Trace formula for products of diagonal matrix elements in chaotic systems

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We derive a trace formula for $\Sigma_n A_{nn} B_{nn} \ldots \delta(E-E_n)$, where A_{nn} is the diagonal matrix element of the operator A in the energy basis of a chaotic system. The result takes the form of a smooth term plus periodic-orbit corrections; each orbit is weighted by the usual Gutzwiller factor times $A_p B_p \ldots$, where A_p is the average of the classical observable A along the periodic orbit p. This structure for the orbit corrections was previously proposed by Main and Wunner [Phys. Rev. E **60**, 1630 (1999)] on the basis of numerical evidence.

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I. INTRODUCTION

In a recent paper [1], Main and Wunner introduced the weighted density of states

$$\rho^{(A,B,\ldots)} \equiv \sum_n A_{nn} B_{nn} \ldots \delta(E-E_n). \tag{1}$$

Here $A, B, \ldots$ are operators with smooth classical limits (Weyl symbols), and $A_{nn} = \langle n|A|n \rangle$ is the diagonal matrix element of A in the energy basis. This is a simple generalization of $\rho^{(A)} \equiv \Sigma_n A_{nn} \delta(E-E_n)$, which has been studied extensively [2–9]. For chaotic systems, Main and Wunner proposed that

$$\rho^{(A,B,\ldots)} = \rho_0^{(A,B,\ldots)} + \frac{1}{\pi\hbar} \sum_p A_p B_p \ldots w_p, \tag{2}$$

where the sum is over all primitive periodic orbits p with energy E, and

$$A_p \equiv \frac{1}{\tau_p} \int_0^{\tau_p} A(\mathbf{X}_p(t)) dt \tag{3}$$

is the average value of the Weyl symbol of A along the orbit; here, τ_p is the period of the orbit, and $\mathbf{X}=(\mathbf{q},\mathbf{p})$ denotes both coordinates and momenta. Also,

$$w_p \equiv \mathrm{Re} \sum_{r=1}^{\infty} \frac{\tau_p e^{i(S_p/\hbar - \mu_p \pi/2)r}}{|\det(M_p^r - I)|^{1/2}} \tag{4}$$

is the Gutzwiller weight factor; S_p, μ_p, and M_p are respectively the action, Maslov index, and monodromy matrix of the orbit. The first term on the right-hand side of Eq. (2) represents the part that remains smooth in the semiclassical limit; it should be $O(\hbar^{-f})$, where f is the number of freedoms. However, Main and Wunner do not give an explicit formula for it.

If we set $B = \ldots = I$ in Eq. (1), and hence $B_p = \ldots = 1$ in Eq. (2), then we recover the trace formula for $\rho^{(A)}$ [4–9].

If we set $A=I$ as well, we recover the original Gutzwiller trace formula for the density of states [2]. This is the essential motivation of Main and Wunner for Eq. (2). They provide strong numerical evidence in favor of it, but they do not give an analytic derivation.

In this paper, we remedy this situation by deriving Eq. (2) from a generalization of a trace formula originally due to Wilkinson [3] (see also [5,8]). Furthermore, we provide an explicit expression for the smooth term.

II. ANALYSIS

We first consider the case of two operators, A and B, and extend the results to an arbitrary number in Sec. III. Following Wilkinson [3], we define

$$S(E,\Delta) \equiv \sum_{nm} A_{nm} B_{mn} \delta_1(E-\tfrac{1}{2}(E_n+E_m))$$
$$\times \delta_2(\Delta-(E_n-E_m)). \tag{5}$$

Here $\delta_1(E)$ and $\delta_2(E)$ are smeared δ functions. Rigorous results concerning $S(E,\Delta)$ have been proven in the case that the Fourier transforms of these smeared δ functions have compact support [8,9]. We will therefore make the simple choice

$$\delta_i(E) \equiv \int_{-\tau_i}^{+\tau_i} \frac{dt}{2\pi\hbar} e^{iEt/\hbar} \tag{6}$$

$$= \frac{\sin(E\tau_i/\hbar)}{\pi E}, \tag{7}$$

where τ_i, $i=1,2$, is a time cutoff. Our results will come from various manipulations of $S(E,\Delta)$ with $\Delta=0$.

