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Trace identities and their semiclassical implications

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Abstract. The compatibility of the semiclassical quantization of area-preserving maps with some exact identities which follow from the unitarity of the quantum evolution operator is discussed. The quantum identities involve relations between traces of powers of the evolution operator. For classically *integrable* maps, the semiclassical approximation is shown to be compatible with the trace identities. This is done by the identification of stationary phase manifolds which give the main contributions to the result. The compatibility of the semiclassical quantization with the trace identities demonstrates the crucial importance of non-diagonal contributions. The same technique is not applicable for *chaotic* maps, and the compatibility of the semiclassical theory in this case remains unsettled. However, the trace identities are applied to maps which appear naturally in the theory of quantum graphs, revealing some features of the periodic orbit theory for these paradigms of quantum chaos.

1. Introduction

This paper focuses on quantum maps which are represented by unitary evolution operators U on an M-dimensional Hilbert space. The quantum map propagates any initial state ψ_0 in the Hilbert space by

$$\psi_{t+1} = U\psi_t = U^{t+1}\psi_0. \tag{1}$$

Traces of powers of U will be the main object of our study. They will be denoted by $t_n \equiv \mathrm{tr}\, U^n$. The fact that U is unitary imposes various relations amongst the t_n which should be satisfied *identically*. In this paper I would like to study a certain class of identities, the simplest version of which reads

$$\lim_{\epsilon\to 0} \epsilon \sum_{n=n_0}^{\infty} t_n^* t_{n+\nu} \mathrm{e}^{-n\epsilon} = t_\nu$$

for arbitrary integers n_0 and ν. The traces t_n can be expressed as sums over periodic orbit contributions. In most cases of interest the periodic orbit expressions are only valid within the semiclassical approximation. However, in the theory of quantum graphs, the periodic orbit expressions are exact. The purpose of the present paper is to study the consequences of the trace identities in periodic orbit theory. When periodic orbit expressions are only approximate, the compatibility of the semiclassical approximation is the main issue. We shall show that for integrable maps, the compatibility results from special correlations between contributions of certain periodic orbits. These methods cannot be used in the study of chaotic maps. However, the theory of quantum graphs is a convenient paradigm of quantum chaotic systems. Here,

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the trace identities can be reduced to express exact correlations between families of periodic orbits.

The trace identities will be proved and discussed in detail in section 2. Before doing this, it is instructive to review a few other identities, which involve the t_n, and which were used in past investigations of the semiclassical approximation [1–4].

The first class of identities can be derived by studying the properties of the characteristic polynomial

$$p_U(z) \equiv \det(I - zU) = \sum_{m=0}^{M} a_m z^m. \tag{2}$$

Since $p_U(U^\dagger) = 0$,

$$a_0 = 1 = -\sum_{m=1}^{M} a_m (U^\dagger)^m. \tag{3}$$

Multiplying by U^n $(n > M)$ and taking the trace one obtains

$$t_n = -\sum_{m=1}^{M} a_m t_{n-m}. \tag{4}$$

By successive applications of the above relation, all the traces t_n with $n > M$ can be expressed in terms of the traces of the M lowest powers.

An important consequence of the unitarity of U is the *inversive symmetry* of the coefficients a_m,

$$a_m = \mathrm{e}^{\mathrm{i}\Theta} a^*_{M-m} \tag{5}$$

where $\det(-U) \equiv \mathrm{e}^{\mathrm{i}\Theta}$. One can utilize the inversive symmetry to obtain identities between the t_n by invoking Newton's identities. They relate the traces t_n and the coefficients of the secular polynomial a_m,

$$a_m = -\frac{1}{m}\left(t_m + \sum_{k=1}^{m-1} a_k t_{m-k}\right). \tag{6}$$

Since $a_m = 0$ for $m > M$, the t_n for all $n > M$ depend linearly on the lower $m \leqslant M$ traces, which is consistent with our previous observation. Successive iterations yield explicit expressions for the coefficients a_m in terms of the t_n, and one can substitute them in (4) or in (5).

The significance of such relations in the semiclassical context is due to the fact that t_n are expressed semiclassically as sums over n-periodic orbits of the classical map. Thus, the compatibility with the exact identities implies that there exist identities relating sums over periodic orbits of *different* periods which are satisfied within the margins of semiclassical accuracy. The resulting identities between the t_n become complicated as n and M increase, and therefore their compatibility with the semiclassical approximation was seldom tested [5].

Another set of identities which will be shown to be closely related to this paper was introduced by Berry in [6]. He considered the spectral density of a quantum Hamiltonian

$$d(E) = \sum_{n=1}^{\infty} \delta(E - E_n) \tag{7}$$

and its smooth approximant

$$d_\epsilon(E) = \sum_{n=1}^{\infty} \delta_\epsilon(E - E_n) \qquad \text{with} \quad \delta_\epsilon(x) = \frac{1}{\pi}\frac{\epsilon}{\epsilon^2 + x^2}. \tag{8}$$

Assuming that the spectrum has no degeneracies ($E_n \neq E_m$ when $n \neq m$), one finds

$$2\pi \lim_{\epsilon\to 0} \epsilon d_\epsilon^2(E) = d(E). \tag{9}$$

Substituting the semiclassical trace formula in both sides of (9) one sees that the left-hand side is quadratic while the right-hand side is linear in the periodic orbit amplitudes. Integrating (9) over a sufficiently large energy domain, the contributions of long orbits to the right-hand side can be made arbitrarily small, while their contribution to the left-hand side will not be smoothed out. This observation led Berry to conclude that the long periodic orbits must contain information about the short periodic orbits if the semiclassical approximation is compatible with (9). This information is stored as correlations between actions of periodic orbits, because pairs of *distinct* periodic orbits combine together to give an amplitude of order ϵ^{-1} in $d_\epsilon^2(E)$, which, upon multiplying by ϵ reproduce the periodic orbit contributions to the oscillatory parts of $d(E)$. This is a highly 'non-diagonal' effect, which needs very special correlations between the actions to find the correct result. This observation shows that the use of identities of this type comes naturally in the context of the study of classical action correlations and their effect on the statistics of the quantum spectra [9–11].

