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Semiclassical initial-value representation of the transfer operator

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The ability of semiclassical initial-value representation (IVR) methods to determine approximate energy levels for bound systems is limited due to problems associated with long classical trajectories. These difficulties become especially severe for large or classically chaotic systems. This work attempts to overcome such problems by developing an IVR expression that is classically equivalent to Bogomolny's formula for the transfer matrix [E. B. Bogomolny, Nonlinearity **5**, 805 (1992); Chaos **2**, 5 (1992)] and can be used to determine semiclassical energy levels. The method is adapted to levels associated with states of desired symmetries and applied to two two-dimensional quartic oscillator systems, one integrable and one mostly chaotic. For both cases, the technique is found to resolve all energy levels in the ranges investigated. The IVR method does not require a search for special trajectories obeying boundary conditions on the Poincaré surface of section and leads to more rapid convergence of Monte Carlo phase space integrations than a previously developed IVR technique. It is found that semiclassical energies can be extracted from the eigenvalues of transfer matrices of dimension close to the theoretical minimum determined by Bogomolny's theory. The results support the assertion that the present IVR theory provides a different semiclassical approximation to the transfer matrix than that of Bogomolny for $\hbar \neq 0$. For the chaotic system investigated the IVR energies are found to be generally more accurate than those predicted by Bogomolny's theory.

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I. INTRODUCTION

Semiclassical initial-value representation (IVR) techniques have become useful and popular tools for treating the dynamics of molecules, atoms, and electrons [1,2]. A characteristic feature of these techniques is that they describe quantum mechanical quantities of interest (such as the time-dependent propagator [3,4], the energy-dependent Green's function [5] and its trace [6], time-independent wave functions [7,8], and the S matrix [9,10]) as integrals over phase space variables. These variables serve as initial conditions for the classical trajectories that are needed to describe the quantum properties. Thus such techniques avoid cumbersome nonlinear searches for special trajectories obeying particular boundary conditions at initial and final times, which are needed for more conventional semiclassical methods. This makes it possible to treat much larger physical systems than feasible with the usual semiclassical techniques. Apart from this practical advantage, properly designed IVR methods are superior semiclassical approximations [4,11], avoiding problems associated with caustics encountered in the usual semiclassical theories and producing uniform semiclassical approximations for wave functions and related properties.

However, existing IVR treatments suffer from a severe computational obstacle: The number of classical trajectories needed to achieve satisfactory convergence of the phase space integrals is often impractically large, especially for systems that are classically chaotic. The root of this difficulty is the rapid variation in the phase of the IVR integrand as a function of initial conditions, a phenomenon that becomes increasingly pronounced at long time in the presence of classical chaos. These rapid phase changes are accompanied by prefactors that increase exponentially with time, as necessary to prevent vanishing of the integral due to phase cancellation. This combination of rapid phases and large prefactors makes the numerical integration over phase space very difficult. As a result, the number of trajectories needed for convergence of IVR calculations of chaotic systems typically grows exponentially with time, making applications of these techniques impractical for the calculation of the long-time quantum evolution of such systems.

A number of methods have been proposed to alleviate this long-trajectory problem. For the calculation of time correlation functions, in the case of systems that are not too chaotic, the so-called forward-backward techniques [12–15] are sometimes effective. For more general chaotic systems integral conditioning (filtering) methods [16–18] can be applied. A cruder, but equally effective, method [19,20] is to terminate classical trajectories once they become too chaotic, as determined by IVR prefactors that are larger than a predetermined value. However, such treatments do not eliminate the exponential growth rate in the number of trajectories needed to maintain accuracy of the calculations, but only cause a decrease in the factor multiplying the exponential. Thus, in practice, IVR calculations of systems with even a mild degree of chaos are limited to the treatment of short-time phenomena, e.g., ultrafast chemical reactions and low-resolution spectra. If the chaos is sufficiently strong, such calculations may already become substantially inaccurate beyond a single cycle of motion, even for two-dimensional systems [19]. For the treatment of energy quantization, the restriction to short times means that the calculated energy spectrum is broad and not all individual levels can be resolved [6,19]. This restriction has also prevented numerical investigation of fundamental questions concerning the IVR treatment of chaotic systems such as the convergence of the IVR integrals at long times and the ultimate accuracy of the resulting energy spectrum.

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A hint as to how the above difficulties might be overcome in a more fundamental and effective way comes from semiclassical periodic orbit theory, where a seemingly analogous long-trajectory problem affects the Gutzwiller trace formula [21–23] for the energy quantization of chaotic systems. This formula expresses the trace $g(E)$ of Green's function as an infinite sum over the periodic orbits of the classical system. However, since the number of such orbits proliferates exponentially with their length, this sum is not, in general, absolutely convergent for real values of the energy E [24]. One solution to this problem [25,26] is to employ Gaussian smoothing, which effectively damps the influence of long periodic orbits in a manner reminiscent of the practice of terminating long trajectories in the IVR case [19,20]. However, a more satisfactory approach has been developed. It involves shifting focus from the trace $g(E)$ to the semiclassical zeta function [27–31]

$$\zeta_{\mathrm{S}}(E) = e^{i\pi N_{\mathrm{TF}}(E)} \exp\left[\int^{E} dE' g(E')\right], \tag{1}$$

where N_{TF} is the integrated mean level density. The energy eigenvalues of a bound system are obtained from this function by finding the values of E that make $\zeta_{\mathrm{S}}(E) = 0$. An expansion of the ζ function in terms of periodic orbits [27–31] allows a resummation of the Gutzwiller periodic orbit series that is convergent since the dominant effect of long orbits in each term is canceled by portions of shorter orbits. In fact, it has been argued that only short orbits with periods less than half the Heisenberg time are actually needed in the ζ function expansion [31].

These considerations suggest that it should be possible to overcome the IVR long-trajectory problem, at least for the purposes of energy quantization, by developing an IVR formulation of the periodic orbit expansion of the ζ function. An alternative approach, which we explore here, is to derive an IVR approximation that, in the classical limit, becomes equivalent to an explicit formula for the ζ function proposed by Bogomolny [32,33]. Bogomolny's expression represents $\zeta_{\mathrm{S}}(E)$ as the Fredholm determinant $\det(\mathbf{1} - \mathbf{T}_E)$, where elements $T_E(\mathbf{q}',\mathbf{q})$ of the transfer matrix $\mathbf{T}_E$ define a semiclassical mapping between points $\mathbf{q}$ and $\mathbf{q}'$ on a Poincaré surface of section (PSS). The energy eigenvalues of the system can then be determined as values of E that make this determinant vanish. Such a calculation does not involve an expansion in terms of periodic orbits but avoids the long-trajectory problem because the formation of $\mathbf{T}_E$ requires only short trajectories that return to a PSS after a single iteration of the classical Poincaré map.

Bogomolny's method has been applied successfully to both integrable [34–39] and chaotic systems [33,35,37,40,41] and has been used to obtain wave functions [37,40,42] as well as energy levels. Although Bogomolny's theory is semiclassical in nature, it has been more firmly rooted in quantum theory by the development of exact quantum Poincaré maps that tend to those of Bogomolny in the classical limit [43–46].

Because Bogomolny's semiclassical expression for $T_E(\mathbf{q}',\mathbf{q})$ requires identification of special classical trajectories that satisfy boundary conditions on the PSS, most applications of his method have been limited to billiards and integrable systems for which trajectories can be determined without a numerical solution of the equations of motion. For similar reasons, this method has been applied only to systems with two or (in special cases) three degrees of freedom [39,47]. However, Haggerty [42] has presented a numerical method that allows the transfer matrix to be constructed for arbitrary smooth potentials, allowing extension of this treatment to systems for which such analytical expressions for the dynamics are not available. He has applied this method to a two-dimensional system with a smooth nonscalable potential and used it to determine the values of $\hbar$ that yield quantized energy eigenvalues for two fixed values of the energy: one corresponding to the integrable regime for the classical motion and one to the chaotic regime.

From the present perspective, Haggerty's numerical technique can be recognized as a simple IVR method. However, it differs from the more modern and general IVR approximation investigated here in two crucial ways: First, the IVR expression of Haggerty for $T_E(\mathbf{q}',\mathbf{q})$ does not include Gaussian coherent state factors in the integrand and, second, it is designed to be exactly equivalent to Bogomolny's formula for the transfer operator. The present inclusion of Gaussian factors in the IVR formulas is known, in other contexts, to yield more accurate wave functions that are free from caustic singularities [4,11]. Additionally, this inclusion has been shown to greatly reduce the number of classical trajectories required to evaluate the IVR expressions, especially when the phase space integrations are performed by Monte Carlo methods [4,48]. The latter property is important because it is a key to making transfer matrix calculations practicable for larger systems. Furthermore, the present approach, which demands equivalence of the IVR expression to Bogomolny's formula only in the classical limit, produces a semiclassical approximation that is not necessarily identical to that of Bogomolny for nonzero $\hbar$. This leaves open the possibility that the IVR expressions developed here may provide values for energy levels that are less or even more accurate than those obtained from the existing theory. In this paper we investigate the possible advantages of the present IVR treatment by comparing its results to those obtained with existing methods and theories.

The remainder of this paper is organized as follows. In Sec. II we obtain an expression for the IVR transfer operator from a previously derived IVR approximation for Green's function [5,6]. Additionally, we develop a version of the IVR formula that allows determination of energy levels for states of specific symmetries and establish the relationship of the present treatment to that of [42]. In Sec. III we describe how the IVR approximation is applied numerically to the two-dimensional classically integrable and chaotic systems treated here. In Sec. IV we present the results of the calculations and compare them to those obtained using the former IVR method of [42] and the theory of Bogomolny. Finally, in Sec. V we summarize our conclusions and present closing remarks.

