The Gutzwiller Trace Formula and the Quantum-Classical Correspondence

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In this expository article, we review the periodic-orbit quantization method and its use in verifying the BGS (Bohigas-Giannoni-Schmit) Conjecture[7] of random matrix universality for chaotic quantum systems. We first illustrate the periodic orbit quantization method by explaining the structure of the Gutzwiller trace formula[2], which determines the leading order semiclassical approximation to the quantum energy spectrum in terms of classical periodic orbits. We begin by guiding the reader through the explicit derivation of the Gutzwiller trace formula for a nonrelativistic particle in two Euclidean dimensions, before presenting the trace formula for arbitrary d. We then introduce the spectral form factor and explain how the Gutzwiller trace formula can be used to verify[5,6] that the (full perturbative) semiclassical approximation to the spectral form factor (suitably averaged over a small time interval) of a quantum system with a chaotic classical limit agrees with the predictions of random matrix theory, in accord with the BGS conjecture.

I. THE GUTZWILLER TRACE FORMULA[2]

A key issue one encounters in quantum chaology is the fact that many of the "standard" methods for studying the semiclassical regime, such as Bohr-Sommerfeld quantization, are *not* actually applicable to chaotic systems[1,2], since the application of such conditions generally requires that the system be multiply-periodic (i.e. capable of being decomposed into a product of systems with one degree of freedom each), which in turn generally requires that the system be integrable (i.e. have one conserved quantity for each degree-of-freedom).

One method for studying the semiclassical regime of nonintegrable systems is the periodic orbit quantization method pioneered by Gutzwiller in the 1970's[2,3]. The crux of this method is the determination, to leading order in $1/\hbar$, of the spectrum of the quantum mechanical Hamiltonian in terms of the behavior of periodic solutions to the classical equations of motion ("periodic orbits" in the classical phase space).

The cornerstone of periodic orbit quantization is the *Gutzwiller trace formula*[2] eq. (23), which expresses the semiclassical (ie. leading order in $1/\hbar$) approximation to the quantum system's resolvent (and hence the semiclassical approximation to the quantum energy spectrum) in terms of a sum of one-loop amplitudes, one for each periodic orbit of the underlying classical system.

We will begin in section I A by deriving in some detail the Gutzwiller trace formula for the case of a single nonrelativistic particle in two Euclidean spacetime dimensions, before turning in section I B to an explanation of the generalization to an arbitrary number of Euclidean spatial dimensions. We will then go on in section II

A. Derivation in $d = 2$

In what follows, we will restrict our consideration to the quantization of systems of nonrelativistic particles. Since we only seek to illustrate the general logic of the GTF, we will also, for convenience, restrict our attention to the case of a single particle in two Euclidean spatial dimensions.

Following[2], we begin by considering the Semiclassical approximation, $R_{\mathrm{sc}}(E)$, to the resolvent

$$R(E) \; = \; \mathrm{Tr}\left(\frac{1}{E-H}\right) \; = \sum_{\text{eigenstates}} \frac{1}{E-E_i} \tag{1}$$

given by

$$R_{\mathrm{sc}}(E) = \int \mathrm{d}\mathbf{q}\, G_{\mathrm{sc}}(\mathbf{q},\mathbf{q},E) \tag{2}$$

where H is the Hamiltonian and G_{sc} is the semiclassical approximation to the Green's function (see appendix A below). The resolvent is a useful quantity since its discontinuity across the real axis can be used to obtain the density of states

$$R(E+\mathrm{i}\epsilon) - R(E-\mathrm{i}\epsilon) = -2\pi\mathrm{i}\rho(E) \tag{3}$$

and so we can consider the determination of the semiclassical resolvent as equivalent to the semiclassical determination of the quantum energy spectrum.

Recall from appendix A that (ignoring for now the "classical" term G_0)

$$\mathrm{i}\hbar G_{\mathrm{sc}}(\mathbf{q}'', \mathbf{q}', E) = \sum_{\substack{\text{classical}\\ \text{trajectories}}} \sqrt{\frac{|D_s|}{(2\pi \mathrm{i}\hbar)^3}} \exp\left[\frac{\mathrm{i}}{\hbar} S_\gamma(E) - \frac{\mathrm{i}\pi}{2} m_\gamma\right] \tag{4}$$

where γ is a classical trajectory connecting $\mathbf{q}'$ and $\mathbf{q}''$ with energy $H|_\gamma = E$,

$$S_\gamma(E) := \int_\gamma \mathbf{p}(\mathbf{q}, \dot{\mathbf{q}}) \cdot \mathrm{d}\mathbf{q} \tag{5}$$

is the classical action along γ, m_γ is the *Maslov index* counting the number of conjugate points along γ, and

$$D_s = \det \begin{pmatrix} \dfrac{\partial^2 S}{\partial \mathbf{q}'' \partial \mathbf{q}'} & \dfrac{\partial^2 S}{\partial \mathbf{q}'' \partial E} \\ \dfrac{\partial^2 S}{\partial E \partial \mathbf{q}'} & 0 \end{pmatrix} \tag{6}$$

is the one-loop determinant.

