Big)\,\mathrm{e}^{-x\tau_0} \qquad \text{semiclassical (large-}x\text{) expansion}$$

$$F_{\mathrm{B}}(\tau) \;\stackrel{\text{def}}{=}\; \sum_m \frac{f_m}{m!}\,(\tau-\tau_0)^m \quad (\textit{Borel transform}) \text{ converges } (= \text{holomorphic}) \text{ near } \tau_0,$$

moreover can be *endlessly analytically continued*
(thus F_{B} has a Riemann surface $\mathcal{S}$ with only isolated singularities); and

$$F(x) = x\int_{\tau_0}^{\infty} F_{\mathrm{B}}(\tau)\,\mathrm{e}^{-x\tau}\;\mathrm{d}\tau \qquad \text{for some path on } \mathcal{S} \text{ (Laplace transform).}$$

Singularities of $F_{\mathrm{B}}(\tau)$ can:

at least be *located*, and have their germs *expanded*, thanks to underlying *classical propagation* principles;

in some cases, have their germs *explicitly interrelated*:
(*resurgence equations* aka *bridge equations*: Écalle 1981).

Sometimes, description is *rich enough* to *quantum-integrate* $\hat{H}\psi = E\psi$ (analytical solvability of a sort):
e.g., for *1D polynomial potentials* $V(q)$ - an ODE case. (V. 1999)

***

The world is not 1D.

Propagation principles $\Leftarrow$ the *quantum–classical correspondence.*

The question is then: how much of the above can be done for

$$\hat{H}\psi = E\psi, \qquad (n\text{D Schrödinger equation})$$

when $n > 1$ *genuinely* - a PDE case, nonseparable, nonintegrable?

The nD quantum resurgence puzzle

1D treatment of Schrödinger eq.:
exact complex WKB method.
For nD: *inapplicable*
already in the real domain.

nD integral approach:
exact saddle-point method.
Irrelevant to the Schrödinger eq.
(save for ∞D path integral).

$\hat{H}\psi = E\psi$
nD Schrödinger eqn
$n > 1$ genuinely

nD singularity analysis:
Poisson formula on manifolds.
Only for the *real* domain (mod C^∞)
and *homogeneous* operators.

nD singularity analysis:
Balian–Bloch approach.
Attains complex singularities,
but *doesn't reach* full solution.

Ideas from 1D

In general for a (confining) potential $V(q)$, the *partition function* $\mathrm{Tr}\ \mathrm{e}^{-\tau \hat{H}} \equiv \sum_k \mathrm{e}^{-\tau E_k}$ will only be holomorphic for $\mathrm{Re}\ \tau > 0$.

Harmonic potential $V(q) = q^2$ (spectrum $\{E_k = 2k+1\}_{k=0,1,2,\ldots}$):

$$\sum_k \mathrm{e}^{-\tau E_k} \equiv \frac{1}{2\sinh \tau} \qquad \text{is } \textit{meromorphic for all complex } \tau$$

(the identity = the basic *Poisson summation formula*).

Whereas for $V(q) = |q|^N$, $N > 2$, the spectrum $\{E_k\} \propto k^{\frac{2N}{N+2}}$ has vanishing density for $k \to \infty$, hence

$$\sum_k \mathrm{e}^{-\tau E_k} \qquad \text{holomorphic for } \mathrm{Re}\ \tau > 0$$

has $\{\mathrm{Re}\ \tau = 0\}$ as *natural boundary* (cf. Jacobi θ-functions for $N = \infty$).