II. THE IVR TREATMENT OF THE TRANSFER OPERATOR

A. Preliminaries

Elements $T_E(\mathbf{q}',\mathbf{q})$ of Bogomolny's transfer matrix $\mathbf{T}_E$ can be regarded as representatives of a semiclassically defined transfer operator $\hat{T}_E$ in the basis of position variables $\mathbf{q}'$ and $\mathbf{q}$ on a Poincaré surface Σ of a system at energy E. Here $\hat{T}_E$ is conceptually similar to the quantum time evolution operator $\exp[-i(\hat{H}-E)t/\hbar]$ except that it propagates functions specified on the PSS for one iteration of the classical Poincaré map. In rough analogy to the evolution operator, $\hat{T}_E$ is unitary in the classical limit. For arbitrary energy, application of $\hat{T}_E$ to a function on the PSS produces a different function on the same PSS. However, when E is an eigenvalue of the Hamiltonian and ψ is a corresponding eigenstate, $\hat{T}_E$ transforms ψ into itself, i.e., $\hat{T}_E\psi = \psi$ or, equivalently,

$$\psi(\mathbf{q}) = \int_\Sigma T_E(\mathbf{q},\mathbf{q}')\psi(\mathbf{q}')d\mathbf{q}'. \tag{2}$$

Thus ψ is an eigenstate of $\hat{T}_E$ with eigenvalue 1 and the energy levels of a system can be determined by solving the secular equation

$$\det(\mathbf{1}-\mathbf{T}_E) = 0. \tag{3}$$

Bogomolny [32,33] established the equivalence between the Fredholm determinant in this secular equation and the semiclassical ζ function, i.e.,

$$\zeta_{\mathrm{S}}(E) = \det(\mathbf{1}-\mathbf{T}_E), \tag{4}$$

so (3) corresponds to the known quantization condition $\zeta_{\mathrm{S}}(E)=0$ for the ζ function. Bogomolny [32,33] further derived an expression for the function $T_E(\mathbf{q}',\mathbf{q})$ as a sum over all trajectories corresponding to the classical Poincaré map from $\mathbf{q}$ to $\mathbf{q}'$. Such a trajectory starts from $\mathbf{q}$ on the PSS with, say, a positive value for the component of the velocity normal to the surface, crosses the surface once with a negative normal velocity component, and ends at $\mathbf{q}'$ on the PSS, again with a positive normal velocity component. The expression for a system of f degrees of freedom is given by

$$T_E(\mathbf{q}',\mathbf{q}) = \sum_{\substack{\text{classical}\\ \text{trajectory}}} \frac{1}{(2\pi i\hbar)^{(f-1)/2}}\left|\det\left[\frac{\partial^2 W_E(\mathbf{q}',\mathbf{q})}{\partial\mathbf{q}'\partial\mathbf{q}}\right]\right|^{1/2} \times \exp[iW_E(\mathbf{q}',\mathbf{q})/\hbar - i\nu\pi/2]. \tag{5}$$

Here

$$W_E(\mathbf{q}',\mathbf{q}) = \int_{\mathbf{q}}^{\mathbf{q}'} \mathbf{p}(\mathbf{x})^T d\mathbf{x} \tag{6}$$

is the reduced action, calculated along a classical trajectory with energy E connecting the points $\mathbf{q}$ and $\mathbf{q}'$, and ν is the Maslov index.

In practical calculations, one must discretize the continuous variables $(\mathbf{q}',\mathbf{q})$ by dividing them into cells of volume $\Delta\mathbf{q}_i$ about points $\mathbf{q}_i$ to produce a finite matrix $\mathbf{T}_E$ with elements

$$(\mathbf{T}_E)_{i,j} = (\Delta\mathbf{q}_i)^{1/2}T_E(\mathbf{q}_i,\mathbf{q}_j)(\Delta\mathbf{q}_j)^{1/2}. \tag{7}$$

Bogomolny showed that the minimum dimension $\tilde{N}(E)$ of this matrix needed to calculate energy eigenvalues up to energy E is

$$\tilde{N}(E) = \frac{A(E)}{(2\pi\hbar)^{f-1}}, \tag{8}$$

where $A(E)$ is the volume of the classically allowed region on the PSS. Thus $\tilde{N}(E)$ coincides with the number of "Planck cells" in this allowed region. To obtain accurate results, however, it is necessary, in practice, to choose the dimension $N(E)$ of the transfer matrix to be larger than this theoretical minimum. For sufficiently large values of $N(E)$, approximately $\tilde{N}(E)$ eigenvalues of $\mathbf{T}_E$ are found to lie near the unit circle in the complex plane, consistent with an approximate form of unitarity for $\mathbf{T}_E$, while the remaining eigenvalues are found to be small and lie near the origin [40,42].

Instead of discrete coordinates, as above, the matrix $\mathbf{T}_E$ can be constructed in a discrete basis $\{\phi_i\}$ obeying a relation of the form $\sum_i |\phi_i)(\phi_i| = \hat{1}$ so that its elements are given by

$$(\mathbf{T}_E)_{i,j} = (\phi_i|\hat{T}_E|\phi_j) = \int_\Sigma d\mathbf{q}'\int_\Sigma d\mathbf{q}\,\phi_i(\mathbf{q}')^* T_E(\mathbf{q}',\mathbf{q})\phi_j(\mathbf{q}). \tag{9}$$

The above comments concerning matrix dimensions apply in such cases as well.

B. The IVR formula for the transfer function

Calculation of $T_E(\mathbf{q}_i,\mathbf{q}_j)$ via Eq. (5) requires identifying all classical trajectories that begin at coordinate $\mathbf{q}_j$ on the Poincaré surface and end at coordinate $\mathbf{q}_i$ after a single cycle of motion. This requires a numerical search that can be difficult for nontrivial systems, especially for those of high dimensionality. This motivates development of an IVR expression for this function.

Our IVR formula for $T_E(\mathbf{q}',\mathbf{q})$ is most simply obtained from an analogous IVR expression for the Green's function $G_E(\mathbf{x}',\mathbf{x})$. For the case that positions $\mathbf{x}'$ and $\mathbf{x}$ both lie on a particular Poincaré surface, it has been shown that this function can be semiclassically approximated as [5,6]

$$\begin{aligned} G_E(\mathbf{x}',\mathbf{x}) = {} & \frac{1}{i\hbar}\left(\frac{1}{2\pi\hbar}\right)^{f-1}\sum_{\sigma=\pm1}\sum_{l=0}^{\infty} a_l \int d\mathbf{y}^{(0)} \\ & \times \int d\mathbf{p}_y^{(0)}\big(\mathbf{q}'|\mathbf{y}^{(l)}\mathbf{p}_y^{(l)}\big)_{\Gamma'} \\ & \times \frac{C}{|\dot{z}_l\dot{z}_0|^{1/2}}\, e^{(i/\hbar)W_E(\mathbf{y}^{(l)},\mathbf{y}^{(0)})}\big(\mathbf{y}^{(0)},\mathbf{p}_y^{(0)}|\mathbf{q}\big)_{\Gamma}, \end{aligned} \tag{10}$$

where the prefactor C is given as [6]

$$C = [\operatorname{sgn}(\dot{z}_l\dot{z}_0)\det(2\boldsymbol{\Gamma}/\pi\hbar)\det(\partial\boldsymbol{\zeta}^{(l)}/\partial\boldsymbol{\zeta}^{(0)})]^{1/2}. \tag{11}$$

In our notation $\mathbf{x} = (z,\mathbf{q})$ is a coordinate in the f-dimensional configuration space. It is resolved into a component z perpendicular to the Poincaré surface (the surface is defined by the condition $z=0$) and components $\mathbf{q}$ along the surface. The quantities $\boldsymbol{\Gamma}$ and $\boldsymbol{\Gamma}'$ are $f\times f$ symmetric matrices that have positive real parts but are otherwise arbitrary. The quantities $(\mathbf{q}|\mathbf{y},\mathbf{p}_y)_\Gamma$ are unnormalized coherent states on the PSS, defined by

$$(\mathbf{q}|\mathbf{y},\mathbf{p}_y)_\Gamma \equiv \exp\left[-(\mathbf{q}-\mathbf{y})^T\boldsymbol{\Gamma}(\mathbf{q}-\mathbf{y})/\hbar + i\mathbf{p}_y^T(\mathbf{q}-\mathbf{y})/\hbar\right]. \tag{12}$$

The $(\mathbf{y}^{(0)},\mathbf{p}_y^{(0)})$ determine coordinates and conjugate momenta on the surface that serve as initial conditions for classical trajectories and $(\mathbf{y}^{(l)},\mathbf{p}_y^{(l)})$ are phase space points for the lth intersection with the PSS. Additionally, $\dot{z}_0$ and $\dot{z}_l$ are the velocity components perpendicular to the surface at the initial time and at the lth return and $\sigma = \pm 1$ is the sign of $\dot{z}_0$, determining the initial direction of the trajectory normal to the surface. In addition, a_l is defined as $1-(1/2)\delta_{l,0}$. The matrix $\partial\boldsymbol{\zeta}^{(l)}/\partial\boldsymbol{\zeta}^{(0)}$ is given by

$$\frac{\partial\boldsymbol{\zeta}^{(l)}}{\partial\boldsymbol{\zeta}^{(0)}} = \frac{1}{2}\frac{\partial\mathbf{p}_y^{(l)}}{\partial\mathbf{p}_y^{(0)}} - i\boldsymbol{\Gamma}'\frac{\partial\mathbf{y}^{(l)}}{\partial\mathbf{p}_y^{(0)}} + \frac{i}{4}\frac{\partial\mathbf{p}_y^{(l)}}{\partial\mathbf{y}^{(0)}}\boldsymbol{\Gamma}^{-1} + \frac{1}{2}\boldsymbol{\Gamma}'\frac{\partial\mathbf{y}^{(l)}}{\partial\mathbf{y}^{(0)}}\boldsymbol{\Gamma}^{-1}, \tag{13}$$

where the partial derivatives (monodromy matrix elements) on the right-hand side are evaluated for fixed energy and fixed final PSS. The phase of the complex prefactor C is determined by the requirement that it be continuous with respect to time. For this purpose, it is important to keep the time-dependent versions of $\text{sgn}(\dot{z}_l\dot{z}_0)$ and $\partial\boldsymbol{\zeta}^{(l)}/\partial\boldsymbol{\zeta}^{(0)}$ together in the square root appearing in Eq. (11) during the dynamical calculations.

The above formula was derived by requiring that a stationary phase approximation to the integrals in (10) yield the Gutzwiller's formula for $G_E(\mathbf{x}',\mathbf{x})$ [21]. For the case considered, this can be expressed as [49]

$$G_E(\mathbf{x}',\mathbf{x}) = \frac{1}{i\hbar}\frac{1}{(2\pi i\hbar)^{(f-1)/2}}\sum_{\substack{\text{classical}\\ \text{trajectory}}}\left|\frac{1}{\dot{z}'\dot{z}}\det\left[\frac{\partial^2 W_E}{\partial\mathbf{q}'\partial\mathbf{q}}\right]\right|^{1/2} \times \exp\left(\frac{i}{\hbar}W_E - i\nu\frac{\pi}{2}\right). \tag{14}$$

Here the sum is taken over all trajectories of energy E connecting the point $\mathbf{x}$ at an initial time to the point $\mathbf{x}'$ at a later time. As before, an f-dimensional coordinate $\mathbf{x}$ is resolved into one variable z perpendicular to the Poincaré surface and a set of $f-1$ coordinates $\mathbf{q}$ along the surface. The condition that (10) reduces to (14) upon application of the stationary phase approximation ensures that the IVR expression is a semiclassical treatment since both the stationary phase approximation and Gutzwiller's formula become exact in the classical limit.

The close similarity between (14) for G_E and (5) for T_E allows us to deduce an IVR formula for the transfer function by making minor adjustments to the IVR formula for the Green's function presented in (10). These modifications are designed to cause a stationary phase evaluation of the integrals in the resulting IVR expression for T_E to yield Bogomolny's formula, in analogy with the condition obeyed by the IVR expression for G_E. The specific procedure is guided by the observation that a stationary phase treatment of an integral results in an expression in which a pre-exponential factor in the integrand is evaluated at the critical points where the exponent is stationary. Thus there is a simple and obvious correspondence between the prefactor in the integral and the resulting prefactor obtained by the stationary phase approximation.

