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Discrete symmetries and semiclassical quantization

W T Strunz, G Alber and J S Briggs
Fakultät für Physik, Universität Freiburg, Hermann Herder Strasse 3, D-79104 Freiburg i. Br., Federal Republic of Germany

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Abstract. With the help of a graph and an associated adjacency matrix the problem of semiclassical quantization is discussed for physical systems with a discrete symmetry. A general expression for the symmetry-reduced zeta-functions is derived in terms of symmetry-reduced moments of the adjacency operator. As an application the uniform semiclassical quantization conditions of the Hecht Hamiltonian are discussed within this approach.

1. Introduction

During the last few years the problem of semiclassical quantization, in particular of quantum systems which are not integrable classically, has received considerable attention because this approach yields direct insight into the connection between quantum and classical mechanics. Thereby the theoretical concept of a dynamical zeta-function which is associated with a physical system and whose zeros determine the semiclassical energy eigenvalues of the corresponding Hamiltonian has proved useful [1–3].

There exist two equivalent ways of defining such a dynamical zeta-function which are related by an analytic continuation procedure. In the first place it may be defined with the help of a cycle expansion as an infinite product over all primitive cycles of the physical system under consideration [1]. In general, the evaluation of a dynamical zeta-function with the help of such a cycle expansion constitutes a considerable task even for one-dimensional, classically integrable systems as soon as effects of quantum mechanical tunnelling are taken into account in a uniform way [4]. This is due to the fact that in this approach contributions of infinitely many primitive cycles have to be taken into account. But typically due to (approximate) cancellations between contributions of certain long primitive cycles and products of contributions of smaller cycles in the end only a finite number of permutation cycles [1, 3] is relevant for the semiclassical quantization. In the second place, the zeta-function of a physical system may be defined by a determinant involving the unitary adjacency matrix of a graph which is approximated by a finite number of vertices. Thereby the graph contains all the information about the topology of relevant (semi-)classical paths of the physical system which is needed for the evaluation of semiclassical energy eigenvalues. This approach offers the advantage that the cancellations between contributions of primitive cycles are taken into account automatically by the finite rank of the adjacency matrix and the contributions of the finite number of relevant permutation cycles is obtained in a straighforward and simple way.

If a physical system is invariant with respect to group operations of a discrete group it is known that the corresponding dynamical zeta-function factorizes with one factor for each irreducible representation. However, so far explicit expressions for these symmetry-reduced zeta-functions have been derived with the help of cycle expansions only by implementing the discrete symmetry cycle by cycle with the help of the concept of a 'symmetry-reduced phase space' [2,5]. In this paper the problem of semiclassical quantization of physical systems with a discrete symmetry is approached from the point of view of a given graph and an associated adjacency matrix. As a main result, general expressions for symmetry-reduced zeta-functions are derived in terms of symmetry-reduced moments of the relevant adjacency matrix. These symmetry-reduced moments can be evaluated in a straightforward way with the help of the group characters. In particular, for this purpose neither a knowledge of irreducible representation matrices of the group nor the concept of a 'symmetry-reduced phase space' [2,5] is required. Furthermore, by considering the special case of quantization of the (classically integrable) Hecht Hamiltonian [6] it is shown that, for graphs which constitute regular representations of the discrete symmetry group, the evaluation of the symmetry-reduced zeta-functions is particularly simple and the non-trivial effects of quantum mechanical tunnelling can easily be taken into account in a uniform way.

The paper is organized as follows. For convenience, in section 2 basic properties of dynamical zeta-functions and their connection with semiclassical quantization are summarized. In section 3 general expressions for symmetry-reduced zeta-functions are derived in terms of symmetry-reduced moments of the relevant adjacency matrix. As an example for the practical relevance of this approach, in section 4 these results are applied to the semiclassical quantization of the Hecht Hamiltonian.

2. Semiclassical quantization and dynamical zeta-functions

In this section we summarize some basic facts about semiclassical quantization of physical systems with the help of a dynamical zeta-function by concentrating on the simple but non-trivial case of dynamics of a particle in a double-minimum potential.

