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Displacement Echoes: Classical Decay and Quantum Freeze

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Motivated by neutron scattering experiments, we investigate the decay of the fidelity with which a wave packet is reconstructed by a perfect time-reversal operation performed after a phase space displacement. In the semiclassical limit, we show that the decay rate is generically given by the Lyapunov exponent of the classical dynamics. For small displacements, we additionally show that, following a short-time Lyapunov decay, the decay freezes well above the ergodic value because of quantum effects. Our analytical results are corroborated by numerical simulations.

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The fidelity with which a wavefunction is reconstructed after an imperfect time-reversal operation was originally introduced as a measure of reversibility in quantum mechanics [1]. Re-dubbed the Loschmidt Echo, it has received much attention in recent years in the context of decoherence and the quantum classical correspondence [2, 3, 4, 5, 6]. For a generic perturbation of the Hamiltonian, four different decay regimes were found: the Gaussian perturbative regime, the Fermi Golden Rule (FGR) regime, the Lyapunov regime, and the regime of classically large perturbations. Of special interest is the Lyapunov regime where the purely quantum mechanical fidelity decays with the Lyapunov exponent of the classical dynamics. It suggests the existence of a universal regime of environment-independent decoherence rate [2, 7, 8].

In this letter we analyze the decay of the Loschmidt echo under a new, non-generic perturbation, namely an instantaneous phase space displacement. Our investigations are mostly motivated by neutron scattering experiments where the phase space displacement is a momentum boost [9], but also to some extent by electronic transitions in molecules and solids, where the displacement is along the position axis, with very little change in the potential [10, 11]. Under this non-generic perturbation, we find that the decay rate of the fidelity is always set by the Lyapunov exponent. Moreover, for small displacements, the initial Lyapunov decay is followed at larger times by a quantum freeze of the fidelity at a displacement-dependent saturation value. The freeze persists up to infinitely large times.

As our starting point, we recall that the differential cross section for incoherent neutron scattering can be calculated from the following correlation function [12, 13] (from now on we set $\hbar \equiv 1$)

$$Y_{jj}\left(\mathbf{P},\mathbf{t}\right) = \left\langle e^{-i\mathbf{P}\cdot\hat{\mathbf{r}}_{\mathbf{j}}} e^{i\hat{H}t} e^{i\mathbf{P}\cdot\hat{\mathbf{r}}_{\mathbf{j}}} e^{-i\hat{H}t}\right\rangle. \quad (1)$$

Here, the brackets represent an ensemble average, $\hat{\mathbf{r}}_{\mathbf{j}}$ are the position operators of the nuclei and $\hat{H}$ is the typical Hamiltonian of the target system. The ensemble average of the correlation function can be written [9]:

$$Y_{jj}\left(\mathbf{P},\mathbf{t}\right) \approx \frac{1}{Q}\int\left(\frac{d^{2N}\alpha}{\pi^N}\right)\Phi\left(\alpha\right) \times \left\langle\alpha\right| e^{-i\mathbf{P}\cdot\hat{\mathbf{r}}_{\mathbf{j}}} e^{i\hat{H}t} e^{i\mathbf{P}\cdot\hat{\mathbf{r}}_{\mathbf{j}}} e^{-i\hat{H}t}\left|\alpha\right\rangle, \quad (2)$$

where $|\alpha\rangle$ are coherent states with N degrees of freedom, $Q = \mathrm{Tr}\left[e^{-\beta\hat{H}}\right]$, and $\Phi\left(\alpha\right)$ is a thermal weight, which tends to $e^{-\beta H_{cl}(\alpha)}$ at high temperatures. The notation $e^{i\hat{H}_{\mathbf{P}}t} = e^{-i\mathbf{P}\cdot\hat{\mathbf{r}}_{\mathbf{j}}} e^{i\hat{H}t} e^{i\mathbf{P}\cdot\hat{\mathbf{r}}_{\mathbf{j}}}$ suggests that we identify the kernel of the integral $I\left(t\right) = \left\langle\alpha\right| e^{-i\mathbf{P}\cdot\hat{\mathbf{r}}_{\mathbf{j}}} e^{i\hat{H}t} e^{i\mathbf{P}\cdot\hat{\mathbf{r}}_{\mathbf{j}}} e^{-i\hat{H}t}\left|\alpha\right\rangle$ with the kernel of a Loschmidt echo problem, we thus introduce the momentum *displacement echo*

$$M_{\mathrm{D}}\left(t\right) = |I(t)|^2 = \left|\left\langle\alpha\right| e^{i\hat{H}_{\mathbf{P}}t} e^{-i\hat{H}t}\left|\alpha\right\rangle\right|^2. \quad (3)$$

