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1988 J. Phys. A: Math. Gen. 21 685

(http://iopscience.iop.org/0305-4470/21/3/023)

J. Phys. A: Math. Gen. 21 (1988) 685-692. Printed in the UK

Unstable periodic orbits and semiclassical quantisation

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Received 14 July 1987

Abstract. The Bohr-Sommerfeld quantisation condition has a meaningful extension to classically chaotic systems whose periodic (unstable) orbits are isolated. It provides a semiclassical Euler factorisation for the functional determinant of the quantal Hamiltonian, in contrast to the Hadamard infinite product over the eigenvalues by which the exact determinant is defined.

It is a long-standing unsolved problem to find a semiclassical eigenvalue formula which would compute the levels of a quantised Hamiltonian arising from a non-integrable and, in particular, ergodic, classical motion (Einstein 1917). By contrast, the Bohr-Sommerfeld quantisation rules are able to locate quite reliably the levels of integrable systems in terms of their classical invariant tori (and those rules appear to extend to certain quasi-integrable systems as well).

Here we shall develop our statement (Voros 1987a) that an Euler infinite product expansion for the quantum determinant is the counterpart of the Bohr-Sommerfeld formulae for exponentially unstable chaotic systems. For simplicity we shall discuss the case of two degrees of freedom, with special emphasis upon the quantisation of the geodesic flow on a compact surface of constant negative curvature, but our conclusions should hold irrespective of dimension.

Let $\hat{H}(q, -\mathrm{i}\hbar\nabla_q)$ denote a quantum Hamiltonian operator with two degrees of freedom, and $H(q, p)$ denote the corresponding ($\hbar \to 0$) classical Hamiltonian. Later it will be assumed that the classical motion in phase space is highly chaotic by virtue of the following properties (reviewed by Alexeev and Yakobson 1981): each constant energy surface $\{H(q, p) = E\}$ is bounded, and neighbouring trajectories upon it separate exponentially in time with rate $\omega(E) > 0$ (ω is the Lyapunov exponent).

Our analysis will rely on a critical discussion of the periodic orbit expansion method. This is usually presented as follows (Gutzwiller 1971, Balian and Bloch 1972, 1974, Berry 1983). Consider the trace of the Green function,

$$R(E) = \mathrm{Tr}(E - \hat{H})^{-1} = \sum_m (E - E_m)^{-1} \tag{1}$$

whose poles $\{E_m\}$ are the exact quantal levels which we seek. By a purely formal semiclassical argument, this trace can be expressed as a sum of terms labelled by the classical periodic orbits γ of $H(q, p)$ having the energy E.

Here we assume that all those periodic orbits are isolated; then the expansion consists of an important contribution $R_0(E)$ from the null orbits (Balian and Bloch

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1971a, b), which will however play no role in this discussion, and of a summation indexed by the distinct primitive (i.e. non-repeated) oriented periodic orbits γ,

$$R(E) \simeq R_0(E) + \sum_{\gamma} R_\gamma(E) \tag{2}$$

with $R_\gamma(E)$ itself subsuming all r-fold repetitions of the primitive orbit γ,

$$R_\gamma(E) = -\hbar^{-1} T \sum_{r=1}^{\infty} (\det(\mathbb{1} - P^r))^{-1/2} \exp[\mathrm{i}r(\hbar^{-1}S - \tfrac{1}{2}\nu\pi)]. \tag{3}$$

Here the following classical quantities are involved (being implicitly labelled by the orbit γ, which in turn depends smoothly upon E in some energy interval see Gutzwiller (1971)):

$$S = \oint_\gamma p\, \mathrm{d}q \qquad \text{(the classical Maupertuis action around } \gamma) \tag{4}$$

$$T = \partial S / \partial E \qquad \text{(the classical period of } \gamma) \tag{5}$$

$$\nu = \text{the number of conjugate points of } \gamma \tag{6}$$

(see Cushman (1978) for general formulae)

$$P = \text{the linearised Poincaré return map around } \gamma. \tag{7}$$

(This map P describes how an infinitesimally small transversal section across γ is mapped onto itself by the classical motion through one turn near and around γ. In two degrees of freedom, P is a 2×2 matrix having eigenvalues $\mathrm{e}^{\pm \mathrm{i}v}$ if the orbit γ is stable, where v is the stability angle of γ, or $\mathrm{e}^{\pm u}$ if the orbit is unstable, where $u > 0$ is the instability exponent of γ; as usual we exclude the exceptional eigenvalues ± 1.)

