Periodic Orbit Quantization by Harmonic Inversion of Gutzwiller's Recurrence Function

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Semiclassical eigenenergies and resonances are obtained from classical periodic orbits by harmonic inversion of Gutzwiller's semiclassical recurrence function, i.e., the trace of the propagator. Applications to the chaotic three disk scattering system and, as a mathematical model, to the Riemann zeta function demonstrate the power of the technique. The method does not depend on the existence of a symbolic code and might be a tool for a semiclassical quantization of systems with nonhyperbolic or mixed regular-chaotic dynamics as well. [S0031-9007(97)03694-6]

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Since the development of *periodic orbit theory* by Gutzwiller [1,2] it has become a question as to how individual semiclassical eigenenergies and resonances can be obtained from periodic orbit quantization for classically chaotic systems. A major problem is the exponential proliferation of the number of periodic orbits with increasing period, resulting in a divergence of Gutzwiller's trace formula at real energies and below the real axis where the poles of Green's function are located. As a consequence, in a direct summation of periodic orbit contributions, smoothing techniques must be applied, resulting in low resolution spectra for the density of states [3]. To extract individual eigenstates, the semiclassical trace formula has to be analytically continued to the region of the quantum poles. This can be achieved by reformulating the eigenvalue problem as finding the zeros of a dynamical zeta function, i.e., an infinite product over entries from classical cycles and by analytic continuation of the Euler product applying *cycle expansion* techniques [4–7]. However, the cycle expansion requires the existence and knowledge of a symbolic code for the periodic orbits and is therefore restricted to a small class of systems. In particular, it is a nontrivial task to apply this concept to systems with a mixed regular-chaotic classical dynamics.

In this Letter we present a new technique for periodic orbit quantization based on the *harmonic inversion* of the semiclassical trace formula for the propagator, which is the Fourier transform of the semiclassical response function. The method requires only the knowledge of all orbits up to a sufficiently long but finite period and does not rely on, e.g., the existence of a symbolic code for the orbits. It may therefore be applied in general to a large variety of systems with an underlying chaotic, mixed, or even regular classical dynamics.

Following Gutzwiller [1,2] the semiclassical response function for chaotic systems is given by

$$g^{\mathrm{sc}}(E) = g_0^{\mathrm{sc}}(E) + \sum_{\mathrm{po}} A_{\mathrm{po}} e^{iS_{\mathrm{po}}}, \tag{1}$$

where $g_0^{\mathrm{sc}}(E)$ is a smooth function and the S_{po} and A_{po} are the classical actions and weights (including phase information given by the Maslov index) of periodic orbit contributions. Equation (1) is also valid for integrable [8] and near-integrable [9] systems, but with different expressions for the amplitudes A_{po}. The eigenenergies and resonances are the poles of the response function, but unfortunately, its semiclassical approximation (1) does not converge in the region of the poles; thus the problem is the analytic continuation of $g^{\mathrm{sc}}(E)$ to this region.

In the following we assume that the classical system has a scaling property; i.e., the shape of periodic orbits does not depend on the scaling parameter, w, and the classical action scales as $S_{\mathrm{po}} = ws_{\mathrm{po}}$. Examples of scaling systems are billiards, Hamiltonians with homogeneous potentials, Coulomb systems, or the hydrogen atom in external magnetic and electric fields. Quantization yields bound states or resonances, w_k, for the scaling parameter. For scaling systems the semiclassical response function $g^{\mathrm{sc}}(w)$ can be Fourier transformed easily to obtain the semiclassical trace of the propagator

$$C^{\mathrm{sc}}(s) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} g^{\mathrm{sc}}(w)e^{-isw}\,dw = \sum_{\mathrm{po}} A_{\mathrm{po}}\,\delta(s - s_{\mathrm{po}})\,. \tag{2}$$