As introduction to our semiclassical calculation of the displacement echo $M_{\mathrm{D}}(t)$, we first discuss the validity of the diagonal approximation used in Ref. [2] for the semiclassical approach to the Loschmidt echo and point out why this approximation is even better for the displacement echo. The diagonal approximation for the Loschmidt echo equates each classical trajectory γ generated by an unperturbed Hamiltonian H with a classical trajectory γ_V generated by a perturbed Hamiltonian $H_V = H + V$. This procedure is not justified a priori in chaotic systems where one expects that an infinitesimally small perturbation generates trajectories diverging exponentially fast taway from their unperturbed counterpart. It was however pointed out by Cerruti and Tomsovic [4], and later by Vaniček and Heller [5], that structural stability theorems [14, 15] justify this approximation. Roughly speaking one can show that, given a uniformly hyperbolic Hamiltonian system H, and a generic perturbation V, each classical trajectory γ'_V generated by the (still hyperbolic) perturbed Hamiltonian $H + V$ is almost always arbitrarily close to one unperturbed trajectory γ.

In general, however, the two trajectories do not share common endpoints. This is illustrated in the left panel of Fig. 1. The semiclassical expression for the kernel of the Loschmidt echo involves a double sum over both the perturbed and the unperturbed classical trajectories, so that both γ'_V and γ are included. After a stationary phase condition, this double sum is reduced to a single sum where γ'_V and γ are equated. In other words, a semiclassical particle follows γ in the forward direction, and γ'_V in the backward direction because this is the best way to minimize the action. The action difference is simply given by the integral of the perturbation along the backward trajectory, and it is in general time-dependent.

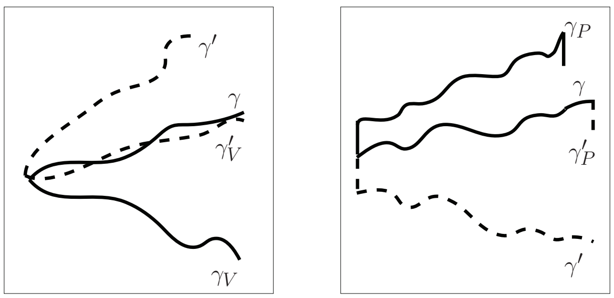

FIG. 1: Illustrative view of structural stability. Left panel: generic perturbations. γ and γ' are two orbits of the unperturbed Hamiltonian, γ_V is the orbit of the perturbed Hamiltonian with the same initial condition as γ, while γ'_V is the orbit of the perturbed Hamiltonian with the same initial condition as γ'. Right panel: phase space displacements. Labels are the same as in the left panel, with $\mathbf{P}$ replacing V as subscript for perturbed trajectories. Note that $\gamma'_\mathbf{P}$ and γ lie on top of each other.

In the present case of a uniform phase-space displacement, the diagonal approximation becomes exact. This is so because any classical trajectory of the unperturbed Hamiltonian is obviously also a trajectory of the perturbed Hamiltonian, up to displacements at both ends of the trajectory. This is illustrated in the right panel of Fig. 1. The fact that the action difference is here time-independent has the important consequence that the FGR decay is replaced by a time-independent saturation term. The Lyapunov decay term is left almost unaffected, as it depends on the classical measure of nearby trajectories with perturbed initial conditions and does not depend on quantum action phases. We also note that for displacement echoes there is no Gaussian perturbative decay, since phase space displacements do not change the spectrum of the system aside from some possible but irrelevant global shift.

