Entire Fredholm Determinants for Evaluation of Semiclassical and Thermodynamical Spectra

Predrag Cvitanović and Gábor Vattay*
Niels Bohr Institute, Blegdamsvej 17, DK-2100 Copenhagen Ø, Denmark
(Received 30 June 1993)

Proofs that Fredholm determinants of transfer operators for hyperbolic flows are entire can be extended to a large new class of multiplicative evolution operators. We construct such operators both for the Gutzwiller semiclassical quantum mechanics and for classical thermodynamic formalism, and introduce a new functional determinant which is expected to be entire for Axiom A flows, and whose zeros coincide with the zeros of the Gutzwiller-Voros zeta function.

PACS numbers: 05.45.+b, 03.20.+i, 03.65.Sq

It has been established recently [1–3] that the Gutzwiller-Voros zeta function [4] derived from the Gutzwiller semiclassical trace formula [5] is in general not an entire function. In this Letter we construct a new classical evolution operator (5) whose Fredholm determinant (9) is entire for the Axiom A flows, and whose spectrum contains the semiclassical Gutzwiller spectrum. Many physically realistic chaotic scattering systems [6,7] are of the Axiom A type, and for them the new determinant has better convergence properties than the Gutzwiller-Voros and Ruelle type zeta functions utilized previously [7,8].

The main idea, extending the dynamical system to the tangent space of the flow, is suggested by one of the standard numerical methods for evaluation of Lyapunov exponents [9]: Start at x_0 with an initial vector $\xi(0)$, and let the flow transport it to $\xi(t)$ along the trajectory $x(t) = f^t(x_0)$. The growth rate of this vector is multiplicative along the trajectory

$$\frac{|\xi(t+t')|}{|\xi(0)|} = \frac{|\xi(t+t')|}{|\xi(t)|}\frac{|\xi(t)|}{|\xi(0)|}, \qquad (1)$$

and can be represented by the trajectory of a "unit" vector $\mathbf{u}(t)$ multiplied by the factor $|\xi(t)|/|\xi(0)|$. For asymptotic times and for almost every initial $(x_0, \xi(0))$, this factor converges to the leading eigenvalue of the linearized stability matrix for the flow.

We implement this multiplicative evaluation of stability eigenvalues by adjoining [10] the d-dimensional transverse tangent space $\xi \in TU_x$, $\xi(x)\cdot\mathbf{v}(x) = 0$ to the $(d+1)$-dimensional dynamical evolution space $x \in U \subset \mathbf{R}^{d+1}$. The dynamics in the $(x,\xi) \in U \times TU_x$ space is governed by the system of equations of variations [11]:

$$\dot{x} = \mathbf{v}(x), \quad \dot{\xi} = \mathbf{D}\mathbf{v}(x)\xi.$$

Here $\mathbf{D}\mathbf{v}(x)$ is the transverse derivative matrix of the flow. We write the solution as

$$x(t) = f^t(x_0), \quad \xi(t) = \mathbf{J}^t(x_0)\cdot\xi_0, \qquad (2)$$

with the tangent space vector ξ transported by the transverse stability matrix $\mathbf{J}^t(x_0) = \partial x(t)/\partial x_0$. In order to determine the length of the vector ξ we introduce a *signed norm*, a differentiable scalar function $g(\xi)$ with the property $g(\Lambda\xi) = \Lambda g(\xi)$ for any number Λ. While in general such a norm is a space dependent function $g(\xi, x)$, we shall assume here for reasons of notational simplicity that g is a function of ξ only. An example is the function

$$g\begin{pmatrix}\xi_1\\ \xi_2\\ \cdots\\ \xi_d\end{pmatrix} = \xi_d.$$

Any vector $\xi \in TU_x$ can now be represented by the product $\xi = \Lambda\mathbf{u}$, where $\mathbf{u}$ is a "unit" vector in the sense that its signed norm is $g(\mathbf{u}) = 1$, and the factor

$$\Lambda^t(x_0, \mathbf{u}_0) = g(\xi(t)) = g(\mathbf{J}^t(x_0)\cdot\mathbf{u}_0) \qquad (3)$$

is the multiplicative "stretching" factor introduced in (1)

$$\Lambda^{t'+t}(x_0, \mathbf{u}_0) = \Lambda^{t'}(x(t), \mathbf{u}(t))\,\Lambda^t(x_0, \mathbf{u}_0).$$

