

Periodic orbit quantization

There are several central subfields in the study of quantum chaos:

- Quantum Chaology: quantization of classically chaotic systems in semiclassical regimes, mainly bounded autonomous systems with discrete spectra. The main quest is to find signatures of classical chaos on the quantum level. Lyapunov exponents are not well-defined, one has to look for generalizations.
 - Periodic Orbit Quantization. Can be used to compute quantum energy levels based on only classical input. Alternatively, one can extract classical parameters from a known quantum spectrum. The number of terms increases exponentially in the chaotic regime.
 - Random Matrix Theory
- Semiclassical Quantization (a.k.a. semiquantum chaos): classical subsystems coupled to quantum mechanical ones. This describes exponential sensitivity in the semiquantal regime. For instance, vibrating quantum billiards are a very important and widely applied example. This is a type of “wave chaos”: quantum systems with classical boundaries, where classicality is not an approximation, unlike in Quantum Chaology.
- True Quantum Chaos: fully quantized systems with exponential sensitivity and infinite recurrence. Since there is no natural definition of Lyapunov exponents, the question of the existence of such systems remains open.

Today we will talk about the periodic orbit quantization, pioneered by Gutzwiller around 1990.

Prelude: integrable systems

Write the QM density of states using a regular function Γ in the positive quadrant of the space of quantum numbers:

$$\rho(E) = \sum_{\mathbf{n}} \delta(E - \Gamma(\hbar\mathbf{n})), \quad (1)$$

then use the Poisson summation formula to rewrite this as

$$\rho(E) = \hbar^{-f} \sum_{\mathbf{m}} \int d^f \mathbf{I} \delta(E - \Gamma(\mathbf{I})) e^{2\pi i(\mathbf{m}, \mathbf{I})/\hbar}. \quad (2)$$

The $\mathbf{m} = 0$ term gives the classical density of states. The fluctuation part can be evaluated in the semiclassical limit by the stationary phase method. Stationary phase points are the ones where (\mathbf{m}, \mathbf{I}) is extremized when restricted to the surface $\Gamma(\mathbf{I}) = E$. Using the Lagrange multiplier method, this is equivalent to

$$0 = \mathbf{m} + \lambda \nabla_{\mathbf{I}} H(\mathbf{I}) = \mathbf{m} + \lambda \boldsymbol{\omega}, \quad (3)$$

$$E = H(\mathbf{I}), \quad (4)$$

which implies that all frequencies are integer multiples of $\omega_0 = \lambda^{-1}$, that is, $\omega_j = m_j \omega_0$. Therefore the leading contributions come from the *classical periodic orbits*. If we pick $I_1 = H$, we have

$$\bar{\rho}(E) = \hbar^{-d} \sum_{\mathbf{m} \neq 0} (\hbar \omega_0)^{\frac{d-1}{2}} \frac{\exp(2\pi i(\mathbf{m}, \mathbf{I}_0)/\hbar)}{|\nabla_{\mathbf{I}} H| \sqrt{\det M}} = \sum_{\mathbf{m} \neq 0} A(E, \mathbf{m}) e^{2\pi i(\mathbf{m}, \mathbf{I}_0)/\hbar}, \quad M = \left. \frac{\partial^2 H}{\partial I_j \partial I_k} \right|_{j,k>1}. \quad (5)$$

Assuming a discrete spectrum, we see that this sum gives an infinity iff the components of \mathbf{I}_0 are integer multiples of \hbar – reproducing the Bohr-Sommerfeld quantization condition.

Semiclassical wave function

Recall that the classical probability density on the configuration space evolves according to

$$\rho(q(t), t) d\mathbf{q} = \rho(q', 0) d\mathbf{q}', \quad (6)$$

so

$$\rho(q(t), t) = \left| \det \frac{\partial \mathbf{q}'}{\partial \mathbf{q}} \right| \rho(q', 0). \quad (7)$$

This means that the semiclassical evolution of the wave function needs to be normalized by the square root of this factor:

$$\psi_{sc}(q, t) = \sqrt{\det \frac{\partial \mathbf{q}'}{\partial \mathbf{q}}} e^{iS(q, q', t)/\hbar} \psi(q', 0). \quad (8)$$

This remains true for sufficiently small t , until the Lagrangian submanifold $(q(t), p(t) = \partial_q S(q, t))$ develops folds and the value of the phase S is no longer unique. Then more than one classical trajectory will connect q' and q with different phases S . When there is a fold at q_0 , the Jacobian $\frac{\partial \mathbf{q}'}{\partial \mathbf{q}}$ diverges like $1/\sqrt{q_0 - q(t)}$ along a trajectory approaching q_0 . After the folding the orientation of $d\mathbf{q}'$ has changed, and moreover, S became multivalued, so q can now be the image of multiple points q' .