To carry out this program, we must identify the differences between (14) for G_E and (5) for T_E. One such difference is the the presence of the factor $(i\hbar|\dot{z}'\dot{z}|^{1/2})^{-1}$ that appears in the Green's function but not in the transfer function. Thus, to form an IVR expression for the transfer function, we remove the corresponding factors $(i\hbar)^{-1}$ and $(\dot{z}_l\dot{z}_0)^{-1/2}$ appearing in the IVR formula for the Green's function. Additional differences between (14) and (5) concern the nature of the summations in the two expressions. In the Green's function they include trajectories that leave the Poincaré surface with any sign of $\dot{z}$ and return to the surface any number of times and with any sign for $\dot{z}'$, while in the transfer function these trajectories leave the surface with a particular sign for $\dot{z}$ (say, $\dot{z} > 0$) and return to the surface exactly once with the same sign for $\dot{z}'$. To adjust the IVR expression for G_E, we remove the summations over σ and l, implicitly restricting the values to $\sigma = 1$ and $l = 2$ (so that $a_2 = 1$).

With these modifications, we obtain the following IVR formula for the transfer function:

$$T_E(\mathbf{q}',\mathbf{q}) = \left(\frac{1}{2\pi\hbar}\right)^{f-1}\int d\mathbf{p}_y \times \int d\mathbf{y}(\mathbf{q}'|\mathbf{y}'\mathbf{p}_y')_{\Gamma'}Ce^{(i/\hbar)W_E(\mathbf{y}',\mathbf{y})}(\mathbf{y},\mathbf{p}_y|\mathbf{q})_{\Gamma}, \tag{15}$$

where we have removed superscripts (0) and replaced superscripts (l) on $\mathbf{y}$ and $\mathbf{p}_y$ by primes. All trajectories needed to compute T_E by this formula are determined by initial conditions $(\mathbf{y},\mathbf{p}_y)$ on the Poincaré surface that, together with the requirements $H(\mathbf{x},\mathbf{p}) = E$ and $\dot{z}_0 > 0$, fix the value of the momentum normal to surface. Therefore, in contrast to (5), calculations using the IVR formula do not require searches for trajectories satisfying specific boundary conditions on the PSS. As in (5), trajectories need not be continued after their first return to the surface with positive normal velocity.

As argued above for the Green's function, the present IVR formula for the transfer function is a semiclassical approximation since it reduces to Bogomolny's formula in the classical limit, where both Bogomolny's expression and the stationary phase approximation become exact. However, for arbitrary width matrices $\boldsymbol{\Gamma}$ and $\boldsymbol{\Gamma}'$ and nonzero $\hbar$, the IVR expression is not identical to Bogomolny's formula. Rather, the IVR and Bogomolny expressions should be regarded as different semiclassical approximations. It should be mentioned that purely quantum mechanical analogs of the transfer function have been developed [43–46] and, consistent with other cases [11,50], it may be possible to derive our IVR expression directly from such treatments, avoiding references to Bogomolny's formula.

C. The δ function limit

Despite the above remarks concerning the general nonequivalence of the IVR and Bogomolny approximations, the present IVR formula does become identical to Bogomolny's expression in the limiting case that the Gaussian width matrices are chosen to have the forms $\boldsymbol{\Gamma} = \boldsymbol{\Gamma}' = \gamma\mathbf{1}$ with $\gamma \to \infty$. Then one can show that

$$(\mathbf{q}|\mathbf{y},\mathbf{p}_y) \to (\pi\hbar/\gamma)^{(f-1)/2}\delta(\mathbf{y}-\mathbf{q}), \tag{16}$$

$$(\mathbf{q}|\mathbf{y}',\mathbf{p}_y') \to (\pi\hbar/\gamma)^{(f-1)/2}\delta(\mathbf{y}'-\mathbf{q}'), \tag{17}$$

and [6]

$$C \to \left(\frac{-2i\gamma^2}{\pi\hbar}\right)^{(f-1)/2}\left|\det\frac{\partial\mathbf{y}'}{\partial\mathbf{p}_y}\right|^{1/2}e^{-i\pi\nu/2}, \tag{18}$$

so that integration over $\mathbf{y}$ casts (15) in the form

$$T_E(\mathbf{q}',\mathbf{q}) = \left(\frac{1}{2\pi i\hbar}\right)^{(f-1)/2} \int d\mathbf{p}_y \delta(\mathbf{y}'-\mathbf{q}') \times \left|\det\frac{\partial \mathbf{y}'}{\partial \mathbf{p}_y}\right|^{1/2} e^{iW_E(\mathbf{y}',\mathbf{q})/\hbar - i\pi\nu/2}. \tag{19}$$

In this equation, $\mathbf{y}'$ is regarded as a function of $\mathbf{p}_y$ and evaluating the remaining integral over that variable immediately gives Bogomolny's expression, Eq. (5).

Equation (19) is an f-dimensional generalization of Haggerty's IVR expression for the transfer function [42]. It cannot be used in its integral form for numerical calculations of $T_E(\mathbf{q}_i,\mathbf{q}_j)$, with discrete values for the coordinates, due to the singular nature of the integrand. However, it can be applied to calculate the transfer matrix in a basis of continuous functions, as in Eq. (9), since the δ function is then integrated over $\mathbf{q}'$, yielding a finite-valued result.

These considerations show that we can perform calculations that effectively use Haggerty's numerical method and obtain semiclassical results that are equivalent to those of Bogomolny's theory by applying our IVR technique to $\langle\phi_i|\hat{T}_E|\phi_j\rangle$ with sufficiently large width matrices. We make use of this observation to compare the results of various theoretical and numerical methods in Sec. IV C.

D. Symmetry-projected transfer operator

For systems with discrete symmetries, one may wish to determine energy levels for states that transform as a specific irreducible representation of the symmetry group. Here we present a version of the IVR formula for T_E that makes this possible and allows treatment of more general symmetry groups than a previous approach [42]. Since our treatment is practically identical to that of [6] for the Green's function, we omit a detailed derivation and present only the final results.

We begin by recalling the operator [51]

$$\hat{P}_j = \frac{d_j}{|G|}\sum_{R\in G}\chi_j(R)\hat{R}$$

that projects onto those energy eigenstates that are a basis for a particular irreducible representation (IR) j. Here the G is the group formed by the symmetry operators $\hat{R}$ of the physical system, $|G|$ is the order of the group, d_j is the dimension of IR j, and $\chi_j(R)$ is the character of $\hat{R}$ in this IR. We wish to form the symmetry-projected transfer function

$$T_E^j(\mathbf{q}',\mathbf{q}) = \frac{d_j}{|G|}\sum_{R\in G}\chi_j(R)T_E^R(\mathbf{q}',\mathbf{q}), \tag{20}$$

where $T_E^j \equiv \hat{P}_j T_E$ and $T_E^R \equiv \hat{R}T_E$. It will then be possible to obtain energy eigenvalues for states with symmetry j from the zeros of $\det(\mathbf{1}-\mathbf{T}_E^j)$.

For simplicity, we restrict the width matrices to the diagonal forms $\mathbf{\Gamma} = \gamma\mathbf{1}$ and $\mathbf{\Gamma}' = \gamma'\mathbf{1}$. The symmetry operators are taken to act on the final variables $\mathbf{x}' = (z,\mathbf{q}')$ according to $\hat{R}\mathbf{x}' = \mathbf{R}\mathbf{x}'$, where $\mathbf{R}$ is an f-dimensional square orthogonal matrix. As shown in Appendix C of [6], the operators $\hat{R}$ may be transferred from $\mathbf{x}'$ to the variables $(z',\dot{z}',\mathbf{y}',\mathbf{p}_y')$ describing the final intersection of the trajectory with the Poincaré surface in the IVR expression for T_E. The operator $\hat{R}$ generally changes the position of the Poincaré surface for this intersection from $z'=0$ to $z_r'=0$, where $z_r' \equiv \hat{R}z'$, and changes the corresponding normal velocity from $\dot{z}'$ to $\dot{z}_r' = \hat{R}\dot{z}'$. Similarly, it transforms the dynamical variables describing the intersection point on the Poincaré surface from $\mathbf{y}'$ and $\mathbf{p}_y'$ to $\mathbf{y}_r' = \hat{R}\mathbf{y}'$ and $\mathbf{p}_{yr}' = \hat{R}\mathbf{p}_y'$, respectively. We thus obtain

$$T_E^R(\mathbf{q}',\mathbf{q}) = \left(\frac{1}{2\pi\hbar}\right)^{f-1}\int d\mathbf{y}\int d\mathbf{p}_y(\mathbf{q}'|\mathbf{y}_r'\mathbf{p}_{yr}')C^R \times e^{iW_E(\mathbf{y}_r',\mathbf{y})/\hbar}(\mathbf{y},\mathbf{p}_y|\mathbf{q}), \tag{21}$$

where the prefactor is given by

$$C^R = [\mathrm{sgn}(\dot{z}_r'\dot{z}_0)(2\gamma/\pi\hbar)^{f-1}\det(\partial\boldsymbol{\zeta}_r'/\partial\boldsymbol{\zeta})\det\mathbf{R}]^{1/2}, \tag{22}$$

with

$$\frac{\partial\boldsymbol{\zeta}_r'}{\partial\boldsymbol{\zeta}} = \frac{1}{2}\frac{\partial\mathbf{p}_{yr}'}{\partial\mathbf{p}_y} - i\gamma'\frac{\partial\mathbf{y}_r'}{\partial\mathbf{p}_y} + \frac{i}{4\gamma}\frac{\partial\mathbf{p}_{yr}'}{\partial\mathbf{y}} + \frac{\gamma'}{2\gamma}\frac{\partial\mathbf{y}_r}{\partial\mathbf{y}}. \tag{23}$$

Turning attention to (20) and recognizing that trajectories contributing to the various T_E^R generally cross different symmetry-transformed Poincaré surfaces in various directions, one finds that T_E^j can be expressed as

$$T_E^j(\mathbf{q}',\mathbf{q}) = \left(\frac{1}{2\pi\hbar}\right)^{f-1}\sum_s\sum_{\sigma=\pm}\int d\mathbf{y}\int d\mathbf{p}_y{\sum_R}' a_j(R) \times(\mathbf{q}'|\mathbf{y}_r'\mathbf{p}_{yr}')C^R e^{iW_E(\mathbf{y}_r',\mathbf{y})/\hbar}(\mathbf{y},\mathbf{p}_y|\mathbf{q}), \tag{24}$$

where the summation over s is over first crossings of all Poincaré surfaces $z_r'=0$, obtained by applying all $\hat{R}\in G$ to the initial surface $z'=0$, 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 $\dot{z}'>0$ to z_r' and $\dot{z}_r'$ with the specified s and σ. Finally, the coefficient $a_j(R)$ is defined as $d_j\chi_j(R)/|G|$.

