Appendix O

Noise/quantum corrections

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The Gutzwiller trace formula is only a good approximation to the quantum mechanics when $\hbar$ is small. Can we improve the trace formula by adding quantum corrections to the semiclassical terms? A similar question can be posed when the classical deterministic dynamics is disturbed by some way Gaussian white noise with strength D. The deterministic dynamics then can be considered as the weak noise limit $D \to 0$. The effect of the noise can be taken into account by adding noise corrections to the classical trace formula. A formal analogy exists between the noise and the quantum problem. This analogy allows us to treat the noise and quantum corrections together.

O.1 Periodic orbits as integrable systems

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We saw in chapter 29 that the noise problem can be reformulated in a "quantum" way. ⇑PRIVATE From now on, we use the language of quantum mechanics, since it is more convenient to visualize the results there. Where it is necessary we will discuss the difference between noise and quantum cases.

First we would like to introduce periodic orbits from an unusual point of view, which can convince you, that chaotic and integrable systems are in fact not as different from each other, than we might think. If we start orbits in the neighborhood of a periodic orbit and look at the picture on the Poincaré section we can see a regular picture. For stable periodic orbits the points form small ellipses around the center and for unstable orbits they form hyperbolas (See Fig. O.1).

Figure O.1: Poincaré section close to a stable and an unstable periodic orbit

The motion close to a periodic orbits is regular in both cases. This is due to the fact, that we can linearize the Hamiltonian close to an orbit, and linear systems are always integrable. The linearized Hamilton's equations close to the periodic orbit $(q_p(t)+q, p_p(t)+p)$ look like

$$\begin{aligned} \dot{q} &= +\partial^2_{pq} H(q_p(t), p_p(t))q + \partial^2_{pp} H(q_p(t), p_p(t))p, & \text{(O.1)} \\ \dot{p} &= -\partial^2_{qq} H(q_p(t), p_p(t))q - \partial^2_{qp} H(q_p(t), p_p(t))p, & \text{(O.2)} \end{aligned}$$

where the new coordinates q and p are relative to a periodic orbit. This linearized equation can be regarded as a d dimensional oscillator with time periodic frequencies. These equations are representing the equation of motion in a redundant way since more than one combination of q, p and t determines the same point of the phase space. This can be cured by an extra restriction on the variables, a constraint the variables should fulfill. This constraint can be derived from the time independence or stacionarity of the full Hamiltonian

$$\partial_t H(q_p(t)+q, p_p(t)+p) = 0. \tag{O.3}$$

Using the linearized form of this constraint we can eliminate one of the linearized equations. It is very useful, although technically difficult, to do one more transformation and to introduce a coordinate, which is parallel with the Hamiltonian flow ($x_\|$) and others which are orthogonal. In the orthogonal directions we again get linear equations. These equations with $x_\|$ dependent rescaling can be transformed into normal coordinates, so that we get tiny oscillators in the new coordinates with constant frequencies. This result has first been derived by Poincaré for equilibrium points and later it was extended for periodic orbits by V.I. Arnol'd and co-workers. In the new coordinates, the Hamiltonian reads as

$$H_0(x_\|, p_\|, x_n, p_n) = \frac{1}{2}p_\|^2 + U(x_\|) + \sum_{n=1}^{d-1} \frac{1}{2}(p_n^2 \pm \omega_n^2 x_n^2), \tag{O.4}$$

which is the general form of the Hamiltonian in the neighborhood of a periodic orbit. The $\pm$ sign denotes, that for stable modes the oscillator potential is positive while for an unstable mode it is negative. For the unstable modes, ω is the Lyapunov exponent of the orbit

$$\omega_n = \ln \Lambda_{p,n}/T_p, \tag{O.5}$$

where $\Lambda_{p,n}$ is the expanding eigenvalue of the Jacobi matrix. For the stable directions the eigenvalues of the Jacobi matrix are connected with ω as

$$\Lambda_{p,n} = e^{-i\omega_n T_p}. \tag{O.6}$$

The Hamiltonian close to the periodic orbit is integrable and can be quantized by the Bohr-Sommerfeld rules. The result of the Bohr-Sommerfeld quantization for the oscillators gives the energy spectra