The $\mathbf{u}$ evolution constrained to $ET_{g,x}$, the space of unit tangent vectors transverse to the flow $\mathbf{v}$, is given by rescaling of (2):

$$\mathbf{u}' = R^t(x, \mathbf{u}) = \frac{1}{\Lambda^t(x, \mathbf{u})}\mathbf{J}^t(x)\cdot\mathbf{u}. \qquad (4)$$

Equations (2), (3), and (4) enable us to define a *multiplicative* evolution operator on the extended space $U \times ET_{g,x}$,

$$\mathcal{L}^t(x', \mathbf{u}'; x, \mathbf{u}) = e^{h(x)}\delta(x' - f^t(x))\frac{\delta(\mathbf{u}' - R^t(x, \mathbf{u}))}{|\Lambda^t(x, \mathbf{u})|^{\beta-1}}, \qquad (5)$$

where h is a function additive along the trajectory, and β is a number. This should be contrasted to "thermodynamic" [12–14] operators of the form

$$\mathcal{L}^t(x', x) = e^{h(x)}\delta(x' - f^t(x))\frac{1}{|\Lambda^t(x)|^{\beta-1}},$$

with $\Lambda^t(x)$ an eigenvalue of $\mathbf{J}^t(x)$. Such operators are

0031-9007/93/71(25)/4138(4)$06.00

in general *not* multiplicative in two or more transverse dimensions, for the simple reason that the eigenvalues of successive stability matrices are in general not multiplicative:

$$\Lambda_{ab} \neq \Lambda_a \Lambda_b.$$

Here $\mathbf{J}_{ab} = \mathbf{J}_a \mathbf{J}_b$ is the stability matrix of the trajectory consisting of consecutive segments a and b, $\mathbf{J}_a$ and $\mathbf{J}_b$ are the stability matrices for these segments separately, and Λ's are their eigenvalues. In particular, this lack of multiplicative property for Λ's had until now frustrated attempts [15] to construct evolution operators whose spectrum contains the semiclassical Gutzwiller spectrum. (The Selberg zeta function [16] for geodesic flows on surfaces of constant negative curvature is an exception: Multiplicativity is guaranteed by the Bowen-Series map [17], which reduces the two-dimensional flow to a direct product of one-dimensional maps, and makes it possible to construct the associated transfer operators in terms of one variable [18].)

In order to derive the trace formula for the operator (5) we need to evaluate $\mathrm{Tr}\,\mathcal{L}^t = \int dx\, d\mathbf{u}\, \mathcal{L}^t(\mathbf{u}, x; \mathbf{u}, x)$. The $\int dx$ integral yields [19] a weighted sum over primitive periodic orbits p and their repetitions r:

$$\mathrm{Tr}\,\mathcal{L}^t = \sum_p T_p \sum_{r=1}^{\infty} \frac{e^{rh_p}\delta(t - rT_p)}{|\det(1 - \mathbf{J}_p^r)|} \Delta_{p,r},$$
$$\Delta_{p,r} = \int_g d\mathbf{u}\, \frac{\delta(\mathbf{u} - R^{T_p r}(x_p, \mathbf{u}))}{|\Lambda^{T_p r}(x_p, \mathbf{u})|^{\beta - 1}}, \qquad (6)$$

where $\mathbf{J}_p$ is the prime cycle p transverse stability matrix. As we shall see below, $\Delta_{p,r}$ is intrinsic to cycle p, and independent of any particular cycle point x_p.

