The Diagonal Approximation for Non-Time-Reversal-Symmetric Systems

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We present a simple, heuristic justification for the diagonal approximation in the periodic orbit theory of long-range spectral statistics for chaotic systems without time reversal symmetry. For ergodic systems, this extends the validity of the approximation beyond the $\log(1/\hbar)$ time, where it is supported by more elementary arguments, to times of the order of the Heisenberg time $T_H = 2\pi\hbar\overline{d}$. This is in agreement with eigenvalue correlations in the Gaussian Unitary Ensemble (GUE) of Random Matrix Theory (RMT). For diffusive systems, the same argument suggests that the diagonal approximation breaks down on a time scale consistent with that expected on the basis of the scaling theory of localization.

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Random matrix theory (RMT) models the universal behaviour of quantum systems that are chaotic in the classical limit [1, 2, 3, 4]. Consider, for example, the form factor

$$K(T) = \frac{1}{\bar{d}} \int_{-\infty}^{\infty} R(\epsilon) e^{\ i c T/\hbar} d\epsilon, \tag{1}$$

where

$$R(\epsilon) = \langle d(E + \frac{1}{2}\epsilon) d(E - \frac{1}{2}\epsilon) \rangle_E - \langle d(E) \rangle_E^2 \tag{2}$$

is the two-point correlation function of the density of states $d(E)$, $\langle ... \rangle_E$ is an average over an energy range around E that is large compared to the mean level spacing and small compared to E itself, and the mean density $\bar{d} = \langle d(E) \rangle_E$ is of the order of $\hbar^{-f}$ in a system with f degrees of freedom. It has been found that $K(T)$ is well approximated by RMT in most regimes of time T; that is, it is *universal*, being determined solely by symmetries. Specifically, systems with no time reversal symmetry are modelled by the Gaussian Unitary Ensemble (GUE), for which

$$K(T) = \begin{cases} T/T_H & for \ \ 0 < T \leq T_H \\ 1 & for \ \ \ \ T > T_H \end{cases} \tag{3}$$

where the Heisenberg time $T_H = 2\pi\hbar\bar{d}$ is conjugate to the mean level separation.

Deviations from (3) are appreciable in ranges of size T_c around $T = 0$ and $T = T_H$, where T_c is the characteristic time scale for the decay of correlations in the corresponding classical system (related to the smallest non-vanishing eigenvalue of the Frobenius-Perron operator) [5, 6, 7]. T_c is analogous to the Thouless time in disordered systems and is purely classical; thus in the semiclassical limit $T_c/T_H \to 0$ and $T_c/T_E \to 0$, where T_E is the Ehrenfest time, which is of the order $\log(1/\hbar)$ for chaotic systems.

A semiclassical approximation to the density of states is given by the Gutzwiller trace formula [2, 8]

$$d(E) = \bar{d} + \Re \frac{1}{\pi\hbar} \sum_p A_p \ e^{\frac{i}{\hbar} S_p}, \tag{4}$$

where the sum is over periodic orbits with action S_p (defined here to include the Maslov index) and amplitude $A_p = \frac{T_p}{|\det(\mathcal{M}_p - I)|^{1/2}}$, T_p being the period and $\mathcal{M}_p$ the monodromy matrix. Substituting this into (1) and (2) then gives [5] :

$$K(T) = \frac{1}{T_H} \langle \sum_{p,p'} A_p A_{p'} e^{\frac{i}{\hbar}(S_p - S_{p'})} \delta \left(T - \frac{T_p + T_{p'}}{2} \right) \rangle_E. \tag{5}$$

This sum over orbit pairs is unfortunately intractable to analytic calculations for typical systems. The standard approach is to make the diagonal approximation, which for non-time-reversal symmetric systems takes the form

$$K(\tau) \approx K^{(diag)}(T) = \frac{1}{T_H} \sum_p A_p^2 \ \delta\left(T - T_p\right). \tag{6}$$