For a quantitative approach to the problem, we semiclassically evaluate $M_\mathrm{D}(t)$ for the case of an initial Gaussian wavepacket, $\langle \mathbf{r} \mid \alpha(\mathbf{r}_0, \mathbf{q}_0) \rangle = \left(\pi\sigma^2\right)^{-\frac{d}{4}} \exp[i\mathbf{p}_0 \cdot (\mathbf{r}-\mathbf{r}_0) - (\mathbf{r}-\mathbf{r}_0)^2/2\sigma^2]$. Following Ref. [16], we semiclassically propagate $|\alpha\rangle$ with the help of the van Vleck propagator, linearly expanding around $\mathbf{r_0}$:

$$\langle \mathbf{r}' | \, e^{-i\hat{H}t} \, |\alpha\rangle_\mathrm{sc} \simeq \left(-\frac{i\sigma}{\sqrt{\pi}}\right)^{\frac{d}{2}} \times \sum_\gamma \sqrt{C_\gamma} \exp[iS_\gamma - i\pi\nu_\gamma/2 - \sigma^2 \left(\mathbf{p}_\gamma - \mathbf{p}_0\right)/2]. \tag{4}$$

Here, the sum runs over all possible classical trajectories γ connecting $\mathbf{r}_0$ and $\mathbf{r}'$ in the time t, $\mathbf{p}_\gamma = -\partial S_\gamma/\partial\mathbf{r}|_{\mathbf{r}=\mathbf{r}_0}$ is the initial momentum on γ, S_γ is the classical action accumulated on γ, ν_γ is the Maslov index and $C_\gamma = \left|-\partial^2 S_j\left(\mathbf{r}, \mathbf{r}'; t\right)/\partial r_i \partial r'_\gamma\right|_{\mathbf{r}=\mathbf{r}_0}$. The kernel $I(t)$ of $M_\mathrm{D}(t)$ involves a double sum over classical trajectories, γ and γ', and can be interpreted as the overlap between a wavepacket that is boosted and subsequently propagated with a wavepacket that is first propagated and subsequently boosted [9]. Enforcing a stationary phase condition kills all but the contributions with the smallest actions. They correspond to $\gamma = \gamma'$ and one has

$$I(t) = \left(-\frac{\sigma^2}{\pi}\right)^{\frac{d}{2}} \int \mathrm{d}\mathbf{r}' \sum_\gamma e^{i\mathbf{P}\cdot(\mathbf{r}'+\mathbf{r}_0)} \, C_\gamma \times \exp - \frac{\sigma^2}{2}\Big[\left(\mathbf{p}_\gamma - \mathbf{p}_0\right)^2 + \left(\mathbf{p}_\gamma - \mathbf{p}_0 - \mathbf{P}\right)^2 \Big]. \tag{5}$$

Taking the squared amplitude $|I(t)|^2$ one obtains the semiclassical expression for the displacement echo

$$\begin{aligned} M_\mathrm{D}(t) &= \left(\frac{\sigma^2}{\pi}\right)^d \int \mathrm{d}\mathbf{r} \, \mathrm{d}\mathbf{r}' \sum_{\gamma,\gamma'} e^{i\mathbf{P}\cdot(\mathbf{r}-\mathbf{r}')} \, C_\gamma \, C_{\gamma'} \\ &\times \; \exp - \frac{\sigma^2}{2}\Big[\left(\mathbf{p}_\gamma - \mathbf{p}_0\right)^2 + \left(\mathbf{p}_\gamma - \mathbf{p}_0 - \mathbf{P}\right)^2 \Big] \\ &\times \; \exp - \frac{\sigma^2}{2}\Big[\left(\mathbf{p}_{\gamma'} - \mathbf{p}_0\right)^2 + \left(\mathbf{p}_{\gamma'} - \mathbf{p}_0 - \mathbf{P}\right)^2 \Big]. \end{aligned} \tag{6}$$

We calculate $\langle M_\mathrm{D}(t) \rangle$, the ensemble-averaged displacement echo over a set of initial Gaussian wavepackets with varying center of mass $\mathbf{r}_0$. There are two qualitatively different contributions to $\langle M_\mathrm{D}(t) \rangle$. The first contribution $\langle M_\mathrm{D}(t) \rangle_\mathrm{c}$ comes from pairs $\gamma \approx \gamma'$ of correlated trajectories that remain within a distance $\lesssim \sigma$ of each other for the whole duration t of the experiment, while the second contribution $\langle M_\mathrm{D}(t) \rangle_\mathrm{u}$ arises from pairs of uncorrelated trajectories (γ, γ'). For the first contribution, we write $\exp[i\mathbf{P}(\mathbf{r}-\mathbf{r}')] \approx 1$, which is true in the semiclassical limit where $\sigma \to 0$, and set $\gamma = \gamma'$. One then has