Equation (24) allows one to calculate the projected transfer function T_E^j by launching trajectories from an initial PSS and considering the first intersection of each trajectory with each Poincaré surface generated by applying the group symmetry operators to the initial surface. For each such intersection, the symmetry operators $\hat{R}$ that carry the intersection surface to the initial PSS with positive transverse velocity must be identified and the corresponding summand in ${\sum_R}'$ must be evaluated.

III. CALCULATIONS

A. System

We illustrate our IVR treatment with numerical calculations for systems of two degrees of freedom with the Hamiltonian [52–54]

$$H = \frac{1}{2}(p_x^2+p_y^2) + \frac{\alpha}{2}(x^2y^2) + \frac{\beta}{4}(x^4+y^4), \tag{25}$$

where α and β are parameters that can greatly influence the nature of the classical behavior. For example, the choice of $\alpha=0$ and $\beta>0$ leads to completely integrable dynamics since the Hamiltonian then describes two independent quartic oscillators in coordinates x and y, while the choice of $\alpha>0$ and $\beta=0$ results in classical behavior that is almost completely chaotic at all energies [52,53]. Thus, by choosing different values for these parameters, we can investigate the IVR method for a variety of dynamical cases.

The symmetry of the potential energy function allows classification of the energy eigenstates of this system according to the IRs of the C_{4v} point group. In the present calculations, we focus on the energy levels of states belonging to the totally symmetric representation A_1. These are obtained by solving $\det(\mathbf{1} - \mathbf{T}_E^j) = 0$, where $\mathbf{T}_E^j$ is constructed using (24) with $j = A_1$.

B. Scaling property

The system described in (25) is especially convenient for the present treatment since the potential energy function is a homogeneous polynomial of fourth degree, i.e., $V(\lambda\mathbf{x}) = \lambda^4 V(\mathbf{x})$. This property implies a one-to-one correspondence between each classical trajectory $[\tilde{\mathbf{x}}(\tilde{t}),\tilde{\mathbf{p}}(\tilde{t})]$ at a fixed arbitrary energy $\tilde{E}$ and a particular trajectory $[\mathbf{x}(t),\mathbf{p}(t)]$ at any other energy E. The latter trajectory is obtained by scaling $\tilde{\mathbf{x}}$, $\tilde{\mathbf{p}}$ and $\tilde{t}$ according to [23]

$$\mathbf{x} = \left(\frac{E}{\tilde{E}}\right)^{1/4}\tilde{\mathbf{x}}, \quad \mathbf{p} = \left(\frac{E}{\tilde{E}}\right)^{1/2}\tilde{\mathbf{p}}, \quad t = \left(\frac{E}{\tilde{E}}\right)^{-1/4}\tilde{t}, \tag{26}$$

which also implies that $W_E = (E/\tilde{E})^{3/4} W_{\tilde{E}}$. Since the arbitrary width matrix Γ has the dimension of momentum divided by position, it is convenient to choose it to scale as $\Gamma = (E/\tilde{E})^{1/4}\tilde{\Gamma}$.

Thus, choosing $\tilde{E} = 1$ and noting that $f = 2$ for the present systems, (21) becomes

$$T_E^R(q',q) = \frac{1}{2\pi\hbar}\int d\tilde{y}\int d\tilde{p}_y E^{7/8}\tilde{C}^R \exp(iE^{3/4}\phi/\hbar), \tag{27}$$

where the integration is over a Poincaré surface at energy $\tilde{E}$. Here $\tilde{C}^R$ is the prefactor C^R of (22) evaluated at energy $\tilde{E}$ and ϕ is defined as

$$\begin{aligned}\phi = {}& i\tilde{\gamma}'(\tilde{q}' - \tilde{y}_r')^2 + \tilde{p}_{yr}'(\tilde{q}' - \tilde{y}_r') + W_{\tilde{E}}(\tilde{y}_r',\tilde{y}) \\ & + i\tilde{\gamma}(\tilde{q} - \tilde{y})^2 - \tilde{p}_y(\tilde{q} - \tilde{y}),\end{aligned} \tag{28}$$

where $\tilde{\gamma} = \tilde{\Gamma}$ and $\tilde{\gamma}' = \tilde{\Gamma}'$ are one-dimensional width "matrices." This expression allows one to recalculate T_E^R for any energy E by simply rescaling two functions in the integrand. Consequently, the IVR calculation can be efficiently repeated for a large number of energies without the need to recompute trajectories.

An additional quantity with scaling properties for our system is the phase space area $A(E)$ on the PSS classically accessible at energy E, which scales as $(E/\tilde{E})^{3/4}$. Thus the minimum dimension (8) of the transfer matrix can be expressed for the present cases (with $\tilde{E} = 1$) as

$$\tilde{N}(E) = E^{3/4}\frac{A(\tilde{E} = 1)}{2\pi\hbar}. \tag{29}$$

In our work we choose the Poincaré surfaces to lie along the line $x = y\tan\varphi$ that passes through the origin in configuration space at an angle φ from the y axis. Then it is straightforward to evaluate $A(1)$ analytically as

$$A(1) = \frac{2B(1/4,3/2)}{[\beta + 2(\alpha - \beta)\sin^2\varphi\cos^2\varphi]^{1/4}}, \tag{30}$$

where $B(1/4,3/2) \approx 3.4961$ is the beta function.

C. Finding energy eigenvalues

According to Bogomolny's theory, energy eigenvalues semiclassically obey the condition $\det(\mathbf{1} - \mathbf{T}_E) = 0$, so it apparently should be possible to determine the energy levels by searching for values of E that cause the determinant to vanish. However, this condition is strictly obeyed only in the classical limit. Additionally, the determinant is complex valued so, in practice, it does not generally vanish at or near energy eigenvalues when $\hbar \neq 0$. One popular method to overcome this problem is to estimate energy eigenvalues from minima of the function $|\det(\mathbf{1} - \mathbf{T}_E)|$ (see, e.g., [35,36,40,41,47]). Another approach [35] is to estimate semiclassical energies from the zeros of the function $\mathrm{Re}\, D_E$ where the functional determinant D_E is defined as $\exp[-i\pi N_{\mathrm{TF}}(E)]\det(\mathbf{1} - \mathbf{T}_E)$, $N_{\mathrm{TF}}(E)$ being the integrated mean level density (the Thomas-Fermi staircase function). This method is expected to succeed because D_E is known to become real in the classical limit[31–33,35]. However, in agreement with the comments in [42], our experience has been that the above techniques do not reliably detect all energy eigenvalues for the systems treated here.

Haggerty [42] has proposed an alternative way to obtain energy eigenvalues from $\mathbf{T}_E$ that we have found to be successful for the present systems. His approach is based on the behavior (mentioned in Sec. II A) of the complex eigenvalues $\lambda_j \exp(i\theta_j)$ of $\mathbf{T}_E$, as the energy E or the value of Planck's constant $\hbar$ is varied. When the dimension of the transfer matrix exceeds $\tilde{N}(E)$, approximately $\tilde{N}(E)$ eigenvalues, which are relevant for quantization, lie near the unit circle of the complex plane ($\lambda_j \approx 1$), consistent with the expected unitarity of the transfer matrix, while the remaining eigenvalues are clustered about the origin ($\lambda_j \ll 1$). As the energy increases or $\hbar$ decreases, the eigenvalues move around the origin of the complex plane, generally in the counterclockwise sense. Under these conditions $\tilde{N}(E)$ also increases and, to maintain the condition that $\tilde{N}(E)$ eigenvalues lie near the unit circle, eigenvalues that were formerly near the origin spiral outward until their moduli become approximately one. Although away from the classical limit it is not true that an eigenvalue of $\mathbf{T}_E$ becomes exactly unity at a quantum energy level, an eigenvalue of this matrix does cross the positive real axis close to the unit circle near such a quantum energy. Thus quantum levels can be reliably estimated from the energies at which $\theta_j = 0$ and λ_j are sufficiently large.

We note that this quantization criterion becomes equivalent to the exact condition $\det(\mathbf{1} - \mathbf{T}_E) = 0$ in the classical limit since the moduli λ_j then become unity for all relevant eigenvalues j. It can therefore be argued that use of the quantization condition $\theta_j = 0$ is consistent with the semiclassical treatment of the matrix $\mathbf{T}_E$, which is also exact only in the classical limit.

Determining energies that satisfy $\theta_j = 0$ would seem to require following individual eigenvalues of the transfer operator around the complex plane as the energy is varied. This is tedious and difficult since the paths of different eigenvalues can cross. We therefore seek a practical way to automate the process of locating semiclassical energy levels. We begin by defining a minimum modulus a, on the order of unity, for the relevant eigenvalues and use it to define the function

$$Z_1(E) \equiv \prod_{\lambda_j > a} \sin \frac{\theta_j}{2}. \tag{31}$$

Then the condition $Z_1(E) = 0$ identifies energies at which at least one of these eigenvalues crosses the positive real axis. Unfortunately, this product becomes discontinuous when the modulus of an eigenvalue, formerly close to the origin, becomes larger than a and joins the relevant set. As a step toward improving this situation, we smoothly introduce the influence of eigenvalues with moduli between b and a (where $b < a$) by multiplying the above product by the strictly positive quantity

$$Z_2(E) \equiv \prod_{b \leqslant \lambda_j \leqslant a} \left[(1 - x_j)^2 + \left(x_j \sin \frac{\theta_j}{2} \right)^2 \right]^{1/2}, \tag{32}$$

where

$$x_j = \frac{\lambda_j - b}{a - b}. \tag{33}$$

Thus we identify semiclassical energy levels as the zeros of the function

$$Z(E) \equiv Z_1(E) Z_2(E). \tag{34}$$

This construction guarantees that the absolute value of $Z(E)$ is a continuous function of the energy. However, the sign of $Z(E)$ can still change discontinuously at certain values of E and this may seem to cause potential difficulties in detecting true zeros. One reason for a sign change is that when the value of a particular λ_k increases through a and $\sin \theta_k/2 < 0$, the positive factor corresponding to index k, formerly in Z_2, becomes negative when it is transferred to Z_1. A second reason concerns the multivalued nature of the angles θ_j describing the phase of an eigenvalues of $\mathbf{T}_E$. In principle, the branch of each $\theta_j(E)$ should be chosen to make it a continuous function of the energy E. This angle is, however, numerically obtained in a particular interval, typically $(-\pi,\pi)$, and its continuity is difficult to ensure due to the crossing of paths for eigenvalues in the complex plane. For this choice of branch and θ_j near $\pm\pi$, a small variation in the energy may cause the calculated sign of θ_j to abruptly change, causing the sign of the factor $\sin \theta_j/2$ to change and leading to an overall sign discontinuity in $Z(E)$. Fortunately, the problems described here are minor since it is easy to distinguish discontinuities from continuous and smooth passages through zero. When $Z(E)$ is found to change discontinuously, its continuity can be restored by simply inverting its sign.

