A fundamental characteristic of quantum systems that are chaotic in their classical limit is universality. It is observed that diverse systems behave identically when statistics of energy levels or wave functions are considered, provided that they have the same symmetries. These universal statistics agree with those of random matrix theory, i.e. with the statistics of eigenvalues and eigenvectors of large random matrices [1]. Support for this random matrix hypothesis comes from a large number of numerical and experimental investigations which have been carried out on a great variety of systems [2]. However, it remains an open question to understand the origin of this universality, and its relation to the underlying classical dynamics.

One theoretical approach by which such an understanding may be attempted is the semiclassical method. Semiclassical approximations are asymptotically valid in the limit $\hbar \to 0$ where universality is expected to hold. Moreover, they directly connect quantum properties with properties of the corresponding chaotic classical system. They have been applied in particular to statistical distributions of the energy levels which are bilinear in the density of states, one example being the spectral form factor $K(\tau)$. One of the successes of the semiclassical approach has been to show that the spectral statistics do indeed agree with the random matrix statistics in the limit of long-range correlations; specifically the correct leading order behaviour of $K(\tau)$ as $\tau \to 0$ has been derived [3].

An extension of this result requires knowledge of correlations between different periodic orbits [4]. The relevant mechanisms by which periodic orbits are correlated have to be identified, and the contributions of correlated orbits to the spectral form factor have to be evaluated. Based on an analogy with disordered systems [5] and with diffractive corrections [6] it has been suggested that the next term in the expansion of $K(\tau)$ for small τ originates from 'two-loop orbits': orbits that have a self-intersection with small crossing angle and neighbouring orbits without self-intersection [7]. There is strong numerical evidence that in systems with time-reversal symmetry these orbit pairs indeed yield the next-order-term in agreement with the expectation based on random matrix theory.

In the following we present a derivation of the next to leading order term in the expansion of the spectral form factor for small τ. We evaluate analytically the contributions of the two-loop orbits to the form factor for uniformly hyperbolic systems with time-reversal symmetry, and we show that the result indeed agrees with random matrix theory. The calculation makes clear the properties of classical trajectories which are responsible for the universal result.

We consider the spectral form factor, which is defined as the Fourier transform of the two-point correlation function of the density of states

$$K(\tau) = \int_{-\infty}^{\infty} \frac{d\eta}{\bar{d}(E)} \left\langle d_o\Big(E + \frac{\eta}{2}\Big)\, d_o\Big(E - \frac{\eta}{2}\Big)\right\rangle_E e^{2\pi i \eta \tau \bar{d}(E)} \tag{1}$$

where the density of states $d(E) = \sum_n \delta(E - E_n)$ is divided into a mean part $\bar{d}(E)$ and an oscillatory part $d_o(E)$. For systems with time-reversal symmetry, or more generally an anti-unitary symmetry, it is expected that the form factor agrees in the semiclassical limit ($\hbar \to 0$) with that of the Gaussian Orthogonal Ensemble (GOE) of random matrix theory which has the expansion

$$K^{\mathrm{GOE}}(\tau) = 2\tau - 2\tau^2 + \mathcal{O}(\tau^3) \quad \text{as} \quad \tau \to 0\,. \tag{2}$$

The semiclassical approximation for the form factor is obtained by inserting Gutzwiller's trace formula for the density of states into (1) and evaluating the integral in leading order of $\hbar$. The result is an approximation in terms of a double sum over all periodic orbits of the classical

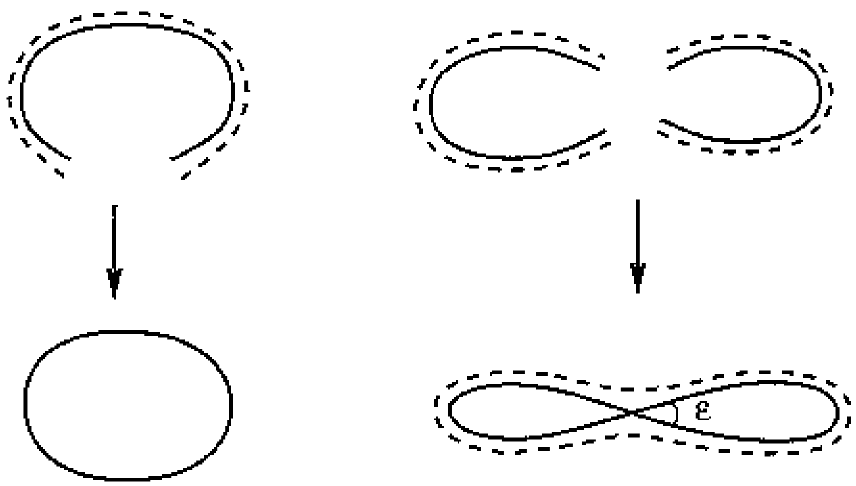

Figure 1: The pairs of orbits considered here consist of different segments. In each segment one orbit is very close to the other (or its time reverse), but they can differ in the way the segments are connected.

system

$$K(\tau) \approx \frac{1}{h\bar{d}(E)} \left\langle \sum_{\gamma\gamma'} A_\gamma A^*_{\gamma'} e^{\frac{i}{\hbar}(S_\gamma - S_{\gamma'})}\, \delta\!\left(T - \frac{T_\gamma + T_{\gamma'}}{2}\right)\right\rangle_E \tag{3}$$

where $\tau = T/(h\bar{d}(E))$ and $h = 2\pi\hbar$. Furthermore, A_γ is an amplitude, generally complex-valued, which depends on the stability and the Maslov index of the periodic orbit γ, and S_γ and T_γ are its action and period.

The double sum in (3) runs over all possible pairings of periodic orbits. However, most of these pairs do not contribute in the semiclassical limit. Periodic orbits which are located in different regions in phase space are uncorrelated, and when summed over, the contributions from different pairs cancel each other. It is expected that the relevant semiclassical contributions come from a relatively small number of pairs of orbits which are correlated. The key problem is then to identify the mechanism which is behind these correlations.

The basic assumption we make is that only those periodic orbits which are almost everywhere close to one another, or to the time-reverse of the other orbit, are correlated [7]. In order for two orbits to be different but nevertheless close they must have special forms which can be constructed in the following way. The orbits are composed of different segments during which one orbit follows very closely the other orbit (or its time-reverse). However, the orbits can differ in the way in which the segments are connected.

The two simplest possibilities are shown in Fig. 1. If orbits are composed of only one segment then the two ends can be connected in only one way. It then follows that the two neighbouring orbits are either identical or one is the time-reverse of the other. Including only these pairs in the double sum corresponds to the diagonal approximation, which yields the correct leading order behaviour $K(\tau) \sim 2\tau$ as $\tau \to 0$ [3].

Two segments, on the other hand, can be connected in two ways, leading to orbits with or without self-intersection at the connection point, as shown in Fig. 1. In order for these pairs to exist and to be close, the crossing angle ε has to be small. Then it can be shown in a linearized approximation, that one orbit is indeed in the neighbourhood of the other.

In the following we evaluate the contributions of such pairs of orbits to the spectral form factor. In order to avoid further assumptions and to keep the calculations simple we restrict attention now to systems with uniformly hyperbolic dynamics, specifically we consider the representative example of the geodesic motion on Riemann surfaces with constant negative curvature [8]. Then the quantities A_γ, S_γ and T_γ in (3) depend only on the length of an orbit, and A_γ is positive. We assume that the systems have no further symmetries and are non-arithmetic so that the typical degeneracy of a length of a periodic orbit is two. For these systems the action difference for the pairs of orbits being considered here has been calculated in the linearized approximation for small crossing angle ε in [7] and is given by

$$\Delta S(\varepsilon) \approx \frac{p^2 \varepsilon^2}{2m\lambda} \tag{4}$$

where λ is the Lyapunov exponent of the system, and p and m are momentum and mass of the particle.

The sum over these pairs of orbits can be evaluated by summing over all self-intersections of periodic orbits with small crossing angle ε, because for every such self-intersection there exists a neighbouring periodic orbit with action difference $\Delta S(\varepsilon)$. The self-intersections are determined by introducing a function which selects them. This is done in the following way. A self-intersection of a periodic orbit with period T divides the orbit into two loops. It can be characterized by the crossing angle ε and the total time t along the shorter of the two loops, $t \leq T/2$. Furthermore, we introduce an angle variable ϕ that specifies the direction of the velocity, and a variable t' that measures the time along a periodic orbit. If at any time t' along a periodic orbit $\boldsymbol{q}(t'+t) = \boldsymbol{q}(t')$ and $\phi(t'+t) = \phi(t') - \pi + \varepsilon$ then this periodic orbit has a self-intersection with opening angle ε, and traversing the corresponding shorter loop takes time t.

Correspondingly, we can express the contribution from pairs of the two-loop orbits to the form factor as

$$\begin{aligned} K^{(2)}(\tau) = \; & \tfrac{4}{\hbar \bar{d}(E)} \operatorname{Re} \textstyle\int_{-\pi}^{\pi} d\varepsilon \, \int_0^{T/2} dt \, \sum_\gamma A_\gamma^2 \, e^{\frac{i}{\hbar}\Delta S(\varepsilon)} \\ & \times \delta(T - T_\gamma) \, \textstyle\int_0^T dt' \, f_{\varepsilon,t}(\boldsymbol{q}(t'), \boldsymbol{p}(t')) \end{aligned} \tag{5}$$

where the function $f_{\varepsilon,t}$ is given by

$$\begin{aligned} f_{\varepsilon,t}(\boldsymbol{q}(t'), \boldsymbol{p}(t')) = \; & |J| \, \delta(\phi(t'+t) - \phi(t') + \pi - \varepsilon) \\ & \times \delta(\boldsymbol{q}(t'+t) - \boldsymbol{q}(t')) \end{aligned} \tag{6}$$

Here $|J| = v^2 \, |\sin \varepsilon| / \sqrt{g}$ is the Jacobian for the transformation from the arguments of the three delta functions to the three integration variables, where v is the speed of the particle and g is the determinant of the metric tensor. The three integrals give a contribution each time that t' is at the beginning of a loop with time t and opening angle ε. The choice of the limits of the integral over ε is not important since the main contribution in the semiclassical limit $\hbar \to 0$ comes from the asymptotic behaviour of the integrand at $\varepsilon = 0$. In (5) the amplitudes and the periods of the neighbouring orbits were set to be equal since the difference does not contribute to the leading semiclassical order.

One of the important properties of long periodic orbits is their uniform distribution on the energy surface in phase space. It implies that the average of a given phase space function

$f(\boldsymbol{q},\boldsymbol{p})$ along all periodic orbits of a certain period T can be replaced, in the limit $T \to \infty$, by an average of this function over the energy surface in phase space [9]. More accurately, the following asymptotic relation holds as $T \to \infty$

$$\begin{array}{cl} & \sum_\gamma |A_\gamma|^2 \delta(T - T_\gamma) \int_0^T dt' \, f(\boldsymbol{q}(t'), \boldsymbol{p}(t')) \\ \sim & \frac{T^2}{\Sigma(E)} \int d^2q \, d^2p \, \delta\left(E - \frac{p^2}{2m}\right) \, f(\boldsymbol{q},\boldsymbol{p}) \end{array} \tag{7}$$

where $\Sigma(E)$ is the volume of the energy surface in phase space.

The relation (5) is in the form in which this property of the periodic orbits can be applied. The semiclassical limit $\hbar \to 0$ is performed with the condition that $\tau/\hbar \to \infty$. The mean density of states being $\bar{d}(E) \sim \Sigma(E)/(2\pi\hbar)^2$, this implies that $T \to \infty$ and thus the leading order semiclassical behaviour arises from the large T behaviour. Applying the uniformity of the periodic orbit distribution and performing the integral over the energy delta-function one obtains

$$K^{(2)}(\tau) \sim \frac{4p^2T^2}{mh\bar{d}(E)} \,\mathrm{Re} \int_{-\pi}^{\pi} d\varepsilon \; \mathrm{e}^{\frac{ip^2\varepsilon^2}{2m\hbar\lambda}} \sin|\varepsilon| \int_0^{T/2} dt \, p_E(\varepsilon, t) \tag{8}$$

where

$$p_E(\varepsilon, t) = \int \frac{d^2q_0 \, d\phi_0}{\Sigma(E)} \, \delta(\boldsymbol{q}(t) - \boldsymbol{q}_0) \, \delta(\phi(t) - \phi_0 + \pi - \varepsilon) \tag{9}$$

and $\boldsymbol{q}(t)$ and $\phi(t)$ are the coordinates of a particle at time t, whose initial conditions at $t = 0$ are specified by $\boldsymbol{q}_0$, ϕ_0 and energy E.

The quantity $p_E(\varepsilon, t)$ has a direct classical interpretation. It is the probability density for a particle with energy E to return after time t to its starting point with a velocity that deviates from the initial velocity by an angle $\varepsilon - \pi$. In the same way as for the diagonal approximation, one thus finds that the periodic orbit sum is related to a transition probability density in phase space [10].

Our aim is to determine the leading order behaviour of (8) as $\hbar \to 0$ which, as remarked above, depends on the long-time behaviour of $p_E(\varepsilon, t)$. For long times $p_E(\varepsilon, t)$ approaches one over the volume of the energy shell in phase space, because the particle is equally likely to be found anywhere on the energy shell, i.e. $p_E(\varepsilon, t) \sim 1/\Sigma(E)$ as $t \to \infty$. Inserting this into (8) and applying the method of stationary phase yields

$$\frac{p^2\tau^3\Sigma(E)}{m\pi^2\hbar^2} \,\mathrm{Re} \int_0^\infty d\varepsilon \; \exp\left(\frac{ip^2\varepsilon^2}{2m\hbar\lambda}\right) \, \varepsilon = 0 \tag{10}$$

and so the leading order term as $\hbar \to 0$ vanishes. This implies that one has to take into account the next order terms. A closer analysis of (5) shows that the important term to consider is the next to leading order behaviour of $p_E(\varepsilon, t)$ as $t \to \infty$. Quite surprisingly, the two-loop contribution does not originate from the ergodic limit of the probability density $p_E(\varepsilon, t)$ but from the approach to this limit.