For a chaotic system with Lyapunov exponent $\omega > 0$, every (non-zero) periodic orbit γ is unstable and isolated, and satisfies

$$u_\gamma = \omega(E) T_\gamma. \tag{8}$$

It is instructive to follow the stable and unstable cases in parallel as far as possible, and for that purpose we make the identification $u \equiv \mathrm{i}v$.

The idea is now to find the poles in the terms $R_\gamma(E)$ of the right-hand side of equation (2), and to treat them as semiclassical eigenvalues (no poles arise from $R_0(E)$). This is accomplished through the successive transformations applied to equation (3):

$$R_\gamma(E) = -\mathrm{i}\hbar^{-1} T \sum_{r=1}^{\infty} \frac{\exp[\mathrm{i}r(\hbar^{-1}S - \frac{1}{2}\nu\pi)]}{2 \sinh \frac{1}{2} r u} \tag{9}$$

$$= -\mathrm{i}\hbar^{-1} T \sum_{r=1}^{\infty} \sum_{n=0}^{\infty} \exp[-r(n + \tfrac{1}{2})u] \exp[\mathrm{i}r(\hbar^{-1}S - \tfrac{1}{2}\nu\pi)] \tag{10}$$

$$= -\mathrm{i}\hbar^{-1} T \sum_{n=0}^{\infty} \{\exp[-\mathrm{i}(\hbar^{-1}S - \tfrac{1}{2}\nu\pi) + (n + \tfrac{1}{2})u] - 1\}^{-1}. \tag{11}$$

The final expression (11) exhibits poles for $R_\gamma(E)$ at the locations specified by the implicit equation (where N, n are non-negative integers)

$$S(E) = \oint_\gamma p\, \mathrm{d}q = [2\pi N - (n + \tfrac{1}{2})\mathrm{i}u + \tfrac{1}{2}\nu\pi]\hbar. \tag{12}$$

This treatment was developed by Gutzwiller (1971) (who used a simplified form of (12) with $n \equiv 0$). With the two quantum numbers present, equation (12) formally qualifies as a semiclassical quantisation condition in two degrees of freedom. However, the stable and unstable cases require sharply different interpretations from now on.

In the stable case where $-\mathrm{i}u = v$ is real, equation (12) yields a sequence of real levels indexed by two quantum numbers N, n. The complete formula (12) in the stable case, with a general expression for the index ν, was obtained in 1974 as a limiting case of the better understood torus quantisation (Voros 1975, 1976), then rederived independently using Gutzwiller's formalism (Dashen *et al* 1974, Miller 1975). It is also proven in many cases that the levels approximated by equation (12) exist, corresponding to eigenfunctions which tend to concentrate upon the stable periodic orbit as $\hbar \to 0$ (see, for instance, Ralston 1976, Colin de Verdière 1977). Consequently, it is correct to view equation (12) as the Bohr–Sommerfeld quantisation formula arising from a stable periodic orbit. (Its range of approximate validity is N large and n small; see Voros (1975).)