$$\begin{aligned} E_n &= \hbar\omega_n \left(j_n + \frac{1}{2}\right) \text{for stable modes,} \\ E_n &= -i\hbar\omega_n \left(j_n + \frac{1}{2}\right) \text{for unstable modes,} \end{aligned} \tag{O.7}$$

where $j_n = 0, 1, \ldots.$ It is convenient to introduce the index $s_n = 1$ for stable and $s_n = -i$ for unstable directions. The parallel mode can be quantized implicitly trough the classical action function of the mode:

$$\frac{1}{2\pi}\oint p_\| dx_\| = \frac{1}{2\pi} S_\|(E_m) = \hbar\left(m + \frac{m_p \pi}{2}\right), \tag{O.8}$$

where m_p is the topological index of the motion in the parallel direction. This latter condition can be rewritten by a very useful trick into the equivalent form

$$(1 - e^{iS_\|(E_m)/\hbar - i m_p\pi/2}) = 0. \tag{O.9}$$

The eigenenergies of a semiclassically quantized periodic orbit are all the possible energies

$$E = E_m + \sum_{n=1}^{d-1} E_n. \tag{O.10}$$

This relation allows us to change in (O.9) E_m with the full energy minus the oscillator energies $E_m = E - \sum_n E_n$. All the possible eigenenergies of the periodic orbit then are the zeroes of the expression

$$\Delta_p(E) = \prod_{j_1,\ldots,j_{d-1}} (1 - e^{iS_\|(E - \sum_n \hbar s_n\omega_n(j_n+1/2))/\hbar - i m_p\pi/2}). \tag{O.11}$$

If we Taylor expand the action around E to first order

$$S_{\|}(E+\epsilon) \approx S_{\|}(E) + T(E)\epsilon, \tag{O.12}$$

where $T(E)$ is the period of the orbit, and use the relations of ω and the eigenvalues of the Jacobi matrix, we get the expression of the Selberg product

$$\Delta_p(E) = \prod_{j_1,\cdots,j_{d-1}} \left(1 - \frac{e^{iS_p(E)/\hbar - im_p\pi/2}}{\prod_n \Lambda_{p,n}^{(1/2+j_n)}}\right). \tag{O.13}$$

If we use the right convention for the square root we get exactly the d dimensional expression of the Selberg product formula we derived from the Gutzwiller trace formula in ? . Just here we derived it in a different way! The function $\Delta_p(E)$ is the semiclassical zeta function for one prime orbit.

Now, if we have many prime orbits and we would like to construct a function which is zero, whenever the energy coincides with the BS quantized energy of one of the periodic orbits, we have to take the product of these determinants:

$$\Delta(E) = \prod_p \Delta_p(E). \tag{O.14}$$

The miracle of the semiclassical zeta function is, that if we take infinitely many periodic orbits, the infinite product will have zeroes not at these energies, but close to the eigenenergies of the whole system !

So we learned, that both stable and unstable orbits are integrable systems and can be individually quantized semiclassically by the old Bohr-Sommerfeld rules. So we almost completed the program of Sommerfeld to quantize general systems with the method of Bohr. *Let us have a remark here. In addition to the Bohr-Sommerfeld rules, we used the unjustified approximation (O.12). Sommerfeld would never do this ! At that point we loose some important precision compared to the BS rules and we get somewhat worse results than a semiclassical formula is able to do. We will come back to this point later when we discuss the quantum corrections.* To complete the program of full scale Bohr-Sommerfeld quantization of chaotic systems we have to go beyond the linear approximation around the periodic orbit.

The Hamiltonian close to a periodic orbit in the parallel and normal coordinates can be written as the 'harmonic' plus 'anharmonic' perturbation

$$H(x_{\|}, p_{\|}, x_n, p_n) = H_0(x_{\|}, p_{\|}, x_n, p_n) + H_A(x_{\|}, x_n, p_n), \tag{O.15}$$

where the anharmonic part can be written as a sum of homogeneous polynomials of x_n and p_n with $x_\parallel$ dependent coefficients:

$$\begin{aligned} H_A(x_\parallel, x_n, p_n) &= \sum_{k=3} H^k(x_\parallel, x_n, p_n) && \text{(O.16)} \\ H^k(x_\parallel, x_n, p_n) &= \sum_{\sum l_n + m_n = k} H^k_{l_n, m_n}(x_\parallel) x_n^{l_n} p_n^{m_n} && \text{(O.17)} \end{aligned}$$

This classical Hamiltonian is hopeless from Sommerfeld's point of view, since it is non integrable. However, Birkhoff in 1927[3] introduced the concept of normal form, which helps us out from this problem by giving successive integrable approximation to a non-integrable problem. Let's learn a bit more about it!