We have to consider $p_E(\varepsilon, t)$ in more detail. It is a classical transition probability density and can be expressed in terms of classical trajectories. These trajectories are all time t loops with opening angle ε. Consider one such loop as shown in Fig. 2a. Every point in the vicinity of its starting point is the starting point of another loop, one example being shown by the dashed line. To determine how angle ε and time t change with the initial point we introduce a local

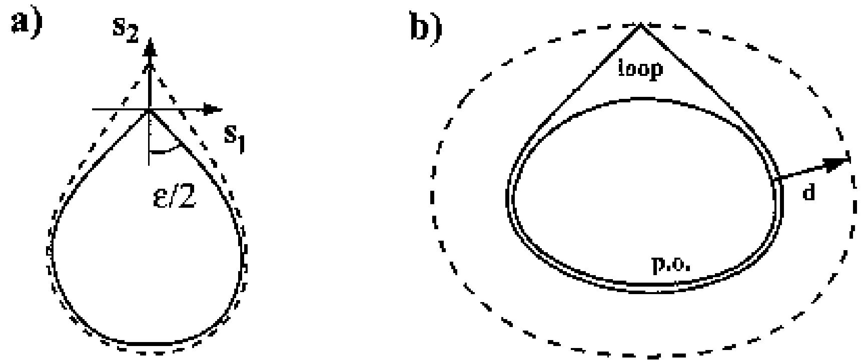

Figure 2: a) A loop with opening angle ε (full line), and the local coordinate system at its starting point. b) Loops with the same opening angle ε whose traversal takes time t form a continuous family which have their starting points on a curve of constant distance d from a periodic orbit.

coordinate system (see Fig. 2a) and linearize the motion in the vicinity of the loop. The result is

$$v\, dt = 2 \cos \frac{\varepsilon}{2}\, ds_2\,, \quad v\, d\varepsilon = -2\lambda \sin \frac{\varepsilon}{2} \tanh \frac{\lambda t}{2}\, ds_2 \tag{11}$$

One finds that angle and time change only in the s_2 direction, but not in the s_1 direction. This is a particular property of the uniformly hyperbolic dynamics. After integrating the equations (11) one arrives at the following conclusion. The loops with fixed ε and t form continuous one-parameter families. All the initial points of the loops within a family lie on a curve which has a constant distance (denoted by d) from a periodic orbit as shown schematically in Fig. 2b. The relation between the loops and the periodic orbit is given by

$$\cosh \frac{\lambda t}{2} \sin \frac{|\varepsilon|}{2} = \cosh \frac{\lambda t_0}{2} \tag{12}$$

where t_0 is the period of the periodic orbit. It is a remarkable property that any loop is uniquely related to a periodic orbit into which it can be continuously deformed through a series of other loops. Put another way, this implies that any self-intersection of any arbitrary classical trajectory is uniquely related to a periodic orbit, because a self-intersection is the initial point of a loop.

We examined this property numerically. We chose a large number of long random trajectories on a Riemann surface with constant negative curvature [11] and recorded all their self-intersections. For every self-intersection a point is plotted in the (ε, t)-plane, where ε and t are the opening angle and traversal time of the corresponding loop. The result is shown in Fig. 3. As expected, the points form continuous lines that start at the periods of the periodic orbits (the t-values at $\varepsilon = \pi$). One can observe a logarithmic divergence of the curves at $\varepsilon = 0$ which is implied by Eq. (12). The full line in Fig. 3 is an evaluation of Eq. (12) for the second family of loops, and it is found to be in perfect agreement with the numerical result.

We continue by expressing $p_E(\varepsilon, t)$ in terms of the classical trajectories. By evaluating the integrals over the delta-functions in (9), $p_E(\varepsilon, t)$ can be written as a sum over all families of loops with opening angle ε, which are labelled by ξ in the following. Alternatively, by using

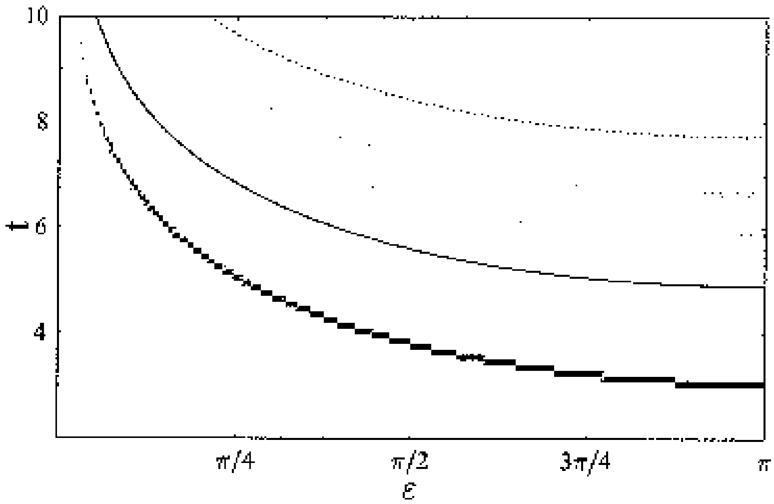

Figure 3: Numerical result of the search for loops with opening angle ε and time t. Grey scales are proportional to the number of loops found in bins in the (ε, t)-plane.

the relation (12), $p_E(\varepsilon, t)$ can also be expressed in terms of the periodic orbits labelled by ξ_0.

$$\begin{aligned} p_E(\varepsilon, t) = & \frac{1}{\Sigma(E)} \sum_{\xi} \frac{T_{\xi_0} \cosh(\lambda d/v)\, \delta(t-T_\xi)}{\sin|\varepsilon/2|\,(\mathrm{Tr}\, M_\xi - 2)} \\ = & \frac{1}{\Sigma(E)} \sum_{\xi_0} \frac{T_{\xi_0}\, \delta(t-T_\xi)}{\sqrt{(\mathrm{Tr}\, M_{\xi_0}-2)(\mathrm{Tr}\, M_{\xi_0}-2+4\cos^2\frac{\varepsilon}{2})}} \end{aligned} \tag{13}$$

where M_ξ and M_{ξ_0} denote the stability matrices. We remark that a further use of Eq. (12) yields

$$p_E(\varepsilon, t) = p_E(\pi, t_0)\ . \tag{14}$$

This means that the distribution $p(\varepsilon, t)$ is identical to the return probability density $p(\pi, t_0)$ at a shifted time t_0, the relation between t and t_0 being given by Eq. (12).

Eq. (13) is now applied to find the next to leading order behaviour of the time integral over $p_E(\varepsilon, t)$ as $t \to \infty$. We assume that from a certain time $T_0(\varepsilon)$ on we can replace $p_E(\varepsilon, t)$ by its ergodic limit $(2\pi m A)^{-1}$. This time $T_0(\varepsilon)$ is chosen to have the same ε-dependence as the time of the families of loops (like, for example, the dashed line in Fig. 3). Thus $T_0(\varepsilon)$ is related to $T_0(\pi)$ by an equation identical to that between t and t_0 (Eq. (12)). For $t < T_0(\varepsilon)$ we replace $p_E(\varepsilon, t)$ by its exact form, Eq. (13). The approximation can be made asymptotically exact by letting $T_0(\pi) \to \infty$ as $T \to \infty$. We find

$$\begin{aligned} \int_0^{T/2} dt\, p_E(\varepsilon, t) \sim & \int_{T_0(\varepsilon)}^{T/2} dt\, \frac{1}{\Sigma(E)} + \sum_{T_{\xi_0} < T_0(\pi)} B_{\xi_0}(\varepsilon) \\ = & \frac{T/2 - T_0(\varepsilon)}{\Sigma(E)} + \text{const} + \mathcal{O}(\varepsilon^2) \end{aligned} \tag{15}$$

where here and in the following constant denotes independence of ε. In the semiclassical limit only the asymptotic behaviour of Eq. (15) as $\varepsilon \to 0$ is relevant and from the analog of Eq. (12) we find $T_0(\varepsilon) \sim -\frac{2}{\lambda}\log\varepsilon + \text{const}$. This logarithmic divergence can be interpreted as follows.

For small ε the two legs of a loop need a certain minimal time in order to separate enough to enable the loop to close. This time can be estimated by requiring that $\varepsilon \exp(\lambda t/2)$ is of order one, yielding the logarithmic dependence above. Substitution into (8) results in

$$\begin{aligned} K^{(2)}(\tau) \sim & \frac{8p^2T^2}{m\hbar d(E)} \operatorname{Re} \int_0^\infty d\varepsilon \, e^{\frac{ip^2 \varepsilon^2}{2m\hbar\lambda}} \, \frac{2\varepsilon(\log\varepsilon + \text{const.})}{\lambda\Sigma(E)} \\ = & \frac{16\tau^2}{\pi} \operatorname{Re} \int_0^\infty d\varepsilon' \, e^{i\varepsilon'^2} \, \varepsilon' \log(\varepsilon') \, . \end{aligned} \tag{16}$$

Evaluating the real part of the last integral finally yields $K^{(2)}(\tau) \sim -2\tau^2$ in agreement with the τ^2-term of the GOE form factor in (2).

In conclusion, we have shown that the off-diagonal contributions to the spectral form factor from two-loop orbits yield a τ^2-term in agreement with random matrix theory. Its origin can be traced to properties of loops with small opening angle ε. It is expected that higher-order terms in the expansion of $K(\tau)$ are related to multi-loop orbits, a point which is under investigation.

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Correlations between Periodic Orbits and their Rôle in Spectral Statistics

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Abstract

We consider off-diagonal contributions to double sums over periodic orbits that arise in semiclassical approximations for spectral statistics of classically chaotic quantum systems. We identify pairs of periodic orbits whose actions are strongly correlated. For a class of systems with uniformly hyperbolic dynamics, we demonstrate that these pairs of orbits give rise to a τ^2 contribution to the spectral form factor $K(\tau)$ which agrees with random matrix theory. Most interestingly, this contribution has its origin in a next-to-leading-order behaviour of a classical distribution function for long times.

1. Introduction

Quantum systems with disorder or with a chaotic classical counterpart share the remarkable property that energy levels, eigenfunctions, transition amplitudes, or transport quantities exhibit universal features. They are independent of the details of the individual system and depend only on its symmetries. In order to see this universality, it is necessary to consider statistical properties, such as fluctuations in the distributions of energy levels. It was originally conjectured [1] and is by now numerically well established that the spectral correlations of classically chaotic quantum systems, in the semiclassical limit $\hbar \to 0$, agree with correlations between eigenvalues of random matrices [2].

While such a connection with random matrix theory has been proven for disordered systems using field theoretical methods [3] (in the so-called ergodic regime), it remains an outstanding problem in the theory of clean (disorder-free) quantum systems with a chaotic classical limit. It has been proposed to extend the field theoretical approaches for disordered conductors in order to treat clean chaotic systems as well [4,5]. However, computing energy level statistics for a given single chaotic system requires to replace the ensemble average over impurity configurations, inherent to disordered devices, by an average over an appropriate range of energy. This causes difficulties which are still discussed controversially (for a recent collection of related review articles see Ref. [6]).

Semiclassical theory being based on the Gutzwiller trace formula [7] represents the other approach towards an understanding of spectral statistics. It provides the most direct link between spectral quantities of the quantum Hamiltonian and properties of the chaotic dynamics of the corresponding classical system. In view of the fact that semiclassical theory can approximate quantum energy levels with a precision at least of the order of the mean level spacing, semiclassics should be appropriate to cope with spectral correlations, at least on energy scales larger than the mean level distance.

A central quantity to characterize spectral statistics is the spectral two-point correlation function, $R(\eta)$, involving a product of two densities of states with energy separation η. A semiclassical approach to $R(\eta)$ is based on approximating the densities of states by the trace formula, which expresses them by sums over contributions from classical periodic trajectories. Hence a computation of $R(\eta)$ involves the evaluation of a double sum over classical trajectories. Along this line, semiclassical theory has been applied [8–10] to better understand the observed universality in quantum energy spectra. It was shown [9] that by including only pairs of orbits with themselves or their time-reversed partner, the so-called diagonal approximation, and by employing mean properties of classical trajectories [8], the energy level correlator agrees with random matrix theory in the limit of long-range correlations. These results were extended in Ref. [10] to describe the leading oscillatory behaviour of $R(\eta)$ by linking it to the diagonal approximation. To access the spectral regime beyond these asymptotic results, the subject of this article, requires the direct calculation of off-diagonal contributions from pairs of different classical paths, and necessitates further insight into classical correlations between trajectories. Although the existence of such correlations has been observed in several systems [11–13], a deeper understanding of the origin of these correlations in generic systems and a systematic semiclassical evaluation of the correlation function $R(\eta)$ or its Fourier transform, the spectral form factor $K(\tau)$, is still missing.

With this article we approach this open question and point out classical correlations between periodic orbits and their rôle for spectral statistics in the semiclassical limit. We present pairs of different, but closely related periodic orbits in two-dimensional systems, and we provide evidence that they are relevant for the first correction to the diagonal approximation for the spectral form factor. These orbit pairs involve trajectories which exhibit self-intersections with small intersection angles. They resemble ballistic analogues of corresponding objects in disordered systems [14,15], i.e. diffusons and cooperons that are connected at Hikami boxes [16]. We note, however, that we deal here with entirely classical paths, while the notion of the Hikami box involves (quantum) scattering, i.e. non-classical processes [15].

We first compute for a given pair of paths the difference in their classical actions. Employing statistics for the self-crossings of the trajectories we then semiclassically evaluate their contribution to the form factor. We find that this contribution vanishes when the leading long-time behaviour of the crossing statistics is applied. We then show that the next-order correction to the long-time asymptotics is important for spectral statistics. By numerical examinations on a Riemannian surface with constant negative curvature we find that this correction has indeed the form that is required for an agreement of spectral statistics with random matrix theory.

2. Off-diagonal contributions to the form factor

Gutzwiller's trace formula provides a link between the energy spectrum of a quantum system and the periodic orbits of its classical limit. It is a representation for the density of states in the form [7]

$$d(E) = \sum_n \delta(E - E_n) \approx \bar{d}(E) + \frac{1}{\pi\hbar} \mathrm{Re} \sum_\gamma A_\gamma e^{iS_\gamma(E)/\hbar}, \qquad (1)$$

where $\bar{d}(E)$ is the mean density of states and γ labels the periodic orbits of the classical system that is assumed to be chaotic. Each orbit contributes in terms of its classical action S_γ and its amplitude A_γ which depends on period, stability, and the number of self-conjugate points of the orbit.

