Initial-value representation of the semiclassical zeta function

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This work casts the semiclassical zeta function in a form suitable for practical calculations of energy levels for rather general systems. To accomplish this, the zeta function is approximated by applying an initial-value representation (IVR) treatment to the traces of the transfer matrix that appear when the function is expanded in cumulants. Because this approach does not require searches for periodic orbits or special trajectories obeying double-ended boundary conditions, it is easily applicable to multidimensional systems with smooth potentials. Calculations are presented for the energy levels of three two-dimensional systems, including one that is classically integrable, one having mixed phase space, and one that is almost fully chaotic. The results show that the present treatment is far more numerically efficient than a previously proposed IVR method for the zeta function [Barak and Kay, Phys. Rev. E **88**, 062926 (2013)]. The approach described here successfully resolves nearly all energy levels in the range investigated for the first two systems as well as energy levels in spectral regions that are not too highly congested for the highly chaotic system.

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I. INTRODUCTION

The semiclassical zeta function is one of the most successful tools for the semiclassical estimation of the quantum energy levels of bound, chaotic systems. In this paper we develop an approximation to this function that allows its practical calculation for rather general systems, including those with many degrees of freedom and smooth potentials.

Historically, theories of the semiclassical zeta function [1–5] were developed in the context of Gutzwiller's [6,7] semiclassical treatment of the trace of Green's function for classically chaotic systems. This trace, given quantum mechanically by $g(E) = \mathrm{Tr}(E^+ - H)^{-1} = \sum_n (E^+ - E_n)^{-1}$ for a bound system, has poles at real values of E that correspond to energy levels E_n. To develop a semiclassical approximation for such levels of a chaotic system, Gutzwiller derived a semiclassical expression for $g(E)$ as an infinite sum over classical periodic orbits. However, straightforward application of this treatment encountered problems because Gutzwiller's formula does not converge absolutely for real E [8]. The source of this difficulty is the exponential proliferation of periodic orbits with increasing length for chaotic systems. Although this problem could be partly circumvented by analytically continuing the trace formula to complex E, or otherwise damping the contributions of long orbits in $g(E)$ [9,10], these methods limit the resolution of the spectral levels, preventing estimation of quantum energies when the level density is high.

A better solution to the convergence problem was found by formulating the eigenvalue determination in terms of the semiclassical zeta function $\zeta^{-1}(E)$. This function can be expressed in the form $\exp[i\pi\bar{N}(E)]D(E)$, where $D(E)$ is a semiclassical approximation to the spectral determinant, $\det(E - H) = \prod_n (E - E_n)$, and $\bar{N}(E)$ is the mean level staircase function. Thus, like $D(E)$, the zeta function has (approximate) zeros at the quantum energy levels $E = E_n$. An explicit expression for the zeta function can be obtained by substituting Gutzwiller's formula for $g(E)$ in the relation $D(E) = \exp[\int^E g(E')dE']$. The result can be written as $\prod \exp(F)$ where the product is over primitive periodic orbits and F can be expressed in terms of actions and monodromy matrices for repetitions of such orbits. Although this formula for the zeta function is still not absolutely convergent, it can be effectively resummed to yield a cycle expansion [2–4,11] that groups together long periodic orbits with combinations of shorter orbits of the same total length. Such an expansion converges because contributions of long orbits are largely canceled by those arising from the combinations of shorter orbits. This convergence allows determination of energy eigenvalues even for dense portions of the energy spectrum where the damped versions of Gutzwiller's formula fail.

Despite the importance of the cycle expansion, its application is limited. Use of the expansion for a chaotic system requires the determination and enumeration of all orbits with periods up to a certain maximum length. Such a calculation requires a numerical search that is generally not feasible for systems with more than two degrees of freedom. Apart from this practical matter, the cycle expansion is appropriate only for systems whose periodic orbits are all isolated, e.g., fully chaotic systems. It cannot be used for systems that are integrable or, more importantly, generic systems with mixed chaotic and regular phase space regions. It is, therefore, desirable to develop a numerically useful semiclassical treatment of the zeta function that is free from such limitations.

We note that the effective restrictions of the cycle expansion to small chaotic systems are also shared by Gutzwiller's formula for the trace $g(E)$. In a previous publication [12], these problems were overcome for $g(E)$ by developing a semiclassical initial-value representation (IVR) treatment of this function. The possibility of solving analogous problems for the zeta function motivates the present development of an IVR approximation for $\zeta^{-1}(E)$.

An IVR treatment [13–16] is a semiclassical approximation to a desired quantity as an integral over phase space variables that serve as initial conditions for classical trajectories. Such a treatment does not require a search for special trajectories

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obeying double-ended boundary conditions or periodic orbits, and is therefore suitable for large systems. Additionally, previously developed IVR approximations have been found to be equally applicable to chaotic and nonchaotic systems. In several cases, IVR expressions can be demonstrated to provide uniform semiclassical approximations [16–19] and, thus, to be more accurate than conventional semiclassical formulas that are expressed explicitly in terms of special trajectories.

IVR treatments have previously been developed for the time-dependent propagator [15–17], the time-independent wave function [18,20], the S matrix [21,22], the Green's function [19], and its trace [12]. Recently, and most relevant to the present work, a particular kind of IVR approximation was also proposed for the zeta function [23]. That treatment was based on Bogomolny's [24,25] representation of the zeta function as a Fredholm determinant $\det(\mathbf{1}-\mathbf{T}_E)$, involving the so-called transfer matrix $\mathbf{T}_E$. Bogomolny derived a semiclassical approximation that expresses elements of this matrix in terms of classical trajectories that begin at a specified position on a Poincaré surface of section (PSS) and return to another specified position upon their first crossing of this surface in the initial direction. In the IVR treatment of Ref. [23] this matrix was more conveniently formulated as an integral over points on the PSS that serve as initial conditions for classical trajectories that may end up anywhere on the surface.

With this approach, the quantization condition $\det(\mathbf{1}-\mathbf{T}_E)=0$ was applied to obtain energy eigenvalues for an integrable and a highly chaotic system with a smooth potentials. The IVR treatment was found to resolve and provide good approximations for all eigenvalues in the ranges investigated.

Despite these favorable properties, the IVR treatment of Ref. [23] suffers from some disadvantages that are shared by other numerical treatments which are based directly on the expression of the zeta function as $\det(\mathbf{1}-\mathbf{T}_E)$ [26]. First, the technique is numerically inefficient because determination of each energy level satisfying the quantization condition requires repeated evaluation of the determinant $\det(\mathbf{1}-\mathbf{T}_E)$, or diagonalization of the matrix $\mathbf{T}_E$, for several values of E near the quantum value. Since the dimension of $\mathbf{T}_E$ is necessarily large for systems with many degrees of freedom or high energies, such calculations can be very numerically intensive and time-consuming, especially when several levels need to be determined. Second, more as a matter of principle, the reliance on the diagonalization or the calculation of determinants for large matrices suggests that the approach should be classified as a hybrid quantum-semiclassical method, rather than a purely semiclassical treatment.

