Number of propagating modes of a diffusive periodic waveguide in the semiclassical limit

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We study the number of propagating Bloch modes N_B of an infinite periodic billiard chain. The asymptotic semiclassical behavior of this quantity depends on the phase-space dynamics of the unit cell, growing linearly with the wave number k in systems with a non-null measure of ballistic trajectories and going like $\sim \sqrt{k}$ in diffusive systems. We have calculated numerically N_B for a waveguide with cosine-shaped walls exhibiting strongly diffusive dynamics. The semiclassical prediction for diffusive systems is verified to good accuracy and a connection between this result and the universality of the parametric variation of energy levels is presented.

I. INTRODUCTION

According to the Bohigas-Giannoni-Schmit conjecture [1], a system with chaotic phase-space dynamics is expected to show universal quantum level statistics in the semiclassical limit, consistent with the predictions of random matrix theory (RMT). For instance, the two-point level correlation of closed chaotic systems has been shown experimentally and numerically to agree with the Gaussian orthogonal ensemble (Gaussian unitary ensemble) for systems with (without) time-reversal symmetry [2,3]. Analytical results supporting this universality have also been achieved using the semiclassical trace formula, first by means of the diagonal approximation and more recently including nondiagonal terms verifying full agreement of the semiclassical form factor with RMT [4].

Much less is known for spatially extended chaotic systems. In the case of systems that relax by a diffusion process, the spectral properties deviate from random matrix theory in a particular way. Dittrich *et al.* [5,6] considered the statistical properties of the energy bands $E_{n,\theta}$ of a closed periodic diffusive system with N chaotic unit cells and analyzed the signatures of chaotic diffusion in the form factor (the Fourier transform of the two-point level correlation function). They showed that their semiclassical results agree nicely with those of Simons and Altshuler [7,8] who proposed that the fluctuations of the energy bands $E_{n,\theta}$ or in fact any parametric variation of the energy levels is universal within the appropriate Dyson ensemble (depending on time-reversal symmetry). Simons and Altshuler calculated the universal two-point level correlation function for a disordered system under the influence of an external perturbation—for instance, in the form of an Aharonov-Bohm flux—and showed that the response of the spectrum to those parameter variations was universal after a suitable scaling with two system specific

parameters. Dittrich *et al.* [5,6] identified one of these parameters with the diffusion coefficient of the chain.

These correlation functions or form factors provide a detailed description of the statistical properties of the spectrum. In this work we consider a particular quantity directly related to the correlation function and of great practical importance for wave propagation in periodic media: the number of propagating modes $N_B(E)$ with energy E. In a periodic system the propagating modes are given by the Floquet-Bloch modes, which are quasiperiodic solutions of the Schrodinger equation. They propagate ballistically through the system with constant (group) velocity and are the only modes allowed to transport energy. For instance, the dimensionless Landauer's conductance of a long periodic sample fluctuates closely to the number of these modes propagating in a given direction. In [9], Faure studied this quantity for quasi-one-dimensional periodic systems in the small Plank constant limit $h = 2\pi\hbar \rightarrow 0$. He showed that if the phase space displays tori in the transverse stroboscopic Poincare section, corresponding to trajectories that propagate ballistically through the system, then $N_B \sim h^{-1}$ but, on the other hand, for fully chaotic and diffusive systems $N_B \sim h^{-1/2}$.

We study $N_B(E)$ numerically for periodic waveguides with diffusive classical dynamics and finite horizon in the semiclassical regime. The paper is organized as follows. In Sec. II we review Faure's derivation of the number of propagating Bloch modes in a waveguide. In Sec. III we define the billiard where the predictions are tested. The results are summarized in Sec. IV Then in Sec. V we discuss in further detail our results and its relation to previous works and present some conclusions.

II. NUMBER OF BLOCH MODES FOR $\hbar \rightarrow 0$

In order to be self-contained, we start reviewing the essential results of [9]. First, in an infinite periodic waveguide,
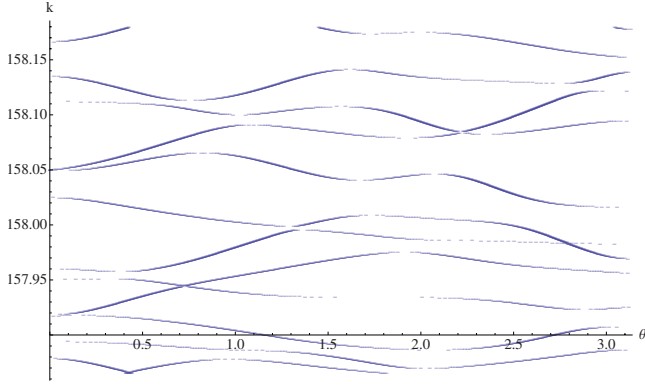
FIG. 1. (Color online) Part of the spectrum $k_n(\theta)$ for the billiard studied in Sec. IV. Note that for the statistics of $N_B(k)$ the computation considers values of k considerably larger than the ones of this figure.

the distribution of quantum velocities $P_\hbar(v,E)$ determines the number of propagating modes $N_B(E)$ with positive velocity [see Eq. (5)]. Second is the asymptotic form of the average $\langle N_B(E) \rangle$ for $\hbar \to 0$, obtained using a semiclassical approximation of $\langle P_\hbar(v,E) \rangle$ [see Eq. (13)].