Assuming that $\frac{\exp(\mathrm{i}S_{\mathrm{cl}}/\hbar)}{\sqrt{|D_s|}}$ is rapidly varying in $\mathbf{q}'$, the integral eq. (2) over $\mathbf{q}'$ is dominated by classical periodic orbits. This simply follows from the fact that

$$\begin{aligned} &\frac{\partial S(\mathbf{q}, \mathbf{q}, E)}{\partial \mathbf{q}} \\ &= \left(\frac{\partial S(\mathbf{q}'', \mathbf{q}', E)}{\partial \mathbf{q}'} + \frac{\partial S(\mathbf{q}'', \mathbf{q}', E)}{\partial \mathbf{q}''}\right)\Bigg|_{\mathbf{q}} &(7)\\ &= \mathbf{p}'' - \mathbf{p}' &(8) \end{aligned}$$

so that the rapid oscillation assumption implies that the integral eq. (2) is dominated by paths with $\mathbf{p}' = \mathbf{p}''$, i.e. (when $\mathbf{q}' = \mathbf{q}''$) by periodic orbits. The integration over $\mathbf{q}' = \mathbf{q}'' = \mathbf{q}$ can thus be accomplished term-by-term by invoking, for each orbit γ, a coordinate system $\{q^i\}$ with q^1 running along the orbit and q^2 locally orthogonal to the orbit.

For a given point $\mathbf{q}_0$ on the periodic orbit, we can expand

$$\begin{aligned} &S(\mathbf{q}, \mathbf{q}, E) - S(\mathbf{q}_0, \mathbf{q}_0, E) \\ &= \frac{1}{2}\left(\frac{\partial^2 S}{\partial q_2' \partial q_2'} + 2\frac{\partial^2 S}{\partial q_2' \partial q_2''} + \frac{\partial^2 S}{\partial q_2'' \partial q_2''}\right)\Bigg|_{\mathbf{q}_0} \delta q_2' \delta q_2'' + \dots \end{aligned} \tag{9}$$

Assuming that the RHS of eq. (9) is singular only for isolated values of $\mathbf{q}_0$, we can approximate the integration over q^2 (in the semiclassical regime $S/\hbar \to \infty$) by stationary phase to find

$$R_{\mathrm{sc}}(E) \underset{S/\hbar\to\infty}{\sim} -\frac{1}{\hbar} \sum_{\substack{\text{periodic}\\ \text{orbits, }\gamma}} \oint_\gamma \mathrm{d}q^1 \sqrt{|D_s|} \frac{\exp\left[\frac{\mathrm{i}}{\hbar} S_\gamma(E) - \frac{\mathrm{i}\pi}{2}\left(m_\gamma + \frac{1}{2} \pm \frac{1}{2}\right)\right]}{\sqrt{\left|\frac{\partial^2 S}{\partial q_2' \partial q_2'} + 2\frac{\partial^2 S}{\partial q_2' \partial q_2''} + \frac{\partial^2 S}{\partial q_2'' \partial q_2''}\right|}} + \dots \tag{10}$$

where $\pm$ is the sign of the RHS of eq. (9). With some work (see e.g. Section 2 of[2]), we can show, furthermore that

$$D_s = \frac{1}{|\dot{q}_1|^2} \frac{\partial^2 S}{\partial q_2' \partial q_2''} \tag{11}$$

A key fact that we must now use is that the Hamiltonian flow fixes the two-dimensional (more generally $2(d-1)$-dimensional) submanifold of phase space with $(E, q^1) = \big(E(\gamma), q^1(\gamma)\big)$. This automorphism is volume preserving, fixes γ, and can be approximated in a neighborhood of γ by a linear transformation (specifically, by the restriction of the monodromy matrix of γ to this submanifold) with characteristic polynomial $P(\lambda)$. It is straightforward, though somewhat technical (see Sections 3 and 4 of[2]) to show that the ratio of the determinants appearing in the integrand of eq. (10) is simply given by $P(1)$, i.e. that

$$R_{\mathrm{sc}}(E) \underset{S/\hbar\to\infty}{\sim} -\frac{1}{\hbar} \sum_{\substack{\text{periodic}\\ \text{orbits, }\gamma}} \oint_\gamma \frac{\mathrm{d}q^1}{|\dot{q}^1|} \sqrt{P(1)} \exp\left[\frac{\mathrm{i}}{\hbar} S_\gamma(E) - \frac{\mathrm{i}\pi}{2} m_\gamma + \frac{1}{2} \pm \frac{1}{2}\right] + \dots \tag{12}$$

which follows from writing the monodromy matrix of γ in terms of derivatives of S.

