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Spectral signatures of chaotic diffusion in systems with and without spatial order

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Abstract

We investigate the two-point correlations in the spectra of extended systems exhibiting chaotic diffusion in the classical limit, in presence and in absence of spatial order. For periodic systems, we express the spectral two-point correlations in terms of form factors with the unit-cell index as a discrete spatial argument. For times below the Heisenberg time, they contain the full space–time dependence of the classical propagator. They approach constant asymptotes via a regime of quantum ballistic motion. In the opposite regime of strong disorder with localized eigenstates, we derive a semiclassical approximation of the form factor that spans the entire transition from metallic to isolating behaviour. The regime of weak breaking of periodicity is accessed from the side of exact order by a perturbation theory for the sets of, without disorder, symmetry-related periodic orbits. © 2001 Elsevier Science B.V. All rights reserved.

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Applying quantum chaos to the physics of disordered solids could merely mean to replace static disorder by chaotic dynamics, as an alternative model of randomness. Here, we think of a theory of classically chaotic motion in extended quantum systems, *simultaneously present* with order or disorder in the potential. On the classical level, this faces us with a notion that does not apply to either bound or scattering systems: chaotic (deterministic) diffusion. In quantum mechanics, the presence or absence of spatial translation symmetry determines whether the eigenstates are extended or localized and thus whether the spectrum is continuous or discrete. Classical and quantum features are relevant on different time scales. A comprehensive theory should therefore contain the crossover, in time, from quasiclassical diffusion to either ballistic, Bloch-tunneling-like motion or to localization.

Our approach is largely based on semiclassical methods. We attempt, in particular, to understand the signatures of chaotic diffusion in the two-point correlations of the quantum spectrum. The application to extended systems requires a refinement of the semiclassical tools: In order to relate spectral

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correlations to classical quantities, we reduce double sums over periodic orbits by means of the diagonal approximation, based on the distinction between pairs of identical and of different orbits. This distinction becomes ambiguous for systems with an exact or approximate spatial symmetry. We show how to systematically account for all pairs of symmetry-related, but non-identical periodic orbits in the spectral statistics. As a surplus, we thus gain a coarse-grained *spatial* resolution of the spectral form factor.

Dealing with disordered systems, we need a relation between spectral statistics and classical mechanics that also on the classical side, is based on statistical quantities rather than individual periodic orbits. We first Fourier transform from the spectral density $d(E)$ to a time-domain quantity, $a(t) = \mathrm{tr}[\hat{U}(t,0)] = \int \mathrm{d}q\, K(\boldsymbol{q},t;\boldsymbol{q},0)$. It can be interpreted as an amplitude to return. A semiclassical approximation is achieved by replacing the quantum propagator $K(\boldsymbol{q}',t;\boldsymbol{q},0)$ with the van-Vleck propagator. Squaring, we arrive at a return *probability*, expressed as a double sum over periodic orbits. As the crucial steps of our approach, we neglect the off-diagonal terms in the sum expressing quantum interferences [1], and generalize the Hannay–Ozorio de Almeida sum rule [2] to establish a relation between the spectral two-point correlations and the probability to return for the corresponding classical dynamics [1,3],

$$K(\tau) = \begin{cases} \gamma\tau P(\tau t_{\mathrm{H}}) & \text{chaotic systems,} \\ \gamma P(\tau t_{\mathrm{H}}) & \text{integrable systems.} \end{cases} \tag{1}$$

Here, $K(\tau) = (1/\Delta r)\langle |a(\tau) - \delta_{1/\Delta r}(\tau)|^2\rangle$ is the spectral form factor, the Fourier transform of the spectral cluster function [3]. $P(\tau t_{\mathrm{H}})$ is a classical return probability, normalized so that $\lim_{t\to\infty} P(t) = 1$. We employ dimensionless times τ and energies r in units of the Heisenberg time $t_{\mathrm{H}} = 2\pi\hbar\langle d\rangle$ and the inverse mean spectral density $1/\langle d\rangle$, respectively. The finite total extension $\Delta r \gg 1$ of the spectrum should be narrow on classical scales. It results in a finite temporal resolution $1/\Delta r$. Presence or absence of time-reversal symmetry enters via a degeneracy factor, $\gamma = 2$ or 1, respectively.