In the present work we develop a more numerically efficient, "purely semiclassical," IVR treatment of the zeta function that avoids explicit calculation or manipulation of large matrices. Like the former method, the present approach is equally applicable to chaotic and nonchaotic systems but, in contrast to that treatment, it scales favorably with system size, making it more suitable for systems with several degrees of freedom. To proceed, we express $\zeta^{-1}(E)$ in terms of the scalar quantities $\mathrm{Tr}(\mathbf{T}_E^n)$, $n=1,2,\ldots$ by means of a cumulant expansion of $\det(\mathbf{1}-\mathbf{T}_E)$. We then express each such trace in an IVR form involving trajectories which return to the PSS n times in the initial normal direction. Finally, we determine semiclassical energy levels as values of E that minimize the resulting approximation to $|\zeta^{-1}(E)|$. We test the method with calculations for three systems, including one that is completely integrable, one that is highly chaotic, and one that is intermediate in nature, having mixed regular and chaotic portions of phase space.

Section II presents our treatment more fully and derives the requisite IVR formulas. Section III describes the systems treated and numerical details of the test calculations. Section IV reports the results of the computations and Sec. V summarizes this work and presents concluding remarks.

II. IVR TREATMENT OF THE ZETA FUNCTION AND ITS CUMULANT EXPANSION

A. Bogomolny's expression of $\zeta^{-1}(E)$ as a Fredholm determinant

To develop our treatment of the zeta function, we recall Bogomolny's formula [24,25]

$$\zeta^{-1}(E)=\det(\mathbf{1}-\mathbf{T}_E), \tag{1}$$

which expresses the zeta function in terms of a Fredholm determinant involving the transfer matrix $\mathbf{T}_E$. The quantum energy levels are, thus, values of E which satisfy the condition

$$\det(\mathbf{1}-\mathbf{T}_E)=0. \tag{2}$$

Each element $T_E(\mathbf{q}',\mathbf{q})$ of the transfer matrix plays the role of a semiclassical propagator that evolves a point on a PSS at position $\mathbf{q}$ to a new point on this surface at position $\mathbf{q}'$. It can be regarded a the semiclassical analog of the Poincaré mapping that carries a point on the PSS to one that classically evolves from it as it crosses the PSS for the first time in the initial normal direction.

Bogomolny [24,25] derived a semiclassical formula for such matrix elements which, for a system with f degrees of freedom, reads

$$T_E(\mathbf{q}',\mathbf{q})=\left(\frac{1}{2\pi i\hbar}\right)^{(f-1)/2}\sum_{\substack{\text{classical}\\ \text{traj}}}\left|\det\left[\frac{\partial^2 W_E(\mathbf{q}',\mathbf{q})}{\partial\mathbf{q}'\partial\mathbf{q}}\right]\right|^{\frac{1}{2}} \times\exp[iW_E(\mathbf{q}',\mathbf{q})/\hbar-i\nu\pi/2]. \tag{3}$$

The sum is over classical trajectories with energy E that connect points $\mathbf{q}$ and $\mathbf{q}'$ after a single crossing of the PSS in the initial direction, corresponding to an application of the Poincaré map. The quantity

$$W_E(\mathbf{q}',\mathbf{q})=\int_{\mathbf{q}}^{\mathbf{q}'}\mathbf{p}(\mathbf{x})^T d\mathbf{x} \tag{4}$$

is the reduced action calculated along such a trajectory and ν is the Maslov index.

A key property of the transfer matrix is that elements

$$T_E^n(\mathbf{q}',\mathbf{q})=\int T_E(\mathbf{q}',\mathbf{q}_{n-1})\cdots T_E(\mathbf{q}_2,\mathbf{q}_1)\,T_E(\mathbf{q}_1,\mathbf{q})d\mathbf{q}_1 d\mathbf{q}_2\cdots d\mathbf{q}_{n-1}, \tag{5}$$

of the matrix $\mathbf{T}_E^n\equiv(\mathbf{T}_E)^n$ are again given semiclassically by Eq. (3) for $T_E(\mathbf{q}',\mathbf{q})$, with the provision that the sum is taken over classical trajectories that connect points $\mathbf{q}$ and $\mathbf{q}'$ after n

crossings of the PSS in the initial direction. Such trajectories are associated with the nth iteration of the Poincaré map.

B. Cumulant expansion of the zeta function

To cast the zeta function in a form suitable for the desired IVR treatment, we apply the identity $\det(\mathbf{A}) = \exp[\mathrm{Tr}\ln\mathbf{A}]$ to the determinant in Eq. (1) and formally expand $\log(\mathbf{1}-\mathbf{T}_E)$ in a Taylor series to obtain

$$\zeta^{-1}(E) = \exp\left[-\sum_{n=1}^{\infty}\frac{1}{n}\,\mathrm{Tr}\,\mathbf{T}_E^n\right]. \tag{6}$$

Further expansion of the exponential function in a Taylor series and rearrangement of terms yields a cumulant expansion whose first terms are given by [11,27]

$$\begin{aligned}\zeta^{-1}(E) = {} & 1 - \mathrm{Tr}\,\mathbf{T}_E - \tfrac{1}{2}\left[\mathrm{Tr}\,\mathbf{T}_E^2 - (\mathrm{Tr}\,\mathbf{T}_E)^2\right] \\ & - \tfrac{1}{3}\left[\mathrm{Tr}\,\mathbf{T}_E^3 - \tfrac{3}{2}\,\mathrm{Tr}\,\mathbf{T}_E^2\ \mathrm{Tr}\,\mathbf{T}_E + \tfrac{1}{2}(\mathrm{Tr}\,\mathbf{T}_E)^3\right]\cdots.\end{aligned} \tag{7}$$

The general form of this expansion can be written as

$$\zeta^{-1}(E) = \sum_{m=0}^{\infty} c_m(E), \tag{8}$$

where the cumulant (or curvature) terms, c_m, are given by the recursion formula

$$c_m = -\frac{1}{m}\sum_{j=0}^{m-1}\mathrm{Tr}\,\mathbf{T}_E^{m-j}c_j, \tag{9}$$

with $c_0 = 1$. Equivalently, these results can be obtained directly by applying the Plemelj-Smithies formula [28] to the determinant $\det(\mathbf{1}-\mathbf{T}_E)$ in Eq. (1).