Since the orientation changes at every fold, the eigenvalues of the Jacobian change sign too. We can keep track by writing the Jacobian as

$$\det \frac{\partial \mathbf{q}'}{\partial \mathbf{q}} \Big|_j = e^{-i\pi m_j(q, q', t)} \left| \frac{\partial \mathbf{q}'}{\partial \mathbf{q}} \right|_j, \quad (9)$$

where m_j counts the number of sign changes of the determinant along the j -th trajectory from q to q' . It is called Maslov index and is a topological invariant in a proper sense. Thus in general the wave function is a sum over possible trajectories from all possible q' to q :

$$\psi_{sc}(q, t) = \int d\mathbf{q}' \sum_j \left| \det \frac{\partial \mathbf{q}'}{\partial \mathbf{q}} \right|_j^{1/2} e^{iS(q, q', t)/\hbar - \frac{i\pi}{2} m_j(q, q', t)} \psi(q'_j, 0). \quad (10)$$

Semiclassical Green's function (Van Vleck)

Recall that the free particle propagator is precisely given by

$$K(q, q', t) = \left(\frac{m}{2\pi i \hbar t} \right)^{d/2} e^{im(q-q')^2/2\hbar t}. \quad (11)$$

However, in general we can only write this for infinitesimal times:

$$K_{sc}(q, q', \delta t) \approx \left(\frac{m}{2\pi i \hbar \delta t} \right)^{d/2} e^{\frac{i}{\hbar} \left(\frac{m(q-q')^2}{2\delta t} - V(q)\delta t \right)}. \quad (12)$$

The prefactor $(m/\delta t)^{d/2}$ can be interpreted as the Jacobian of the transformation from the final position q to the initial momentum p' :

$$\frac{\partial p}{\partial q} = -\frac{\partial^2 S}{\partial q \partial q'} = -\frac{\partial p'}{\partial q} = \frac{m}{\delta t}, \quad S \approx \frac{m(q-q')^2}{2\delta t}, \quad (13)$$

that is,

$$K_{sc}(q, q', \delta t) \approx \left(\frac{1}{2\pi i \hbar} \right)^{d/2} \left(\det \frac{\partial p'}{\partial q} \right)^{1/2} e^{\frac{i}{\hbar} S(q, q', \delta t)}. \quad (14)$$

Now we simply evolve this short time representation according to (10)

$$K_{sc}(q'', q', t' + \delta t) = \sum_j \left| \det \frac{\partial q}{\partial q''} \right|_j^{1/2} e^{\frac{i}{\hbar} S_j(q'', q, t') - \frac{i\pi}{2} m_j(q'', q', t')} K(q, q', t) = \quad (15)$$

Now we use

$$\det \frac{\partial q}{\partial q''} \Big|_t \det \frac{\partial p'}{\partial q} \Big|_{q', \delta t} = \det \frac{\partial p'}{\partial q''} \Big|_{q', t' + \delta t} \quad (16)$$

to rewrite

$$K_{sc}(q, q', t) = \sum_j \left(\frac{1}{2\pi i \hbar} \right)^{d/2} \left| \det \frac{\partial p'}{\partial q} \right|_j^{1/2} e^{\frac{i}{\hbar} S_j(q, q', t) - \frac{i\pi}{2} m_j(q, q', t)}. \quad (17)$$

Note that this propagator is complicated due to the summation over classical trajectories which proliferate at longer times, and it satisfies the group property only approximately, unlike the exact propagator:

$$K_{sc}(q, q', t_1 + t_2) \approx \int dq'' K_{sc}(q, q'', t_2) K_{sc}(q'', q', t_1), \quad (18)$$

and this connection can be made precise by applying the stationary phase method to the integral on the r.h.s.. The stationary phase condition reads

$$\partial_{q''} S(q, q'', t_2) + \partial_{q''} S(q'', q', t_1) = 0, \quad (19)$$

which is equivalent to

$$p''_- = p''_+ \text{ at } t_1, \quad (20)$$

i.e. there is no “break” in the trajectory at q'' . Therefore the semiclassical propagation contains this additional constraint of $p_{out} = p_{in}$.

The propagator can also be derived from the Feynman path integral by yet another stationary phase argument.

The Green function is defined by

$$G(q, q', E) = (i\hbar)^{-1} \int_0^\infty dt e^{iEt/\hbar} K(q, q', t). \quad (21)$$

We evaluate the semiclassical Green function by applying the stationary phase method to (17). Recall that the standard stationary phase approximation for Fresnel integrals reads

$$\int A(\mathbf{x}) e^{is\Phi(\mathbf{x})} d\mathbf{x} \approx \sum_{\mathbf{x}_0} \left(\frac{2\pi i}{s} \right)^{d/2} |\det \Phi''(\mathbf{x}_0)|^{-1/2} A(\mathbf{x}_0) e^{is\Phi(\mathbf{x}_0) - \frac{i\pi}{2} m(\mathbf{x}_0)}, \quad (22)$$

where $m(\mathbf{x}_0)$ counts the number of negative eigenvalues of $\Phi''(\mathbf{x}_0)$.