Keating [7] (see also [8]) generalized (9) and used it in his studies of the spectrum of the Riemann zeros. The 'non-diagonal' correlations which are necessary to prove the identities are introduced by using the Hardy–Littlewood conjecture on the correlations between primes.

Bogomolny [12] tested (9) for the spectrum of a rectangular billiard with periodic boundary conditions and of integrable systems in general. By considering carefully the stationary phase manifolds in the sums over periodic orbits which arise from the left-hand side, he was able to perform the summations and to demonstrate the compatibility of the semiclassical approximation with (9). Bogomolny's methods [12] are used here to prove the compatibility of the semiclassical approximation with the trace identities for integrable systems. The version of (9) which is appropriate for maps, is given in (15) below. It is obtained from the trace identities (10) by multiplying by $e^{i\nu\theta}$ and summing over ν. Thus, testing the semiclassical compatibility with the trace identities, offers a check for each individual ν, rather than a global test of their sum.

This manuscript is arranged in the following way. The trace identities will be derived in the next section. The semiclassical quantization of area-preserving maps will be reviewed in section 3 and the compatibility of the semiclassical approximation will be demonstrated in section 4 for integrable maps. The close relation between the compatibility problem and the correlations between actions of periodic orbits will be addressed at the end of this section. The difficulties encountered in attempting to use the same methods to study the compatibility in the case of hyperbolic maps are discussed as well. Some progress in this direction can be made, by considering maps which appear naturally in the analysis of quantum graphs [19–21]. The periodic orbit theory for these maps is exact, and the trace identities can be used to derive certain relations which must exist amongst *families* of periodic orbits. This will be discussed in section 5. The combinatorial nature of the periodic orbit theory of quantum graphs was emphasized in [21], and the trace identities, when applied for a particular problem, are shown in the appendix to lead to new combinatorial identities which involve Krawtchouk polynomials [13, 14]. The latter are important building blocks in the theory of error-correcting codes [15], and the identities might be of use in this branch of mathematics.

2. Trace identities

Consider a unitary matrix U of dimension M. Its spectrum consists of M points on the unit circle $\{e^{i\theta_m}, m = 1, \ldots, M\}$, where the eigenphases are real and are assumed to be distinct. Recalling the notation $t_n \equiv \mathrm{tr}\, U^n$, the following identities hold for arbitrary integers n_0 and ν:

$$\lim_{\epsilon\to 0} \epsilon \sum_{n=n_0}^{\infty} t_n^* t_{n+\nu} e^{-n\epsilon} = t_\nu. \tag{10}$$

To prove these relations one substitutes $t_n = \sum_{m=1}^{M} e^{in\theta_m}$ and after summing the geometric series, one uses

$$\lim_{\epsilon\to 0} \frac{\epsilon}{1 - e^{i(\theta_m - \theta_{m'}) - \epsilon}} = \left\{ \begin{array}{lll} 1 & \text{for} & (\theta_m - \theta_{m'}) = 0 \\ 0 & \text{for} & (\theta_m - \theta_{m'}) \neq 0 \end{array} \right\} = \delta_{m,m'}. \tag{11}$$

The condition that there are no degeneracies in the spectrum of U is used to justify the rightmost equality in (11).

A few points are worth noting.

(a) The $\epsilon \to 0$ limit of the sum weighted by $e^{-n\epsilon}$ can be interpreted as a time average

$$\lim_{\epsilon\to 0} \epsilon \sum_{n=n_0}^{\infty} (\cdot)_n e^{-n\epsilon} = \lim_{N\to\infty} \frac{1}{N} \sum_{n=n_0}^{n_0+N} (\cdot)_n. \tag{12}$$

(b) For $\nu = 0$, and using $t_0 = M$, one finds

$$\lim_{\epsilon\to 0} \epsilon \sum_{n=0}^{\infty} \frac{1}{M} |t_n|^2 e^{-n\epsilon} = 1. \tag{13}$$

Thus, the time average of $|t_n|^2/M$ approaches 1, a result familiar from the study of the spectral form-factor for unitary matrices [16].

(c) The spectral density of U on the unit circle can be written as

$$d(\theta) = \sum_{l=1}^{M} \delta_{2\pi}(\theta - \theta_l) = \lim_{\epsilon\to 0} d_\epsilon(\theta) \qquad d_\epsilon(\theta) \equiv \frac{1}{2\pi} \sum_{m=-\infty}^{\infty} t_m e^{-im\theta - \epsilon|m|}. \tag{14}$$

Using (10), one can easily derive

$$2\pi \lim_{\epsilon\to 0} \epsilon d_\epsilon^2(\theta) = d(\theta) \tag{15}$$

which is the analogue of (9) for the spectrum of unitary operators.

The following identities which involve products of more than two traces can be proven with the help of (11):

$$t_\nu = \lim_{\epsilon_1\to 0} \cdots \lim_{\epsilon_k\to 0} \epsilon_1 \cdots \epsilon_k \sum_{n_1=n_{1_0}}^{\infty} \cdots \sum_{n_k=n_{k_0}}^{\infty} t_{n_1}^* \cdots t_{n_k}^* t_{(n_1+\cdots+n_k)+\nu} \exp\left(-\sum_{i=1}^{k} n_i \epsilon_i\right) \tag{16}$$

where the n_{i_0} are arbitrary integers. The identities (16) can also be written as

$$t_{\nu_1+\cdots+\nu_k} = \lim_{\epsilon_1\to 0} \cdots \lim_{\epsilon_k\to 0} \epsilon_1 \cdots \epsilon_k \sum_{n_1=n_{1_0}}^{\infty} \cdots \sum_{n_k=n_{k_0}}^{\infty} t_{n_1+\cdots+n_k}^* t_{n_1+\nu_1} \cdots t_{n_k+\nu_k} \exp\left(-\sum_{i=1}^{k} n_i \epsilon_i\right). \tag{17}$$

The equivalence of (16) and (17) can be shown by taking the complex conjugate of (17), denoting $\nu_1 + \cdots + \nu_k = -\nu$ and shifting the summation variables n_i by ν_i. The shifts do not affect the result since they can be absorbed in the arbitrary $\{n_{i_0}\}$.

