Abstract

Reader will be guided through basic steps toward the important result of the semiclassical theory, Gutzwiller trace formula. All results will be developed entirely in the context of 2D chaotic billiards, but ideas could be understood as general. Main motivation is to show, how semiclassical part of the energy spectrum is treated within semiclassical approximations.
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1 Introduction

In quantum mechanics we are always facing the problem of obtaining the spectrum of quantum-mechanical observables (operators), the most important of which is the spectrum of the Hamiltonian. Except the trivial school examples, almost all quantum systems lack the existence of explicit formulas which would reproduce the series of eigenvalues. Therefore numerical computation is indispensable. But numerical work is always limited with computational time. Since energy spectrum is infinite, there is no theoretical possibility to compute it as whole. But on the other hand this would be of no practical use. We are always focused in the special part of the spectrum, say a few lowest eigenvalues. The lower part of the spectrum was of main importance since the beginning of the quantum mechanics. These is understandable if we are to explain the world in its stable form. Eventually the new area of physics arises which has its origins in the classical mechanics, the theory of chaos. Chaos has a clear definition in the context of classical mechanics. Its emergence is due to nonlinearity of dynamical equations leading to hyper-sensitivity to perturbations. But definition through nonlinearity is inconsistent with quantum mechanics which is linear by construction. There are a lot of conjectures that classically chaotic systems are distinguishable also on the quantum level. Believing so, we have to find the signatures of chaos in quantum mechanics. Here is where all our purposes enter. Many important conjectures are related to statistical properties of the energy spectrum. But for honest statistic we must deal with large number of eigenvalues. Obtaining a sufficiently large sample proves to be a great computational challenge. And suddenly here comes the Gutzwiller trace formula as a big relief. I have chosen the simple 2D chaotic billiard system as a generic representative of the wider class of chaotic systems, to perform the derivation of this important formula.

2 Density of states

So, the key quantity of interest is the density of states $d(E)$, defined so that

$$\int_{E_a}^{E_b} d(E) dE$$

is the number of states with energy levels between $E_a$ and $E_b$. Thus,

$$d(E) = \sum_i \delta(E - E_i).$$

(1)
In practice it is hard to resolve the discrete structure of the spectrum when working in the semiclassical regime. Therefore it is reasonable to suppress spectrum into its smoothed representation. We have smoothed density of states defined as

\[ \bar{d}(E) = \frac{1}{2\Delta} \int_{E-\Delta}^{E+\Delta} d(E) dE \]  

(2)

And the corresponding smoothed cumulative density

\[ \bar{N}(E) = \int_{-\infty}^{E} \bar{d}(E) dE \]  

(3)

The smoothing scale \( \Delta \) will be taken to be much less than any typical energy of the classical system but much larger than \( \hbar/T_{\text{min}} \), where \( T_{\text{min}} \) is the shortest characteristic time for orbits of the classical problem.

### 2.1 Weyl formula

The volume of classical phase space corresponding to system energies less than or equal to some value \( E \) is

\[ V(E) = \int U(E - H(p, q)) d^Dq d^Dp. \]

where \( U(x) \) is the Heaviside unit step function. We assume that the average phase space volume occupied by a state is \( (2\pi\hbar)^D \). Thus the smoothed number of states with energy less than \( E \) is

\[ \bar{N}(E) = \frac{V(E)}{(2\pi\hbar)^D} \]

and since the smoothed density of states is \( \bar{d}(E) = d\bar{N}(E)/dE \), we have

\[ \bar{d}(E) = \frac{1}{(2\pi\hbar)^D} \int \delta(E - H(p, q)) d^Dq d^Dp. \]  

(4)

This result is also known as Weyl formula. For our case of two-dimensional billiard Hamiltonian, \( H = p^2/2m \) we obtain

\[ \bar{d}(E) = \frac{mA}{2\pi\hbar^2} \]  

(5)

where \( A \) is the area of the billiard. We note that the spacing between two adjacent states in the semiclassical regime is of order \( 1/\hbar^2 \) for the case of 2D billiards, so the restriction ensures that in the semiclassical regime there are many states in our smoothing interval \( \Delta \). If we were to examine the density of states on the finer scale, then the resulting smoothed density of states would fluctuate around \( \bar{d}(E) \). Now we focus just in that direction.
3 Derivation of trace formula

An important and fundamental connection between the classical mechanics of a system and its semiclassical quantum wave properties is provided by trace formula originally derived by Gutzwiller (1967, 1969, 1980) and by Balian and Bloch (1970, 1971, 1972).

