The Trace Formula and Spectral Statistics : Beyond the Diagonal Approximation

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Abstract

We calculate the 2-point spectral correlation function for classically chaotic systems in the semiclassical limit using Gutzwiller's trace formula. The off-diagonal contributions from pairs of non-identical periodic orbits are evaluated by relating them to the diagonal terms. The behaviour we find is similar to that recently discovered to hold for disordered systems using non-perturbative supersymmetric methods. Our analysis generalizes immediately to include parametric statistics, higher-order correlations, and to the study of the semiclassical distribution of matrix elements.

Gutzwiller's trace formula [1] leads to a semiclassical representation for the density of states $d(E) = \sum_n \delta(E - E_n)$ of a quantum system in terms of the periodic orbits of the underlying classical dynamics:

$$d(E) = \bar{d}(E) + \frac{1}{\pi\hbar} \sum_p \sum_{n=1}^{\infty} T_p A_{p,n} \cos(nS_p/\hbar), \tag{1}$$

where $\bar{d}$ is the mean density ($\bar{d} = O(\hbar^{-f})$ if the system has f degrees of freedom), and the periodic orbits, labelled p, have action S_p (defined here to include the Maslov index), period $T_p = dS_p/dE$, and stability amplitude $A_{p,n} = |\det(M_p^n - I)|^{-1/2}$, M_p being the monodromy matrix that describes the local flow linearized about the pth orbit. This expression provides a natural tool with which to investigate the conjectured link [2, 3] between the statistical distribution of the energy levels of classically chaotic systems and the eigenvalue correlations of random matrix theory (RMT). For example, one easily obtains from it a semiclassical approximation for the 2-point spectral correlation function

$$R_2(x) = \langle d(E + x_1) d(E + x_2) \rangle, \tag{2}$$

where $x = x_1 - x_2$ and $\langle \ldots \rangle$ denotes an energy average, in the form of a sum over all pairs of periodic orbits. The main questions to be answered are then: which properties of chaotic orbits are related to the universal features exhibited by complex spectra, such as level repulsion and rigidity, and how can the precise form of the results for the three symmetry-related RMT ensembles - the unitary ensemble (GUE), the orthogonal ensemble (GOE), and the symplectic ensemble (GSE) - be recovered?

The principal development in this direction was Berry's theory [4] for the form-factor

$$K(T) = \int_{-\infty}^{\infty} R_2(x) \exp(ixT/\hbar) dx. \tag{3}$$

His analysis was based largely on the diagonal approximation, which involves keeping only the contributions from pairs of orbits that are identical modulo symmetries. These diagonal terms may be evaluated using the Hannay-Ozorio de Almeida sum rule for ergodic flows [5], and when $T \ll T_H = 2\pi\hbar\bar{d}$ the results coincide with the corresponding RMT expressions. Unfortunately, to calculate $K(T)$ outside this range necessarily involves the evaluation of the off-diagonal terms associated with pairs of non-identical orbits. The

problem is that these are connected with correlations between the actions and stabilities of different orbits, about which we have no a priori knowledge [6], except in a few non-generic examples [7], or in the case of the Riemann zeta function [8].

Our aim here is to outline a method for evaluating the off-diagonal contributions indirectly, but explicitly, by relating them to the diagonal terms. Specifically, we derive expressions for them in terms of a classical zeta function whose analytic structure, associated with the Hannay-Ozorio de Almeida sum rule, determines their form in the semiclassical limit.

The results we obtain are very closely related to ones found recently for ensembles of disordered systems using nonperturbative supersymmetric methods [9, 10]. Indeed, making certain simplifying approximations we recover those precisely. This then represents further strong evidence of the deep connections between the quantum properties of individual deterministically chaotic systems and of ensembles of randomly disordered systems. Furthermore, it also emphasizes the close formal relationship between the semiclassical approach, based on the trace formula, and the sypersymmetric techniques associated with nonlinear σ-models.