We now want to deal with the phase factors and explicit factor of $P(1)$ in eq. (12). For unstable orbits $P(\lambda)$ will have two real roots $\lambda = e^{\pm u}$, while for stable orbits $P(\lambda)$ will have two roots on the unit circle $\lambda = e^{\pm \mathrm{i}v}$, i.e.

$$P(1) = \begin{cases} +4\left(\sin(v/2)\right)^2 & \text{if } \gamma \text{ is stable} \\ -4\left(\sinh(u/2)\right)^2 & \text{if } \gamma \text{ is unstable} \end{cases} \tag{13}$$

Since this is independent of q^1, we can perform the integration $\oint \mathrm{d}q^1/|\dot{q}^1|$ over the orbit to simply get an overall factor of T_γ, the (primitive) period of γ, giving

$$R_{\mathrm{sc}}(E) \underset{S/\hbar\to\infty}{\sim} -\frac{1}{\hbar}\sum_{\substack{\text{periodic}\\ \text{orbits, } \gamma}} T_\gamma \sqrt{P(1)} \exp\left[\frac{\mathrm{i}}{\hbar}S_\gamma(E) - \frac{\mathrm{i}\pi}{2}m_\gamma + \frac{1}{2} \pm \frac{1}{2}\right] + \dots \tag{14}$$

1. Contribution of Stable Orbits

In order to finish evaluating eq. (14), we begin by considering the contribution to $R_{\mathrm{sc}}(E)$ from stable periodic orbits, for which $P(1) > 0$ (see eq. (13) above). The number of conjugate points along a given stable periodic orbit, s, is even (odd) provided the sign of D_s is positive (negative); thus, for stable periodic orbits, the amplitude factor $\exp\left[-\frac{\mathrm{i}\pi}{2}(\dots)\right]$ due to the phase delay in eq. (14) is always real-valued.

Consider now a particular stable periodic orbit s, which is "primitive" in the sense that it cannot be written as a (nonunit) integer number of traversals of another periodic orbit. The sum over orbits in eq. (14) counts multiple traversals of the same orbit as distinct, so there is one contribution to eq. (14) for each r-traversal of s, with $r \in \mathbb{Z}_+$. Such terms come in with the same overall factor of T_s (since the integration that leads to it is over coordinate space rather than time) but do not contribute equally to the amplitude, since the number of conjugate points along the r-traversal of s varies with r; luckily, it does so in a way that is simply related to the "stability angle" v which enters the amplitude via eq. (13): indeed, we have that[2]

$$\#\text{ of conjugate points } = \lfloor v/\pi \rfloor \tag{15}$$

However, we also have that

$$v_{(r\text{ traversals})} = r \cdot v_{(\text{one traversal})} \tag{16}$$

Using that, additionally

$$S_{(r\text{ traversals})} = r \cdot S_s(E) \tag{17}$$

we find that the net contribution of s (including all its r-traversals) to $R_{\mathrm{sc}}(E)$ is given by

$$R_{\mathrm{sc}}(E) \supseteq -\frac{T_s}{\hbar}\sum_{r=1}^{\infty} \frac{1}{2\sin(rv/2)}\, e^{\mathrm{i}nS_s(E)/\hbar} \tag{18}$$

Note that we have been able to absorb the conjugate-point "bookkeeping" of the $\pm$'s into the sign of the denominator of eq. (18). Assuming that s is sufficiently isolated from other orbits, one can interpret the above sum as describing the interference of waves which run around the stable periodic orbit r times[2].