It has been shown recently that, in the semiclassical approximation, energy eigenvalues of quantum systems may be obtained in a convenient way with the help of a finite graph and an associated adjacency or transfer matrix $\langle k|\mathcal{A}(E)|i\rangle$ [3]. Thereby the energy eigenvalues are determined by the zeros of the corresponding dynamical zeta-function

$$\zeta(E) = \mathrm{e}^{-\mathrm{i}S/2}\mathrm{Det}\{1 - \mathcal{A}(E)\}. \tag{1}$$

For convenience the phase factor $\mathrm{e}^{\mathrm{i}S} = \det\{-\mathcal{A}\}$ in (1) is chosen in such a way that the unitarity of $\langle k|\mathcal{A}(E)|i\rangle$ implies real values of $\zeta(E)$ for real values of the energy E.

As far as the determination of the energy eigenvalues of a quantum system is concerned this adjacency or transfer matrix contains all the required information. Physically speaking, this matrix and its corresponding graph characterize the topology of the dynamical flow of the physical system. One of the simplest non-trivial examples of such a graph which determines the uniform quantization conditions of a particle which moves in a double-minimum potential is shown in figure 1. The corresponding adjacency matrix is given by [4,7]

$$\mathcal{A}(E) = \begin{pmatrix} 0 & \rho\mathrm{e}^{\mathrm{i}(S_1-\pi/2)} & \sqrt{1-\rho^2}\mathrm{e}^{\mathrm{i}S_1} & 0 \\ \mathrm{e}^{\mathrm{i}(S_1-\pi/2)} & 0 & 0 & 0 \\ 0 & 0 & 0 & \mathrm{e}^{\mathrm{i}(S_2-\pi/2)} \\ 0 & \sqrt{1-\rho^2}\mathrm{e}^{\mathrm{i}S_2} & \rho\mathrm{e}^{\mathrm{i}(S_2-\pi/2)} & 0 \end{pmatrix}.$$

The quantities S_1 and S_2 are modified classical actions which characterize the dynamics inside the potential wells 1 and 2 and take into account effects of the potential barrier. The real-valued reflection coefficient is denoted ρ. With each reflection there is associated a Maslov index of 1 which leads to the additional phase contributions of magnitude $e^{-i\pi/2}$. Explicit expressions for these quantities are given in [7], for example. Here the vertices of the graph correspond to the real-(or complex-)valued classical turning points. Its edges are elementary classical (or non-classical tunnelling) paths which connect these turning points. The adjacency matrix element $\langle k|\mathcal{A}(E)|i\rangle$ may be interpreted as the semiclassical probability amplitude for the transition of the physical system from a quantum mechanical state $|i\rangle$ which is localized around vertex i to state $|k\rangle$ which is localized around vertex k along an elementary classical path. If two vertices are not connected by an elementary path the corresponding transition probability amplitude is zero. Analogously, the matrix element $\langle k|\mathcal{A}^n(E)|i\rangle$ is the sum of all probability amplitudes for transitions from state $|i\rangle$ to state $|k\rangle$ along (composite) paths of length n. The adjacency operator $\mathcal{A}(E)$ may be viewed as a linear operator acting in the vector space $\mathcal{V}$ which is spanned by the localized states $\{|i\rangle\}$.

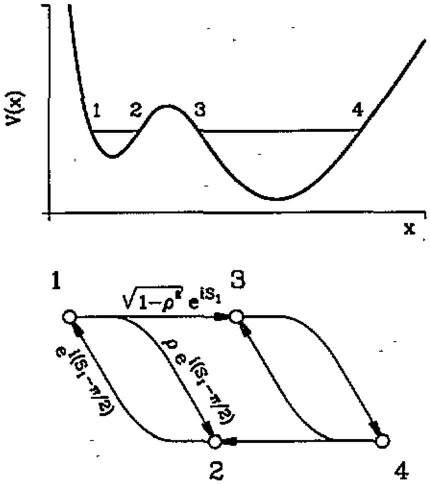

Figure 1. Double-minimum potential and corresponding graph.