We now outline the basic ideas behind our calculation. We begin with the trace formula (1), truncated (smoothly if necessary) so as to include only orbits with periods $T_p < T^*$, where T^* is a parameter whose value will be fixed later in the analysis. Denoting the resulting density by $d_{T^*}(E)$, one can then define corresponding approximations to the eigenvalues via the quantization condition [11, 12]

$$N_{T^*}(E_n(T^*)) = n + 1/2, \tag{4}$$

where $N_{T^*}(E) = \int_0^E d_{T^*}(E')dE' = \bar{N}(E) + N_{T^*}^{(osc)}(E)$ is the associated staircase (counting function),

$$N_{T^*}^{(osc)}(E) = \frac{1}{\pi} \sum_{T_p<T^*} \sum_{n=1}^{\infty} \frac{1}{n} A_{p,n} \sin(nS_p), \tag{5}$$

and for simplicity we have set $\hbar = 1$. (Henceforth, the semiclassical limit will correspond to $\bar{d} \to \infty$.) Clearly $d_{T^*}(E)$ represents a semiclassical approximation to the exact density of states smoothed on the energy scale $\sim h/T^*$; thus if $T^* \sim T_H$ it can be used to calculate faithful approximations to the

true eigenvalues (i.e. $E_n(T^\star) \simeq E_n$ for $T^\star \geq T_H$) and to study the *average* behaviour of the spectral correlations over ranges $x \gg \bar{d}^{-1}$. However, it misses the correlation information related to the singular structure of the exact density of states on scales small compared to the mean level separation. To overcome this difficulty, we define a new *bootstrapped density* $D_{T^\star}(E) = \sum_n \delta(E - E_n(T^\star))$, which may in principle also be calculated using only those orbits with $T_p \leq T^\star$, but which does not involve any energy-smoothing. We call it a bootstrapped density because its Fourier transform clearly has structure for all times T, not just for $T < T^\star$, the role of the *effective orbits* introduced beyond $T^\star$ being to generate the correct analytic properties associated with the discreteness of the quantum spectrum. Rewriting $D_{T^\star}$ in the form

$$\begin{aligned} D_{T^\star}(E) &= d_{T^\star}(E) \sum_n \delta(N_{T^\star}(E) - n - 1/2) \\ &= d_{T^\star}(E) \sum_{k=-\infty}^{\infty} (-1)^k \exp(2\pi i k N_{T^\star}(E)), \end{aligned} \tag{6}$$

and substituting into (2) then gives

$$\begin{aligned} R_2(x) = \langle & d_{T^\star}(E+x_1) d_{T^\star}(E+x_2) \\ & \sum_{k_1,k_2} (-1)^{k_1-k_2} \exp(2\pi i (k_1 N_{T^\star}(E+x_1) - k_2 N_{T^\star}(E+x_2))) \rangle, \end{aligned} \tag{7}$$

which is the equation upon which our analysis will be based.

Consider first the $k_1 = k_2 = 0$ term, which we write in the form

$$\langle d_{T^\star}(E+x_1) d_{T^\star}(E+x_2) \rangle = \bar{d}^2 + R_2^{(diag)}(x), \tag{8}$$

where

$$R_2^{(diag)}(x) = \frac{1}{4\pi^2} \frac{\partial^2}{\partial x_1 \partial x_2} \ln \Delta(x_1, x_2), \tag{9}$$

and

$$\ln \Delta(x_1, x_2) = 4\pi^2 \langle N_{T^\star}^{(osc)}(E+x_1) N_{T^\star}^{(osc)}(E+x_2) \rangle. \tag{10}$$

Because only orbits with $T_p < T^\star \sim T_H$ contribute, we assume that the resulting sum over orbit-pairs may be replaced by the diagonal terms, for

which the pairing involves orbits with exactly the same action and stability [4]. The result can then be expressed in the form $\Delta(x) = |Z_g(ix)|^2$, where

$$Z_g(s) = \exp\Big(\sum_{T_p \le T^\star} \sum_{n=1}^{\infty} \frac{g_p}{n^2} |A_{p,n}|^2 e^{nT_p s}\Big) \tag{11}$$

and g_p is the number of orbits with period T_p and amplitude A_p. In generic systems the multiplicity g_p is the same for almost all orbits and so, if its value is denoted g, $Z_g = (Z(s))^g$, where $Z(s)$ is defined by (11) with $g_p = 1$. For systems without time-reversal invariance $g = 1$, and for systems whose dynamics is time-reversal symmetric $g = 2$ [4]. Furthermore, using the Hannay-Ozorio de Almeida sum rule it is easy to demonstrate that if $s \to 0$ but $sT^\star \to \infty$, then $Z(s) \to \gamma/s$, and hence one obtains the appropriate RMT expressions: $R_2^{(diag)} \to -1/(2\pi^2 x^2)$ when $g = 1$ (GUE) and $R_2^{(diag)} \to -1/(\pi^2 x^2)$ when $g = 2$ (GOE). Since we anticipate taking $T^\star \sim T_H$, this result effectively emerges in the limit $x \to 0$, $x\bar{d} \to \infty$. We note in passing that there are non-generic examples of strongly chaotic systems for which $Z(s)$ has a simple pole at $s = 0$, but the multiplicities are not constant [7]. In these cases it is known that the level statistics do not obey the RMT conjecture. Clearly this then implies that it is not only the analytic properties of Z, but the multiplicity structure as well, that determine the behaviour of the spectral statistics.