(Here the energy average has been assumed implicitly, and the symbol $\langle ... \rangle_E$ omitted.) One justification is that as $\hbar \to 0$ the phase of the exponential in (5) oscillates rapidly and consequently averages to zero unless $S_p = S_{p'}$. This is clearly valid if otherwise $|S_p - S_{p'}| > \hbar$. However, because of the exponential proliferation of periodic orbits in chaotic systems, this condition can only hold for times T that are less than T_E; that is, for times that are $\mathcal{O}(\log(1/\hbar))$. Even so, when the sum in (6) is evaluated using the Hannay-Ozorio de Almeida sum rule [9], one finds

$$K^{(diag)}(T) = \frac{T}{T_H} \tag{7}$$

when $T > T_c$, which coincides with the GUE expression (3) up to Heisenberg time T_H, which is of the order of $\hbar^{1-f}$. It is therefore natural to ask why the approximation works so far outside its obvious range of validity. Our purpose here is to present one possible explanation. In addition, we will also show that our argument leads to predictions for the time-scale on which the diagonal approximation (equivalent to diagrammatic perturbation theory [10]) breaks down in diffusive systems that are in agreement with the scaling theory of localization.

Our approach makes explicit use of the conjectured universality of the quantum spectral statistics in classically chaotic systems of spinless particles without time reversal (or any other anti-unitary) symmetry in the following way. For simplicity, we consider a two dimensional billiard with no geometrical symmetry threaded by Aharonov-Bohm flux lines [11], and average over the fluxes. It will be assumed that the form factor, being universal, is invariant under this operation. We will then show that this implies the exactness of the diagonal approximation in the range $T_c < T < T^*$, where T^* is of the same order as T_H. (The range $0 \leq T \leq T_c$ is already covered by the argument given after (6), because $T_c/T_E \to 0$ as $\hbar \to 0$).

Before we start, it is worth noting explicitly that flux lines are central to our approach; we cannot use a smooth magnetic field. The motion of a charged particle is different in the two cases in several important respects. First, the classical motion is not disturbed at all by the flux lines, whereas it is in a smooth magnetic field. Second, quantum wave functions are diffracted by the flux lines and, by virtue of the boundary conditions, vanish on each of them; hence their morphology is completely different from that encountered in a smooth magnetic field. Third, all physical quantities are periodic in each flux, and so any analogy with a real magnetic field can only hold when the fluxes are much smaller than one fluxon. In the present work we make essential use of this periodicity.

Let the billiard be threaded by $N+1$ flux lines with fluxes ϕ_j (in units of one fluxon), where $j = 0, 1, 2...N$. The action of the periodic orbit p then satisfies

$$\frac{S_p}{\hbar} = \frac{S_p^0}{\hbar} + 2\pi \sum_{j=0}^{N} \phi_j \omega_{j,p} \tag{8}$$

where S_p^0 is the action of the pth orbit in the absence of the flux lines, and $\omega_{j,p}$ is its winding number with respect to the position of the j-th flux line. Hence the semiclassical approximation to the form factor (5) can be written

$$K(T;\phi_0,\Phi) = \frac{1}{T_H} \sum_{p,p'} A_p A_{p'} e^{\frac{i}{\hbar}(S_p^0 - S_{p'}^0) + i2\pi \sum_{j=0}^{N} \phi_j (\omega_{j,p} - \omega_{j,p'})} \delta\left(T - \frac{T_p + T_{p'}}{2}\right) \tag{9}$$

where Φ denotes the set of fluxes ϕ_j with $j = 1, 2, ..., N$. If ϕ_0 is sufficiently large, the system belongs to the class of systems described by general Hamiltonians where time reversal symmetry is broken [12], independently of the values of ϕ_0 and ϕ_j for $j \neq 0$ (the restrictions on this statement will be discussed below). Averaging over all ϕ_j with $j > 0$ will thus not affect $K(T)$ in the universal regime, and so