The signal $C^{\mathrm{sc}}(s)$ has δ peaks at the positions of the classical recurrences $s = s_{\mathrm{po}}$ of periodic orbits and with peak heights (recurrence strengths) A_{po}; i.e., $C^{\mathrm{sc}}(s)$ is Gutzwiller's periodic orbit recurrence function. Consider now the quantum mechanical counterparts of $g^{\mathrm{sc}}(w)$ and $C^{\mathrm{sc}}(w)$ taken as the sums over the poles w_k of Green's function,

$$g^{\mathrm{qm}}(w) = \sum_k \frac{d_k}{w - w_k + i\epsilon}\,, \tag{3}$$

$$C^{\mathrm{qm}}(s) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} g^{\mathrm{qm}}(w)e^{-isw}\,dw = -i\sum_k d_k e^{-iw_k s}, \tag{4}$$

with d_k being the multiplicities of resonances, i.e., $d_k = 1$ for nondegenerate states. Extraction of the frequencies,

w_k, and amplitudes, d_k, from the signal $C^{\mathrm{qm}}(s)$ defined on a finite segment is known as *harmonic inversion* with a large variety of applications in various fields [10]. Recently the method was applied to analyze quantum spectra by fitting them to the functional form of Gutzwiller's trace formula [11]. It is the main issue of this Letter to show that this procedure can be reverted and *semiclassical* eigenvalues and resonances can be extracted by fitting Gutzwiller's semiclassical periodic orbit recurrence signal $C^{\mathrm{sc}}(s)$ to the functional form of Eq. (4). This means that the method of harmonic inversion can be successfully applied for periodic orbit quantization. The frequencies, w_k, obtained by harmonic inversion of $C^{\mathrm{sc}}(s)$ are the semiclassical approximation to the poles of Green's function in (3).

The harmonic inversion problem can be formulated as a nonlinear fit (see, e.g., Ref. [10]) of the signal $C(s)$ defined on an equidistant grid,

$$c_n \equiv C(n\tau) = \sum_k d_k e^{-in\tau w_k}, \qquad n = 0, 1, 2, \ldots, N, \tag{5}$$

with the set of generally complex variational parameters $\{w_k, d_k\}$. [In this context the discrete Fourier transform scheme would correspond to a linear fit with N amplitudes d_k and fixed real frequencies $w_k = 2\pi k/N\tau$, $k = 1, 2, \ldots, N$. The latter implies the so-called "uncertainty principle"; i.e., the resolution, defined by the Fourier grid spacing, Δw, is inversely proportional to the length, $s_{\max} = N\tau$, of the signal C(s).] The "high resolution" property associated with Eq. (5) is due to the fact that there is no restriction for the closeness of the frequencies w_k as they are variational parameters. In Ref. [12] it was shown how this nonlinear fit problem can be recasted as a linear algebra one using the filter-diagonalization procedure. The crucial idea was to associate the signal c_n with an autocorrelation function of a suitable dynamical system,

$$c_n = \langle \Phi_0 | e^{-in\tau\hat{\Omega}} | \Phi_0 \rangle, \tag{6}$$

with the effective complex symmetric Hamiltonian $\hat{\Omega}$ whose eigenvalues are the frequencies, w_k, of interest. $\langle \cdots | \cdots \rangle$ corresponds to the complex symmetric inner product (i.e., no complex conjugation). The "initial state" Φ_0 is defined implicitly by identifying the amplitudes d_k with the overlaps $\langle \Phi_0 | \Phi_n \rangle^2$ of Φ_0 with the eigenvectors, Φ_k, of $\hat{\Omega}$. This establishes an equivalence between the problem of extracting spectral information from the signal with the one of diagonalizing the evolution operator $\hat{U} = e^{-i\tau\hat{\Omega}}$ (or the Hamiltonian $\hat{\Omega}$) of the fictitious underlying dynamical system. The filter-diagonalization method is then used for extracting the eigenvalues of $\hat{\Omega}$ in any chosen small energy window. Operationally this is done by solving the small generalized eigenvalue problem,

$$\mathbf{U}^{(p)} \mathbf{B}_k = u_k^p \mathbf{U}^{(0)} \mathbf{B}_k, \tag{7}$$

whose eigenvalues $u_k^p = \exp[-ip\tau w_k]$ and eigenvectors $\mathbf{B}_k$ yield the frequencies w_k with their amplitudes d_k for a chosen frequency interval. The converged w_k and d_k should not depend on p. This condition allows one to identify spurious or nonconverged frequencies by comparing the results with different values of p (e.g., with $p = 1$ and $p = 2$). In periodic orbit quantization the amplitudes d_k are the multiplicities of semiclassical resonances and also allow one to check the convergence of the calculations. Eigenvalues with amplitudes d_k close to 1 are assumed to be well-converged nondegenerate states. The knowledge of the operator $\hat{U}$ (or $\hat{\Omega}$) itself is not required as for a properly chosen basis its matrix representation $\mathbf{U}^{(p)}$ can be expressed only in terms of c_n. The advantage of the filter-diagonalization procedure is its numerical stability with respect to both the length and complexity (the number and density of the contributing frequencies) of the signal. Here we apply the method of Ref. [13] which is an improvement of the filter-diagonalization method of Ref. [12] in that it allows one to significantly reduce the required length of the signal.