The choice of parameter b in $Z_2(E)$ is not critical since its value does not affect the zeros of $Z(E)$. A suitable choice of parameter a is also not difficult in practice since the distribution of λ_j values for $\theta_j = 0$ forms distinct peaks for the relevant and irrelevant eigenvalues of $\mathbf{T}$, separated by a gap containing few, if any, eigenvalues [42]. We find that examination of the moduli λ_j, of eigenvalues crossing the positive real axis in the complex plane, for a relatively small range of energies, is sufficient to determine a value of a that successfully divides the eigenvalues into the relevant and irrelevant sets for *all* energies studied. The specific values of a and b used in our calculations will be presented in Sec. IV.

D. Basis functions

Although most of our calculations are carried out using a finite set of points y_i to represent the transfer matrix [as in (7)], we also perform some calculations in which this matrix is represented in a basis of continuous functions on the PSS [see (9)]. As discussed in Sec. II C, this allows us to perform comparative calculations that effectively use Haggerty's numerical technique and provide energy levels consistent with Bogomolny's theory. We choose this basis to consist of harmonic oscillator wave functions

$$\phi_j(q) = \frac{1}{\sqrt{2^j j!}} \left(\frac{2\sigma}{\pi\hbar} \right)^{1/4} e^{-\sigma q^2/\hbar} H_j \left(\sqrt{\frac{2\sigma}{\hbar}} q \right), \tag{35}$$

where the H_j are Hermite polynomials. We further choose the harmonic oscillator width parameter σ to scale as $\sigma = (E/\tilde{E})^{1/4}\tilde{\sigma}$, in a manner similar to the coherent state width parameter γ.

When (15) is substituted into (9), the expression for matrix elements $(\mathbf{T}_E)_{ij}$ is found to involve the quantities $(yp_y|\phi_j)$ and $(\phi_i|y'p'_y)$. With the above basis, the formula [55]

$$\int_{-\infty}^{\infty} e^{-(x-y)^2} H_n(\alpha x) dx = \pi^{1/2} (1 - \alpha^2)^{n/2} H_n \left[\frac{\alpha y}{(1 - \alpha^2)^{1/2}} \right] \tag{36}$$

can be used to express such inner products in the analytical form

$$(yp_y|\phi_j) = \frac{1}{\sqrt{2^j j!}} \left(\frac{\gamma - \sigma}{\gamma + \sigma} \right)^{j/2} \times H_j \left[\left(\frac{2\gamma\sigma}{\gamma^2 - \sigma^2} \right)^{1/2} z \right] g(y,p_y), \tag{37}$$

where

$$g(y,p_y) = \left[\frac{2\pi\hbar\sigma}{(\gamma + \sigma)^2} \right]^{1/4} \times \exp \left[-\left(\gamma\sigma y^2 + p_y^2/4 - i\sigma y p_y \right) / (\gamma + \sigma)\hbar \right] \tag{38}$$

and

$$z = (\gamma/\hbar)^{1/2} y - i(4\gamma\hbar)^{-1/2} p_y. \tag{39}$$

The functions $f_j = (yp_y|\phi_j)$ for $j = 1,2,3,\ldots$ can be conveniently generated by the recursion formula

$$f_j = \sqrt{\frac{4\gamma\sigma}{(\gamma + \sigma)^2}} \left(\frac{z}{\sqrt{j}} \right) f_{j-1} - \sqrt{\frac{j - 1}{j}} \left(\frac{\gamma - \sigma}{\gamma + \sigma} \right) f_{j-2}, \tag{40}$$

with $f_0 = g(y,p_y)$.

E. Other details

The value of $\hbar$ is set to unity in all our calculations. Quantum mechanical energy eigenvalues are determined by diagonalizing the Hamiltonian operator in a large harmonic oscillator basis set, as discussed in [54].

Although the phase space integrations in the IVR expression (24) can be carried out by ordinary quadrature methods for the present low-dimensional system, they are performed here by a Monte Carlo technique to explore the feasibility of the general IVR treatment for larger systems, where quadrature techniques are impractical. To generate random y and p_y values for the Monte Carlo integration, a rectangular portion of the Poincaré plane, containing the classically allowed region, is uniformly sampled and points falling outside this region are rejected. The accepted points serve 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.

Because all classical trajectories needed for the calculations are short, chaos does not impede convergence of the Monte Carlo sums. Thus, in contrast to previous IVR calculations for highly chaotic systems, all sampled trajectories in the classically allowed region are retained and there is no need to impose numerical filtering or trajectory termination procedures to achieve convergence in the present work.

IV. RESULTS

A. Integrable case

We first consider results of our treatment for an integrable system defined by the Hamiltonian (25) with the parameters $\alpha = 0$ and $\beta = 0.01$. The Poincaré surface is chosen as the line $y = x$ passing through the origin in configuration space, corresponding to the rotational angle $\varphi = \pi/4$ in (30). The transfer matrix is constructed as in (7), where the discrete values q_k are chosen as N equally spaced points between the minimum and maximum classically allowed positions on the PSS. The Gaussian width parameters are chosen as $\tilde{\gamma} = \tilde{\gamma}' = 0.5$ and energies of the 47 states of A_1 symmetry with $E < 12$ are investigated.

Figure 1 plots the difference $\Delta E = E_{\rm qm} - E_{\rm sc}$, between the accurate quantum energies $E_{\rm qm}$ and the semiclassical energies $E_{\rm sc}$, as a function of the dimension N of matrix $\mathbf{T}_E$, for levels with $11 < E < 12$. The phase space integrals in the IVR expression were evaluated with 5×10^4 classical trajectories (Monte Carlo points). The results show that the computed energies essentially converge for $N \approx 38$, which is only about 40% higher than the theoretical minimum value $\tilde{N}(E) \approx 27$ for these states. We have observed similar convergence behavior for other energy ranges examined for this system. As discussed above, calculations based on Bogomolny's transfer matrix usually require dimensions on the order of 10 times $\tilde{N}(E)$ in order to obtain converged energies using the conditions $|\det(\mathbf{1} - \mathbf{T}_E)| = 0$ or $\mathrm{Re}\, D_E = 0$. The success of the present calculations with much smaller matrix dimensions can be attributed to the use of the alternate method described in Sec. III C for the determination of the energies.

Figure 2 examines the dependence of the computed energies on $N_{\rm tr}$, the number of classical trajectories that are used to evaluate the integrals over the PSS. These calculations were performed using $N = 38$ for the same levels as in Fig. 1. The convergence with respect to $N_{\rm tr}$ is seen to be very slow. This behavior can be understood in terms of the results presented in Appendix A, which establish that the semiclassical energies obtained in our calculations can be expressed as Monte Carlo averages over contributions from the $N_{\rm tr}$ randomly sampled trajectories. The slow improvement in the precision of the energies observed here is consistent with the $N_{\rm tr}^{-1/2}$ convergence that characterizes such Monte Carlo averages. Despite this unfavorable feature, the calculations already appear to be converged to a reasonable degree for $N_{\rm tr} \geqslant 1.2 \times 10^4$ trajectories.

Although the $N_{\rm tr}^{-1/2}$ convergence of the Monte Carlo method is a disadvantage for the determination of accurate

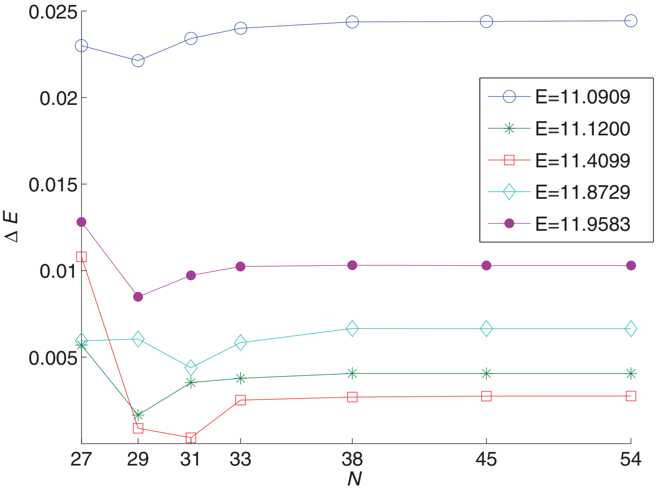

FIG. 1. (Color online) Error in the semiclassical energy eigenvalues in the range $11 < E < 12$ for the integrable system, as a function of the dimension N of the transfer matrix. The ΔE and energies in the legend are expressed in atomic units.

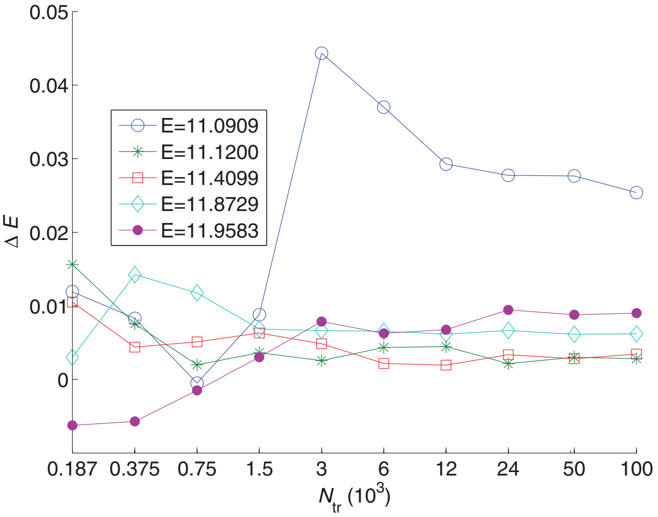

FIG. 2. (Color online) Error in the semiclassical energy eigenvalues in the range $11 < E < 12$ for the integrable system, as a function of the number of trajectories used in the IVR calculations. The ΔE and energies in the legend are expressed in atomic units.