In contrast to Gutzwiller's trace formula for the Green's function, the cumulant expansion converges absolutely for a chaotic system. Therefore, the energy eigenvalues of a system can be obtained from the zeros of Eq. (8), with the sum calculated to a sufficiently high order. This advantageous property results from cancellations that occur in each curvature term between contributions from long periodic orbits and combinations of shorter ones that shadow them. Substitution of Bogomolny's formula for the transfer matrix, Eq. (3), in Eqs. (8) and (9), provides an alternative route to the derivation of the cycle expansion for chaotic systems.

C. IVR formula for the traces of $\mathbf{T}_E^n$

Our treatment requires development of an IVR formula for the traces appearing in Eqs. (8) and (9). To accomplish this, we make use of an IVR approximation

$$\begin{aligned}T_E(\mathbf{q}',\mathbf{q}) = {} & \left(\frac{1}{2\pi\hbar}\right)^{f-1}\int d\mathbf{p}_y\int d\mathbf{y}\,(\mathbf{q}'|\mathbf{y}'\mathbf{p}_y') \\ & \times C\,e^{iW_E(\mathbf{y}',\mathbf{y})/\hbar}\,(\mathbf{y},\mathbf{p}_y|\mathbf{q}),\end{aligned} \tag{10}$$

for the elements of the transfer matrix that was presented in Ref. [23]. In this equation, $\mathbf{p}_y$ and $\mathbf{y}$ are momentum and position variables on the PSS that serve as initial conditions for classical trajectories and $\mathbf{p}_y'$ and $\mathbf{y}'$ are the corresponding variables marking the trajectories' first recrossing of the PSS in the initial normal direction. Quantities $(\mathbf{q}|\mathbf{y}\mathbf{p}_y)$ are unnormalized Gaussian coherent state functions on the PSS,

$$(\mathbf{q}|\mathbf{y},\mathbf{p}_y) = \exp\left(-(\mathbf{q}-\mathbf{y})^T\mathbf{\Gamma}(\mathbf{q}-\mathbf{y})/\hbar + i\mathbf{p}_y^T(\mathbf{q}-\mathbf{y})/\hbar\right), \tag{11}$$

where the $f-1$-dimensional matrix $\mathbf{\Gamma}$ is symmetric with a positive real part but is otherwise arbitrary. To simplify the current treatment (and unlike Ref. [23]), we use the same matrix $\mathbf{\Gamma}$ for both coherent state functions in Eq. (10). The prefactor C is given by

$$C = \left[\mathrm{sgn}(\dot{z}'\dot{z})\det\left(\frac{2\mathbf{\Gamma}}{\pi\hbar}\right)\det\left(\frac{\partial\boldsymbol{\zeta}'}{\partial\boldsymbol{\zeta}}\right)\right]^{1/2}, \tag{12}$$

where $\dot{z}$ and $\dot{z}'$ are the initial and final velocities normal to the PSS and the matrix $\partial\boldsymbol{\zeta}'/\partial\boldsymbol{\zeta}$ is given by

$$\frac{\partial\boldsymbol{\zeta}'}{\partial\boldsymbol{\zeta}} = \frac{1}{2}\frac{\partial\mathbf{p}_y'}{\partial\mathbf{p}_y} - i\mathbf{\Gamma}\frac{\partial\mathbf{y}'}{\partial\mathbf{p}_y} + \frac{i}{4}\frac{\partial\mathbf{p}_y'}{\partial\mathbf{y}}\mathbf{\Gamma}^{-1} + \frac{1}{2}\mathbf{\Gamma}\frac{\partial\mathbf{y}'}{\partial\mathbf{y}}\mathbf{\Gamma}^{-1}. \tag{13}$$

The partial derivatives (monodromy matrix elements) on the right-hand side of this equation are evaluated for fixed energy and position of the final PSS. The phase of the complex prefactor C is determined by the requirement that it be continuous with respect to time. It is, therefore, important to calculate the time-dependent analog of $\mathrm{sgn}(\dot{z}'\dot{z})\partial\boldsymbol{\zeta}'/\partial\boldsymbol{\zeta}$ along each trajectory so that phase of the square root appearing in Eq. (12) can be monitored and its continuity can be ensured.

Equation (10) was obtained in Ref. [23] by imposing the requirement that it reduce to Bogomolny's expression, Eq. (3), when the integrals are approximated by the stationary phase approximation. One consequence is that, like Eq. (3), the expression for $T_E(\mathbf{q}',\mathbf{q})$ appearing in Eq. (10) is also valid for $T_E^n(\mathbf{q}',\mathbf{q})$ if $\mathbf{y}'$ and $\mathbf{p}_y'$ are interpreted as the variables on the Poincaré surface at the nth return of the trajectory to the PSS in the initial direction.

Despite its derivation from Bogomolny's formula, the IVR and Bogomolny approximations are not equivalent, except in the classical limit. For example, the numerical results in Ref. [23] suggested that use of the IVR approximation, Eq. (10), to calculate energy eigenvalues via Eqs. (1) and (2), generally produced more accurate results for the chaotic system investigated than Bogomolny's theory.

Given the result in Eq. (10) it is simple to obtain an IVR expression for the traces needed in a calculation of the cumulant expansion. Indeed, integration over $\mathbf{q}' = \mathbf{q}$ immediately gives

$$\mathrm{Tr}\,\mathbf{T}_E^n = \left(\frac{1}{2\pi\hbar}\right)^{f-1}\int d\mathbf{p}_y\int d\mathbf{y}\,(\mathbf{y},\mathbf{p}_y|\mathbf{y}',\mathbf{p}_y')C\,e^{iW_E(\mathbf{y}',\mathbf{y})/\hbar}, \tag{14}$$

where the prime again denotes the nth intersection with the PSS in the initial normal direction. Energy levels can now be estimated by substituting this expression into the cumulant expansion and identifying the values of E that cause $|\zeta^{-1}(E)|$ to be near zero.