$$K(T) = \langle K(T;\phi_0,\Phi)\rangle_\Phi = \frac{1}{T_H} \sum_{p,p'} A_p A_{p'} e^{\frac{i}{\hbar}(S_p^0 - S_{p'}^0) + i2\pi\phi_0(\omega_{0,p} - \omega_{0,p'})} \prod_{j=1}^{N} \delta_{\omega_{j,p},\omega_{j,p'}} \delta\left(T - \frac{T_p + T_{p'}}{2}\right) \tag{10}$$

where $\delta_{i,j}$ is the Kronecker δ-symbol.

At this stage we divide the periodic orbits into 2 classes, corresponding to those that are self retracing and those that are not. For orbits that are self retracing, all winding numbers vanish. The fraction of these compared to the set of all orbits of period T is of the order of $e^{-h_t T/2}$, where h_t is the topological entropy. Therefore their contribution to the form factor can be ignored in the universal regime where we shall work.

Of the orbits that are not self retracing, many pairs (p, p') will not contribute to (10) because they have different winding numbers. Moreover, assuming for the moment that there is no restriction on the number of flux lines (such a restriction will, however, be discussed below), the periodic orbits of a given period can be uniquely determined by their winding numbers. To see this, take two different periodic orbits, p_1 and p_2, with the same winding numbers around the flux lines already in place. A new flux line j_{12} can always be introduced in the space between the two orbits about which they will have different winding numbers $\omega_{j_{12},p_1} \neq \omega_{j_{12},p_2}$. Hence if the density of flux lines is unbounded, all non-diagonal contributions to the form factor can be removed, for any given fixed T, by the averaging procedure described above; that is, the diagonal approximation can be shown to be exact for all T.

We are now in the position of having proved too much, because the diagonal approximation is in fact only exact up to $T = T_H$. The question is, therefore, what determines the breakdown of the flux line argument? To answer this, it is helpful to place the flux lines at the vertices of a lattice with spacing a. Knowledge of all the winding numbers determines the orbits with resolution a. The key point is that the approach described above can only be applied when a is large compared to the de-Broglie wavelength λ. There are three ways to see this. First, the semiclassical trace formula (4) is only valid when $\lambda \ll a$, otherwise non-classical diffractive orbits must be included. (The only length-scale in the scattering of plane waves by a single flux line is λ, and the amplitude of the diffracted waves decreases as $\sqrt{\lambda/r}$, where r is the distance from the flux line). Second, the quantum wave functions can only resolve the flux lines if their separation is large compared to λ. Third, because the wavefunctions must vanish on the flux lines, they typically cannot extend over the billiard if $\lambda > a$. (This is analogous to the situation for channels, where if the wavelength is smaller than the width the wave is evanescent.) Thus as a is varied there is a sharp transition in their morphology at $\lambda = a$.

The fact that one must have $\lambda \ll a$ sets a restriction on the ability of the flux lattice to resolve periodic orbits. The corresponding limit of resolution in the time regime may be estimated as follows. The probability density for an ergodic orbit of length l not to pass through a given lattice cell $\mathcal{S}$ of size $a \times a$ is proportional to e^{-l/l^*}, where the mean free path is $l^* = \mathcal{A}/a$, and $\mathcal{A}$ is the area of the billiard. (Usually the mean free path is

$1/n\sigma$ where n is the density of scatterers and σ is their cross section; in the present case there is one scatterer, the region $\mathcal{S}$, so $n = 1/\mathcal{A}$, and in two dimensions σ is the linear size of $\mathcal{S}$, therefore $\sigma \approx a$.) The probability density for an orbit of period T not to pass through $\mathcal{S}$ is therefore proportional to e^{-T/T^*}, where, taking a of the order of (but much larger than) λ,

$$T^* = \eta_1 \frac{\mathcal{A}m}{\lambda p} = \eta T_H \tag{11}$$

Here η and $\eta_1 = 2\pi\eta$ are (undetermined) constants, m is the mass of the particle and p is its momentum.

