Classical, semiclassical, and quantum investigations of the four-sphere scattering system

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A genuinely three-dimensional system, viz. the hyperbolic four-sphere scattering system, is investigated with classical, semiclassical, and quantum mechanical methods at various center-to-center separations of the spheres. The efficiency and scaling properties of the computations are discussed by comparisons to the two-dimensional three-disk system. While in systems with few degrees of freedom modern quantum calculations are, in general, numerically more efficient than semiclassical methods, this situation can be reversed with increasing dimension of the problem. For the four-sphere system with large separations between the spheres, we demonstrate the superiority of semiclassical versus quantum calculations, i.e., semiclassical resonances can easily be obtained even in energy regions which are unattainable with the currently available quantum techniques. The four-sphere system with touching spheres is a challenging problem for both quantum and semiclassical techniques. Here, semiclassical resonances are obtained via harmonic inversion of a cross-correlated periodic orbit signal.

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I. INTRODUCTION

The breakthrough for the semiclassical quantization of chaotic systems was the development of periodic orbit theory [1,2]. In Gutzwiller's trace formula the density of states is expressed as an infinite sum over all isolated periodic orbits of the classical system. Although the periodic orbit theory is in principle valid for systems with an arbitrary number of degrees of freedom, applications have, for practical reasons, so far mostly been restricted to two-dimensional systems. The main difficulties are, first, the numerical periodic orbit search, which becomes more difficult in multidimensional systems, and, second, the fact that the semiclassical trace formula usually does not converge. The convergence problems can be solved, e.g., with cycle expansion [3–5] or harmonic inversion [6–8] techniques, and both methods have been successfully applied to the three-disk billiard as a prototype model of a two-dimensional hyperbolic scattering system. Practical applications of periodic orbit theory to three-dimensional systems are very rare. For the three-dimensional Sinai billiard extensive quantum computations have been performed and the quantum spectra have been analyzed in terms of classical periodic orbits [9,10]. However, no semiclassical eigenstates have been calculated from the set of periodic orbits. Semiclassical resonances have been obtained for the three-dimensional two- and three-sphere scattering systems [11] but for these systems all periodic orbits lie in a one- or two-dimensional subspace.

In this paper we investigate the scattering of a particle on four equal spheres centered at the corners of a regular tetrahedron. Classical and semiclassical as well as quantum mechanical methods will be applied to the four-sphere system at various center-to-center separations of the spheres. The four-sphere system can be regarded as the simplest extension of the three-disk repellor to three-dimensional space with a set of genuinely three-dimensional periodic orbits. Chaotic properties of the four-sphere system have been verified experimentally by the observation of fractal structures via optical light-scattering on the spheres [12,13].

When solving two- and three-dimensional systems with both quantum and semiclassical methods it is interesting to study the scaling properties of the quantization methods with the number of degrees of freedom, and to compare the efficiency of the various algorithms. The numerical effort for the quantization of nonintegrable systems usually increases strongly with the number of degrees of freedom, and therefore efficient quantization techniques are highly desirable. A large variety of quantum mechanical and semiclassical methods have been developed. The direct solution of Schrödinger's equation is possible, e.g., by time-dependent wave packet expansions or numerical diagonalization of the Hamiltonian in a complete basis set. Exact quantum mechanical calculations usually require storage of multidimensional wave functions and a computational effort that grows exponentially with the number of coupled degrees of freedom. These methods are therefore feasible for systems with relatively few degrees of freedom. As an alternative to exact quantum calculations, approximate, e.g., semiclassical, methods can be used. Gutzwiller's trace formula can be applied to systems with an arbitrary number of degrees of freedom, however, the number of periodic orbits and the numerical effort needed to find them usually increases very rapidly with increasing dimension of the phase space. As a matter of fact, Gutzwiller's periodic orbit theory has been applied almost exclusively to systems with two degrees of freedom, viz. the anisotropic Kepler problem [1,14], the hydrogen atom in a magnetic field [15], and two-dimensional billiards [3,4,16,17]. For these systems direct quantum mechanical computations are usually more powerful and efficient than the semiclassical calculation of spectra by means of periodic orbit theory. The four-sphere system is an example where semiclassical methods turn out to be superior to direct quantum mechanical computations [18], i.e., semiclassical resonances can easily be obtained even in energy regions which are unattainable with the presently known quantum techniques.
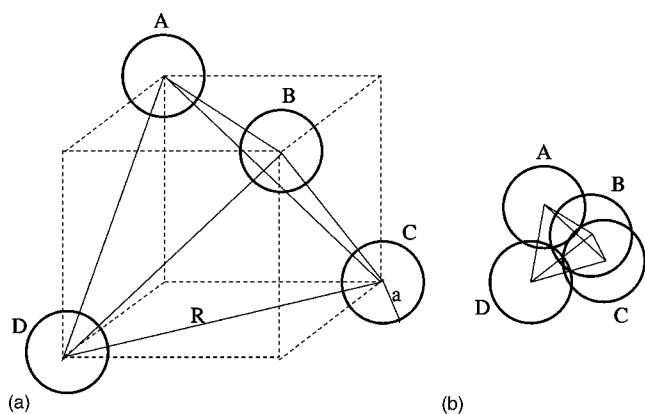
FIG. 1. The four-sphere system consists of four equal spheres centered at the corners of a regular tetrahedron. (a) Large center-to-center separation $R \gg 2a$. (b) Touching four-sphere system with $R = 2a$.

The paper is organized as follows. In Sec. II we investigate the classical dynamics of the four-sphere system. The symbolic code is introduced and its symmetry reduction by means of the tetrahedra group T_d is discussed. The periodic orbits are found in a systematic way by an efficient numerical periodic orbit search, and the pruning of orbits at small separations of the spheres is analyzed. In Sec. III we introduce the semiclassical techniques for periodic orbit quantization, viz. the cycle-expansion method, the harmonic inversion method, and the extension of harmonic inversion to cross-correlated periodic orbit signals. In Sec. IV we present the method applied for the exact quantum mechanical calculation of the resonances. In Sec. V we show the results for the semiclassical and quantum resonances at various separations of the spheres. The results are discussed with special emphasis on the comparison of the efficiency of the various methods. Some concluding remarks are given in Sec. VI.

II. CLASSICAL DYNAMICS: THE PERIODIC ORBITS OF THE FOUR-SPHERE SYSTEM

The four-sphere system is a genuinely three-dimensional billiard where the systematic periodic orbit search is a nontrivial task. In this section we first develop the symbolic dynamics of orbits and the symmetry reduction using the tetrahedra group, and then discuss the numerical periodic orbit search and the calculation of the periodic orbit parameters.

A. Symbolic code and symmetry reduction

The four-sphere system discussed here consists of four equal spheres with radius a centered at the corners of a regular tetrahedron. We choose $a = 1$ in what follows. The system is then solely determined by the center-to-center separation R. The four-sphere system with large center-to-center separation $R \gg 2a$ and with touching spheres ($R = 2a$) are shown in Figs. 1(a) and 1(b), respectively.