Consider a periodic waveguide in the Cartesian (x,y) plane, with $x \in \,]-\infty,+\infty[$ (the propagation axis) and y bounded for every x between the wave boundaries that we define as hard walls. The waveguide is composed of cells with length L. In the waveguide particles are free; hence, Schrodinger's equation reduces to Helmholtz equation, i.e.,

$$(\nabla^2 + k^2)\psi(x,y) = 0, \qquad (1)$$

with $\psi(x,y)$ satisfying Dirichlet boundary conditions at the walls. The reader can have in mind several physical contexts where this is valid such as optical, microwave, or acoustic cavities or degenerate electron gases in mesoscopic devices. The classical analog of the quantum system under consideration is given by the free particle Hamiltonian $H(x,p_x,y,p_y) = (p_x^2 + p_y^2)/2$ (we consider particles of unit mass), plus perfect elastic walls as the waveguide boundaries. The results we present below hold for general periodic Hamiltonian systems (not only billiards) where the confining potential in the transversal direction y could be soft. Equation (13) is the general result for that case whereas the particular result for hard-wall billiards is given by Eq. (15), which is the expression we use in the rest of the paper.

Let us consider the phase-space surface of constant energy in one unit cell $\Sigma_E = \{(x,p_x,y,p_y)/0 \le x \le L, \; h_1(x) \le y \le h_2(x), \; H(x,p_x,y,p_y) = E\}$, where $h_1(x)$ and $h_2(x)$ define the lower and upper walls of the waveguide, respectively. Since the boundaries of the guide are periodic and Σ_E is compact, we have from Bloch theorem that the solutions of Schrodinger's equation [Eq. (1)] form bands, i.e., its spectrum has the form $E_{n,\theta}$ with $n \in \mathbb{N}$ as the band index and $\theta = qL \in [-\pi,\pi]$, where q is the Floquet-Bloch wave number. Figure 1 illustrates this spectrum for a chaotic periodic waveguide. An important consequence of Bloch theorem is that the propagation in a periodic system is ballistic with a group velocity [10]

$$v_{n,\theta} = \frac{L}{\hbar} \frac{dE_{n,\theta}}{d\theta}. \qquad (2)$$

Since $N = \int_a^b dx \, \delta(C - f(x))\Theta(f'(x))\frac{df}{dx}$ is the number of points such that $f(x) = C$ with positive derivative in the interval (a,b), Faure expressed the number of Bloch modes with energy E propagating with positive velocity, $N_B(E)$, as

$$N_B(E) = \sum_n \int_{-\pi}^{\pi} d\theta \, \delta(E - E_{n,\theta}) \Theta(v_{n,\theta}) \frac{dE_{n,\theta}}{d\theta}, \qquad (3)$$

where $\delta(\cdot)$ is the Dirac delta function and $\Theta(\cdot)$ is the Heaviside step function. Considering the distribution of quantum velocities $P_\hbar(v,E)$ defined as [9,11]

$$P_\hbar(v,E) = h^2 \sum_n \int \frac{d\theta}{2\pi} \delta(v - v_{n,\theta}) \delta(E - E_{n,\theta}), \qquad (4)$$

with $v_{n,\theta}$ defined in Eq. (2), one obtains

$$N_B(E) = \frac{1}{hL} \int_0^\infty v P_\hbar(v,E) dv. \qquad (5)$$

The normalization over v of $P_\hbar(v,E)$ is

$$\int dv P_\hbar(v,E) = h^2 \int \frac{d\theta}{2\pi} \rho(E,\theta), \qquad (6)$$

with $\rho(E,\theta) = \sum_n \delta(E - E_{n,\theta})$ as the density of states. We note that Eq. (5) is an exact result, a particular case of the Kac-Rice formula [12], valid for quasi-one-dimensional periodic systems [9].

The number of propagating Bloch modes is a rapidly fluctuating quantity as a function of E at scales near the mean level spacing $\Delta E = 1/\bar{\rho}_E$, where $\bar{\rho}_E$ is the mean density of states. These fluctuations are eliminated by considering the average of $N_B(E)$ over an energy interval δE such that $E \gg \delta E \gg \Delta E$ (i.e., quantum mechanically large but classically small), which is the same definition used to determine $\bar{\rho}_E$ from $\rho(E,\theta)$. This procedure is supposed to play a similar role to the ensemble average for disordered systems. Note that we can write

$$\langle N_B(E) \rangle = \frac{1}{hL} \int_0^\infty v \langle P_\hbar(v,E) \rangle dv. \qquad (7)$$

As follows from Eq. (6), $\langle P_\hbar(v,E) \rangle$ is normalized to $h^2 \bar{\rho}_E = \nu_E$, where ν_E is the Liouville measure of the constant energy surface Σ_E (Weyl law).

The expression at the right-hand side of Eq. (7) will be used for the theoretical semiclassical analysis of $\langle N_B(E) \rangle$ but not as a recipe to implement a numerical computation because it is difficult to properly sample small velocities to generate the velocity distribution. However, we are not concerned with the numerical evaluation of this distribution but with the average of $N_B(E)$ which can be computed in different ways. In Sec. III B we describe a numerical method that allows us to compute $\langle N_B(E) \rangle$ accurately bypassing the computation of $P_\hbar(v,E)$. (See in particular the last paragraph at the end of the aforementioned section.)