So, switch to the operator $f(\hat{H}) = \hat{H}^{\frac{N+2}{2N}}$ of spectrum $\{E_k^{\frac{N+2}{2N}}\}$:

$$\mathrm{Tr}\ \mathrm{e}^{-\tau f(\hat{H})} = \sum_k \mathrm{e}^{-\tau E_k^{\frac{N+2}{2N}}} .$$

More precisely: in terms of a single scaled variable,

$$(2\pi\hbar)^{-1}\oint_{p^2+|q|^N=E} p\,\mathrm{d}q = c_N E^{\frac{N+2}{2N}}/\hbar \equiv x,$$

complete Bohr–Sommerfeld quantization condition:

$$\text{for some } F(x) \sim x + \frac{b_1}{x} + \frac{b_2}{x^3} + \cdots : \qquad F(x_k) = k + \tfrac{1}{2}.$$

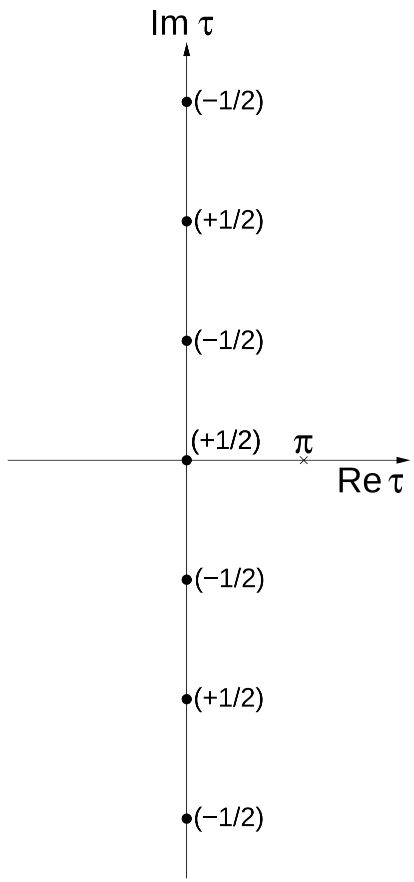
Spectral functions of $\{x_k\}$: $\mathcal{N}(x) \stackrel{\text{def}}{=} \sum_k \theta\big[F(x) - (k+\frac{1}{2})\big]$, $\Theta(\tau) \stackrel{\text{def}}{=} \sum_k \mathrm{e}^{-\tau x_k}$:

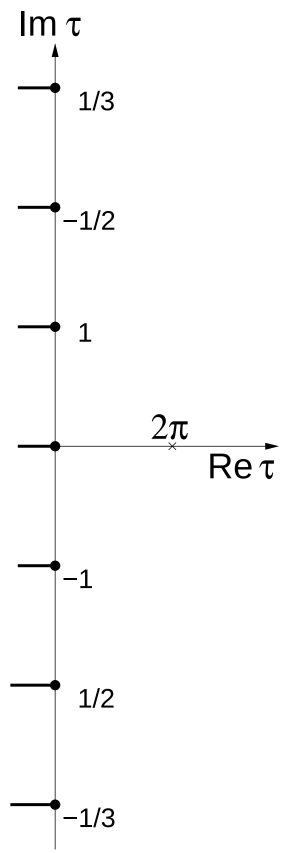
$$\mathcal{N}(x) \equiv F(x) + \sum_{r\neq 0} \frac{(-1)^r}{2\pi \mathrm{i} r}\,\mathrm{e}^{2\pi \mathrm{i} r F(x)} \qquad \text{(Poisson summation formula)}$$

$$= x + \frac{\log\Phi(x)}{2\pi\mathrm{i}} + \sum_{r\neq 0} \frac{(-1)^r}{2\pi \mathrm{i} r}[\Phi(x)]^r\,\mathrm{e}^{2\pi \mathrm{i} r x}, \qquad \Phi(x) \stackrel{\text{def}}{=} \mathrm{e}^{2\pi\mathrm{i}\left[\frac{b_1}{x}+\frac{b_2}{x^3}+\cdots\right]}$$

$$\mathcal{N}(x) \equiv \frac{1}{2\pi\mathrm{i}}\int_{-\mathrm{i}\infty}^{+\mathrm{i}\infty} \frac{\Theta(\tau)}{\tau}\,\mathrm{e}^{x\tau}\,\mathrm{d}\tau \quad \Leftarrow \quad \Theta(\tau) = \int_0^\infty \mathrm{e}^{-\tau x}\,\mathrm{d}\mathcal{N}(x) \quad \text{(Borel)}$$