One of the main reasons for the interest in the trace formula in recent years has been that it allows one to investigate theoretically the conjectured universality in the statistical distribution of energy levels. Consider, for example, the spectral form factor that is defined as the Fourier transform of the spectral two-point correlator,

$$K(\tau) = \int_{-\infty}^{\infty} \frac{d\eta}{\bar{d}(E)} \langle d_{osc}(E + \eta/2) d_{osc}(E - \eta/2) \rangle_E e^{2\pi i \eta \tau \bar{d}(E)}, \qquad (2)$$

where $d_{osc}(E) = d(E) - \bar{d}(E)$. It is evaluated by averaging over an energy interval that is small in comparison to E but contains a large number of levels. For chaotic systems with time reversal symmetry, which we consider in the following, the form factor is expected to be identical with that of the Gaussian Orthogonal Ensemble (GOE) [2],

$$K^{GOE}(\tau) = \begin{cases} 2\tau - \tau \log(1 + 2\tau) & \text{if } \tau < 1, \\ 2 - \tau \log \dfrac{2\tau + 1}{2\tau - 1} & \text{if } \tau > 1, \end{cases} \qquad (3)$$

if τ is in the so-called universal regime $\tau > \tau_{erg}$ (where $\tau_{erg} = \mathcal{O}(\hbar^{d-1})$ in d dimensions). For small values of τ it has the expansion

$$K^{GOE}(\tau) = 2\tau - 2\tau^2 + \dots . \qquad (4)$$

The semiclassical theory of spectral statistics has been developed in order to find an explanation for the observed agreement with random matrix statistics. Its aim is to attribute this universal property of the quantum system to generic properties of trajectories of the corresponding classical system. For the spectral form factor the semiclassical approximation is obtained by inserting the trace formula (1) into Eq. (2) and evaluating the Fourier transform in leading order of $\hbar$. This leads to a double sum over periodic orbits,

$$K(\tau) \approx \frac{1}{2\pi\hbar\bar{d}(E)} \sum_{\gamma,\gamma'} \left\langle A_\gamma A_{\gamma'}^* e^{i(S_\gamma - S_{\gamma'})/\hbar} \delta\left(T - \frac{T_\gamma + T_{\gamma'}}{2}\right) \right\rangle_E, \qquad (5)$$

where $T_\gamma = \partial S_\gamma / \partial E$ is the period of an orbit, and $\tau = T/(2\pi\hbar\bar{d}(E))$. Due to the exponential proliferation of the number of periodic orbits with their period, the double sum contains a huge number of pair terms. Most of the pairs consist of periodic orbits with actions that are uncorrelated, and their contributions cancel each other when summed over. It is expected that the non-vanishing contributions come from a relatively small number of pairs of orbits which are correlated.

The strongest correlation occurs between orbits which have identical actions. In the diagonal approximation only those pairs of orbits are considered which are identical or related by time inversion. Their contribution to the form factor can be evaluated by applying a classical sum rule for periodic orbits [8]. In this way one obtains the leading term of the GOE form factor for small values of τ: $K(\tau) \approx 2\tau$ [9].

To go beyond the diagonal approximation requires the evaluation of pairs of different orbits which are not related by any symmetry. In this article we wish to provide an explanation where these off-diagonal contributions come from. In particular, we will discuss in detail the next term in the expansion (4) of the form factor for small τ, namely the term $-2\tau^2$. We will provide evidence that it can be obtained in two-dimensional systems from pairs of self-intersecting orbits with small opening angles and orbits in their close vicinity.

We start with some general considerations. For a chaotic system it is reasonable to expect that correlations exist only between periodic orbits which are close in coordinate space. One therefore needs a mechanism by which two or more periodic orbits can be obtained which are different but which are located almost everywhere in close vicinity to each other in coordinate space. Hints on their topology can be obtained from diagrams in perturbation theory for disordered systems [15,17], or from classical correlations between periodic and diffractive orbits [18]. The basic idea is that the periodic orbits consist of different segments. In each segment, an orbit follows very closely its neighbouring orbit or the time-reverse of this orbit, but the orbits differ in how these segments are connected. In order that the segments can be connected in different ways they must form loops. Thereby, one obtains a semiclassical loop expansion in close analogy to the loop expansion in diagrammatic perturbation theory.

Let us consider the simplest example. It consists of a pair of two periodic orbits with two loops in coordinate space as depicted in Fig. 1. The two orbits follow one loop in the same direction and the other loop in the opposite direction. For that reason these pairs can exist only in systems with time-reversal invariance.

In the following we argue that such pairs of classical periodic orbits indeed exist. Let us assume that the opening angle ε (we also call it crossing angle) is very small. As we will see later, it is sufficient to consider only this case. For small ε one can describe the outer orbit by linearizing the motion in the vicinity of the inner self-intersecting orbit. This leads to the following conditions for the outer periodic orbit:

$$\begin{pmatrix} \delta_2 \\ p(\gamma_2 + \varepsilon/2) \end{pmatrix} = R \begin{pmatrix} \delta_1 \\ p(\gamma_1 - \varepsilon/2) \end{pmatrix}, \\ \begin{pmatrix} -\delta_2 \\ p(\gamma_2 - \varepsilon/2) \end{pmatrix} = L \begin{pmatrix} -\delta_1 \\ p(\gamma_1 + \varepsilon/2) \end{pmatrix}. \qquad (6)$$

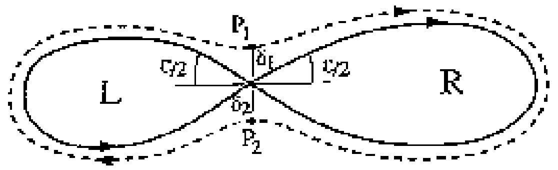

Fig. 1. An example of a self-intersecting classical periodic orbit with small opening angle ε, and its neighbouring periodic orbit. The local coordinate system is oriented along the middle of the opening angle ε.

L and R denote the two stability matrices of the left and right loop of the inner orbit, respectively, and p is the absolute value of the momentum at the crossing. The distances δ_1 and δ_2 are shown in the figure, and γ_1 and γ_2 denote the angles between the horizontal line and the tangents to the outer orbit in the points P_1 and P_2, respectively. The expression (6) consists of four inhomogeneous linear equations for the four unknown quantities δ_1, δ_2, γ_1, and γ_2 and can be solved. Therefore, the outer periodic orbit exists in the linearized approximation. A closer examination shows that it behaves in the following way. In point P_1 the outer orbit is exponentially close to the stable direction of the right inner loop. In the following, it approaches the inner loop exponentially fast for some time (for about half the loop) until it starts to deviate from it again. In point P_2 it then almost reaches the stable direction of the time-reverse of the left inner orbit, and again approaches it exponentially fast until it starts to deviate from the left loop again at about half the loop.

The action difference between both orbits can be obtained in the linearized approximation by expanding the action up to second order around the inner orbit. One finds

$$\Delta S(\varepsilon) \approx \frac{p\varepsilon}{2}(\delta_1 + \delta_2) . \tag{7}$$

The common solution of the equations in (6) leads to a linear relation between the angle ε and the distance $\delta_1 + \delta_2$,

$$\delta_1 + \delta_2 = \frac{R_{12}(\mathrm{Tr}L + 2) + L_{12}(\mathrm{Tr}R + 2)}{\mathrm{Tr}(L^i R) - 2}\, p\varepsilon , \tag{8}$$

so that the action difference in Eq. (7) depends quadratically on ε. In Eq. (8), L^i denotes the stability matrix for the time-inverse of the inner left loop. In terms of the matrix elements of L it is given by

$$L^i = \begin{pmatrix} L_{22} & L_{12} \\ L_{21} & L_{11} \end{pmatrix} . \tag{9}$$

The action difference $\Delta S(\varepsilon)$ predominantly originates from the region around the self-intersection.

To summarize, there is the following recipe for finding pairs of orbits as shown in Fig. 1. One has to look for periodic orbits which have self-intersections with a small crossing angle ε. The self-intersection divides an orbit into two loops. The prediction is that there exists a neighbouring periodic orbit which follows one loop in the same and the other loop in the opposite direction, and that it has a small action difference given by Eqs. (7) and (8). We tested this prediction for classical chaotic motion in the hyperbola billiard, for which we have a long list of periodic orbits available [19]. We looked for orbits with small crossing angles and checked whether the neighbouring orbits exist and have the predicted action difference. We found that this is indeed the case. For example, for an orbit pair involving a long orbit with a crossing angle of 2.6° we found the two lengths (corresponding to scaled actions) $l_1 = 24.08676$ and $l_2 = 24.08469$. The difference is $\Delta l = 0.00207$, compared to the theoretical value of $\Delta l_{th} = 0.00208$ obtained from Eqs. (7) and (8).

In order to proceed we have to evaluate the number of self-intersections of periodic orbits and the distribution of the crossing angles. We start by calculating these quantities for general, non-periodic trajectories. The corresponding results for periodic orbits can be inferred by using the principle of uniformity [20,21]. According to it, averages of a quantity along generic non-periodic orbits lead to the same result as averages over all periodic orbits, if the latter are performed with relative weights which take into account the different stabilities of the periodic orbits. The derivation for the crossing angles is performed in the appendix by using the ergodic property of chaotic systems. As a result we find for a trajectory with time T that the average number of self-intersections with an opening angle in an interval $\mathrm{d}\varepsilon$ around ε ($0 \le \varepsilon \le \pi$) is given by

$$P(\varepsilon, T)\,\mathrm{d}\varepsilon \sim \frac{T^2 \langle v^2 \rangle}{\pi A} \frac{\sin\varepsilon}{2}\,\mathrm{d}\varepsilon \qquad \text{for} \qquad T \to \infty . \tag{10}$$

Here, $P(\varepsilon, T)$ is the density of crossings of opening angle ε for trajectories of time T, A is the accessible area at energy E, and $\langle v^2 \rangle$ is the average of the velocity square over A (see the appendix for an accurate definition.) By an integration over ε it follows from Eq. (10) that the total number of self-intersections of a trajectory of time T increases as

$$N(T) \sim \frac{\langle v^2 \rangle T^2}{\pi A} \qquad \text{for} \qquad T \to \infty . \tag{11}$$

We want to use this classical information to evaluate the contribution of the pairs of double-loop orbits to the spectral form factor. For general chaotic systems this requires further assumptions, in particular that the crossing-angle distribution is independent of elements of the stability matrices. Then one can show that the contribution to the form factor vanishes if the leading behaviour for large T, Eq. (10), is used. We will not perform this calculation for general systems. Instead, we will focus from now on onto a particular class of systems with uniformly hyperbolic dynamics for which the calculations are simpler and no further assumption is needed. This is the motion on Riemann surfaces of constant negative curvature [22]. There the periodic orbits do not have conjugate points, and they all possess the same Lyapunov exponent. These systems have the additional advantage that averages along periodic orbits need not be weighted in order to be identical to averages along generic trajectories. In these systems the stability matrix of an orbit of time T has the simple form

$$M = \begin{pmatrix} \cosh\lambda T & (m\lambda)^{-1}\sinh\lambda T \\ m\lambda\sinh\lambda T & \cosh\lambda T \end{pmatrix} , \tag{12}$$

where m is the mass of the particle and λ the Lyapunov exponent of the system. With Eq. (12) the action difference, Eq. (7) with (8), simplifies to

$$\Delta S(\varepsilon) \approx \frac{p^2 \varepsilon^2}{2m\lambda} . \tag{13}$$

By using Eqs. (10) and (13), we can evaluate the contribution of the pairs of orbits to the spectral form factor. We do this by summing over all intersections of angle ε that occur in periodic orbits, and then integrate over ε. We account for an additional degeneracy factor of two in Eq. (5) owing to time reversal invariance. Furthermore, we take twice the real part, since there is a corresponding complex conjugate term in the double sum over periodic orbits. Altogether we obtain the following expression:

$$\begin{aligned} K^{(2)}_{\text{off}}(\tau) &\approx \frac{4}{2\pi\hbar\bar{d}(E)} \mathrm{Re} \int_0^\infty \mathrm{d}\varepsilon \sum_\gamma |A_\gamma|^2 P(\varepsilon, T) \\ &\quad \times \exp(\mathrm{i}\Delta S(\varepsilon)/\hbar)\delta(T - T_\gamma) \\ &\approx \frac{4}{2\pi\hbar\bar{d}(E)} \mathrm{Re} \int_0^\infty \mathrm{d}\varepsilon \int_0^\infty \mathrm{d}T' \rho(T') \frac{T'^2}{\exp(\lambda T')} P(\varepsilon, T) \\ &\quad \times \exp(\mathrm{i}\Delta S(\varepsilon)/\hbar)\delta(T - T') \\ &\approx \frac{4}{2\pi\hbar\bar{d}(E)} \mathrm{Re} \int_0^\infty \mathrm{d}\varepsilon \frac{v^2 T^3}{\pi A} \frac{\varepsilon}{2} \exp\left(\frac{\mathrm{i}p^2\varepsilon^2}{2\hbar m\lambda}\right) \\ &= 0 \end{aligned} \tag{14}$$

It has been evaluated by replacing the sum over periodic orbits by an integral with density

$$\rho(T) \sim \frac{\exp(\lambda T)}{T} \quad \text{for} \quad T \to \infty , \tag{15}$$

and by using $|A_\gamma|^2 \approx T_\gamma^2 \exp(-\lambda T_\gamma)$. In the limit $\hbar \to 0$, the main contribution to the integral comes from angles ε close to zero. For obtaining the leading semiclassical contribution we could therefore take only the first term in the Taylor expansion of $\sin \varepsilon$. Furthermore, we extended the integral to infinity. (For convergence questions it should be considered with a momentum p that has a small positive imaginary part that is sent to zero after the integral is performed.) The result vanishes since the result of the integration is purely imaginary.

After a closer inspection of expression (14) it is, however, not surprising that the result gives zero. In order to perform the semiclassical limit, one has to translate the time T into τ by the relation $T = 2\pi\hbar\bar{d}(E)\tau$, and then take the limit $\hbar \to 0$. Since in two-dimensional systems $\bar{d}(E) \sim mA/(2\pi\hbar^2)$, one finds that the expression in (14) is of order $\mathcal{O}(\hbar^{-1})$. Without taking the real part the expression would diverge in the limit $\hbar \to 0$. Moreover, it would be of order τ^3 whereas we believe that it should be the lowest-order off-diagonal contribution and thus be of order τ^2.