We now turn to obtain the leading-order term of the semiclassical expansion of $\langle N_B(E)\rangle$. Asch and Knauf [11] proved the asymptotic convergence of $\langle P_\hbar(v,E)\rangle$ toward the classical asymptotic velocity distribution $P_a(v,E)$, i.e.,

$$P_\hbar(v,E) = P_a(v,E) \quad \text{when } \hbar \to 0, \qquad (8)$$

which holds for test functions independent of $\hbar$, i.e., over intervals of order $\delta v \sim 1$, $\delta E \sim 1$, a coarse graining consistent with Eq. (7). In the right-hand side of Eq. (8) $P_a(v,E)$ is the probability density of the asymptotic mean velocity,

$$v_a = \lim_{t\to\infty} \frac{x(t)}{t}, \qquad (9)$$

where $x(t)$ is the longitudinal position at time t of a free particle in the waveguide whose initial condition was taken randomly with a uniform probability distribution on the surface Σ_E. When the classical dynamics is not purely ergodic, i.e., there are some tori associated with ballistic trajectories in the stroboscopic Poincare section, the leading-order term in the semiclassical limit of N_B can be obtained just using equivalence (8) in the integrand of Eq. (7). On the other hand, in the case when the dynamics is completely ergodic, $P_a(v,E)dv$ is a punctual measure at $v=0$ because $v_a=0$ almost surely. To obtain the leading semiclassical contribution in $\langle N_B(E)\rangle$, it is necessary to quantify more precisely how the quantum level velocity distribution approaches the classical asymptotic velocity distribution as $\hbar \to 0$, that is, we need a refinement of Eq. (8).

When the classical dynamics is fully ergodic and the mixing rate is rapid enough, we expect that (almost) any initial ensemble of particles in the system will relax by diffusion, with a Gaussian density profile spreading according to $\langle x(t)^2\rangle = D_E t$ for large times, with D_E as the diffusion coefficient for Σ_E. Hence, the mean velocity distribution at time t is given by

$$P_t(v,E) = \frac{\nu_E}{\sqrt{2\pi}\bar{\sigma}_t} \exp\left(-\frac{v^2}{2\bar{\sigma}_t^2}\right), \qquad (10)$$

where $\bar{\sigma}_t^2 = D_E/t$. In the limit $t \to \infty$, $P_t(v,E)$ converges to a punctual measure at $v=0$. It has been shown [13], using the Gutzwiller trace formula and also with RMT arguments, that in systems with hyperbolic classical dynamics the variance of a quantum operator in the semiclassical limit is equal to the variance of the associated classical observable at time $t=t_H/g$, with $t_H=h/\Delta E=\nu_E/h$ as the Heisenberg time of the unit cell and g as a factor depending on the antiunitary symmetries of the system. For the billiard we study in Sec. III the factor $g=2$ due to the transversal mirror reflection symmetry of the unit cell [28] (see the discussion in Sec. V). Then, we have a relation between the variance $\sigma_\hbar^2 = \langle v_{n,\theta}^2\rangle$ of the quantum level velocity and the variance of the classical mean velocity $\bar{\sigma}_t$,

$$\sigma_\hbar^2 = \frac{gD_E}{t_H} = \bar{\sigma}_{t_H/g}^2 \quad \text{for } \hbar \to 0. \qquad (11)$$

This relation between level velocity variance and the classical diffusion coefficient D_E for the energy shell Σ_E was studied in detail for the kicked rotor [14] where the diffusion

coefficient displays a nontrivial behavior as a parameter is varied. In a different context, [15] explores the relation between classical diffusion coefficient and quantum evolution properties.

Inspired by Eq. (11), Faure conjectured a higher-order semiclassical equivalence between the averaged distribution of quantum velocities $\langle P_\hbar(v,E)\rangle$ and the classical mean velocity distribution at time $t=t_H/g$, i.e.,

$$P_\hbar(v,E) = P_{t=t_H/g}(v,E) \quad \text{when } \hbar \to 0, \qquad (12)$$

over widths of order $\delta E \sim 1$, $\delta v \sim \sqrt{h}$. This conjecture is based on result (11) and the quantum ergodicity theory [16]. It can also be seen as a consequence of the universality in the parametric variation of energy levels discovered by Simons and Altshuler [8], as we discuss in Sec. V Using Eq. (12) in the integral of Eq. (7) we have, for a purely diffusive waveguide,

$$\langle N_B(E)\rangle = \frac{1}{\sqrt{h}} \sqrt{\frac{g\,\nu_E D_E}{2\pi L^2}} + o(\sqrt{1/h}). \qquad (13)$$

Equation (13) was derived in [9] without the factor g and was checked numerically for the kicked Harper model.

Billiards are a particular class of systems with the simplifying property that their phase-space dynamics is the same on every energy shell except for a change of time scale. For two-dimensional billiards $\nu_E = 2\pi A_c$ depends only on A_c, the area of the unit cell. Hence, the semiclassical limit $\hbar \to 0$ is equivalent to $k \to \infty$ due to the relation $\hbar^2 k^2 = 2E$. In Σ_E the upper bound of the mean asymptotic speed is $\sqrt{2E}$. Considering the change of variables $v = \sqrt{2E}u$ we have [from Eqs. (7) and (8)] $\langle N_B(E)\rangle = \frac{\sqrt{2E}}{hL} \int_0^1 u P_a(u)du$ with $P_a(u)$ as the classical asymptotic velocity distribution in $\Sigma_{1/2}$ where the particles move with constant unit speed. Since $\sqrt{2E} = \hbar k$,

$$\langle N_B(k)\rangle = \frac{k}{2\pi L} \int_0^1 v P_a(v)dv. \qquad (14)$$

Thus, for ballistic waveguides $[P_a(v) \neq \nu_E \delta(v)]$ the average number of propagating Bloch modes goes asymptotically for k going to infinity as $\sim \mu_{bal} k/2\pi + o(k)$, where μ_{bal} is the measure of ballistic trajectories in a stroboscopic cross section of the waveguide as defined in [9]. For diffusive billiard chains, the diffusion coefficient satisfies $D_E = |v|D_1$ with speed $|v| = \sqrt{2E}$ and D_1 as the diffusion coefficient in the energy shell $\Sigma_{1/2}$ where particles move with unit speed. Then, using $|v| = \hbar k$ and $\nu_E = 2\pi A_c$ in Eq. (13) we have that the average number of propagating modes in a diffusive wave guide is

$$\langle N_B(k)\rangle = \frac{\sqrt{gA_c D_1}}{\sqrt{2\pi}L}\sqrt{k} + o(\sqrt{k}). \qquad (15)$$

In the following sections we will study how well this result applies to a version of the cosine waveguide, where many semiclassical results for quantum systems have been tested [17,18].