The compatibility of the semiclassical approximation for t_n with the identities (10) and (16) will be investigated in section 4, after the semiclassical approximation for t_n which will be reviewed in the following section.

3. Semiclassical quantization of maps

The quantum unitary operator U to be investigated, is assumed to be the quantum version of an area-preserving map $\mathcal{F}$ acting on a finite phase space domain $\mathcal{M}$ with area $|\mathcal{M}|$. (For the sake of simplicity the maps to be considered to act on manifolds with $f = 1$, and will be assumed to have the twist property.) The dimension of the Hilbert space, M, is related to the classical phase space volume $|\mathcal{M}|$ by

$$M = \left[\frac{|\mathcal{M}|}{(2\pi\hbar)^f} \right] \tag{18}$$

where $[\,\cdot\,]$ stands for the integer part and f is the number of classical freedoms.

The phase space coordinates are denoted by $\gamma = (q, p)$ and γ is mapped to $\bar{\gamma} \equiv \mathcal{F}(\gamma)$. Area-preserving maps can be derived from a generating function (action) $\Phi(q, \bar{q})$

$$p = -\frac{\partial \Phi(q, \bar{q})}{\partial q} \qquad \bar{p} = \frac{\partial \Phi(q, \bar{q})}{\partial \bar{q}}. \tag{19}$$

The explicit mapping function $\bar{\gamma} = \mathcal{F}(\gamma)$ is obtained by solving the implicit relations (19). The twist condition ensures that the implicit equations (19) have a unique solution.

In the case where the map is integrable, let I be the invariant momentum (action variable) under the action of the map and ϕ the canonically conjugate angle variable. The domain of the map is the annulus $I \in [I_{\min}, I_{\max}]$, $\phi \in [0, 2\pi)$ and $|\mathcal{M}| = 2\pi(I_{\max} - I_{\min})$. In this representation, the generating function must take the form $\Phi(\phi, \bar{\phi}) = \Phi(\bar{\phi} - \phi)$. The explicit map is

$$\bar{I} = I \qquad \Delta\phi = \bar{\phi} - \phi = f(I). \tag{20}$$

Here $f(I)$ (the angular velocity) is the inverse of the generating relation $I = \Phi'(\Delta\phi)$, which gives $\Delta\phi$ in terms of I. The twist condition is fulfilled if $\Phi''(\Delta\phi) \neq 0$.

The semiclassical quantization of $\mathcal{F}$ provides an approximation to the exact quantum map. In the q representation it is [3, 17]

$$\langle q|U|\bar{q}\rangle_{\text{scl}} = \left(\frac{1}{2\pi\hbar \mathrm{i}} \right)^{1/2} \left[\frac{\partial^2 \Phi(q, \bar{q})}{\partial q \partial \bar{q}} \right]^{1/2} \mathrm{e}^{(\mathrm{i}/\hbar)\Phi(q, \bar{q})}. \tag{21}$$

It can be shown to preserve the composition property $U_{\text{scl}}^{t+s} = U_{\text{scl}}^{t} U_{\text{scl}}^{s}$ and unitarity $U_{\text{scl}}(U_{\text{scl}})^\dagger = I$ within the accuracy margin of the semiclassical approximation.

The semiclassical approximation for t_n involves the periodic manifolds of the classical map. For hyperbolic maps [3, 18],

$$[t_n]_{\text{scl}} = \sum_{p \in \mathcal{P}_n} \frac{n_p \mathrm{e}^{\mathrm{i}r(\Phi_p/\hbar - \nu_p \pi/2)}}{|\det(I - T_p^r)|^{1/2}}. \tag{22}$$

The semiclassical approximation for t_n involves the set of n-periodic orbits $\mathcal{P}_n$ which are repetitions of primitive periodic orbits of $\mathcal{F}$, with periods n_p which are divisors of n, so that $n = n_p r$. The monodromy matrix is denoted by T_p. Each periodic orbit contribution is endowed with a phase which is the action summed along the periodic orbit,

$$\Phi_p = \sum_{j=1}^{n_p} \Phi(q_j, q_{j+1}) \qquad (\text{with} \quad q_{n_p+1} = q_1) \tag{23}$$

and of the Maslov contribution $-\nu_p \pi/2$.

For integrable maps, the action-angle variables (I, ϕ) will be used, where I is the classical invariant. In the quantum picture, I is quantized to integer multiples of $\hbar$ so that $I_j = j\hbar$ and $1 \leqslant j \leqslant M$. The matrix U is diagonal in the action representation. The semiclassical approximation for the eigenphases can be carried out directly,

$$[\theta_j]_{\rm scl} = \frac{1}{\hbar}\left[\Phi(f(I_j)) - I_j f(I_j)\right] \tag{24}$$

where $f(I)$ is the angular frequency (20). Thus,

$$[t_n]_{\rm scl} = \sum_{j=1}^{M} {\rm e}^{{\rm i}n[\theta_j]_{\rm scl}}. \tag{25}$$

This semiclassical expression is not of the desired form, because it does not express t_n in terms of the periodic orbits. However, performing the j sum using Poisson summation, one finds

$$[t_n]_{\rm scl} = \left(\frac{2\pi}{n\hbar}\right)^{1/2} {\rm e}^{-{\rm i}(n+\frac{1}{2})\pi/2} \sum_{m=1}^{n} \left[\Phi''(\Delta\phi = 2\pi m/n)\right]^{1/2} {\rm e}^{({\rm i}/\hbar)n\Phi(\Delta\phi=2\pi m/n)}. \tag{26}$$

Now, t_n is expressed as a sum over the periodic manifolds of period n and winding number m. They occur at values of I for which the angular frequency is rational $f(I_{n,m}) = 2\pi m/n$.