These considerations indicate that the correct contribution to the form factor might arise from a $1/T$ correction to the asymptotic law (10) for the classical density $P(\varepsilon, T)$. In the following we first show that a multiplicative correction term of the form

$$1 - \frac{4\Delta T}{T} \qquad \text{with} \qquad \Delta T = -\frac{1}{\lambda}\log(c\varepsilon) , \tag{16}$$

where c is an arbitrary constant, leads to the random matrix result. We then confirm numerically that such a correction indeed exists.

Multiplying the integrand in Eq. (14) by $(-4\Delta T/T)$ leads to

$$\begin{aligned} K^{(2)}_{\text{off}}(\tau) &\approx \frac{4}{2\pi\hbar\bar{d}(E)} \mathrm{Re} \int_0^\infty \mathrm{d}\varepsilon \frac{v^2 T^3}{\pi A} \frac{\varepsilon}{2} \exp\left(\frac{\mathrm{i}p^2\varepsilon^2}{2\hbar m\lambda}\right) \frac{4\log(c\varepsilon)}{\lambda T} \\ &= \frac{4}{2\pi\hbar\bar{d}(E)} \mathrm{Re} \int_0^\infty \mathrm{d}\eta \frac{2\mathrm{i}\hbar T^2}{\pi m A} \exp(-\eta) \log\sqrt{\mathrm{i}} \\ &= -2\tau^2 , \end{aligned} \tag{17}$$

where, after the change of the integration variable, all further arguments of the logarithm could be neglected since they lead to a vanishing contribution. The final result agrees with the random matrix expression in Eq. (4).

In the following we examine numerically whether a correction to the law (10) of the form (16) exists. For that purpose we consider a Riemannian surface in form of an octagon. We choose random trajectories, follow them for a fixed length L and determine the mean density of the intersection angles. Since we are interested in the correction to the asymptotic form of this density we need to have good statistics. The numerics is carried out with 50 million randomly chosen trajectories of length $L = 100$, and half a million trajectories of length $L = 1000$ (the area of the system is $A = 4\pi$). We use dimensionless units in which $v = \lambda = 1$ and $L = T$.

First we test the asymptotic law (10) by calculating

$$p(\varepsilon, T) := P(\varepsilon, T) \frac{\pi A}{T^2 \langle v^2 \rangle} . \tag{18}$$

For long times this function should agree with a normalized distribution of crossing angles of the form $\sin(\varepsilon)/2$, and we compare it to this curve in Figs. 2(a) and (c). In the first of these two figures the results for trajectories of length $L = 100$ are presented. Here one can still see a small difference between the two curves. When going to the results for longer trajectories of length $L = 1000$ in Fig. 2(c), however, this difference cannot be discerned any more.

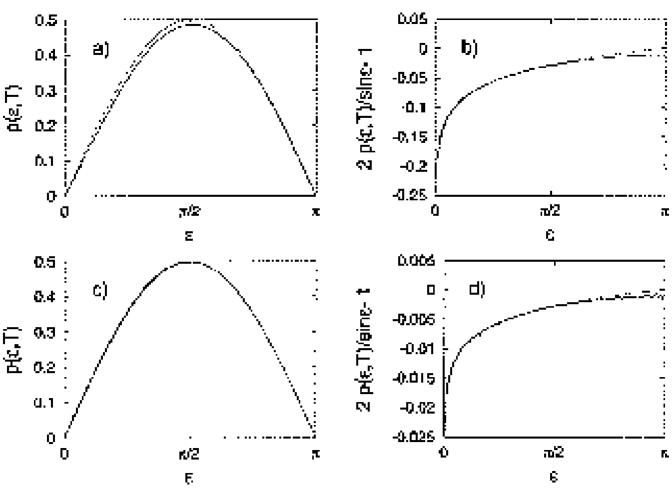

Fig. 2. (a) and (c): The distribution of crossing angles $p(\varepsilon, T)$ (full line) in comparison to $\sin(\varepsilon)/2$ (dashed line), evaluated along trajectories of length $L = 100$ and $L = 1000$, respectively. (b) and (d): The deviation of $p(\varepsilon, T)$ from $\sin(\varepsilon)/2$ (full line) in comparison with the log-distribution (dashed line) that is described in the text, evaluated along trajectories of length $L = 100$ and $L = 1000$, respectively.

In Figs. 2(b) and (d) we investigate the deviation from the asymptotic law (10). We do this by plotting the distribution $2p(\varepsilon, T)/\sin\varepsilon - 1$. As argued above we expect that this deviation is responsible for the τ^2 term of the spectral form factor. In order to obtain an agreement with random matrix theory, the plotted function must have the form $(4\log\varepsilon + \text{const})/(\lambda T)$ for small ε as follows from Eq. (16). This expression contains only one free additive parameter, which is of no relevance for the form factor. We fitted this parameter and plotted this curve also (dashed lines in Figs. 2(b) and (d)).

The agreement between the different curves in Fig. 2(b) and also in Fig. 2(d) is remarkable. The random matrix prediction requires only an agreement for small values of ε, but there is an excellent agreement almost over the whole range $0 \le \varepsilon \le \pi$. In our opinion this result is the first clear indication on the origin of the off-diagonal contributions to the form factor in the perturbative regime near $\tau = 0$.

3. Discussion and Conclusions

This clear-cut numerical result suggests to draw the following conclusions:

(*i*) It is possible to systematically evaluate off-diagonal contributions to the spectral form factor by the semiclassical method.
(*ii*) The τ^2 term of the spectral form factor is indeed related to the eight-shaped orbits in Fig. 1
(*iii*) The τ^2 term originates from the next-to-leading asymptotic form of the distribution of crossing angles for large T.

For general systems the calculations will be more complicated. One reason is that Maslov indices are present. A second reason is that the stabilities of the orbits are, in general, different. As a consequence, it is not the pure distribution of crossing angles which matters, but a distribution which depends also on Maslov indices and elements of the stability matrices along the loops. A complete analytical derivation of the τ^2 contribution, purely on the basis of classical chaotic dynamics, remains to be performed.

The fact that the contribution (14) vanishes in the semiclassical limit and that only the term (17) arising from corrections to the long-time distribution of crossing angles prevails, shows at least a formal analogy with the situation when evaluating two-loop corrections to the density correlator for a diffusive system using diagrammatic perturbation theory. There, the contribution from dressed square Hikami boxes vanishes to leading order and only the next-order expansion in energy leads to the final result [15].

The problem to compute off-diagonal contributions to the spectral form factor is closely related to corresponding questions which involve energy averages over products of advanced and retarded Green functions. One prominent example is mesoscopic quantum transport. For clean chaotic systems a semiclassical theory, which adequately and quantitatively describes weak localization, is still lacking [23–25]. The question to obtain the τ^2 term in the spectral form factor has much in common with this long-lasting problem to semiclassically compute weak-localization corrections in ballistic quantum transport. There, it was already suggested to consider certain pairs of initially close classical orbits [24,26]. Proceeding in the same way as for the pairs of correlated periodic two-loop orbits we have computed the action difference for orbit pairs relevant to quantum transport. It also scales quadratically with the self-intersection angle ε, but with a different prefactor. Again deviations from the asymptotic form of crossing distributions must be included to get non-zero results [27].

Another field of application of our findings are mesoscopic Andreev billiards, i.e. ballistic cavities coupled to superconducting leads. Semiclassical approaches to the proximity effect in these systems so far rely on the diagonal approximation [28–30] and an extension to off-diagonal paths along the lines presented here appears promising.

To conclude, we have shown that in chaotic systems a class of off-diagonal pairs of periodic orbits exists which evidently exhibit action correlations. We have demonstrated for systems with uniformly hyperbolic dynamics that in the perturbative regime (corresponding to the small τ expansion) these orbit pairs yield a τ^2 contribution to the spectral form factor which agrees with the random matrix result. Our results for the two-loop orbits demonstrate that the semiclassical theory is a powerful tool to deal with spectral statistics of individual disorder-free quantum systems. We believe that, for systems with time-reversal symmetry, the higher-order contributions to the form factor involve periodic orbits with three and more loops. For systems without time-reversal symmetry the considered two-loop orbits do not exist, and contributions from orbits with more loops should cancel mutually. A systematic computation of higher-order contributions from multi-loop periodic-orbit configurations remains as a challenging future program.

Acknowledgements

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4. Appendix: The density of angles of self-intersection

In this appendix we derive the leading asymptotic form of the density $P(\varepsilon, T)$ for long times T. The quantity $P(\varepsilon, T)\,\mathrm{d}\varepsilon$ is defined as the average number of self-intersections with an opening angle in an interval $\mathrm{d}\varepsilon$ around ε of trajectories of time T in a chaotic system. For the derivation we employ the ergodicity theorem which can be formulated in the form

$$\int_0^T \mathrm{d}t\, f(q(t), p(t)) \sim T\, \frac{\int \mathrm{d}^2q\, \mathrm{d}^2p\; \delta(E - H(q,p))\, f(q,p)}{\int \mathrm{d}^2q\, \mathrm{d}^2p\; \delta(E - H(q,p))}\,, \qquad T \to \infty\,. \tag{19}$$

It states that for almost all initial conditions the integration of a sufficiently smooth function f along a trajectory of time T is, asymptotically for large T, given by T times the phase space average of this quantity. We choose in this appendix a simple, heuristic derivation by employing the ergodicity theorem for a function f that has the form of a delta-function. A rigorous derivation would require the use of smoothed quantities.

The density $P(\varepsilon, T)$ is defined as

$$
\begin{aligned}
&P(\varepsilon, T) \\
&= \left\langle \frac{1}{2}\int_0^T \mathrm{d}t \int_0^T \mathrm{d}t' \, |J| \, \delta(q(t) - q(t')) \, \delta(\varepsilon - |\angle[v(t), v(t')]|) \right\rangle
\end{aligned} \tag{20}
$$

where the average is taken over different initial conditions and $\angle[v(t), v(t')]$ denotes the angle between $v(t)$ and $v(t')$. The quantity J is the Jacobian for the transition from the argument of the first delta-function to t and t'

$$
\begin{aligned}
|J| &= |\dot{x}(t)\dot{y}(t') - \dot{x}(t')\dot{y}(t)| = |v(t) \times v(t')| \\
&= v(t)\, v(t') \sin|\angle[v(t), v(t')]| \, .
\end{aligned} \tag{21}
$$

We apply the ergodicity theorem twice to replace the time integrals by phase space averages. In the following we are more general than in the remaining article by allowing Hamiltonians of the form $H = (1/2m)(p - (e/c)A)^2 + V(q) = (m/2)v^2 + V(q)$ with the possibility of a vector potential that breaks time reversal symmetry. Inserting Eq. (19) into Eq. (20) results in

$$
\begin{aligned}
&P(\varepsilon, T) \sim \frac{T^2}{2} \times \\
&\frac{\int \mathrm{d}^2q\mathrm{d}^2p\mathrm{d}^2q'\mathrm{d}^2p'\delta(E - H(q,p))\delta(E - H(q',p'))|v \times v'|\delta(q - q')\delta(\varepsilon - |\angle[v, v']|)}{\int \mathrm{d}^2q\mathrm{d}^2p\mathrm{d}^2q'\mathrm{d}^2p'\delta(E - H(q,p))\delta(E - H(q',p'))} \\
&= \frac{T^2}{2}\frac{\int \mathrm{d}^2q v\mathrm{d}v\mathrm{d}\phi\mathrm{d}^2q' v'\mathrm{d}v'\delta(E - H(q,p))\delta(E - H(q',p'))2vv'\sin\varepsilon\delta(q - q')}{\int \mathrm{d}^2q v\mathrm{d}v\mathrm{d}\phi\mathrm{d}^2q' v'\mathrm{d}v'\mathrm{d}\phi'\delta(E - H(q,p))\delta(E - H(q',p'))} \\
&= \frac{T^2}{2\pi A^2}\sin\varepsilon \int \mathrm{d}^2q \frac{2}{m}(E - V(q)).
\end{aligned} \tag{22}
$$

Here the integration variables have been changed from Cartesian coordinates for the momenta to polar coordinates for the velocities. A is the accessible area at energy E and we define $\langle v^2 \rangle$ as average of the velocity square over A:

$$
A = \int_{V(q) \le E} \mathrm{d}^2q \, , \qquad \langle v^2 \rangle = \frac{1}{A}\int_{V(q) \le E} \mathrm{d}^2q \, \frac{2}{m}(E - V(q)) \, . \tag{23}
$$

With this definition we arrive at the final result

$$
P(\varepsilon, T) \sim \frac{T^2 \langle v^2 \rangle}{\pi A}\frac{\sin\varepsilon}{2} \, , \qquad T \to \infty \, , \tag{24}
$$

where ε varies between 0 and π. The T^2-dependence of the total number of crossings (without explicit prefactor) has been proven in Ref. [32].

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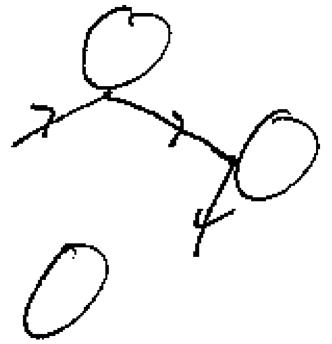
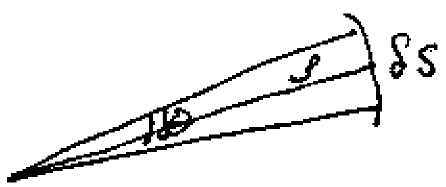
The Lorentz Gas - Classical Chaos + Quantum Dynamics: The Ehrenfest time



electrons moving among fixed hard ball scatterers.