The stationary points t^* of the integrand in (21) are given by

$$\partial_t S(q, q', t^*) + E = 0, \quad (23)$$

whose solutions are exactly the lengths of the classical trajectories from q' to q at energy E . The second derivative is just $\partial_t^2 S(q, q', t^*) = (\partial E / \partial t)_{q', q}$, so we have for one classical trajectory j

$$G_j(q, q', E) = \frac{1}{i\hbar (2\pi i\hbar)^{\frac{f-1}{2}}} \left| \left(\det \frac{\partial p'}{\partial q} \right)_{t, q'} \left(\det \frac{\partial t}{\partial E} \right)_{q', q} \right|_j^{1/2} e^{\frac{i}{\hbar} S_j - \frac{i\pi}{2} m_j} = \quad (24)$$

$$= \frac{1}{i\hbar (2\pi i\hbar)^{\frac{f-1}{2}}} \left| \left(\det \frac{\partial (p', t)}{\partial (q, E)} \right)_{q'} \right|_j^{1/2} e^{\frac{i}{\hbar} S_j - \frac{i\pi}{2} m_j} \quad (25)$$

where now the index m_j includes also the sign flips of $\partial_t^2 S$. Furthermore, it is convenient to choose the coordinates so that q_{\parallel} is the coordinate along the trajectory, and $q_{\perp i}$ are the perpendicular directions. In this case

$$\det \frac{\partial (p', t)}{\partial (q, E)} = \frac{1}{\dot{q}\dot{q}'} \det D_{\perp}(q, q', E), \quad D_{\perp} = -\frac{\partial^2 S}{\partial q_{\perp} \partial q'_{\perp}}. \quad (26)$$

Putting everything together,

$$G_j(q, q', E) = \frac{1}{i\hbar (2\pi i\hbar)^{\frac{d-1}{2}}} \frac{1}{|\dot{q}\dot{q}'|^{1/2}} |\det D_{\perp}|_j^{1/2} e^{\frac{i}{\hbar} S_j - \frac{i\pi}{2} m_j}, \quad (27)$$

where the topological index now counts the number of changes of sign $\det D_{\perp}$ along the trajectory. Finally, the total Green function is

$$G_{sc}(q, q', E) = G_0 + \sum_j G_j, \quad (28)$$

where G_0 is the contribution of “short” trajectories: the stationary phase method cannot be used at small t^* because the amplitude of K_{sc} diverges:

$$G_0(q, q', E) = \frac{1}{i\hbar} \int_0^\infty dt \left(\frac{m}{2\pi i\hbar t} \right)^{n/2} e^{\frac{i}{\hbar} \left(Et + \frac{(q-q')^2}{2t} - V(q)t \right)}. \quad (29)$$

Instead G_0 can be approximated in terms of the Hankel special functions. This approximation is valid when $S_0(q, q', E) \lesssim \hbar$.

Trace formula (Gutzwiller)

Van Vleck formula is assumed to be valid for chaotic Hamiltonians. The problem is finding the trajectories from q to q' , and this is too difficult. Next we can try to take the trace of G_c . The trace contains contributions from “long” classical trajectories labeled by j , and “zero length” trajectories whose lengths approach zero as $q' \rightarrow q$.

$$\text{tr } G_{sc}(E) = \int d\mathbf{q} G_{sc}(q, q, E) = \text{tr } G_0(E) + \sum_j \int d\mathbf{q} G_j(q, q, E), \quad (30)$$

$$\text{tr } G_j(E) = \frac{1}{i\hbar (2\pi\hbar)^{\frac{d-1}{2}}} \oint_j \frac{dq_{\parallel}}{\dot{q}} \int_j d\mathbf{q}_{\perp} |\det D_{\perp}^j|^{1/2} e^{\frac{i}{\hbar} S_j - \frac{i\pi}{2} m_j}. \quad (31)$$

The stationary phase condition is

$$0 = \partial_q S(q, q, E) = \partial_{q'} S(q', q, E) + \partial_q S(q', q, E) |_{q'=q} = p' - p, \quad (32)$$

i.e. there is destructive interference unless the trajectory is exactly periodic. Therefore the calculation is reduced to summation over all periodic orbits. It is natural to split the integration into a longitudinal part along the trajectory, and the transversal part. The actions and topological indices don't depend on q_{\parallel} , so the longitudinal integration is very straightforward.

The density varies smoothly, so we can approximate it by its value at the (stationary) classical trajectory, $q_{\perp} = 0$. Note that $m_j(q_{\parallel}, q_{\perp}, E) = m_j(E)$ since it doesn't depend on q_{\parallel} and is topologically invariant, i.e. locally constant in q_{\perp} .