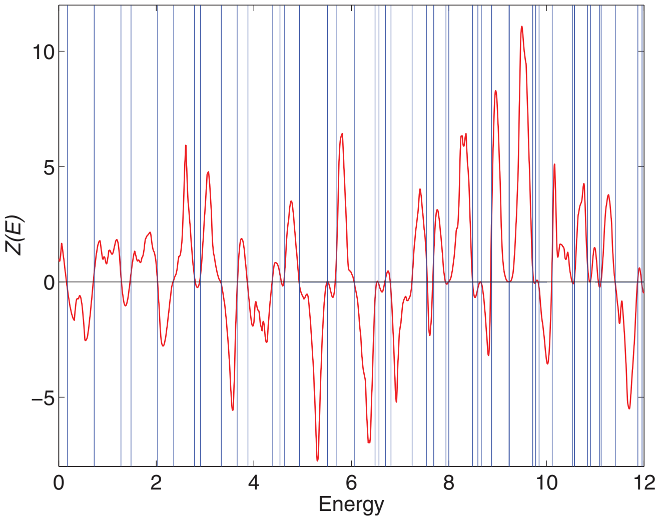

FIG. 3. (Color online) Plot of $Z(E)$ versus energy for A_1 states of the integrable system. Vertical lines indicate the quantum energy levels. Energies are expressed in atomic units.

results, it makes it possible to obtain qualitatively correct estimates with only a few trajectories. Thus the calculations are seen to predict the existence of the correct number of quantum levels in the energy range explored using fewer than 200 trajectories. The convergence rate of the Monte Carlo method improves significantly for lower energies due to the factor $E^{3/4}$ appearing in the exponential of Eq. (27), which reduces the fluctuations in the integral. Interestingly, we have found that the IVR transfer matrix for this system already predicts the correct number of energy levels in the interval $0 < E < 2.5$ using as few as two trajectories. Of course, the success of this method with such a small number of random integration points involves an element of luck.

Figure 3 displays the function $Z(E)$ defined in (34) for the full range of energies investigated. These calculations were performed using 5×10^4 trajectories and matrix dimension $N = 38$. Values $a = 0.8$ and $b = 0$ were used for the parameters in the expression for $Z(E)$ throughout the energy range. The magnifications in Fig. 4 confirm that there exists a one-to-one correspondence between the zeros of $Z(E)$ and the quantum energy levels in the entire range. Considering the near degeneracies of many of the levels, the successful resolution of all the quantum energies here is remarkable.

Figure 5 examines the accuracy of the calculations for this system by plotting the error $\Delta E = E_{\rm qm} - E_{\rm sc}$ (in units of the mean level spacing) for the semiclassical energies $E_{\rm sc}$ obtained in Figs. 3 and 4. A solid line connects points with the largest negative errors in Fig. 5. These points can be shown to correspond to states with quantum numbers $(2n,2n)$, $n = 0,1,2,\ldots,$ for the two degrees of freedom of the separable Hamiltonian. Similarly, a dashed line connects the points with the next-largest negative errors, corresponding to states with quantum numbers $(2n,2n+2)$. The formation of such distinct families of error points is also evident in the results of Haggerty [42] for the near-integrable case treated there. As in the present calculations, the largest errors are found for states with the greatest excitation along the PSS. Biechele *et al.* [36] also reported difficulties for such states in their treatment of the two-dimensional harmonic oscillator. A qualitative explanation for the exceptionally large errors in these cases was proposed in [42].

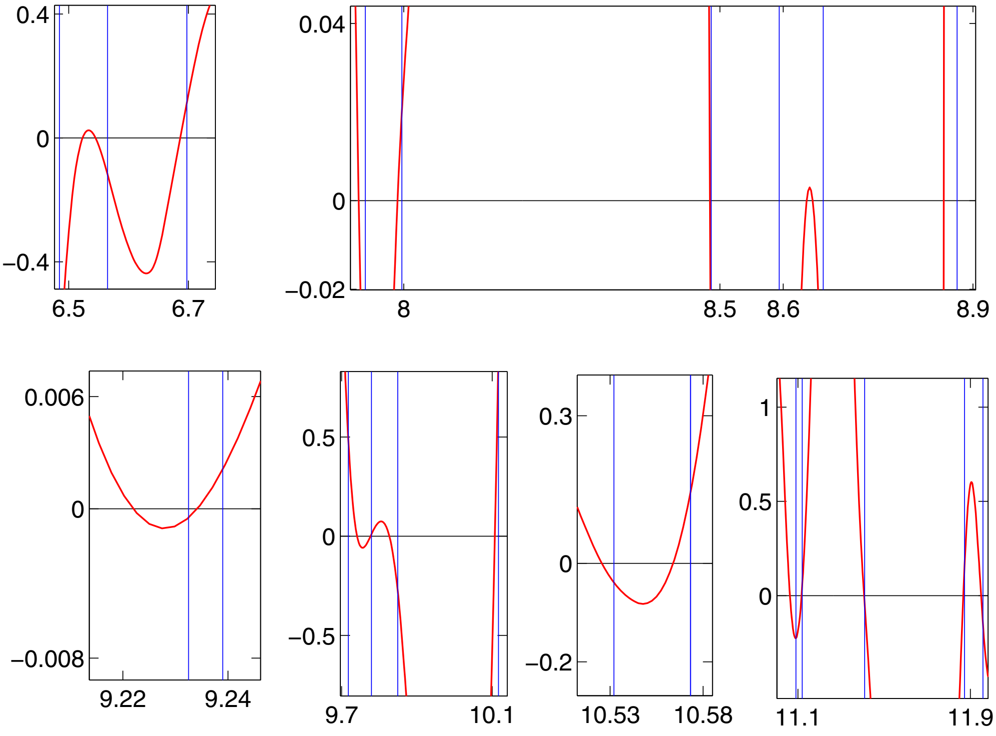

FIG. 4. (Color online) Magnified view of the function $Z(E)$ for A_1 states of the integrable system in regions of near degeneracies. Energies on the abscissa are expressed in atomic units. Vertical lines indicate the quantum energy levels.

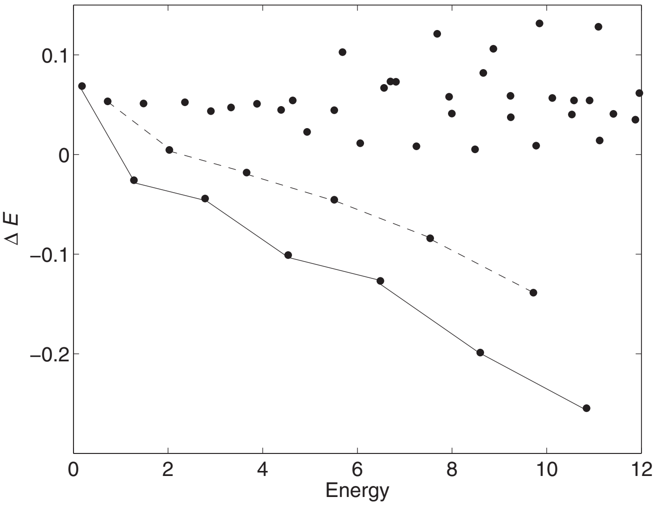

FIG. 5. Error (in units of the mean level spacing) for the semiclassical energy eigenvalues of the integrable system, plotted as a function of the energy. The energies on the abscissa are expressed in atomic units.

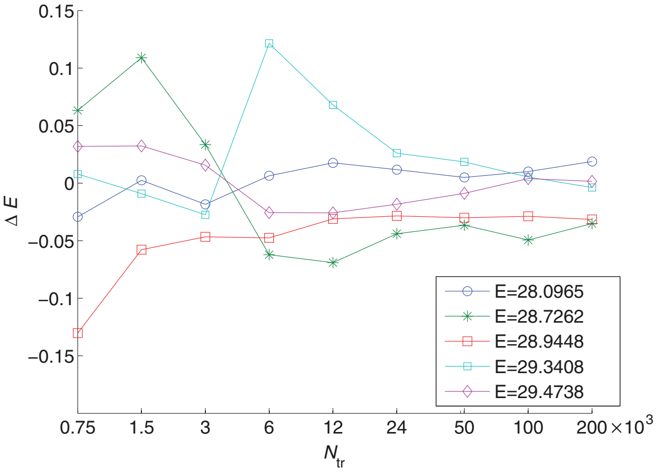

FIG. 7. (Color online) Error in the semiclassical energy eigenvalues in the range $28 < E < 30$ for the chaotic system, as a function of the number of trajectories used in the IVR calculations. The ΔE and energies in the legend are expressed in atomic units.

B. Chaotic case

To make the system almost completely chaotic with large Lyapunov numbers, the parameters in the Hamiltonian (25) are chosen to have the values $\alpha = 1.00$ and $\beta = 0.01$ [54]. Calculations of the transfer matrix are carried out using a PSS defined by the condition $x = 0$, corresponding to the rotational angle $\varphi = 0$ in (30). Here $\mathbf{T}_E$ is constructed in the position representation in the same manner as for the integrable system and once again the Gaussian width parameters are chosen as $\tilde{\gamma} = \tilde{\gamma}' = 0.5$. The energies of 61 states of A_1 symmetry with $E < 35$ are studied.

The error in the semiclassical energies for the range $28 < E < 30$ is plotted as a function of the dimension N of the transfer matrix in Fig. 6 for calculations using 5×10^4 trajectories. It can be seen that the IVR results converge to a very good accuracy for $N \approx 60$, which is only 33% larger than the theoretical minimum $\tilde{N} \approx 45$. Similar results are obtained at other energies. This once again contrasts with the much larger matrix dimensions found necessary in most other calculations.

Figure 7 examines the error in the semiclassical calculations as a function of the number of classical trajectories N_{tr} for levels with $28 < E < 30$ and the fixed matrix dimension $N = 60$. The convergence of the Monte Carlo treatment is found to be even slower than observed for the integrable case in Fig. 2. As a result, the statistical errors in the computed energy eigenvalues are greater than for the integrable system with comparable values of N_{tr}.

The function $Z(E)$ is displayed for the full range of energies investigated in Figs. 8 and 9. The calculations were carried

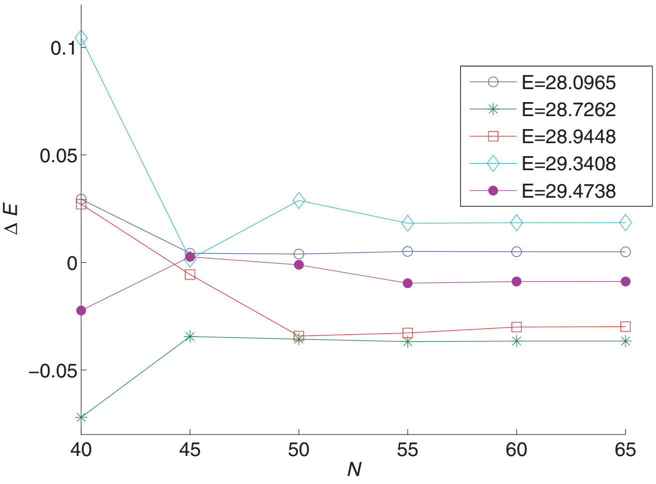

FIG. 6. (Color online) Error in the semiclassical energy eigenvalues in the range $28 < E < 30$ for the chaotic system, as a function of the dimension N of the transfer matrix. The ΔE and energies in the legend are expressed in atomic units.