We begin by writing

$$S(E,0) = \delta_2(0) \sum_n A_{nn} B_{nn} \delta_1(E_n-E)$$
$$+ \frac{1}{\pi} \sum_{n,m \neq n} A_{nm} B_{mn} \frac{\sin(\omega_{nm}\tau_2)}{E_n-E_m}$$
$$\times \delta_1(E-\tfrac{1}{2}(E_n+E_m)), \tag{8}$$

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where $\omega_{nm} \equiv (E_n - E_m)/\hbar$. The first term on the right-hand side is the one we want; except for the factor of $\delta_2(0) = \tau_2/\pi\hbar$, it is the same as the right-hand side of Eq. (1), in the limit as $\tau_1 \to \infty$. To get rid of the unwanted second term, we take τ_2 to be much greater than the Heisenberg time $\tau_H \equiv 2\pi\hbar\rho_0$; here

$$\rho_0 \equiv \int \frac{d^{2f}X}{(2\pi\hbar)^f} \delta(E - H(\mathbf{X})) \quad (9)$$

is the Weyl formula for the mean density of states. If $\tau_2 \gg \tau_H$, then we typically have $|\omega_{nm}|\tau_2 \gg 1$. In this case, $\sin(\omega_{nm}\tau_2)$ varies erratically as n and m are varied. Furthermore, the factor of $1/(E_n - E_m)$ can be written as $\rho_0/(n - m) = (\tau_H/2\pi\hbar)/(n - m)$, up to a factor which also varies erratically. We then have

$$S(E,0) = \frac{\tau_2}{\pi\hbar} \sum_n A_{nn}B_{nn}\delta_1(E_n - E)$$
$$+ \frac{\tau_H}{2\pi^2\hbar} \sum_{n,m \neq n} \frac{A_{nm}B_{mn}R_{nm}}{n - m} \delta_1(E - \tfrac{1}{2}(E_n + E_m)), \quad (10)$$

where we can think of R_{nm} as a random number. Provided that $|A_{mn}|$ and $|B_{mn}|$ do not tend to increase as $|m - n|$ increases (in general, a decrease is to be expected), the sum in the second term should quickly converge. Then we have

$$\frac{\pi\hbar}{\tau_2} S(E,0) = \sum_n A_{nn}B_{nn}\delta_1(E_n - E) + O(\tau_H/\tau_2). \quad (11)$$

The first term on the right-hand side is the same as the right-hand side of Eq. (1), provided $\tau_1 \gg \tau_H$, and the second term is small if $\tau_2 \gg \tau_H$.

We now wish to evaluate $S(E,\Delta)$ semiclassically. We first use Eq. (6) in Eq. (5) to get

$$S(E,\Delta) = \int_{-\tau_2}^{+\tau_2} \frac{dt}{2\pi\hbar} e^{-i\Delta t/\hbar} \int_{-\tau_1}^{+\tau_1} \frac{dt'}{2\pi\hbar} e^{+iEt'/\hbar} F(t,t'), \quad (12)$$

where we have defined

$$F(t,t') \equiv \sum_{nm} A_{nm}B_{mn} e^{-i(E_n + E_m)t'/2\hbar} e^{+i(E_n - E_m)t/\hbar}. \quad (13)$$

The key point is that we can write $F(t,t')$ as a single trace,

$$F(t,t') = \text{Tr } U(-t + \tfrac{1}{2}t')A U(t + \tfrac{1}{2}t')B, \quad (14)$$

where $U(t) = e^{-iHt/\hbar}$ is the time-evolution operator.

To simplify our exposition, we temporarily make the (otherwise unnecessary) assumption that the Weyl symbols of A and B are functions of only the coordinates $\mathbf{q}$ and not the momenta $\mathbf{p}$. We can then evaluate the trace by inserting two complete sets of position eigenstates, leading to

$$F(t,t') = \int d^f q_1 d^f q_2 \langle \mathbf{q}_1 | U(-t + \tfrac{1}{2}t') | \mathbf{q}_2 \rangle$$
$$\times A(\mathbf{q}_2)\langle \mathbf{q}_2 | U(t + \tfrac{1}{2}t') | \mathbf{q}_1 \rangle B(\mathbf{q}_1). \quad (15)$$