D. Symmetry-projected traces

For systems with high energy or many degrees of freedom, energy levels are dense and may be difficult to resolve completely using the treatment described above. This problem can be partially alleviated for systems with discrete symmetries by adapting the IVR approximation of the zeta function to specific irreducible representations (irreps) of the symmetry point group. The treatment is similar to that detailed in Ref. [12] for the analogous case of the trace of Green's function. The first step is to apply the projection operator for a particular irrep j to the final position variables in Eq. (10), to produce the symmetry-projected matrix element $\mathbf{T}_{E,j}$. The resulting IVR formula for this quantity was presented in Ref. [23]. Its immediate generalization to $\mathbf{T}^n_{E,j}$ is

$$T^n_{E,j}(\mathbf{q}',\mathbf{q}) = \left(\frac{1}{2\pi\hbar}\right)^{f-1} \sum_s \sum_{\sigma=\pm} \int d\mathbf{y} \int d\mathbf{p}_y \sum_R{}' a_j(R) \times (\mathbf{q}'|\mathbf{y}'_r\mathbf{p}'_{yr}) C^R e^{iW_E(\mathbf{y}'_r,\mathbf{y})/\hbar} (\mathbf{y},\mathbf{p}_y|\mathbf{q}). \quad (15)$$

This result is based on the following understandings [12,23]. The Poincaré surface used to initiate the trajectories is described by the condition $z = 0$, where z is one of the position variables, and the initial velocity normal to the PSS, $\dot{z}$, is taken to be positive. The symmetry operators $\hat{R}$ belonging to the system's point group are considered to act on the final coordinates $(z',\mathbf{q}')$. Of course, like z and $\dot{z}$, the primed variables obey $z' = 0$ and $\dot{z}' > 0$, but the symmetry operator $\hat{R}$ generally changes the condition defining the "final PSS" to $z'_r = \hat{R}z' = 0$ and changes the velocity normal to the PSS from $\dot{z}'$ to $\dot{z}'_r = \hat{R}\dot{z}_r$, which may be positive or negative. Additionally, the operator can be taken to apply to the dynamical variables along the surface $(\mathbf{y}',\mathbf{p}'_y)$ instead of $\mathbf{q}'$, transforming them to $(\mathbf{y}'_r,\mathbf{p}'_{yr}) = (\hat{R}\mathbf{y}',\hat{R}\mathbf{p}'_y)$ [12].

Thus, in Eq. (15), the summation over s is over the nth crossings of all Poincaré surfaces $z'_r = 0$ generated by applying operators $\hat{R}$ in the point group to the surface $z' = z = 0$, and the summation over σ is over the two possible signs of $\dot{z}'_r$ at the crossing. The summation over R is restricted to those symmetry operators that transform z' and $\dot{z}'$ to z'_r and $\dot{z}'_r$, respectively, with the specified s and σ. The coefficient $a_j(R)$ is defined as $d_j\chi_j(R)/|G|$, where d_j is the dimension of irrep j, $\chi_j(R)$ is the character of R in this irrep, and $|G|$ is the order of the group. Finally, the prefactor C^R in Eq. (15) is given by

$$C^R = [\mathrm{sgn}(\dot{z}'_r\dot{z})\det(2\mathbf{\Gamma}/\pi\hbar)\det(\partial\boldsymbol{\zeta}'_r/\partial\boldsymbol{\zeta})\det\mathbf{R}]^{1/2}, \quad (16)$$

where $\mathbf{R}$ is the f-dimensional matrix representing $\hat{R}$ in the basis of position variables $(z',\mathbf{q}')$, and $\partial\boldsymbol{\zeta}'_r/\partial\boldsymbol{\zeta}$ is as defined in Eq. (13) with $(\mathbf{y}',\mathbf{p}'_y)$ replaced by $(\mathbf{y}'_r,\mathbf{p}'_{yr})$.

Setting $\mathbf{q}'$ equal to $\mathbf{q}$ and integrating over this variable gives the desired IVR formula for the trace,

$$\mathrm{Tr}\,\mathbf{T}^n_{E,j} = \left(\frac{1}{2\pi\hbar}\right)^{f-1} \sum_s \sum_{\sigma=\pm} \int d\mathbf{y} \int d\mathbf{p}_y \sum_R{}' a_j(R) \times (\mathbf{y},\mathbf{p}_y|\mathbf{y}'_r\mathbf{p}'_{yr}) C^R e^{iW_E(\mathbf{y}'_r,\mathbf{y})/\hbar}. \quad (17)$$

This equation allows one to calculate the trace of the projected transfer operator by launching trajectories from an initial PSS and following them as they intersect, for the nth time, each Poincaré surface generated by applying the group symmetry operators to the initial surface. Each such intersection contributes to terms in the sums in Eq. (17) with particular values of s and σ and R. The R values for such contributions correspond to symmetry operators $\hat{R}$ that carry the final intersection surface to the initial PSS with positive transverse velocity. These operators must be identified in order to evaluate the factors appearing after $\sum'_R$ in Eq. (17).

III. CALCULATIONS

A. The system

As in previous publications [12,18,19,23,29], we test our IVR treatment with numerical calculations for the two-dimensional quartic oscillator system with the Hamiltonian [30–32]

$$H = \frac{1}{2}\left(p_x^2 + p_y^2\right) + \frac{\alpha}{2}(x^2y^2) + \frac{\beta}{4}(x^4 + y^4). \quad (18)$$

The parameters α and β in this expression can be adjusted to vary the classical dynamics of the system from almost fully chaotic ($\alpha > 0$, $\beta = 0$), to nonintegrable with mixed phase space ($\alpha > 0$, $\beta > 0$), to fully integrable ($\alpha = 0$, $\beta > 0$). The symmetry of the potential energy function allows the wave functions of the system to be classified according to the irreps of the C_{4v} point group. In the present calculations, we focus on the energy levels of states belonging to the one-dimensional irreps A_1, A_2, B_1, and B_2.

Conveniently, the potential energy function for this system is a homogeneous polynomial, obeying $V(\lambda\mathbf{x}) = \lambda^4 V(\mathbf{x})$. As a result, a one-to-one relationship exists between each classical trajectory $(\mathbf{x}(t),\mathbf{p}(t))$ at an energy E and a particular trajectory $(\tilde{\mathbf{x}}(\tilde{t}),\tilde{\mathbf{p}}(\tilde{t}))$ at an arbitrary reference energy $\tilde{E}$ [7]. This relationship is expressed as

$$\mathbf{x} = \left(\frac{E}{\tilde{E}}\right)^{1/4}\tilde{\mathbf{x}}, \quad \mathbf{p} = \left(\frac{E}{\tilde{E}}\right)^{1/2}\tilde{\mathbf{p}}, \quad \text{and} \quad t = \left(\frac{E}{\tilde{E}}\right)^{-1/4}\tilde{t}. \quad (19)$$