O.2 The Birkhoff normal form

Birkhoff studied the canonical perturbation theory close to an equilibrium point of a Hamiltonian. Equilibrium point is where the potential has a minimum $\nabla U = 0$ and small perturbations lead to oscillatory motion. We can linearize the problem and by introducing normal coordinates x_n and conjugate momentums p_n the quadratic part of the Hamiltonian will be a set of oscillators

$$H_0(x_n, p_n) = \sum_{n=1}^{d} \frac{1}{2}(p_n^2 + \omega_n^2 x_n^2). \tag{O.18}$$

The full Hamiltonian can be rewritten with the new coordinates

$$H(x_n, p_n) = H_0(x_n, p_n) + H_A(x_n, p_n), \tag{O.19}$$

where H_A is the anharmonic part of the potential in the new coordinates. The anharmonic part can be written as a series of homogeneous polynomials

$$\begin{aligned} H_A(x_n, p_n) &= \sum_{j=3}^{\infty} H^j(x_n, p_n), && \text{(O.20)} \\ H^j(x_n, p_n) &= \sum_{|l|+|m|=j} h^j_{lm} x^l p^m, && \text{(O.21)} \end{aligned}$$

[3]It is really a pity, that in 1926 Schrödinger introduced the wave mechanics and blocked the development of Sommerfeld's concept.

where h^j_{lm} are real constants and we used the multi-indices $l := (l_1, ..., l_d)$ with definitions

$$|l| = \sum l_n, x^l := x_1^{l_1} x_2^{l_2} ... x_d^{l_d}.$$

Birkhoff showed, that that by successive canonical transformations one can introduce new momentums and coordinates such, that in the new coordinates the anharmonic part of the Hamiltonian up to any given n polynomial will depend only on the variable combination

$$\tau_n = \frac{1}{2}(p_n^2 + \omega_n^2 x_n^2), \tag{O.22}$$

where x_n and p_n are the new coordinates and momentums, but ω_n is the original frequency. This is called the Birkhoff normal form of degree N:

$$H(x_n, p_n) = \sum_{j=2}^{N} H^j(\tau_1, ..., \tau_d), \tag{O.23}$$

where H^j are homogeneous degree j polynomials of τ-s. This is an integrable Hamiltonian, the non-integrability is pushed into the remainder, which consists of polynomials of degree higher than N. We run into trouble only when the oscillator frequencies are commensurate e.g. it is possible to find a set of integers m_n such that the linear combination

$$\sum_{n=1}^{d} \omega_n m_n,$$

vanishes. This extra problem has been solved by Gustavson in 1966 and we call the the object Birkhoff-Gustavson normal form. The procedure of the successive canonical transformations can be computerized and can be carried out up to high orders (~ 20).

Of course, we pay a price for forcing the system to be integrable up to degree N. For a non-integrable system the high order terms behave quete widely and the series is not convergent. Therefore we have to use this tool carefully. Now, we learned how to approximate a non-integrable system with a sequence of integrable systems and we can go back and carry out the BS quantization.

O.3 Bohr-Sommerfeld quantization of periodic orbits

There is some difference between equilibrium points and periodic orbits. The Hamiltonian (O.4) is not a sum of oscillators. One can transform the parallel part, describing circulation along the orbit, into an oscillator Hamiltonian, but this would make the problem extremelly difficult. Therefore, we carry out the canonical transformations dictated by the Birkhoff procedure only in the orthogonal directions. The $x_{\|}$ coordinate plays the role of a parameter. After the tasformation up to order N the Hamiltonian (O.17) is