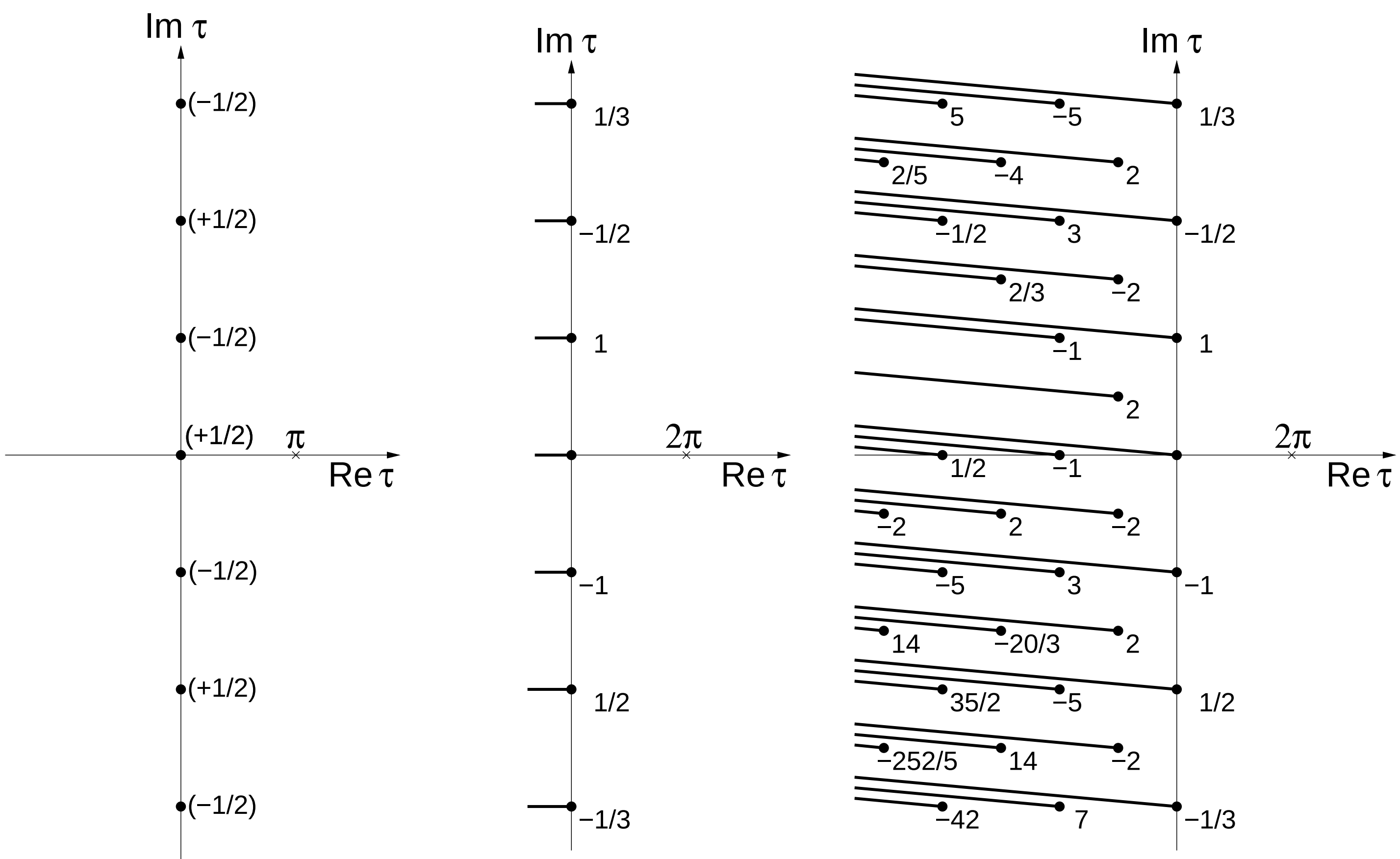
So, $$\frac{1}{2\pi\mathrm{i}}\int_{-\mathrm{i}\infty}^{+\mathrm{i}\infty}\frac{\Theta(\tau)}{\tau}\,\mathrm{e}^{x\tau}\,\mathrm{d}\tau = x + \frac{\log\Phi(x)}{2\pi\mathrm{i}} + \sum_{r\neq 0}\frac{(-1)^r}{2\pi\mathrm{i}r}[\Phi(x)]^r\,\mathrm{e}^{2\pi\mathrm{i}rx}$$