$$\langle M_\mathrm{D}(t) \rangle_\mathrm{c} = \left(\frac{\sigma^2}{\pi}\right)^d \int \mathrm{d}\mathbf{r}\mathrm{d}\mathbf{r}' \, \delta_\sigma(\mathbf{r}-\mathbf{r}') \times \sum_\gamma C_\gamma^2 \, e^{-\sigma^2\left[(\mathbf{p}_\gamma - \mathbf{p}_0)^2 + (\mathbf{p}_\gamma - \mathbf{p}_0 - \mathbf{P})^2\right]}, \tag{7}$$

where $\delta_\sigma(\mathbf{r}-\mathbf{r}')$ restricts the integrals to $|\mathbf{r}-\mathbf{r}'| \leq \sigma$. The calculation of (7) is straightforward. The integral over $\mathbf{r}'$ gives a factor σ^d. One then replaces one C_γ by its asymptotic value, $C_\gamma \propto \exp[-\lambda t]$, and uses the second C_γ to perform a change of integration variable $\int \mathrm{d}\mathbf{r} \sum_\gamma C_\gamma = \int \mathrm{d}\mathbf{p}$. After a Gaussian integration, one finally gets the correlated contribution to $\langle M_\mathrm{D}(t)\rangle$ as

$$\langle M_\mathrm{D}(t)\rangle_\mathrm{c} \;=\; \alpha \, \exp[-(\mathbf{P}\sigma)^2/2] \, \exp[-\lambda t]. \qquad (8)$$

Here, α is a weakly time-dependent number of order one [2].

For the uncorrelated part, an ergodicity assumption is justified at sufficiently large times, under which one gets

$$\langle M_\mathrm{D}(t)\rangle_\mathrm{u} \;=\; f(\mathbf{P}) \, \langle \tilde{M}_\mathrm{D}(t)\rangle_\mathrm{u}, \qquad (9a)$$

$$f(\mathbf{P}) \;=\; \frac{1}{\Omega^2} \int \mathrm{d}\mathbf{r}\mathrm{d}\mathbf{r}' \exp[i\mathbf{P}\cdot(\mathbf{r}-\mathbf{r}')], \qquad (9b)$$

$$\langle \tilde{M}_\mathrm{D}(t)\rangle_\mathrm{u} \;=\; \left(\frac{\sigma^2}{\pi}\right)^d \Big(\int \mathrm{d}\mathbf{x} \sum_\gamma C_\gamma \qquad (9c)$$

$$\times \; \exp -\frac{\sigma^2}{2}\Big[\,(\mathbf{p}_\gamma-\mathbf{p}_0)^2 + (\mathbf{p}_\gamma-\mathbf{p}_0-\mathbf{P})^2\,\Big]\Big)^2,$$

with the system's volume $\Omega \propto L^d$. It is straightforwardly seen that $\langle \tilde{M}_\mathrm{D}(t)\rangle_\mathrm{u} = \exp[-(\mathbf{P}\sigma)^2/2]$, and $f(\mathbf{P}) = g(|\mathbf{P}|L)/(|\mathbf{P}|L)^2$, in term of an oscillatory function $g(|\mathbf{P}|L) = 4\sin^2(|\mathbf{P}|L/2)$ for $d=1$ and $g(|\mathbf{P}|L) = 4J_1^2(|\mathbf{P}|L)$ for $d=2$. For $d=3$, g is given by Bessel and Struve functions. The uncorrelated contribution to the displacement echo reads

$$\langle M_\mathrm{D}(t)\rangle_\mathrm{u} \;=\; \exp[-(\mathbf{P}\sigma)^2/2] \; g(|\mathbf{P}|L)\Big/(|\mathbf{P}|L)^2, \qquad (10)$$

which, together with Eq. (8) gives the average displacement echo as

$$\langle M_\mathrm{D}(t)\rangle = \exp[-(\mathbf{P}\sigma)^2/2] \, \left[\alpha \, e^{-\lambda t} + \frac{g(|\mathbf{P}|L)}{(|\mathbf{P}|L)^2}\right]. \qquad (11)$$

In addition, as is the case for Loschmidt echoes, $\langle M_\mathrm{D}(t)\rangle \geq N^{-1}$ where N is the size of Hilbert space.