Note that the diagonalization of small matrices in (7) does not imply that the results of periodic orbit quantization are more "quantum" in any sense than those obtained, e.g., from a cycle expansion. The eigenvalues are solutions of nonlinear equations, and the diagonalization is equivalent to the search for zeros of the dynamical zeta function in the cycle expansion technique. Numerical calculation of the zeros is also a nonlinear problem, and in contrast to the matrix diagonalizations there might be a problem of missing roots.

As a first example we now apply the method of harmonic inversion to the three disk scattering problem which has served as a model system for periodic orbit quantization in many investigations during recent years [4,14–16]. The radius of the disks is normalized to $R = 1$, and the system is characterized by the distance d between the disks. In billiards the scaled action s is given by the length L of orbits ($s = L$), and the quantized parameter is the absolute value of the wave vector $k = |\mathbf{k}| = \sqrt{2mE}/\hbar$. In Fig. 1 we present results for $d = 6$. Figure 1(a) shows the trace of the semiclassical propagator $C^{\mathrm{sc}}(L)$. The groups with oscillating sign belong to periodic orbits with different cycle lengths in the symbolic code of Cvitanović and Eckhardt [4]. To obtain a smooth function on an equidistant grid, required for our harmonic inversion method, the δ functions in (2) are convoluted with a Gaussian function. This does not change the underlying spectrum. The result of the high resolution spectral analysis of this signal is shown in Fig. 1(b). The crosses represent semiclassical poles for which the amplitudes d_k are very close to $d_k = 1$, mostly within one percent. Because the amplitudes converge much slower than the frequencies, these resonance positions are assumed to be very accurate within the semiclassical approximation. In fact, a perfect agreement to many significant digits is achieved for these poles with the results obtained by cycle expansion [16]. For the diamonds the amplitudes deviate from $d_k = 1$ within 5% to maximal 50%. Figure 2 presents results for a shorter

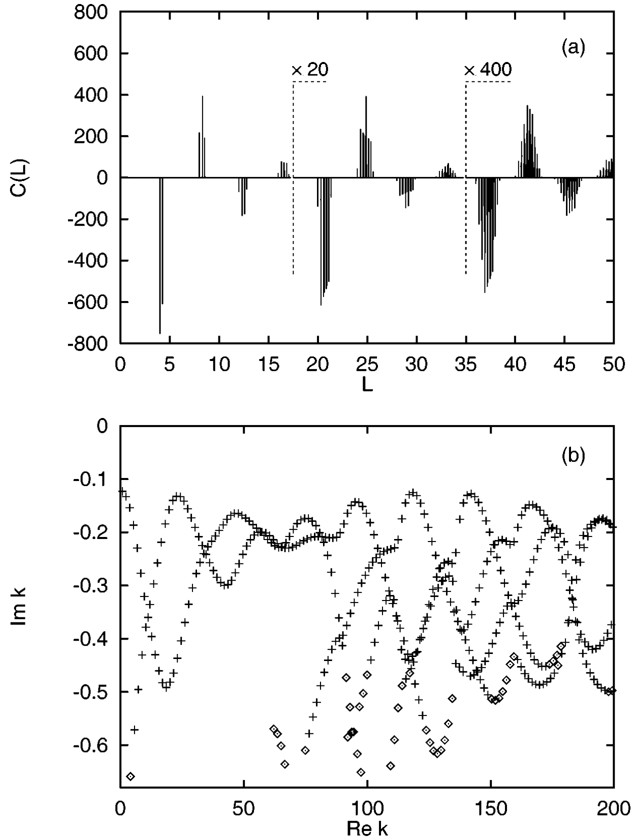

FIG. 1. Three disk scattering system (A_1 subspace) with $R = 1$, $d = 6$. (a) $C(L)$, trace of the semiclassical propagator. The signal has been convoluted with a Gaussian function of width $\sigma = 0.0015$. (b) Semiclassical resonances. The resonance positions marked by diamonds might be less accurate (see text).