Here we have made the additional approximation that $nv \notin 2\pi\mathbb{Z}$, which physically means that we are ignoring the behavior of the Green's function at focal points (where the approximation eq. (4) breaks down). Since eq. (18) is finite near odd conjugate points, and using evidence from certain special examples for the behavior of the amplitude near even conjugate points (where the amplitude remains finite but only attains half the expected phase), we are led to conjecture the following correction[2] to eq. (18):

$$R_{\mathrm{sc}}(E) \supseteq -\frac{T_s}{2\hbar}\sum_{r=1}^{\infty} \exp\left[\mathrm{i}n\left(\frac{S_s(E)}{\hbar} - \frac{v}{2}\right) + \frac{\mathrm{i}\pi}{2}\right] \tag{19}$$

One can evaluate the resulting geometric series to find that $R_{\mathrm{sc}}(E)$ has a simple pole of residue 1 whenever

$$S_s(E)/\hbar = 2\pi m + v/2 \tag{20}$$

i.e. that the semiclassical density of states has a δ-function singularity of strength one for each stable classical periodic orbit satisfying eq. (20). This condition is considered[2] to be the generalization of the Bohr-Sommerfeld quantization condition to non-integrable systems.

2. Contribution of Unstable Orbits

Consider now the contribution to $R_{\mathrm{sc}}(E)$from unstable periodic orbits, for which $P(1) < 0$ (see eq. (13) above). For unstable periodic orbits, the amplitude factor due to factor $\exp\left[-\frac{\mathrm{i}\pi}{2}(\dots)\right]$ due to the phase delay in eq. (14) is always purely imaginary.

A given unstable primitive periodic orbit $\tilde{s}$ will again yield one contribution to eq. (14) for each r-traversal of $\tilde{s}$, $r \in \mathbb{Z}_+$. Thus, if there are l conjugate points along $\tilde{s}$, there will be $r \cdot l$ conjugate points along an r-traversal of $\tilde{s}$; as before, the instability exponent for the r-traversal will be $ru_{\text{one traversal}}$ and the action of the r-traversal will be $r \cdot S_{\tilde{s}}(E)$, and, in analogy to eq. (18), we find that the net contribution of $\tilde{s}$ (including all its r-traversals) to $R_{\mathrm{sc}}(E)$ is given by

$$R_{\mathrm{sc}}(E) \supseteq -\frac{\mathrm{i}T_{\tilde{s}}}{\hbar}\sum_{r=1}^{\infty} \frac{1}{2\sinh(ru/2)}\, e^{\mathrm{i}n\left(\frac{S}{\hbar} - \frac{l\pi}{2}\right)} \tag{21}$$

This formula suffers from the same issues as eq. (18) above, and the analog of the conjectured correction eq. (19) is

$$R_{\rm sc}(E) \supseteq -\frac{\mathrm{i}T_{\tilde{s}}}{2\hbar}\sum_{r=1}^{\infty}\exp\left[\mathrm{i}n\left(\frac{S_{\tilde{s}}(E)}{\hbar}-\frac{l\pi}{2}+\frac{\mathrm{i}u}{2}\right)\right] \tag{22}$$

B. The Gutzwiller Trace Formula for Arbitrary d

Having now spent some time acquainting ourselves with the $d=2$ case, it is helpful to zoom out and consider the Gutzwiller formula for general d, which reads[4]

$$R_{\rm sc}(E) \underset{\hbar\to 0}{\sim} \frac{1}{\mathrm{i}\hbar}\sum_{\substack{\text{primitive}\\ \text{orbits, } p}} T_p \sum_{r=1}^{\infty}\frac{\exp\left(\frac{\mathrm{i}}{\hbar}S_p(E)-\frac{\mathrm{i}\pi}{2}\tilde{m}_p\right)}{\sqrt{\left|\det\left(1-(\mathbf{M}_p)^r\right)\right|}} \tag{23}$$

Here p labels primitive classical periodic orbits, r enumerates repetitions of a given periodic orbit, $\mathbf{M}_p$ is the monodromy matrix of p, and $\tilde{m}_p$ is the Maslov index of p (see appendix A). Note that unlike similar trace formulas found in mathematics (such as the Selberg trace formula, see[11] for a review), the Gutzwiller trace formula is *not* exact, but rather the leading term in a semiclassical expansion.