$\frac{1}{2\sinh\tau}$ $[V(q)=q^2]$ General 1D $\frac{\Theta(\tau)}{\tau}$ (formally): [pole + log] singularities

$$\frac{1}{2\pi\mathrm{i}}\int_{-\mathrm{i}\infty}^{+\mathrm{i}\infty}\frac{\Theta(\tau)}{\tau}\,\mathrm{e}^{x\tau}\,\mathrm{d}\tau = x + \frac{\log\Phi(x)}{2\pi\mathrm{i}} + \sum_{r\neq 0}\frac{(-1)^r}{2\pi\mathrm{i}r}[\Phi(x)]^r\,\mathrm{e}^{2\pi\mathrm{i}rx}$$



$\frac{1}{2\sinh\tau}$ $[V(q)=q^2]$ General 1D $\frac{1}{\tau}\sum_k \mathrm{e}^{-\tau x_k}$ $[V(q)=q^4]$ (V. 1981, 1983)

Poisson relation on nD manifolds (compact, Riemannian)

(Chazarain 1974, Duistermaat–Guillemin 1975)

For Δ the Laplacian operator, $\{x_k\}$ = the spectrum of $\sqrt{-\Delta}$,

$$T(t) \stackrel{\text{def}}{=} \operatorname{Tr} \mathrm{e}^{-\mathrm{i}t\sqrt{-\Delta}} = \sum_k \mathrm{e}^{-\mathrm{i}tx_k} \qquad (t \text{ real})$$

is a distribution singular only at $\pm$(*lengths of* real *periodic geodesics*) (including 0, where the singularity is strongest).

Generalization: for P a positive elliptic ΨDO of order $m > 0$, $\{x_k\}$ = the spectrum of $f(P) = P^{1/m}$ (of order 1),

$$T(t) \stackrel{\text{def}}{=} \operatorname{Tr} \mathrm{e}^{-\mathrm{i}tf(P)} = \sum_k \mathrm{e}^{-\mathrm{i}tx_k} \qquad (t \text{ real})$$

is a distribution singular only at $\pm$(*periods of closed bicharacteristics*).

The singular-part expansions are in principle computable, e.g., using *quantum Birkhoff normal forms* (QBNF).

Selberg trace formula on 2D compact hyperbolic surfaces

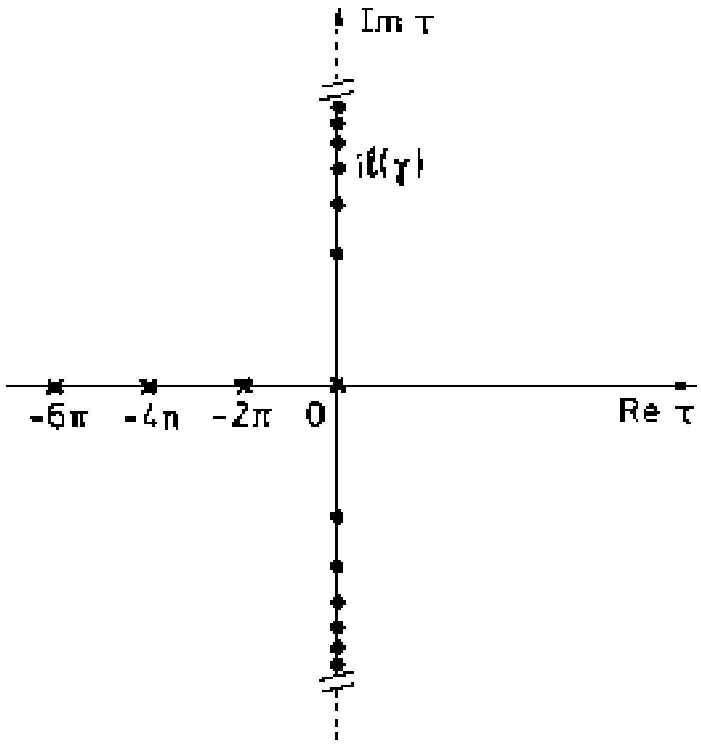
(Cartier–V. 1988)