The expressions for t_n in terms of periodic manifolds in the cases of classically integrable and classically chaotic maps are the necessary building blocks for the discussions which follows.

4. Compatibility of the semiclassical approximation

The compatibility of the semiclassical approximation for t_n with the trace identities will now be shown for *integrable* maps. This is done by applying Bogomolny's method [12]. Turning first to (10), the semiclassical expression (26) for t_n is substituted into the right-hand side of (10), resulting in

$$\begin{aligned}\epsilon \sum_{n=n_0}^{\infty} \left[t_n^* t_{n+\nu}\right]_{\rm scl} {\rm e}^{-n\epsilon} &= \epsilon {\rm e}^{-{\rm i}\nu\pi/2} \frac{2\pi}{\hbar} \sum_{n=n_0}^{\infty} \frac{{\rm e}^{-n\epsilon}}{(n(n+\nu))^{1/2}} \\ &\quad \times \sum_{m=1}^{n} \sum_{m'=1}^{n+\nu} \left(\Phi''\left(2\pi\frac{m}{n}\right)\Phi''\left(2\pi\frac{m'}{n+\nu}\right)\right)^{1/2} {\rm e}^{({\rm i}/\hbar)[(n+\nu)\Phi(2\pi m'/(n+\nu)) - n\Phi(2\pi m/n)]}.\end{aligned} \tag{27}$$

The sum above runs over the periodic manifolds (tori) of the map. It is important to respect the integer character of n, m, m', since only for integer values are the classical orbits periodic. Had we turned these sums to integrals by, for example, Poisson summation, we would have lost this feature. To get a finite contribution for (27) we must collect all the terms which contribute coherently to the sum. Summing over these terms (weighted by ${\rm e}^{-\epsilon n}$) should provide a pole at $\epsilon = 0$, so that the final multiplication by ϵ will yield the residue at the pole. Inspecting (27) we immediately notice that, for example, the terms for which $m'/(n+\nu) = m/n = \alpha(\nu)$ (where $\alpha(\nu)$ depends only on ν) yield a contribution of the desired nature, because the net phase $\nu\Phi(2\pi\alpha(\nu))$ is common to all the summed terms. To find these contributions in a consistent way, we shall identify them as the points where the first variation of the phase of the summand vanishes:

$$\delta\{\text{phase}\} = \delta n\Bigg[\left(\Phi\left(2\pi\frac{m'}{n+\nu}\right) - \Phi\left(2\pi\frac{m}{n}\right)\right)$$
$$-2\pi\left(\frac{m'}{n+\nu}\Phi'(2\pi\frac{m'}{n+\nu}\right) - \frac{m}{n}\Phi'\left(2\pi\frac{m}{n}\right)\Bigg)\Bigg]$$
$$+\delta m'\left[2\pi\Phi'\left(2\pi\frac{m'}{n+\nu}\right)\right] - \delta m\left[2\pi\Phi'\left(2\pi\frac{m}{n}\right)\right]. \tag{28}$$

The phase is stationary with respect to variations in n when

$$\frac{m'}{n+\nu} = \frac{m}{n}. \tag{29}$$

One should consider only the solutions in the range $m \leqslant n$ and $m' \leqslant n+\nu$, consistently with the range of the sums over m and m'. The solution of (29) in integers is

$$\begin{aligned} n &= N\nu \qquad \text{with} \quad N = N_0, \ldots, \infty \\ m &= Nk \qquad \text{with} \quad k = 1, \ldots, \nu \\ m' &= (N+1)k. \end{aligned} \tag{30}$$

The arbitrary integer n_0 is replaced by another arbitrary constant N_0 which fixes the lower limit of the n sum. This solution is the general solution for the generic cases. One can always invent maps for which other stationary points exist. For each value of k, the points of stationary phase form a grid. Near each grid point, the summation variables will be replaced by local variables

$$n = N\nu + \delta n \qquad m = Nk + \delta m \qquad m' = (N+1)k + \delta m' \tag{31}$$

with

$$|\delta n| \leqslant \tfrac{1}{2}\nu \qquad |\delta m| \leqslant \tfrac{1}{2}k \qquad |\delta m'| \leqslant \tfrac{1}{2}k. \tag{32}$$

The range of variation of the local variables is chosen such that each point in the original sum will be counted once. The contribution of the domain about each grid point will be computed by using the stationary phase approximation. The phase cannot be made stationary with respect to independent variations of m and m' because there is no guarantee that $\Phi'(2\pi m'/(n+\nu)) = 0$ and $\Phi'(2\pi m/n) = 0$ have solutions when n, m and m' are integers. However, when (29) is satisfied, the phase is stationary on the manifold $\delta m = \delta m'$. Thus, the sum over n, m, m' in (27) is replaced by

$$\sum_{n=n_0}^{\infty}\sum_{m=1}^{n}\sum_{m'=1}^{n+\nu} \to \sum_{k=1}^{\nu}\sum_{N=N_0}^{\infty}\left\{\sum_{\delta n=-\nu/2}^{\nu/2}\ \sum_{\delta m=-k/2}^{k/2}\ \sum_{\delta m'=-k/2}^{k/2}\delta_{\delta m,\delta m'}\right\} \tag{33}$$

where the curly brackets on the right enclose the contribution of the vicinity of a single grid point, restricted to the line $\delta m = \delta m'$. On this line the summand is constant and therefore the summation amounts to multiplication by k. The δn sum can be computed by considering the quadratic approximation to the phase near the stationary points and retaining the leading term in the result. It is determined by the curvature of the phase at the point where it is stationary

$$\left.\frac{\partial^2\{\text{phase}\}}{\partial n^2}\right| = -(2\pi)^2\frac{k^2}{N(N+1)\nu^3}\Phi''\left(2\pi\frac{k}{\nu}\right). \tag{34}$$