We now make use of the semiclassical approximation [2,10] to get

$$\int d^f q_2 \langle \mathbf{q}_3 | U(-t + \tfrac{1}{2}t') | \mathbf{q}_2 \rangle A(\mathbf{q}_2)\langle \mathbf{q}_2 | U(t + \tfrac{1}{2}t') | \mathbf{q}_1 \rangle$$
$$\cong \sum_{\text{paths}} K_{\text{path}}(\mathbf{q}_3, \mathbf{q}_1; t') A(\mathbf{q}_{\text{path}}(t + \tfrac{1}{2}t')). \quad (16)$$

Here the sum is over all classical paths that go from $\mathbf{q}_1$ at time zero to $\mathbf{q}_3$ at time t', $\mathbf{q}_{\text{path}}(\tau)$ is the position reached at time τ along a particular path, and $K_{\text{path}}(\mathbf{q}_3, \mathbf{q}_1; t')$ is the contribution of that path to the propagator $\langle \mathbf{q}_3 | U(t') | \mathbf{q}_1 \rangle$ in the semiclassical limit.

We now perform the integrals over $d^f q_1$ in Eq. (15) and over dt' in Eq. (12) by stationary phase [2–9]. We get a contribution from zero-length paths (for which $t' = 0$ at the point of stationary phase), and a sum over contributions from periodic orbits (for which $t' = \tau_p$ at the point of stationary phase). The result is

$$S(E,\Delta) = \int_{-\tau_2}^{+\tau_2} \frac{dt}{2\pi\hbar} e^{-i\Delta t/\hbar} \left[\rho_0 C_0(t) + \frac{1}{\pi\hbar} \sum_{\tau_p < \tau_1} w_p C_p(t) \right], \quad (17)$$

where the sum is over all primitive periodic orbits with period less than τ_1. Also, we have introduced the energy-surface correlation function

$$C_0(t) \equiv \frac{1}{\rho_0} \int \frac{d^{2f}X}{(2\pi\hbar)^f} \delta(E - H(\mathbf{X}))A(\mathbf{X}(t))B(\mathbf{X}), \quad (18)$$

and the orbit correlation function

$$C_p(t) \equiv \frac{1}{\tau_p} \int_0^{\tau_p} d\tau A(\mathbf{X}_p(\tau + t + \tfrac{1}{2}\tau_p))B(\mathbf{X}_p(\tau)). \quad (19)$$

Next, we must separate out a possible constant term in $C_0(t)$. To do so, we take the microcanonical average of $A(\mathbf{X})$ on a surface of constant energy E,

$$A_0 \equiv \frac{1}{\rho_0} \int \frac{d^{2f}X}{(2\pi\hbar)^f} \delta(E - H(\mathbf{X}))A(\mathbf{X}), \quad (20)$$

and define $\tilde{A}(\mathbf{X}) \equiv A(\mathbf{X}) - A_0$ and $\tilde{B}(\mathbf{X}) \equiv B(\mathbf{X}) - B_0$. We then have $C_0(t) = A_0 B_0 + \tilde{C}_0(t)$, where

$$\tilde{C}_0(t) \equiv \frac{1}{\rho_0} \int \frac{d^{2f}X}{(2\pi\hbar)^f} \delta(E - H(\mathbf{X}))\tilde{A}(\mathbf{X}(t))\tilde{B}(\mathbf{X}). \quad (21)$$

Since the system is chaotic (and hence mixing), $\tilde{C}_0(t) \to 0$ as $t \to \pm\infty$. We now have

$$S(E,\Delta) = \rho_0 A_0 B_0 \delta_2(\Delta) + \int_{-\tau_2}^{+\tau_2} \frac{dt}{2\pi\hbar} e^{-i\Delta t/\hbar} \left[\rho_0 \widetilde{C}_0(t) \right.$$

$$\left. + \frac{1}{\pi\hbar} \sum_{\tau_p < \tau_1} w_p C_p(t) \right]. \quad (22)$$

Next, we use the fact that $C_p(t)$ is periodic in t with period τ_p, which allows us to write [3]

$$C_p(t) = \sum_{k=-\infty}^{+\infty} \Gamma_{pk} e^{+2\pi ikt/\tau_p}, \quad (23)$$

where

$$\Gamma_{pk} = \frac{1}{\tau_p} \int_0^{\tau_p} dt\, e^{-2\pi ikt/\tau_p} C_p(t). \quad (24)$$

We note in particular that

$$\Gamma_{p0} = A_p B_p. \quad (25)$$

Now using Eq. (23) in Eq. (22), we get

$$S(E,\Delta) = \rho_0 A_0 B_0 \delta_2(\Delta) + \rho_0 \int_{-\tau_2}^{+\tau_2} \frac{dt}{2\pi\hbar} e^{-i\Delta t/\hbar} \widetilde{C}_0(t)$$

$$+ \frac{1}{\pi\hbar} \sum_{\tau_p < \tau_1} w_p \sum_{k=-\infty}^{+\infty} \Gamma_{pk} \delta_2(\Delta - 2\pi\hbar k/\tau_p). \quad (26)$$

This result is a slight generalization of Wilkinson's [3].

