

Bohr-Sommerfeld Quantization of Periodic Orbits

Gábor Vattay*

Division de Physique Théorique, Institut de Physique Nucléaire,

F-91406 Orsay Cedex, France

e-mail:vattay@ipncls.in2p3.fr

(October 29, 2018)

Abstract

We show, that the canonical invariant part of \hbar corrections to the Gutzwiller trace formula and the Gutzwiller-Voros spectral determinant can be computed by the Bohr-Sommerfeld quantization rules, which usually apply for integrable systems. We argue that the information content of the classical action and stability can be used more effectively than in the usual treatment. We demonstrate the improvement of precision on the example of the three disk scattering system.

Gutzwiller trace formula for chaotic systems is often presented as the counterpart of the Bohr-Sommerfeld (BS) quantization of integrable systems [1]. Consequently, corrections of the trace formula proportional with powers of \hbar are usually associated with quantum corrections [3]. In this letter we would like to show, that a part of \hbar corrections is not connected to deep quantum effects and they can be calculated with some precision from purely semiclassical BS arguments. Then we propose a new trace formula and spectral determinant which is more precise than the usual trace formula although it uses only the linear stability and action as an input data, just like the original trace formula.

First we would like to introduce periodic orbits from an unusual point of view. Chaotic and integrable systems on the level of periodic orbits are in fact not as different from each other as 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 pattern. For stable periodic orbits the points form small ellipses around the center and for unstable orbits they form hyperbola. 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 a periodic orbit, and linear systems are always integrable. Based on Poincaré's idea, Arnold and coworkers have shown [4], that the Hamiltonian close to a periodic orbit can be brought to a very practical form. One has to introduce new coordinates: one which is parallel with the orbit (x_{\parallel}) and others which are orthogonal. In the orthogonal directions we get linear equations. These equations with x_{\parallel} dependent rescaling can be transformed into normal coordinates so that we get tiny oscillators, or inverse oscillators, in the new coordinates with constant, frequencies. In the new coordinates, the Hamiltonian is

$$H_0(x_{\parallel}, p_{\parallel}, x_n, p_n) = \frac{1}{2}p_{\parallel}^2 + U(x_{\parallel}) + \sum_{n=1}^{d-1} \frac{1}{2}(p_n^2 \pm \omega_n^2 x_n^2), \quad (1)$$

which is one possible normal 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. Since the eigenvalues of the monodromy or Jacobi stability matrix of a periodic orbit are invariant under the transformations we made sofar, the oscillator frequencies can be expressed for unstable modes with the Ljapunov exponent of the orbit

$$\omega_n = \ln |\Lambda_{p,n}|/T_p, \quad (2)$$

where $\Lambda_{p,n}$ is the expanding eigenvalue of the Jacobi matrix and T_p is the period of the orbit. Also, for stable directions the eigenvalues of the Jacobi matrix are connected with ω as

$$\Lambda_{p,n} = e^{-i\omega_n T_p}. \quad (3)$$

The Hamiltonian (1) is integrable and can be semiclassically quantized by the BS rules. The result of the BS quantization for the oscillators gives the energy spectra

$$\begin{aligned} E_n &= \hbar\omega_n \left(j_n + \frac{1}{2} \right) \quad \text{for stable modes,} \\ E_n &= -i\hbar\omega_n \left(j_n + \frac{1}{2} \right) \quad \text{for unstable modes,} \end{aligned} \quad (4)$$

where $j_n = 0, 1, \dots$. 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 through the classical action function :

$$\frac{1}{2\pi} \oint p_{\parallel} dx_{\parallel} = \frac{1}{2\pi} S_{\parallel}(E_m) = \hbar \left(m + \frac{\mu_p \pi}{2} \right), \quad (5)$$

where μ_p is the Maslov index of the motion in the parallel direction. This latter condition can be rewritten in the equivalent form

$$(1 - e^{iS_{\parallel}(E_m)/\hbar - i\mu_p\pi/2}) = 0. \quad (6)$$

The eigenenergies of a semiclassically quantized periodic orbit [5] are all the possible energies

$$E = E_m + \sum_{n=1}^{d-1} E_n. \quad (7)$$

This relation allows us to change in (6) 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

$$\Delta_p^{BSH}(E) = \prod_{j_1, \dots, j_{d-1}} (1 - e^{iS_{\parallel}(E - \sum_n \hbar s_n \omega_n(j_n + 1/2))/\hbar - i\mu_p\pi/2}). \quad (8)$$