3.1 The meaning of trace

We consider the Green function for the quantum wave equation corresponding to a classical Hamiltonian $H(p, q)$,

$$H(-i\hbar \nabla, q)G(q, q'; E) - EG(q, q'; E) = -\delta(q - q')$$  \hspace{1cm} (6)

If we express Green function in terms of the complete orthonormal basis $\phi_j$ we get

$$G(q, q'; E) = \sum_j \phi_j^*(q')\phi_j(q) \frac{1}{E - E_j}$$  \hspace{1cm} (7)

The above is singular as $E$ passes through $E_j$ for each $j$. To define this singularity we make use of causality. This leads to replacing $E$ by $E + i\epsilon$, where $\epsilon$ goes to zero through positive values. That is,

$$\lim_{\epsilon \to 0^+} \frac{1}{E - E_j} = P\left(\frac{1}{E - E_j}\right) - i\pi \delta(E - E_j)$$

Here $P(1/x)$ signifies that, when the function $1/x$ is integrated with respect to $x$, the integral is to be taken as the principal part integral at the singularity $x = 0$. Term $-i\pi \delta(E - E_j)$ results from integration around the infinitesimal semicircle skirting the pole. Relation is easy to understand if you remind the Cauchy integral theorem. Note that minus sign arise because of the integration in the opposite sense. We get additional $-i\pi$ term when taking the closed path integral over the infinite semicircle in the lower half of the complex plane. Now taking just imaginary part of the Green function yields

$$\text{Im} G(q, q'; E) = -\pi \sum_j \phi_j^*(q')\phi_j(q) \delta(E - E_j),$$

which upon setting $q = q'$ and integrating results in

$$\text{Im} \int G(q, q'; E)d^2q = -\pi \sum_j \delta(E - E_j).$$
This integral is formally called the trace of the Green function, Trace \((G)\). If we remember the definition for the density of states \((1)\), we can immediately write \(d(E) = -\frac{1}{\pi} \text{Im}[\text{Trace } (G)]\) \((8)\).

Hence we obtain the exact formula for the density of states in terms of the trace of the Green function.

### 3.2 Semiclassical Green function

For case of infinite 2D domain the solution for the Green function is known exactly:

\[
G_0(q, q'; E) = -\frac{i}{4} \frac{2m}{\hbar^2} H_0^{(1)}(k|q - q'|) \tag{9}
\]

where \(H_0^{(1)}\) is the zero order Hankel function of the first kind. To interpret the result for \(G_0\) we do the large argument approximation of \(H_0^{(1)}\):

\[
H_0^{(1)}(k|q - q'|) \sim \left(\frac{2}{\pi}\right)^{1/2} \exp \left(-\frac{i\pi}{4}\right) \frac{\exp [ik|q - q'|]}{\sqrt{k|q - q'|}} \tag{10}
\]

That is, \(G_0\) is an outward propagating cylindrical wave originating from the point \(q = q'\). Since bounded domains are of interest, namely 2D billiards, we have to include indirect trajectories due to bouncing from the walls, which contribute to the exact Green function. Let us separate our billiard on two regions; first we choose the disc in \(q\)-space about the point \(q = q'\) so that the radius of the disc \(R\) satisfies \(kR \gg 1\) and the remaining region is the exterior of the disc. Since \(k|q - q'| \gg 1\) on the boundary of the disc, waves leaving the disc may be thought of as local plane waves (the wavelength is much shorter than the radius of curvature of the wavefronts). Thus, the geometrical optics ray approximation is applicable for \(q\) outside the disc. So for points outside the disc, the Green function \(G\) consists of geometrical optics contribution from each of the ray paths connecting \(q\) to \(q'\),