An immediate application of Eq. (1) is one-dimensional systems with static disorder [3]. Here, $P(t)$ is obtained from a solution of the classical diffusion equation with Neumann boundary conditions. Its asymptotes are

$$P(t) = \begin{cases} \sqrt{t_{\mathrm{d}}/2t} & t \ll t_{\mathrm{d}} \quad \text{(free diffusion),} \\ 1 & t \gg t_{\mathrm{d}} \quad \text{(saturation).} \end{cases} \tag{2}$$

The Thouless (diffusion) time $t_{\mathrm{d}} = L^2/\pi D$, with L, the overall length of the system, and the diffusion constant D, establishes a classical time scale independent of t_{H}. The spectral statistics is determined solely by their ratio, the dimensionless conductance $g = t_{\mathrm{H}}/t_{\mathrm{d}} \sim \xi/L$, where ξ is the mean localization length. Inserting Eq. (2) into Eq. (1), we obtain for the form factor (in the unitary case) [3],

$$K(\tau) = \begin{cases} \sqrt{\tau/2g} & \text{regime 1,} \\ \tau & \text{regime 2,} \\ 1 & \text{regime 3.} \end{cases} \tag{3}$$

In the case of *weak disorder*, $g > 1/2$, free diffusion (regime 1) saturates beyond $\tau \approx 2/g$ (regime 2). For *strong disorder*, $g < 1/2$, diffusion is limited by localization at $\tau \approx 2g$, regime 2 is never reached. The quantum long-time asymptote where the discreteness of the spectrum is resolved and $K(\tau)$ saturates (regime 3), is approached for $\tau \gg 1$ and $\tau \gg 2g$ in the respective two limits. It is not obtained from our semiclassical approach, but connected "by hand" to the short-time regime by extrapolation to the point of intersection. Eq. (3) interpolates between the spectral statistics of the GUE for $g \gg 1$, the metallic limit, and Poissonian statistics in the isolating limit $g \ll 1$.

In spatially periodic systems (we assume a finite chain of N unit cells with cyclic boundary conditions), the presence of a unitary symmetry allows to order the spectrum according to the associated conserved quantity, the Bloch angle $\theta_m = 2\pi m/N$ (or quasimomentum $k_m = \hbar\theta_m N/a$), $a = L/N$, $m = 0, \ldots, N-1$. Restricting the spectral statistics to the representation-specific subspectra, however, discards information contained in the correlations *across* the Brillouin zone. We therefore perform, on top of the transformation to the time domain that results in amplitudes $\tilde{a}_m(\tau)$, a discrete Fourier transformation from the quasimomentum to the unit-cell-number space [4]. The corresponding amplitude $a_n(\tau) = N^{-1}\sum_{m=0}^{N-1} \exp(\mathrm{i}n\theta_m)\tilde{a}_m(\tau) = \int_{\text{unit cell}} \mathrm{d}q\, K(\boldsymbol{q} + n\boldsymbol{a}, \tau t_{\mathrm{H}}; \boldsymbol{q}, 0)$ now refers to returning only up to shifts by integer multiples of $\boldsymbol{a}$, the vector generating the discrete translation group. The semiclassical expressions for the representation-specific density [5] carry Bloch factors $\exp(\mathrm{i}n_j\theta_m)$

as additional, non-classical phases. The integer n_j is the number of times a generalized periodic orbit runs around the unit cell before returning, i.e., a winding number. By transforming to the unit-cell-number domain, the Bloch factor is converted to a Kronecker delta that restricts the orbits contributing to $a_n(\tau)$ to those with $n_j = n$. Proceeding along similar lines as above, we obtain as a generalization of Eq. (1) [6,7],

$$K_n(\tau) = \gamma_n \tau P_n(\tau t_{\mathrm{H}}), \tag{4}$$

where $P_n(t) = \int_{\text{unit cell}} \mathrm{d}q\, K^{\mathrm{cl}}(\boldsymbol{q} + n\boldsymbol{a}, t; \boldsymbol{q}, 0)$ is the winding-number distribution. The degeneracy γ_n now takes the value 2 at points of twofold symmetry of the lattice and 1 else. With the classical propagator $K^{\mathrm{cl}}(\boldsymbol{q}', t; \boldsymbol{q}, 0)$, the generalized form factors contain the full spatio-temporal information on the classical spreading, coarse grained on the scale of the lattice constant. In the present case, they are given by $K_n(\tau) = \gamma_n \tau \mathrm{Ga}^{(\mathrm{mod}\, N)}(n, g_{\mathrm{uc}}\tau)$, with $\mathrm{Ga}^{(\mathrm{mod}\, p)}(x, \Delta)$ a normalized Gaussian of period p and width Δ. The appropriate scaling parameter here, $g_{\mathrm{uc}} = N^2 t_{\mathrm{H}}/t_{\mathrm{d}}$, is a conductance per unit cell, where t_{H} now refers to the density of *bands*. If $g_{\mathrm{uc}} \gg N^2$, classical spreading saturates before t_{H}. The discreteness of the spectrum is then too coarse to resolve the band structure. Only for $g_{\mathrm{uc}} \ll N^2$, the "weak-coupling" or "tight-binding" limit, proper bands are formed, reflected in the central form factor $K_0(\tau)$ as a marked peak at $\tau = 1$. The case $N = 2$ – systems with two identical, weakly coupled cells – is extreme but has a wide range of applications [8].