The implication is that all the classical trajectories for an IVR treatment can be calculated at the single energy $\tilde{E}$. To further simplify the numerical computations, we choose the one-dimensional width "matrix" $\mathbf{\Gamma}$ to scale with the energy as $\mathbf{\Gamma} = (E/\tilde{E})^{1/4}\tilde{\gamma}$, where $\tilde{\gamma}$ has a fixed, positive value. With the choice $\tilde{E} = 1$, this allows Eq. (14) for the present system to be expressed as

$$\mathrm{Tr}\,\mathbf{T}^n_E = \frac{1}{2\pi\hbar}\sqrt{\frac{\pi\hbar}{2\gamma}} \int d\tilde{y} \int d\tilde{p}_y\, E^{3/4}\,\tilde{C}\exp(iE^{3/4}\phi/\hbar), \quad (20)$$

where the integration is over a Poincaré surface at energy $\tilde{E}$, $\tilde{C}$ is the prefactor defined in Eq. (12) at energy $\tilde{E}$, and ϕ is given by

$$\phi = \frac{i\tilde{\gamma}}{2}(\tilde{y}' - \tilde{y})^2 + \frac{i}{8\tilde{\gamma}}(\tilde{p}'_y - \tilde{p}_y)^2 - \frac{1}{2}(\tilde{y}' - \tilde{y})(\tilde{p}_y{}' + \tilde{p}_y) + W_{\tilde{E}}(\tilde{y}',\tilde{y}). \quad (21)$$

This result allows one to recalculate the quantities $\mathrm{Tr}\,\mathbf{T}^n_E$, needed to form the cumulant expression for the zeta function,

at any energy E, by simply rescaling two functions in the integrand. Therefore, classical trajectories determined at energy $\tilde{E} = 1$ can be used to perform IVR calculations at all energies. An entirely analogous simplification occurs for the symmetry-adapted traces of Eq. (17).

B. Numerical details

As in Refs. [12,13], the phase space integrations in our IVR formulas for $\mathrm{Tr}\,\mathbf{T}_E^n$ [Eqs. (14) or (17)] are carried out by the Monte Carlo method with uniform sampling of a PSS. To generate random $\tilde{y}$ and $\tilde{p}_y$ values for the Monte Carlo integration, a rectangular portion of a Poincaré plane, containing the classically allowed region at $\tilde{E} = 1$, is uniformly sampled and points falling outside this region are rejected. The accepted points are used as initial conditions for Hamilton's equations of motion and these, along with the linearized equations of motion for the stability matrices and a differential equation for the action W_E, are integrated as a function of time until the trajectories cross the required symmetry-related Poincaré surfaces in each normal direction a preselected maximum number of times, n_p. This allows evaluation of $\mathrm{Tr}\,\mathbf{T}_E^n$ for $n = 1,2,\ldots,n_p$ and, thus, the zeta function to order n_p in the cumulant expansion, Eq. (8).

Semiclassical energy levels are estimated from minima in plots of the computed quantities $|\zeta^{-1}(E)|$ as a function of E. Quantum mechanical energy eigenvalues used for comparison are obtained by diagonalizing the Hamiltonian operator in a large harmonic oscillator basis set (for states with A_1 symmetry) or from values tabulated in Ref. [32] (for states with B_1, B_2, and A_2 symmetries).

IV. RESULTS

A. Integrable case

We begin by presenting results for the treatment of an integrable system obtained by setting the parameters in the Hamiltonian of Eq. (18) to $\alpha = 0$, $\beta = 0.01$. The Poincaré surface was taken as the line $y = x$ passing through the origin in configuration space and the Gaussian width parameter $\tilde{\gamma}$ was chosen as 0.5. Energy levels for states with A_1 symmetry and $E < 27$ were investigated.

Figures 1–3 display the numerical results for the function $|\zeta^{-1}(E)|$, obtained by applying the IVR expression, Eq. (17), to the traces $\mathrm{Tr}\,\mathbf{T}_E^n$ in the cumulant expansion (8). These calculations were performed using 2.5×10^4 trajectories (Monte-Carlo points on the PSS) and a maximum of $n_p = 40$ returns to the PSS. Practically identical results were obtained with $n_p = 20$. Apart from a few exceptions, these figures display a nearly one-to-one correspondence between the minima of $|\zeta^{-1}(E)|$ and the quantum energy levels in the range examined. Considering the near degeneracies of many of the levels, the successful resolution of the quantum energies here is remarkable. Although the former IVR treatment of Ref. [23] for this system was able to resolve *all* energy levels in the range considered, it is important to bear in mind that the work there was restricted to lower energies, $E < 12$, and required a factor of 20–25 more computational time than the present treatment for the same energy range.

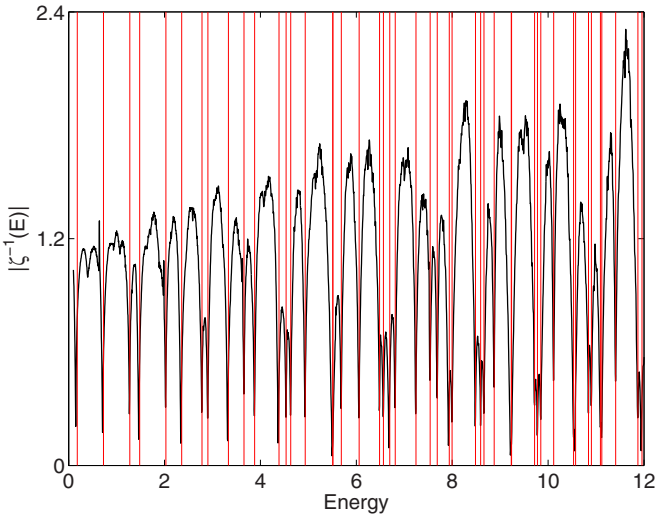

FIG. 1. (Color online) $|\zeta^{-1}(E)|$ vs energy for A_1 states of the integrable system for $0 \leqslant E \leqslant 12$. Vertical lines indicate quantum mechanical energy levels.

B. Intermediate case

We now apply our IVR treatment to a system whose phase space has an intermediate, mixed, nature, with regions of chaotic dynamics coexisting with those of regular behavior, characterized by invariant tori. To achieve this situation we choose values $\alpha = 1, \beta = 0.25$ for the parameters in Eq. (18). The composite Poincaré surface in Fig. 4 verifies that substantial portions of phase space are occupied by chaotic trajectories and by regular classical trajectories for this case. The energy in this figure is chosen as $E = 1$ but the classical scaling properties of the Hamiltonian of Eq. (18) imply that the Poincaré surface of the section has a similar appearance at any energy.