For energies well above the potential barrier the semiclassical reflection coefficient ρ becomes exponentially small and contributions from the elementary paths $1 \to 2$ and $4 \to 3$ tend to zero. Similarly, for energies well below the potential barrier, the contributions of the non-classical tunnelling paths $1 \to 3$ and $4 \to 2$ become exponentially small. Thus the graph of figure 1 and its adjacency matrix yield via the zeros of the corresponding dynamical zeta-function, i.e.

$$\zeta(E) = \cos(S_1 + S_2) + \rho\cos(S_1 - S_2) = 0 \tag{2}$$

in a simple way the well known uniform quantization condition for a double-minimum potential.

Alternatively the dynamical zeta-function of a physical system may be evaluated by applying a so-called cycle expansion to a product representation of equation (1) in terms of primitive cycles [3]. This product representation is obtained from (1) with the help of the relation

$$\det(1 - \mathcal{A}(E)) = \exp\{\ln \mathrm{Det}(1 - \mathcal{A}(E))\} = \exp\left\{-\sum_{n=1}^{\infty} \mathrm{Tr}(\mathcal{A}^n(E))/n\right\}. \tag{3}$$

Thereby the trace operation $\mathrm{Tr}(\mathcal{A}^n(E))$ implies that $\ln \mathrm{Det}(1-\mathcal{A}(E))$ is expressed as a sum of contributions of all *closed paths* of the physical system. Introducing the concept of a primitive cycle, we thus obtain from (1) the product representation

$$\zeta(E) = \mathrm{e}^{-\mathrm{i}S/2} \prod_{[\gamma^p]} [1 - w(\gamma^p)] \tag{4}$$

with $w(\gamma^p)$ denoting the semiclassical probability amplitude of the primitive cycle γ^p. (A cycle is a closed path of the corresponding graph modulo starting point; a primitive cycle cannot be represented by a repetition of any shorter cycles.) In general, the number of primitive cycles is infinite so that equation (4) involves an infinite product. This implies that for real values of the energy E the product representation of (4) is not applicable directly because it is not convergent. (For the graph shown in figure 1 it may be shown explicitly that (1) and (4) are only equivalent for energies with a positive imaginary part [4].) For real values of energy the product representation of (4) is equal to (1) only in the sense of an analytic continuation procedure. This analytic continuation can be achieved by the mechanism of the so-called cycle expansion [1, 2]. Thereby the infinite product of (4) is expanded formally, i.e.

$$\prod_{[\gamma^p]} [1 - w(\gamma^p)] = 1 - \sum_{[\gamma^p]} w([\gamma^p]) + \sum_{[\gamma_1^p][\gamma_2^p]} w([\gamma_1^p]) w([\gamma_2^p]) - \dots \tag{5}$$

and is evaluated in such a way that contributions from certain long primitive cycles are cancelled by products of contributions of smaller cycles. Thus finally all but a finite number of terms which correspond to permutation cycles [3] remain.

Evaluating the dynamical zeta-function directly from equation (1) by characterizing a physical system by a graph and an associated adjacency matrix offers the advantage that the contributions of the finite number of permutation cycles is obtained directly by evaluating the determinant involving the adjacency matrix. Thereby the finite dimension of the adjacency matrix takes into account automatically the infinitely many relations between contributions of certain long primitive cycles and corresponding products of smaller primitive cycles which cancel each other in the cycle expansion [3, 4]. Explicit expressions for adjacency or transfer matrices have been derived recently for one-dimensional [4, 7] and two-dimensional [3] physical systems.

3. Discrete symmetries and symmetry-reduced dynamical zeta functions

In this section general expressions for symmetry-reduced dynamical zeta-functions are derived in terms of symmetry-reduced moments of the adjacency matrix of an arbitrary graph which is symmetric with respect to a discrete symmetry group. As a main result, semiclassical quantization conditions are obtained by this method in a simple, straightforward way from a knowledge of the group characters only, without any reference to the concept of a 'symmetry-reduced phase space' [2, 5].