We note next that if the trajectory $f^t(x)$ is periodic with period T, the tangent space contains d periodic solutions

$$\mathbf{e}_i(x(T + t)) = \mathbf{e}_i(x(t)), \quad i = 1, ..., d,$$

corresponding to the d unit eigenvectors $\{\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_d\}$ of the transverse stability matrix, with "stretching" factors (3) given by its eigenvalues

$$\mathbf{J}_p(x) \cdot \mathbf{e}_i(x) = \Lambda_{p,i}\, \mathbf{e}_i(x), \quad i = 1, ..., d.$$

The $\int d\mathbf{u}$ integral in (6) picks up contributions from these periodic solutions. In order to compute the stability of the ith eigendirection solution, it is convenient to expand the variation around the eigenvector $\mathbf{e}_i$ in the stability matrix eigenbasis $\delta\mathbf{u} = \sum \delta u_\ell \mathbf{e}_\ell$. The variation of the map (4) at a complete period $t = T$ is then given by

$$\delta R^T(\mathbf{e}_i) = \frac{\mathbf{J} \cdot \delta\mathbf{u}}{g(\mathbf{J} \cdot \mathbf{e}_i)} - \frac{\mathbf{J} \cdot \mathbf{e}_i}{g(\mathbf{J} \cdot \mathbf{e}_i)^2} \left(\frac{\partial g(\mathbf{e}_i)}{\partial \mathbf{u}} \cdot \mathbf{J} \cdot \delta\mathbf{u} \right)$$
$$= \sum_{k \neq i} \frac{\Lambda_{p,k}}{\Lambda_{p,i}} \left(\mathbf{e}_k - \mathbf{e}_i \frac{\partial g(\mathbf{e}_i)}{\partial u_k} \right) \delta u_k\,. \qquad (7)$$

The δu_i component does not contribute to this sum since $g(\mathbf{e}_i + du_i \mathbf{e}_i) = 1 + du_i$ implies $\partial g(\mathbf{e}_i)/\partial u_i = 1$. Indeed, infinitesimal variations $\delta\mathbf{u}$ must satisfy

$$g(\mathbf{u} + \delta\mathbf{u}) = g(\mathbf{u}) = 1 \quad \Longrightarrow \quad \sum_{\ell=1}^{d} \delta u_\ell \frac{\partial g(\mathbf{u})}{\partial u_\ell} = 0\,,$$

so the allowed variations are of the form

$$\delta\mathbf{u} = \sum_{k \neq i} \left(\mathbf{e}_k - \mathbf{e}_i \frac{\partial g(\mathbf{e}_i)}{\partial u_k} \right) c_k\,, \quad |c_k| \ll 1\,,$$

and in the neighborhood of the $\mathbf{e}_i$ eigenvector the $\int \mathbf{u}$ integral can be expressed as

$$\int_g d\mathbf{u} = \int \prod_{k \neq i} dc_k\,.$$

Inserting these variations into the $\int d\mathbf{u}$ integral we obtain

$$\int_g d\mathbf{u} \;\; \delta(\mathbf{e}_i + \delta\mathbf{u} - R^T(\mathbf{e}_i) - \delta R^T(\mathbf{e}_i) + \cdots)$$
$$= \int \prod_{k \neq i} dc_k\, \delta((1 - \Lambda_k/\Lambda_i)c_k + \cdots)$$
$$= \prod_{k \neq i} \frac{1}{|1 - \Lambda_k/\Lambda_i|}\,,$$

and the $\int d\mathbf{u}$ trace (6) becomes

$$\Delta_{p,r} = \sum_{i=1}^{d} \frac{1}{|\Lambda_{p,i}^r|^{\beta-1}} \prod_{k \neq i} \frac{1}{|1 - \Lambda_{p,k}^r/\Lambda_{p,i}^r|}\,. \qquad (8)$$