We now set $\Delta = 0$. For the $k=0$ term in the sum over orbit modes, we have a factor of $\delta_2(0) = \tau_2/\pi\hbar$; for the $k \neq 0$ terms, we use Eq. (7). After dividing through by $\delta_2(0)$, and using $\rho_0 = \tau_H/2\pi\hbar$, the result is

$$\frac{\pi\hbar}{\tau_2} S(E,0) = \rho_0 A_0 B_0 + \frac{\tau_H}{2\tau_2} \int_{-\tau_2}^{+\tau_2} \frac{dt}{2\pi\hbar} \widetilde{C}_0(t)$$

$$+ \frac{1}{\pi\hbar} \sum_{\tau_p < \tau_1} w_p \Gamma_{p0}$$

$$+ \frac{1}{\pi\hbar} \sum_{\tau_p < \tau_1} \frac{\tau_p}{\tau_2} w_p \sum_{k \neq 0} \frac{\Gamma_{pk} \sin(2\pi k\tau_2/\tau_p)}{2\pi k}. \quad (27)$$

If we assume $\tau_2 \gg \tau_1$, the last term can be neglected. Comparing Eqs. (11) and (27), and recalling Eq. (25), we verify Eq. (2). This is our key result.

There is, however, an important caveat. We have taken both τ_1 and τ_2 to be much greater than $\tau_H \sim \hbar^{-(f-1)}$. The rigorous treatment of [8,9], on the other hand, requires τ_1 and τ_2 to remain fixed as $\hbar \to 0$. This suggests that a compromise of $\tau_{1,2} \sim \tau_H$ might be optimal, which is consistent with other analyses of the trace formula [11–14]. To further investigate this issue, we consider the special case $A = B$. The magnitude of fluctuations in the values of the diagonal matrix elements of an operator A have been previously evaluated [4,6,7,15,16], with the result that

$$\rho_0^{(A,A)} = \rho_0 A_0^2 + g \int_{-\tau_H}^{+\tau_H} \frac{dt}{2\pi\hbar} \widetilde{C}_0(t). \quad (28)$$

Here $g = 2$ if the system is time reversal invariant, and $g = 1$ if it is not. Equation (28) is consistent with Eqs. (11) and (27) if we set $\tau_2 = \tau_H/2g$. We therefore conclude that, in the more general case where $A \neq B$,

$$\rho_0^{(A,B)} = \rho_0 A_0 B_0 + g \int_{-\tau_H}^{+\tau_H} \frac{dt}{2\pi\hbar} \widetilde{C}_0(t). \quad (29)$$

If we also set $\tau_1 = \tau_2$, then the final term in Eq. (27) will be negligible for short periodic orbits (although it may become significant as the orbit period τ_p approaches τ_2). This provides a theoretical explanation for the numerical results of Main and Wunner [1].

Equation (29) is an explicit formula for the smooth term. However, for $\tau_{1,2} \sim \tau_H$, it is an uncontrolled approximation, since the neglected terms in Eqs. (11) and (27) are not formally suppressed. Nevertheless, the agreement of Eq. (28) with the results of [4,6,7,15,16] leads us to believe that Eq. (29) is correct.

III. EXTENSIONS

We now return to Eq. (1) and consider a string of diagonal matrix elements of N operators, $A, B, \ldots, Z$. We can find a trace formula for Eq. (1) by starting from

$$F(t_1, \ldots, t_N) = \operatorname{Tr} U(t_1) A U(t_2) B \ldots U(t_N) Z. \quad (30)$$

We then make Fourier transforms with respect to suitable linear combinations of the t_i's to construct

$$S(E, \Delta_2, \ldots, \Delta_N)$$

$$= \sum_{nml\ldots} A_{nm} B_{ml} \ldots \delta_1\left(E - \frac{1}{N}(E_n + E_m + \ldots)\right)$$

$$\times \delta_2(\Delta_2 - (E_n - E_m)) \delta_3(\Delta_3 - (E_m - E_l)) \ldots. \quad (31)$$

A straightforward generalization of the analysis in Sec. II then leads to a result analogous to Eqs. (11) and (27), thus verifying Eq. (2).