FIG. 2. Portion of the infinite cosine waveguide with a trajectory's segment inside.

III. COSINE BILLIARD CHAIN

A. Definition and classical dynamics

We consider a periodic bidimensional waveguide with cosine-shaped hard walls [19]. The unit cell is defined for $-1 \leq x \leq 1$ with the upper boundary given by $h_2(x) = 1 + (A_2/2)[1 + \cos(\pi x)]$ and the lower boundary defined by $h_1(x) = \frac{1}{2}[1 + \cos(\pi x)]$. The waveguide is constructed as an infinite one-dimensional chain of these unit cells as shown in Fig. 2. Such a billiard has finite horizon, i.e., it does not have unbounded collision-free trajectories. Note the aforementioned unit-cell mirror symmetry in the transversal axis ($x = 0$). We focus on a few values of A_2 in the range $0.3 \leq A_2 \leq 0.60$, where we found that the dynamics is strongly chaotic. Very small tori are observed for $A_2 = 0.38$ and 0.45 in the longitudinal Poincare section over $y = h_1(x)$. For the other values of A_2 considered the phase space looks fully ergodic to the naked eye. In all cases the connected ergodic component makes up at least about 95% of phase-space volume and the most important property for our purposes, exponential decay of the instantaneous velocity autocorrelation $\langle v_x(t)v_x(0) \rangle$, was observed for all values of A_2 explored (Fig. 3). This implies that the system exhibits normal diffusion, i.e., that

$$\tilde{x} = \lim_{t \to \infty} \frac{x(t) - x(0)}{\sqrt{t}} \equiv \lim_{t \to \infty} \tilde{x}_t \qquad (16)$$

is a stationary Gaussian random variable, with zero mean and variance $\langle \tilde{x}^2 \rangle = D_1$. In Fig. 4 we plot the distribution of the normalized displacement $\tilde{x}$ for $A_2 = 0.3$ showing remarkably good convergence to a normal distribution. This holds true for the other values of A_2 that we consider. Another way to support our conclusion that $\tilde{x}$ is normal distributed and
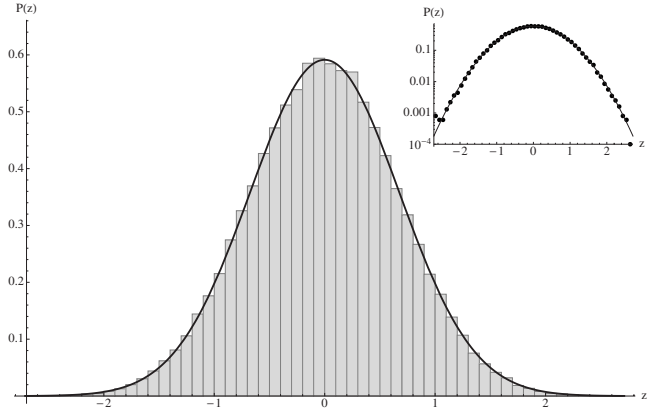
FIG. 4. Histogram of the normalized displacement $\tilde{x}_t$ for a waveguide with $A_2 = 0.3$ at time $t = 50\,000$ using an ensemble of 10^5 initial conditions. The best Gaussian fit is plotted over it. The inset shows the same histogram (dots) in logarithmic scale where convergence to a Gaussian (full line) is more evident to be achieved even deep in the tails.

that there is convergence for at least the first two moments [20] comes from the fact that $\frac{\pi}{2}\langle|\tilde{x}_t|\rangle^2 = \langle \tilde{x}_t^2 \rangle$ for large enough time as observed in Fig. 5. Note that, for instance, an anomalous diffusive system with ergodic phase space but with infinite horizon trajectories could have convergence in distribution to a Gaussian for an appropriate normalized displacement, but it would fail to satisfy this relation between first and second moments for any finite time approximation of $\tilde{x}$ [21].

B. Bloch basis

The propagating states of a periodic waveguide are given by the Bloch modes with unitary eigenvalues. The Bloch basis of a given waveguide can be defined by the solutions of a generalized eigenvalue problem as follows [22]. Consider only one unit cell between two infinite plane leads. The wave function can be written as

$$\psi(x,y) = \sum_{i=1}^{\infty} [c_i^+(x) + c_i^-(x)]\phi_i(x,y), \qquad (17)$$