Now, we show how one can derive the Gutzwiller trace formula from (8). We have to expand the action around E to first order $S_{\parallel}(E + \epsilon) \approx S_p(E) + T_p(E)\epsilon$, where $T_p(E)$ and $S_p(E)$ are the period and the action of the orbit, and we have to use the relations of ω -s and the eigenvalues of the Jacobi matrix, we get

$$\Delta_p(E) = \prod_{j_1, \dots, j_{d-1}} \left(1 - \frac{e^{iS_p(E)/\hbar - i\nu_p\pi/2}}{\prod_n |\Lambda_{p,n}|^{1/2} \Lambda_{p,n}^{j_n}} \right), \quad (9)$$

where ν_p is the Maslov index of the orbit. Now, if we have many primitive orbits and we would like to construct a function formally, 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:

$$\Delta(E) = \prod_p \Delta_p(E). \quad (10)$$

This is exactly the Gutzwiller-Voros [10,2] spectral determinant, which is the regularized semiclassical expression for the spectral determinant

$$\Delta(E) = \det(E - \hat{H})$$

of the Hamilton operator of the system. The logarithmic derivative of this quantity gives the trace of the Green's function and the oscillating part of the trace formula in semiclassical approximation

$$Tr G(q', q', E) = -\frac{d}{dE} \log \Delta(E) \approx \frac{1}{i\hbar} \sum_{p,r} T_p(E) \frac{e^{irS_p(E) - ir\nu_p\pi/2}}{|\det(1 - J_p^r)|^{1/2}}, \quad (11)$$

where the summation goes for the primitive periodic orbits and their repetitions, J_p is the monodromy or Jacobi matrix of the periodic orbit. The construction of the spectral determinant (8) described above is not unique in the sense, that we can multiply each periodic orbit's spectral determinant with a smooth function which does not have zeroes and poles on the complex energy plane. However, the logarithmic derivative of such a smooth function will not contribute to the oscillating part of the trace formula and can be considered as a part of its smooth part.

From this derivation we can see, that the Gutzwiller trace formula is recovered only if we linearize the action. This is a very bad approximation for low energies, where the ratio $T_p(E)/S_p(E) \sim 1/E$, is large. In that regime we might expect that the spectral determinant (8) works better than the Gutzwiller-Voros formula (9).

That this is the case, we have checked on the example of the three disk scattering system [13,14] at the standard parameters of disk separation 6 compared to the radius of the disks. This is a billiard system, where the parallel action is $S(E) = kL_p$, where $k = \sqrt{E}$ is the wave number (with mass unit $m = 1/2$) and L_p is the geometrical length of the the orbit. There is only one unstable oscillator mode with oscillator energies

$$E_{p,j}(k) = -i\hbar \frac{2k \log |\Lambda_p|}{L_p} (j + 1/2).$$

The new spectral determinant as a function of the wave number is

$$\Delta^{BSH}(k) = \prod_p \prod_j (1 - e^{iL_p \sqrt{k^2 - E_{p,j}(k)}/\hbar - i\nu_p \pi/2}). \quad (12)$$

If we expand the exponent in \hbar we can see that it gives corrections to the leading action and stability term. We can compare the first \hbar correction with the exact \hbar correction computed in Ref. [3] and Ref. [6]. The \hbar corrected spectral determinant with the exact correction is defined as

$$\Delta^{ex}(k) = \prod_p \prod_j (1 - e^{ikL_p/\hbar - i\nu_p \pi/2 - (j+1/2) \ln |\Lambda_p| + i\hbar C_{p,j}^{ex(1)}/k + \dots}), \quad (13)$$

where $C_{p,j}^{ex(1)}$ the exact first \hbar correction. The first correction coming from (12) is

$$C_{p,j}^{BSH(1)} = (j + 1/2)^2 (\ln |\Lambda_p|)^2 / L_p.$$

On Fig. 1 we can see, that this accounts for about 80% of the exact correction. As we will see later, this is not the whole first \hbar correction which comes from the BS quantization, it illustrates only that by using (12) we already take into account a whole series of \hbar corrections. We also compared the exact quantum mechanical resonances [7] with those computed [9] from the Gutzwiller-Voros spectral determinant and with the Gutzwiller-Voros spectral determinant with the first \hbar correction [6] and plotted the results on the complex wave number plane. We can see on Fig. 2, that for large k the Gutzwiller-Voros spectral determinant, its \hbar corrected version and the new BS type expressions approximate the resonances accurately, with a few percent error. However, the lowest resonances are approximated better by the new expression and the \hbar corrected Gutzwiller-Voros determinant is even worse than the

uncorrected. This is because the Gutzwiller-Voros determinant and its corrected version are asymptotic series expanded in the powers of $1/k$, while the new formula approximates the eigenenergies of the individual periodic orbits for small values of k also correctly. We can conclude, that by using (12) or in general (8) we can considerably improve the Gutzwiller-Voros theory for low energies by using exactly the same input data (stability, action, Maslov index) in a more economic way.