Eq. (11) is our main result. It states that $M_\mathrm{D}(t)$ is the sum of a time-dependent decaying term of classical origin and a time-independent term of quantum origin. The prefactor $\exp[-(\mathbf{P}\sigma)^2/2] \to 1$ in the semiclassical limit and is thus of little importance. We see that generically, $M_\mathrm{D}(t)$ follows a classical exponential decay, possibly interrupted by a quantum freeze as long as the displacement is not too large, $g(|\mathbf{P}|L)\Big/(|\mathbf{P}|L)^2 > N^{-1}$ [17]. We note that in the semiclassical limit, $M_\mathrm{D}(t\to 0) \to 1$, because of the saturation of $\alpha(t \to 0) \to 1$ and the disappearance of uncorrelated contributions at short times. Most importantly, there is no displacement-dependent decay, i.e. no counterpart to the FGR decay nor the perturbative Gaussian decay for $M_\mathrm{D}(t)$, because phase-space displacements leave the spectrum unchanged, up to a possible homogeneous shift [18].

We numerically check our predictions. We specialize to the kicked rotator model with Hamiltonian

$$H_0 = \frac{\hat{p}^2}{2} + K\cos\hat{x} \sum_n \delta(t-n). \qquad (12)$$

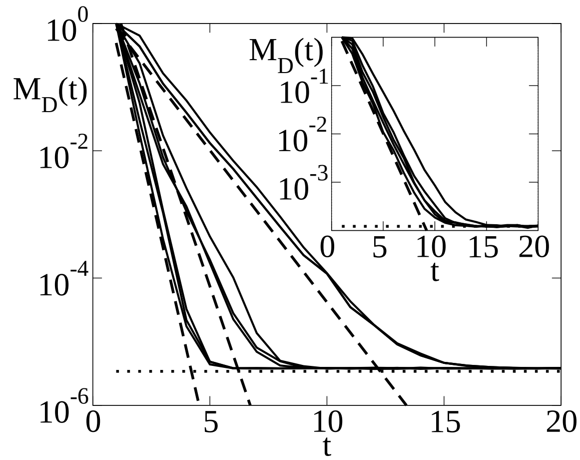

FIG. 2: Main plot : Displacement echo $M_\mathrm{D}(t)$ for the kicked rotator model with $N = 262144$, and displacements $P = m \times 2\pi/N$, $m = 10$, 20, 30. Averages have been performed over a set of 10000 different initial coherent states. The full lines correspond to kicking strengths $K = 10.09$, 50.09 and 200.09 (from right to left) and the dashed lines (slightly shifted for clarity) give the predicted exponential decay given by the reduced Lyapunov exponent $\lambda_0 = 1.1$, 2.5, 3.7. The dotted line gives the saturation at N^{-1}. Inset : Displacement echo for $N = 8192$, $K = 10.09$, and displacements $P = 2\pi/N, 4\pi/N, \ldots 10\pi/N$. Data are obtained from 1000 different initial coherent states. The dashed line gives the predicted exponential decay given by the reduced lyapunov exponent $\lambda_0 = 1.1$. The dotted line gives the minimal saturation value at N^{-1}.

We focus on the regime $K > 7$, for which the dynamics is fully chaotic with Lyapunov exponent $\lambda = \ln[K/2]$. We quantize this Hamiltonian on a torus, which requires to consider discrete values $p_l = 2\pi l/N$ and $x_l = 2\pi l/N$, $l = 1, \ldots N$. In these units, one has $L = N$. The displacement echo of Eq. (3) is computed for discrete times $t = n$, as

$$M(n) = \left|\langle\psi_0| \exp^{-iP\hat{x}} \left(\mathcal{U}^\dagger\right)^n \exp^{iP\hat{x}} \left(\mathcal{U}\right)^n |\psi_0\rangle\right|^2, \qquad (13)$$

with $P = |\mathbf{P}|$. Here, we used the unitary Floquet time-evolution operator $\mathcal{U}$ whose matrix elements in $x-$representation are given by

$$\mathcal{U}_{l,l'} \;=\; \frac{1}{\sqrt{N}} \exp\left[i\frac{\pi(l-l')^2}{N}\right] \exp\left[-i\frac{NK}{2\pi}\cos\frac{2\pi l'}{N}\right].$$

Numerically, the time-evolution of ψ_0 in Eq. (13), is calculated by recursive calls to a fast-Fourier transform routine, which allowed us to reach very large system sizes up to $N = 262144 = 2^{18}$.