\[
G(q, q'; E) \simeq -\frac{1}{\hbar^{3/2}} \sum_{j=1}^{\infty} a_j(q, q'; E) \exp \left[\frac{i}{\hbar} S_j(q, q'; E) + i\phi_j\right] \tag{11}
\]

where \(j\) labels a ray path. Quantity \(S_j\) is the action along the path \(j\), \(\phi_j\) is a phase factor, the meaning of which will be discussed in following sections, and \(a_j\) is the wave amplitude whose determination takes into account the spreading and convergence of the nearby rays. We emphasize that \(S_j, a_j\) and \(\phi_j\) are independent of \(\hbar\) and are determined purely by consideration of the
classical orbits.
To calculate $a_j$ in two spatial dimensions consider Figure 1. In this case we show two infinitesimally separated rays originating from the source point $q'; l$ denotes the distance along the ray; the radius $r_0$ is chosen so that the circle lies in the disc and satisfies $kr_0 \gg 1$; $ds(l)$ denotes the differential arclength along the wavefront (perpendicular to the rays). By conservation of probability flux we have

$$|a(r_0)|^2 \dot{q}(r_0) ds(r_0) = |a(l)|^2 \dot{q}(l) ds(l),$$

where $\dot{q} = |\partial H/\partial p|$ is the particle speed. Since in billiards speed of the particle is constant of the motion we have

$$|a(l)| = |a(r_0)| \left[ \frac{ds(r_0)}{ds(l)} \right]^{1/2}.$$  \hspace{1cm} (12)

Because $r_0$ lies within the disc and satisfies $kr_0 \gg 1$, we can find $q(r_0)$ by using the large argument approximation of $H_0^{(1)}(kr)$ (10) and comparing it with (11) we obtain

$$a(r_0) = \frac{m \exp(-i\pi/4)}{(2\pi r_0)^{1/2}} (2mE)^{-1/4}.$$  \hspace{1cm} \hspace{1cm} (12)

Knowing $a(r_0)$ we can use (12) to calculate $a_j(q, q'; E)$ at any point along a classical trajectory. Special consideration of wave effects, not included in the
geometrical ray picture, is necessary at points where \( ds(l) = 0 \). Note that for chaotic trajectories nearby orbits separate exponentially, with the consequence that \( ds(r_0)/ds(l) \) and hence also \( a_j \), on average decrease exponentially with the distance \( l \) along the orbit.

### 3.3 Semiclassical trace formula

Now we are ready to calculate the trace of the green function which should be more properly written as

\[
\int \lim_{q \to q'} \text{Im}[G(q, q'; E)]d^2q.
\]

For \( q \) very close to \( q' \), there is the short path directly from \( q' \) to \( q \), plus many long indirect paths. For the short direct path, the geometrical optics approximation is not valid, but we may use \( G_0 \) to obtain these contribution. For the indirect paths the geometrical optics approximation is valid. Thus we write

\[
d(E) = d_0(E) + \tilde{d}(E),
\]

where \( d_0(E) \) and \( \tilde{d}(E) \) represent the direct and indirect contributions respectively;

\[
d_0(E) = -\frac{1}{\pi} \int \lim_{q \to q'} \text{Im}[G_0(q, q'; E)]d^2q, \quad (13)
\]

\[
\tilde{d}(E) = \frac{1}{\pi \hbar^{3/2}} \text{Im} \int \sum_j a_j(q, q'; E) \exp[iS_j(q, q'; E)/\hbar + i\phi_j]d^2q. \quad (14)
\]

It is easy to show that the direct contribution gives the Weyl result for \( \bar{d}(E) \). We just take the real part of the Hankel function, which is regular at the origin and show that

\[
-\frac{1}{\pi} \int \lim_{q \to q'} \text{Im} \left[ \frac{im}{2\hbar^2} H_0^{(1)}(k|q-q'|) \right]d^2q = \frac{m}{2\pi \hbar^2} \int \lim_{q \to q'} J_0(k|q-q'|)d^2q = \frac{mA}{2\pi \hbar^2}
\]

is indeed (5). Since these is so, then the quantity \( \tilde{d}(E) \) yields the fluctuations of \( d(E) \) about its smoothed average \( \bar{d}(E) \).