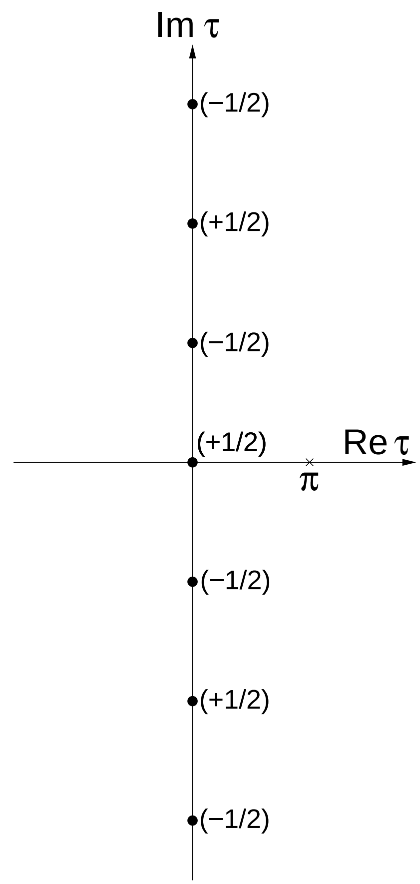
(Assuming constant negative curvature $\equiv -1$) For Δ the Laplacian operator, $\{x_k\}$ = the spectrum of $f(\Delta) \stackrel{\mathrm{def}}{=} \sqrt{-\Delta - 1/4}$,

$$\Theta(\tau) \stackrel{\mathrm{def}}{=} \operatorname{Tr} \mathrm{e}^{-\tau f(\Delta)} = \sum_k \mathrm{e}^{-\tau x_k} \qquad \text{(holomorphic for } \operatorname{Re} \tau > 0)$$

has a *meromorphic continuation for all complex* τ, which is singular only at $\pm$(*lengths of periodic geodesics*), **real and complex**.

No branch cuts: an exceptional feature; the statement follows from a Selberg Trace formula, which is analytically exact (a nongeneric fact, in analogy to the exact Bohr–Sommerfeld quantization for the 1D harmonic oscillator).





$$\Theta(\tau) \stackrel{\text{def}}{=} \mathrm{Tr}\, \mathrm{e}^{-\tau\sqrt{-\Delta-1/4}}$$

2D Hyperbolic Laplacian

$$\sum_k \mathrm{e}^{-\tau(2k+1)} = \frac{1}{2\sinh\tau}$$

1D harmonic oscillator

Also for 2D *quantum billiards*: high orders of Weyl series reflect real/complex periodic orbits (Berry–Howls 1994).

Balian–Bloch representation of quantum mechanics

(1974)

Write Green's function $G_E(q,q';\hbar) \stackrel{\text{def}}{=} \langle q|(\hat{H}_\hbar - E)^{-1}|q'\rangle$ in Fourier representation wr to $x = 1/\hbar$:

$$G_E(q,q';\hbar) = \frac{x^2}{2\pi\mathrm{i}} \int_{-\infty}^{+\infty} \Omega_E(q,q';s)\, \mathrm{e}^{\mathrm{i}xs}\, \mathrm{d}s,$$

then the Schrödinger equation amounts to an *integral equation* for Ω_E,

$$\Omega_E(q,q';s) = \frac{A(q,q')}{s - S_E(q,q')} + \frac{1}{2\pi\mathrm{i}} \int_{-\infty}^{+\infty} \mathrm{d}s' \int \mathrm{d}^n q''\, \frac{\Omega_E(q,q'';s')\, \Delta A(q'',q')}{s - s' - S_E(q'',q')}$$

which locates the s-plane singularities of $\Omega_E(q,q';s)$ at the *actions* $S_E(q,q')$ of **real and complex** *classical trajectories* of energy E from q to q'.