The amplitude of the result depends on N, but when it is substituted in (27) it exactly cancels the N-dependent coefficient. The phase of the δn sum is $\nu\Phi(2\pi k/\nu)$, which is also independent of N. Thus, the resulting terms of the N sum depend on N only through $\mathrm{e}^{-\epsilon\nu N}$. Summing and taking the limit $\epsilon \to 0$ results in a factor ν^{-1}. Collecting all the factors, one finds that (27) is approximated by

$$\lim_{\epsilon\to 0} \epsilon \sum_{n=n_0}^{\infty} \left[t_n^* t_{n+\nu}\right]_{\mathrm{scl}} \mathrm{e}^{-n\epsilon} = \left(\frac{2\pi}{\nu\hbar}\right)^{1/2} \mathrm{e}^{-\mathrm{i}(\nu+\frac{1}{2})\pi/2} \sum_{k=1}^{\nu} \left[\Phi''\left(2\pi\frac{k}{\nu}\right)\right]^{1/2} \mathrm{e}^{(\mathrm{i}/\hbar)\nu\Phi(2\pi k/\nu)} = [t_\nu]_{\mathrm{scl}}\,. \tag{35}$$

This completes the proof that the trace identities (10) are compatible with the semiclassical approximation.

The more complex relations (16) or the equivalent (17) can be checked using the same technique. As an example, the compatibility of the identity

$$\lim_{\epsilon_1,\epsilon_2=0} \epsilon_1\epsilon_2 \sum_{n_1,n_2} t^*_{n_1+n_2} t_{n_1+\nu_1} t_{n_2+\nu_2} \mathrm{e}^{-n_1\epsilon_1-n_2\epsilon_2} = t_{\nu_1+\nu_2} \tag{36}$$

will be demonstrated in some detail.

Substituting in (36) the semiclassical approximation (26) for t_n, one has to consider the sum

$$\begin{aligned}
&\epsilon_1\epsilon_2 \mathrm{e}^{-\mathrm{i}(\nu_1+\nu_2)\pi/2} \left(\frac{2\pi}{\hbar}\right)^{3/2} \sum_{n_1,n_2} \mathrm{e}^{-n_1\epsilon_1-n_2\epsilon_2} \left(\frac{1}{n_1+n_2}\frac{1}{n_1+\nu_1}\frac{1}{n_2+\nu_2}\right)^{1/2} \\
&\quad\times \sum_{m_1=1}^{n_1+\nu_1}\sum_{m_2=1}^{n_2+\nu_2}\sum_{m_{12}=1}^{n_1+n_2} \left[\Phi''\left(2\pi\frac{m_1}{n_1+\nu_1}\right)\Phi''\left(2\pi\frac{m_2}{n_2+\nu_2}\right)\Phi''\left(2\pi\frac{m_{12}}{n_1+n_2}\right)\right]^{1/2} \\
&\quad\times \exp\left\{\frac{\mathrm{i}}{\hbar}\left[(n_1+\nu_1)\Phi\left(2\pi\frac{m_1}{n_1+\nu_1}\right) + (n_2+\nu_2)\Phi\left(2\pi\frac{m_2}{n_2+\nu_2}\right)\right.\right. \\
&\quad\left.\left. -(n_1+n_2)\Phi\left(2\pi\frac{m_{12}}{n_1+n_2}\right)\right]\right\}.
\end{aligned} \tag{37}$$

The phase of (37) can be made stationary with respect to variations of n_1 and n_2 under the following conditions:

$$\begin{aligned}
-\Phi_{12} + \Phi_1 + \frac{m_{12}}{n_1+n_2}\Phi'_{12} - \frac{m_1}{n_1+\nu_1}\Phi'_1 = 0 \\
-\Phi_{12} + \Phi_2 + \frac{m_{12}}{n_1+n_2}\Phi'_{12} - \frac{m_2}{n_2+\nu_2}\Phi'_2 = 0
\end{aligned} \tag{38}$$

where the short-hand notation $\Phi_1 = \Phi(2\pi m_1/(n_1+\nu_1))$ and $\Phi'_1 = 2\pi\Phi'(2\pi m_1/(n_1+\nu_1))$, etc was used. The conditions (38) are satisfied by solutions in integers of

$$\frac{m_{12}}{n_1+n_2} = \frac{m_1}{n_1+\nu_1} \leqslant 1 \qquad \text{and} \qquad \frac{m_{12}}{n_1+n_2} = \frac{m_2}{n_2+\nu_2} \leqslant 1. \tag{39}$$

The general solutions depend on three integers N_1, N_2 and k so that

$$\begin{aligned}
&n_1 = (N_1-1)\nu_1 + N_1\nu_2 && \text{with} \quad N_1 = N_0,\ldots,\infty \\
&n_2 = N_2\nu_1 + (N_2-1)\nu_2 && \text{with} \quad N_2 = N_0,\ldots,\infty \\
&m_{12} = (N_1+N_2-1)k && \text{with} \quad 1 \leqslant k \leqslant \nu_1+\nu_2 \\
&m_1 = N_1 k \\
&m_2 = N_2 k.
\end{aligned} \tag{40}$$

Again, for each value of k the points of stationary phase form a grid and one computes separately the contribution from the vicinity of each grid point. The summation volume about each grid point is of size

$$|\delta n_1, \delta n_2| \leqslant \tfrac{1}{2}(\nu_1+\nu_2) \qquad |\delta m_1, \delta m_2| \leqslant \tfrac{1}{2}k \qquad |\delta m_{12}| \leqslant k. \tag{41}$$