In full coordinate space each orbit can be described by the infinite sequence of spheres where the orbit is scattered. By labeling the spheres as $\{A, B, C, D\}$, it is possible to code a periodic orbit as the infinite cycles of a limited length string consisting of the sphere labels which we call here the itinerary code of the orbit. For a given string length, all combinations of the letters $\{A, B, C, D\}$ correspond to a physical orbit, with the exception that two consecutive letters in the itinerary code cannot be identical and, for short center-to-center separation $R \gtrsim 2a$, some orbits may be excluded by pruning (see Sec. II C). Several itinerary code strings may represent the same periodic orbit or a similar orbit obtained by a symmetry operation, i.e., rotation or reflection. For example, the itinerary codes ABC and BCA correspond to the same periodic orbit by cyclic permutations, and the orbits ABC, ACD, ABD, and BCD can be mapped onto each other by rotations.

By using the symmetry properties T_d of the tetrahedron the system can be reduced to its fundamental domain. The symmetry reduced orbits can be described by a ternary alphabet of symbols "0," "1," and "2," which are the three fundamental orbits, i.e., the symmetry reductions of the shortest orbits scattered between two, three, and four spheres, respectively. Therefore, we shall use the symbol 0 for returning back to the previous sphere after one reflection, symbol 1 for the reflection to the other third sphere in the same reflection plane of the orbit, and symbol 2 for the reflection to the other forth sphere out of the reflection plane of the orbit. The reflection plane is defined by the centers of the first three *different* spheres toward back in the history of the itinerary code of the orbit. The primitive periodic orbits of cycle length n_p in the fundamental domain are now given by those periodic sequences of n_p symbols 0, 1, and 2 which are free of subcycles (e.g., the code $\overline{0101}$ with subcycle $\overline{01}$ is not primitive, we will neglect the line indicating periodicity in the following). The periodic orbits do not change by cyclic permutations of the code. We will choose the code word with the lowest numerical value as the representative (e.g., 0112 instead of 1120). With these rules every symmetry reduced periodic orbit of the four-sphere system is uniquely described by a symbolic code. However, at small separations of the spheres some physical orbits are pruned as discussed below in Sec. II C.

From the $\{0,1,2\}$ code of the symmetry reduced orbits the $\{A,B,C,D\}$ itinerary code can be obtained as follows. We choose the plane spanned by the spheres (A,B,C) as the initial reflection plane and start the journey with the sequence AB. Then the rules given above are applied for the symbols 0, 1, and 2 to guide the orbit to the subsequent spheres. Note that symbolic codes which contain only the symbols 0 and 1 lie in the two-dimensional (A,B,C) plane, i.e., they correspond to the set of orbits with a binary symbolic code, which has been well established for the three-disk [3,4] and three-sphere system [11]. Orbits including the symbol 2 are genuinely three-dimensional orbits. In Table I we present the symbolic codes of all periodic orbits up to cycle lengths $n_p = 3$ of the symmetry reduced code. Note that no subcycles and cyclic permutations exist on the list. In the second column, the corresponding itinerary codes $\tilde{p}$ of the symbolic codes of column 1 are given, which have been obtained by following the rules explained above. The last column in Table I shows the symmetry classes of the orbits.

TABLE I. Symbolic code p of the symmetry reduced periodic orbits with cycle lengths $n_p \leq 3$ and the itinerary codes $\tilde{p}$ of the orbits in full coordinate space. The column $h_{\tilde{p}}$ gives the symmetry type of the orbits.

p	$\tilde{p}$	$h_{\tilde{p}}$
0	AB	σ_d, C_2
1	ABC	C_3
2	ABDC	S_4
01	ABAC	σ_d
02	ABADAC	C_3
12	ABCDBADC	S_4
001	ABABCBCAC	C_3
002	ABABDBDCDCAC	S_4
011	ABACBC	σ_d
012	ABACDC	C_2
021	ABADBDCBC	C_3
022	ABADCDBABCDC	S_4
112	ABCADC	σ_d
122	ABCDACBDC	C_3

The T_d group has 1 e, 3 C_2, 8 C_3, 6 S_4, and 6 σ_d, in total 24 different symmetry elements. Each orbit (except the one represented by 0) can be assigned by one and only one of the symmetry elements $\{e, \sigma_d, C_2, C_3, S_4\}$ of the group T_d. Note that periodic orbits in the fundamental domain, and thus their symmetry reduced symbolic codes, are two-, three-, or four-times shorter than the orbits (and the itinerary codes) in the full coordinate space when they belong to the symmetry class $\{\sigma_d, C_2\}$, C_3, or S_4, respectively. The symbolic length of orbits belonging to symmetry class e, i.e., the identity is unchanged under symmetry reduction.

B. Numerical periodic orbit search

Each trajectory of the four-sphere system is completely determined by the reflection points on the surfaces of the spheres, which on each sphere can be described by two spherical coordinates θ and ϕ. For a given itinerary code arbitrarily chosen reflection points on the spheres connected by straight lines in the correct order result in a periodic but not necessarily a physical orbit. The true physical orbit, for which the incident and reflection angle at each reflection point must coincide, can be obtained by direct application of Hamilton's principle, i.e., the orbital length, which is proportional to the classical action, becomes a minimum when the reflection points are varied. The length function of an orbit with a total number of N reflection points depends on the $2N$ variables $\{\theta_i, \phi_i\}$ with $i = 1, \ldots, N$. Numerically, the minimizing of the length

$$L = L(\theta_1, \phi_1, \theta_2, \phi_2, \ldots, \theta_N, \phi_N) \tag{1}$$

can be achieved by applying the well established quasi-Newton method [19], which is implemented, e.g., in the NAG-library [20]. The required gradient of the length function ∇L has been derived analytically.

As mentioned above the length of periodic orbits in full coordinate space can be two, three, or four times the length of the corresponding symmetry reduced orbit in the fundamental domain (see Table I). As the required computational effort for the quasi-Newton method increases rapidly with the dimensionality of the problem, it is desirable to exploit the symmetry properties of the tetrahedra group and to directly search for the periodic orbits in the fundamental domain. To this end for a symmetry reduced orbit with cycle length n_p the reflection point on the sphere $n_p + 1$ is associated with the reflection point on the first sphere by an appropriate transformation, i.e., one of the 24 possible symmetry transformations of the tetrahedra group T_d. The length minimization is now applied to the trajectory segments between the first sphere and sphere $n_p + 1$, i.e., the dimensionality of the length minimization of periodic orbits in the fundamental domain is reduced to $2n_p$ for all primitive orbits with cycle length n_p.