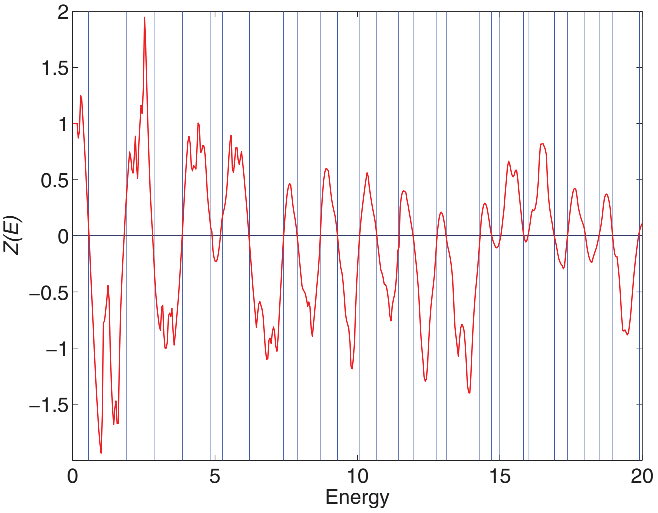

FIG. 8. (Color online) Plot of $Z(E)$ versus energy for the chaotic potential for the range $E = 0$–20. Vertical lines indicate the quantum energy levels. Energies are expressed in atomic units.

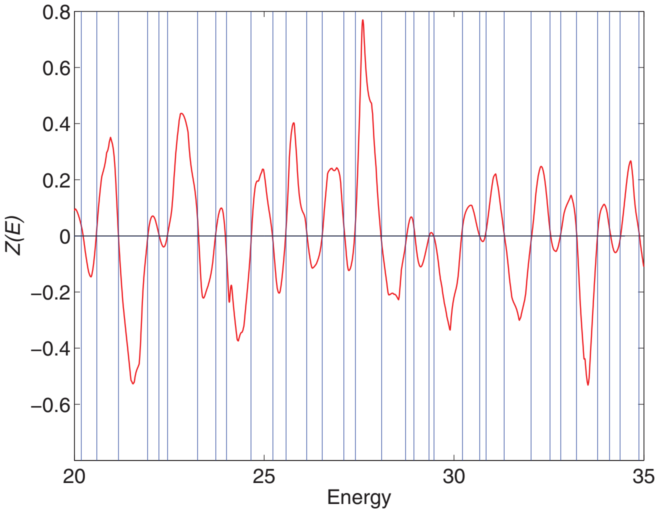

FIG. 9. (Color online) Plot of $Z(E)$ versus energy for the chaotic potential for the range $E = 20$–35. Vertical lines indicate the quantum energy levels. Energies are expressed in atomic units.

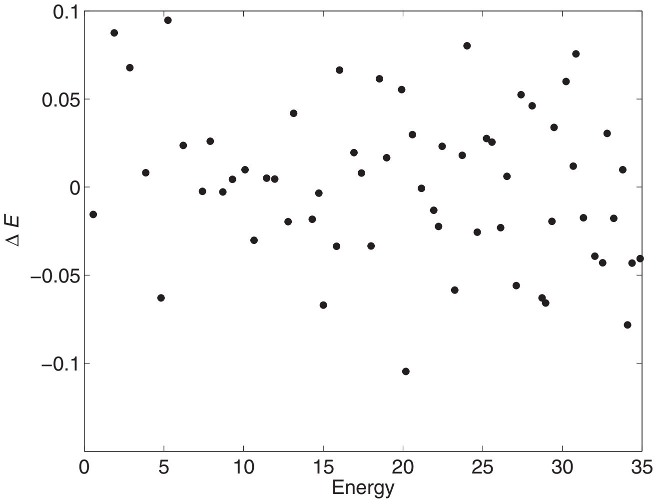

FIG. 10. Error (in units of mean level spacing) for the semiclassical energy eigenvalues of the chaotic system, plotted as a function of the energy. The energies on the abscissa are expressed in atomic units.

out using $N = 60$, $N_{\rm tr} = 5 \times 10^4$, and constant values $a = 1.0$ and $b = 0.0$ for the parameters in $Z(E)$ throughout the energy range. As in the integrable case, there is a one-to-one relationship between the zeros of $Z(E)$ and the quantum levels in the entire energy range investigated, so all such levels are unambiguously resolved. In contrast, previous semiclassical IVR calculations for the trace of Green's function for this system [6,19] display false peaks where there are no quantum levels and some ambiguously weak peaks near actual quantum levels. Additionally, these previous calculations are unable to resolve all levels for energies greater than about 14.0, due to the high level density and spectral peak broadening caused by the termination of long trajectories. Thus, in a sense, the present calculations successfully overcome the long-trajectory IVR problem for this system.

Figure 10 presents the error (in units of the mean level spacing) in the semiclassical energy levels obtained from Figs. 8 and 9. Unlike Fig. 5 for the integrable system, the distribution of errors seems random with no evidence of the formation of families with regular error patterns, or states with anomalously large errors, or a systematic increase in mean error with energy. In drawing these conclusions, however, it must be remembered that the statistical uncertainties in the calculations, associated with the Monte Carlo integration, are relatively large and may partially mask such trends, particularly at high energies.

C. The δ function limit

We wish to compare the numerical efficiency of our IVR treatment (as applied with finite values of γ) to that of Haggerty's method and the accuracy of our semiclassical approximation to that of Bogomolny's theory. As explained in the Sec. II C, we accomplish this by applying our IVR formula to the transfer matrix in a basis of continuous functions [see Eqs. (15) and (9)] with a very large value for the Gaussian width parameter γ that effectively converts the Gaussian functions to δ functions. In this section we describe such calculations using the harmonic oscillator basis discussed in Sec. III D. We treat the chaotic system described in Sec. IV B and choose the large value of $\tilde{\gamma}$ (for $\tilde{E} = 1$) as 1000. Tests show that order-of-magnitude increases or decreases in this value barely affect the IVR results so, for practical purposes, this choice achieves the required δ function limit.

These calculations are compared to those with the same harmonic oscillator basis but using $\tilde{\gamma} = 0.5$, as in Sec. IV B. These are found to produce energies and standard deviations (see below) that are practically identical to those of Sec. IV B with the same value $N_{\rm tr}$, as expected for treatments that differ only in the matrix representation.

The same sample of trajectories is used in the calculations for both values of γ. To obtain sufficient precision for unambiguous comparisons, the number of trajectories is chosen to be 4×10^5. Since the value of $N_{\rm tr}$ needed to maintain the required degree of convergence increases steeply with E, the present investigations are limited to the 19 energy levels with $E < 15$.

The width parameter for the harmonic oscillator basis is chosen as $\tilde{\sigma} = 0.5$ for $\tilde{E} = 1$. It is found that this basis is less efficient than the position representation used in Secs. IV A and IV B and the matrix dimension N needs to be about 2.6 times the minimum theoretical dimension $\tilde{N}$ to achieve convergence in the present cases. For the energy levels investigated here, $\tilde{N}$ is less than 27 and N is chosen as 80.

Figure 11 compares results for the two calculations. The statistical uncertainty in the semiclassical energies is indicated by error bars corresponding to two standard deviations in the computed results. As explained in Appendix B, the standard deviation is estimated as the absolute difference of the energies obtained with 4×10^5 and 2×10^5 trajectories. Although the relative sizes of the individual error bars for the two calculations vary with the energy level, the average statistical errors for the large γ results are a factor of 2.25 greater than those for the $\tilde{\gamma} = 0.5$ case. Given the expected $N_{\rm tr}^{-1/2}$ dependence for the convergence of Monte Carlo techniques,

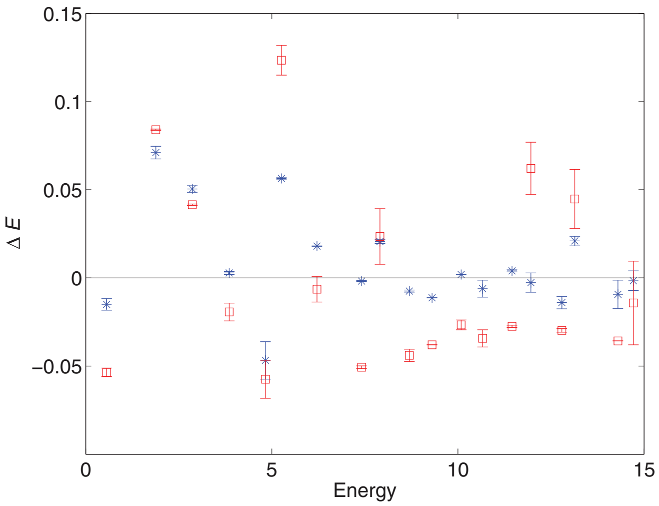

FIG. 11. (Color online) Comparison of errors in the semiclassical energies obtained using $\tilde{\gamma} = 0.5$ (stars) and $\tilde{\gamma} = 1000$ (squares). The two calculations use identical classical data and harmonic oscillator basis sets. The ΔE and energies on the abscissa are expressed in atomic units.

the number of trajectories in the calculation with large γ would have to be increased by a factor of about 5 to achieve the same degree of convergence as for small γ. This confirms that the present IVR treatment, which advocates Gaussian factors of finite and nonzero width, is significantly more numerically efficient than the method proposed in [42].

In all but three cases, the results of the two calculations displayed in Fig. 11 fall outside the mutual error bars. This verifies that the present treatment produces semiclassical energies that are different from those of the Bogomolny theory. More surprisingly, eliminating the above three uncertain cases, the absolute errors of the $\tilde{\gamma} = 0.5$ calculation are smaller than those obtained with $\tilde{\gamma} = 1000$ for 14 of the 16 energies examined. This implies that the accuracy of the present IVR treatment, with finite and nonzero Gaussian widths, is better than that of Bogomolny's method for most of the states investigated for the present system. Further remarks are presented in the following section.

V. SUMMARY AND REMARKS

This work describes an attempt to overcome the long-trajectory problem that limits the usefulness of IVR methods, especially for systems that are chaotic or large. For this purpose we formulated Bogomolny's transfer matrix as an IVR expression. Additionally, we adapted the expression to allow determination of energy levels for bound states of a desired symmetry. We found that the technique indeed overcomes the problem of long trajectories so it successfully resolves all energy levels of a chaotic system.

The approach described here has advantages, relative to the direct application of Bogomolny's method, that are especially crucial for the treatment of large systems with smooth potentials. Particularly, the present method does not require searches for special trajectories obeying boundary conditions on the PSS. Although this favorable property is shared by Haggerty's method, the present technique requires significantly fewer trajectories to converge the IVR integrations by the Monte Carlo procedure. This advantage will become especially important for treatment of larger systems where integration by the Monte Carlo technique is practically unavoidable.

In this work the semiclassical energy levels are obtained from the eigenvalues of the transfer matrix by the method described in Sec. III C, which is a variation of a technique developed by Haggerty. With this approach it is found that the dimension N of the transfer matrices need not be much larger than the theoretical minimum $\tilde{N}$, determined by Bogomolny's theory. Since this dimension is much smaller than that used in most previous calculations of $\mathbf{T}_E$ and since the numerical effort to diagonalize matrices or calculate determinants scales as N^3, this result has substantial numerical implications.