The phase cannot be made stationary with respect to independent variations of m_1, m_2 and m_{12}. However, as in the previous case, the phase is constant for

$$\delta m_{12} = \delta m_1 + \delta m_2. \tag{42}$$

The sums in (37) are rewritten in terms of the local variables for each grid point, and the curly brackets encloses the sums over individual domains (41),

$$\sum_{n_1=n_0}^{\infty}\sum_{n_2=n_0}^{\infty}\sum_{m_1=1}^{n_1+\nu_1}\sum_{m_2=1}^{n_2+\nu_2}\sum_{m_{12}=1}^{n_1+n_2} \to \sum_{k=1}^{\nu_1+\nu_2}\sum_{N_1=N_0}^{\infty}\sum_{N_2=N_0}^{\infty}\left\{\sum_{\delta n_1}\sum_{\delta n_2}\sum_{\delta m_1}\sum_{\delta m_2}\delta_{\delta m_{12},\delta m_1+\delta m_2}\right\}. \tag{43}$$

The last Kronecker δ is due to the restriction (42). Since the summands in the δm_1, δm_2 sums are constant, they contribute a factor of k^2. The δn_1, δn_2 sum is performed again by expanding the phase to second order and retaining the leading term in the result. The determinant of second derivatives at the point of stationary phase is

$$\det\left(\frac{\partial^2\{\text{phase}\}}{\partial n_i \partial n_j}\right) = -\left(2\pi\frac{k}{\nu_1+\nu_2}\right)^4\left(\Phi''(2\pi\frac{k}{\nu_1+\nu_2})\right)^2\frac{\nu_1+\nu_2}{(n_1+n_2)(n_1+\nu_1)(n_2+\nu_2)} \tag{44}$$

where n_1 and n_2 take the values (40). Collecting all the factors, and performing the N_1 and N_2 sums while taking the limit $\epsilon_1, \epsilon_2 \to 0$, one remains with the sum over k which can be easily identified as $\left[t_{\nu_1+\nu_2}\right]_{\text{scl}}$.

This method can be extended to identities involving higher powers. The procedure becomes much more cumbersome and will not be reproduced here.

The essence of the derivations outlined above is that the phase of the summands is constant on an infinite grid of integers. Only when all of them are summed together do they provide the necessary singularity which is cancelled against the ϵ factors and gives the correct answer.

The compatibility of the trace identities with the semiclassical approximation demonstrates the importance of 'non-diagonal' correlations which are essentially due to the repetitive nature of the distribution of periodic orbits for integrable maps. As a matter of fact, had one applied the standard diagonal approximation where repetitions are neglected, to the sums (27) and (37) one would obtain a vanishing result when ν or $(\nu_1 + \nu_2) \neq 0$. The condition (29) picks up (non-diagonal) pairs of n-periodic and $n + \nu$ periodic manifolds which coincide, since the action variable $I_{n,m}$ is the same. This feature is effective in integrable systems since the periodic manifolds are specified completely by integers (the period n and the winding number m), and it is responsible for the compatibility of the trace identity with the semiclassical approximation. The condition (40) expresses a similar coincidence of three periodic manifolds. In chaotic systems, repetitions do exist but they play a much less important role, because apart from the period n there exists no other integer which would replace m to specify the periodic orbits. This is why the method described in the present section fails for the chaotic case. For systems which are chaotic in the classical limit, attempts to identify the classical correlations which are implied by the trace identities have failed, so far, to give a definite answer.

An alternative way to explain the compatibility of the trace identities with the semiclassical quantization of integrable maps is to note that the semiclassical expressions (25) for t_n have the formal structure as a trace of a unitary matrix. Since the trace identities are based exclusively on this form, they are ensured automatically. This observation does not detract from the work presented above because it gives new insight into the interplay between the trace identities and the correlations in the spectrum of classical actions. A similar argument can be applied to explain the analogous result in Bogomolny's work [12]. There, the trace formula is derived starting with the EBK expression for the spectrum which is manifestly *real* and *discrete*. The identity (9) is valid automatically for such a spectrum, irrespective of the actual value of the energies.

5. Trace identities and quantum maps on graphs

So far, any attempt to assess the compatibility of the trace identities with the semiclassical approximation for classically chaotic systems ended in failure. Even for maps on graphs, where the periodic orbit expansion of t_n is exact [19–21], I was unable to derive the trace identities starting from the exact, periodic orbit expressions. In the present section, I use a different approach and study the consequences of the trace identities on the periodic orbit theory for graphs. The resulting identities will be shown to express correlations between families of periodic orbits.

In the following paragraphs the definition of the quantum map on a graph will be sketched. A complete exposition can be found in [21]. A graph is a collection of V vertices connected by B bonds. The number of bonds emerging from the vertex i is denoted by v_i. To each bond $b = (i, j)$ we assign a length L_b, and assume that the lengths are rationally independent. The Schrödinger operator for the graph is the one-dimensional Laplacian on each bond supplemented with appropriate boundary conditions on the vertices. The most general solution of the Schrödinger equation consists of counter-propagating waves on the bonds. They are completely specified by the $2B$ amplitudes $a_b, a_{\hat{b}}$ of these waves. The boundary conditions at the vertices, must be chosen in a way which guarantees that the resulting operator is self-adjoint. This can be done, for example, by assigning to each vertex a *unitary* 'vertex scattering matrix' $\sigma^{(i)}_{b,b'}$, whose indices b, b' run over the v_i bonds which emerge from i. The boundary conditions are imposed by requiring that at each vertex, the amplitudes of the waves which impinge on the vertex and scatter from it, are related by $\sigma^{(i)}$.