We now focus our attention on obtaining the semiclassical expression for fluctuation about \( \bar{d}(E) \), namely \( \tilde{d}(E) \). Since the semiclassical regime corresponds to very small \( \hbar \), the factor \( \exp(iS_j/\hbar) \) in the integrant of (14) varies very rapidly with \( q \). Thus one may use the stationary phase approximation to evaluate the integral. The idea of stationary phase bases on assumption
that due to rapidly varying phase the integral is averaged to zero everywhere except at the points where phase is stationary, $\nabla S_j(q, q'; E) = 0$; this condition equals

$$[\nabla_q S_j(q, q'; E) + \nabla_{q'} S_j(q, q'; E)]_{q = q'} = 0.$$  

From the definition of action this yields $p(q) - p'(q) = 0$ where $p'(q) \equiv p(q')|_{q' = q}$. We see that the stationary phase condition selects out classical periodic orbits. On Figure 2 we see two different cases: (a), the stationary phase condition is not satisfied and (b), the stationary phase condition is satisfied. Thus, we have the important result that fluctuation of the density of states reduces to a sum over all periodic orbits of the classical problem.

For the case of isolated stable periodic orbits and unstable periodic orbits the following result is obtained after the integration of (14), using the stationary phase approximation

$$\hat{d}(E) = \frac{1}{\pi \hbar} \sum_j \sum_{r=1}^{\infty} \frac{T_j}{[\det(M_j - I)]^{1/2}} \cos \left[ r S_j(E)/\hbar - rm_j \pi/2 \right]. \quad (15)$$

These is the famous Gutzwiller trace formula derived in 1969 by Gutzwiller. We have expressed $a_j$ in terms of the stability matrix $M_j$ and the time $T_j$, needed by the classical particle to perform a primitive cycle. Also the phase factor has been written in its definite form, where $m_j$ is the Maslov index. We will refer to a single traversal of a closed ray path as a primitive periodic orbit. Note that we have to include all periodic orbits in the sum.
Summation is organized as follows. Index $j$ labels the primitive periodic orbit while index $r$ counts its repetitions, since the $r$-th round trip of the primitive periodic orbit is the periodic orbit as well. Primitive periodic orbit is the base orbit for the infinite set of non-primitive periodic orbits with the same topological structure. So it is advantageous to organize summation that way while there are simple algebraic relations between the classical invariants of the composite (non-primitive) periodic orbit and the classical invariants of its underlying primitive periodic orbit. Action $S$ and phase factor $m\pi/2$ are both additive quantities, whereas stability matrix $M$ is multiplicative. Having the composite periodic orbit $r$ as the $r$-th round trip of the primitive periodic orbit $j$ we find, $S_{r,j} = rS_j$, $m_{r,j}\pi/2 = rm_j\pi/2$ and $M_{r,j} = M_j^r$. Note that $T_j$ is a primitive period independent of $r$.

4 Trace formula in practice

4.1 Search for periodic orbits

In search for periodic orbits we get use of the principle of least action. In the case of the billiard, action is proportional to the orbit length since the modulus of the momentum is a constant of motion. Orbit is uniquely defined with its sorted bounce points $s_i$, as there is only one straight line connecting them. Choosing $N$ bounce orbit we have to find $\tilde{s} = (s_1, s_2, \ldots, s_N)$ so that $\partial_s L(s)|_{s=\tilde{s}} = 0$ if

$$L(s) = d(s_N, s_1) + \sum_{i=1}^{N-1} d(s_i, s_{i+1})$$

and $d(x, y)$ is the length of the path connecting boundary points $x$ and $y$. If we can find symmetry properties of the orbit, which are in fact the symmetry properties of the billiard, we can add constrains to reduce the dimensionality of the problem. It depends on the numerical method and strategy, but it can happen that solution is not a primitive periodic orbit. We learned from the previous section that non-primitive periodic orbit is trivially related to the underlying primitive periodic orbit. Searching for them would be a waste of time. Solution must be also checked for pruning and in that case must be ruled out. The problem of pruning is typical for non-convex billiards.