Once a periodic orbit has been found its orbital parameters required for semiclassical periodic orbit quantization can be calculated. The most important ones are the monodromy matrix and the Maslov index of the orbit. The Maslov index increases by 2 at each reflection on a hard sphere, i.e., $\mu_{po} = 2n_p$ for an orbit with cycle length n_p. The calculation of the monodromy matrix $\mathbf{M}_{po}$ for the periodic orbits of three-dimensional billiards has been investigated in Refs. [9,21]. $\mathbf{M}_{po}$ is a symplectic (4×4) matrix with eigenvalues λ_1, $1/\lambda_1$, λ_2, and $1/\lambda_2$. For the hyperbolic four-sphere system λ_1 and λ_2 are either both real or the orbits are loxodromic, i.e., the eigenvalues of $\mathbf{M}_{po}$ are a quadruple $\{\lambda, 1/\lambda, \lambda^*, 1/\lambda^*\}$ with λ being a complex number. For the four-sphere system with radius $a = 1$ and center-to-center separation $R = 6$ the orbital lengths and stability parameters for all primitive periodic orbits with cycle length $n_p \leq 3$ are presented in Table II. For that sphere separation $(R = 6a)$ we have calculated the complete set of primitive periodic orbits with symbol lengths $n_p \leq 14$, numbering 533 830 orbits in total. For sphere separation $R = 2.5a$ we also calculated all primitive periodic orbits with symbol lengths $n_p \leq 14$, and in addition all orbits with symbol lengths $n_p \leq 22$ and physical lengths $L \leq 12$, which allows for the construction of a periodic orbit signal with length $L_{max} = 12$ used for the semiclassical quantization in Sec. V B.

C. Pruning of orbits

For center-to-center separations $R > 2.0482a$ between the spheres there is a one to one correspondence between the symbolic codes and the primitive periodic orbits. However, when the separation is reduced below that value some orbits become unphysical, i.e., the symbolic dynamics is pruned. The pruning of orbits has been investigated in detail for the three-disk scattering system [22,23]. For the four-sphere system the mechanism is similar: As illustrated in Fig. 2, an orbital segment may (a) pass through one of the spheres, or (b) a reflection may occur inside one of the spheres. For a periodic orbit search at small separation between the spheres all orbits obtained numerically by minimizing the length must be checked whether pruning occurs or not. For touch-

TABLE II. Parameters of the symmetry reduced primitive periodic orbits p with cycle length $n_p \leqslant 3$ of the four-sphere system with radius $a=1$ and center-to-center separation $R=6$.

p	h_p	L	$Re\lambda_1$	$Im\lambda_1$	$Re\lambda_2$	$Im\lambda_2$
0	σ_d, C_2	4.000000	9.89898	0.00000	9.89898	0.00000
1	C_3	4.267949	−11.7715	0.00000	9.28460	0.00000
2	S_4	4.296322	−4.52562	9.49950	−4.52562	−9.49950
01	σ_d	8.316529	−124.095	0.00000	88.4166	0.00000
02	C_3	8.320300	−37.1479	98.0419	−37.1479	−98.0419
12	S_4	8.567170	117.644	0.00000	−102.992	0.00000
001	C_3	12.321747	−1240.54	0.00000	868.915	0.00000
002	S_4	12.322138	−353.853	976.176	−353.853	−976.176
011	σ_d	12.580808	1449.55	0.00000	824.981	0.00000
012	C_2	12.617350	1192.83	0.00000	−1020.66	0.00000
021	C_3	12.584068	1201.43	0.00000	−996.800	0.00000
022	S_4	12.619948	−755.582	804.976	−755.582	−804.976
112	σ_d	12.835715	−496.339	1038.46	−496.339	−1038.46
122	C_3	12.863793	−1100.56	0.00000	1219.28	0.00000

ing spheres ($R=2a$) all pruned orbits with symbol lengths $n_p \leqslant 7$ and their pruning types a or b are presented in Table III. Pruning exists for orbits with symbol lengths $n_p \geqslant 5$, i.e., the symbolic dynamics is complete only for $n_p \leqslant 4$. Furthermore, periodic orbits with long heads of 0 symbols in the code can have accumulation points at finite values of the physical length L. It is impossible to find all orbits beyond the first accumulation point. We have searched for all periodic orbits of the touching four-sphere system with physical lengths $L \leqslant L_{max}=3.6$, symbol lengths $n_p \leqslant 60$, and with the total number of 1 and 2 symbols in the symbolic code restricted to $n_1+n_2 \leqslant 10$, resulting in about 2.8×10^6 primitive periodic orbits.

The semiclassical quantization by harmonic inversion of a cross-correlated periodic orbit signal (see Sec. III C) requires the knowledge of the expectation values of various linearly independent classical observables A along the periodic orbits [24,25]. We have chosen the observables $A_1=r^2$ and $A_2=L^2$, i.e., we have calculated the averaged squared distance and squared angular momentum of the periodic orbits of the touching four-sphere system.

III. SEMICLASSICAL PERIODIC ORBIT THEORY

We now wish to calculate semiclassically the resonances of the four-sphere scattering system by application of periodic orbit theory. Gutzwiller's trace formula [1] expresses the quantum mechanical response function

$$g_{qm}(E) = \sum_n \frac{1}{E - E_n + i\epsilon} \qquad (2)$$

in terms of the periodic orbits of the underlying classical system, i.e.,

$$g_{scl}(E) = g_0(E) + \sum_{po} A_{po}(E) e^{iS_{po}(E)/\hbar}, \qquad (3)$$

where $g_0(E)$ is a smooth function of the energy and $A_{po}(E)$ and $S_{po}(E)$ are the periodic orbit amplitudes (including phase information given by the Maslov indices) and classical actions, respectively. For billiards the classical action depends linearly on the length of the trajectory and the wave number

TABLE III. All pruned orbits with cycle length $n_p \leqslant 7$ and their pruning types a or b (see Fig. 2) of the four-sphere system with touching spheres, $R=2a$.

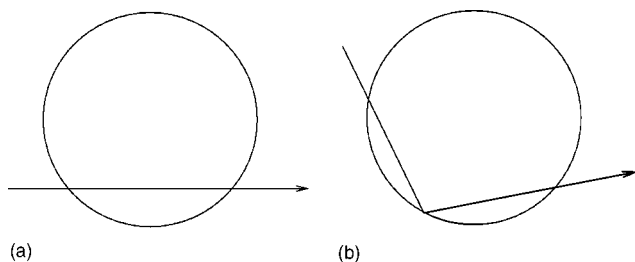| Symbolic code	Pruning type
00021	a
000011	a
000021	a
000002	b
0000001	b
0000011	a
0000021	a
0000002	b

(a)   (b)

FIG. 2. Sketch of the two types of pruning occurring in the four-sphere system at small separation between the spheres: (a) An orbital segment passes through one of the spheres. (b) A reflection occurs inside a sphere.

TABLE IV. Weight factors w_p for the periodic orbit sum [Eq. (4)] of the four-sphere system with symmetries of the tetrahedra group T_d.