Fig. 2 shows the behavior of the echo for displacements in the range $P \gg 2\pi/N$ for which $\langle M_\mathrm{D}(t)\rangle_\mathrm{u} \ll N^{-1}$ and thus plays no role. It is seen that the decay rate of the displacement echo strongly depends on the kicking strength K, but is largely independent of the displacement P. We quantitatively found that in that regime,

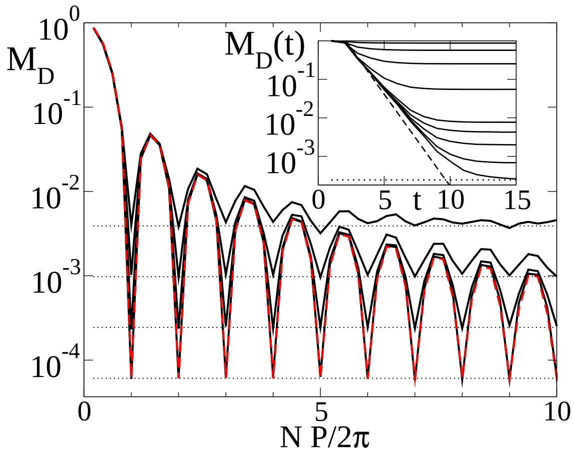

FIG. 3: (color online) Main plot: Saturation value $M_{\rm D}(\infty)$ of the displacement echo as a function of the rescaled displacement $NP/2\pi$ for the kicked rotator model with $N = 256$, 1024, 4096, 16384 (full lines, from top to bottom). Data are obtained from 1000 different initial coherent states. The dotted lines give the saturation at N^{-1}. The red dashed line gives the theoretical prediction $M_{\rm D}(\infty) = {\rm Max}(4\exp[-(\sigma P)^2/2]\sin^2(PL/2)\big/(PL)^2, N^{-1})$ for $N = 16384$. Inset: Quantum freeze of the displacement echo for kicking strength $K = 10.09$, $N = 4096$, and $P \in [0, 2\pi/N]$. The dashed line gives the decay with the reduced Lyapunov exponent $\lambda_0 = 1.1$ (see text).

$M_{\rm D}(t) \approx \exp[-\lambda_0 t]$, in term of the reduced Lyapunov exponent λ_0 [19]. The inset shows moreover, that lowering the displacement to the regime $P = m2\pi/N$ with $m \leq 5$ does not affect the decay rate of $M_{\rm D}(t)$, i.e. there is no FGR decay for the displacement echo.

We focus in Fig. 3 on smaller displacements $P \leq 2\pi/N$. The behavior of $\langle M_{\rm D}(t)\rangle$ clearly satisfies Eq. (11), with a quantum freeze at a displacement-dependent value following a decay with a slope given by the Lyapunov exponent. We show in the main panel the P-dependence of the value at which $M_{\rm D}(t)$ freezes. The data unambiguously confirm the algebraically damped oscillations predicted in Eq. (8).

In summary, we have presented a semiclassical calculation of phase-space displacement echoes. We showed that they are generically given by the sum of a classical decay and a quantum freeze term (11). Because phase-space displacements do not generate time-dependent action differences, and because they vanish in first order perturbation theory, there is no other time-dependent decay, in contrast to Loschmidt echoes [1, 2, 3, 4, 5].

To conclude, we note that neutron scattering correlation functions are given by the average $\langle I(t)\rangle$ of the kernel of $M_{\rm D}(t)$. Starting back from Eq. (5), one gets

$$|Y_{jj}\,(\mathbf{P},\mathbf{t})\,| \simeq \exp[-(\mathbf{P}\sigma)^2/4]\,\frac{g^{1/2}(|\mathbf{P}|L)}{|\mathbf{P}|L}, \qquad (14)$$

i.e. $|Y_{jj}|$ is given by the quantum freeze term only. This is so, since the correlations between pairs of trajectories that are necessary for the existence of the Lyapunov term appear only once $I(t)$ is squared. The Lyapunov decay is in this sense similar to diffuson and cooperon correlators in disordered electronic systems, which appear in averages over *products* of Green's functions, but cannot be traced back to the impurity-averaged Greens function.

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