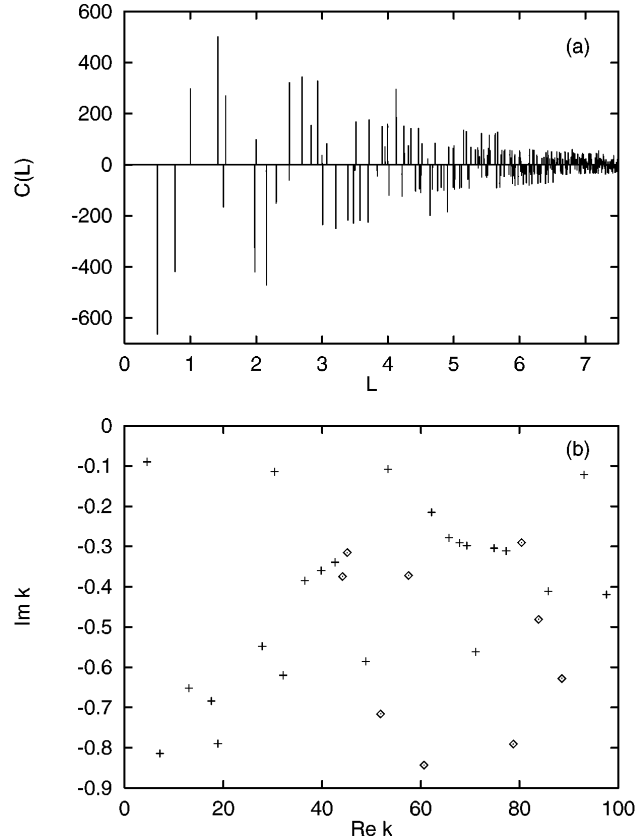

FIG. 2. Same as Fig. 1 but with separation ratio $R : d = 1 : 2.5$ and convolution of $C^{\mathrm{sc}}(L)$ with a Gaussian function of width $\sigma = 0.0003$.

distance $d = 2.5$ between the disks. For large L groups of orbits with the same cycle length of the symbolic code strongly overlap and cannot be recognized in Fig. 2(a). In this case the convergence of the conventional cycle expansion is rather slow because the semiclassical Selberg zeta function has poles [15]. The total number of converged semiclassical resonances obtained at $d = 2.5$ is small compared to the scattering system with $d = 6$ because the length of the signal is by a factor of 7 shorter than that in Fig. 1(a). More resonances at higher k values might be obtained from a longer signal.

As a second example we apply the method of harmonic inversion to the famous Riemann zeta function [17]. As pointed out by Berry [18], the density of zeros of the zeta function $\zeta(z)$ along the line $z = \frac{1}{2} - iw$ can be written in formal analogy to Gutzwiller's trace formula (1) as a nonconvergent series with $S_{p,m} = wm\ln(p)$ and $A_{p,m} = i\ln(p)/p^{m/2}$. Here the "periodic orbits" are the prime numbers, p, and $m = 1, 2, \ldots$ formally counts the "repetitions." Applying our method of harmonic inversion to the signal

$$C(s) = i \sum_p \sum_{m=1}^{\infty} \frac{\ln(p)}{p^{m/2}}\, \delta[s - m\ln(p)], \qquad (8)$$

we obtained about 80 zeros converged to 6 digit precision from a signal with $s_{\max} = \ln(1000) = 6.91$ (168 prime numbers) and about 2500 zeros converged to 12 digits from a signal with $s_{\max} = \ln(10^6) = 13.82$ (78498 prime numbers). Note that these results have been obtained directly from analyzing the signal (8) without using the functional equation for the Riemann-Siegel formula [17,18]. In general, the number of frequencies (here Riemann zeros) which can be converged depends on the length of the signal. The required signal length, $s_{\max}$, for harmonic inversion is related to the average density of frequencies, $\overline{\varrho}(w)$, by $s_{\max} \sim 4\pi\overline{\varrho}(w)$. More details will be given elsewhere [19].