1. An Aside: The Monodromy Matrix

For completeness, we remind the reader that the monodromy matrix, $\mathbf{M}_\gamma$, of a periodic orbit γ is defined as follows: We begin by considering a trajectory, γ', which is contained within a neighborhood of γ. Letting $(\mathbf{q},\mathbf{p})$ and $(\mathbf{q}',\mathbf{p}')$ to be canonical coordinates constructed relative to γ and γ' as described above, we set $\boldsymbol{\xi}'=\mathbf{q}'-\mathbf{q}$ and $\boldsymbol{\eta}'=\mathbf{p}'-\mathbf{p}$. After a time T_γ, the particle described by γ' will evolve to the point $(\mathbf{q}''=\mathbf{q}+\boldsymbol{\xi}'',\mathbf{p}''=\mathbf{p}+\boldsymbol{\eta}'')$, linearly related to $(\mathbf{q}',\mathbf{p}')$ by the *monodromy matrix*, $\mathbf{M}_\gamma$, i.e.

$$\begin{pmatrix}\boldsymbol{\xi}''\\ \boldsymbol{\eta}''\end{pmatrix} = \mathbf{M}_\gamma\begin{pmatrix}\boldsymbol{\xi}'\\ \boldsymbol{\eta}'\end{pmatrix} \tag{24}$$

II. SEMICLASSICAL TESTS OF RANDOM MATRIX UNIVERSALITY

A useful arena for learning how to diagnose the presence of quantum chaos is the semiclassical regime of quantum systems with chaotic classical limits. One hopes that a proper understanding of this situation will help us understand which properties of the quantum theory might reflect the presence of chaos in the classical limit, and so understand which properties of a quantum mechanical system might diagnose the presence of chaos (nonintegrability) more generally.

One of the most well-understood diagnostics of quantum chaos, which does not depend on the presence of any additional structure beyond quantum mechanics and nonintegrability, is the notion of “fine-grained” or “late-time” chaos, as captured by the celebrated *BGS (Bohigas-Giannoni-Schmit) Conjecture*[7] of Random Matrix Universality. The BGS conjecture posits that the excited energy levels of a chaotic quantum system should—when averaged over small energy windows and viewed at scales sightly coarser than that of the average energy spacing—be distributed like those in a random matrix theory. The particular universality class of random matrix theory describing the spectrum is expected to be determined only by the basic discrete symmetry properties of the system (such as e.g. the presence or absence of time-reversal symmetry). The BGS conjecture is supported by an overwhelming amount of numerical and experimental evidence[4], but its underlying theoretical foundations are to date poorly understood.

As we have seen above, the periodic-orbit quantization of Gutzwiller is a viable method for probing the semiclassical approximations to the spectra of quantum systems with chaotic classical limits, and so a natural use might be to verify the BGS conjecture in the semiclassical regime. We will now give a rough sketch for how one does this, following the work of Altland, Braun, Haake, Heusler, and Müller[5,6].

A. The Spectral Form Factor

A key diagnostic tool in the study of late-time quantum chaos is the *spectral form factor*, which is defined as follows: One begins by choosing some free parameter (e.g. a time interval) over which to average observables in our system, and then calculates the two-point correlation function of the density of states with respect to this averaging procedure $\langle\rho(E)\rho(E')\rangle$ (here and in what follows, $\langle\,\cdot\,\rangle$ denotes averaging with respect to e.g. small time intervals or within random matrix theory, rather than a quantum expectation value). This gives a quantity which probes the distribution of the system's energy levels and which can be easily compared to the predictions of random matrix theory.

The *spectral form factor* (SFF), $K(\tau)$, is defined to be the Fourier transform of the normalized connected density-density correlator

$$K(\tau) \coloneqq \int \mathrm{d}\varepsilon\, e^{\frac{\mathrm{i}}{\hbar}\varepsilon t}\,\frac{\langle\,\rho(E+\varepsilon/2)\rho(E-\varepsilon/2)\,\rangle_c}{\rho(E)} \tag{25}$$

viewed as a function of the dimensionless time variable:

$$\tau = t/T_H \tag{26}$$

where

$$T_H = 2\pi\hbar\,\rho(E) \tag{27}$$

is the *Heisenberg time*, with semiclassical approximation

$$T_{H\,\mathrm{sc}} = \frac{\Omega(E)}{(2\pi\hbar)^{d-1}} \tag{28}$$

where $\Omega(E)$ is the symplectic volume of the energy shell and, here, d is the number of degrees of freedom. Note that conventions for the normalization, units, and notation for the SFF and its argument differ across disciplines.

According to the BGS conjecture, we expect a chaotic system with Hamiltonian H to fall into one of three classes[4]: unitary (no time reversal symmetry), orthogonal (time-reversal symmetry squaring to the identity), or symplectic (time-reversal symmetry squaring to minus the identity), with random matrix theory predictions[8]

$$K(\tau) = \begin{cases} \tau & \text{(Unitary)} \\ 2\tau - \tau\log(1+2\tau) & \text{(Orthogonal)} \\ \frac{1}{2}\tau - \frac{1}{4}\tau\ln(1-\tau) & \text{(Symplectic)} \end{cases} \tag{29}$$

for $|\tau| < 1$. The spectral form factor reflects the "rigidity" of chaotic spectra, in which nearby energy levels tend to repel one another and adhere to a consistent spacing (for the classes above, given by the so-called "Wigner surmise"). For chaotic systems, it is expected that the SFF eq. (25) will begin to resemble the random matrix theory prediction eq. (29) for τ larger than a nonuniversal time-scale known as the "ramp" or "Thouless" time[9].