Classically it is chaotic with positive Lyapunov exponents. To see this, examine two infinitesimally close trajectories:



$$\delta S = \rho\, \delta\theta$$

$$\delta S(t+\tau) = \rho(t+\tau)\, \delta\theta$$

$$= \left[\rho_0(\tau) + v t\right] \delta\theta$$

$$\delta\theta = \frac{\delta S(\tau)}{\rho_0(\tau)}$$

$$\frac{\delta S(t+\tau)}{\delta S(\tau)} = 1 + \frac{v t}{\rho_0(\tau)} \quad \text{Free motion}$$

$$\frac{1}{\rho_-} = \frac{1}{\rho_+} + \frac{2}{a \cos\phi}$$

Consider a sequence of collisions at time $t_1, t_2, t_3, \dots t_N$, ~~fast~~ $t_N < t < t_{N+1}$

$$S(t) = S(0)\,\frac{\rho^-_{t_1}}{\rho_0}\,\frac{\rho^-_{t_2}}{\rho^+_{t_1}}\cdots\frac{\rho^-_{t_N}}{\rho^+_{t_{N-1}}}\cdot\frac{\rho_t}{\rho^+_{t_N}}$$

$$\frac{\rho^-_{t_j}}{\rho^+_{t_{j-1}}} = \frac{\rho^+_{t_{j-1}} + v(t_j - t_{j-1})}{\rho^+_{t_{j-1}}} = \exp\int_{t_{j-1}}^{t_j}\frac{v\,d\tau}{\rho^+_{t_{j-1}} + v(\tau - t_{j-1})}$$

$$= \exp\int_{t_{j-1}}^{t_j}\frac{v\,d\tau}{\rho_\tau}$$

$$S(t) = S(0)\,e^{v\int_0^t \frac{d\tau}{\rho(\tau)}} \to S(0)\,e^{\lambda t}$$

$$\lambda = \frac{1}{t}\int_0^t \frac{v\,d\tau}{\rho(\tau)} \qquad t\to\infty$$

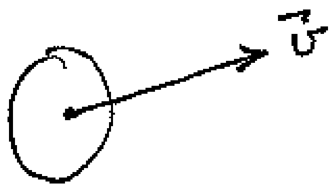
This can be evaluated numerically or in some cases analytically.

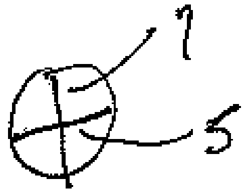
What about Q.M? Look at the propagation of a wave packet.

$$\psi(\vec{r},t) = \int dr' \langle \vec{r}| e^{-\frac{i}{\hbar} t H} | r' \rangle \langle r' | 0 \rangle$$

$$G(\vec{r}, \vec{r}'; t) = \left(\frac{1}{2\pi i \hbar}\right)^{d/2} \sum_{\text{paths}} |D|^{1/2} e^{\left[\frac{i}{\hbar} S(\vec{r}, r'; t) + \frac{i\nu\pi}{2}\right]}$$

For $\langle r'|0\rangle$ we take a Gaussian





We treat η + ζ separately

$$\psi(r;0) = \langle r'|0\rangle = \frac{1}{(2\pi \sigma_{\parallel 0} \sigma_{\perp 0})} e^{\left[\frac{i\zeta}{\lambda_0} - \frac{\zeta^2}{4\Omega_{\parallel,0}} - \frac{\eta^2}{4\Omega_{\perp,0}}\right]}$$

$$\lambda_0 = \frac{\hbar}{|p_0|}$$

Free motion Propagator

$$G_F(\vec{r},\vec{r}';t) = \left(\frac{m}{2\pi i \hbar t}\right)^{d/2} e^{\frac{i}{\hbar}\frac{m}{2}\frac{(\vec{r}-\vec{r}')^2}{t}}$$

$$S = \int_0^t L\,dt \qquad L = T - V = T = \frac{P^2}{2m}$$

$$\vec{P} = \frac{m(\vec{r}-\vec{r}')}{t} = m\vec{v}$$

$$\psi(\vec{r},t) = \int d\vec{r}_0\; G_F(\vec{r},\vec{r}_0;t)\,\psi_0(\vec{r}_0)$$

We pick $\psi_0(\vec{r})$ to be a Gaussian W.P. with center at $\vec{r}_0$ and width smaller than radius of scatterer and smaller than distance from $\vec{r}_0$ to any scatterer. When this integral is done

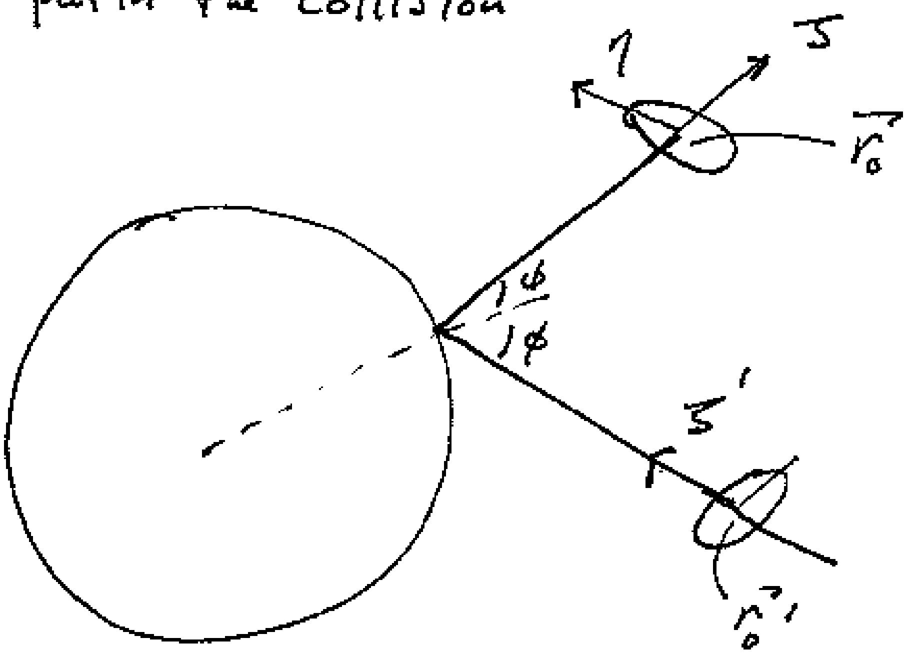
$$\Omega_{11,0} \to \Omega_{11,t} = \Omega_{11,0} + \frac{i}{2}\,\lambda_D v t$$

$$\Omega_0 \to \Omega_t = \Omega_0 + \frac{i}{2}\,\lambda_D v t$$

$$\lambda_D = \frac{\hbar}{|P_0|}, \quad v = \frac{|P_0|}{m}$$

Center moves to $\vec{r}_0 + \frac{\vec{P}_0}{m} t$

Now we put in the collision

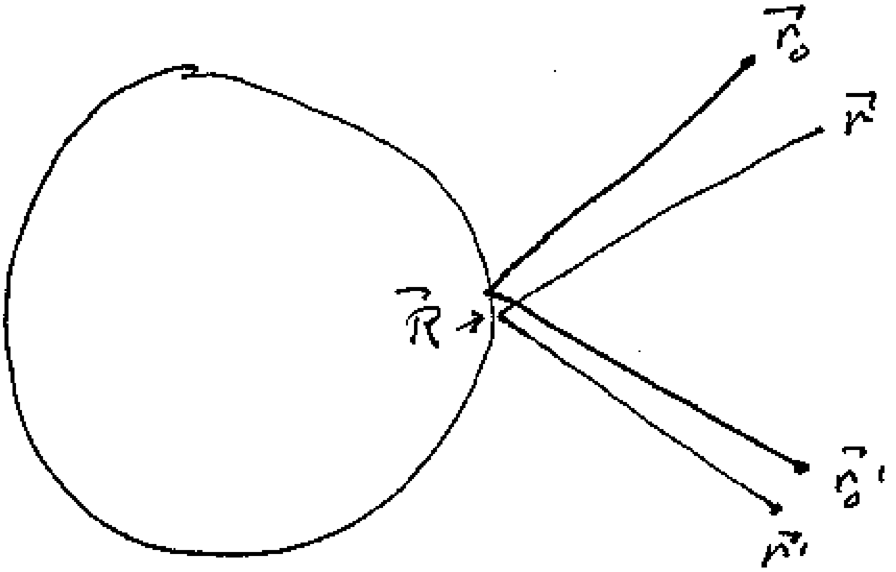


Need to locate the point of collision for a point at $\vec{r}' = \vec{r}_0' + \delta\vec{r}'$ colliding at $\vec{R}$ and arriving at $r = \vec{r}_0 + \delta\vec{r}$ $\quad |\delta\vec{r}| < |\vec{r}_0|$, $|\delta r'| < |r_0'|$

Center of coordinates at ~~center of scatterer~~ location of classical collision

$$S_R = \frac{m}{2t}\left(|\vec{r}' - \vec{R}| + |\vec{R} - \vec{r}| \right)^2$$

Find the extremum w.r.t. $\vec{R} = (\bar{X}, \bar{Y})$



We find

$$\underline{X} = -\frac{1}{2a}\left(\frac{xy'+x'y}{x+x'}\right)^2 + O(\delta^2)$$

$$\underline{Y} = \frac{xy'+x'y}{x+x'} - \frac{1}{2a}\,\frac{x-x'}{y-y'}\left(\frac{xy'+x'y}{x+\cancel{x}'}\right)^2 + O(\delta$$

Note: For classical trajectory

$$x = l\cos\phi \qquad x' = l'\cos\phi$$
$$y = l\sin\phi \qquad y' = -l\sin\phi \qquad \to \underline{Y} = 0, \quad \underline{X} = 0$$

$$\delta \sim \frac{|\delta\vec{r}|}{a},\ \frac{|\delta\vec{r}|}{r},\ \frac{|\delta\vec{r}\,'|}{r'}$$

$$S_R(\vec{r},\vec{r}';t) = \frac{m}{2t}\Big[(x+x')^2 + (y-y')^2 +$$

$$+\frac{2}{a}\frac{(xy'+x'y)^2}{(x+x')} + O(\delta^2)\Big]$$

Note: We assume that r is not in geometrical shadow of $\vec{r}'$

From this we find that at the collision, there is an instantaneous change in the wave packet whereby $\Omega_{\parallel}$ (associated with ξ variable in direction of motion) satisfies

$$\Omega_{\parallel}^{+} = \Omega_{\parallel}^{-}$$

And for Ω (associated with η)

$$\frac{1}{\Omega^+} = \frac{1}{\Omega^-} - \frac{4i}{\hbar a \cos\phi}$$

The classical equations are recovered if we write

$$\Omega_{\parallel} = \frac{i}{2}\lambda \rho_{\parallel} \,, \quad \Omega = \frac{i}{2}\lambda \bar{\rho}$$

Then for free motion

$$\bar{\rho}_t = \bar{\rho}_0 + vt$$

and at collision

$$\frac{1}{\bar{\rho}^+} = \frac{1}{\bar{\rho}^-} + \frac{2}{a\cos\phi}$$

In any case

$$\rho_{\parallel t} = \rho_{\parallel 0} + vt$$

whether or not there is a collision

If one considers a sequence of collisions the width of the wave packet satisfies

$$\sigma_t^2 = \frac{1}{\mathrm{Re}\left(\frac{1}{\Omega_t}\right)} = \frac{\lambda}{2\,\mathrm{Im}\left(\frac{1}{\rho_t}\right)}$$

At collision

$$\frac{1}{\rho_t^+} = \frac{1}{\rho_t^-} + \frac{2}{a \sin\phi}$$

$$\mathrm{Im}\,\frac{1}{\rho_t^+} = \mathrm{Im}\,\frac{1}{\rho_t^-} \qquad \text{so} \quad \sigma_{t_j}^{+2} = \sigma_{t_j}^{-2}$$

If there is a collision at time t_j then at time t, later but before the next collision

$$\sigma_t = \sigma_{t_j} \left| \frac{\rho_{t_j} + v(t-t_j)}{\rho_{t_j}} \right| = \sigma_{t_j}\, e^{v \,\mathrm{Re} \int_{t_j}^{t} \frac{dz}{\rho_z}}$$

So after a series of collisions, provided the wave packet stays small

$$\sigma_t = \sigma_0\, e^{v\,\mathrm{Re}\int_0^t \frac{dz}{\rho_z}} = \sigma_0\, e^{\lambda_Q^{(t)} t}$$

$$\lambda_Q(t) = \frac{v}{t}\int_0^t \frac{dz}{\rho_z}$$

There are quantum corrections in $\lambda_Q(t)$ apart from the finite time part.

For free streaming one has

$$\sigma_t = \frac{\sigma_0}{\rho}\left[(\rho_0 + v t)^2 + \varepsilon_0 (v t)^2\right]^{1/2}$$

$$\varepsilon_0 = \left(\frac{\lambda \rho_0}{2\sigma_0^2}\right)^2 \approx \hbar^2$$

The quantum corrections are due to uncertainty

Suppose wave packet is of size σ_0, then

$$\Delta p_0 \, \sigma_0 \approx \hbar$$

$$\Delta p_0 \approx \frac{\hbar}{\sigma_0}$$

In time t this spread becomes

$$\frac{\Delta p_0}{m} t = \frac{\hbar t}{m\sigma_0} = \frac{\hbar}{m v \sigma_0}(v t) = \frac{\lambda v t}{\sigma_0}$$

So $\sigma_t = \left[\sigma_{cl}^2 + \sigma_Q^2\right]^{1/2}$

The difference between λ_{cl} + $\lambda_Q \approx \hbar^2$

All this is OK for $t < t_{Ehr}$

t_{EHR} = time for packet to spread to size of scatterer

$$a \sim \sigma_0 e^{\lambda t_{Ehr}}$$

$$t_{Ehr} = \frac{1}{\lambda} \log \frac{a}{\sigma_0}$$

What do we take for σ_0 – typically on the order of a de Broglie w.l.