Hence for Im Tr G_E (giving the spectral density), Im Tr $\Omega_E(s)$ is singular at the *actions* $S_{E,\gamma}$ of **real and complex** *classical trajectories* γ of energy E that are *periodic.*

The Gutzwiller trace formula (1971)

It is a *real*-periodic-orbit expansion for the integrated density of states of the operator $\hat{H}$, or "spectral staircase" $\mathcal{N}(E;\hbar) \stackrel{\text{def}}{=} \sum_k \theta(E - E_k(\hbar))$:

$$\mathcal{N}(E;\hbar) \sim \sum_{\{\gamma\}} \Big(\sum_m A_{\gamma,m}(E) \hbar^m \Big) \mathrm{e}^{\mathrm{i} S_{E,\gamma}/\hbar} \qquad (\{\gamma\} = \textit{ real} \text{ periodic orbits}).$$

But: *all* summations diverge, making "$\sim$" is most ill-defined.

Resurgent remedy: cures the pathologies of the formula (formally), and inversely the cured formula suggests a resurgent structure in nD quantum mechanics. Problem: it's still *conjectural* (formal reasonings).

Based on: Balian–Bloch transform of $\mathcal{N}(E;\hbar)$ (i.e., wr to $x = 1/\hbar$),

$$\mathcal{N}(E;\hbar) \equiv \frac{1}{2\pi \mathrm{i}} \int_{-\mathrm{i}\infty}^{+\mathrm{i}\infty} \frac{\Theta_E(\tau)}{\tau} \mathrm{e}^{x\tau} \, \mathrm{d}\tau, \qquad \Theta_E(\tau) \stackrel{\text{def}}{=} \sum_k \mathrm{e}^{-\tau x_k(E)},$$

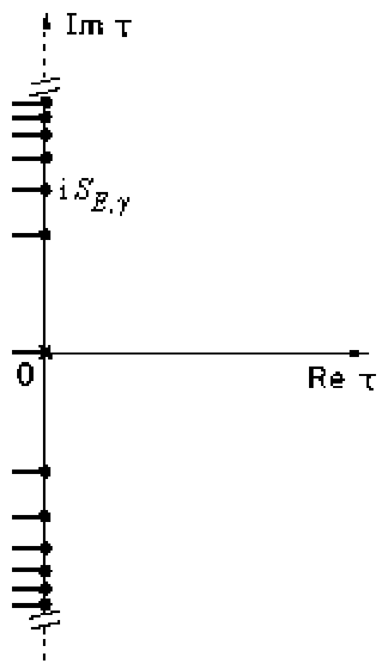
as $\mathcal{N}(E;\hbar) \equiv \sum_k \theta(x - x_k(E))$, $\quad \{x_k(E)\} \stackrel{\text{def}}{=} (1/\hbar)$-spectrum at fixed E,

i.e., a *generalized eigenvalue problem*, not just a function $f(\hat{H})$ as above.

So, $$\frac{1}{2\pi \mathrm{i}} \int_{-\mathrm{i}\infty}^{+\mathrm{i}\infty} \frac{\Theta_E(\tau)}{\tau}\, \mathrm{e}^{x\tau}\, \mathrm{d}\tau \sim \sum_{\{\gamma\}} \Big(\sum_m A_{\gamma,m}(E) \hbar^m \Big)\, \mathrm{e}^{\mathrm{i} S_{E,\gamma}/\hbar}$$