The semiclassical analysis outlined above can be done in a more general framework by the systematic application of the normal form theory of Birkhoff and Gustavson. This can be considered as a generalization of the normal form quantization of Swimm, Delos and Robnik [8] from equilibrium points to the periodic orbits. The full Hamiltonian expanded close to a periodic orbit can be written as the ‘harmonic’ plus an ‘anharmonic’ perturbation

$$H(x_{\parallel}, p_{\parallel}, x_n, p_n) = H_0(x_{\parallel}, p_{\parallel}, x_n, p_n) + H_A(x_{\parallel}, x_n, p_n), \quad (14)$$

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

$$H_A(x_{\parallel}, x_n, p_n) = \sum_{k=3}^{\infty} H^k(x_{\parallel}, x_n, p_n), \quad (15)$$

$$H^k(x_{\parallel}, x_n, p_n) = \sum_{\sum_n l_n + m_n = k} h_{l_n, m_n}^k(x_{\parallel}) x_n^{l_n} p_n^{m_n}. \quad (16)$$

We can carry out the canonical transformations introduced by Birkhoff and Gustavson [11,8,1] and the Hamiltonian can be brought to normal form in the orthogonal directions. The x_{\parallel} coordinate plays the role of a parameter. After the transformation up to order N the Hamiltonian (16) is

$$H(x_{\parallel}, p_{\parallel}, \tau_1, \dots, \tau_{d-1}) = H_0(x_{\parallel}, p_{\parallel}, \tau_1, \dots, \tau_{d-1}) + \sum_{j=2}^N U^j(x_{\parallel}, \tau_1, \dots, \tau_{d-1}) + h.o.t, \quad (17)$$

where U^j is a j -th order homogeneous polynomial of τ -s with x_{\parallel} dependent coefficients and $\tau_n = \frac{1}{2}(p_n^2 \pm \omega_n^2 x_n^2)$ is the Hamiltonian function of the original oscillator. This Hamiltonian truncated at order N is integrable, the nonintegrability is pushed to the higher order terms (h.o.t). The orthogonal part can then be BS quantized by quantizing the individual oscillators, replacing τ -s as we did in (5). This leads to a one dimensional effective potential indexed by the *quantum numbers* j_1, \dots, j_{d-1}

$$H(x_{\parallel}, p_{\parallel}, j_1, \dots, j_{d-1}) = \frac{1}{2} p_{\parallel}^2 + U(x_{\parallel}) + \sum_{n=1}^{d-1} \hbar s_n \omega_n (j_n + 1/2) + \sum_{k=2}^N U^k(x_{\parallel}, \hbar s_1 \omega_1 (j_1 + 1/2), \hbar s_2 \omega_2 (j_2 + 1/2), \dots, \hbar s_{d-1} \omega_{d-1} (j_{d-1} + 1/2)), \quad (18)$$

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

$$\begin{aligned}
S_p(E, j_1, \dots, j_{d-1}) &= \oint p_{\parallel} dx_{\parallel} = \\
&= \oint dx_{\parallel} \sqrt{2 \left(E - \sum_{n=1}^{d-1} \hbar s_n \omega_n(j_n + 1/2) - U_{eff}(x_{\parallel}, j_1, \dots, j_{d-1}) \right)} = 2\pi\hbar \left(m + \frac{\mu_p \pi}{2} \right),
\end{aligned} \tag{19}$$

where U_{eff} contains all the x_{\parallel} dependent terms of the Hamiltonian. The spectral determinant becomes

$$\Delta^{BSA}(E) = \prod_p \prod_{j_1, \dots, j_{d-1}} (1 - e^{iS_p(E, j_1, \dots, j_{d-1})/\hbar - i\nu_p \pi/2}). \tag{20}$$

Here one can see, that the indices j , which were just auxiliary indices in the Gutzwiller-Voros approach, now can be interpreted as "orthogonal quantum numbers". Formally, the integrability of the Hamiltonian is maintained in each level of the approximation and the Ruelle [12] type zeta functions

$$\zeta_{j_1, j_2, \dots, j_{d-1}}^{-1}(E) = \prod_p (1 - e^{iS_p(E, j_1, \dots, j_{d-1})/\hbar - i\nu_p \pi/2}),$$

corresponding to a given j configuration, can be interpreted as the factorization of the total spectral determinant according to subspaces with fixed quantum numbers. 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 corrections to the Gutzwiller-Voros spectral determinant 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 $s_n \omega_n(j_n + 1/2)$. We mention here Ref. [15] as a good example, where the superiority of the method outlined here can be demonstrated above the pure periodic orbit theory and the comparison of \hbar expansion and BS quantization can be clearly studied.