An orbit that does not pass through the cell $\mathcal{S}$ differs by at least one winding number from an orbit that does. Because of the exponential nature of the probability density, nearly all of the orbits with period $T < T^*$ are uniquely determined by their winding numbers and there the diagonal approximation holds. Conversely, almost all orbits with period $T > T^*$ cannot be resolved in this way and then the diagonal approximation can no longer be justified. It is striking that T^* is of exactly the same order as the time T_H on which the approximation is known to break down.

Our argument is equivalent to the following suggestive procedure. Take a typical trajectory of length vT, where v is the velocity and T is the evolution time. Now give the trajectory a width of a de Broglie wavelength λ. The above discussion implies that the diagonal approximation is justified for times up to the order of T^*, when the area swept out is equal to the total area of the billiard; that is, T^* is the solution of $\frac{h}{mv} vT^* = \mathcal{A}$. This generalizes immediately to billiards of arbitrary dimension f. Then T^* is the solution of $(\frac{h}{mv})^{f-1} vT^* = \mathcal{V}$, where $\mathcal{V}$ is the total volume. This clearly gives $T^* = \mathcal{V}(2E)^{\frac{f}{2}-1} m^{\frac{f}{2}}/h^{f-1}$, which is again of the same order as the Heisenberg time. In a similar way, the argument also extends trivially to smooth scalar potentials.

It seems reasonable to assume that there is no time scale between T^* and T_H, and that therefore η is of order unity, but we cannot find its value from the present arguments. The most that we can conclude semiclassically is that in the region $T_c \ll T \ll T^* = \mathcal{O}(T_H)$,

$$T_H \frac{dK(T)}{dT} = 1. \tag{12}$$

for non-time-reversal-symmetric ergodic systems. This extends the range of validity beyond the $\log(1/\hbar)$ time that previously set the limit. For $T < T_c$ the form factor is not

universal and the assumptions underlying the flux-line argument do not hold. However, the first argument, given in the paragraph after (6) does then apply, because $T_c/T_E \to 0$ as $\hbar \to 0$, and so again the diagonal terms should be semiclassically exact.

Our approach can also be extended to diffusive systems. Consider first the case of a quasi-one-dimensional billiard, in which the motion is diffusive in one dimension. Again the flux-line method provides a justification of the diagonal approximation up to a time of the order of T^*, when the area swept out by an orbit given a width λ, hT^*/m, is equal to the total area explored. This second area is proportional to the mean distance traveled in the direction of diffusion, namely $\sqrt{DT^*}$ where D is the diffusion constant, and to the billiard width w. Hence $T^* \sim m^2w^2D/h^2$. More generally, for diffusion in f dimensions

$$(\frac{h}{mv})^{f-1}T^*v \sim \mathcal{V}_f(T^*) \tag{13}$$

where $\mathcal{V}_f(T)$ is the volume explored by a typical orbit after a time T. If we take for $\mathcal{V}_f$ the corresponding volume for a random walk [13], then, for example, $T^* \sim \exp(\alpha_2/\hbar)$ when $f = 2$, and $T^* \sim |\alpha_f\hbar^{f-1} - c|^{-\frac{2}{f-2}}$ for $2 < f < 4$, where c is a constant and α_f depends on m, v, D and the volume scale in system. The diagonal approximation is expected to work for $T < T^*$, in which range one has the classical result [10]

$$K^{(diag)} \approx P(T)\frac{T}{T_H} \qquad for \quad T_c < T < T^*. \tag{14}$$

where $P(T)$ is the probability density for a typical orbit to return to its starting point after a time T. For $T > T^*$ quantum interference becomes important. It is interesting to note that T^* is of exactly the same order as the break time derived from the scaling theory of localization. The flux line argument thus provides a semiclassical basis for Allen's estimate for the parametric dependence of the localization length [14]. In addition, if we assume that the time scale T^* translates under Fourier transform in the variable $1/\hbar$ into a length scale for action correlations [15], then we also have a justification for the corresponding assumptions made in [16].