The quantum evolution on the graph corresponds to a free propagation along the bonds, and scattering at the vertices. It is effected by the unitary $2B \times 2B$ matrix

$$S_{d',d}(k) = \mathcal{C}_{d',d}\mathrm{e}^{\mathrm{i}L_{d'}k}\sigma^{(i_d)}_{d',d}(k). \tag{45}$$

Here d, d' go over the set of $2B$ directed bonds, $\mathcal{C}_{d',d}$ is the directed-bond connectivity matrix, which takes the value 1 when the end vertex of d (denoted by i_d) coincides with the start vertex of d'. Otherwise, $\mathcal{C}_{d',d} = 0$. k is the wavenumber at which the evolution is considered. One can show that this evolution operator has a 'classical' counterpart which describes a mixing evolution on an appropriately defined Poincaré section.

The relevance of graphs for the present discussion follows from the fact that tr $S^n(k)$ can be written in terms of n-periodic loops on the graph in close analogy to (22). Namely,

$$\mathrm{tr}\, S^n(k) = \sum_{p\in\mathcal{P}_n} n_p \mathcal{A}_p^r \mathrm{e}^{\mathrm{i}krl_p}\mathrm{e}^{\mathrm{i}\mu_p r} \tag{46}$$

where the sum is over the set $\mathcal{P}_n$ of primitive periodic orbits whose period n_p is a divisor of n, with $r = n/n_p$. $l_p = \sum_{b\in p} L_b$ is the length of the periodic orbit. μ_p is the phase accumulated from the vertex matrix elements along the orbit, and it is the analogue of the Maslov index. The amplitudes $\mathcal{A}_p$ are given by

$$\mathcal{A}_p = \prod_{d=1}^{n_p} \left|\sigma^{(i_d)}_{d+1,d}\right| \equiv \mathrm{e}^{-\frac{1}{2}\gamma_p n_p} \tag{47}$$

where d runs over the directed bonds traversed by the periodic orbit, and γ_p appears naturally in the classical description of the graph as the stability exponent. The main difference between (22) and (47) is that the former is an approximation while the latter is *exact*.

The number of n-periodic orbits on the graph proliferate exponentially with n, in complete analogy with the n-periodic orbits of area-preserving and hyperbolic maps. The length spectrum of n-periodic orbits is highly degenerate: given a set of B non-negative integers

$$\vec{q} = (q_1, \ldots, q_B) \qquad \sum_{b=1}^{B} q_b = n \tag{48}$$

all the periodic orbits which are obtained by traversing the bonds b q_b times but in a different order are *isometric* with $l_{\vec{q}} = \sum_{b=1}^{B} q_b L_b$. Note that not all the possible partitions of n into B non-negative integers correspond to legitimate periodic orbits, since the orbits must be *connected*. The amplitudes of isometric orbits contribute coherently to the trace (46). Grouping together the amplitudes of the isometric lengths we obtain

$$s_n(k) \equiv \operatorname{tr} S^n(k) = \sum_{\vec{q}} A(n, \vec{q})\, \mathrm{e}^{\mathrm{i}kl_{\vec{q}}} \qquad A(n, \vec{q}) = \sum_{p \in \vec{q}} n_p \mathcal{A}_p^r \mathrm{e}^{\mathrm{i}\mu_p r}. \tag{49}$$

If $\vec{q}$ is compatible with the connectivity, then the right sum extends over all the isometric n-periodic orbits characterized by $\vec{q}$. Otherwise, $A(n, \vec{q}) = 0$. This convention will be used henceforth, and all sums over vectors of integers (such as the left-hand sum in (49)) go over all the possible $\vec{q}$ according to (48).

Expression (49) for $s_n(k)$ can now be substituted into the trace identity (10),

$$\lim_{\epsilon \to 0} \epsilon \sum_{n=n_0}^{\infty} \sum_{\vec{f}, \vec{g}} A^*(n, \vec{f}) A(n+\nu, \vec{g})\, \mathrm{e}^{\mathrm{i}k(l_{\vec{g}} - l_{\vec{f}})} \mathrm{e}^{-n\epsilon} = \sum_{\vec{h}} A(\nu, \vec{h})\, \mathrm{e}^{\mathrm{i}kl_{\vec{h}}}. \tag{50}$$

Here, $\vec{f}$, $\vec{g}$ and $\vec{h}$ are vectors of non-negative integers which sum up to n, $n+\nu$ and ν, respectively. Since (50) is valid for every k, and utilizing the fact that the lengths of the bonds are rationally independent, we find that for any $\vec{h}$,

$$\lim_{\epsilon \to 0} \epsilon \sum_{n=n_0}^{\infty} \sum_{\vec{f}} A^*(n, \vec{f}) A(n+\nu, \vec{f} + \vec{h})\, \mathrm{e}^{-n\epsilon} = A(\nu, \vec{h}). \tag{51}$$

This identity is valid for arbitrary $\vec{h}$. However, only if $\vec{h}$ is compatible with the connectivity, $A(\nu, \vec{h}) \neq 0$. The above identity is the main result of this section. The amplitudes $A(n, \vec{q})$ are formed as a coherent superposition of contributions of the isometric periodic orbits which constitute *families*. As such, they depend crucially on the relative phases of the amplitudes of the individual periodic orbits. These phases are not random (see, e.g., [22]) and only due to their delicate imbalance can the identities (51) be satisfied.

To clarify the structure of (51), consider a few examples. If $\nu = 0$ (and $\vec{h} = 0$), one obtains the analogue of (13), which is now expressed as a condition on the family amplitudes,

$$\lim_{\epsilon \to 0} \epsilon \sum_{n=n_0}^{\infty} \sum_{\vec{q}} |A(n, \vec{q})|^2 \mathrm{e}^{-n\epsilon} = 2B. \tag{52}$$

When $\nu = 1$, the right-hand side of (51) vanishes for graphs without loops because the shortest periodic orbits are 2-periodic. The left-hand side vanishes because one cannot construct simultaneously a pair of n- and $(n+1)$-periodic orbits which differ from each other by the addition of a *single* traversal of one of the bonds. Hence either $A(n, \vec{q})$ or $A(n+1, \vec{q} + \vec{1})$ vanish.