B. The Spectral Form Factor From Periodic Orbits

Its a remarkable fact that, for chaotic systems with ergodic and hyperbolic classical dynamics, one can actually derive the pectral form factor eq. (29) directly from the Gutzwiller trace formula eq. (23)[5,6] in the semiclassical limit. One does this by using eq. (23) to yield the semiclassical expansion of the density of states

$$\rho_{\mathrm{sc}}(E) = \frac{1}{\pi\hbar}\,\mathrm{Re}\sum_{\gamma} A_\gamma\, e^{\mathrm{i}S_\gamma(E)/\hbar} \tag{30}$$

giving

$$K_{\mathrm{sc}}(\tau) = \left\langle \sum_{\gamma,\gamma'} A_\gamma A^*_{\gamma'}\, e^{\frac{\mathrm{i}}{\hbar}\left(S_\gamma - S_{\gamma'}\right)}\, \delta\Big(\tau - \frac{T_\gamma + T_{\gamma'}}{2T_H}\Big) \right\rangle \tag{31}$$

and then taking the semiclassical limit $\hbar \to 0$, $T_H \to \infty$, $T_\gamma/T_H = \mathrm{const.}$ In this limit, the leading (perturbative in $1/\hbar$) contributions to eq. (31) come from families of pairs of orbits (γ,γ') with small action difference $|S_\gamma - S_{\gamma'}| \sim \hbar$; all other contributions are nonperturbatively suppressed by the rapidly oscillating phase factor.

The primary assumptions are ergodicity and hyperbolicity of the classical dynamics and finiteness of all classical relaxation times (as determined by Ruelle-Pollicott resonances and Lyapunov exponents). The latter condition is needed to ensure that the shortest time scale of relevance (the Ehrenfest time) is still much larger than any classical time scale.

For systems described by the unitary or orthogonal classes (for simplicty and brevity, we ignore systems described by the symplectic class, which are covered in[6]), we can recover the first term of eq. (29) from the leading order term of eq. (31), yielded by restricting the double sum to a single sum over pairs of orbits with $S_\gamma = S_{\gamma'}$, For systems without time reversal symmetry, this is simply given by taking $\gamma' = \gamma$. Classical ergodicity allows us to apply the Hannay-Ozorio de Almeida (HOdA) sum rule[12]

$$\left\langle \sum_\gamma |A_\gamma|^2\, \delta\big(\tau - T_\gamma/T_H\big) \right\rangle = \tau \tag{32}$$

($\langle\,\cdot\,\rangle$ denoting averaging over a small time interval) and so we find that

$$\langle K_{\mathrm{sc}}(\tau)\rangle \underset{\hbar\to 0}{\approx} \tau \qquad \text{(without time reversal)} \tag{33}$$

as predicted in eq. (29). This is the famous "diagonal" approximation of Berry[10]. For systems with time reversal symmetry T (since we are considering systems with conventional classical limits, i.e. Bosons, we will necessarily have $\mathsf{T}^2 = 1$), there is an overall factor of 2

$$\langle K_{\mathrm{sc}}(\tau)\rangle \underset{\hbar\to 0}{\approx} 2\tau \qquad \text{(with time reversal)} \tag{34}$$

which comes from an additional, equal contribution to eq. (31) from pairs with $\gamma' = \mathsf{T}\gamma$; this matches the prediction of eq. (29) for the orthogonal class.

The remaining terms in the power series expansion of eq. (29)

$$K(\tau) = \begin{cases} \tau \;+\; \displaystyle\sum_{n=2}^{\infty} 0 & \text{(Unitary)} \\ 2\tau + \displaystyle\frac{1}{2}\sum_{n=2}^{\infty}\frac{(-1)^n 2^n}{n-1}\,\tau^n & \text{(Orthogonal)} \end{cases} \tag{35}$$

can be obtained as follows: The condition that we only consider pairs of orbits with small action difference means that we should only consider the contribution to eq. (31) from pairs (γ,γ') where γ and γ' differ from one another only within a close l-encounter[5,6], where a close l-encounter is a short stretch of configuration space along which two distinct segments of a given orbit run alongside one another (before they begin to diverge exponentially due to chaotic Lyapunov behavior). In the special case of a close 2-encounter, we call (γ,γ') a *Sieber-Richter pair* (see fig. 1).