The transversal stationary phase integral is evaluated

$$\text{tr } G_j(E) = \frac{1}{i\hbar} \oint \frac{dq_{\parallel}}{\dot{q}} \sqrt{\left| \frac{\det D_{\perp j}(q_{\parallel}, 0, E)}{\det D'_{\perp j}(q_{\parallel}, 0, E)} \right|} e^{\frac{i}{\hbar} S_j - \frac{i\pi}{2} m_j}, \quad (33)$$

where we introduced

$$\det D_{\perp} = \left\| \frac{\partial p'_{\perp}}{\partial q_{\perp}} \right\| = \left\| \frac{\partial (q'_{\perp}, p'_{\perp})}{\partial (q_{\perp}, q'_{\perp})} \right\| \quad (34)$$

$$\det D'_{\perp} = \left\| \frac{\partial (p_{\perp} - p'_{\perp}, q_{\perp} - q'_{\perp})}{\partial (q_{\perp}, q'_{\perp})} \right\|, \quad (35)$$

$$\frac{\det D'_{\perp}}{\det D_{\perp}} = \left\| \frac{\partial (p_{\perp} - p'_{\perp}, q_{\perp} - q'_{\perp})}{\partial (q'_{\perp}, p'_{\perp})} \right\| = \left\| \frac{\partial (x_{\perp} - x'_{\perp})}{\partial x'_{\perp}} \right\| = \det(M - I), \quad (36)$$

where M is the monodromy matrix for a transversal section to the orbit of the constant energy shell. This ratio of determinants enforces the periodic boundary conditions (“stability factor”).

Then we have

$$\text{tr } G_j(E) = \frac{1}{i\hbar} \sum_{j,r} \frac{1}{\sqrt{|\det(1 - M_j)|}} e^{r(\frac{i}{\hbar} S_j - \frac{i\pi}{2} m_j)} \oint \frac{dq_{\parallel}}{\dot{q}_{\parallel}}. \quad (37)$$

This takes a long time to explain using only quantum mechanics, but the spatial integral includes only one traversal of every trajectory. Thus for a *primitive* cycle p ,

$$\int_0^{L_p} \frac{dq_{\parallel}}{\dot{q}_{\parallel}} = \int_0^{T_p} dt = T_p. \quad (38)$$

The monodromy matrix of a repeated cycle is simply the r th power of the primitive matrix M_p . We arrived at the Gutzwiller trace formula

$$\boxed{\text{tr } G_{sc}(E) = \text{tr } G_0(E) + \frac{1}{i\hbar} \sum_p T_p \sum_{r=1}^{\infty} \frac{1}{\sqrt{|\det(1 - M_p^r)|}} e^{r\left(\frac{i}{\hbar} S_p - \frac{i\pi}{2} m_p\right)},} \quad (39)$$

where the first summation is over all *classical primitive periodic orbits*.

The topological Maslov index m_p counts the number of changes of sign of the matrix of second derivatives along the prime periodic orbit p . For instance, the index of a closed $2n$ -dimensional curve is the number of times the partial derivatives $\partial p_i / \partial q_i$ for each conjugate pair change their signs as one traverses the curve (no sum on i).

Note 1. Since we assumed that periodic orbits are isolated and don't form continuous families (as in integrable systems or KAM tori with mixed phase space), these formulas so far are only valid for hyperbolic and elliptic orbits.

Note 2. For deterministic flows and number theory, spectral determinants and zeta functions become exact.

Average density of states

Since the trace of G is the Cauchy transform of the density of states, we can invert this to find the density from the trace:

$$\frac{i}{2\pi} \lim_{\epsilon \rightarrow 0} \int d\mathbf{q} (G(\mathbf{q}, \mathbf{q}, E + i\epsilon) - G(\mathbf{q}, \mathbf{q}, E - i\epsilon)) = \rho(E) = \sum_j \delta(E - E_j). \quad (40)$$

The real part of $\text{tr } G_0$ is infinite, but the imaginary part is not and it encodes the density of states:

$$\rho_0(E) = -\frac{1}{\pi} \int d\mathbf{q} \text{Im } G_0(\mathbf{q}, \mathbf{q}, E). \quad (41)$$

One can give an interpretation of this as the number of quantum states accommodated up to energy E , provided that the volume of one quantum cell is h^n :

$$\rho_0(E) = \frac{d}{dE} N(E) = \frac{V_n}{(2\pi\hbar)^n} \int d\mathbf{p} \delta\left[E - \frac{p^2}{2m}\right] = \left(\frac{2m}{\hbar^2}\right)^{n/2} \frac{V_n \Omega_n}{2(2\pi)^n} E^{(d-2)/2}, \quad (42)$$

which is Weyl's law.

From the Gutzwiller formula, the fluctuating part of the density is

$$\boxed{\rho_{fl}(E) \sim \frac{1}{\pi\hbar} \sum_p T_p \sum_{r=1}^{\infty} \frac{\cos\left(r\frac{S_p(E)}{\hbar} - rm_p\frac{\pi}{2}\right)}{\sqrt{|\det(1 - M_p^r)|}},} \quad (43)$$

$$N_{fl}(E) \sim \frac{1}{\pi} \sum_{p,r} \frac{\sin\left(r\frac{S_p(E)}{\hbar} - rm_p\frac{\pi}{2}\right)}{r\sqrt{|\det(1 - M_p^r)|}}, \quad (44)$$

The Green function itself can be regularized by subtracting off the singular term in the short-distance asymptotics. Then we can define the regularized spectral determinant as

$$\det(H - E) = \exp\left(-\int^E dE' \operatorname{tr} G_{reg}(E')\right). \quad (45)$$

This gives the semiclassical zeta function

$$\det(H - E)_{sc} = e^{i\pi N_{sc}(E)} \exp\left(-\sum_p \sum_{r=1}^{\infty} \frac{1}{r} \frac{e^{ir\left(\frac{S_p}{\hbar} - m_p \frac{\pi}{2}\right)}}{|\det(1 - M_p^r)|^{1/2}}\right). \quad (46)$$

This can be evaluated by means of cycle expansions.