The symmetry of a physical system with respect to a discrete symmetry group $\mathcal{G}$ manifests itself in the symmetry of the corresponding graph. Thereby each group operation g leads to a permutation of the vertices of the graph. The corresponding linear transformations $U(g)$ $(g \in \mathcal{G})$ in the vector space $\mathcal{V}$ which is spanned by the localized quantum states $\{|i\rangle\}$ form a representation of the group $\mathcal{G}$. Thus the discrete symmetry implies

$$[\mathcal{A}, U(g)] = 0 \qquad (g \in \mathcal{G}) \tag{6}$$

and the adjacency matrix may be brought into block diagonal form by a unitary transformation. This implies that the dynamical zeta-function of (1) factorizes, i.e.

$$\zeta(E) = \prod_{j=1}^{r} [\zeta_j(E)]^{d_j} \tag{7}$$

with each factor $\zeta_j(E)$ originating from an irreducible representation of the discrete symmetry group. The integer r counts the number of inequivalent irreducible representations of dimension d_j and equals the number of classes of the group [8]. For graphs with a large number of vertices, in general this block diagonalization constitutes a considerable task and besides a knowledge of the group characters also the irreducible representation matrices of the group have to be known.

Expressions for symmetry-reduced zeta-functions have been derived recently by starting from the product representation of (4) [2]. With the help of the concept of a symmetry-reduced phase space the discrete symmetry has been implemented cycle by cycle. Thus product representations for the corresponding symmetry-reduced zeta-functions are obtained. From the practical point of view the evaluation of symmetry-reduced zeta-functions with this approach constitutes a considerable task even in the simple case of one-dimensional quantum systems as soon as effects of tunnelling have to be taken into account in a uniform way. Thus it seems desirable to derive explicit expressions for symmetry-reduced zeta-functions directly from a given graph and an associated adjacency operator. For this purpose we start from equation (3) and decompose the basis vectors $|i\rangle$ which correspond to the vertices of a given graph into irreducible components according to [8]

$$|i\rangle = \sum_{j=1}^{r} \frac{d_j}{N} \sum_{g\in\mathcal{G}} \chi^{(j)*}(g)\{U(g)|i\rangle\}. \tag{8}$$

In this notation $\chi^{(j)}(g)$ is the character of the group element g in the jth irreducible representation. The dimension of this representation is d_j and r is equal to the number of classes of the group. The order of the group is denoted N. Evaluating the trace $\mathrm{Tr}(\mathcal{A}^n(E))$ in (3) with the help of the symmetry projection of (8) we thus find the reduced zeta-functions

$$\zeta_j(E) = \mathrm{e}^{-\mathrm{i}S_j/2} \exp\left\{ -\sum_{n=1}^{\infty} \langle \mathcal{A}_j^n(E)\rangle / n \right\}. \tag{9}$$

Thereby the nth symmetry-reduced moment of the adjacency operator is defined by

$$\langle \mathcal{A}_j^n(E)\rangle = \mathrm{Tr}\left[\sum_{g\in\mathcal{G}} \frac{1}{N} \chi^{(j)*}(g) U(g) \mathcal{A}^n \right]. \tag{10}$$

The evaluation of the reduced zeta-function of (9) can be simplified considerably by taking into account the finite rank of the unitary adjacency matrix. This may be achieved in a convenient way by introducing the quantities $\langle \mathcal{A}^n(E)\rangle_c$ which are defined by the generating function

$$\exp\left\{ -\sum_{n=1}^{\infty} z^n \langle \mathcal{A}_j^n(E)\rangle / n \right\} = \sum_{n=0}^{\infty} \frac{(-z)^n}{n!} \langle \mathcal{A}_j^n(E)\rangle_c. \tag{11}$$