T_d	e	C_3	C_2	S_4	σ_d
A_1	1	1	1	1	1
A_2	1	1	1	-1	-1
E	2	-1	2	0	0
T_1	3	0	-1	1	-1
T_2	3	0	-1	-1	1

$k=\sqrt{2ME}/\hbar$ with M being the particle mass. For the three-dimensional four-sphere system the periodic orbit sum as a function of the wave number k reads

$$g(k) = \sum_p \sum_{r=1}^{\infty} \frac{w_p(-1)^{rn_p}L_p e^{ikrL_p}}{\sqrt{|(2-\lambda_{p,1}^r-\lambda_{p,1}^{-r})(2-\lambda_{p,2}^r-\lambda_{p,2}^{-r})|}}, \quad (4)$$

where n_p is the cycle length, L_p the physical length, $\lambda_{p,i}$ are the eigenvalues of the monodromy matrix, and r is the repetition number of the primitive periodic orbit p. The weight factors w_p result from the symmetry decomposition of the system [26] and depend on the chosen irreducible subspace of the spectrum and the symmetry of the periodic orbits. For the tetrahedra group T_d the values of the weight factors w_p are given in Table IV. In the following we will concentrate on the subspace A_1, where the weight factors of all orbits are $w_p=1$.

The semiclassical resonances of the four-sphere system are given by the poles of the function $g(k)$. However, it is well known that the periodic orbit sum (4) does not converge in those regions where the physical poles are located, and special techniques must be applied to obtain an analytical continuation of the periodic orbit sum (4). For the three-disk system with large center-to-center separation $R=6a$ the cycle-expansion method [3,4,27] and harmonic inversion techniques [6,7] have proven to be powerful approaches for overcoming the convergence problems of the periodic orbit sum, and both methods can also be successfully applied to the four-sphere system. However, when pruning of orbits sets in at small separations, and in particular in the case of touching disks or spheres, the situation is much more difficult and subtle, since the direct application of the cycle-expansion method fails. The two-dimensional closed three-disk billiard is a bound system, where a few semiclassical eigenenergies have been obtained in Ref. [14] using the cycle expansion in combination with a functional equation. This method is not valid for open systems and cannot be extended to the four-sphere system which remains open even in the case of touching spheres [12,13]. Nevertheless, the harmonic inversion of cross-correlated periodic orbit signals [24,25] has been successfully applied to the closed three-disk system [28,29] and this method will also serve as a powerful tool for the three-dimensional four-sphere system. We will now introduce the quantization methods. Applications to the four-sphere system and comparisons with quantum mechanical results will be presented in Sec. V.

A. The cycle-expansion method

The periodic orbit sum in Gutzwiller's trace formula does usually not converge in the energy regions of physical interest. However, for some systems, e.g., the three-disk scattering billiard, semiclassical energies, or resonances can be obtained with the help of the cycle-expansion method [3–5]. If the periodic orbits can be associated to a symbolic dynamics the Gutzwiller-Voros ζ function [1,30] can be expanded according to increasing cycle length of the orbits. In this expansion the contributions of long periodic orbits may be approximately shadowed by the combined contributions of shorter orbits. In this case the cycle expansion can converge rapidly.

For billiards the Gutzwiller-Voros zeta function can be written as

$$Z_{GV}(k;z) = \exp\left\{-\sum_p \sum_{r=1}^{\infty} \frac{1}{r} \frac{(-z)^{rn_p}e^{irkL_p}}{\sqrt{|\det(\mathbf{M}_p^r - 1)|}}\right\}, \quad (5)$$

with an additional parameter z which must be set to $z=1$. The cycle expansion is achieved by taking z as a bookkeeping variable and expanding Eq. (5) as a truncated power series in z. The semiclassical resonances are obtained as the zeros (in the variable k) of the cycle-expanded ζ function (5) with again $z=1$. In our computations for the four-sphere system we use cycle expansions up to order $n_{\max}=12$.

B. Semiclassical quantization by harmonic inversion

An alternative method for semiclassical quantization is based on the observation that the extraction of eigenvalues from Gutzwiller's trace formula can be reformulated as a signal processing task [6–8]. The harmonic inversion method is briefly explained as follows. The Fourier transform of the function $g(k)$ in Eq. (4) yields the semiclassical signal

$$C^{sc}(L) = \sum_p \sum_{r=1}^{\infty} \frac{(-1)^{rn_p}L_p}{\sqrt{|\det(\mathbf{M}_p^r - 1)|}}\delta(L - rL_p), \quad (6)$$

as a sum of δ functions. The central idea of semiclassical quantization by harmonic inversion is to adjust the semiclassical signal $C^{sc}(L)$ with finite length $L \leq L_{\max}$ to its quantum mechanical analog

$$C^{qm}(L) = \frac{i}{2\pi}\int_{-\infty}^{+\infty}\sum_n \frac{d_n}{k-k_n+i\epsilon}e^{-ikL}dk = \sum_n d_n e^{-ik_n L},$$
$$(7)$$

where the amplitudes d_n and the semiclassical eigenvalues k_n are free adjustable complex parameters. This is achieved by signal processing [31,32] of the semiclassical signal $C^{sc}(L)$. Numerical recipes for extracting the parameters $\{d_n,k_n\}$ by harmonic inversion of the δ function signal (6) are given in Refs. [8,33].

Note that the cycle expansion does usually not work for systems that are highly pruned because the condition that contributions of longer orbits are shadowed by combinations of short orbits is not fulfilled. The shadowing is, however, not required for the harmonic inversion method which is

based on signal processing of the semiclassical periodic orbit signal $C^{sc}(L)$ in Eq. (6), with L the orbit length. Therefore the periodic orbits are naturally arranged and truncated by the orbit length rather than symbolic length or Maslov indices as for the cycle-expansion method.

C. Harmonic inversion of cross-correlated periodic orbit signals

The method of semiclassical quantization by harmonic inversion of cross-correlated periodic orbit signals is a generalization of the quantization scheme presented in Sec. II B. The idea is to use the classical average values of a set of linearly independent classical observables to construct a cross-correlated signal, whose informational content is significantly increased as compared to the one-dimensional signal, and therefore should lead to semiclassical spectra with improved resolution.

The numerical tools for the harmonic inversion of cross-correlated periodic orbit signals have already been well established [25], and therefore we only briefly review the basic ideas and refer the reader to the literature for details. For simplicity but without loss of generality, we focus on billiard systems, where the shape of the orbits is independent of the energy E, and the classical action of orbits reads $S = \hbar k L$, with k the wave number and L the physical length. The starting point is to introduce a weighted response function in terms of k

$$g_{\alpha\alpha'}(k) = \sum_n \frac{b_{\alpha n} b_{\alpha' n}}{k - k_n + i\epsilon}, \tag{8}$$

where k_n is the eigenvalue of the wave number of eigenstate $|n\rangle$ and

$$b_{\alpha n} = \langle n | \hat{A}_\alpha | n \rangle \tag{9}$$

are the diagonal matrix elements of a chosen set of N linearly independent operators $\hat{A}_\alpha$, $\alpha = 1, 2, \ldots, N$. The Fourier transform of Eq. (8) yields the $N \times N$ cross-correlated signal

$$C_{\alpha\alpha'}(L) = \frac{i}{2\pi} \int_{-\infty}^{+\infty} g_{\alpha\alpha'}(k) e^{-ikL} dk = \sum_n b_{\alpha n} b_{\alpha' n} e^{-ik_n L}. \tag{10}$$