One-/two-dimensional systems

There is no monodromy matrix in the 1D case, so

$$\rho(E) = \frac{T_p}{2\pi\hbar} + \sum_r \frac{T_p(E)}{\pi\hbar} \cos\left(r \frac{S_p(E)}{\hbar} - rm_p \frac{\pi}{2}\right) = \frac{T_p(E)}{2\pi\hbar} \sum_n \delta\left(\frac{S_p(E)}{2\pi\hbar} - m_p(E)/4 - n\right), \quad (47)$$

which recovers the Bohr-Sommerfeld quantization condition. We also have that

$$N_{sc}(E_n + \epsilon) = n - \frac{1}{2} = \frac{S_p}{2\pi\hbar} - \frac{m_p}{4} - \frac{1}{2}, \quad (48)$$

so the spectral determinant is

$$\det(H - E)_{sc} = \exp\left(-\frac{i}{2\hbar} S_p + \frac{i\pi}{2} m_p\right) \exp\left(-\sum_r \frac{1}{r} e^{\frac{i}{\hbar} r S_p - \frac{i\pi}{2} r m_p}\right) = 2 \sin\left(\frac{S_p(E)}{\hbar} - \frac{m_p(E)}{4}\right), \quad (49)$$

whose zeros are the Bohr-Sommerfeld energies.

In 2D, M has two eigenvalues Λ and Λ^{-1} . We distinguish three important cases:

- elliptic case: $\Lambda = e^{i\chi}$, $\chi \in \mathbb{R}$,
- hyperbolic case: $\Lambda = e^\chi$, $\chi > 0$,
- inverse-hyperbolic case: $\Lambda = -e^\chi$, $\chi > 0$.

Then

$$|\det(I - M_p^r)|^{1/2} = |\Lambda_p^r|^{1/2} (1 - \Lambda_p^{-r}) = \begin{cases} 2 \left|\sin \frac{r\chi}{2}\right|, \\ 2 \sinh \frac{r\chi}{2}, \\ 2 \cosh \frac{r\chi}{2}, \end{cases} \quad (50)$$

$$|\det(I - M_p^r)|^{-1/2} = \sum_{k=0}^{\infty} |\Lambda_p|^{-r/2} \Lambda_p^{-kr}, \quad (51)$$

therefore the sum over r inside the exponential can be recognized as a logarithm, and we have simply

$$\det(H - E)_{sc} = e^{i\pi N_{sc}(E)} \prod_p \prod_{k=0}^{\infty} \left(1 - \frac{e^{\frac{i}{\hbar} S_p - \frac{i\pi}{2} m_p}}{|\Lambda_p|^{1/2} \Lambda_p^k}\right). \quad (52)$$

Long orbits approximation

Note that in the purely hyperbolic case M has eigenvalues of the form $e^{\lambda p}$. These exponents are the appropriate generalizations of the Lyapunov exponents to quantum systems. The determinant can be approximated for long orbits in terms of the instability exponent λ_p and the (large) period $T_p = \partial_E S_p$:

$$\det(M_p^r - I) \approx e^{r\lambda_p T_p}, \quad (53)$$

so the trace formula takes the form

$$N_{fl}(E) \sim \frac{1}{\pi} \sum_{p,r} \frac{e^{-\frac{1}{2}r\lambda_p T_p}}{r} \sin\left(rS_p(E) - \frac{rm_p\pi}{2}\right). \quad (54)$$

This is exactly the limit that brings together the universal conclusions exhibited by the Random Matrix Theory approach and individual asymptotics provided by Gutzwiller's formula. Indeed, long orbits determine the short distance structure of the eigenvalues (high frequency terms in the series), which is where RMT works well. The deviations from RMT behavior caused by short periodic orbits are a numerical fact.

Convergence problems

The number of closed orbits proliferates exponentially with the length:

$$|\{l(p) < x\}| \sim \frac{e^{hx}}{x}, \quad x \rightarrow \infty, \quad (55)$$

where h is the topological entropy. The decay of the terms in the sum is not enough to compensate for this growth, even in the hyperbolic case. However, techniques have been developed that allow useful applications of Gutzwiller's formula.

If we consider E with an imaginary part of at least h , the sum will become convergent. This is called the *entropy barrier*. This means that by analytic continuation we should be able to extend it to larger domains. One way to rearrange the sum is by using the zeta function.