In conclusion, we have introduced harmonic inversion as a new and general tool for semiclassical periodic orbit quantization and finding the roots of dynamical zeta functions. The method requires the complete set of periodic orbits up to a given maximum period as input, but does not depend on special properties of the orbits, as, e.g., the existence of a symbolic code or a functional equation. Therefore, the method might also be a tool for the semiclassical quantization of systems with mixed regular-chaotic classical dynamics, which still is a challenging and unsolved problem. The signal $C^{\mathrm{sc}}(s)$ can be composed as the sum of a signal related to the irregular part of the classical phase space with periodic orbit amplitudes given by Gutzwiller's trace formula [2] and a signal related to stable [8] or nearly integrable [9] torus structures. It should also be possible to include, e.g., creeping orbits [20], ghost orbit contributions [11,21,22], and higher order $\hbar$ corrections [23] into the signal $C^{\mathrm{sc}}(s)$, which can then be inverted to reveal the semiclassical poles.

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[1] M.C. Gutzwiller, J. Math. Phys. **8**, 1979 (1967); **12**, 343 (1971).
[2] M.C. Gutzwiller, *Chaos in Classical and Quantum Mechanics* (Springer, New York, 1990).
[3] D. Wintgen, Phys. Rev. Lett. **61**, 1803 (1988).
[4] P. Cvitanović and B. Eckhardt, Phys. Rev. Lett. **63**, 823 (1989).
[5] G.S. Ezra, K. Richter, G. Tanner, and D. Wintgen, J. Phys. B **24**, L413 (1991); D. Wintgen, K. Richter, and G. Tanner, Chaos **2**, 19 (1992).
[6] G. Tanner, P. Scherer, E.B. Bogomolny, B. Eckhardt, and D. Wintgen, Phys. Rev. Lett. **67**, 2410 (1991).
[7] G. Tanner, K.T. Hansen, and J. Main, Nonlinearity **9**, 1641 (1996).
[8] M.V. Berry and M. Tabor, Proc. R. Soc. London A **349**, 101 (1976).
[9] S. Tomsovic, M. Grinberg, and D. Ullmo, Phys. Rev. Lett. **75**, 4346 (1995); D. Ullmo, M. Grinberg, and S. Tomsovic, Phys. Rev. E **54**, 136 (1996).
[10] S. Marple, Jr., *Digital Spectral Analysis with Applications* (Prentice-Hall, Englewood Cliffs, NJ, 1987).
[11] J. Main, V.A. Mandelshtam, and H.S. Taylor, Phys. Rev. Lett. **78**, 4351 (1997).
[12] M.R. Wall and D. Neuhauser, J. Chem. Phys. **102**, 8011 (1995).
[13] V.A. Mandelshtam and H.S. Taylor, Phys. Rev. Lett. **78**, 3274 (1997).
[14] P. Gaspard and S.A. Rice, J. Chem. Phys. **90**, 2225, 2242, and 2255 (1989).
[15] B. Eckhardt and G. Russberg, Phys. Rev. E **47**, 1578 (1993).
[16] B. Eckhardt, P. Cvitanović, P. Rosenqvist, G. Russberg, and P. Scherer, in *Quantum Chaos,* edited by G. Casati and B.V. Chirikov (Cambridge University Press, Cambridge, 1995), p. 405.
[17] H.M. Edwards, *Riemann's Zeta function* (Academic Press,New York, 1974).
[18] M.V. Berry, in *Quantum Chaos and Statistical Nuclear Physics,* edited by T.H. Seligman and H. Nishioka, Lecture Notes in Physics, Vol. 263 (Springer, Berlin, 1986), p. 1; M.V. Berry and J.P. Keating, J. Phys. A **23**, 4839 (1990).
[19] J. Main, V.A. Mandelshtam, G. Wunner, and H.S. Taylor, Nonlinearity (to be published).
[20] A. Wirzba, Chaos **2**, 77 (1992).
[21] M. Kuś, F. Haake, and D. Delande, Phys. Rev. Lett. **71**, 2167 (1993).
[22] J. Main and G. Wunner, Phys. Rev. A **55**, 1743 (1997).
[23] P. Gaspard and D. Alonso, Phys. Rev. A **47**, R3468 (1993).