Figure 5 displays the function $|\zeta^{-1}(E)|$ for A_1 states of this system with energies $E < 57$. Here (and in the chaotic

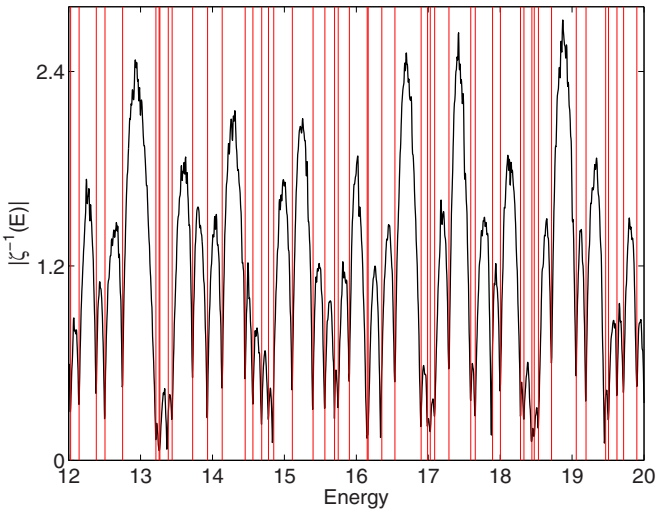

FIG. 2. (Color online) $|\zeta^{-1}(E)|$ vs energy for A_1 states of the integrable system for $12 \leqslant E \leqslant 20$. Vertical lines indicate quantum mechanical energy levels.

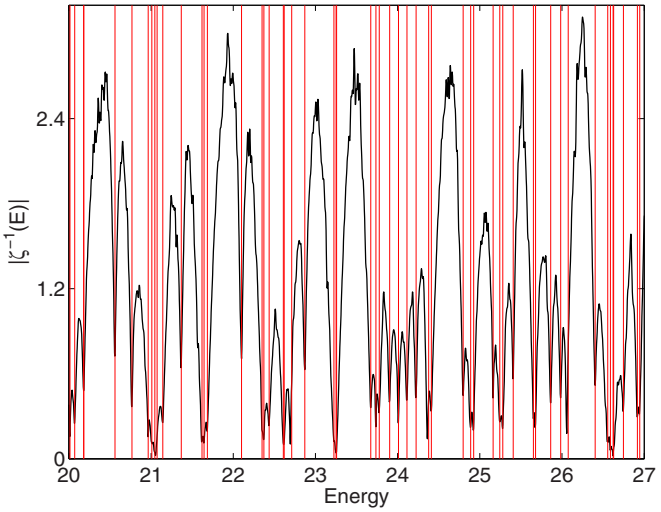

FIG. 3. (Color online) $|\zeta^{-1}(E)|$ vs energy for A_1 states of the integrable system for $20 \leqslant E \leqslant 27$. Vertical lines indicate quantum mechanical energy levels.

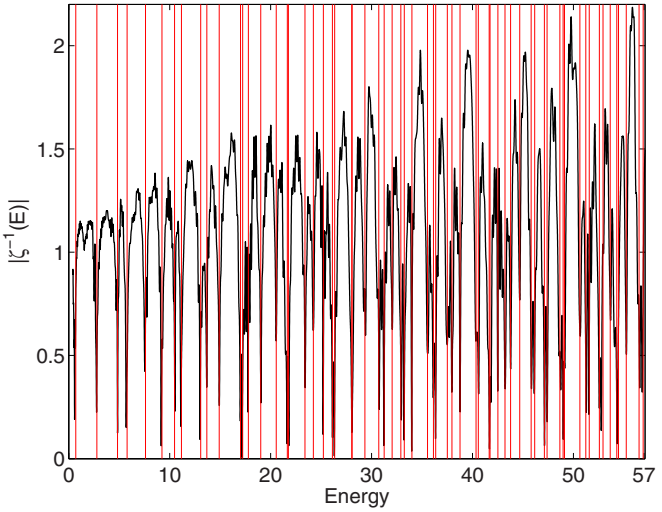

FIG. 5. (Color online) $|\zeta^{-1}(E)|$ vs energy for A_1 states of the system with mixed phase space. Vertical lines indicate quantum mechanical energy levels.

case below), the Poincaré plane was chosen as $x = 0$ to obtain the most rapidly converging results. The calculations were carried out by using $\tilde{\gamma} = 0.5$, $n_p = 12$, and 5×10^4 trajectories (although effective convergence was already achieved with half this number). As in the integrable case, the results show that nearly all energy levels in the investigated range are resolved and that the semiclassical energy estimates (the minima of $|\zeta^{-1}(E)|$) are in very good agreement with the quantum energy levels.

C. Chaotic case

We now turn our attention to the parameter choice $\alpha = 1.0$, $\beta = 0.01$, which is known to result in strongly chaotic classical dynamics (characterized by large Lyapounov numbers) that extends throughout almost all portions of phase space [30–32].

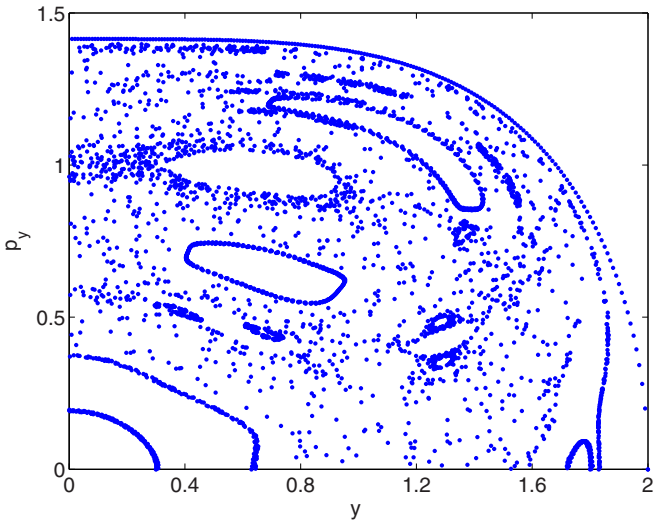

FIG. 4. (Color online) Poincaré surface of section ($x = 0$, $p_y > 0$) for the classical Hamiltonian (18) with $\alpha = 1.0$, $\beta = 0.25$. Due to the symmetry only one quadrant is shown.

These parameters were previously used to test the former IVR treatment of the zeta function [23] and the IVR approximation for the trace of Green's function [12].

In common with most other IVR treatments for chaotic systems, the high instability of the classical trajectories in this case poses a serious challenge for the present IVR treatment. Specifically, this instability makes the complex exponent in the IVR formula [e.g., the function ϕ in Eq. (20)] very sensitive to variations in the initial conditions at long times, causing the phase of the integrand to fluctuate rapidly with changes in the integration variables. The large Lyapounov numbers also cause the modulus $|C|$ of the prefactor to grow, on the average, exponentially with time. These combined effects make numerical evaluation of the IVR integral very difficult for long-time dynamics, requiring a very large number of trajectories for convergence. Thus, for the present system, a straightforward Monte Carlo calculation of $\mathrm{Tr}\,\mathbf{T}_E^n$ or c_n is found to be practically unfeasible for $n > 2$.