One method (due to Cvitanovich) uses the fact that contributions from orbits and pseudo-orbits of the same lengths tend to cancel. Rearranging the sum by lengths would therefore make it rapidly converging. The method is based on the principle that long orbits can be decomposed into small fundamental cycles. This technique is applicable only if there is a symbolic dynamics, i.e. every orbit can be labelled by a symbolic sequence and for every symbolic sequence there is an orbit. Non-Euclidean billiards on spaces of constant negative curvature are perfect examples. This method gives surprisingly good values of the energy levels, for instance, in the anisotropic Kepler problem.

Note 3. For instance, the collinear three-body problem ($l = l_1 = l_2 = 0$ states of the Helium atom) is generically chaotic and turns out to have a simple symbolic dynamics, so the trace formula was successfully applied to compute an important part of the spectrum with reasonable accuracy. Unlike a direct numerical calculation, this method gives more insight into the structure of the spectrum.

Selberg trace formula

We will now consider geodesic motion on manifolds of constant negative curvature. It is known that the geodesic flow in this case is ergodic. Similarly to how the approximation to the heat kernel becomes exact in the Euclidean case, Gutzwiller's formula will become exact here. The resulting formula is the Selberg trace formula.

We will discuss one of the simplest special cases of the formula. Let $\Gamma \backslash \mathbb{H}$ be a hyperbolic surface, where Γ is a subgroup of the isometry group of the Poincaré metric $dV = dx dy / y^2$, $\mathrm{PSL}_2(\mathbb{R})$. For the Laplace-Beltrami operator $\Delta = y^2 \Delta_{flat}$, we consider the boundary value problem

$$(\Delta + \lambda_n) u_n(z) = 0, \quad z \in \mathbb{H}, \quad (56)$$

$$u_n(gz) = u_n(z) \quad g \in \Gamma. \quad (57)$$

In other words, we are finding the spectrum of the Laplace-Beltrami operator on the fundamental domain \mathcal{D} with natural "periodic" boundary conditions. To state the trace formula, we need an arbitrary analytic function h on $|\mathrm{Im} z| < \frac{1}{2} + \delta$ which is even, bounded and decreasing as $h(z) = O(z^{-2-\delta})$, $z \rightarrow \infty$.

Theorem. *Setting $\lambda_k = s_k(1 - s_k)$, $s_k = \frac{1}{2} + ir_k$, then*

$$\sum_{k=0}^{\infty} h(r_k) = \frac{\mathrm{Vol}(\mathcal{D})}{2\pi} \int_{\mathbb{R}} x h(x) \tanh(\pi x) dx + \sum_{p \in \mathcal{P}, m \geq 1} \frac{l(p)}{2 \sinh\left(\frac{ml(p)}{2}\right)} \hat{h}(ml(p)), \quad (58)$$

where $\hat{h}(k) = \frac{1}{2\pi} \int e^{-ixk} h(x) dx$, \mathcal{P} is the set of all primitive periodic orbits and l is the geodesic length functional.

Proof.

$$\rho(\lambda) = -\frac{1}{\pi} \int_{\mathcal{D}} \mathrm{Im} G(z, z, \lambda) dV(z), \quad (59)$$

$$G(z, z', \lambda) = \sum_{g \in \Gamma} G_{\mathbb{H}}(gz, z', \lambda). \quad (60)$$

The geodesic distance is well-known, so we have an explicit formula for $G_{\mathbb{H}}$:

$$\rho(\lambda) = \frac{1}{2^{3/2} \pi^2} \sum_{g \in \Gamma} \int_{\mathcal{D}} dV(z) \int_{l(z, gz)}^{+\infty} \frac{\sin(rx)}{\sqrt{\cosh x - \cosh l(z, gz)}} dx, \quad (61)$$

where $\lambda = \frac{1}{4} + r^2$. The mean density corresponds to $g = \mathrm{id}$, giving

$$\rho_0(\lambda) = \frac{\mathrm{Vol}(\mathcal{D})}{4\pi} \tanh(\pi r). \quad (62)$$

A group element is called *primitive* if it cannot be expressed in terms of powers of other group elements. Thus there is a correspondence between such elements and periodic orbits. However, multiple primitive elements correspond to each orbit, because the choice of the starting point is irrelevant. *Conjugacy classes* of primitive elements, on the other hand, correspond to periodic

orbits in a one-to-one manner. Moreover, every conjugacy class of Γ contains a simple power of a primitive element p^m , corresponding to a periodic orbit repeated m times.