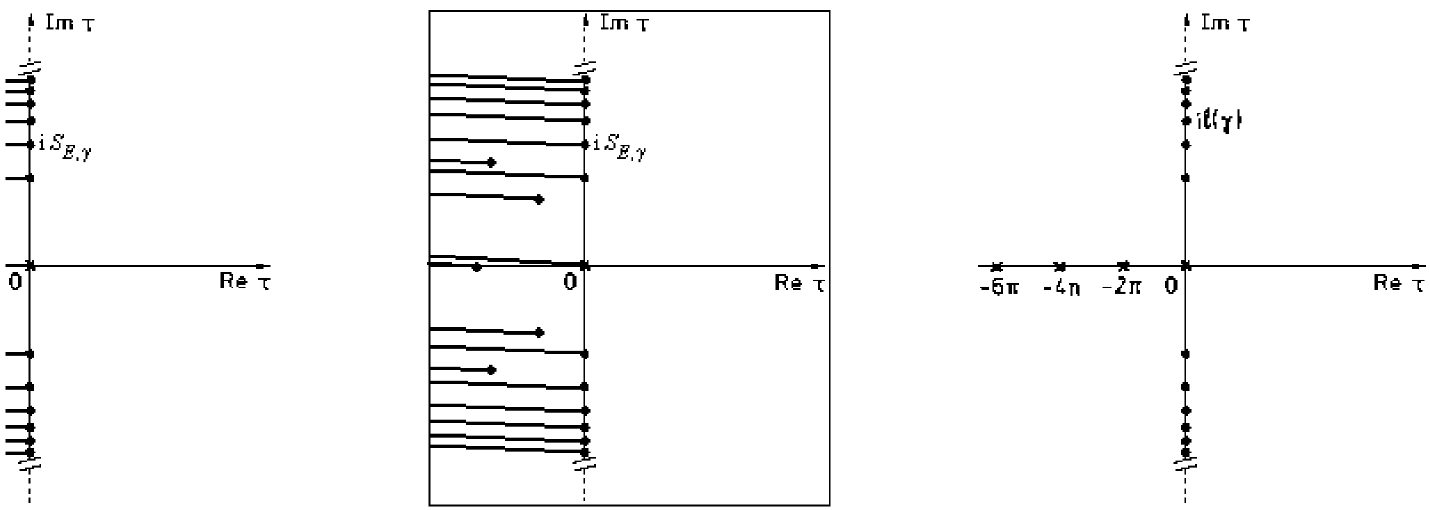
where $\{\gamma\}$ = the *real* classical periodic orbits of energy E; $S_{E,\gamma}$ = their actions (including 0 where the expansion is more singular, $O(\hbar^{-n})$). This

- says: $\Theta_E(\tau) \stackrel{\mathrm{def}}{=} \sum_k \mathrm{e}^{-\tau x_k(E)}$ is singular on $\{\mathrm{Re}\, \tau = 0\}$ at $\{\tau = \mathrm{i} S_{E,\gamma}\}$;
- encodes a *singular decomposition* for $\Theta_E(\tau)$ on that imaginary τ-axis (the expansion coefficients $A_{\gamma,m}(E)$ are in principle reachable).



Conjecture (V. 1986): (if $\{S_{E,\gamma}\}$ is a discrete set) $\Theta_E(\tau) = \sum_k \mathrm{e}^{-\tau x_k(E)}$ continues analytically in τ with singularities at $\{\tau = \mathrm{i}S_{E,\gamma}\}$ where now $\{\gamma\}$ = *real and complex* classical periodic orbits of energy E.

Open questions: prove (conditionally: $V(q)$ complex-analytic, ...?) that $\Theta_E(\tau)$ is a *resurgent function*; find resurgence equations, and a richer resurgence algebra. Expect *genuine branch cuts* in general: the *topologies* of the Riemann surfaces then have to be found (as done in 1D), so the periodic orbits won't just naively *add* as in trace formulae.



Gutzwiller T.F. $\Rightarrow$ More general $\Theta_E(\tau)$ $\Leftarrow$ Hyperbolic Δ (2D)
(*our conjecture*)

Concrete examples of generalized spectra $\{x_k(E)\}$

(scaled-energy spectroscopy, or $(1/\hbar)$-spectroscopy)

1) the H-atom in a uniform B-field reduces to the 3D Hamiltonian $\hat{H}(x,g) = -\hbar^2\Delta - r^{-1} + g^2r^2/8 \equiv x^2\hat{H}(1, x^6g^2)$; hence $\{x_k(E)\} \equiv$ the $g^{-1/3}$-spectrum at fixed $(Eg^{-2/3},\ x)$.

