Chaotic dynamics in an elastic medium with surface disorder

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We investigate the dynamics of an elastic medium described by a two-dimensional network of nodes of equal mass connected by springs whose force constants are equal inside the network and chosen at random at its surface. The system can be considered a billiard in the sense that the network is ordered all throughout its bulk. Being an eigenvalue problem its complexity is manifested in a frequency statistics which, in most of the spectrum, can be described by the Wigner-Dyson distribution. At low frequencies the dispersion relation is linear in the wave number and the network shows regular behavior (frequency statistics according to Poisson distribution). We study the dynamical behavior of this model by investigating how the system escapes from a normal mode of the ordered network, and calculate the Lyapunov exponent λ in different frequency regions. [S1063-651X(97)12410-2]

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I. INTRODUCTION

Quantum analogs of classical systems which show chaotic behavior have spectra whose short-range statistical properties are adequately described by random matrix theory [1–4]. If the system is rotationally invariant and has time reversal symmetry, some of the features of its spectrum are closely simulated by random matrices of the Gaussian orthogonal ensemble (GOE). In particular, their nearest-level spacings are distributed according to the Wigner-Dyson distribution. Many quantum systems which satisfy this picture [1,2] have already been identified.

We have recently proposed a model of quantum chaotic billiards in two and three dimensions [5,6] which consists of a tight-binding Hamiltonian in which the energies of the atomic orbitals at the surface sites are chosen at random. This model, in contrast with the more standard geometric billiards [1], has two length scales: the system size L and the lattice constant a. In the macroscopic limit ($L/a \rightarrow \infty$) microscopic roughness remains and affects quantum particles, i.e., particles characterized by a wavelength of the order of a. As a consequence, in the macroscopic limit all levels are distributed according to Wigner-Dyson statistics [7].

In this work we investigate the dynamics of a two-dimensional (2D) network of nodes of equal mass connected among themselves by springs that have the same force constant within the bulk of the network, and to rigid walls through springs whose force constants are chosen at random. Like the model Hamiltonian described above, this system can be considered a billiard as it is ordered throughout its bulk, whereas complex (chaotic) behavior is expected to be derived from the disorder introduced at its surface. Being an eigenvalue problem its complexity will result in a frequency statistics of the Wigner-Dyson type in most of the spectrum (see below). In the quantum limit, this model can be regarded as the phonon counterpart of the electron Hamiltonian investigated in [5]. The model presented here is an interesting system to investigate chaotic dynamics as its behavior significantly varies through the band of normal modes. In fact, at low frequencies the velocity is dispersionless, and a more regular behavior is expected in this frequency region. The study of the dynamics is carried out by investigating how the system escapes from a normal mode of the ordered network [8,9]. This allows us to calculate the Lyapunov exponent.

II. MODEL AND METHODS

The model whose dynamics will be investigated in this work is characterized by the same type of parameters as the electron Hamiltonian discussed in Ref. [5]. The energies of the atomic levels at the boundary sites in the tight-binding Hamiltonian [5] and the surface force constants in the elastic network are random variables which are used to describe surface disorder (either topological or compositional). In the former case the disorder is diagonal whereas in the model presented here it is nondiagonal. We do not expect, however, that this should imply any significant difference in their behaviors. In fact, we have recently checked that, if the surface hopping integrals in the tight-binding Hamiltonian, instead of the energies of the surface atomic orbitals, are chosen at random, the behavior of the system is essentially the same. Both the electron Hamiltonian and the elastic network are billiards in the sense that their bulks are completely ordered, whereas complexity is expected to be derived from surface disorder. Those parameters describe the amount in which the system deviates from integrability in a more natural way than in more standard two- or three-dimensional geometrical billiards, such as Sinai, stadium, or Africa billiards [1,2,10]. In

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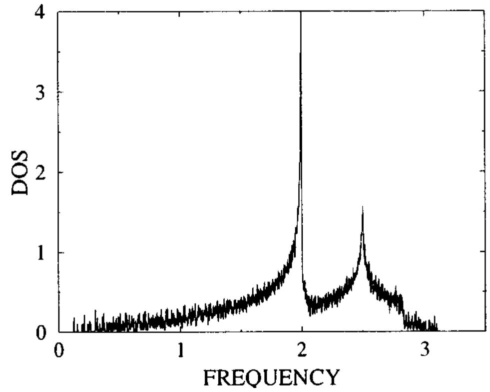

FIG. 1. Density of states (DOS) in a surface disordered spring network of size $L=40$, as a function of frequency for the model investigated in this work (see text). The force constants at the surface were randomly chosen in the range 0.0–2.0. In the calculations an imaginary part, equal to the average intermode spacing, was added to the frequency.

the following we briefly discuss the Hamiltonian used in this work and the procedures we have followed to investigate the statistics of the frequencies of the normal modes and the dynamics of the model.