4.2 Stability matrix

Linear stability matrix describes the deformation of an infinitesimal neighborhood in the co-moving frame of periodic orbit by performing one cycle.
Deformation is characterized by the time evolution of the distance of infinitesimally close phase space points. Since the distance along the trajectory is invariant of the cycle, we have to consider only its perpendicular variations. We end up with $2 \times 2$ matrix describing the evolution of variational vector $\delta r_\perp = (\delta q_\perp, \delta p_\perp)$. Stability matrix is composed of two kinds of partial stability matrices $M_t$ and $M_r$, where first denotes the matrix of the free motion between two successive reflections and second is the matrix for a reflection. They have the following form

$$M_t = \begin{pmatrix} 1 & l/p \\ 0 & 1 \end{pmatrix}, \quad M_r = \begin{pmatrix} -1 & 0 \\ -2p/(r \cos \theta) & -1 \end{pmatrix},$$

where $l$ is the length of a trajectory between two reflections, $r$ is the radius of curvature at a reflection point, $\theta$ is the angle of incidence and $p$ is the modulus of the momentum. Stability matrix for a cycle is than a product of stability matrices corresponding to successive sections of the periodic orbit:

$$M = M_r^{s_1} M_t^{s_1-s_2} M_r^{s_2} M_t^{s_2-s_3} \ldots M_r^{s_N} M_t^{s_N-s_1}.$$ 

Note that $\det M = 1$, and so there are three possibilities for pairs of eigenvalues and consequently three types of periodic orbit: elliptic ($\lambda, 1/\lambda = \exp(\pm i\phi)$), hyperbolic ($\lambda, 1/\lambda > 0$) and hyperbolic with reflection ($\lambda, 1/\lambda < 0$). Last two cases lead to linear instability of periodic orbit, which is necessary for amplitude finiteness in equation (15). This is obvious if we look at the stationary phase integral as the interference phenomenon as there is an exponential reduction of orbits that contribute to the interference.

### 4.3 Phase factor

The origin of the Maslov index can most easily be understood in the one-dimensional case. Semiclassically, one approximates the wave functions to lowest order by plane waves with the local wave number $k(x) = \sqrt{E - V(x)}$. This approximation obviously breaks down at classical turning points where $E = V(x)$ and the wavelength diverges. Expanding the wave function around classical turning points and matching the solutions to the plane-wave solutions far from the turning points leads to additional phases in the semiclassical quantization. In the limit $\hbar \to 0$ these are independent of the detailed shape of the potential. Each reflection at a soft turning point gives a phase of $-\pi/2$, whereas each reflection on an infinite potential wall gives a phase of $-\pi$. Writing these phase as $-m\pi/2$, one usually calls $m$ the Maslov index.
4.4 Convergence

When trying Gutzwiller trace formula in practice the problem of divergence usually arise, mainly as a consequence of the rapid proliferation of periodic orbits with growing period. We can make the useful estimation by expanding a single term in the sum about some energy $E_0$,

$$\exp\left(\frac{iS_k(E)}{\hbar}\right) \approx \exp\left(\frac{iS_k(E_0)}{\hbar} + \frac{iT_k(E - E_0)}{\hbar}\right),$$

we see that the periodic orbit $k$ contributes a term to $\tilde{d}(E)$ that oscillates with energy period $\delta E_k \sim 2\pi\hbar/T_k$. As we include longer and longer period orbits in the sum, we see that the resolved scale of $\tilde{d}(E)$ becomes shorter. Hence, if we only desire a representation of $\tilde{d}(E)$ smoothed over some scale $\Delta$, we only need to include finite number of periodic orbits whose period is not larger than $2\pi\hbar/\Delta$. But still it is not always the case that such a restriction insures the finiteness of the number of periodic orbits. Various techniques have been developed to circumvent the convergence problem of periodic orbit theory. I will mention just two most popular, the cycle expansion technique [3] and the analytical continuation with harmonic inversion [4]. Cycle expansion works only if there exists the complete symbolic dynamics while harmonic inversion is quite general. Basic ideas and use, reader can find in references.