We want quantum effects to be small so

$$\varepsilon_0 = \left(\frac{\hbar \rho_0}{2 \sigma_0^2} \right)^2 < 1$$

suppose $\rho_0 \sim a$

then $\sigma_0 > (\hbar a)^{1/2}$

$$t_{Ehr} \approx \frac{1}{2\lambda} \log \frac{a}{\hbar}$$

Lyap   de Broglie

Scattering Resonances & the two disk billiard

Consider $G(E) = \int_0^\infty dt\, e^{\frac{iEt}{\hbar}} e^{-\frac{itH}{\hbar}} e^{-\epsilon t}$

$$E = E + i\epsilon$$

$$G_\epsilon(E) = \frac{1}{E - H + i\epsilon}$$

Suppose we have a particle moving among many scatterers $i = 1, 2, \ldots N$

$$H = H_0 + V, \quad V = \sum_{i=1}^{N} V_i(r)$$

$$G_\epsilon = \frac{1}{E - H_0 - \sum V_i + i\epsilon}$$

We can expand this in powers of the potential but it is better to use a <u>binary collision expansion</u> which sums many terms in the V-series

Consider 1 scatterer

$$G_z^{(1)} = \frac{1}{E - H_0 - V_1 + i\varepsilon} = G_0 + G_0 V_1 G_0 + G_0 V_1 G_0 V_1 G_0 + \cdots$$

$$\equiv G_0 + G_0 T_1 G_0 \qquad G_0 = \frac{1}{E - H_0 + i\varepsilon}$$

$$T_1 = V_1 + V_1 G_0 V_1 + \cdots$$

Then

$$G(E) = G_0 + \sum_i G_0 T_i G_0 + \sum_{i \neq j} G_0 T_i G_0 T_j G_0$$

$$+ \sum_{\substack{i \neq j \\ k \neq j}} G_0 T_i G_0 T_j G_0 T_k G_0 + \cdots$$

$k = i$ is allowed

Let's calculate $\langle \varphi_0 | G | \varphi_0 \rangle$ for some $|\phi_0\rangle$

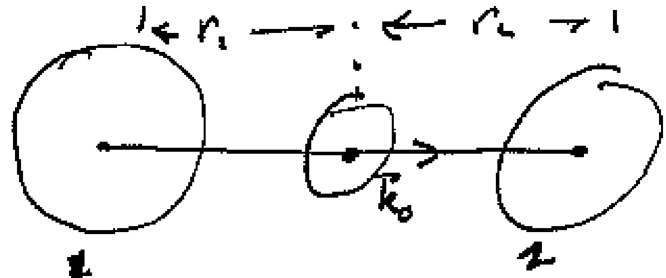
$$\langle \varphi_0 | G(E) | \varphi_0 \rangle = \langle \varphi_0 | G_0 | \varphi_0 \rangle + \sum_{i,k,k'} \langle \phi_0 | G_0 | k \rangle \langle k | T_i | k' \rangle \langle k' | G_0 | k' \rangle \langle k' | \varphi_0 \rangle$$

$$+ \sum_{i \neq j} \langle \varphi_0 | G_0 | k \rangle \langle k | T_i | k' \rangle \langle k' | G_0 | k' \rangle \langle k' | T_j | k'' \rangle \langle k'' | G_0 | k'' \rangle \langle k'' | \varphi_0 \rangle + \cdots$$

Write

$$\langle \varphi_0 | G(E) | \varphi_0 \rangle = \langle \varphi_0 | G_0 | \varphi_0 \rangle + S(E)$$

Let us consider a two ball system



Wave packet initially on axis with $\vec{k}_0$

The series is

$$G_0 (T_1 + T_2) G_0 + G_0 T_1 G_0 T_2 G_0 + G_0 T_2 G_0 T_1 G_0$$

$$+ \cdots$$

Look at series that starts with T_2

$$\langle \varphi_0 | G_0 | k \rangle \langle k | T_2 | k' \rangle \langle k' | G_0 | \varphi_0 \rangle$$

$$+ \langle \varphi_0 | G_0 | k \rangle \langle k | T_1 | k' \rangle \langle k' | G_0 | k'' \rangle \langle k'' | T_2 | k''' \rangle$$

$$\langle k''' | G_0 | \varphi_0 \rangle + \cdots$$

For hard disk scatterers, the matrix elements can be evaluated

$$\langle \vec{k} | T | \vec{k}' \rangle = 2\pi a \frac{\hbar^2}{2m} e^{-i(\vec{k}-\vec{k}')\cdot R} \sum_{l=-\infty}^{\infty} e^{il(\theta_k - \theta_{k'})} \left\{ \frac{k'^2 - \kappa^2}{k^2 - k'^2} \left[k' J_l(ka) J_{l-1}(k'a) - k J_{l-1}(ka) J_l(k'a) \right] + k' J_l(ka) J_{l-1}(k'a) - \kappa J_l(ka) J_l(k'a) \frac{H^{(1)}_{l-1}(\kappa a)}{H^{(1)}_l(\kappa a)} \right\}$$

$$E = \frac{\hbar^2 \kappa^2}{2m}$$

For our $|\phi_0\rangle$ there is a positive overlap in this series if before & after a chain of scatterers the packet is heading to the right.

We need

$$\int dk' \ldots dk''' \langle \varphi_0 | G_0 | k \rangle \langle k | T_1 | k' \rangle \underbrace{\langle k' | G_0 | k'' \rangle}^{A(k') \, \delta(k'-k'')} \langle k'' | T_2 | k''' \rangle \langle k''' | G_0 | \varphi_0 \rangle$$

$$= \int dk \int dk_1 \int dk_2 \; \langle \varphi_0 | G_0 | k \rangle \langle k | T_1 | k_1 \rangle A(k_1) \langle k_1 | T_2 | k_2 \rangle \langle k_2 | G_0 | \varphi_0 \rangle$$

Now $\vec{k}, \vec{k}_2 \approx \vec{k}_0$ due to overlaps

Next important term is

$$\langle \varphi_0 | G_0 T_1 G_0 T_2 G_0 T_1 G_0 T_2 G_0 | \varphi_0 \rangle$$

$$= \int \cdots \int \langle \varphi_0 | G_0 | k \rangle \langle k | T_1 | k_1 \rangle A(k_1) \langle k_1 | T_2 | k_2 \rangle A(k_2) \langle k_2 | T_1 | k_3 \rangle A(k_3) \langle k_3 | T_2 | k_4 \rangle \langle k_4 | G_0 | \varphi_0 \rangle$$

$\vec{k}, \vec{k}_4 \approx \vec{k}_0$

Note that this series is of the form

$$\langle \phi_0 | \; G_0 T_1 G_0 T_2 G_0 + G_0 T_1 G_0 T_2 G_0 T_1 G_0 T_2 G_0 + \ldots \; | \phi_0 \rangle$$

$$= \langle \phi_0 | \left[\frac{1}{1 - G_0 T_1 G_0 T_2} - 1 \right] G_0 | \phi_0 \rangle$$

In the high energy diffraction regime

$$\frac{2a^2}{R}, \frac{(a+\sigma)^2}{R} \ll \lambda \ll a, \sigma$$

The Fourier integrals can be done & one obtains

$$S(E) = \frac{-m}{\hbar^2} \left(\frac{iR}{2\pi k v_1 v_2} \right)^{1/2} \frac{| \varphi_0(k, h_0) |^2}{1 - \left(f_k(\pi) \frac{e^{ikR}}{\sqrt{R}} \right)^2}$$

$$f_k(\theta) = - \left(\frac{2}{\pi i k} \right)^{1/2} \sum_{l=-\infty}^{\infty} e^{il\theta} \frac{J_l(ka)}{H_l^{(1)}(ka)}$$

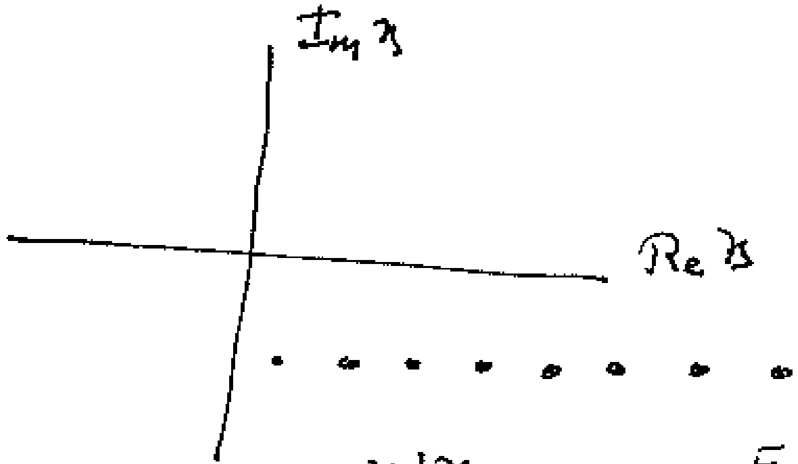
Or for ~~[illegible]~~ $ka \gg 1$

$$f_k(\theta) = -\left[\frac{a}{2}\left|\sin\frac{\theta}{2}\right|\right]^{1/2} e^{-2ika|\sin\theta/2|}$$

$$f_k(\pi) = -\sqrt{\frac{a}{2}}\, e^{-2ika}$$

The denominator has poles at

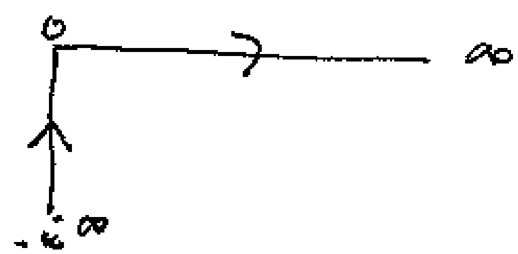
$$k_n = \frac{\pi n}{R-4a} - \frac{i}{2R-4a}\ln\frac{2R}{a} \approx \frac{\pi n}{R} - \frac{i}{2R}\ln\frac{2R}{a}$$



$$E = \frac{\hbar^2 k^2}{2m}$$

$$S(t) = \int_\Gamma \underbrace{dE}_{k\,dk}\, e^{-\frac{iEt}{\hbar}} S(E)$$

$\Gamma =$



$$S(t) \approx e^{-i\frac{E_0 t}{\hbar}} \, e^{-\frac{1}{2}\lambda^{(2)} t} \overbrace{\sum_n e^{-\frac{ivt}{R}\pi n}}^{\text{strong when } vt = 4}$$

$$\lambda^{(2)} = \frac{v}{R} \ln \frac{2R}{a} = \text{classical Lyap of 2 disk scatterer}$$

This is an example of Gaspard & Rice Quantum escape rate formula.

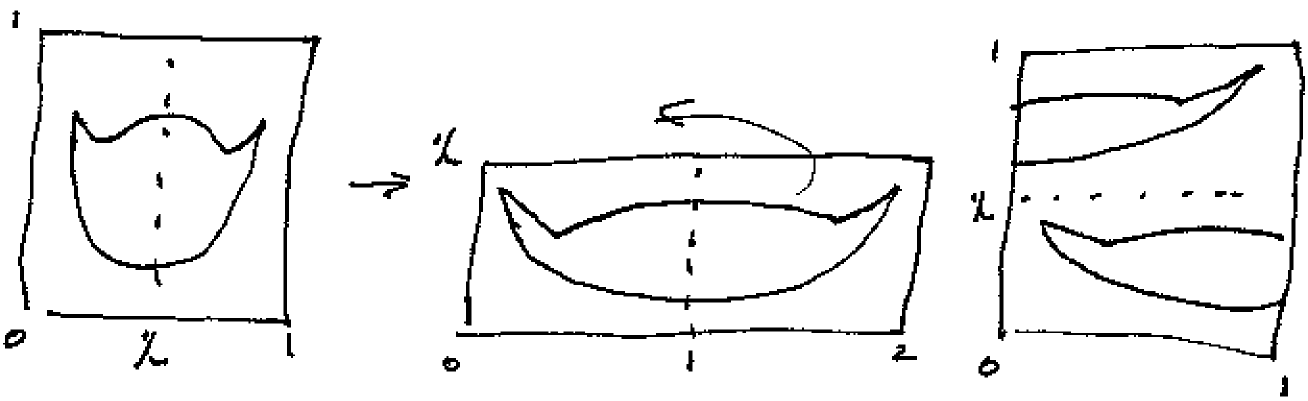
Decays occur as $\underline{\lambda - 2h_{KS}}$ rather than $\lambda - h_{KS}$ as in classical escape rate

Here $h_{KS} = 0$ but for other case  $h_{KS} \neq 0$

Slower decay in QM than classically due to constructive interference of w.v.

Baker + Multibaker Maps, Classical + Quantum

Baker Map – Classical



$$B: \quad \begin{matrix} x' \\ y' \end{matrix} = \begin{matrix} 2x \\ \frac{y}{2} \end{matrix} \quad 0<x<\tfrac{1}{2} \qquad \begin{matrix} x' \\ y' \end{matrix} = \begin{matrix} 2x-1 \\ \frac{y+1}{2} \end{matrix} \quad \tfrac{1}{2}<x<1$$

Area preserving map. Discrete Liouville eq.

$$\rho_n(x,y) = \rho_{n-1}(B^{-1}(x,y))$$

$$B^{-1}: \quad \begin{matrix} x' \\ y' \end{matrix} = \begin{matrix} \frac{x}{2} \\ 2y \end{matrix} \quad 0<y<\tfrac{1}{2} \qquad \begin{matrix} \frac{x+1}{2} \\ 2y-1 \end{matrix} \quad \tfrac{1}{2}<y<1$$

$$\rho_n(x,y) = \rho_{n-1}\left(\tfrac{x}{2}, 2y\right)\Theta\left(\tfrac{1}{2}-y\right) +$$

Perron-Frob. Eq.

$$+\ \rho_{n-1}\left(\tfrac{x+1}{2}, 2y-1\right)\ \Theta\left(y-\tfrac{1}{2}\right)$$

$$W_n(x) = \int_0^1 dy\, \rho_n(x,y)$$

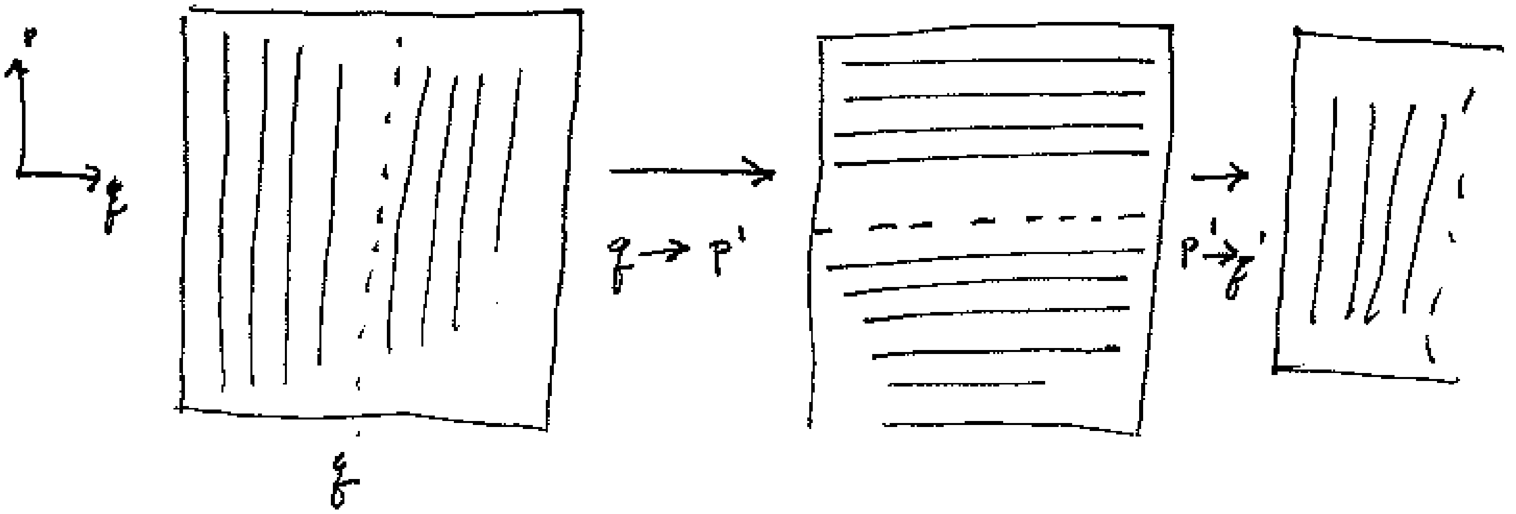
$$W_n(x) = \int_0^{1/2} dy\, \rho_{n-1}\left(\frac{x}{2}, 2y\right) + \int_{1/2}^1 dy\, \rho_n\left(\frac{x+1}{2}, 2y-1\right)$$

$$= \frac{1}{2}\left[W_{n-1}\left(\frac{x}{2}\right) + W_{n-1}\left(\frac{x+1}{2}\right)\right]$$

Decays to eq.