In all our simulations the 2D elastic medium is represented by a square network of nodes of equal mass m connected by Hookean springs. In particular, we take clusters of the square lattice containing $L\times L$ nodes, joined by first and second nearest-neighbor springs [11]. The Hamiltonian is

$$H=m\sum_{i=1}^{N}\ddot{\mathbf{u}}_i+\sum_{i,j=1}^{N}k_{i,j}[(\mathbf{u}_i-\mathbf{u}_j)\cdot\hat{\mathbf{r}}_{i,j}]^2, \tag{1}$$

where $N=L^2$. $k_{i,j}=k_1,k_2$ if i and j are first and second nearest neighbors, respectively, and zero otherwise. $\mathbf{u}_i$ is the displacement of node i and $\hat{\mathbf{r}}_{i,j}$ is the unit vector in the i-j direction. In these calculations we take the mass of the nodes (m) and the force constants of the bulk springs equal to one $(m=k_1=k_2=1)$, whereas the force constants of the surface springs (those which join the network to the rigid walls) were chosen at random in the range $k_1^s,k_2^s\in[k_{\rm min},k_{\rm max}]$. Calculations have been carried out for network sizes up to $L=80$ (note that the system has $S=2L^2$ normal modes). The Schwarz algorithm for symmetric matrices was used to compute the whole spectrum [12]. Averaging sets include up to 50 000 modes. The density of states (normal modes) is illustrated in Fig. 1. The low frequency region in which the density of states is very small is characterized by a dispersion relation approximately proportional to the wave number [11], which gives a dispersionless velocity.

To characterize the statistical properties of the spectra, each real spectrum of frequencies ω_i is mapped onto an unfolded spectrum Ω_i through $\Omega_i=\overline{N(\omega_i)}$, where $\overline{N(\omega)}$ is the average number of modes up to a frequency ω. This averaged magnitude is obtained after calculating the mean density of states in small frequency intervals that contain a large number of modes in spite of being small. This is always possible in our model since the number of disorder realizations can be taken as large as necessary. Thus the averaged density of states can be considered as a continuous function of ω. Finally, $\overline{N(\omega)}$ is obtained by integrating the averaged density of states from the bottom of the frequency band up to ω.

The dynamics of this system is studied by investigating how the system escapes from a normal mode of the ordered network. Specifically, we launch (at $t=0$) the disordered network into a normal mode of the ordered (o) network and calculate the correlation function of the displacement field as a function of time. We further assume that the velocity of the nodes at $t=0$ is zero. The displacement vector at $t=0$ of a node i of the disordered system is then given by

$$\mathbf{u}_i(0)=\mathbf{u}_{i\beta}^o=\sum_{\alpha=1}^{S}\mathbf{A}_{i\alpha}c_{\alpha\beta}, \tag{2}$$

where $\mathbf{A}_{i\alpha}$ are the amplitudes (vector) of the normal modes α of the disordered network and $c_{\alpha\beta}$ are constants which are obtained from

$$c_{\alpha\beta}=\sum_{i=1}^{N}\mathbf{A}_{i\alpha}\cdot\mathbf{A}_{i\beta}^o, \tag{3}$$

where $\mathbf{A}_{i\beta}^o$ are the amplitudes of the normal mode β of the ordered network. The $c_{\alpha\beta}$ form a distribution whose variance (σ) depends on the ordered normal mode on which the disordered network is launched. This variance will be an essential parameter in the discussion of the dynamical behavior of the system.

The displacement field in the disordered network is given by

$$\mathbf{u}_i(t)=\sum_{\alpha=1}^{S}\mathbf{A}_{i\alpha}c_{\alpha\beta}\cos(\omega_\alpha t), \tag{4}$$

ω_α being the frequencies of the normal modes. To investigate how the network escapes from its initial vibrational state we calculate the correlation function, namely,

$$C(t)=\sum_{i=1}^{N}\mathbf{u}_i(0)\cdot\mathbf{u}_i(t)=\sum_{\alpha=1}^{S}c_{\alpha\beta}^2\cos(\omega_\alpha t). \tag{5}$$

The results presented in the next section indicate that vibrational states showing a chaotic behavior are characterized by a correlation function which at short times decreases as

$$C(t)=\cos(\omega_\beta^o t)\exp(-\lambda t), \tag{6}$$

where λ is the Lyapunov exponent and ω_β^o is the frequency of the normal mode of the ordered system into which the disordered network was launched at $t=0$.