$$H(x_{\|}, p_{\|}, \tau_1, ... \tau_{d-1}) = H_0(x_{\|}, p_{\|}, \tau_1, ..., \tau_{d-1}) + \sum_{j=2}^{N} U^j(x_{\|}, \tau_1, ..., \tau_{d-1}), \quad (O.24)$$

where U^j is a jth order homogeneous polynomial of τ-s with $x_{\|}$ dependent coefficients. The orthogonal part can be BS quantized by quantizing the individual oscillators, replacing τ-s as we did in (O.8). This leads to a one dimensional effective potential indexed by $j_1, ..., j_{d-1}$

$$\begin{aligned} H(x_{\|}, p_{\|}, j_1, ..., j_{d-1}) &= \frac{1}{2}p_{\|}^2 + U(x_{\|}) + \sum_{n=1}^{d-1} \hbar s_n \omega_n (j_n + 1/2) + \qquad (O.25) \\ &+ \sum_{k=2}^{N} U^k(x_{\|}, \hbar s_1 \omega_1 (j_1 + 1/2), \hbar s_2 \omega_2 (j_2 + 1/2), ..., \hbar s_{d-1} \omega_{d-1} (j_{d-1} + 1/2)), \end{aligned}$$

where j_n can be any non-negative integer. The term with index k is proportional with $\hbar^k$ due to the homogeneity of the polynomials.

The parallel mode now can be BS quantized for any given set of j-s

$$\begin{aligned} S_p(E, j_1, ..., j_{d-1}) &= \oint p_{\|} dx_{\|} = \qquad (O.26) \\ &= \oint dx_{\|} \sqrt{E - \sum_{n=1}^{d-1} \hbar s_n \omega_n (j_n + 1/2) - U(x_{\|}, j_1, ..., j_{d-1})} = 2\pi\hbar(m + m_p/2), \end{aligned}$$

where U contains all the $x_{\|}$ dependent terms of the Hamiltonian. The spectral determinant becomes

$$\Delta_p(E) = \prod_{j_1, ..., j_{d-1}} (1 - e^{iS_p(E, j_1, ..., j_{d-1})/\hbar - m_p \pi/2}). \quad (O.27)$$

This expression completes the Sommerfeld method and tells us how to quantize chaotic or general Hamiltonian systems. Unfortunately, quantum mechanics postponed this nice formula until our book.

This formula has been derived with the help of the semiclassical Bohr-Sommerfeld quantization rule and the classical normal form theory. Indeed, if we expand S_p in the exponent in the powers of $\hbar$

$$S_p = \sum_{k=0}^{N} \hbar^k S_k,$$

we get more than just a constant and a linear term. This formula already gives us corrections to the semiclassical zeta function in all powers of $\hbar$. There is a very attracting feature of this semiclassical expansion. $\hbar$ in S_p shows up only in the combination $\hbar s_n \omega_n (j_n + 1/2)$. A term proportional with $\hbar^k$ can only be a homogeneous expression of the oscillator energies $s_n \omega_n (j_n + 1/2)$. For example in two dimensions there is only one possibility of the functional form of the order k term

$$S_k = c_k(E) \cdot \omega_n^k (j + 1/2)^k,$$

where $c_k(E)$ is the only function to be determined.

The corrections derived sofar are *doubly* semiclassical, since they give semiclassical corrections to the semiclassical approximation. What can quantum mechanics add to this ? As we have stressed in the previous section, the exact quantum mechanics is not invariant under canonical transformations. In other context, this phenomenon is called the operator ordering problem. Since the operators $\hat{x}$ and $\hat{p}$ do not commute, we run into problems, when we would like to write down operators for classical quantities like $x^2 p^2$. On the classical level the four possible orderings $xpxp$, $ppxx$, $pxpx$ and $xxpp$ are equivalent, but they are different in the quantum case. The expression for the energy (O.26) is not exact. We have to go back to the level of the Schrödinger equation if we would like to get the exact expression.

O.4 Quantum calculation of $\hbar$ corrections

The Gutzwiller trace formula has originally been derived from the saddle point approximation of the Feynman path integral form of the propagator. The exact trace is a pathsum for all closed paths of the system

$$\mathrm{Tr} G(x, x', t) = \int dx G(x, x, t) = \int \mathcal{D}x e^{iS(x,t)/\hbar}, \qquad \text{(O.28)}$$