These quantities are universal polynomials of the symmetry-reduced moments $\langle \mathcal{A}_j^n(E)\rangle$. Explicit expressions for them for $n \leqslant 4$ are given in table 1. Without symmetry-reduction the relation between moments of $\mathcal{A}$ and these universal polynomials as given in (11) has already been used by various authors [3, 9]. Inserting (11) into (9) we finally obtain

$$\zeta_j(E) = \mathrm{e}^{-\mathrm{i}S_j/2} \sum_{n=0}^{n_j} \frac{(-1)^n}{n!} \langle \mathcal{A}_j^n(E)\rangle_{\mathrm{c}}. \tag{12}$$

Now the symmetry-reduced zeta-function is represented as a finite sum involving symmetry-reduced moments of the adjacency operator. The upper limit of summation n_j is related to the rank d_{A} of the unitary adjacency operator by

$$d_{\mathrm{A}} = \sum_{j=1}^{r} n_j d_j. \tag{13}$$

This relation may be obtained from (1) by formally multiplying each adjacency matrix element by a factor z. Then the finite rank d_{A} of the unitary adjacency operator implies that $\mathrm{Det}(1 - \mathcal{A}(E))$ is a polynomial in the variable z of order $z^{d_{\mathrm{A}}}$ which, together with equation (7), implies (13). Similarly, the phase S_j in (12) may be obtained from (7) by considering the limit $z \to \infty$, thus obtaining

$$\mathrm{e}^{\mathrm{i}S_j} = \frac{(-1)^{n_j}}{n_j!} \langle \mathcal{A}_j^{n_j}(E)\rangle_{\mathrm{c}} \tag{14}$$

which implies $S = \sum_{j=1}^{r} d_j S_j$. Thus all quantities $\langle \mathcal{A}_j^n(E)\rangle_{\mathrm{c}}$ with $n > n_j$ are zero. From the point of view of the cycle expansion of the dynamical zeta-function these infinitely many relations between symmetry-reduced moments of the adjacency operator reflect the fact that an adjacency matrix of finite rank implies automatically that contributions of certain long primitive cycles are cancelled by contributions of certain shorter ones [2–4]. The general expression for the factorization of the dynamical zeta-function, which is obtained from (7) and (10)–(12), is the main result of this section. It allows the evaluation of the reduced dynamical zeta-function directly from the group characters and the given graph. A knowledge of the irreducible representation matrices of the group or the concept of a 'symmetry-reduced phase space' [2, 5] is not required. Furthermore, in cases in which the number of vertices of the graph equals the order of the discrete group the evaluation of the symmetry-reduced moments is greatly simplified. In this case the graph constitutes a regular representation of the symmetry group and any vertex of the graph can be reached from an arbitrarily chosen vertex, for example vertex $|1\rangle$, by one of the group operations. Thus, equation (10) reduces to

$$\langle \mathcal{A}_j^n(E)\rangle = \sum_{g\in\mathcal{G}} \chi^{(j)*}(g) \langle 1|U(g)\mathcal{A}^n|1\rangle. \tag{15}$$

In the following section we discuss the semiclassical quantization of a classically integrable physical system which may be represented by such a graph. In particular, it is shown that this approach allows to take into account the non-trivial effects of quantum mechanical tunnelling in a straightforward and uniform way.

Table 1. Explicit expressions for the first few polynomials $\langle\mathcal{A}_j^k\rangle_c$ in terms of the corresponding symmetry-reduced moments of the adjacency operator $\langle\mathcal{A}_j^k\rangle$.

k	$\langle\mathcal{A}_j^k\rangle_c$
1	$\langle\mathcal{A}_j\rangle$
2	$\langle\mathcal{A}_j\rangle^2 - \langle\mathcal{A}_j^2\rangle$
3	$\langle\mathcal{A}_j\rangle^3 - 3\langle\mathcal{A}_j\rangle\langle\mathcal{A}_j^2\rangle + 2\langle\mathcal{A}_j^3\rangle$
4	$\langle\mathcal{A}_j\rangle^4 - 6\langle\mathcal{A}_j\rangle^2\langle\mathcal{A}_j^2\rangle + 3\langle\mathcal{A}_j^2\rangle^2 + 8\langle\mathcal{A}_j\rangle\langle\mathcal{A}_j^3\rangle - 6\langle\mathcal{A}_j^4\rangle$