The sum over g can now be rewritten as a sum over all conjugacy classes $[g]$:

$$\rho(\lambda) = \rho_0(\lambda) + \sum_{[g]} \rho_{[g]}(\lambda) = \rho_0(\lambda) + \sum_{[p]} \sum_{m \geq 1} \rho_{[p^m]}(\lambda), \quad (63)$$

$$\rho_{[g]}(\lambda) = \frac{1}{2^{3/2} \pi^2} \int_{\text{FD}([g])} dV(z) \int_{l(z, gz)}^{+\infty} \frac{\sin(rx)}{\sqrt{\cosh x - \cosh l(z, gz)}} dx, \quad (64)$$

where $\text{FD}([g])$ is the fundamental domain of the centralizer S_g of $g \in [g]$. S_g is generated by an element g_0 , $S_g = \{g_0^m\}_{m \in \mathbb{Z}}$. The summation over all conjugacy classes is therefore equivalent to a summation over all powers of the primitive elements g_0^m . Then a tedious calculation gives

$$\rho_{[p^m]}(\lambda) = \frac{l(p)}{4\pi \sinh\left(\frac{ml(p)}{2}\right)} \cos(ml(p)), \quad (65)$$

where $l(p)$ is defined by $2 \cosh l(p) = \text{tr } p$ (and we have the identity $2 \cosh ml(p) = \text{tr } p^m$).

An independent calculation shows that $l(p^m)$ is also the distance between z and $p^m z$. Hence they are the lengths of the unique (up to conjugation) periodic orbits associated to p^m . The proof can be made rigorous by integrating $\rho(\lambda)$ against a test function h . \square

Treating the formula in a distributional sense, we get the ‘‘physical’’ version of the formula

$$\rho(r) = \sum_k \delta(r - r_k) = \frac{\text{Vol}(\mathcal{D})}{2\pi} r \tanh \pi r + \frac{1}{2\pi} \sum_{[p], m} \frac{l(p)}{\sinh \frac{ml(p)}{2}} \cos ml(p) r. \quad (66)$$

We see that quantum geodesic motion on $\Gamma \backslash \mathbb{H}$ possesses a trace formula closely related to the Gutzwiller formula. In fact, it is a special case of the Gutzwiller formula that turns out to be exact.

Weil formula for the Riemann zeta

There is an identity by Weil that holds for the same class of test functions h as the Selberg formula:

$$\sum_n h(\gamma_n) - 2h\left(\frac{i}{2}\right) = \frac{1}{2\pi} \int_{\mathbb{R}} h(x) \left(\frac{\Gamma'(x)}{\Gamma(x)} \left(\frac{1}{4} + \frac{i}{2}x \right) - \ln \pi \right) dx - 2 \sum_{p \in \mathcal{P}, m \geq 0} \frac{\ln p}{p^{m/2}} \hat{h}(m \ln p), \quad (67)$$

where \mathcal{P} is the set of prime numbers and $\frac{1}{2} + i\gamma_n$ are the non-trivial zeros of ζ (not assuming the Riemann hypothesis).

We see a strong similarity between (58) and (67), where prime numbers correspond to primitive orbits of lengths $\ln p$. As a consequence of the Selberg trace formula, the number of primitive orbits of length less than x is

$$|\{l(p) < x\}| \sim \frac{e^x}{x}, \quad x \rightarrow \infty, \quad (68)$$

which is also analogous to the prime number theorem

$$|\{\ln p < x\}| \sim \frac{e^x}{x}, \quad x \rightarrow \infty. \quad (69)$$

Assuming the Euler product formula for $\zeta(z)$ in $z \in (\frac{1}{2}, 1)$ (its validity is related to the Riemann hypothesis), we can formally write for the counting function of the zeros of ζ

$$\langle N^\zeta(t) \rangle = \frac{t}{2\pi} \ln \frac{t}{2\pi e} + \frac{7}{8} + O(t^{-1}), \quad (70)$$

$$N_{fl}^\zeta(t) = \frac{1}{\pi} \arg \zeta \left(\frac{1}{2} + it \right) = \frac{1}{\pi} \operatorname{Im} \ln \zeta \left(\frac{1}{2} + it \right) = -\frac{1}{\pi} \sum_{p,r} \frac{e^{-\frac{1}{2}r \ln p}}{r} \sin(tr \ln p). \quad (71)$$

A comparison of this with (54) gives a formal definition of stability for the zeta zeros:

Eigenvalues	energy levels	zeta zeros	
asymptotics	$\hbar \rightarrow 0$	$t \rightarrow \infty$	
actions	$\frac{rS_p}{\hbar}$	$rt \ln p$	(72)
periods	rT_p	$r \ln p$	
stabilities	λ_p	1	

Finding a quantum system with these parameters would be a huge step forward for number theory and physics alike.

Semiclassical sum rule (Hannay and Ozorio de Almeida)

Using Gutzwiller's formula, we compute the spectral autocorrelation function. Note that it cannot be computed via the diagonal approximation for non-integrable systems. Let us normalize the mean level spacing to one, so that the autocorrelation is

$$C(E) = \left\langle \left(\rho \left(\bar{E} + \frac{1}{2}E \right) - 1 \right) \left(\rho \left(\bar{E} - \frac{1}{2}E \right) - 1 \right) \right\rangle. \quad (73)$$

Brackets denote an average over $\bar{E} \in \Delta \bar{E}$. From the trace formula,

$$C(E) = \sum_{n,m} A_n A_m^* \left\langle \exp \left\{ \frac{i}{\hbar} \left(S_n \left(\bar{E} + \frac{E}{2} \right) - S_m \left(\bar{E} - \frac{E}{2} \right) \right) \right\} \right\rangle. \quad (74)$$