As in other IVR treatments [12,29,33], we partially overcome this problem by terminating trajectories when the square modulus of the integrand becomes larger than a predetermined cutoff, chosen here to be 1.3×10^6. This makes it possible to converge the Monte Carlo integrations with a reasonable number of classical trajectories. However, as will become apparent below, the price of such a restriction to the length of highly chaotic trajectories is a broadening of certain minima in the function $|\zeta^{-1}(E)|$ and a consequent loss of resolution in the energy spectrum.

The termination of trajectories also creates some apparent difficulties for the calculation of the symmetry-adapted traces $\mathrm{Tr}\,\mathbf{T}_{E,j}^n$ via Eq. (17). The numerical procedure described in Sec. II D requires a trajectory to intersect each symmetry-related Poincaré surface in each direction n times in order for it to contribute to this trace. However, the termination procedure often cuts off trajectories after completion of only some, but not all, of these intersections. If the contributions from such partial completions are discarded, very few Monte Carlo points remain for the convergence of the integrals

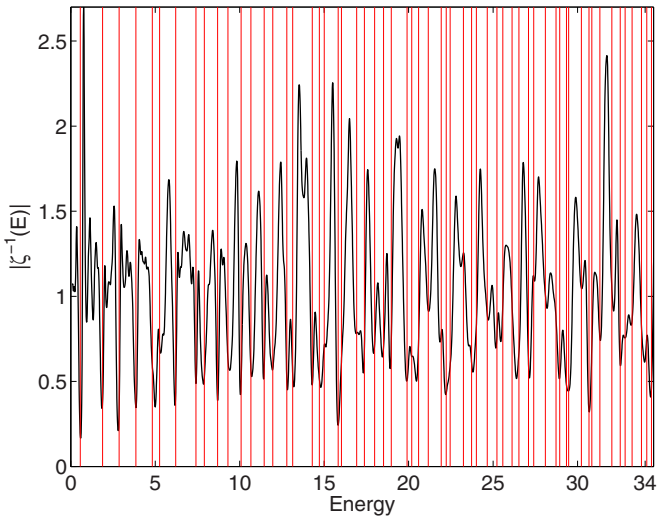

FIG. 6. (Color online) $|\zeta^{-1}(E)|$ vs energy for A_1 states of the chaotic system. Vertical lines indicate quantum mechanical energy levels.

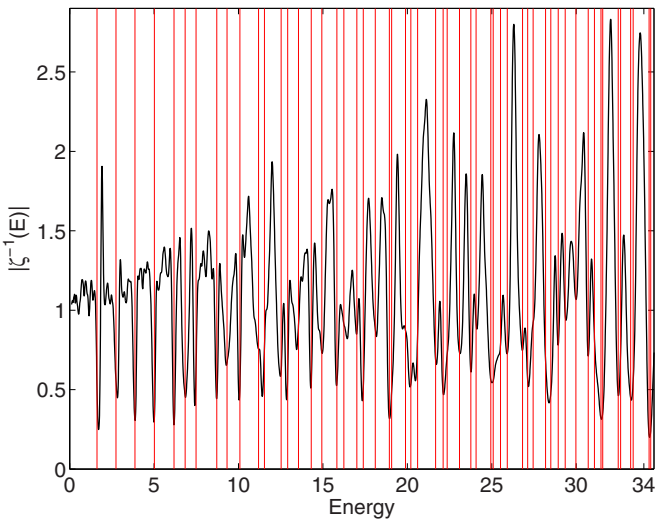

FIG. 8. (Color online) $|\zeta^{-1}(E)|$ vs energy for B_1 states of the chaotic system. Vertical lines indicate quantum mechanical energy levels.

representing traces so that, again, calculations are impractical even for moderate values of n.

In the present work we simply retain contributions from all such partial completions. Although one may worry that this would ruin the symmetry projection, the numerical results for the zeta functions, presented below, do not display signs of any significant symmetry contamination. A possible explanation is that the various trajectories in the Monte Carlo calculations undergo complementary completed and missed intersections so that each symmetry-related intersection occurs statistically an equal number of times.

Numerical calculations of the zeta function for symmetry species A_1, A_2, B_1, and B_2 are presented in Figs. 6–9, respectively. The calculations were performed with $\tilde{\gamma} = 0.5$, 1.0×10^5 trajectories, and $n_p = 25$. Increasing n_p to 200 caused no visible change the computed results. In each figure, the minima of $|\zeta^{-1}(E)|$ are found to be in good agreement with the quantum energy levels for low energies but there are clear signs of resolution loss at higher energies where the quantum spectrum becomes dense. Comparison of the A_1 semiclassical levels with those obtained from an IVR treatment of the trace of Green's function [12] indicate that the two techniques yield comparable (but not identical) results. The trajectory truncation procedure limits the energy resolution in a similar way for both cases. More will be said about this matter in the next section.

V. SUMMARY AND REMARKS

The cycle expansion of the semiclassical zeta function has been one of the most successful tools for the semiclassical

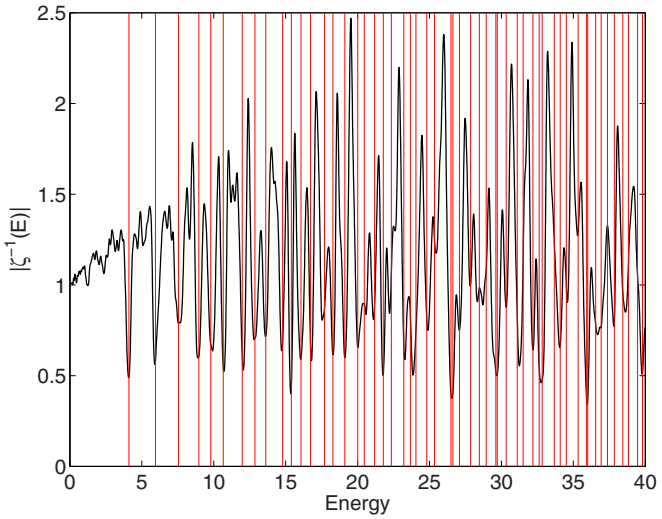

FIG. 7. (Color online) $|\zeta^{-1}(E)|$ vs energy for A_2 states of the chaotic system. Vertical lines indicate quantum mechanical energy levels.