2) in a quantum kicked top, effects of real *and complex* periodic orbits.

FIG. 1. Fourier transformed trace $T_1(\omega; j_0 = 1, M = 100)$ of the Floquet operator of the kicked top for various values of the control parameter k : (a) below $k_c = 12.73$ with a ghost peak at $\omega = 0.51$ and three peaks corresponding to real periodic orbits; (b) slightly above k_c where the highest peak corresponds to an unresolved doublet due to two real periodic orbits; (c) sufficiently far above k_c where the doublet is resolved.

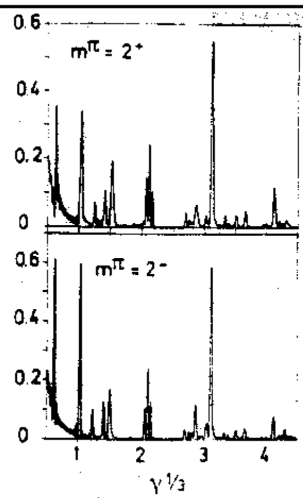
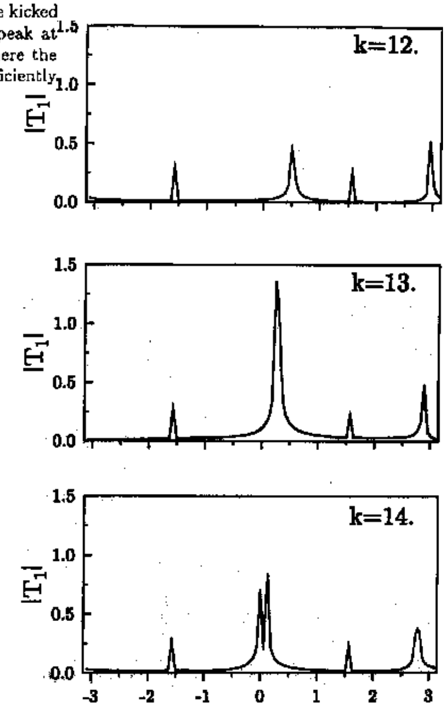


FIG. 1. Squared, normalized Fourier transforms of the quantum spectra in the $m=2$ subspaces for $\epsilon=-0.2$. The lowest 300 levels in each subspace have been included in the transformation.



1) Wintgen 1987 2) Kuś–Haake–Delande 1993

Some references

R. Balian & C. Bloch, Ann. Phys. (NY) **85** (1974) 514–545

M.V. Berry & C.J. Howls, Proc. Roy. Soc. Lond. **A447** (1994) 527–533

P. Cartier & A.V., C. R. Acad. Sci. (Paris) **307**, Série I (1988) 143–148

J. Chazarain, Invent. Math. **24** (1974) 65–82

J.J. Duistermaat & V.W. Guillemin, Invent. Math. **29** (1975) 39–79

J. Écalle, Les Fonctions Résurgentes I, Publ. Math. Univ. Paris-Sud (Orsay) **81-05** (1981)

M.C. Gutzwiller, J. Math. Phys. **12** (1971) 343–358

M. Kuś, F. Haake & D. Delande, Phys. Rev. Lett. **71** (1993) 2167–2170

A.V., C. R. Acad. Sci. (Paris) **293**, Série I (1981) 709–712;
and Ann. Inst. H. Poincaré **A39** (1983) 211–338

A.V., in: Path Integrals from meV to MeV (Proceedings, Bielefeld 1985), eds. M.C. Gutzwiller *et al.*, World Scient., Singapore (1986) 173–195 (§6); and in: YKIS'93 (Proceedings, Kyoto 1993), Prog. Theor. Phys. Suppl. **116** (1994) 17–44 (§3) *(references for this talk)*

A.V., J. Phys. **A32** (1999) 5993–6007 [corrigendum: **A33** (2000) 5783–5784]

D. Wintgen, Phys. Rev. Lett. **58** (1987) 1589–1592