where $i \in \mathbb{N}$ labels the local transverse modes $\phi_i(x,y)$ which satisfy the waveguide boundary conditions at each x. In the particular case we are considering (hard-wall billiard chain) $\phi_n(x,y) = \sqrt{\frac{2}{h(x)}}\sin\{n\pi[y - h_1(x)]/h(x)\}$ with $h(x) = h_2(x) - h_1(x)$. Inserting Eq. (17) in Eq. (1), the wave equation becomes a system of ordinary differential equations for the $c_i^{\pm}(x)$ which after suitable transformation can efficiently determine transmission and reflection matrices [23,24]. Let a_i^+ (a_i^-) be the right (left) going wave on the left lead and b_i^+ (b_i^-) be the right (left) going wave on the right lead [identified with $c_i^{\pm}(x)$ evaluated at the left x_l and right x_r boundaries of the cell, respectively] as illustrated in Fig. 6. If t and r (t' and r') are the left-to-right (right-to-left) transmission and reflection matrices then outgoing waves are linked to ingoing waves by
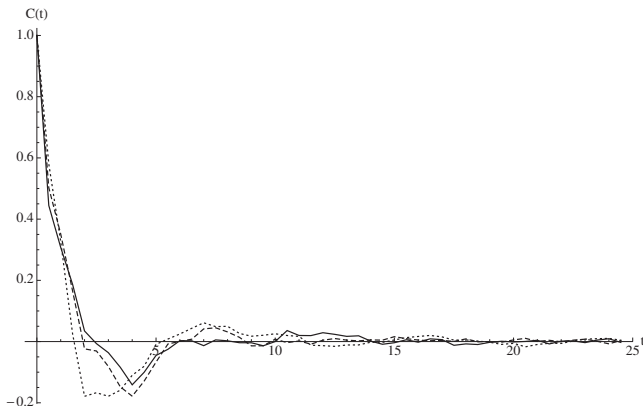
$$ta^+ + r'b^- = b^+,$$

FIG. 3. Velocity autocorrelation function $C(t) = \langle v_x(t)v_x(0) \rangle$ for an ensemble of 20 000 particles in three billiards with $A_2 = 0.6, 0.45, 0.3$ (full, dashed, and dotted lines, respectively). The decay to noise level is quite fast in all cases, at around $t \sim 15$, which is approximately 30 collisions.
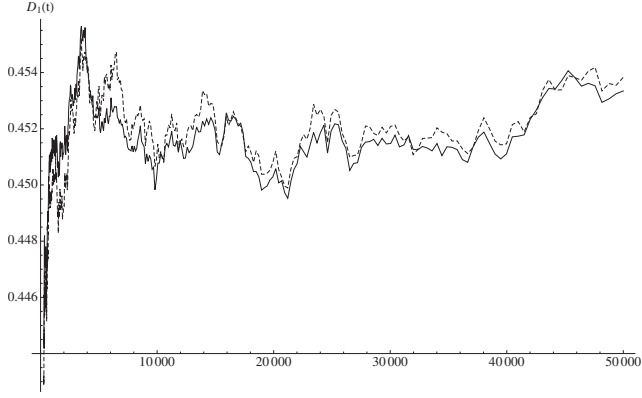
FIG. 5. Finite time approximations of the diffusion coefficient $D_1(t) = \langle x_t^2 \rangle / t$ for the $A_2 = 0.3$ cosine waveguide calculated from the variance (second moment) of the sample's displacements (black line) and from the first moment using $\frac{\pi}{2} \langle |\tilde{x}_t| \rangle^2 = \langle \tilde{x}_t^2 \rangle$, as expected for Gaussians (dashed line) for an ensemble of 10^5 initial conditions. To obtain the diffusion coefficient D_1 we average $D_1(t)$ for times after the transient relaxation regime. The diffusion coefficients obtained in this way from the first and second moments of x_t are the same up to standard error.

$$ra^+ + t'b^- = a^-. \tag{18}$$

We can recast this (infinite) system of equations as

$$M_1 \begin{bmatrix} a^+ \\ a^- \end{bmatrix} = M_2 \begin{bmatrix} b^+ \\ b^- \end{bmatrix}, \tag{19}$$

where

$$M_1 = \begin{pmatrix} t & 0 \\ -r & I \end{pmatrix}, \quad M_2 = \begin{pmatrix} I & -r' \\ 0 & t' \end{pmatrix}. \tag{20}$$

Now, we impose Bloch condition, namely, that the wave function is equal on both lead boundaries up to a complex factor λ,

$$\begin{bmatrix} a^+ \\ a^- \end{bmatrix} = \lambda \begin{bmatrix} b^+ \\ b^- \end{bmatrix}, \tag{21}$$

where $\lambda = \exp(i\theta) = \exp(iqL)$. Then, the Bloch basis is defined as the set of modes that satisfy Eq. (21), i.e., they are the solutions $\mathbf{v}_n$ of the unit cell's generalized transfer matrix eigenvalue problem

$$M_1 \mathbf{v}_n = \lambda_n M_2 \mathbf{v}_n. \tag{22}$$

The propagating Bloch modes are such that $|\lambda_n| = 1$; the other modes are evanescent and decay exponentially in the direction of propagation. In practice, this infinite system of equations must be truncated to a dimension at least equal to the number of propagating Fourier modes in the leads, but in most cases it is necessary to include some evanescent Fourier modes to describe the field adequately. Note that the transmission and reflection matrices used in Eq. (20) are evaluated at the (right or left) entry boundary of the unit cell and carry information from these decaying modes in the near field, which in general can couple between unit cells in the chain. Hence, these matrices do not satisfy the usual (energy)

FIG. 6. Illustration of a quasi-one-dimensional waveguide composed of one unit cell (gray) connected to two ideal leads going to infinity. The field [Eq. (17)] at the unit cell's boundaries is given by $[c_i^+(x_0) \ c_i^-(x_0)] = [a_i^+ \ a_i^-]$ and $[c_i^+(x_1) \ c_i^-(x_1)] = [b_i^+ \ b_i^-]$. Solving the scattering problem in this geometry we can obtain the Bloch basis of the infinite periodic chain.

flux conservation relations coming from the unitarity of the scattering matrix in the far field [25]. Moreover, including evanescent modes brings about infinitely fast decaying states (i.e., null eigenvalues λ_n) [26] making matrices (20) noninvertible. In this case the transfer matrix $M = M_2^{-1} M_1$ cannot be defined. Only when the geometry of the unit cell is such that the coupling between evanescent modes is negligible it is possible to truncate t, r, t', and r' to the far-field nondecaying modes and define the transfer matrix.