III. RESULTS

A. Statistics of the frequency spectrum

We have first investigated the nearest-level (mode) statistics of the normalized spectra. The results are illustrated in Fig. 2 for clusters of sizes $L=$ 50 and 80. There is a rather wide frequency range where the variance is close to that of GOE matrices (0.286). The inset of Fig. 2 shows the distribution of nearest-mode spacings in a frequency region where

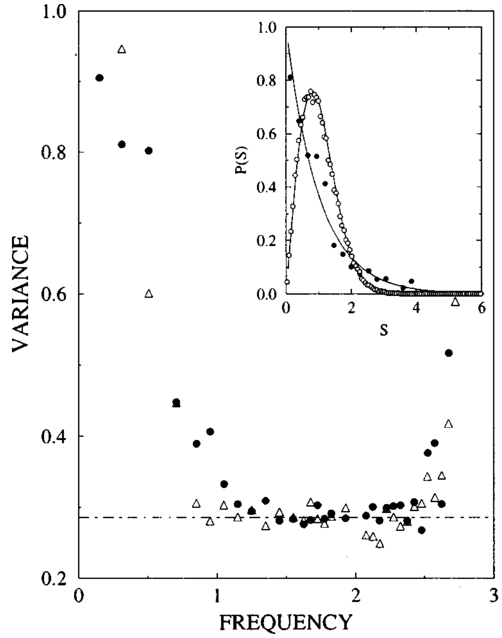

FIG. 2. Variance of the nearest-mode spacings in the whole normalized frequency spectrum. The results correspond to 30 realizations of 50×50 clusters (circles) and five realizations of 80×80 clusters (triangles). Inset: Distribution of nearest-level spacings in 50×50 clusters for frequencies in the ranges 0.0–0.4 (filled circles) and 1.05–1.95 (open circles). For the sake of comparison, the Wigner-Dyson and the Poisson distributions are also shown. The force constants at the surface were randomly chosen in the range 0.0–2.0.

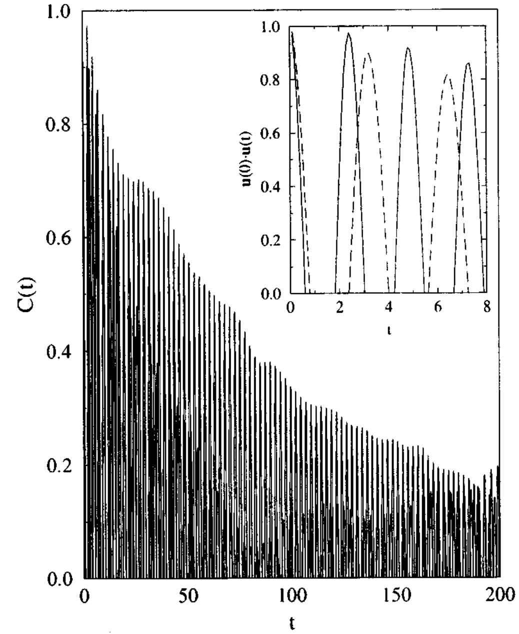

FIG. 3. Correlation function for the displacement field of the disordered network launched at $t=0$ on two different normal modes of the ordered network with frequencies $\omega_\beta^o = 1.9346, 2.5842$. The results correspond to a single realization of a 40×40 cluster with surface force constants chosen at random in the range 0.0–4.0. Inset: short time behavior shown to illustrate how the oscillations of the correlation function have a period which approximately corresponds to that of the normal mode of the ordered network. Only positive values of $C(t)$ are shown.

the variance is ≈ 0.286. As expected, the results closely follow the Wigner-Dyson distribution.

As already found in the quantum case [5], we observe the existence of quasi-ideal states near the band edges: modes that are similar to those found in the ordered network and do therefore follow the Poisson distribution, see inset of Fig. 2. It has to be remarked that the results for frequency regions close to the band edges may not be so accurate due to the very low density of states in that region (see Fig. 1). In the present case there is a rather wide frequency range close to the bottom of the band, where the variance is very different from the Wigner-Dyson value. We have checked that this result is very robust and depends only slightly on the degree of disorder, for the system sizes L reached in this work. The reason for this behavior was already noted in the preceding section, and in fact it is a consequence of the nearly linear dispersion relation in that frequency region: a linear dispersion relation gives an almost constant velocity (independent of the wave number). Elastic waves having such a dispersion relation propagate at a velocity which does not depend on $\mathbf{r}$ and thus average out any surface disorder.