The relatively rapid Monte Carlo convergence of the present IVR technique, as compared with the method of [42], is consistent with previous investigations. For IVR expressions in the position representation, it is known that the presence of Gaussian factors improves the Monte Carlo convergence because it damps out the rapid oscillations of the integrand away from points of stationary phase [4,48]. Semiclassical approximations for energy eigenstates in the coherent state representation [56] can be used to verify that this conclusion also applies to IVR treatments in bases formed by wave functions of integrable systems, e.g., the harmonic oscillator states of Sec. IV C. However, this favorable damping of the integrand occurs only when γ is chosen to have a finite and nonzero value, so the treatment of [42] (where γ is effectively taken as infinite) does not benefit from the increased numerical efficiency.

As stressed earlier in this work, the IVR treatment for the transfer matrix is not generally equivalent to Bogomolny's theory, except in the classical limit. Our numerical treatment of the chaotic system indeed confirms that the energy levels produced by the IVR method, with moderate values of γ, differ from those obtained by Bogomolny's approximation. More intriguingly, the results clearly suggest that the IVR energies are more accurate than those obtained from Bogomolny's theory for most of the states of the system investigated.

This result seems surprising in view of the treatment applied in Sec. II, which derived the IVR expression for the transfer matrix by requiring it to reduce to Bogomolny's formula (the target theory) when the phase space integrals are evaluated by the stationary phase method. This approach is entirely analogous to treatments used to derive IVR expressions for other quantities [4,5,7–10,50]. Though convenient, however, this method of derivation leaves the impression that the resulting IVR expression is an only approximation to the target semiclassical theory, making it a presumably inferior and less accurate approximation. In the case of the IVR formula for the time-dependent propagator, an alternative derivation can be used to show that this conclusion is incorrect: The IVR expression is a uniform semiclassical approximation that remains accurate at caustics provided the Gaussian width parameters are chosen to be finite and nonzero [2,4,11]. It is thus superior to the Van Vleck approximation, which is the target theory in this case. Furthermore, there is numerical evidence that analogous conclusions apply to IVR expressions for the time-independent wave function [7,8,50], the Green's function [5], angular momentum coupling coefficients [57], and (perhaps most highly relevant [44,45]) the S matrix [9,10]. Therefore, despite expedient derivations that do not always do justice to the resulting theories, it may be appropriate to regard IVR treatments, including the present one, as generally different semiclassical approximations and to anticipate that they may be superior to the targets in some respects. Viewed in this way, the numerical results found in Sec. IV C are less surprising.

Despite these remarks, we are not aware of previous numerical evidence suggesting that energy levels of chaotic systems, computed by IVR techniques, may be more accurate than those obtained by more conventional semiclassical methods. The required comparisons have apparently not been possible because of the limited precision of the IVR calculations, brought about by the long-trajectory problem. The high resolution of the energy levels achieved here offers a real opportunity to detect such possible differences in accuracy.

While the higher accuracy for the IVR energies observed in the present work is certainly interesting, it remains only an empirical result since a detailed theoretical explanation is lacking. In addition to further theoretical analysis, calculations applying more strongly convergent integration methods to a larger variety of states and systems are clearly desirable.

The treatment developed here is an encouraging attempt to overcome the long-trajectory problem that plagues IVR calculations by applying techniques related to the semiclassical ζ function. However, as already noted in [42], the extraction of energy levels directly from $\mathbf{T}_E$ involves matrix algebra that confers a quantum mechanical flavor to the approach and introduces an unfavorable scaling with respect to system dimensionality. It might be possible to overcome these disadvantages by developing an IVR treatment based on the expansions of the ζ function used to derive periodic orbit treatments.

APPENDIX A: ENERGY LEVELS AS MONTE CARLO AVERAGES

The phase space integrals in the IVR expressions for the transfer matrix elements are evaluated in this work by a Monte Carlo method. Thus the transfer matrix $\mathbf{T}$, constructed from a sample of M ($\equiv N_{\text{tr}}$) trajectories, is approximated as the average

$$\mathbf{T}^{(M)} = M^{-1}\sum_{j=1}^{M}\mathbf{T}_j, \tag{A1}$$

where $\mathbf{T}_j$ is the contribution from a particular trajectory j, initiated from a random sample of initial conditions on the PSS. Many of our conclusions about the convergence of the calculations with respect to M rest on the claim that each resulting semiclassical energy level $E^{(M)}$, obtained from $\mathbf{T}^{(M)}$, also has the form of a Monte Carlo average

$$E^{(M)} = M^{-1}\sum_{j=1}^{M}E_j, \tag{A2}$$

where the variable E_j can be interpreted as the contribution to the energy level from trajectory j. However, since the semiclassical energies are obtained from the rather indirect condition that (in principle) certain eigenvalues of $\mathbf{T}^{(M)}$ are unity, the above claim is not self-evident and is therefore established here.

We begin by showing that the eigenvalues of the IVR transfer matrix have the form of a Monte Carlo average provided M is large enough that the error in the Monte Carlo approximation can be treated perturbatively. We would like to estimate solutions of the eigenvalue equation

$$\mathbf{T}^{(M)}\mathbf{u}^{(M)} = \tau^{(M)}\mathbf{u}^{(M)}, \tag{A3}$$

where $\tau^{(M)}$ are particular eigenvalues of $\mathbf{T}^{(M)}$ near unity (assumed nondegenerate) and $\mathbf{u}^{(M)}$ are the corresponding eigenvectors. To accomplish this, we apply a perturbative treatment based on the decomposition

$$\mathbf{T}^{(M)} = \mathbf{T} + \Delta\mathbf{T}, \tag{A4}$$

where the unperturbed transfer matrix is calculated by an exact Monte Carlo treatment with $M \to \infty$ and the perturbation $\Delta\mathbf{T}$ is assumed to be small. In terms of the right eigenvector $\mathbf{u}$ and the left eigenvector $\mathbf{v}^T$ of $\mathbf{T}$, for the eigenvalue τ of $\mathbf{T}$ corresponding to $\tau^{(M)}$, standard first-order perturbation theory gives

$$\tau^{(M)} = \tau + \mathbf{v}^T\Delta\mathbf{T}\mathbf{u} = \mathbf{v}^T\mathbf{T}^{(M)}\mathbf{u}. \tag{A5}$$

Substitution of (A1) then expresses $\tau^{(M)}$ as the Monte Carlo average

$$\tau^{(M)} = M^{-1}\sum_{j=1}^{M}\tau_j, \tag{A6}$$

where

$$\tau_j \equiv \mathbf{v}^T\mathbf{T}_j\mathbf{u}. \tag{A7}$$

We recall that all the above matrices, eigenvalues, and eigenvectors are implicitly functions of the energy E. For Monte Carlo calculations using M trajectories, semiclassical levels $E^{(M)}$ are obtained from eigenvalues $\tau^{(M)}$ obeying the condition

$$\tau^{(M)}(E^{(M)}) = 1. \tag{A8}$$

We wish to estimate such energies in terms of the semiclassical levels $\mathcal{E} \equiv E^{(\infty)}$ obtained with an accurate Monte Carlo calculation using an infinite number of trajectories. These energies obey the condition

$$\tau(\mathcal{E}) = 1. \tag{A9}$$

To accomplish this we express $\tau^{(M)}$ as

$$\tau^{(M)}(E) = \tau(E) + \Delta\tau(E), \tag{A10}$$

where $\Delta\tau = \mathbf{v}^T\Delta\mathbf{T}\mathbf{u}$ [see (A5)], and decompose $E^{(M)}$ as

$$E^{(M)} = \mathcal{E} + \Delta E, \tag{A11}$$

which implicitly defines ΔE. Substituting (A11) into (A10) and applying condition (A8) gives

$$\tau(\mathcal{E} + \Delta E) + \Delta\tau(\mathcal{E} + \Delta E) = 1. \tag{A12}$$

Expanding and neglecting terms to second and higher order in the differences yields

$$\tau(\mathcal{E}) + \Delta E\tau'(\mathcal{E}) + \Delta\tau(\mathcal{E}) = 1, \tag{A13}$$

where the prime denotes the energy derivative. Applying (A9) and rearranging the equation now produces

$$\Delta E = -\Delta\tau(\mathcal{E})/\tau'(\mathcal{E}), \tag{A14}$$

which, using (A9)–(A11), can be expressed as

$$E^{(M)} = \mathcal{E} + [1 - \tau^{(M)}(\mathcal{E})]/\tau'(\mathcal{E}). \tag{A15}$$

Finally, applying (A6), Eq. (A15) can be written as the Monte Carlo average of (A2), where

$$E_j \equiv \mathcal{E} + [1 - \tau_j(\mathcal{E})]/\tau'(\mathcal{E}), \tag{A16}$$

thus establishing the desired result.

APPENDIX B: MONTE CARLO ERROR ESTIMATE

Consider IVR calculations of semiclassical energies employing two sets of trajectories for the Monte Carlo integration: the first consisting of M trajectories and the second obtained by adding another M independent trajectories to this set to form a total of $2M$ samples. We would like to establish that the absolute difference $|E^{(2M)} - E^{(M)}|$ between the resulting semiclassical energies is an estimate of the standard deviation $s^{(2M)}$ in the energy $E^{(2M)}$ obtained with $2M$ trajectories.

Since the calculation with $2M$ trajectories effectively pools the results from two separate calculations with M trajectories, we can apply (A2) to express

$$E^{(2M)} = \tfrac{1}{2}(E^{(M)} + E^{(M)'}) \tag{B1}$$

in terms of energies obtained with the first and second sets of M trajectories. Recognizing $E^{(2M)}$ as the mean of these two energies, we can write

$$\begin{aligned} E^{(M)'} &= E^{(2M)} + \tfrac{1}{2}\delta E, \\ E^{(M)} &= E^{(2M)} - \tfrac{1}{2}\delta E, \end{aligned} \tag{B2}$$

where

$$\delta E = E^{(M)'} - E^{(M)} \tag{B3}$$

is assumed positive. Equation (B1) allows us to eliminate $E^{(M)'}$ and express δE as

$$\delta E = 2|E^{(2M)} - E^{(M)}|. \tag{B4}$$

It is now simple to use (B2) to calculate the sample standard deviation for the pair of energies $E^{(M)'}$ and $E^{(M)}$. The result is

$$s^{(M)} = \delta E/\sqrt{2}, \tag{B5}$$

which can also be expressed as

$$s^{(M)} = \sqrt{2}|E^{(2M)} - E^{(M)}| \tag{B6}$$

by applying (B4). The standard deviation defined in this way estimates the statistical error obtained with a sample of M trajectories. Equation (A2), expressing the semiclassical energies as a Monte Carlo average, implies that the standard deviation $s^{(2M)}$, obtained with a sample of $2M$ trajectories, should be smaller than $s^{(M)}$ by a factor of $\sqrt{2}$. This yields the desired estimate

$$s^{(2M)} = |E^{(2M)} - E^{(M)}|. \tag{B7}$$

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