Expanding the action to linear term in energy $S_n \left(\bar{E} \pm \frac{E}{2} \right) = S_n \left(\bar{E} \right) \pm \frac{E}{2} T_n$, we obtain

$$C(E) = \sum_{n,m} A_n A_m^* \left\langle \exp \left\{ \frac{i}{\hbar} \left(S_n - S_m + \frac{T_n + T_m}{2} E \right) \right\} \right\rangle. \quad (75)$$

The spectral formfactor $K(t)$, defined as the Fourier transform of E , is usually expressed in terms of the Heisenberg time $T_H = 2\pi\hbar$:

$$K(\tau T_H) = \sum_{n,m} A_n A_m^* \left\langle \exp \left\{ \frac{i}{\hbar} (S_n - S_m) \right\} \right\rangle \delta \left(\tau - \frac{\tau_n + \tau_m}{2} \right), \quad (76)$$

where $\tau_n = T_n/T_H$.

For integrable systems, we can drop the non-diagonal terms by arguing that due to the averaging over an energy window all nondiagonal terms will vanish. However, this argument cannot be generalized to non-integrable systems because of the exponential proliferation of periodic orbits with length.

Still let us take only the diagonal terms. In systems with time-reversal symmetry, every orbit occurs twice with conjugate stability factors. Otherwise, they occur only once. Thus the diagonal part is

$$K_D(\tau T_H) = g \sum_n |A_n|^2 \delta(\tau - \tau_n), \quad g = 1, 2. \quad (77)$$

For short orbits this gives the length spectrum of periodic orbits. We are instead interested in long orbits, when the separate terms in this sum become indistinguishable.

This has a neat interpretation. Consider the classical probability of return on a periodic orbit n of energy E to the starting position at time t : it can be shown to equal

$$P_n(E, t) = \frac{T_p}{\det(M_n - I)} \delta(t - T_n), \quad (78)$$

where T_p is the period of the corresponding primitive orbit (this is a probability distribution over t and n). Then we find

$$\sum_n |A_n|^2 \delta(\tau - \tau_n) = \frac{1}{2\pi\hbar} \sum_n T_p P_n(E, t) \approx \frac{1}{2\pi\hbar} \sum_n T_n P_n(E, t) = \frac{t}{2\pi\hbar} \sum P_n = \tau P(E, t). \quad (79)$$

The error produced by replacing T_p with T_n is only algebraically large, whereas the number of orbits grows exponentially with length. $P(E, t)$ is the total return probability on the energy shell,

$$P(E, t) = \int dpdq \delta(H - E) \delta(\mathbf{q} - \mathbf{q}(t)). \quad (80)$$

We conclude that in chaotic systems the phase space distribution of the very long orbits is uniform on the energy surface – *principle of uniformity*. This allows us to approximate the delta function by its average, i.e. the reciprocal of the area of the energy surface, giving

$$P(E, t) \approx \frac{1}{\Omega_E} \int dpdq \delta(H - E) = 1. \quad (81)$$

Collecting the results,

$$\boxed{\sum_n |A_n|^2 \delta(\tau - \tau_n) = \tau.} \quad (82)$$

This is the sum rule of *Hannay and Ozorio de Almeida*. Since the spectral form factor cannot increase unboundedly, this shows that the diagonal part cannot describe K for chaotic systems besides small τ . For integrable systems, the diagonal approximation can be related to eigenvalue statistics Random Matrix Ensembles.

Another argument can provide the short-distance structure (Michael Berry):

$$K(\tau T_H) \rightarrow 1, \quad \tau \rightarrow \infty. \quad (83)$$

From these two regimes, Sir Berry computed the spectral rigidity:

$$\Delta_3(L) = \frac{1}{2\pi^2} \int_0^\infty \frac{d\tau}{\tau^2} K(\tau T_H) G(\pi L \tau) \approx \frac{g}{2\pi^2} \ln L + \text{const}, \quad (84)$$

$$G(x) = 1 - f^2(x) - 3(f'(x))^2, \quad f(x) = \frac{\sin x}{x}. \quad (85)$$

This matches precisely the spectral rigidity for the GOE ($g = 2$) and GUE ($g = 1$). In fact, even the constant term matches for the GUE. This proved the link between RMT and periodic orbit theory on the level of two-point correlation function. The two main ingredients are the *principle of uniformity*, giving the short time K , and an *analytic bootstrap* giving the asymptotic behavior of K .

References

- [1] Stöckmann, Quantum chaos: an introduction
- [2] Bourgade, Keating, “Quantum chaos, random matrix theory, and the Riemann ζ -function”
<http://www.bourbaphy.fr/keating.pdf>
- [3] Cvitanović, Artuso et.al., Chaos classical and quantum <http://chaosbook.org>
- [4] Keating, Lerner, “PERIODIC ORBITS, SPECTRAL STATISTICS, AND THE RIEMANN ZEROS”