Pollicott Ruelle Resonances

QUANTUM BAKER



N = # of Quantum states = $\frac{\text{Area}}{h} \Rightarrow h = \frac{1}{N}$

N is an integer, we take N even

$|q_n\rangle \qquad n = 0, \ldots, N-1$

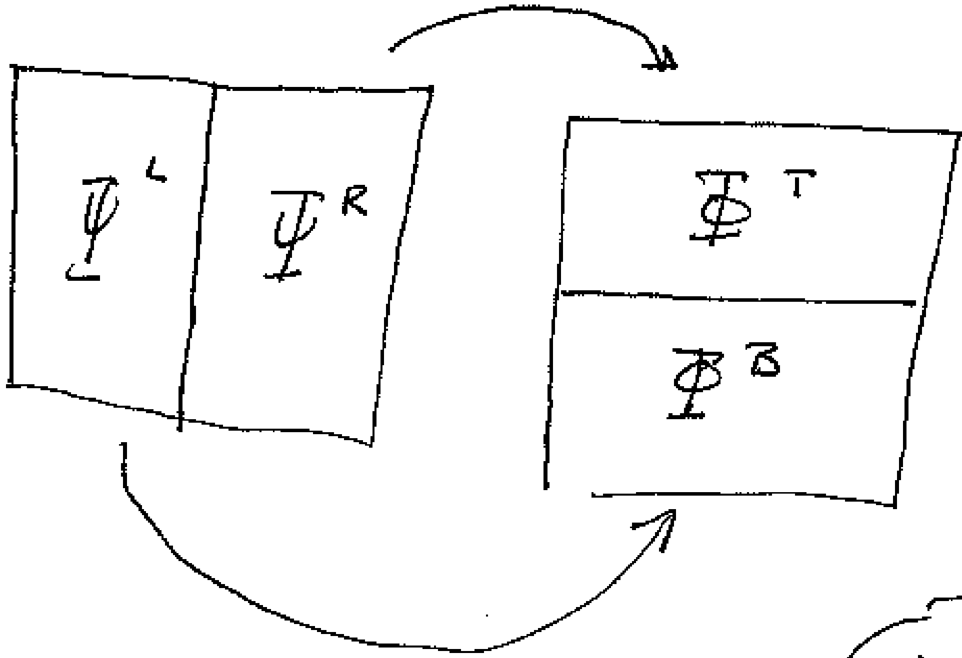
$|p_n\rangle \qquad n = 0, \ldots N-1$

$$\langle q_n | p_m \rangle = \frac{1}{\sqrt{N}} e^{\frac{i q_n p_m}{\hbar}}$$

$$|\Psi\rangle = \sum |q_n\rangle\langle q_n|\Psi\rangle$$

$$|\Psi\rangle = \sum |p_n\rangle\langle p_n|\Psi\rangle$$

$$\Psi_n = \langle q_n|\Psi\rangle, \quad \tilde{\Psi}_m = \langle p_m|\Psi\rangle$$



Stretching of the left side

$$\Phi^B_{2m} = \frac{1}{\sqrt{2}} \Psi^L_m \qquad 0 \le n \le \frac{N}{2} - 1$$

$$\tilde{\Psi}^L_{2m} = \frac{1}{\sqrt{2}} \tilde{\Phi}^B_m \qquad 0 \le n \le \frac{N}{2} - 1$$

In momentum representation Apply stretching Backwards

$$\tilde{\Phi}^B_m = 0 \qquad m \ge N/2$$

$$\Psi^L_n = 0 \qquad n \ge \frac{N}{2}$$

Balasz + Voros show with some algebra that this can be arranged by writing

$$\begin{pmatrix} \tilde{\Phi}_B \\ 0 \end{pmatrix} = \begin{bmatrix} F_{N/2} & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \psi_L \\ 0 \end{bmatrix}$$

NOT CLEAR A PRIORI THAT THERE WAS A SOLUTI

$F_{N/2}$ is a $\frac{N}{2} \times \frac{N}{2}$ matrix of the form

$$\left(F_K \right)_{mn} = \frac{1}{\sqrt{K}} e^{-\frac{2\pi i}{K}(m+\phi_m)(n+\phi_n)}$$

$0 \le \phi_m, \phi_n \le 1$ are arbitrary phases

Similarly

$$\begin{pmatrix} 0 \\ \tilde{\Phi}_T \end{pmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & F_{N/2} \end{bmatrix} \begin{bmatrix} 0 \\ \psi^R \end{bmatrix}$$

OR

$$\begin{pmatrix} \tilde{\Phi}^B \\ \Phi^T \end{pmatrix} = \begin{bmatrix} F_{N/2} & 0 \\ 0 & F_{N/2} \end{bmatrix} \begin{bmatrix} \psi^L \\ \psi^R \end{bmatrix}$$

This transforms L, R → T, B

but in momentum representation. To get back to space-rep, write

$$\begin{pmatrix} \psi^L \\ \psi^R \end{pmatrix}' = B \begin{pmatrix} \psi^L \\ \psi^R \end{pmatrix}$$

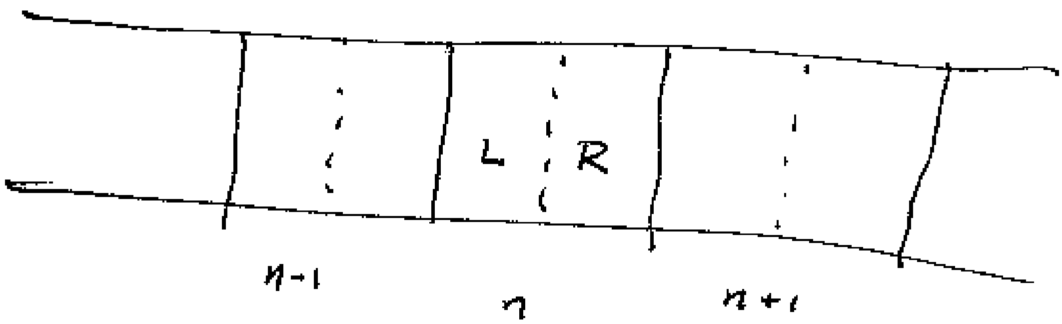
$$\boxed{B = F_N^{-1} \begin{pmatrix} F_{N/2} & 0 \\ 0 & F_{N/2} \end{pmatrix}}$$

Phases B-V $\phi_n = \phi_m = 0$

Saraceno $\phi_n = \phi_m = 1/2$ Preserves ~~this~~ A symmetry

CLASSICAL LIMIT $N \to \infty$, $h \to 0$

CLASSICAL MULTIBAKER - GASPARD



$n, L \to B, n+1$

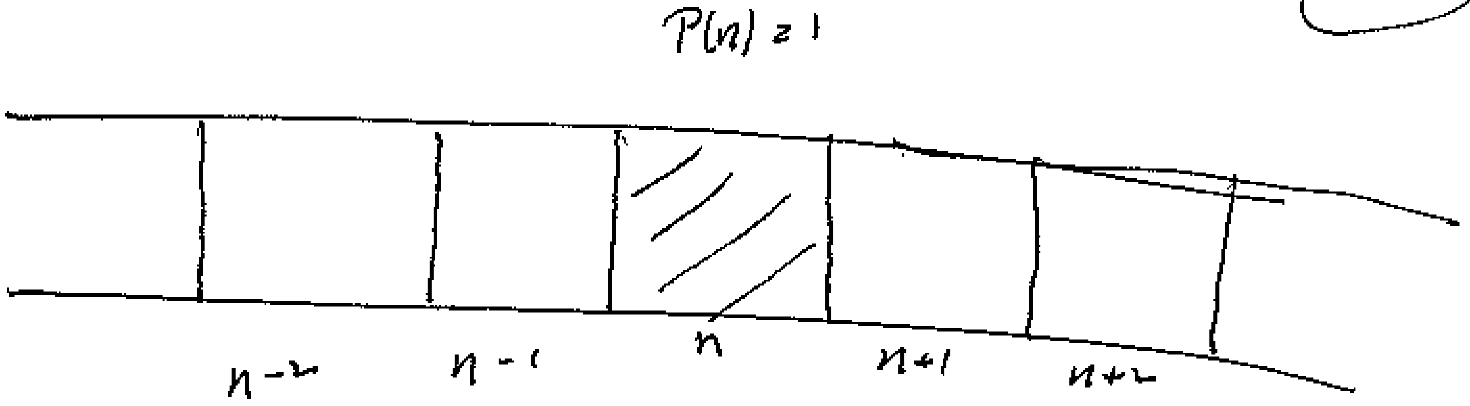
$n, R \to T, n-1$

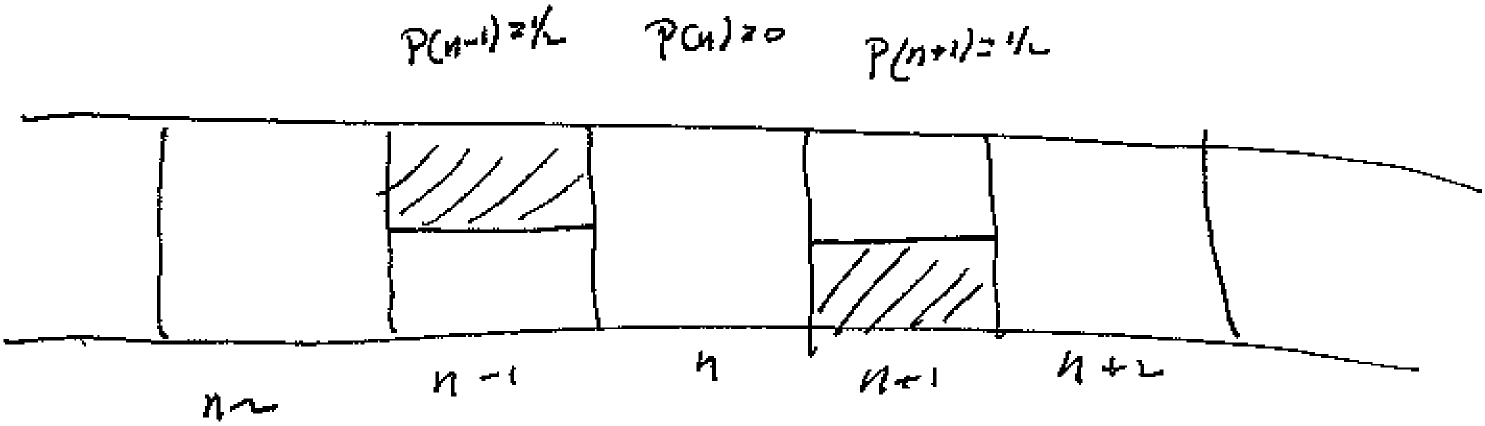
$x = [x] + \tilde{x}$

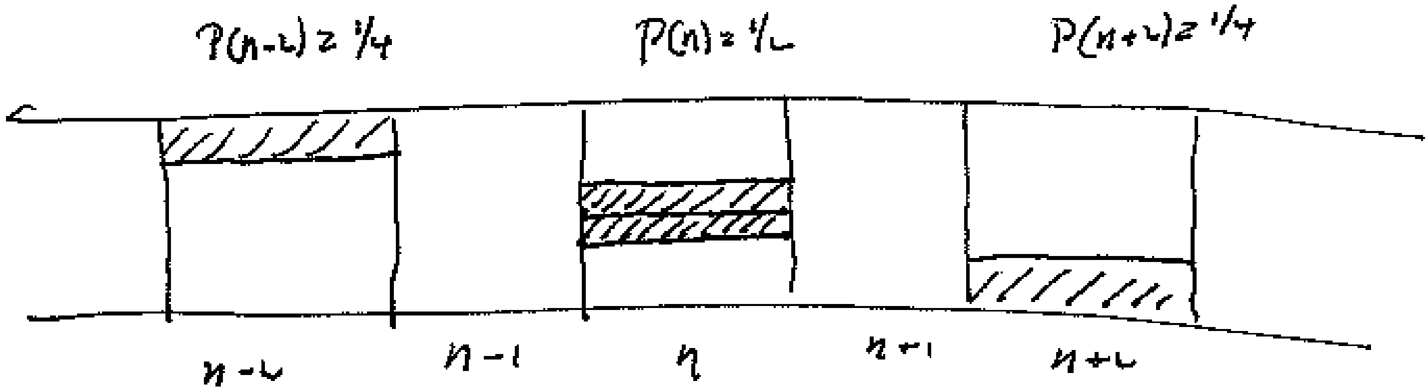
$$M(n, x, y) = \begin{cases} (n+1, 2\tilde{x}, y/2) & 0 \le \tilde{x} < 1/2 \\ (n-1, 2\tilde{x}-1, \frac{y+1}{2}) & 1/2 \le \tilde{x} \le 1 \end{cases}$$

Drop the "~"

Chaotic map with good diffusive properties, deterministic random walk







$D = \frac{1}{2}$ $\qquad \langle (\Delta x)^2 \rangle_t = 2Dt$

After 2-Steps

$$\langle (\Delta x)^2 \rangle = \frac{1}{4} \times 2^2 + \frac{1}{2} \times 0^2 + \frac{1}{4} \times 2^2 = 2 = 2\left(\frac{1}{2}\right) \cdot 2$$

QUANTUM MULTIBAKER

Two steps (can be done in several ways:)

1) Translate $\psi_L(n-1)$ to site n

Translate $\psi_R(n+1)$ to site n

2) Apply baker at site n,

$$\begin{bmatrix} \psi_L(n,t+1) \\ \psi_R(n,t+1) \end{bmatrix} = F_N^{-1}(n) \begin{bmatrix} F_{N/2}(n) & 0 \\ 0 & F_{N/2}(n) \end{bmatrix} \begin{bmatrix} \psi_L(n-1,t) \\ \psi_R(n+1,t) \end{bmatrix}$$

Index n in F's mean that we pick phases in F's for each site separately, but for a given n, all phases in $F_{N/2}$, F_N are the same

The phases give the model a great deal of flexibility. Can have periodic, quasi-periodic, random, ... phases

$$\left(\overline{F}_N(n)\right)_{kj} = \frac{1}{\sqrt{N}} e^{-\frac{2\pi i}{N}(k+\varphi_p(n))(j+\varphi_q(n))}$$

We can suppose there are L sites + each site has N-states so that the w.f. $|\Psi\rangle$ for the system has $L \times N$ components.