Note that our method computes θ as a function of k, i.e., we fix the energy E (or the wave number k) and then we obtain the set of Bloch quasimomenta θ_n for which a propagative solution exists. With this method we can accurately compute the energy average at the left-hand side of Eq. (7).

IV. NUMERICAL RESULTS

We now study numerically the semiclassical behavior of $\langle N_B(k) \rangle$ for the cosine billiard chain. In order to compute the transmission and reflection matrices we employ the admittance multimodal method described in [24], where, for each value of k, the field is described using the local transverse modes (Fourier basis) of the waveguide truncated to a finite number of channels, as described in Sec. III B The number of propagating modes $N_B(k)$ is obtained by counting the solutions of Eq. (22) with $|\lambda_n| = 1$ and positive group velocity. As a function of k, the above number fluctuates at scales $\Delta k = 2\pi/(kA_c)$ [29]. We consider an average of the form

$$\langle N_B(k) \rangle_r = \int N_B(k') f_r(k - k') dk', \tag{23}$$

where $f_r(k)$ is a positive function of unit norm in dk with compact support in an interval of length $r\Delta k$ with $r \gg 1$. The dependence of $\langle N_B(k) \rangle_r$ in the width of $f_r(k)$ is briefly discussed at the end of this section but for what follows we drop explicit reference to r.

In Fig. 7 we show $\langle N_B(k) \rangle$ for $k \in [\pi, 150\pi]$, for $A_2 = 0.3$. For this A_2 value, the phase space does not show noticeable tori. In the k interval explored the number of open transverse modes in the Fourier basis ranges from 1 up to 150 (100 evanescent modes were used for all wave numbers). The dashed line shows a Gaussian smoothed moving average with variance π^2 of $N_B(k)$ for a uniform sampling of wave numbers with spacing $\delta k \sim 0.37\pi$, which is bigger than the
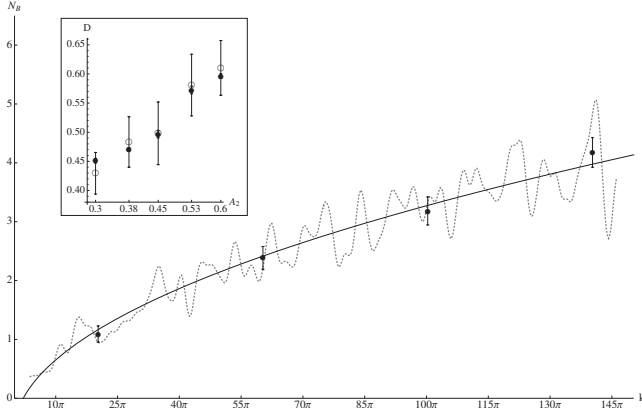
FIG. 7. The dashed line is the Gaussian smoothed moving average (with standard deviation $\sim \pi$) of the number of propagating Bloch modes $N_B(k)$ in the cosine billiard chain with $A_2=0.3$ for a uniform k sampling with increments $\delta k=0.371\,47\pi$. The expected semiclassical result for $\langle N_B(k) \rangle$, plotted in full line, shows good agreement with the moving average. The four black points (with their associated standard error) were computed for the same geometry using a uniform sampling of 153 wave numbers in an interval 300 mean level spacings wide, which constitutes a better statistics than the moving average (a sampling at least 15 times denser). In the inset, the diffusion coefficient calculated classically (black dots) and the one obtained from the best fit following Eq. (15) for the quantum computation of $N_B(k)$ (circles) for five values of A_2 are shown. In all cases, a good agreement with the expected semiclassical behavior [Eq. (15)] is observed.

mean level spacing in the whole k range. The full line is the expected semiclassical result (15) adjusted with an additive constant. This constant appears because in the system under study $\langle N_B(k^*) \rangle = 0$ for some $k^* > 0$ and we are not sufficiently deep in the semiclassical regime for its relative value to be negligible. $N_B(k)$ fluctuates very rapidly with k as expected but the agreement between the moving average and the semiclassically predicted curve is quite good in the whole wavenumber interval explored. We observe similar good results for other configurations of the unit cell with $0.6 \geq A_2 \geq 0.3$ even when there are some small tori in the transverse Poincare sections. This is not surprising because the classical dynamics in those systems is also strongly mixing and for waves to resolve such small structure wave numbers of order $k \gtrsim 2000\pi$ would be needed, a fairly large value compared to the range considered. In the inset of Fig. 7 we show the diffusion coefficient calculated classically (from Monte Carlo simulations) and also the one obtained from the best fit following Eq. (15) for the quantum computation of $N_B(k)$ for five values of A_2.

As mentioned in definition (23) of the mean number of propagating Bloch modes, the width of interval $r\Delta k$ over which we take the average is arbitrary and it is only assumed to be much larger that the mean level spacing Δk and classically small. In order to find out how relevant is this choice we calculate $\langle N_B(k) \rangle_r$ for four different values of k as a function of $r \in [2,300]$ using a uniform k sampling of 153 points around the four wave numbers. In Fig. 8 we see that, after a transient phase in $r \sim 200$, the value of the average reaches an approximately stable region in the four cases. The four

black dots in Fig. 7 show this result for $r=300$, also agreeing nicely with the expected semiclassical curve.

We end this section by remarking how close to the semiclassical regime the presented results are. In our calculations λ/W (the wavelength in units of the waveguide width) is as small as 0.012. We note that the calculations in [5], which are also compared with semiclassical results for periodic billiards, were computed with the parameter $\lambda/W \sim 0.12$.