A point of remarkable relevance is the dependence of these results on the size of the system L. In the case of the electron Hamiltonian, numerical results [5] and qualitative arguments based upon perturbation theory [7] indicated that, in the macroscopic limit, all energy levels should be distributed according to the Wigner-Dyson statistics, no matter the degree of disorder. Although in the present case the larger size of the matrices makes a reliable numerical study difficult, a similar qualitative argument should also be valid in the present case. Thus it is likely that in the thermodynamic limit the Wigner-Dyson statistics should apply in the whole frequency band.

We finally note that, in the quantum limit, and due to the actual linear relationship between energies and frequencies, quantum energy levels will also be distributed according to Wigner-Dyson statistics.

B. Dynamical behavior of the elastic medium

The correlation function $C(t)$ for the displacement field obtained by launching the disordered network at $t=0$ into two different modes of the ordered network are depicted in Fig. 3 [only positive values of $C(t)$ are shown]. As expected, they show an oscillatory behavior, which, at short times, is modulated by an exponential [9]. The frequency of the oscillations is very similar to that of the ordered state into which the disordered system was launched at $t=0$ (ω_β^o). This is further illustrated in Fig. 4 where the numerical results for $C(t)$ are plotted along with the function given in Eq. (6). The agreement for short times is remarkable. The frequency of the oscillation can actually be shifted in an amount which depends on the actual normal mode of the ordered state into which the system was launched (see Table I). These results are in line with those reported in Ref. [9] for correlation functions in geometric chaotic billiards.

At longer times the numerical results for $C(t)$ deviate from the simple behavior of Eq. (6) as can be clearly seen in Fig. 4 for t beyond 30. The time interval in which Eq. (6) holds strongly depends on the frequency ω_β^o. The Lyapunov

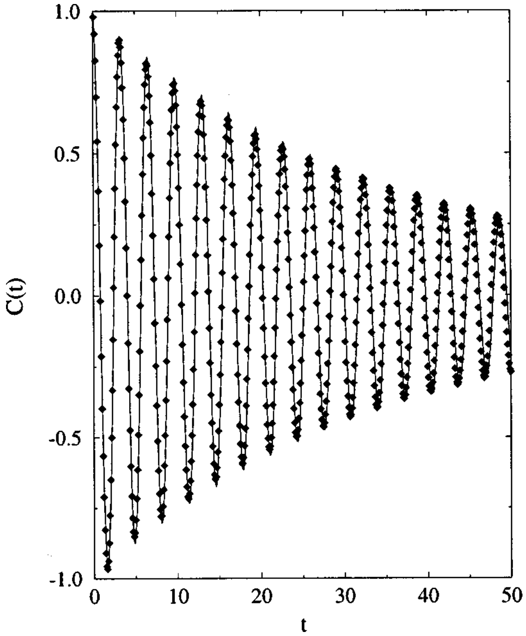

FIG. 4. Short time behavior of the correlation function (filled diamonds) for the displacement field of the disordered network launched at $t=0$ on a normal mode of the ordered network with frequency $\omega_\beta^o=1.9346$. The results correspond to 40×40 clusters with surface force constants chosen at random in the range 0.0–4.0. The continuous curve corresponds to $C(t)=\cos(1.9346t)\exp(-0.027t)$.

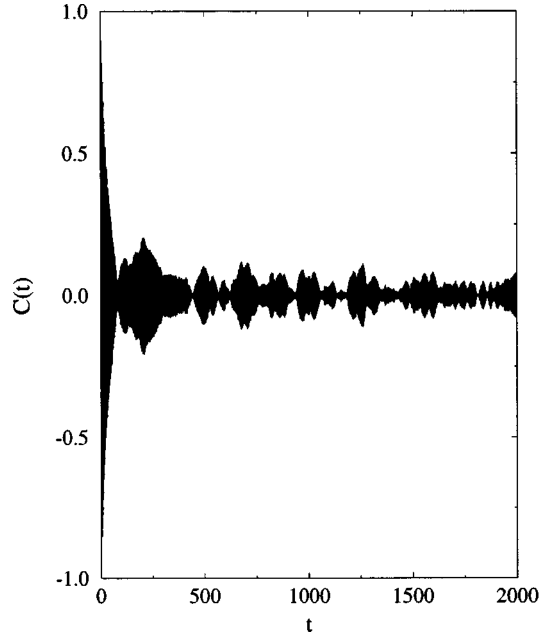

FIG. 5. Long time behavior of the correlation function for the displacement field of the disordered network launched at $t=0$ on a normal mode of the ordered network with frequency $\omega_\beta^o=1.9346$. The results correspond to 40×40 clusters with surface force constants chosen at random in the range 0.0–4.0.

exponent was obtained through a fitting of the numerical results in that interval (see Table I). The long time behavior is in fact very complex as shown in Fig. 5. $C(t)$ shows the typical features of chaotic systems with regions in which it is finite alternating with others where it is very small. It is interesting to note that a behavior like that of Eq. (6) should have only been expected for all t if the distribution of weights $c_{\alpha\beta}$ in Eq. (3), or, alternatively, the Fourier transform of $C(t)$, had a Lorentzian shape, $S(\omega)=\lambda/\pi[\lambda^2+(\omega-\omega_\beta^o)^2]$.