4. Application

As an example, in this section we discuss the semiclassical quantization of the Hecht Hamiltonian [6]

$$H(\boldsymbol{J}) = a\boldsymbol{J}^2 + b(J_x^4 + J_y^4 + J_z^4 - \tfrac{3}{5}\boldsymbol{J}^4) \tag{16}$$

with the help of a graph and an associated adjacency matrix. This model Hamiltonian has been used successfully for the description of rotational spectra of non-rigid octahedral-symmetric molecules like SF_6 [10]. In the case of SF_6 the parameters a and b assume the values $a = 0.091\,083$ cm^{-1} and $b = 1.81 \times 10^{-9}$ cm^{-1}. Here, $\boldsymbol{J}$ is the body-fixed angular momentum operator of the molecule, and both $H(\boldsymbol{J})$ and $\boldsymbol{J}^2$ are conserved quantities. Therefore, on the energy shell and for fixed value of $\boldsymbol{J}^2$ the dynamics are one-dimensional, so that this Hamiltonian describes a classically integrable dynamical system. Classically, at energy $E_s = 0.5b\boldsymbol{J}^2$ the dynamics evolve along separatrices with 12 stable and 12 unstable fixed points. Correspondingly, for energies $E < E_s$ there exist eight stable periodic orbits and for $E > E_s$ their number is reduced to six [10–12]. Semiclassical quantization conditions for this Hamiltonian which are valid either well below or well above this threshold have already been derived by Harter and Patterson [10]. Semiclassical quantization conditions which are valid uniformly across this threshold have been derived recently by Robbins *et al* [11, 12] from the point of view of periodic orbit theory. With the help of elaborate summation techniques these authors derived analytical expressions for the semiclassical energy eigenvalues by determining the poles of the density of states.

Alternatively, these uniform semiclassical quantization conditions may also be obtained in a straightforward and simple way with the help of a suitably chosen graph and an associated adjacency matrix which constitute a regular representation of the octahedral symmetry group. Such a graph can be constructed by inspection of the classical paths of the angular momentum $\boldsymbol{J}$ for fixed values of energy and $\boldsymbol{J}^2$. For energies $E < E_s$ there exist eight classical periodic orbits which describe precession of the system around one of the eight stable fixed points of the angular momentum [12]. They are indicated in figure 2 by dashed lines. The topology of the six classical periodic orbits which exist for energies $E > E_s$ is indicated by solid lines in figure 2. If we characterize these dynamical aspects by a graph which constitutes a regular representation of the octahedral symmetry group, we have to take into account that any vertex must be reachable from any other one by application of one of the group operations. Furthermore, it is a natural requirement that vertices which belong to closed paths and are associated with classical periodic orbits of the physical system are connected by group elements which belong to an Abelian and therefore cyclic subgroup. (In semi-simple Lie groups, for example, this requirement defines the natural geodesics of the group manifold [13].) This implies that the six classical periodic orbits which exist for energies $E > E_s$ may be associated in a natural way with the six different fourfold rotations (usually denoted C_4) of the octahedral symmetry group [8]. Therefore each of these orbits consists of four vertices of the graph which are all connected by only one of the six possible fourfold rotations which generates an Abelian subgroup. A corresponding graph is shown in figure 2. The number of vertices, namely 24, equals the order of the symmetry group. In figure 2 these vertices are visualized by points on the faces of a cube. The six closed paths on these faces whose vertices are connected by solid lines represent the six classical periodic orbits of the physical system which exist for energies $E > E_s$. Analogously, the eight classical periodic orbits which exist for energies $E < E_s$ may be associated with the eight possible threefold rotations (usually denoted C_3) of the octahedral symmetry group [8]. The corresponding closed paths of the graph are indicated by dashed lines in figure 2. For energies $E < E_s$ the solid lines of figure 2 represent non-classical elementary tunnelling paths, whereas the dashed lines represent classically allowed elementary paths. For energies $E > E_s$ the situation is reversed. An adjacency matrix which is symmetric with respect to the octahedral symmetry group may be obtained easily from this graph by associating with each solid line a probability amplitude $\omega_1 = \sqrt{1-\rho^2}e^{i\tilde{S}}$ and with each dashed line a probability amplitude $\omega_2 = \rho e^{i(\tilde{S}-\pi/2)}$. In analogy with the tunnelling problem discussed in section 2, ρ is the reflection coefficient which tends to 1 for energies well below E_s and becomes exponentially small for energies well above E_s. Each reflection implies a Maslov index of 1. The modified classical action $\tilde{S}$ characterizes the dynamics along an elementary path. Explicit expressions for these quantities as a function of energy, suitably continuated for $E > E_s$, are given in [12].