A semiclassical approximation to the cross-correlated signal (10) has been derived in Refs. [24,34]. The cross-correlated periodic orbit signal reads

$$C^{sc}_{\alpha\alpha'}(L) = \sum_p \sum_{r=1}^{\infty} \frac{a_{\alpha,p} a_{\alpha',p} (-1)^{rn_p} L_p}{\sqrt{|\det(\mathbf{M}_p^r - \mathbf{1})|}} \delta(L - rL_p), \tag{11}$$

where r is the repetition number counting the traversals of the primitive orbit, and $\mathbf{M}_p$ is the monodromy matrix of the primitive periodic orbit. The weight factors $a_{\alpha,p}$ are classical averages over the periodic orbits

$$a_{\alpha,p} = \frac{1}{L_p} \int_0^{L_p} A_\alpha[\mathbf{q}(L), \mathbf{p}(L)] dL, \tag{12}$$

with $A_\alpha(\mathbf{q}, \mathbf{p})$ the Wigner transform of the operator $\hat{A}_\alpha$. Semiclassical approximations to the eigenvalues k_n and eventually also to the diagonal matrix elements $\langle n | \hat{A}_\alpha | n \rangle$ are now obtained by adjusting the semiclassical cross-correlated periodic orbit signal (11) to the functional form of the quantum signal (10). The numerical tool for this procedure is an extension of the harmonic inversion method to the signal processing of cross-correlation functions [35,36]. The advantage of using the cross-correlation approach is based on the realization that the total amount of independent information contained in the $N \times N$ signal is $N(N+1)$ multiplied by the length of the signal, while the total number of unknowns (here $b_{\alpha n}$ and k_n) is $(N+1)$ times the total number of poles k_n. Therefore the informational content of the $N \times N$ signal per unknown parameter is increased (as compared to the one-dimensional signal) by roughly a factor of N, and the cross-correlation approach should lead to a significant improvement of the resolution.

IV. QUANTUM CALCULATIONS

Schrödinger's equation for the three-disk or the four-sphere system is a free wave equation in two or three dimensions, $[\Delta + k^2]\Psi(\mathbf{k}) = 0$, with Dirichlet boundary conditions, i.e., $\Psi(\mathbf{k}) = 0$ on the surface of the disks or spheres, respectively. Although the problem looks simple the solution is a nontrivial task and, most importantly, the numerical effort increases extremely rapidly with the dimension of the system.

For the three-disk system the exact quantum resonances can be obtained as roots of the equation [27,37]

$$\det \mathbf{M}(k)_{mm'}^{\text{3-disk}} = 0, \tag{13}$$

with m and m' nonzero integer numbers which can be truncated by an upper angular momentum $m_{max} \gtrsim 1.5ka$ [27]. With matrices $\mathbf{M}(k)_{mm'}^{\text{3-disk}}$ of dimension up to $\sim(400 \times 400)$, Eq. (13) allows for the efficient numerical calculation of resonances in the region $0 \leq \text{Re} ka \leq 250$. The matrix elements of $\mathbf{M}(k)_{mm'}^{\text{3-disk}}$ in Eq. (13) can be written analytically in terms of Bessel and Hankel functions. Explicit expressions are given in Ref. [27]. The quantum resonances are obtained by a numerical root search in the complex k plane [19].

Similarly, exact quantum resonances of the three-dimensional four-sphere scattering system can be obtained as roots of the equation

$$\det \mathbf{M}(k)_{lm,l'm'}^{\text{4-sphere}} = 0, \tag{14}$$

with $0 \leq l, l' \leq l_{max}$ and $m, m' = 0, 3, 6, 9, \ldots, l_{max}$ for the subspace A_1 and A_2. An explicit expression for the matrix elements of $\mathbf{M}(k)_{lm,l'm'}^{\text{4-sphere}}$ has been derived [11] and reads

$$\mathbf{M}(k)_{lm,l'm'}^{4\text{-sphere}} = \delta_{ll'}\delta_{mm'} + \frac{3}{2}\sqrt{4\pi}i^{l'-l}\frac{j_l(ka)}{h_{l'}^{(1)}(ka)}g_m g_{m'}$$

$$\times \sum_{\tilde{l}=0}^{\infty} C(l,m,l',m',\tilde{l};\theta_0,\beta_0)h_l^{(1)}(kR), \quad (15)$$

with

$$C(l,m,l',m',\tilde{l};\theta_0,\beta_0)$$

$$= \sum_{M=-l'}^{l'} i^{\tilde{l}}\sqrt{(2l+1)(2l'+1)(2\tilde{l}+1)}\begin{pmatrix}\tilde{l} & l' & l \\ 0 & 0 & 0\end{pmatrix}(-1)^M$$

$$\times[d_{m'M}^{l'}(\beta_0) \pm (-1)^{m'}d_{-m',M}^{l'}(\beta_0)]$$

$$\times\left[(-1)^m Y_{\tilde{l},m-M}(\theta_0,0)\begin{pmatrix}\tilde{l} & l' & l \\ m-M & M & -m\end{pmatrix}\right.$$

$$\left.\pm Y_{\tilde{l},-m-M}(\theta_0,0)\begin{pmatrix}\tilde{l} & l' & l \\ -m-M & M & m\end{pmatrix}\right], \quad (16)$$

where the $\pm$ signs refer to the subspace A_1 and A_2, respectively. The angles θ_0 and β_0 in Eq. (16) are obtained from

$$\cos(\theta_0) = -\frac{2}{\sqrt{6}}, \quad \sin(\theta_0) = \frac{1}{\sqrt{3}},$$

$$\cos(\beta_0) = -\frac{1}{3}, \quad \sin(\beta_0) = \frac{2}{3}\sqrt{2},$$

and the $d_{mm'}^j(\beta)$ are the matrix elements of finite rotations [38],

$$d_{mm'}^j(\beta) = \langle jm|e^{-i\beta J_y}|jm'\rangle.$$

The large brackets in Eq. (16) refer to $3j$ symbols [38], and the values of g_m are defined as

$$g_m = \begin{cases} 1/\sqrt{2} & \text{for } m=0 \\ 1 & \text{for } m=3,6,9,\dots,l \\ 0 & \text{otherwise.} \end{cases}$$

Note that $g_{m=0}$ should read $g_0=1/\sqrt{2}$ instead of $\sqrt{2}$ in Eq. (38) of Ref. [11]. Similar as for the three-disk system the angular momentum [quantum numbers l and l' in Eq. (14)] can be truncated at $l_{max}\gtrsim 1.5ka$ to achieve convergence of the calculation.

It is important to note that the computation of the quantum mechanical resonances of the three-dimensional four-sphere scattering system becomes much more expensive than for the two-dimensional three-disk system. First of all, the calculation of each matrix element $\mathbf{M}(k)_{lm,l'm'}^{4\text{-sphere}}$ in Eq. (15) requires the summation over quantum numbers $\tilde{l}$ and [via Eq. (16)] M. To accelerate the calculation of the matrix (15) at various values of k we have calculated and stored the values of $C(l,m,l',m',\tilde{l};\theta_0,\beta_0)$ in Eq. (16) separately. Equation (16) does not depend on the sphere separation R, and therefore the stored C values can be used in calculations of spec-

tra with arbitrary R. However, the calculation of the matrix elements in Eq. (15) still requires the summation over $\tilde{l}$.