Since in our approach the $k_1 = k_2 = 0$ term corresponds to the usual diagonal approximation, we identify the other terms as representing the off-diagonal contributions, and so denote them by $R_2^{(off)}(x)$. To evaluate these we note first that the Taylor expansion in powers of x of the mean counting function leads to a term $(k_1 - k_2)\bar{N}(E)$ in the phase which is $O(\hbar^{-f})$. Hence the energy-average renders negligible any contributions with $k_1 \neq k_2$, and so

$$R_2^{(off)}(x) = \frac{\partial^2}{\partial x_1 \partial x_2} \sum_{k \neq 0} \frac{1}{(2\pi k)^2} \exp(2\pi i \bar{d} k (x_1 - x_2)) \Phi_k(x_1, x_2), \tag{12}$$

where

$$\Phi_k(x_1, x_2) = \langle \exp(2\pi i k (N_{T^\star}^{(osc)}(E + x_1) - N_{T^\star}^{(osc)}(E + x_2))) \rangle. \tag{13}$$

We now make the key assumption that in generic systems the orbits up to period $T^\star$ can be treated as being statistically independent modulo exact

degeneracies, and hence that the energy average of any smooth function of $\exp(iS_p(E))$, $\langle f\rangle = \langle f(e^{iS_1(E)},\ldots,e^{iS_M(E)})\rangle$, can be calculated using

$$\langle f\rangle = \int_0^{2\pi}\cdots\int_0^{2\pi} f(e^{i\phi_1},\ldots,e^{i\phi_M})\prod_{j=1}^{M}\frac{d\phi_j}{2\pi}. \tag{14}$$

This is essentially equivalent to a random phase or strict diagonal approximation. The justification is that the diagonal approximation itself is known to be valid for times $T \ll T_H$ [4].

Using the trace formula for N_{T^*} (5) one can thus perform the energy-average in (13) by evaluating the integral in (14). We shall give exact results for certain cases later. First, for clarity, we discuss a simple leading-order approximation to $\Phi_k(x)$ based on the relation $\langle\exp(iG(E))\rangle \simeq \exp(-\langle G^2(E)\rangle/2)$. This is an identity if G is a Gaussian random function with zero mean, and so, since the exponent in (13) behaves like a sum of a large number of independent random terms (cf. (14)) it is expected to be a good approximation for generic systems. From it one obtains

$$\Phi_k(x_1,x_2) = \exp(-2\pi^2k^2\langle(N_{T^*}^{(osc)}(E+x_1) - N_{T^*}^{(osc)}(E+x_2))^2\rangle = \left(\frac{\Delta(x)}{L^2}\right)^{k^2}, \tag{15}$$

where $\Delta(x)$ was defined in (10) and $L = \exp(2\pi^2\langle(N_{T^*}^{(osc)}(E))^2\rangle)$. Using the Hannay-Ozorio de Almeida sum rule, it may be seen that $L \sim (T^*)^g$. Since we anticipate taking $T^* \sim T_H$, it then follows that the terms in the k sum decrease rapidly, as $(\bar{d})^{-2gk^2}$. Hence to leading semiclasssical order, as $x\bar{d}\to\infty$, we may retain just the $k = \pm 1$ contributions. If now we choose T^* so that $L = CT_H^g$ (which essentially corresponds to taking $T^* = T_H$), we then have that $\Phi_{\pm 1}(x) \simeq \Delta(x)/(C\bar{d})^{2g}$, where C is a constant. Thus finally, with an appropriate choice for C,

$$R_2^{(off)}(x) \simeq \frac{\cos(2\pi\bar{d}x)}{2\pi^{2g}\bar{d}^{2g-2}}|\gamma^{-1}Z(ix)|^{2g}, \tag{16}$$

which is directly equivalent to the relationship that was shown by Andreev and Altshuler [9] to hold between the perturbative and non-perturbative parts of R_2 for disordered systems in the limit of large conductance using the sypersymmetric approach. The contribution from the pole of $Z(s)$ at $s = 0$ gives immediately the exact GUE expression when $g = 1$, and the

leading-order GOE result as $x\bar{d} \to \infty$ when $g = 2$. Clearly the structure of Z around the pole determines the semiclassical approach to the RMT limit. We should point out at this stage that the value of γ, the residue at the pole, is in general not known, and hence cannot be determinated by our method.