In the unstable case, all naive interpretations of equation (12) as a quantisation condition fail. With $u > 0$, all the poles given by equation (12) are now complex, hence none qualifies as an eigenvalue, be it approximate. The poles cannot describe resonances either, since none of these exist in a bound system (this interpretation is correct, however, for certain scattering systems; see Ikawa (1983), Gérard and Sjöstrand (1987)). Still, a complex pole lying very close to the real axis (in comparison with the true level spacing), could correspond approximately to an energy level by giving a sharp bump in the level density. This may happen where the level spacing is largest (typically at low energy), and for those poles which are produced by the shortest and least unstable orbits, as observed by Gutzwiller (1971) in the anisotropic Kepler problem. At a slightly higher energy, however, not only the true level spacing decreases below the width of any bump, prohibiting level discrimination, but worse, the poles from all unstable orbits γ in equations (2) and (3) start to proliferate exponentially (like the periodic orbits for an Anosov system; see Alexeev and Yakobson (1981), Hannay and Ozorio de Almeida (1984)), forming a set so dense that we cannot expect the periodic orbit sum to exhibit isolated bumps any longer.

Hence equation (12) may quantise some levels approximately at best in a restricted low-density region, in total contradiction with its putative semiclassical nature.

Thus we see no satisfactory theoretical interpretation of equation (12) as a quantisation condition in the unstable case.

This then suggests that it is the derivation of the periodic orbit expansion itself which requires a re-examination; its formal character, commonly accepted in the literature, may prove critically unsatisfactory in the unstable case.

Without putting the theory on a rigorous basis (a desirable but remote goal), we can suggest one improvement which results in a consistent interpretation of equation (12) in the unstable case.

Specifically, we designate the following as a critical feature of the periodic orbit expansion (2), which offsets its formal elegance and universality: its terms, and the symbol $\simeq$ in between, have a loose mathematical meaning. It may thus happen that the poles on one side seem totally unrelated to the poles on the other side. We claim that (i) this in fact will be the normal situation in the chaotic case; and (ii) nevertheless, an affirmative interpretation of equation (12) is possible.

At first, the problem and our answer will be more visible on the special example of free motion on a compact Riemannian surface of constant negative curvature (-1)

(reviewed by Balazs and Voros 1986). The quantum Hamiltonian is $\hat{H} = -\Delta - \frac{1}{4}$ (with Δ the Laplace-Beltrami operator); the classical Hamiltonian is $H = \|p\|^2$ and induces the geodesic flow, which is an Anosov flow on each energy surface, with Lyapunov exponent $\omega = 2E^{1/2}$. In this case, a special form of the periodic orbit sum is known to be exact (Colin de Verdière 1973, Gutzwiller 1980), being given by the Selberg trace formula (Selberg 1956, Balazs and Voros 1986, § VII):

$$\sum_m \left(\frac{1}{E - E_m} + \frac{1}{E_m}\right) = \text{constant} + \frac{\text{area}}{2\pi}\left(\frac{\Gamma'}{\Gamma}\right)(\tfrac{1}{2} + \sqrt{-E})$$
$$- \sum_\gamma \sum_{n=1}^{\infty} \frac{L_\gamma}{2\sinh\frac{1}{2}nL_\gamma} \frac{\exp(-nL_\gamma\sqrt{-E})}{2\sqrt{-E}} \tag{13}$$

where L_γ is the length of γ; the right-hand sum only converges for $\sqrt{-E} > \frac{1}{2}$. Indeed, if we substitute into equation (9) the appropriate parameter values (using $\|\dot{q}\| = 2\|p\| = 2E^{1/2}$),

$$S_\gamma = \oint_\gamma p\dot{q}\,\mathrm{d}t = E^{1/2}L_\gamma \qquad T_\gamma = L_\gamma/(2E^{1/2}) \qquad u_\gamma = \omega T_\gamma = L_\gamma \qquad \nu_\gamma = 0 \tag{14}$$

(and $\hbar = 1$), we find precisely the contribution of γ in equation (13).