In order to understand the behaviour of the $K_n(\tau)$ beyond the unit-cell Heisenberg time, we calculate the $a_n(\tau)$ in an approximation that becomes exact in the long-time limit [7]. It requires stationarity of phases $2\pi r_\alpha(\theta)\tau - (n \bmod N)\theta$ with respect to the Bloch angle θ, where $r_\alpha(\theta)$ are the exact bands. This condition amounts to a *ballistic* spreading of wavepackets, with a velocity $\sim \mathrm{d}r_\alpha/\mathrm{d}\theta$. For $g_{\mathrm{uc}} \ll N^2$, it implies a decay of $K_0(\tau)$ by a factor N, before the spreading saturates and the form factors reach their asymptotic values γ_n/N. The peak at $\tau = 1$ and $n = 0$ reflects the strong correlation of levels due to the formation of bands. The theoretical $K_n(\tau)$ are shown in Fig. 1a and compared to data for the kicked rotor on a torus [9] in Fig. 1b.

The definition of generalized form factors and periodic orbits allows us to systematically include pairs

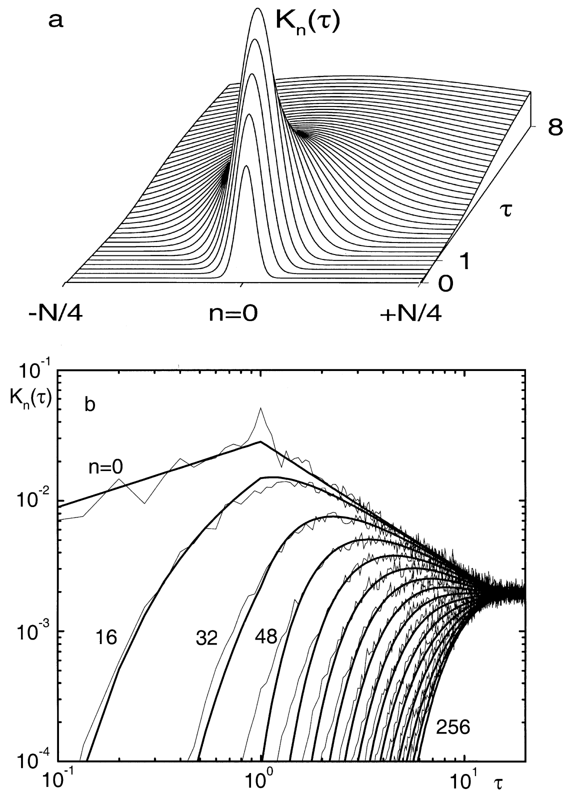

Fig. 1. (a) Space–time dependence of the theoretical prediction for $K_n(\tau)$, (b) form factors $K_n(\tau)$ for the kicked rotor on a torus at selected values of n, compared to the theory (heavy lines). In both panels, $N = 512$ and $g_{\mathrm{uc}} = 200\pi$.

of symmetry-related orbits. It suggests itself to extend this idea to systems with weakly broken translational symmetry where periodic orbits can still be ordered in N-fold quasidegenerate sets, i.e., where their topology remains intact. We then replace amplitudes by their unperturbed values, and treat the action shifts $\Delta S_{j,n} = S'_{j,n} - S_j$, of periodic orbit j in unit cell n, as perturbations. Assuming the $\Delta S_{j,n}$ to be Gaussian random variables with zero mean and variance $\langle (\Delta S)^2 \rangle = \sigma^2 \tau$, σ measuring the deviation from symmetry, we obtain [10]

$$K_{\mathrm{pert}}(\tau, \sigma) = K_0(\tau) \left(N^{-1} + (1 - N^{-1})\, \mathrm{e}^{-\sigma^2 \tau} \right). \tag{5}$$

Eq. (5) describes the decay of the peak in the unperturbed form factor due to the gradual disintegration of the bands with disorder. It fills the gap between the weak-disorder limit of Eqs. (3) and (4), but constitutes a regime of its own, outside the one-parameter scaling of the disordered case: In addition to the (static or dynamic!) disorder *within* the unit cell, characterized by g_{uc}, we here have the (static) breaking of symmetry *among* the cells, measured by σ. Due to its perturbative nature, Eq. (5) does not account for localization.

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