TABLE I. Lyapunov exponent (λ) and time interval $(0,t_0)$ over which it was calculated, for a disordered network of size $L=40$ and surface force constants in the range 0.0–4.0, launched at $t=0$ into several eigenmodes of the ordered network with frequencies ω_β^o. The variance of the distribution of disordered eigenmodes (σ), the average frequency ($\langle\omega\rangle$), and the number of modes N_m within that energy (variance) is also given. The results have been grouped according to σ.

ω_β^o	$\langle\omega\rangle$	σ	N_m	λ	t_0
0.3053	0.3053	0.0622	10	9×10^{-8}	5000
1.9467	1.9467	0.0657	250	0.0076	460
2.7733	2.7782	0.0625	80	0.0037	450
0.5820	0.6002	0.1021	30	0.0001	1200
1.9682	1.9836	0.1023	460	0.0064	250
2.5417	2.5567	0.1023	270	0.0223	100
0.6458	0.6641	0.1110	35	0.0009	1200
1.9927	2.0092	0.1109	440	0.0007	2800
2.5794	2.5970	0.1108	220	0.0308	50
0.8645	0.8966	0.1414	50	0.0041	660
1.8642	1.8942	0.1409	345	0.0087	300
2.1501	2.1839	0.1414	160	0.0053	230

The results discussed above allow us to enter into a question of remarkable interest, namely, whether the Lyapunov exponent is or is not related to the variance of the distribution of the weights of the modes of the disordered network. Had this distribution been a Lorentzian, such as that written above, its variance would have completely determined the decay of $C(t)$. However, our results indicate that this is not the case of the present model (see Table I). In fact, there is no correlation between the Lyapunov exponent and the variance of the distribution of weights. On the other hand, this is consistent with the long time behavior of $C(t)$, which is a consequence of the non-Lorentzian character of $S(\omega)$. As the density of states has also a significant dependence on frequency (see Fig. 1), it is also important to check whether the Lyapunov exponent has some correlation with the average number of modes N_m participating in the construction of a given ordered mode. The results for N_m reported in Table I do also indicate that there is no correlation between N_m and λ. This conclusion is in accordance with recent results for the tight-binding Hamiltonian which indicate that the Lyapunov exponent and the variance σ scale with the size of the system in a significantly different way, namely, as $1/L$ and $1/L^{1/2}$, respectively [13].

The results reported in Table I are in line with those of Fig. 2. In fact, at low frequencies the Lyapunov exponent is very small or even negligible (see the results for $\omega_\beta^o=0.3053$), illustrating the regular behavior expected in this frequency region. The conclusion of this analysis is that the *nature* of the normal modes (whether chaotic or regular) is in fact the key factor in determining the dynamics of the system.

IV. CONCLUDING REMARKS

In this work we have investigated the properties of an elastic network with surface disorder. The model can be considered a billiard in the sense that all scattering centers are located at its surface. The system has a frequency spectrum characterized by nearest-mode spacings distributed according to the Wigner-Dyson distribution. It is widely accepted that this behavior is a clear hallmark of quantum chaotic behavior. The reason the present system shows this feature is the fact that it is also an eigenvalue problem.

We have also investigated its dynamical behavior by studying how the system escapes from a normal mode of the ordered network. At short times the correlation function shows oscillations modulated by an exponential. The frequency of these oscillations almost coincides with that of the normal mode of the ordered network into which the system was launched at $t=0$. On the other hand, the decaying exponential gives the Lyapunov exponent. At longer times $C(t)$ shows a very complex behavior. The results for the Lyapunov exponent indicate that the behavior of this system strongly depends on the frequency of the ordered normal mode, and, in particular, no exponential decay of the correlation function is observed in the lower part of the spectrum. This is ascribed to the fact that in this frequency region the frequency is proportional to the wave number and thus the velocity is dispersionless. It is also shown that the dynamical behavior cannot be completely understood in terms of the variance of the distribution of the weights of the disordered eigenstates needed to build up an ordered one.

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