5 Numerical experiment

Direct use of the Gutzwiller trace formula is problematic, since it is divergent, so in practice its use is always mixed with techniques which help to gain the spectrum before direct computation would run out of control. However, I will show how it works as it is.

5.1 Billiard and symbolic code

I choose a fully chaotic billiard shown on Figure 3. Chaos is assured due to concave boundary which strongly defocuses nearby orbits. Cathetus is of length 1 and radius of curved hypotenuse is 2. We can uniquely name orbit by partitioning the boundary on the smooth topologically distinct regions and generate name upon the series of reflections where every reflection on the specific region holds the letter. We can partition the boundary by finding regions where no successive reflections are possible. In our case we choose letter $a$ to name the reflection on the horizontal cathetus, letter $b$ associated with reflection on vertical cathetus and letter $c$ associated with reflection on
the curved hypothenuse. There are semantic restrictions. Names where letter is followed by the same letter is prohibited (is not physical). Code could be more compact if we are able to name the distinct topological events. I will make a simplification by translating $aca \rightarrow a$, $bcb \rightarrow a$, $abc \rightarrow b$, $bac \rightarrow b$, $acb \rightarrow c$ and $bca \rightarrow c$.

5.2 Orbits

Technique of searching for periodic orbits is treated in previous section. Most of the work is done if we are able to find coding system with as possible simple grammatical rules upon which we can simply determine if orbit is physical. Since grammar is strongly system dependent I will not focus much into these special example as there are no real general rules. On Figure 4 you can see some shortest periodic orbits. Notice, how longer periodic orbits combine motives of shortest one. These is usually followed by shadowing effect and hence with the higher convergence.

5.3 Result

I have included all periodic orbits with symbolic code no longer than 10 into the sum of Gutzwiler trace formula. Obviously, I have to include non-primitive orbits as well. Semiclassical mechanic arises by formally taking the limit of $\hbar$ to zero. To avoid some unnecessary regularization I rather observe the density of states in wave number space:

$$\tilde{d}(k) = \tilde{d}(E) \frac{\partial E}{\partial k},$$
leading to:

\[ \tilde{d}(k) = \frac{1}{\pi} \sum_j \sum_{r=1}^{\infty} \frac{l_j}{[\det(M_j - I)]^{1/2}} \cos [r(l_j k - m_j \pi/2)]. \]

Now result is shown on Figure 5. Notice how good are lower states reproduced by peaks of the density distribution. Notice also the deviations from the levels corresponding to higher \( k \). When we do the projection from the energy eigenvalues to the wave number eigenvalues, density of states changes. If it is constant for the energy levels in the Weyl approximation, we see that it is proportional to \( k \) for wave number levels. Structure becomes thinner, therefore we have to add longer periodic orbits into the sum if we are to represent higher spectra.

6 Conclusions

At first we have shown that the density of states equals the trace of the Green function. Then we make a formal limit of \( \hbar \) to zero, leading to highly oscillatory integral. We assume that integral averages to zero everywhere except where phase is stationary. Stationary phase condition selects out the classically chaotic orbits and the integral reduces to the sum over them. Periodic orbits contribute waves which interfere to reproduce the spectral density distribution. We saw in practical example that the Gutzwiller trace
formula indeed works, but we are also aware of the difficulties to control the convergence. The Gutzwiller trace formula is at first the important theoretical result, whereas there practical applications are limited. Semiclassical theory of chaotic spectra has two complementary extremes, trace formula and random matrix theory. Random matrix theory is able to predict the level spacing statistic with price of losing the information of the shape of the spectrum. On the other hand, with the Gutzwiller trace formula we can obtain the shape of the spectrum, smoothed to some finite scale, but we are not (practically) able to resolve the individual levels. With sophisticated methods physicists were able to refine the basic Gutzwiller trace formula into the powerful practical tool [4]. However, in these areas of research, the Gutzwiller trace formula is an important pedagogical and theoretical starting point.

References