V. DISCUSSION AND CONCLUSIONS

In Sec. II we closely followed Faure derivation of Eq. (13). Here, we provide an alternative argument allowing us to understand better the connection with [6,8]. Proceeding as in Sec. II, we define the probability distribution of level velocity in natural units w,

$$p(w,E) = \frac{1}{2\pi} \sum_n \int_{-\pi}^{\pi} d\theta \, \delta(E - E_{n,\theta}) \delta\left(w - \frac{dE_{n,\theta}}{d\theta}\right), \quad (24)$$

so that

$$N_B(E) = 2\pi \int_0^{\infty} w \, p(w,E) dw. \quad (25)$$

Then, as was noted in [27], the distribution of level velocities satisfies $p(w,E) = \lim_{\phi \to 0} \phi K(w\phi, \phi)$ with $K(\Omega, \phi)$ as the autocorrelation function

$$K(\Omega, \phi) = \langle \rho(E + \Omega, \theta + \phi)\rho(E, \theta) \rangle_{E,\theta} - \bar{\rho}_E^2 \quad (26)$$

of the energy density $\rho(E, \theta) = \Sigma_n \delta(E - E_{n,\theta})$. The average is over θ and over a classically small energy interval around E and $\bar{\rho}_E$ denotes this average for $\rho(E, \theta)$. According to Simons and Altshuler $k(\omega, \chi) = K(\Omega, \phi)/\bar{\rho}_E^2$ is a universal function, where $\omega = \bar{\rho}_E \Omega$ and $\chi = \sqrt{C(0)}\phi$ with $C(0) = \bar{\rho}_E^2 \langle (dE_{n,\theta}/d\theta)^2 \rangle$. They showed this result for disordered systems and verified numerically its validity for chaotic systems in the semiclassical limit. It follows from their expression for $k(\omega, \chi)$ that the probability distribution of level velocity $p(w,E)$ is a Gaussian with variance $C(0)/\bar{\rho}_E^2$. Thus, from Eq. (25), we obtain $N_B(E) = \sqrt{2\pi C(0)}$. The constant $C(0)$ is system dependent and must be computed, for example, semiclassically. In our case it is simply related to the average of the square of the quantum velocity $C(0) = (\bar{\rho}_E^2 \hbar^2/L^2) \langle v_{n,\theta}^2 \rangle$ that is given in Eq. (11), leading to $N_B(E) = \sqrt{\frac{1}{\hbar}(g\nu_E D_E/2\pi L^2)}$. Thus, Faure's result (13) can be seen as a consequence of universality in the parametric level correlations. The validity of the universal correlation function for periodic systems was studied in [6] by Dittrich *et al.* in the semiclassical limit. They computed $K(\Omega, \phi)$ by Fourier transforming their semiclassical expression for the form factor identifying a $C(0)$ that agrees with the previous result.

The universal correlation function $k(\omega, \chi)$ is different for Gaussian orthogonal ensemble (GOE) and Gaussian unitary ensemble (GUE). For periodic systems, when χ plays the role of the Bloch parameter, time-reversal symmetry T is broken for all χ besides three exceptional points [5]. Thus, when no further antiunitary symmetries exist, $k(\omega, \chi)$ moves between GOE and GUE at different parts of the band. In our
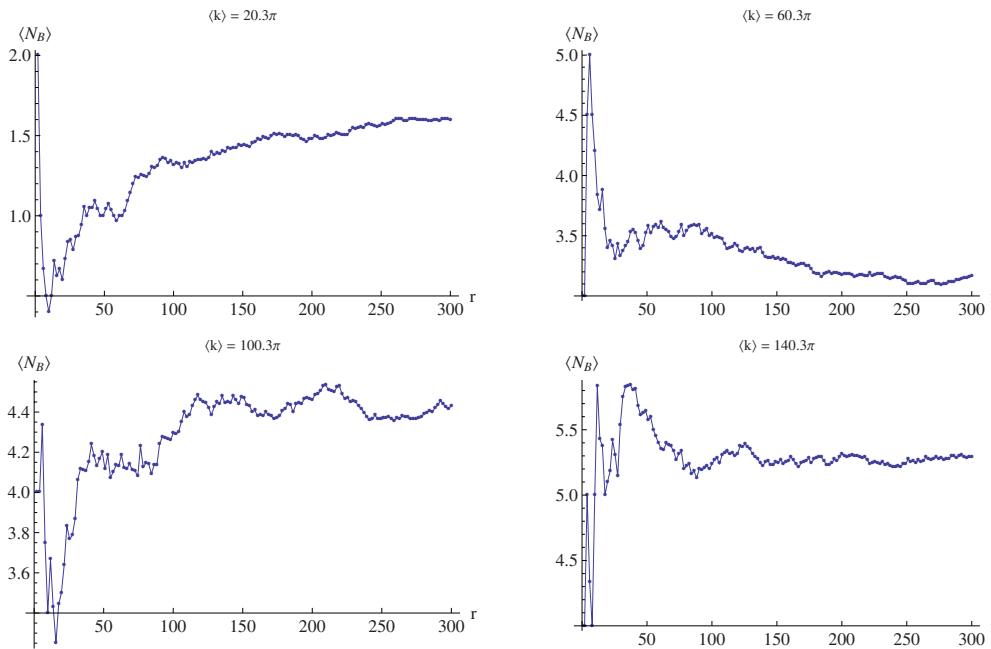
FIG. 8. (Color online) $\langle N_B(k)\rangle_r$ as a function of r for four energies in the $A_2 = 0.3$ cosine billiard. A uniform sampling of 153 wave numbers distributed in a 300 mean-level-spacing wide interval was used. In all cases after $r \sim 200$ the average fluctuations are notably reduced and the result for $\langle N_B(k)\rangle$ is in agreement with the expected semiclassical result (see Fig. 7) indicating that this is a good smoothing window to eliminate the spectrum fluctuations.

case, the unit cell is invariant under the operator S_x that transforms $x \rightarrow -x$ (mirror reflection along the transversal direction). So, even though the unit-cell Hamiltonian does not commute with S_x nor with T, it does commute with the operator TS_x which is antiunitary. Then, as χ is varied, the system always belongs to GOE [28].