The second problem of solving Eq. (14) is the scaling of the dimension of the matrix $\mathbf{M}(k)_{lm,l'm'}^{4\text{-sphere}}$, which is an $N\times N$ matrix with

$$N = \tfrac{1}{6}(l_{max}+2)(l_{max}+3),$$

i.e., N scales as $N\sim k^2$ for the four-sphere system, as compared to $N\sim k$ for the three-disk system, Eq. (13). For example, in the region $ka\approx 200$ the required matrix dimension is $N\gtrsim 300$ for the three-disk system, as compared to $N\gtrsim 15\,000$ for the four-sphere system. For the four-sphere system with center-to-center separations $R=6a$, $R=2.5a$, and the touching spheres $R=2a$ we have computed the quantum resonances in the region $0\leqslant \text{Re } ka\leqslant 60$ by solving Eq. (14) with matrices of dimension up to (1751×1751). The results will be presented in Sec. V. With currently available computer technology it is impossible to significantly extend the quantum calculations for the four-sphere system to the region Re $ka\geqslant 60$ using Eq. (14). The efficiency of the semiclassical and quantum methods for the four-sphere system will be compared and discussed in Sec. V D.

V. RESULTS AND DISCUSSION

We will now present and discuss the results of our semiclassical and quantum computations for the four-sphere system with large sphere separation $R=6a$ intermediate separation $R=2.5a$, and touching spheres $R=2a$. In Sec. V D we will compare and discuss the efficiency of the various quantization methods.

A. Sphere separation $R=6a$

The quantum mechanical and semiclassical A_1 resonances of the four-sphere system with radius $a=1$ and center-to-center separation $R=6$ are presented in Fig. 3. The quantum resonances marked by the squares have been obtained by solving Eq. (14) with matrices $\mathbf{M}(k)_{lm,l'm'}^{4\text{-sphere}}$ of dimension up to (1134×1134), which is sufficient only to obtain converged results in the region Re $k\lesssim 50$ [see Fig. 3(a)]. By contrast, the semiclassical resonances can easily be obtained in a much larger region, e.g., Re $k\leqslant 250$ shown in Fig. 3(b). The crosses mark the zeros of the cycle-expanded Gutzwiller-Voros ζ function (5). The cycle expansion has been truncated at cycle length $n_{max}=7$, which means that a total set of just 508 primitive periodic orbits are included in the calculation. The plus symbols mark the semiclassical resonances obtained by harmonic inversion of the periodic orbit signal (6) with signal length $L_{max}=60$ constructed from the set of 533 830 primitive periodic orbits with cycle lengths $n_p\leqslant 14$.

In the region Re $k\leqslant 50$ [Fig. 3(a)] the quantum and semiclassical resonances agree very well, with a few exceptions. The first few quantum resonances in the uppermost resonance band are narrower, i.e., closer to the real axis than the corresponding semiclassical resonances. A similar discrepancy between quantum and semiclassical resonances has al-
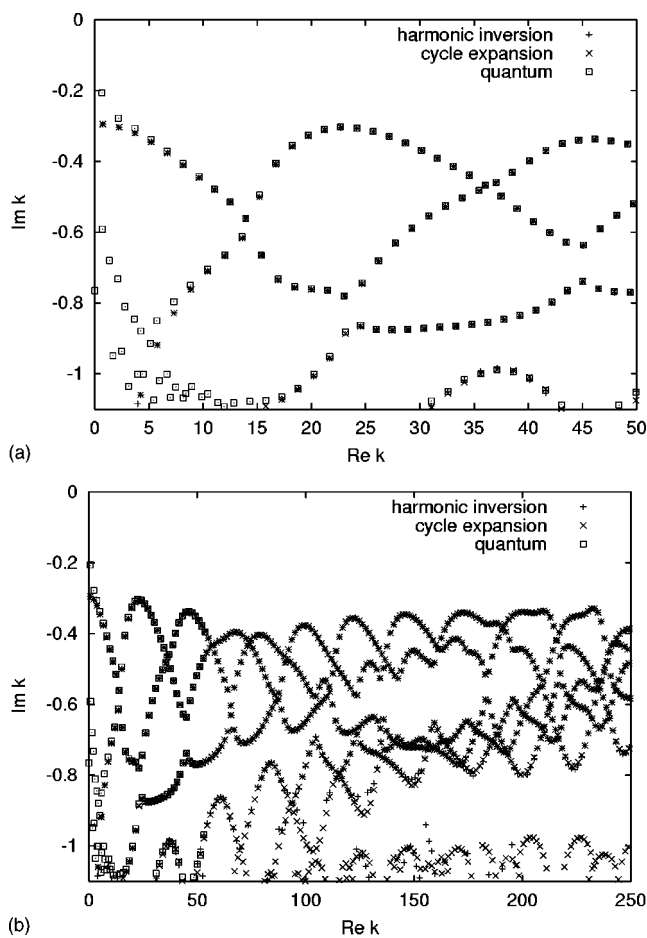
(a)

(b)

FIG. 3. A_1 resonances in the complex k plane of the four-sphere system with radius $a=1$ and center-to-center separation $R=6$. Squares: Quantum computations. Crosses and plus symbols: Semiclassical resonances obtained by cycle expansion and harmonic inversion methods, respectively.
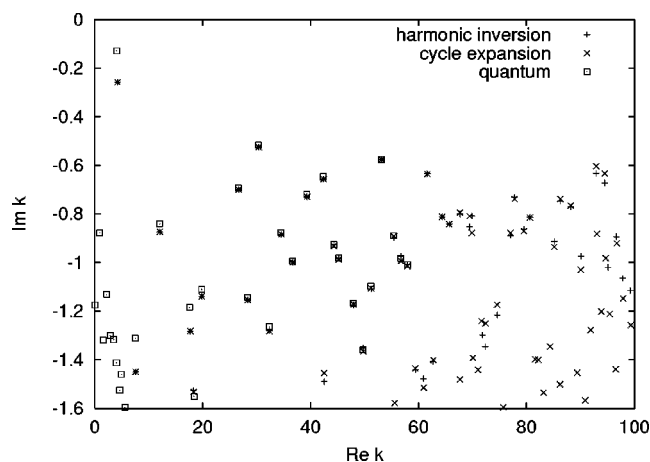

FIG. 4. A_1 resonances in the complex k plane of the four-sphere system with radius $a=1$ and center-to-center separation $R=2.5$. Squares: Quantum computations. Crosses and plus symbols: Semiclassical resonances obtained by cycle expansion and harmonic inversion methods, respectively.

ready been observed in the three-disk system [4,27]. Furthermore, in the region Re $k<15$ and Im $k<-0.5$ several quantum resonances have been found [see the squares in Fig. 3(a)], which seem not to have any semiclassical analog. These resonances are related to the diffraction of waves at the spheres, and its semiclassical description requires an extension of Gutzwiller's trace formula and the inclusion of diffractive periodic orbits [39,40]. The semiclassical resonances obtained by either harmonic inversion or the cycle-expansion method [the plus symbols and crosses in Fig. 3(b), respectively] are generally in perfect agreement, except for the very broad resonances that lie deep in the complex plane, i.e., in the region Im $k \lesssim -0.8$.