Being a rigorous and exact version of the periodic orbit sum in the unstable case, the Selberg trace formula should reveal unambiguously the meaning of the 'Bohr-Sommerfeld rule' (12). We first switch from equation (13) to the determinant product formula (Sarnak 1987, Voros 1986, 1987b)

$$\det(\hat{H} - E) = \mathscr{D}(E)^{-1}\mathscr{Z}(\tfrac{1}{2} + \sqrt{-E}) \tag{15}$$

of which the trace formula is the logarithmic derivative in E. Namely, $\det(\hat{H} - E)$ is the functional determinant of the quantum Hamiltonian,

$$\det(\hat{H} - E) = \exp(\alpha E + \beta) \prod_{m=0}^{\infty} (1 - E/E_m)\exp(E/E_m). \tag{16}$$

The values of the constants α and β (Voros 1987b) are unimportant here since only the eigenvalue condition $\det(\hat{H} - E) = 0$ will matter; likewise, $\mathscr{D}(E)$ is a 'trivial' factor (i.e. it has explicitly known zeros, all at irrelevant locations); and finally, $\mathscr{Z}(s)$ is the Selberg zeta function (Selberg 1956), which expresses the contribution of all (isolated, primitive) periodic geodesics as an Euler infinite product,

$$\mathscr{Z}(s) = \prod_\gamma \left[\prod_{n=0}^{\infty} (1 - \mathcal{N}_\gamma^{-s-n})\right] \qquad \text{with } \mathcal{N}_\gamma = \mathrm{e}^{L_\gamma},\ s = \tfrac{1}{2} + \sqrt{-E}. \tag{17}$$

It is then obvious that the 'quantisation' condition (12), with its parameters specified by equation (14), is perfectly legitimate as giving the enumeration of the zeros of the factors of $\mathscr{Z}(\frac{1}{2} + \sqrt{-E})$ in equation (17).

If the product $\mathscr{Z}(\frac{1}{2} + \sqrt{-E})$ vanished at the zeros of its factors, then so would $\det(\hat{H} - E)$ (because the zeros of $\mathscr{D}(E)$ in equation (15) lie manifestly elsewhere); consequently, the roots of equation (12) would be eigenvalues of $\hat{H}$, but complex ones! This is precisely the paradox to be understood.

Now, the chaotic nature of the classical system is what explains the fallacy of this 'derivation'. As equation (17) constitutes an infinite product, its convergence domain must be specified, and this is only the half-plane $\mathrm{Re}(s) > 1$, precisely because of the exponential proliferation of periodic orbits γ with respect to their lengths L_γ. Now it so happens that both the true zeros of $\mathscr{Z}(s)$, and the zeros of its factors (which we may call the pseudo-zeros of $\mathscr{Z}(s)$), lie inside the complementary region $\mathrm{Re}(s) \leqslant 1$. In this region the true zeros and the pseudo-zeros need not be related to one another, and in fact they are not. (While the process of analytical continuation of equation (17) does establish some form of connection, it is so implicit that we cannot describe it constructively—in any case it provides at best a global relation between the totality of zeros and the totality of pseudo-zeros.)

Still, enumeration of the pseudo-zeros of $\mathscr{Z}(s)$ by equation (12) has one affirmative meaning: it does specify factor by factor the Eulerian expansion (17) of $\mathscr{Z}(s)$. In this way it reveals that the quantum determinant $\det(\hat{H} - E)$, initially defined by a Weierstrass (or Hadamard) infinite product, equation (16), admits in fact a second factorisation, of Euler type this time, arising from equations (15) and (17). Whilst the Hadamard product involves the quantum eigenvalues, the Euler product involves only classical ingredients, revealing its semiclassical nature. The restricted domain of convergence of the Eulerian product however precludes its use to locate its individual zeros (the eigenvalues) in any simple way.

It is well known that the two factorisations of the Selberg zeta function exhibit some striking similarities with those of the Riemann zeta function $\zeta(s)$ (Selberg 1956, Hejhal 1976, Berry 1986). In the latter case, the true zeros are the famous ones of $\zeta(s)$, while the pseudo-zeros involve the logarithms of the prime numbers in place of the primitive periodic orbit lengths. The difficulty to locate the true zeros in the critical strip $0 < \mathrm{Re}\, s < 1$, starting from the Euler product in $\mathrm{Re}\, s < 1$, is well known for both functions (it can also be ascribed to the instability of the analytical continuation process with respect to initial conditions in $\mathrm{Re}\, s > 1$). Berry (1986) has observed that suitably truncated Euler products can nevertheless mimic very accurately the low-lying zeros of $\zeta(s)$; this property reminds one of the approximation of a few low-lying eigenvalues using equation (12), and likewise it needs further quantitative understanding.