The corresponding Fredholm determinant is obtained by observing [19] that the Laplace transform of the trace

$$\mathrm{Tr}\,\mathcal{L}(s) = \int_{0_+}^{\infty} dt\, e^{st}\, \mathrm{Tr}\, \mathcal{L}(t)$$

is a logarithmic derivative $\mathrm{Tr}\,\mathcal{L}(s) = -\frac{d}{ds}\ln F(s)$ of the Fredholm determinant:

$$F(\beta, s) = \exp\left(-\sum_{p,r} \frac{e^{(h_p + sT_p)r}}{r\,|\det(1 - \mathbf{J}_p^r)|} \Delta_{p,r}(\beta) \right). \qquad (9)$$

This determinant is the central result of this paper. Its zeros correspond to the eigenvalues of the evolution operator (5), and can be evaluated by standard cycle expansion methods [3,20].

In the "thermodynamic" formalism [12–14] for classical chaotic systems β is a parameter which plays the role of "inverse temperature," and h_p is the integral of some weight function $h(x)$ evaluated along the prime periodic orbit p. The classical correlation spectra are given by $\beta = 1$ and $h_p = 0$. For two-dimensional Hamiltonian flows the Gutzwiller semiclassical quantization [5] corresponds to

$$\beta = 1/2, \quad h_p = iS_p/\hbar + i\nu_p\pi/2, \quad s = 0\,, \qquad (10)$$

where S_p is the action of the periodic orbit, and ν_p its Maslov index. The derivation of the Fredholm determinant (9) for semiclassical quantization of flows in dimensions higher than 2 follows closely the standard Van Vleck propagator derivation [5] and will be presented elsewhere [21].

The simplest application of (9) is to two-dimensional hyperbolic Hamiltonian flows. The stability eigenvalues are related by $\Lambda_1 = 1/\Lambda_2 = \Lambda$, and the Fredholm determinant is given by

$$F_\sigma(\beta, s) = \exp\left(-\sum_{p,r} \frac{\sigma_p^r}{r \mid \Lambda_p^r \mid} \frac{e^{r(h_p+sT_p)}}{(1-1/\Lambda_p^r)^2} \Delta_{p,r}(\beta)\right),$$

$$\Delta_{p,r}(\beta) = \frac{\mid \Lambda_p^r \mid^{-\beta+1}}{1-1/\Lambda_p^{2r}} + \frac{\mid \Lambda_p^r \mid^{\beta-3}}{1-1/\Lambda_p^{2r}}. \quad (11)$$

The extra multiplicative factor is set to the eigenvalue sign $\sigma = \Lambda/|\Lambda|$ for F_-, and to $\sigma = 1$ for F_+; this will be used below. The Gutzwiller-Voros zeta function corresponds to setting $\Delta_{p,r} = |\Lambda_p^r|^{1/2}(1 - 1/\Lambda_p^r)$, and the "quantum Fredholm determinant" [2] is obtained by setting $\Delta_{p,r} = |\Lambda_p^r|^{1/2}$ in (11).

The main virtue of the determinant (9) is that the theorem of Rugh [22], applicable to multiplicative evolution operators such as (5), implies that this determinant is entire for the Axiom A flows, i.e., free of poles in the entire complex s or complex energy plane. One consequence of this general result is that the cycle expansions of the new Fredholm determinant should converge faster than exponentially with the maximal cycle length truncation, in contrast to the more familiar Gutzwiller-Voros and Ruelle type zeta functions which converge exponentially. This was recently checked by detailed numerical studies [3] of the related quantum Fredholm determinant [2], as well as by direct checks [21] of (11).

Here we illustrate the effectiveness of the new determinant by one numerical example. The dynamical system tested is the Hamiltonian Hénon map $x_{k+1} = 1 - ax_k^2 - x_{k-1}$ at $a = 20$. This map can be interpreted as a normal-form approximation to the Poincaré section of an Axiom A repelling flow with complete binary Markov partition, such as the 3-disk repeller [3]. We assume that the flight time between collisions is constant, so the action of a cycle p is given by $S_p/\hbar = kn_p$, where $k = \sqrt{E}$ is the wave number, and pick as the Maslov phase $\nu_p = 2n_p$, corresponding to the A_1 representation of the 3-disk system. In this model a relatively high number of periodic orbits can be easily computed; in evaluating the zeros of the Gutzwiller-Voros zeta function, the quantum Fredholm determinant of Ref. [3], and the new Fredholm determinant (11) plotted in Fig. 1, cycle expansions were truncated to cycles up to period 18.