B. Sphere separation $R=2.5a$

The semiclassical quantization becomes more and more demanding with decreasing separation between the spheres. The reason is that the shadowing of longer orbits by combinations of shorter orbits in the cycle-expanded Gutzwiller-Voros ζ function becomes less accurate and the construction of the periodic orbit signal of length $L \le L_{max}$ used for the

harmonic inversion method requires more and more periodic orbit data. However, both semiclassical quantization techniques, i.e., cycle expansion and harmonic inversion can still be successfully applied at significantly reduced separation between the spheres.

As an example of an intermediate sphere separation we discuss the case $R=2.5a$, where the spheres are rather close, however, the symbolic dynamics of the periodic orbits is still complete, i.e., no orbits are pruned. The graphical comparison of the quantum mechanical and semiclassical resonances in the region $0 \le \text{Re } ka \le 100$ is given in Fig. 4. The semiclassical resonances shown as plus symbols have been obtained by harmonic inversion of a periodic orbit signal of length $L_{max}=12$. The signal has been constructed using all primitive periodic orbits with symbol lengths $n_p \le 14$ and parts of the orbits with symbol lengths $15 \le n_p \le 22$, in total a set of about 4.6×10^6 orbits. The crosses in Fig. 4 mark the semiclassical resonances obtained by 12th order cycle expansion using the complete set of 69 706 primitive periodic orbits with symbol lengths $n_p \le 12$. The exact quantum resonances have been obtained in the region $0 \le \text{Re } k \le 60$ by solving Eq. (14) with matrix dimensions up to (1751×1751).

In the region Re $k \lesssim 60$ the resonances obtained by the two semiclassical methods are in excellent agreement except for the imaginary parts of some resonances very deep down in the complex plane. In this region the semiclassical resonances agree well with the exact quantum mechanical resonances, the deviations are due to the semiclassical approximation, i.e., the first-order $\hbar$ expansion in the semiclassical trace formula. As in the case $R=6a$ (Sec. V A) some quantum resonances in the region Re $k \lesssim 10$ are related to the diffraction of waves at the spheres and do not have a semiclassical analog without the appropriate extension of the periodic orbit theory [39,40]. At Re $k \gtrsim 60$ the agreement between resonances obtained semiclassically via cycle expansion and harmonic inversion becomes less perfect, especially for some broad resonances with Im $k \lesssim -1.1$. Unfor-

tunately, no quantum results are currently available for Re $k > 60$ to judge the quality and accuracy of the semiclassical computations in that region.

C. Four touching spheres ($R = 2a$)

The semiclassical quantization of the four-sphere system becomes even more difficult when the spheres are further moved together and the symbolic dynamics becomes pruned (see Sec. II C). In particular, the case of touching spheres with $R = 2a$ is a real challenge for the following reason. For touching spheres the symbolic dynamics is pruned in a similar way as in the three-disk problem [23]. The closed three-disk billiard is a bound system, and some eigenenergies have been extracted by either combining the cycle-expansion method with a functional equation [14] or by the harmonic inversion method [28,29]. However, contrary to the closed three-disk system the four touching spheres do not form a bound system, which means that the method of Ref. [14] combining the cycle-expansion method with a functional equation cannot be applied, and thus the touching four-sphere system cannot be quantized with the help of the cycle-expansion method. Nevertheless, we will now demonstrate that the harmonic inversion method applied to a cross-correlated periodic orbit signal can reveal at least some of the low-lying semiclassical resonances.

For the construction of the periodic orbit signal we have calculated about 2.8×10^6 orbits of the touching four-sphere system with lengths $L < L_{max} = 3.6$. (Note that the signal is incomplete as discussed in Sec. II C.) For the application of the cross-correlation technique we use the operators $\hat{A}_1 = 1$ (the identity), the squared angular momentum $\hat{A}_2 = L^2$, and the squared distance from the origin $\hat{A}_3 = r^2$. Because the signal is incomplete and rather short the results of the harmonic inversion are less perfectly converged than for the four-sphere system with larger sphere separation, i.e., the amplitudes d_n in Eq. (7) may deviate from the ideal values $d_n = 1$ for true physical resonances and $d_n = 0$ for spurious resonances which must be omitted. As a criterion to accept resonances we have chosen the condition $|d_n - 1| < 0.5$.

The results of our semiclassical and quantum computations for the four touching spheres are presented in Fig. 5. The crosses mark the semiclassical resonances obtained by harmonic inversion of the one-dimensional periodic orbit signal. The low number of crosses indicates that the convergence of the one-dimensional signal is not very satisfactory. The plus symbols show the resonances obtained by harmonic inversion of the (3×3) cross-correlated periodic orbit signal using the operators $\hat{A}_1 = 1$, $\hat{A}_2 = L^2$, and $\hat{A}_3 = r^2$. With the cross-correlation technique the convergence properties have been significantly improved compared to the analysis of the one-dimensional signal. The real parts of the semiclassical resonances agree well with the real parts of the exact quantum mechanical resonances marked by the squares in Fig. 5. The agreement between the imaginary parts is, however, less perfect. Some quantum resonances in Fig. 5 do not have a semiclassical counterpart. Those resonances with Re $k < 10$ are probably related to the diffraction of waves at the spheres
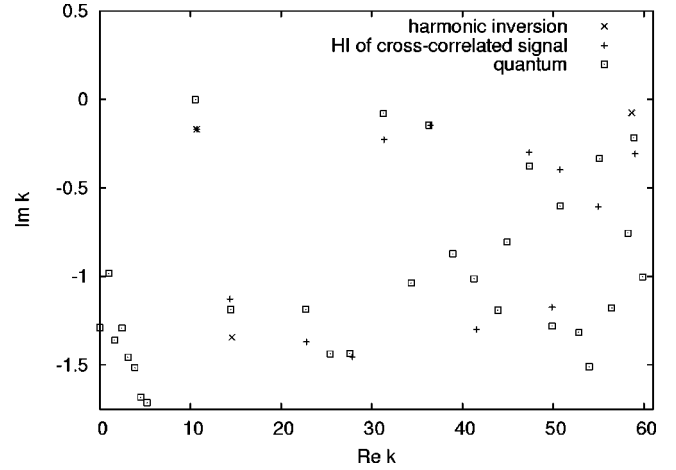

FIG. 5. A_1 resonances in the complex k plane of the touching four-sphere system with radius $a = 1$ and center-to-center separation $R = 2$. Squares: Quantum computations. Crosses: Semiclassical resonances obtained by harmonic inversion without using cross correlation. Plus symbols: Semiclassical resonances obtained by the harmonic inversion of a (3×3) cross-correlated periodic orbits signal using the operators 1 (identity), L^2, and r^2.

as discussed above, i.e., they cannot be explained without extensions of the semiclassical theories applied in this paper.