It is worth noting that in diffusive systems RMT is only applicable if the localization length exceeds the size of the system $\mathcal{L}$, that is when T^* is larger than the Thouless time $\mathcal{L}^2/D$, and that our arguments are being applied in the nonuniversal regime before RMT is valid [17]. The justification relies on there still being an ensemble of systems

with different fluxes all having the same classical limit, and on the assumption that the form factor depends only on the classical dynamics. The fact that in ergodic systems the diagonal approximation applies in the nonuniversal regime when $T < T_c$ provides further support [5, 6, 7].

The simple arguments we have presented support the correctness of the diagonal approximation for systems without time reversal invariance that are modeled by GUE in the universal semiclassical regime, where RMT holds. This results from a pure quantum symmetry: the existence of a continuous family of quantum systems with the same classical limit. The possibility to vary the phases of the contributions of the various periodic orbits without any effect on the classical dynamics leads to the conclusion that the off-diagonal contribution averages to zero for times less than T^*, which is of the order of the Heisenberg time T_H. Unfortunately, our argument does not extend directly to time-reversal-symmetric systems. To do so would require the construction of families of systems with GOE statistics for which off-diagonal terms in the periodic orbits sums could be eliminated by averaging over one or more parameters. It is striking that for such systems the diagonal approximation is not exact, but that it does hold approximately on time scales of the order of T_H (in the sense that it predicts the correct universal slope of the form factor as $T/T_H \to 0$). It would be interesting, therefore, to pursue this line of reasoning further. With this point in mind, we again draw attention to the fact that our flux-line argument does not resolve contributions from self-retracing orbits, or trajectories in their neighborhood, which probably play a central role in the semiclassical theory of time-reversal-symmetric systems [18].

Also with this in mind, we return to make a final comment about (10). In the flux-line construction we left one flux (labeled $j = 0$) fixed and large, to ensure that we stayed within the GUE. However, this is not strictly necessary, because the GOE-GUE transition is semiclassically sharp; specifically, in a billiard with a single flux ϕ, the level statistics are, on the scale of the mean level spacing, GOE when $\phi = 0$ and GUE when $\phi^2 \mu T_H >> 1$, where μT_H is the mean-square winding number of orbits whose period is T_H [12]. (For the form factor to take the GUE form throughout the regime $T_c < T < T^*$ similarly requires $\phi^2 \mu T_c >> 1$.) Thus if the form-factor is averaged over *all* of the fluxes, the result is semiclassically close to the GUE expression. This has interesting

implications. Consider a billiard in which the dynamics is time-reversal-symmetric. The level statistics will then be GOE and one may expect this to be seen in the semiclassical periodic orbit sum (5). Now introduce a set of flux lines, as above, and average over all of them. The result is a similar orbit sum, but contains only those pairs that have the same winding numbers about all of the positions where the flux lines were - this corresponds to (10) without the contribution from the $j = 0$ flux. Note that no fluxes appear in the final expression. This implies that if one sums over all pairs of orbits in (5) one will get the GOE form factor, but if one sums only over those pairs that have the same winding numbers about some arbitrarily chosen set of points, one will be left with the GUE form factor, at least for $T < T^*$. Thus the semiclassical difference between the GOE and the GUE is in orbits that have different winding numbers about one or more such points. One such pairing is between an orbit and its time-reverse, leading to the derivative of $K(T)$ at $T = 0$ being twice the GUE value, but the fact that the $K(T)$ is not exactly linear implies that there are more. It possible that this may be a clue as to the semiclassical origins of weak localization corrections. The fact that orbits in the vicinity of self-retracing trajectories are an exceptional set with respect to the flux line argument again hints at their involvement in these corrections [18].

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