It is also worth noting that, as already discussed in [10], $Z(s)$ may be approximately related to a classical zeta function $Z_{cl}(s)$, since, if the eigenvalues of the monodromy matrix M_p are Λ_p ($|\Lambda_p| > 1$) and Λ_p^{-1} (for simplicity we specialize here to two degree-of-freedom Hamiltonian systems), and ignoring the repetitions (i.e., taking $n = 1$ in (1)), $Z(s) \simeq Z_{cl}(s)$ where

$$\frac{1}{Z_{cl}(s)} = \prod_p \prod_{k=0}^{\infty} \left(1 - \frac{e^{sT_p}}{|\Lambda_p|\Lambda_p^k}\right)^{k+1}. \tag{17}$$

We are now in a position to consider the statistics of the third RME: the GSE. The way in which our method is constructed allows us to make use of a remarkable theorem of Mehta and Dyson [13], which states that if every alternate level is removed from a spectrum in which the correlations are GOE, then the correlations in the resulting sequence are the same as those of the GSE. This can be implemented in our semiclassical scheme by first taking $D_{T^*}(E) = d_{T^*}(E)\sum_n \delta(N_{T^*}(E) - 2n - 1/2)$, second by replacing $\bar{d}$ in the above formula by $2\bar{d}$ (because the original spectrum has twice the density of the new one), and finally by assuming, as in the GOE calculation, that the orbits come in time symmetric pairs. The result when $x\bar{d} \to \infty$ is that

$$R_2^{(diag)}(x) = \frac{1}{4\pi^2}\frac{\partial^2}{\partial x^2}\ln|Z(ix)|, \tag{18}$$

$$R_2^{(off)}(x) = \bar{d}\frac{\cos(2\pi\bar{d}x)}{4}|\gamma^{-1}Z(ix)|, \tag{19}$$

where $Z(s)$ is defined by (11) with $g_p = 1$ or (approximately) by (17). Again, the simple pole at $s = 0$ gives the leading order GSE asymptotics.

The method and results described above generalize in a number of different directions (for a more complete discussion, see [14]). First they extend directly to parametric correlations. Consider, for example, the correlation function

$$R_2(x, \phi) = \langle d(E + x/2, \bar{\phi} + \phi/2)d(E - x/2, \bar{\phi} - \phi/2)\rangle,$$

where ϕ is a parameter in the Hamiltonian and the average extends over both E and $\bar{\phi}$. Semiclassically the main effect of the parametric change is felt in S_p:

$$S_p(E + x/2, \bar{\phi} + \phi/2) \simeq S_p(E, \bar{\phi}) + \frac{x}{2} T_p + \frac{\phi}{2} \frac{\partial S_p}{\partial \phi}. \tag{20}$$

Writing $\partial S_p/\partial\phi = T_p \langle \partial H/\partial\phi \rangle_p$, where H is the Hamiltonian, we assume that the orbit-averaged derivatives $\langle \partial H/\partial\phi \rangle_j$ are Gaussian distributed with zero mean and variance α/T for orbits with $T_p \simeq T$. Averaging over the contributions to the diagonal orbit-sum, we thus have that

$$\langle \cos(xT_p + \phi T_p \langle \frac{\partial H}{\partial \phi} \rangle_p) \rangle \simeq \cos(xT_p) \exp(-\phi^2 T_p \alpha/2).$$

Hence, in terms of the dimensionless parameter $\tilde{\phi} = \phi\sqrt{\alpha/2}$, for all three ensembles the semiclassical approximation to $R_2(x, \phi)$ is obtained by replacing x in $R_2(x)$ by $y = x + i\tilde{\phi}^2$ in Z, but not in the $\cos(2\pi\bar{d}x)$ factor. Interestingly, no new choice for $T^\star$ is required in obtaining this result.

The second generalization is to higher orders of correlation. For example, our method extends immediately to the calculation of the 3-point correlation function

$$R_3(x_1, x_2, x_3) = \langle d(E + x_1) d(E + x_2) d(E + x_3) \rangle. \tag{21}$$

For simplicity we consider the case of non-time-reversal symmetric systems. Substituting $D_{T^\star}$ into (21), one immediately finds that the irreducible off-diagonal contributions are given in terms of the same function Z

$$\begin{aligned} \tilde{R}_3(x_1, x_2, x_3) \;=\; & -\frac{1}{2\pi^3} \sin(2\pi\bar{d}(x_2 - x_3)) |\gamma^{-1} Z(i(x_2 - x_3))|^2 \\ & \mathrm{Im} \left(\frac{Z'(i(x_2 - x_1))}{Z(i(x_2 - x_1))} + \frac{Z'(i(x_1 - x_3))}{Z(i(x_1 - x_3))} \right) + (1 \leftrightarrow 2, 3), \end{aligned}$$

where $(1 \leftrightarrow 2, 3)$ denotes a sum of two terms, each the same as the first, but with x_1 interchaged with x_2 and x_3 respectively. As $x_j \to 0$ this expression is dominated by the pole of $Z(s)$ at $s = 0$ and we recover the exact GUE formula for $\tilde{R}_3$, as above. Again, no new choice for $T^\star$ is required.