The dynamics (4) can be restricted to a u unit eigenvector neighborhood corresponding to the largest eigenvalue of the Jacobi matrix [21]. In this neighborhood the largest eigenvalue of the Jacobi matrix is the only fixed point, and the Fredholm determinant obtained by keeping only the largest term the $\Delta_{p,r}$ sum in (8) is also entire. This observation enables us to show that the Gutzwiller-Voros zeta function $Z(E)$ for Axiom A flows is meromorphic in the complex E plane, as it can be written as a ratio of entire functions; for two-dimensional Hamiltonian systems,

$$Z(E) = \frac{F_+(\frac{1}{2}, E) F_-(\frac{7}{2}, E)}{F_-(\frac{3}{2}, E) F_+(\frac{5}{2}, E)}, \quad (12)$$

where F_σ includes only the first term in the $\Delta_{p,r}$ sum (11). The zeros of the Gutzwiller-Voros zeta function coincide with the ones obtained from $F_+(\frac{1}{2}, E)$, and the leading poles arise from $F_-(\frac{3}{2}, E)$. Such relations [3] follow by inserting into $\Delta_{p,r}$ identities like

$$1 = \frac{1}{1-1/\Lambda^r} - \frac{1}{\Lambda^r}\frac{1}{1-1/\Lambda^r}$$

[σ weight in (11) is needed to account for the $1/\Lambda = \sigma/|\Lambda|$ term in the above indentity].

In conclusion, we have constructed a classical evo-

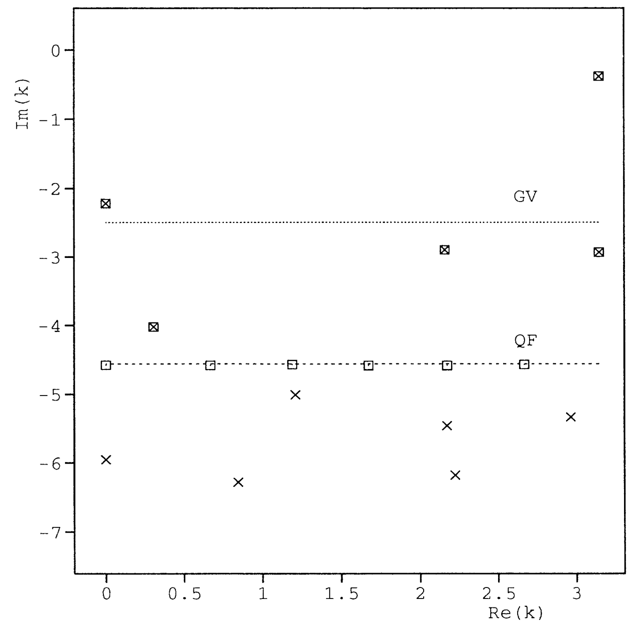

FIG. 1. The leading semiclassical resonances in the k complex wave-number plane ($\times$) for the determinant (9), compared with ($\Box$) the zeros of the "quantum Fredholm determinant" [2,3] for the Hénon map $x_{k+1} = 1 - 20x_k^2 - x_{k-1}$ model repeller flow. While the quantum Fredholm determinant has a finite region of analyticity [the bottom line of zeros reflects a pole expected at $\text{Im}(k) = -4.559843\ldots$, indicated by the dashed line labeled "QF"], the new determinant shows no numerical indication of any poles, and enables us to reach resonances deeper down in the complex plane. The Gutzwiller-Voros zeta function is reliable only down to the line labeled "GV," $\text{Im}(k) = -2.491905\ldots$, the upper bound on the poles of determinant $F_-(\frac{3}{2}, E)$ in (12).

lution operator for semiclassical quantization, and derived a new determinant for periodic orbit quantization of chaotic dynamical systems. We have checked numerically that the new determinant is analytic to the limit of numerical precision of current cycle expansions, and well beyond both the Gutzwiller-Voros zeta function and the quantum Fredholm determinant.