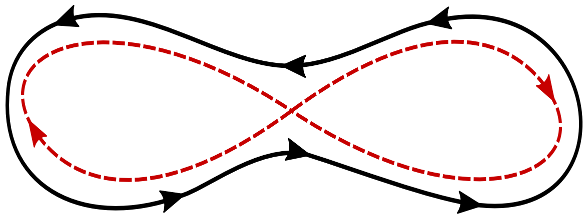

FIG. 1: Sketch of a Sieber-Richter pair in configuration space, inspired by Fig. 1 of[6]. The partner orbits differ noticeably only inside an encounter of two orbit stretches. The sketch greatly exaggerates the difference between the two partner orbits outside the encounter and greatly underemphasizes both the relative and absolute lengths of the orbit stretches outside the encounter.

Let v_l ($l \geq 2$) be the number of close l-encounters within which γ and γ' differ, $V :- \sum_l v_l$ be the total number of close encounters and $L := \sum_l l v_l$ be the total number of orbit stretches within encounters (= the total number of "loops" outside encounters). Then the nth term in eq. (35) is reproduced by the contribution to eq. (31) from all families of pairs with $L - V + 1 = n$. This is worked out in detail for $n = 2, 3$ in[13], and the general combinatoric argument is given in[5,6].

APPENDIX A: THE SEMICLASSICAL GREEN'S FUNCTION[4]

Conservation of phase-space volume under classical Hamiltonian time evolution $\mathbf{q}_0 \mapsto \mathbf{q}(t)$ leads to the condition

$$\rho(\mathbf{q}(t), t) = \left|\frac{\partial \mathbf{q}_0}{\partial \mathbf{q}(t)}\right| \rho(\mathbf{q}_0, 0) \tag{A1}$$

on the classical phase-space density $\rho(\mathbf{q}, t)$. This means that the semiclassical ($S/\hbar \to \infty$) approximation, $\psi_{\rm sc}$, to the quantum-mechanical wavefunction should evolve as

$$\psi_{\rm sc}(\mathbf{q}, t) \underset{\text{small } t}{\approx} \sqrt{\frac{\partial \mathbf{q}_0}{\partial \mathbf{q}}}\, e^{\mathrm{i}S(\mathbf{q},\mathbf{q}_0,t)}\, \psi_{\rm sc}(\mathbf{q}_0, 0) \tag{A2}$$

where in the above expression we take t to be small enough that there is a unique classical solution connecting $\mathbf{q}_0$ to $\mathbf{q}$.

If we relax this restriction on t, there will in general be many such classical trajectories, $\{\gamma\}$, connecting $\mathbf{q}_0$ to $\mathbf{q}$; the orientation of $\mathrm{d}\mathbf{q}_0$ need not be consistent among the distinct classical trajectories, so we must take care to keep track of the sign of the Jacobian via

$$\left.\frac{\partial \mathbf{q}_0}{\partial \mathbf{q}}\right|_\gamma = e^{-\mathrm{i}\pi m_\gamma} \left|\frac{\partial \mathbf{q}_0}{\partial \mathbf{q}}\right|_\gamma \tag{A3}$$

where *the Maslov index*, m_γ, denotes the number of conjugate points along γ. We thus have that

$$\psi_{\rm sc}(\mathbf{q}, t) = \int \mathrm{d}\mathbf{q}_0 \sum_{\substack{\text{classical}\\ \text{trajectories}}} \sqrt{\left|\frac{\partial \mathbf{q}_0}{\partial \mathbf{q}}\right|_\gamma}\, e^{\mathrm{i}S_\gamma - \frac{\mathrm{i}\pi}{2} m_\gamma}\, \psi_{\rm sc}(\mathbf{q}_0, 0) \tag{A4}$$