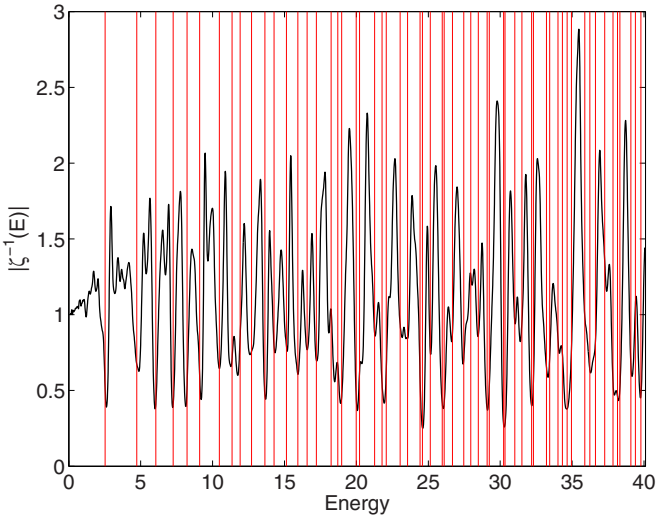

FIG. 9. (Color online) $|\zeta^{-1}(E)|$ vs energy for B_2 states of the chaotic system. Vertical lines indicate quantum mechanical energy levels.

quantization of chaotic systems. However, this treatment is effectively restricted to systems with fully chaotic behavior and requires identification and coding of all periodic orbits, a process that is not feasible for systems with more than two or three degrees of freedom. In the present work, we develop an IVR treatment for the cumulant expansion of $\zeta^{-1}(E)$, a direct precursor of the cycle expansion. This yields a method for calculation of the zeta function that is equally applicable to integrable systems, classically chaotic systems, and generic systems with mixed phase space. This treatment does not require searches for periodic orbits or their enumeration and coding, and is therefore relatively easy to apply to systems with several degrees of freedom and smooth potentials.

The above advantages are shared by the IVR approximation for the zeta function presented in Ref. [23]. However, the approach developed here avoids diagonalization or evaluation of determinants of large matrices, which lend a quantum flavor to the former method and cause computations to scale unfavorably with energy and system size. Consequently, calculations based on the present treatment are far more numerically efficient than those using the former method, requiring computational times that are a factor of at least 20 shorter in the cases examined here. In view of the N^3 scaling for computation times of N-dimensional determinants, this numerical advantage should grow dramatically for larger systems.

The tests of the IVR method presented in Sec. IV are encouraging. The semiclassical calculations for the integrable and intermediate systems provide resolution of all but a few, very closely spaced, levels and yield energies that are in very good agreement with quantum values. There are indications that the remaining, minor, imperfections in the resolution may be related to the limited reliability of using the minima of $|\zeta^{-1}(E)|$ to detect energy levels compared, e.g., with the method based on examination of the eigenvalues of $\mathbf{T}_E$ applied in Refs. [26] and [23].

For the highly chaotic system studied here, our semiclassical technique gives levels that are in generally good agreement with quantum values at low energies, but the method becomes noticeably less capable of resolving all levels as the energy and the spectral density increase. This feature can be traced to the numerical problems associated with long trajectories that affect almost all IVR treatments of chaotic systems. To our knowledge, the only IVR quantization method that is free of such problems is the IVR zeta function method of Ref. [23]. That treatment, though far more computationally demanding that the present one, successfully resolves all energy levels for the present chaotic system because it relies only on short trajectories that undergo a single return to the PSS in the initial direction.

As discussed above, the numerical problems associated with long trajectories in IVR methods are due to the highly oscillatory nature of the phase space integrals. Thus, to apply IVR methods in such cases, it is necessary to reduce these fluctuations. Methods that have been proposed to accomplish this include filtering techniques [33–35] and the simple trajectory termination method applied here [29,33]. Unfortunately, all these methods limit the resolution of the computed energy spectra, reducing the usefulness of the IVR treatments at high energies.

It is interesting to observe that the IVR long trajectory problem is in some ways analogous to the problem of long perodic orbits that prevents the absolute convergence of Gutzwiller's trace formula for chaotic systems. In addition, the trajectory termination method applied here bears some resemblance to techniques that impose convergence upon the Gutzwiller formula by damping terms with long periodic orbits [9,10]. Such methods also lead to a loss of resolution in the computed energy spectra comparable to that observed for the IVR treatment here.

The cumulant expansion of the zeta function effectively solves the problem of long trajectories in the context of Gutzwiller's treatment. It accomplishes this by diminishing the effect of these trajectories, canceling their contributions to the zeta function with those of shorter trajectories. It may, therefore, seem odd that the cumulant expansion does not similarly solve the long trajectory problem for IVR treatments, as evidenced by the need to truncate trajectories and the consequent loss of resolution in the present calculations for the chaotic system.

The reason for this, however, becomes clearer when we recall that each curvature term c_m in the cumulant expansion is itself a sum of terms, each proportional to a product of the form $\prod_n \mathrm{Tr}\,\mathbf{T}_E^n$ with $\sum n = m$. It is among such terms that cancellation of the long trajectories takes place for each c_m. The present IVR treatment calculates this sum by evaluating each of the traces $\mathrm{Tr}\,\mathbf{T}_E^n$, $n = 1,2,\ldots,m$, individually by an IVR expression, calculating each term in c_m separately, and finally combining these terms to form the desired quantity c_m. However, the terms in the expression for c_m are not individually small. Only their combination in c_m is small (for large enough m) so that a curvature term is the small difference of relatively large numbers. Because such a differencing process results in the loss of precision, an accurate calculation of c_m requires an even more accurate calculation of each term in the difference.

However, the present technique is unable to achieve such accuracy for chaotic systems due to the convergence problems of the IVR expressions. Thus, the desired cancellation does not occur. Indeed, unless methods such as termination of trajectories are applied, the lack of numerical convergence for the IVR integrals causes successive terms in the cumulant expansion to grow exponentially rather than decrease, so that the expansion itself diverges strongly.

Nevertheless, it remains possible that a different IVR treatment of the cumulant expansion for $\zeta^{-1}(E)$ may provide a solution to the long trajectory problem that plagues almost all IVR methods for chaotic systems. The analysis above suggests how such an IVR expression would need to be designed. Unlike the present approach, such a treatment would have to express a given curvature term c_m as a whole (and not individual components such as $\mathrm{Tr}\,\mathbf{T}_E^n$) as an IVR integral over initial conditions for classical trajectories. Such a formulation should allow the cancellation associated with long trajectories to occur in each term of a Monte Carlo sum representing the integral. This cancellation can be accomplished accurately since the quantities needed to form each term can be calculated with high precision and no very large numbers need to be differenced. These ideas should be explored in future work.

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