As a final comment, we note that Eq. (14) applies also to classical waves with dispersion relation $\omega = ck$ propagating in a waveguide with speed $c = 1$. We can restore c by noticing that the distribution of group velocities $v_{n,\theta} = Ld\omega_{n,\theta}/d\theta$ is related to our previous distribution by $p_k(v) = \frac{1}{c}P_k(\frac{v}{c})$. With this new $p_k(v)$ the formula becomes

$$N_B(k) = \frac{k}{2\pi cL}\int_0^\infty v p_k(v) dv, \qquad (27)$$

with the normalization $\int dv p_k(v) = \int \frac{dv}{c}P_k(\frac{v}{c}) = 2\pi A_c$ for the group-velocity distribution. The result for the number of propagating modes also applies for these classical waves.

To conclude, we have studied the agreement between numerical computations and a semiclassical approximation of the number of propagating modes in a diffusive periodic waveguide. We also showed the relation between $\langle N_B(E)\rangle$ and previously studied spectral properties of periodic systems. The semiclassical results used in our analysis are previous to the discovery of how to include nondiagonal contributions to correlation functions. Nevertheless, it was noted [13,14] that their role in the computation of the fluctuations in velocity should be very limited. Indeed, besides the average justified by the rapid phase variation, the observable amplitude (the velocity in this case) fluctuates around its null average, further justifying the diagonal approximation.

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[1] O. Bohigas, M. J. Giannoni, and C. Schmit, Phys. Rev. Lett. **52**, 1 (1984).

[2] H.-J. Stöckmann, *Quantum Chaos: An Introduction* (Cambridge University Press, Cambridge, England, 1999).

[3] F. Haake, *Quantum Signatures of Chaos* (Springer, Berlin, 2000).

[4] S. Heusler, S. Müller, A. Altland, P. Braun, and F. Haake, Phys. Rev. Lett. **98**, 044103 (2007).

[5] T. Dittrich, B. Mehlig, H. Schanz, and U. Smilansky, Chaos, Solitons Fractals **8**, 1205 (1997).

[6] T. Dittrich, B. Mehlig, H. Schanz, and U. Smilansky, Phys. Rev. E **57**, 359 (1998).

[7] B. D. Simons and B. L. Altshuler, Phys. Rev. Lett. **70**, 4063 (1993).

[8] B. D. Simons and B. L. Altshuler, Phys. Rev. B **48**, 5422 (1993).

[9] F. Faure, J. Phys. A **35**, 1339 (2002).

[10] C. Kittel, *Introduction to Solid State Physics* (John Wiley & Sons, New York, 1966).

[11] J. Asch and A. Knauf, Nonlinearity **11**, 175 (1998).

[12] M. Wilkinson, in *Supersymmetry and Trace Formulae: Chaos and Disorder*, edited by I. V. Lerner, J. P. Keating, and D. E. Khmelnitskii (Kluwer Academic/Plenum Press, New York, 1999).

[13] B. Eckhardt, S. Fishman, J. Keating, O. Agam, J. Main, and K. Muller, Phys. Rev. E **52**, 5893 (1995).

[14] A. Lakshminarayan, N. R. Cerruti, and S. Tomsovic, Phys. Rev. E **60**, 3992 (1999).

[15] F. Barra and P. Gaspard, Phys. Rev. E **65**, 016205 (2001).

[16] A. Bäcker, R. Schubert, and P. Stifter, Phys. Rev. E **57**, 5425 (1998).

[17] M. Mendoza, P. A. Schulz, R. O. Vallejos, and C. H. Lewenkopf, Phys. Rev. B **77**, 155307 (2008).

[18] J. A. Méndez-Bermúdez, G. A. Luna-Acosta, P. Šeba, and K. N. Pichugin, Phys. Rev. E **66**, 046207 (2002).

[19] G. A. Luna-Acosta, K. Na, L. E. Reichl, and A. Krokhin, Phys. Rev. E **53**, 3271 (1996).

[20] A. Papoulis, *Probability, Random Variables, and Stochastic Process*, 4th ed. (McGraw-Hill, New York, 1994).

[21] D. N. Armstead, B. R. Hunt, and E. Ott, Phys. Rev. E **67**, 021110 (2003).

[22] A. Duclos, D. Lafarge, and V. Pagneux, Eur. Phys. J.: Appl. Phys. **45**, 11302 (2009).

[23] V. Pagneux and A. Maurel, Proc. R. Soc. London, Ser. A **462**, 1315 (2006).

[24] V. Pagneux, J. Comput. Appl. Math. **234**, 1834 (2010).

[25] V. Pagneux and A. Maurel, J. Acoust. Soc. Am. **116**, 1913 (2004).

[26] H. Wu and D. W. L. Sprung, Appl. Phys. A: Mater. Sci. Process. **58**, 581 (1994).

[27] V. E. Kravtsov and M. R. Zirnbauer, Phys. Rev. B **46**, 4332 (1992).

[28] M. Robnik and M. V. Berry, J. Phys. A **19**, 669 (1986).

[29] Δk follows from the Weyl law $N = k^2 A_c/(4\pi)$.

[30] http://www.scat-alfa.eu