Our discussion thus brings no new results on the Selberg zeta function, but it stresses the new nature of the Bohr–Sommerfeld formulae in this context: while they no longer quantise the levels, they should not be discarded because they express the factors of an Euler product decomposition.

The qualitative extension of this exact result to other systems with isolated periodic orbits is immediate. In fact, equations (2) and (11) arise by formally taking to leading order in $\hbar$, the logarithmic derivative of

$$\prod_m (E_m - E) \simeq \prod_\gamma \left(\prod_{n=0}^{\infty} (1 - \exp\{\mathrm{i}[\hbar^{-1} S - \tfrac{1}{2}\nu\pi - (n + \tfrac{1}{2})\mathrm{i}u]\}) \right). \tag{18}$$

This again expresses a property of double factorisation for the determinant of the Schrödinger operator. However, the sign $\simeq$ now implies at least four distinct deviations from rigorous equality:

(i) some regularisation of the determinant on the left-hand side, as before (e.g. Weierstrass or zeta regularisation, both being routine operations);

(ii) the delimitation of the region of convergence D of the right-hand side in the complex-E plane; this domain may just reach the real axis (carrying the exact eigenvalues) in the stable case but not in the unstable case, where actions proliferate exponentially, according to Hannay and Ozorio de Almeida (1974));

(iii) some proportionality factor has to be inserted, its zeros and poles being, however, genuinely unrelated to the eigenvalues $\{E_m\}$ (this factor has to do with the null orbit term in equation (2)).

All three features were already present in the previous example where the periodic orbit sum was rigorously exact, but in general a fourth limitation must be added:

(iv) the relation (18) only holds semiclassically, i.e. in some asymptotic sense (which remains to be qualified) as $\hbar \to 0$. However, we conjecture the existence of an exact identity like (18) where each factor on the right-hand side would include quantal corrections.

Finally, we show that the same double factorisation property is also implied, albeit trivially, by the periodic orbit sum for a one-dimensional, and hence integrable system. In one dimension, the analogue of equation (3) is

$$\sum_m (E-E_m)^{-1} \simeq -\mathrm{i}\hbar^{-1} T \sum_{r=1}^{\infty} \exp[\mathrm{i}r(\hbar^{-1}S - \tfrac{1}{2}\nu\pi)] \tag{19}$$

which is the logarithmic derivative of the relation

$$\prod_m (E_m - E) \simeq \{1-\exp[\mathrm{i}(\hbar^{-1}S - \tfrac{1}{2}\nu\pi)]\}. \tag{20}$$

Here the right-hand side can be viewed as an Euler product with a single factor; its zeros are now the standard Bohr-Sommerfeld eigenvalues, the solutions of

$$S = \oint_\gamma p\,\mathrm{d}q = (2m\pi + \tfrac{1}{2}\nu\pi)\hbar \qquad (m = 0, 1, 2, \ldots) \tag{21}$$

and now they are genuine semiclassical approximations to the eigenvalues E_m. Indeed, the domain of validity of equation (20) may now reach the real energies. Otherwise, the relation (20) is meant in the same loose sense as equation (18) (see points (i), (iii) and (iv) above).