The \hbar corrections derived here are *doubly* semiclassical, since they give semiclassical corrections to the semiclassical approximation. What can quantum mechanics add to this? Since quantum mechanics is not invariant for canonical transformations, the derived \hbar corrections give only the leading behaviour of corrections and the exact corrections can be computed by other methods. The Birkhoff-Gustavson transformations should be replaced by quantum perturbation theory and semiclassical quantum numbers should be replaced by exact quantum numbers. This has been done in Ref. [6] which we are going to publish elsewhere. We don't think, that the semiclassical determination of \hbar corrections in higher orders is a very practical way to compute them, but in predicting the general structure of the corrections it helps us to understand their general behaviour and later probably to sum them up in order to get meaningful formulas also for low energies.

The author thanks the discussions with E. Bogomolny, O. Bohigas, P. Cvitanović, P. E. Rosenqvist, N. Whelan and A. Wirzba. This project has been financed by the EHCM PECO, OTKA F17166 and T17493.

REFERENCES

- * On leave from Eötvös University Budapest, Department of Solid State Physics
- [1] M. C. Gutzwiller, J. Math. Phys. **12**, 343 (1971); *Chaos in Classical and Quantum Mechanics* (Springer-Verlag, New York, 1990)
 - [2] A. Selberg, J. Indian Math. Soc. **20**, 47 (1956)
 - [3] P. Gaspard and D. Alonso, Phys. Rev. **A47**, R3468 (1993); D. Alonso and P. Gaspard, Chaos **3**, 601 (1993); P. Gaspard, Prog. Theor. Phys. Suppl. **116**, 59 (1994)
 - [4] V. I. Arnold, *Geometrical Methods in the Theory of Ordinary Differential Equations*, Springer Verlag, New-York (1993)
 - [5] W. H. Miller, J. Chem. Phys. **63**, 996 (1975); A. Voros, in Colloques Internationaux CNRS no 237, pp 277-286 (1975); A. M. Ozorio de Almeida and J. H. Hannay, J. Phys. **A20** 5873 (1987); K. Stefanski and E. Pollak, J. Chem. Phys. **87**, 1079 (1987)
 - [6] G. Vattay and P. E. Rosenqvist, Orsay preprint, April 1995, unpublished.
 - [7] A. Wirzba, Chaos **2**, 77 (1992)
 - [8] R. T. Swimm and J. B. Delos, J. Chem. Phys. **71**, 1706 (1979); M. Robnik, J. Phys. **A17**, 109 (1984)
 - [9] P. Cvitanović, P. E. Rosenqvist, G. Vattay and H. H. Rugh, CHAOS **3** (4), 619 (1993)
 - [10] A. Voros, J. Phys. **A21**, 685 (1988)
 - [11] F. G. Gustavson, Astron. J. **71**, 670 (1966)
 - [12] D. Ruelle, *Statistical Mechanics, Thermodynamic Formalism* (Addison-Wesley, Reading, MA, 1978)
 - [13] P. Gaspard and S. A. Rice, J. Chem. Phys. **90** 2225, 2242, 2255 (1989) **91** E3279 (1989)
 - [14] P. Cvitanović and B. Eckhardt, Phys. Rev. Lett. **63**, 823 (1989)
 - [15] N. D. Whelan, Phys. Rev. **E51**, 3778 (1995)

FIGURES

FIG. 1. Comparison between the exact \hbar corrections and the BS approximation. We have taken all the periodic orbits p of the three disk system up to 9 bounces. We computed the first \hbar correction for $j = 0$ ($C_{p,0}^{ex}$). Then we computed the quantity $(\ln |\Lambda_p|)^2/4L_p$, which correction comes from the lowest order harmonic approximation of the BS quantization of the periodic orbit ($C_{p,0}^{BSH(1)}$). We plotted here this value versus the exact \hbar correction for each periodic orbit p . We can see, that for the 22 shortest orbits they are almost linearly correlated and about 80% of the exact correction comes from this effect. The rest is coming from the anharmonicity and from deep quantum effects.

FIG. 2. Complex resonances of the 3 disk scattering system. The quantum calculation, the Gutzwiller-Voros approximation, the Gutzwiller-Voros approximation with one \hbar correction added and the BS spectral determinant in harmonic approximation (BSH) . We used all the periodic orbits up to 9 bounces. For small Rek resonances the \hbar correction breaks down, while our approximation is deviating the right way from the Gutzwiller-Voros result.