For $\nu \geqslant 2$, I was not able to disentangle the mechanism which is responsible for the validity of (51). However, the study of graphs emphasizes the classification of periodic orbits into families of strongly correlated orbits. This phenomenon finds its analogue in periodic orbits of area-preserving, chaotic maps.

The computation of the family amplitudes $A(n, \vec{q})$ is a combinatorial problem, which, for particular cases, can be carried out explicitly (see, e.g., [21, 23]). Thus, the trace identities can be used to derive combinatorial identities of a novel type. One example of this class of identities is described in the appendix.

6. Summary

The trace identities introduced in this paper were shown to uncover correlations between periodic orbits. In the integrable case, they are of the same type which was discovered and discussed by Bogomolny [12]. As for hyperbolic maps, at this stage, one can only infer from the study of quantum graphs that the correlations are linked with the partition of the set of periodic orbits into strongly correlated families. This observation is consistent with other studies of periodic orbits correlations [11].

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Appendix. Identities for Krawtchouk polynomials

We consider here the quantum map for a two-star graph which was defined and studied in detail in [21]. It consists of a 'central' vertex out of which emerge two bonds, terminating at vertices (with indices $j = 1, 2$) with valencies $v_j = 1$. The ratio between the bond lengths L_j is assumed to be irrational. This simple model is not completely trivial if the central vertex scattering matrix is chosen as

$$\sigma^{(o)} = \begin{pmatrix} 1/\sqrt{2} & \mathrm{i}/\sqrt{2} \\ \mathrm{i}/\sqrt{2} & 1/\sqrt{2} \end{pmatrix}. \tag{A1}$$

At the two other vertices the vertex scattering matrix is just 1. The Hilbert space is of dimension two and the evolution operator is

$$S(k) = \begin{pmatrix} \mathrm{e}^{2\mathrm{i}kL_1} & 0 \\ 0 & \mathrm{e}^{2\mathrm{i}kL_2} \end{pmatrix} \begin{pmatrix} 1/\sqrt{2} & \mathrm{i}/\sqrt{2} \\ \mathrm{i}/\sqrt{2} & 1/\sqrt{2} \end{pmatrix} \tag{A2}$$

where the diagonal matrix on the left takes care of the free propagation on the bonds and the reflections from the vertices $j = 1, 2$.

One can write an *exact* expression for $s_n(k) = \mathrm{tr}\, S^n(k)$ in terms of periodic orbits on the two-star graph as in (46). There are $2^n/n$ n-periodic orbits. However, their lengths can take only $n + 1$ distinct values: $L(n, q) = 2(qL_1 + (n - q)L_2)$, with $0 \leqslant q \leqslant n$. Thus, one can write

$$s_n(k) = \sum_{q=0}^{n} \mathrm{e}^{\mathrm{i}L(n,q)k} A(n, q) \tag{A3}$$

where $A(n,q)$ is the coherent sum of the amplitudes contributed by the isometric orbits with length $L(n,q)$. It can be computed explicitly [21, 23] in terms of Krawtchouk polynomials

$$A(n,q) = \frac{1}{\sqrt{2^n}} \begin{cases} 1 & \text{for} \quad q = 0 \text{ or } n \\ (-1)^{n+q}\sqrt{\dfrac{n}{q}\dbinom{n}{q}}P_{n-1,n-q}(q) & \text{for} \quad 0 < q < n \end{cases} \tag{A4}$$

and the Krawtchouk polynomials are defined as in [13, 14] by

$$P_{N,k}(x) = \binom{N}{k}^{-1/2} \sum_{\nu=0}^{k} (-1)^{k-\nu} \binom{x}{\nu}\binom{N-x}{k-\nu} \qquad \text{for} \quad 0 \leqslant k \leqslant N. \tag{A5}$$

Substituting (A3) in the trace identity (10), we obtain for any integers ν and n_0

$$\lim_{\epsilon\to 0} \epsilon \sum_{n=n_0}^{\infty} \mathrm{e}^{-n\epsilon} \sum_{q=0}^{n}\sum_{p=0}^{n+\nu} \mathrm{e}^{2\mathrm{i}k[(p-q)L_1+(\nu-(p-q))L_2]} A(n+\nu,\, p)A(n,q)$$
$$= \sum_{\kappa=0}^{\nu} A(\nu,\kappa)\, \mathrm{e}^{2\mathrm{i}k[\kappa L_1+(\nu-\kappa)L_2]}. \tag{A6}$$

This is valid for any value of the wavenumber k. When the lengths L_1 and L_2 are incommensurate, the equality can hold only if the coefficients of the phase factors $\mathrm{e}^{2\mathrm{i}kL(\nu,\kappa)}$ on both sides are equal. This implies

$$\lim_{\epsilon\to 0} \epsilon \sum_{n=n_0}^{\infty} \mathrm{e}^{-n\epsilon} \sum_{q=0}^{n} A(n+\nu, q+\kappa)A(n,q) = A(\nu,\kappa) \tag{A7}$$

with $0 \leqslant \kappa \leqslant \nu$. Restricting to κ to the interval $1 \leqslant \kappa \leqslant \nu - 1$ the identity can be expressed in terms of Krawtchouk polynomials exclusively,

$$\sqrt{\frac{\nu}{\kappa}\binom{\nu}{\kappa}} P_{\nu-1,\nu-\kappa}(\kappa) = \lim_{\epsilon\to 0} \epsilon \sum_{n=n_0}^{\infty} \frac{\mathrm{e}^{-n\epsilon}}{2^n} \sum_{q=0}^{n} \sqrt{\frac{n(n+\nu)}{q(q+\kappa)}\binom{n}{q}\binom{n+\nu}{q+\kappa}}$$
$$\times P_{n-1,n-q}(q) P_{n+\nu-1,n+\nu-q-\kappa}(q+\kappa). \tag{A8}$$

I could not find identities of this kind in the standard books on Krawtchouk polynomials.

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