The leading contribution to the smooth term is of the form $\rho_0 A_0 \ldots Z_0$. There are also subleading contributions that depend on various energy-surface correlation functions. For example, for $N = 3$ we have

$$\rho_0^{(A,B,Z)} = \rho_0 A_0 B_0 Z_0 + \frac{g}{2\pi\hbar} \int_{-\tau_H}^{+\tau_H} dt [A_0 \widetilde{C}_0^{BZ}(t)$$

$$+ B_0 \widetilde{C}_0^{ZA}(t) + Z_0 \widetilde{C}_0^{AB}(t)]$$

$$+ \frac{1}{\rho_0}\left(\frac{g}{2\pi\hbar}\right)^2 \int_{-\tau_H}^{+\tau_H} dt_1 \int_{-\tau_H}^{+\tau_H} dt_2 \widetilde{C}_0^{ABZ}(t_1, t_2). \quad (32)$$

Here $\tilde{C}_0^{AB}(t)$ is given by Eq. (21),

$$\tilde{C}_0^{ABZ}(t_1,t_2) = \frac{1}{\rho_0} \int \frac{d^{2f}X}{(2\pi\hbar)^f}$$
$$\times \delta(E-H(\mathbf{X}))\tilde{A}(\mathbf{X}(t_1))\tilde{B}(\mathbf{X}(t_2))\tilde{Z}(\mathbf{X}),$$
$$(33)$$

and again $g=2$ if the system is time-reversal invariant, and $g=1$ if it is not. This follows from requiring Eq. (32) to reproduce Eq. (29) when we set $Z=I$.

IV. CONCLUSIONS

We have formulated and verified a precise version of Eq. (2), which was originally proposed by Main and Wunner [1] for chaotic systems. Our derivation provides an analytic explanation for their numerical results.

Main and Wunner also proposed an equation analogous to Eq. (2) for integrable systems that generalizes the Berry-Tabor trace formula [17]. We have not attempted to derive this version, but clearly it would be of interest to do so.

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[1] J. Main and G. Wunner, Phys. Rev. E **60**, 1630 (1999).

[2] M. C. Gutzwiller, J. Math. Phys. **8**, 1979 (1967); **12**, 343 (1971).

[3] M. Wilkinson, J. Phys. A **20**, 2415 (1987).

[4] M. Wilkinson, J. Phys. A **21**, 1173 (1988).

[5] B. Eckhardt, S. Fishman, K. Müller, and D. Wintgen, Phys. Rev. A **45**, 3531 (1992).

[6] B. Eckhardt and J. Main, Phys. Rev. Lett. **75**, 2300 (1995).

[7] B. Eckhardt, S. Fishman, J. Keating, O. Agam, J. Main, and K. Müller, Phys. Rev. E **52**, 5893 (1995).

[8] M. Combescure and D. Robert, Ann. Inst. Henri Poincaré Phys. Theor. **61**, 443 (1994); J. Math. Phys. **36**, 6596 (1995).

[9] M. Combescure, J. Ralston, and D. Robert, Commun. Math. Phys. **202**, 463 (1999).

[10] M. V. Berry and K. E. Mount, Rep. Prog. Phys. **35**, 315 (1972).

[11] M. V. Berry and J. P. Keating, J. Phys. A **23**, 4839 (1990).

[12] O. Agam and S. Fishman, J. Phys. A **26**, 2113 (1993).

[13] T. Prosen, Ann. Phys. (N.Y.) **235**, 115 (1994).

[14] H. Primack and U. Smilansky, J. Phys. A **31**, 6253 (1998).

[15] M. Feingold and A. Peres, Phys. Rev. A **34**, 591 (1986).

[16] S. Hortikar and M. Srednicki, Phys. Rev. E **57**, 7313 (1998).

[17] M. V. Berry and M. Tabor, Proc. R. Soc. London, Ser. A **349**, 101 (1976); J. Phys. A **10**, 371 (1977).