For the harmonic oscillator with eigenvalues $(2m+1)\hbar$, equation (20) corresponds to the exact formula (with γ being Euler's constant)

$$\begin{aligned}\prod_{m=0}^{\infty} & (1-E/(2m+1)\hbar)\exp[E/(2m+1)\hbar] \\ &= \tfrac{1}{2}\pi^{-1/2}\exp\{[\log 2 + \tfrac{1}{2}(\gamma - \mathrm{i}\pi)]\hbar^{-1}E\}\Gamma[\tfrac{1}{2}(1+\hbar^{-1}E)] \\ &\quad \times \{1-\exp[\mathrm{i}(\hbar^{-1}\pi E - \pi)]\}.\end{aligned} \tag{22}$$

In the case of an integrable system with more than one degree of freedom, a formula like equation (20) might still hold for the determinants of those quantal observables which become separable in action-angle coordinates, but not for the Hamiltonian itself in general because the corresponding periodic orbit expansion (Berry and Tabor 1976, equation (21)) cannot be resummed in the same way as here. (Moreover, it also exhibits false singularities; see Keating and Berry (1987).)

Factorised forms of the periodic orbit expansion already appear in the works of Gutzwiller (1979, 1982, 1987) on the anisotropic Kepler problem (AKP) and Berry (1986), but in a very different perspective. Both authors aim at alternative, i.e. resummed forms of that expansion which remain convergent at real energies, thereby yielding bona fide quantisation rules. This is an analytical continuation process, and they attempt it upon infinite product forms of the expansion. For any such analytical continuation to be effective, it requires an input of information about certain fine details of the asymptotic distribution of actions for the very large periodic orbits. Specifically, Berry (1986) suggests that the Riemann-Siegel formula can be generalised from the case of $\zeta(s)$. Gutzwiller (1982) replaces the unknown distribution of actions for the AKP by an ansatz, the energy distribution of an Ising chain; his new sum, although quite different from the original periodic sum in some respects, does yield after analytical continuation some very accurate (yet not exactly real) eigenvalues. Only an effective resummation method can achieve such results, but it is as yet unclear to us whether any such procedure can be implemented in general.

By contrast, our approach deals with the periodic orbit expansion as it stands (not resummed). This viewpoint is consistent with the idea that those details of the asymptotic distribution of large periodic orbit actions, which control the analytical continuation of equation (18), may not be available in general (this is even now the case for the distribution of prime numbers, whose details are inferred from the assumed locations of the zeros of $\zeta(s)$, instead of the converse). This ignorance then precludes our extraction of a quantisation formula from equation (18). Even with the advent of powerful resummation methods, this should persist to some extent because two problems are likely to remain unsolved. First, the quantal corrections, however small in the domain of convergence, may grow under the analytical continuation process so much as to make the approximation (18) useless at real, finite energies. Second, the semiclassical regime ($E \to \infty$ or $\hbar \to 0$) requires any asymptotic eigenvalue formula to become increasingly accurate, which in turn requires an infinitely detailed knowledge of the distribution of large actions in the periodic orbit sum. Consequently, we believe that for a general chaotic system there cannot exist a semiclassical quantisation condition more explicit than the specification of the quantised Hamiltonian itself.

In conclusion, we have verified in two extreme cases (Anosov as opposed to one-dimensional systems) that the Bohr-Sommerfeld formula for isolated periodic orbits expresses the property of double factorisation (Hadamard and Euler) for the functional determinant $\Pi_m (E_m - E)$. The defining Hadamard factorisation is exact; the Euler factorisation holds at least semiclassically, being then specified by the generalised Bohr-Sommerfeld quantisation conditions. (We also hope that a system with non-isolated periodic orbits can exhibit a double factorisation property for some determinant). We finally surmise that in the chaotic case the factorisation formula cannot be turned into a semiclassical quantisation condition.

Traditionally, Eulerian infinite products are supposed to reflect the arithmetical properties of those special analytic functions which occur in number theory. The standard example of double factorisation is indeed given by the Riemann zeta function, with its well known Euler and Hadamard product decompositions. Our result suggests that this property of double factorisation will also arise in connection with the spectral theory of quantum Hamiltonian operators; it would then be a more general phenomenon, not being subject to restrictions of an arithmetical nature.

Acknowledgments

We are grateful to M V Berry, B Eckhardt, M C Gutzwiller and the referees for useful suggestions during the revision of this paper.

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