G.V. is indebted to D. Szász and A. Krámli for pointing out the importance of the Bunimovich-Sinai curvatures, to the Széchenyi Foundation and OTKA F4286 for support, and to the Center for Chaos and Turbulence Studies, Niels Bohr Institute, for hospitality. P.C. thanks the Carlsberg Fundation for support.

* On leave from Eötvös University, Budapest, Hungary.

[1] B. Eckhardt and G. Russberg, Phys. Rev. E **47**, 1578 (1993).
[2] P. Cvitanović and P.E. Rosenqvist, in *From Classical to Quantum Chaos, Societá Italiana di Fisica Conference Proceedings*, edited by G. F. Dell'Antonio, S. Fantoni, and V. R. Manfredi (Editrice Compositori, Bologna, 1993), Vol. 41, pp. 57–64.
[3] P. Cvitanović, P.E. Rosenqvist, H.H. Rugh, and G. Vattay, Chaos (to be published).
[4] A. Voros, J. Phys. A **21**, 685 (1988).
[5] M.C. Gutzwiller, *Chaos in Classical and Quantum Mechanics* (Springer, New York, 1990).
[6] P. Gaspard and S.A. Rice, J. Chem. Phys. **90**, 2225 (1989); **90**, 2242 (1989); **90**, 2255 (1989).
[7] P. Cvitanović and B. Eckhardt, Phys. Rev. Lett. **63**, 823 (1989).
[8] P. Gaspard and D. Alonso Ramirez, Phys. Rev. A **45**, 8383 (1992).
[9] G. Bennettin, L. Galgani, and J.-M. Strelcyn, Meccanica **15**, 9 (1980).
[10] A similar extension to the tangent space has been introduced by E. Gozzi, M. Reuter, and W.D. Thacker, Phys. Rev. D **40**, 3363 (1989), and other authors, but with rather different motives and applications in mind.
[11] V.I. Arnold, *Ordinary Differential Equations* (MIT Press, Cambridge, MA, 1978).
[12] D. Ruelle, *Statistical Mechanics, Thermodynamic Formalism* (Addison-Wesley, Reading, MA, 1978).
[13] T.C. Halsey, M.H. Jensen, L.P. Kadanoff, I. Procaccia, and B.I. Shraiman, Phys. Rev. A **33**, 1141 (1986).
[14] P. Szépfalusy, T. Tél, A. Csordás, and Z. Kovács, Phys. Rev. A **36**, 3525 (1987).
[15] Periodic Orbit Theory—theme issue, edited by P. Cvitanović, Chaos **2**, 1–158 (1992).
[16] A. Selberg, J. Ind. Math. Soc. **20**, 47 (1956).
[17] R. Bowen and C. Series, Publ. Math. Inst. Hautes Etud. Sci. **50**, 153 (1979).
[18] D. Mayer, Commun. Math. Phys. **130**, 311 (1990); in "From Phase Transitions to Chaos," edited by G. Györgyi *et al.* (to be published), pp. 521–529; E.B. Bogomolny and M. Caroli, Physica (Amsterdam) **67D**, 88 (1993).
[19] P. Cvitanović and B. Eckhardt, J. Phys. A **24**, L237 (1991).
[20] R. Artuso, E. Aurell, and P. Cvitanović, Nonlinearity **3**, 325 (1990).
[21] G. Vattay (to be published).
[22] H.H. Rugh, Nonlinearity **5**, 1237 (1992). See also Ref. [3] for a discussion of the applicability of the theorem.