The Multibaker map acts as

$$|\Psi'\rangle = M|\Psi\rangle$$

M is the Floquet operator and the ~~the~~ time dependence of any operator Ω is

$$\Omega(t) = (M^{\dagger})^t \Omega M^t$$

If we look at diffusion in the QMB we expect

1. Uniform phases - ballistic motion
2. random phases - localization

TRANSP of QUASI-ENERGIES FOR PERIODIC + RANDOM PHASES + EIGENSTATES FOR RANDOM PHASES.

MEAN SQUARE DISPLACEMENT IN TRANSLATION INVARIANT SYSTEM

Let r be an operator that gives the lattice site index n as an eigenvalue

Let $\vec{v} = M^{+} r M - r$ = velocity operator

The eigenvalues of $\vec{v}$ are ± 1

MSD $\equiv$

$$\langle (\Delta r(t))^2 \rangle_{\Psi} = \langle (\vec{r}(t) - \vec{r})^2 \rangle_{\Psi}$$

$$= \langle (M^{+t} r M^{t} - r)^2 \rangle_{\Psi}$$

$$M^{+t} r M^{t} = M^{+t} r M^{t} - M^{+(t-1)} r M^{(t-1)}$$
$$+ M^{+(t-1)} r M^{t-1} = v_{t-1} + \cdots$$

$$M^{+t} r M^t - r = \sum_{\tau=0}^{t-1} v_\tau$$

$$\langle (\Delta r(t))^2 \rangle_\Psi = \sum_{\tau_1, \tau_2 = 0}^{t-1} \langle v_{\tau_1} v_{\tau_2} \rangle_\Psi$$

Now suppose we impose periodic b.c. & look at eq average (eq = uniform distrib)

$$\rho_{eq} = \frac{1}{NL} \mathbb{1}$$

$$\langle (\Delta r(t))^2 \rangle = \sum_{\tau_1, \tau_2 = 0}^{t-1} \langle v_{\tau_1} v_{\tau_2} \rangle_{eq}$$

$$\langle v_{\tau_1} v_{\tau_2} \rangle = \langle M^{+\tau_1} v M^{\tau_1} M^{+\tau_2} v M^{\tau_2} \rangle$$

$$= \langle v_0 \, v_{\tau_1 - \tau_2} \rangle = C_{\tau_1 - \tau_2}$$

$$\langle (\Delta r(t))^2 \rangle = t C_0 + 2 \sum_{\tau_1 > \tau_2} C_{\tau_1 - \tau_2}$$

$$= t C_0 + 2 \sum_{\tau \geq 1}^{t-1} (t - \tau) C_\tau$$

Now due to the isotropy of lattice (phases are same) + translational invariance, one can show

$$C_2 = \frac{1}{N} \mathrm{Tr}\left[B^{+2} J B^{2} J \right]$$

Baker - not Multibaker

$$J = \begin{bmatrix} \mathbb{1}_{N/2} & 0 \\ 0 & -\mathbb{1}_{N/2} \end{bmatrix}$$

and using the eigenstates of $\underset{\sim}{B}$

$$B|j\rangle = e^{i\varphi_j}|j\rangle$$

$$\langle (\Delta r)^2(t) \rangle = \frac{1}{N} \sum_{j,k} |J_{jk}|^2 \frac{\sin^2\left[\frac{(\varphi_j - \phi_k)t}{2}\right]}{\sin^2\left(\frac{\varphi_j - \phi_k}{2}\right)}$$

One can evaluate this either numerically OR using RMT

To find RMT value for $|J_{jk}|^2$

$$J_{jj} = \langle j | J | j \rangle = \sum_{\alpha=0}^{N-1} |\langle j|\alpha\rangle|^2 - \sum_{\frac{N}{2}}^{N} |\langle j|\alpha\rangle|^2$$

$|\alpha\rangle$ = position ket

If $\quad S_j = \sum_{\alpha=0}^{\frac{N}{2}-1} |\langle\alpha|j\rangle|^2$

and $\quad 1 = \sum_{\alpha=0}^{N/2-1} |\langle\alpha|j\rangle|^2 + \sum_{\frac{N}{2}}^{N} |\langle j|\alpha\rangle|^2$

$$J_{jj} = S_j - (1 - S_j) = 2S_j - 1$$

In RMT the eigenstates are uniformly distributed

$$P(\{\Phi\}) = c\,\delta(1 - |\Phi|^2) = c\,(1 - \sum_{\alpha} |\langle\alpha|\psi\rangle|^2)$$

$$|\langle j|J|j\rangle|^2 \rightarrow 4\langle S^2\rangle - 4\langle S\rangle + 1$$

$\langle S\rangle = \frac{1}{2}$ due to uniform

In COE Ψ is real, in CUE Ψ is complex

$$\langle S^2\rangle = \frac{M+2}{4(M+1)} \; ; \quad M = \frac{N}{k} \quad \begin{cases} k=2 & \text{COE} \\ k=1 & \text{CUE} \end{cases}$$

$$\langle |J_{jj}|^2 \rangle = \frac{k}{N+k}$$

To get $\langle |J_{jk}|^2 \rangle$ use

$$\sum_{j,k} |J_{jk}|^2 = \mathrm{Tr}\, J^2 = N = \sum_j |J_{jj}|^2 + \sum_{j \neq k} |J_{jk}|^2$$

$$\langle |J_{jk}|^2 \rangle = \frac{N}{(N-1)(N+k)} \qquad j \neq k$$

Next

$$\left\langle e^{i(\varphi_1 - \varphi_2)t} \right\rangle = \int_0^{2\pi} d\varphi_1 \int_0^{2\pi} d\varphi_2 \, e^{i(\varphi_1-\varphi_2)t} \, \frac{R(\varphi_1,\varphi_2)}{N(N-1)}$$

$R(\varphi_1, \varphi_2)$ = correlation function of 2 angles

Given in Mehta for COE, CUE

Finally:

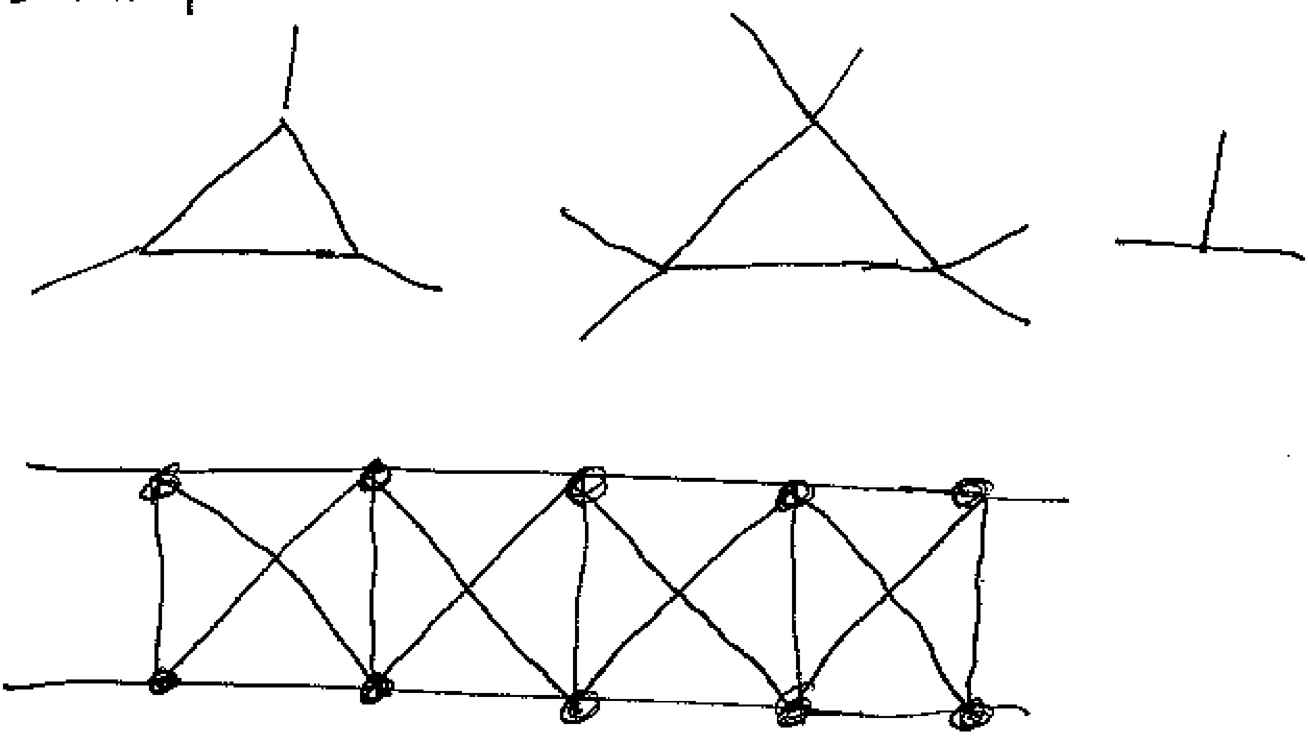
$$\langle (\Delta r(t))^2 \rangle = \begin{cases} t + \dfrac{t(t-1)}{N+k}\left[k-1 + \dfrac{t-2}{3(N-1)}\right] & t \leq N \\[2ex] \dfrac{k}{N+k}\, t^2 + \dfrac{N}{3} - \dfrac{N(k-1)}{3(N+k)} & + \text{small corrections} \end{cases}$$

Diffusive up to $t \sim N$ then

Ballistic, $t \to \infty$, $N \to \infty$ don't commute

QUANTUM GRAPHS - SMILANSKY + KOTTOS
BARRA + GASPARD

Examples



Some open graphs

We have bonds and vertices

On each bond there is a Sch. Eq

$$\cancel{\frac{\hbar^2}{2m}} \; -\frac{d^2}{dx^2}\psi_b(x) = k^2 \psi_b(x)$$

$$\psi_b(x) = \psi_+(b)\, e^{ikx} + \psi_-(b)\, e^{-ikx}$$

If we assign a direction or orientation to each bond, we distinguish the orientation with b and $\hat{b}$

$x_{ij} = 0$ at i
$= l_b$ at j $\quad l_b = l_{\hat{b}}$

$x_{ji} = 0$ at j $\quad x_{\hat{b}} = l_b - x_b$
$= l_b$ at i

$$\psi_{\hat{b}}(x) = \psi_b(l_b - x)$$

Continuity condition

$\psi_b(0) = \phi_i$ for all bonds that start at vertex i

$\psi_b(l_b) = \phi_j$ for all bonds that end at vertex j

We can let derivatives have discontinuities at vertex by writing

$$\sum_{\substack{\text{bonds} \\ \text{that start at vertex } i}} \frac{d}{dx}\psi_b(x)\Big|_{x \to 0} = -\alpha\, \phi_i$$

Let $C_{ij} = C_{ji} = 1$ if vertices i & j are connected
$= 0$ otherwise

Write the b.c. as

$$\psi_{i,j}(x)\Big|_{x=0} = \phi_i \ , \quad \psi_{ij}(x)\Big|_{x=l_{ij}} = \phi_j \quad \text{if } C_{ij} = 1$$

Current equation

$$\sum_{j<i} C_{ij}\left(-\frac{d}{dx}\right)\psi_{j,i}^{(x)}\Big|_{x=l_{j,i}}$$

$$+\sum_{j>i} C_{ij}\,\frac{d}{dx}\,\psi_{ij}(x)\Big|_{x=0} = \lambda_i \phi_i$$

So solutions are of the form

$$\psi_{ij}(x) = \frac{1}{\sin k l_{ij}}\Big[\phi_i \sin k(l_{ij}-x) + \phi_j \sin kx\Big]$$

Fits b.c.

$$\frac{d\psi}{dx} = \frac{k}{\sin k l_{ij}}\Big[-\varphi_i \cos k(l_{ij} - x) + \phi_j \cos kx\Big]$$

$$\left.\frac{d\psi}{dx}\right|_{l_{ij}} = \frac{k}{\sin k l_{ij}}\Big[-\varphi_i + \phi_j \cos k l_{ij}\Big]$$

$$\left.\frac{d\psi}{dx}\right|_{0} = \frac{k}{\sin k l_{ij}}\Big[-\phi_i \cos k l_{ij} + \phi_j\Big]$$

Derivative b.c. is

bonds that begin or end on i

$$-\sum_{j<i} \frac{k C_{ij}}{\sin k l_{ij}}\Big[-\phi_j + \phi_i \cos k l_{ij}\Big]$$

$$+\sum_{i>j} \frac{k C_{ij}}{\sin k l_{ij}}\Big[-\phi_i \cos k l_{ij} + \phi_j\Big] = \lambda_i \varphi_i$$

This provides the secular eq for k's

These models have many interesting properties

1. There is an exact trace formula in terms of classical periodic orbits on the graph
2. There is a classical mechanics with free particle motion on bonds and transition probabilities at the vertices!
3. The classical version has good transport properties.