D. Efficiency of the semiclassical and quantum algorithms

For the four-sphere system as an example of a physical system with three degrees of freedom we now wish to discuss and compare the efficiency of the semiclassical and quantum computations. As mentioned in the Introduction (Sec. I) the efficiency of quantum computations usually decreases rapidly with the number of degrees of freedom of the physical system. It is an interesting and important question whether semiclassical methods can beat the efficiency of quantum computations with increasing dimension of the problem. Although there is not much hope and evidence that this is generally true, because of the exponential proliferation of periodic orbits in chaotic systems, it can be true for certain specific systems. An example for the superiority of semiclassical over quantum mechanical calculations is the four-sphere system with large sphere separation, e.g., $R = 6a$, where semiclassical resonances can easily be obtained even in energy regions which are out of reach for the presently known quantum techniques [18]. To understand this it is instructive to study the expense and scaling properties of the quantum and classical computations for the three-disk and four-sphere system.

As explained in Sec. IV exact quantum resonances of the three-disk and four-sphere systems can be obtained as roots of Eqs. (13) and (14), respectively, with angular quantum numbers truncated at $l_{max} \gtrsim 1.5ka$. The calculation of the matrix elements $\mathbf{M}(k)_{lm,l'm'}^{\text{4-sphere}}$ in Eq. (14) is much more expensive than for the matrix elements $\mathbf{M}(k)_{mm'}^{\text{3-disk}}$ in Eq. (13). However, the serious problem of solving Eq. (14) is the scaling of the dimension of the matrix $\mathbf{M}(k)_{lm,l'm'}^{\text{4-sphere}}$, which is an $N \times N$ matrix with $N = (l_{max} + 2)(l_{max} + 3)/6$, i.e., N scales as $N \sim k^2$ for

the four-sphere system, as compared to $N \sim k$ for the three-disk system, Eq. (13). For example, in the region $ka \approx 200$ the required matrix dimension is $N \gtrsim 300$ for the three-disk as compared to $N \gtrsim 15\,000$ for the four-sphere system. With currently available computer technology it is, therefore, impossible to significantly extend the quantum calculations for the four-sphere system to the region $ka \gtrsim 60$ using Eqs. (14)–(16). Note that the cost of the quantum computations does not depend on the separation R between the disks or spheres.

The expense of the semiclassical quantization is basically given by the required number of periodic orbits which, in chaotic systems, increases exponentially with the symbolic or physical length of the orbits. For the three-disk system the number of symmetry reduced primitive periodic orbits with symbol length n_p is given approximately by $N \sim 2^{n_p}/n_p$ whereas it scales as $N \sim 3^{n_p}/n_p$ for the four-sphere system. Contrary to the quantum computations the numerical expense for the semiclassical quantization, i.e., the required number of orbits depends on the separation R between the disks or spheres. For large separation $R = 6a$ the cycle-expansion method is most efficient for the calculation of a large number of resonances. The reason is that the assumption of the cycle expansion that the contributions of longer periodic orbits in the expansion of the Gutzwiller-Voros ζ function (5) are shadowed by pseudo-orbits composed of shorter periodic orbits is very well fulfilled. The harmonic inversion method also allows for the calculation of a large number of resonances, but requires a larger input set of periodic orbits. While for the two-dimensional three-disk system the semiclassical and quantum computations are very efficient, the semiclassical methods are superior to the quantum techniques for the three-dimensional four-sphere system. The semiclassical calculations can easily be extended to the region Re $ka \gtrsim 60$ where no quantum results are available because of the unfavorable scaling of the dimension of the matrix $\mathbf{M}_{lm,l'm'}$ in Eq. (14). Of course, a more efficient quantum method for the four-sphere system than that of Ref. [11] may in principle exist. However, to the best of our knowledge no such method has been proposed in the literature to date. The four-sphere system therefore is an example of a three-dimensional system where semiclassical methods are presently superior to exact quantum calculations.

At reduced separation $R = 2.5a$ between the disks or spheres the semiclassical quantization requires an increased set of periodic orbits to achieve convergence of the cycle-expansion or harmonic inversion analysis. However, for the four-sphere system the semiclassical methods are still superior to the exact quantum computations, i.e., semiclassical resonances can be obtained in regions which are unattainable with the quantum methods as can be seen in Fig. 4.

The situation is different for touching spheres $R = 2a$, which is a challenging system not only for the quantum but also for the semiclassical computations. The construction of a long periodic orbit signal is impossible because orbits with increasing sequences of consecutive 0 symbols in the code lead to accumulation points in the physical length similar as for the closed three-disk system [28,29]. The semiclassical calculations for the touching spheres are therefore at least about the same or even more expensive than the quantum computations.

VI. CONCLUSIONS

In summary, we have investigated an open system with three degrees of freedom, viz. the four-sphere scattering problem with various sphere separations by means of classical, semiclassical, and quantum mechanical methods. The classical system has genuinely three-dimensional periodic orbits. In the symmetry reduced fundamental domain, they can be associated to a ternary symbolic alphabet, which allows for a systematic periodic orbit search. For large separations between the spheres ($R \gtrsim 2.5a$) semiclassical resonances have been obtained by application of the cycle-expansion technique and the harmonic inversion method. For touching spheres ($R = 2a$), the symbolic dynamics is pruned and the cycle expansion does not converge, however, some semiclassical resonances can be revealed by harmonic inversion of a cross-correlated periodic orbit signal.

Exact quantum mechanical resonances have also been calculated, however, the quantum computations for the three-dimensional four-sphere system are much more expensive than for the two-dimensional analog, viz. the three-disk scattering problem. Therefore, the quantum computations had to be restricted to the region with relatively low wave numbers, i.e., Re $ka < 60$. By analyzing the scaling properties of both the quantum and semiclassical calculations we have demonstrated the superiority of semiclassical methods over quantum computations at least for large sphere separations, i.e., semiclassical resonances can easily be obtained in energy regions which at present are unattainable with the established quantum method. These results may encourage the investigation of other systems with three or more degrees of freedom with the goal of developing powerful semiclassical techniques, which are competitive with or even superior to quantum computations for a large variety of systems.

In those regions where exact quantum results for the four-sphere system are lacking an assessment of the accuracy of the semiclassical resonances is presently impossible. Higher-order $\hbar$ corrections have been calculated for two-dimensional billiard systems [41–43], however, the extension of the theory to three-dimensional systems is a nontrivial task for future work.

Those quantum resonances which are related to diffraction of waves at the spheres have not yet been explained semiclassically. For the three-disk system diffractive resonances have been obtained with an extended periodic orbit theory by including the contributions of creeping orbits [39,40]. It will be interesting to generalize these ideas to the genuinely three-dimensional four-sphere system.

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