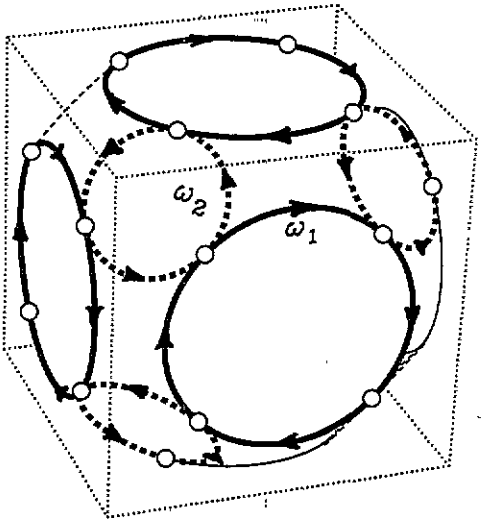

Figure 2. Graph of the Hecht Hamiltonian.

With the help of this graph and the general expression for the reduced zeta-functions as given in (12) and (15), we can easily perform the symmetry reduction and obtain the uniform semiclassical quantization conditions of the Hecht Hamiltonian. The evaluation of the symmetry-reduced moments of the adjacency operator is greatly simplified by noting that only two group elements start from each vertex. This implies that, for $n = 1$ for example, the sum in (15) consists of two terms only. For convenience, in table 2 the characters of the five classes of the octahedral group (rows) are summarized for the five irreducible representations (columns). Furthermore, as we are dealing with a regular representation the integers n_j appearing in (12) are given by $n_j = d_j \leqslant 3$ [8]. Thus we simply obtain the following reduced dynamical zeta-functions

$$\begin{aligned}
\zeta_{A_1}(E) &= 2\sin\left(\frac{\tilde{S}-\beta}{2}\right) \\
\zeta_{A_2}(E) &= 2\cos\left(\frac{\tilde{S}+\beta}{2}\right) \\
\zeta_{E}(E) &= 2\sin(\tilde{S}) + \sin(\beta) \\
\zeta_{T_1}(E) &= 2\sin\left(\frac{3\tilde{S}+\beta}{2}\right) - 2\cos(\beta)\sin\left(\frac{\tilde{S}+\beta}{2}\right) \\
\zeta_{T_2}(E) &= 2\cos\left(\frac{3\tilde{S}-\beta}{2}\right) + 2\cos(\beta)\cos\left(\frac{\tilde{S}-\beta}{2}\right)
\end{aligned} \tag{17}$$

with $\sqrt{1-\rho^2} = \cos(\beta)$. Their zeros determine the well known uniform quantization conditions of the Hecht Hamiltonian [11, 12].

Table 2. Character table of the five classes (rows) of the octahedral group for the five inequivalent irreducible representations (columns).

	E	$8C_3$	$3C_2$	$6C_2$	$6C_4$
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

This example demonstrates that the use of a graph and an associated adjacency matrix provides not only a practical but also a physically illuminating method for semiclassical quantization of systems with a discrete symmetry. Thereby the graph characterizes the topology of the dynamic flow of the physical system. As this approach allows the inclusion of effects of quantum mechanical tunnelling in a straightforward way, it may prove useful in the future development of a uniform semiclassical theory of multidimensional tunnelling.

Acknowledgments

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