Matching to the usual short time expression for the propagator

$$\begin{aligned} &K(\mathbf{q}, \mathbf{q}_0, t) \\ &\underset{\text{small } t}{\approx} \left(\frac{1}{2\pi \mathrm{i}\hbar}\frac{m}{t}\right)^{\frac{d}{2}} \exp\left[\frac{\mathrm{i}}{\hbar}\left(\frac{m(\mathbf{q}-\mathbf{q}_0)^2}{2t} - V(\mathbf{q})t\right)\right] \\ &\approx \left(\frac{1}{2\pi \mathrm{i}\hbar}\right)^{d/2} \sqrt{\left|\frac{\partial S}{\partial \mathbf{q}\partial \mathbf{q}_0}\right|_\gamma}\, e^{\frac{\mathrm{i}}{\hbar}S(\mathbf{q},\mathbf{q}_0,t)} \end{aligned} \tag{A5}$$

gives the identity

$$K_{\rm sc}(\mathbf{q}, \mathbf{q}_0, t) = \sum_{\substack{\text{classical}\\ \text{trajectories}}} \sqrt{\left|\frac{\partial \mathbf{p}_0}{\partial \mathbf{q}}\right|_\gamma}\, e^{\frac{\mathrm{i}}{\hbar}S_\gamma - \frac{\mathrm{i}\pi}{2} m_\gamma} \tag{A6}$$

here we have used that

$$\left(\frac{m}{t}\right)^d \approx \left|\frac{\partial \mathbf{p}}{\partial \mathbf{q}}\right| = \left|\frac{\partial^2 S}{\partial \mathbf{q}\partial \mathbf{q}_0}\right| \tag{A7}$$

The relation between the Green's function and the propagator

$$G(\mathbf{q}, \mathbf{q}_0, E) = \frac{1}{\mathrm{i}\hbar}\int_0^\infty \mathrm{d}t\, e^{\frac{\mathrm{i}}{\hbar}Et}\, K(\mathbf{q}, \mathbf{q}_0, t) \tag{A8}$$

then tells us that the semiclassical approximation to the Green's function can be expanded as

$$G_{\rm sc}(\mathbf{q}, \mathbf{q}_0, E) = G_0(\mathbf{q}, \mathbf{q}_0, E) + \sum_{\substack{\text{classical}\\ \text{trajectories}}} G_{{\rm sc}(\gamma)}(\mathbf{q}, \mathbf{q}_0, E) \tag{A9}$$

where each $G_{{\rm sc}(\gamma)}$ is given by the one-loop approximation

$$\mathrm{i}\hbar\, G_{{\rm sc}(\gamma)} = \sqrt{\frac{D_s}{(2\pi \mathrm{i}\hbar)^d}}\, e^{\frac{\mathrm{i}}{\hbar}S_\gamma - \frac{\mathrm{i}\pi}{2}\tilde{m}_\gamma} \tag{A10}$$

Here

$$D_s = \det\begin{pmatrix} \dfrac{\partial^2 S}{\partial \mathbf{q}\partial \mathbf{q}_0} & \dfrac{\partial^2 S}{\partial \mathbf{q}\partial E} \\ \dfrac{\partial^2 S}{\partial E\partial \mathbf{q}_0} & 0 \end{pmatrix} \tag{A11}$$

is the one-loop determinant and $\tilde{m}_\gamma$ now includes all the sign flips of $\partial_t^2 S$ as well. This one-loop approximation follows immediately from the standard asymptotics

$$\begin{aligned} &\int \mathrm{d}\mathbf{x}\, A(\mathbf{x})\, e^{\mathrm{i}s\Phi(\mathbf{x})} \\ &\underset{s\to\infty}{\sim} \sum_{\substack{\text{stationary}\\ \text{points } \mathbf{x}_0}} \left(\frac{2\pi \mathrm{i}}{s}\right)^{\frac{d}{2}} \frac{A(\mathbf{x}_0)\, e^{\mathrm{i}s\Phi(\mathbf{x}_0) - \frac{\mathrm{i}\pi}{2}m(\mathbf{x}_0)}}{\sqrt{|\det \Phi''(\mathbf{x}_0)|}} \end{aligned} \tag{A12}$$

(where $m(\mathbf{x}_0)$ counts the number of negative eigenvalues of $\Phi''(x_0)$) and the fact that the stationary point, t_*, of (A8) obeys

$$\partial_t S(\mathbf{q}, \mathbf{q}_0, t_*) = E \tag{A13}$$

The "classical" term

$$\begin{aligned} &\mathrm{i}\hbar G_0(\mathbf{q}, \mathbf{q}_0, E) \\ &= \int_0^\infty \mathrm{d}t \left(\frac{m}{2\pi \mathrm{i}\hbar t}\right)^{\frac{d}{2}} \exp\left[\frac{\mathrm{i}}{\hbar}\left((E - V(\mathbf{q}))\, t + \frac{(\mathbf{q}-\mathbf{q}_0)^2}{2t}\right)\right] \end{aligned} \tag{A14}$$

encodes the contributions to G_{sc} from "short" ($T_\gamma \lesssim E/\hbar$) trajectories not covered by the stationary phase method (which requires $t_* \gg E/\hbar$).

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