Our method also applies to correlations involving weighted densities. For example, consider the density of states weighted by the diagonal matrix elements of an operator $\hat{A}$ in the eigenbasis of $\hat{H}$: $d(\hat{A}, E) = \sum_n \langle n|\hat{A}|n\rangle \delta(E -$

E_n). Assuming $\hat{A}$ to be sufficiently smooth, there is a trace formula for $d(\hat{A}, E)$ that corresponds to (1) with $\bar{d}$ multiplied by the microcanonical average of the classical observable $A(p, q)$, and with the p^{th} periodic orbit contribution multiplied by an additional amplitude factor $a_p = \int_0^{T_p} A(p(t), q(t))dt/T_p$ [15]. We can define a bootstapped density $D_{T^*}(\hat{A}, E)$ containing only information from the orbits with period $T_p < T^*$ in the following way. If the T^*-truncated trace formula for $d(\hat{A}, E)$ is denoted by $d_{T^*}(\hat{A}, E)$, a natural approximation to $\langle n|\hat{A}|n\rangle$ is $A_{nn}(T^*) = d_{T^*}(\hat{A}, E_n(T^*))/d_{T^*}(E_n(T^*))$, where $E_n(T^*)$ is the associated approximation to E_n. We then take $D_{T^*}(\hat{A}, E) = \sum_n A_{nn}(T^*)\delta(E - E_n(T^*))$. The point is that this factorizes as $D_{T^*}(\hat{A}, E) = d_{T^*}(\hat{A}, E)D_{T^*}(E)/d_{T^*}(E)$, and so allows us to apply the same formulae as before. One interesting result is that if the microcanonical average of $\hat{A}$ is zero then the off-diagonal contributions to 2-point correlation functions vanish at leading order. This therefore justifies the previous use of the diagonal approximation in this case [16].

Up to now we have based our discussion on the approximate formula (15). Perhaps the most important extension of the method outlined above is that the calculation can also be performed exactly, with the correlations between orbit-repetitions n in (1) included correctly. This may be achieved by noting that $N_{T^*}^{(osc)}(E) = -\mathrm{Im}\ln Z_{T^*}(E)/\pi$, where $Z_{T^*}(E)$ is the semi-classical Selberg-type zeta function with its Euler product truncated at T^*. Substituting this into (13), the integral in (14) can be performed exactly. For example, the result for non-time-reversal-symmetric systems may be written in the form

$$R_2^{(off)} = \frac{1}{2\pi^2}|\gamma^{-1}Z_{cl}(ix)|^2 \mathrm{Re}[\exp(2\pi i\bar{d}x)\prod_p \phi_p(x)], \tag{22}$$

with

$$\phi_p(x) = {}_2\phi_1(a_p, b_p; c_p; q_p, z_p)\frac{|Z_p(0)|^2}{|Z_p(ix)|^2}, \tag{23}$$

where $a_p = b_p = \exp(-iT_p x)$, $c_p = q_p = \Lambda_p^{-1}$, $z_p = |\Lambda_p|^{-1}\exp(iT_p x)$, ${}_2\phi_1(a, b; c; q, z)$ is the q-hypergeometric series [17], and $Z_{cl}(s) = \prod_p Z_p(s)$ is the classical zeta function defined in (17) (for details see [14]). The product in (22) converges when x is real and takes the value 1 when $x = 0$. This result appears to represent a refinement of the expressions presented in [9] and [10] and re-derived above by ignoring correlations between orbit repetitions

in the trace formula. Evidence that such corrections are meaningful is that for the 2-point correlations of the zeros of the Riemann zeta-function $\zeta(s)$ [8] the corresponding result

$$R_2^{(off)}(x) = \frac{1}{2\pi^2}|\zeta(1+ix)|^2 \mathrm{Re}\left[e^{2\pi i\tilde{d}x}\prod_p\left(1-\frac{(1-p^{ix})^2}{(p-1)^2}\right)\right] \qquad (24)$$

can be shown [14] to be exactly equivalent to the Hardy-Littlewood conjecture for the pairwise distribution of the prime numbers [8].

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