A Model for Irregular Scattering in the Presence of Localization

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ABSTRACT

We present a 1-d abstract model for classical and quantum chaotic scattering in which the interacting dynamics is defined by the Standard Map. This model exhibits the three characteristic regimes (ballistic, ohmic, localized) of quantum transport in disordered solids and can be therefore used to investigate transport fluctuations in the framework of chaotic scattering.

1. Scattering phenomena in which transport takes place inside the interaction region have a broad physical relevance. A well known example is electrical conduction in solids at low temperature, that can be described as a quantum process of scattering of electron waves by a conducting sample[1,2]. Other examples are disintegration or ionization processes in which the decay of a metastable state is determined by some sort of diffusion eventually leading into a continuum of free states[3]; typical among these is the microwave ionization of highly excited hydrogen atoms[4].

Since classical transport in the absence of external random agents requires a chaotic dynamics, problems involving 'diffusive scattering' are naturally related to chaotic scattering, where quantum coherence effects have been shown to produce characteristic Ericson-like fluctuations of the scattering amplitudes[5]. In the case of diffusive scattering however one more coherence effect has to be taken into account, namely quantum localization.

The investigation of diffusive scattering within the theoretical framework of chaotic scattering requires the formulation of appropriate models that must be amenable to both classical and quantum analysis. There are many physically meaningful models for classical chaotic transport and also for quantum transport in the presence of localization, but most of them are not quite convenient for a direct comparison of classical and quantum properties. For example, the quantum simulation of classical models such as the Lorentz gas with an appropriately large number of scatterers presents considerable computational problems; on the other hand, quantum tight-

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binding models of the Anderson type, though very well suited to the analysis of localization effects, do not possess a well-defined classical limit.

Here we present a scattering model that, in spite of a rather abstract character, displays the essential features of diffusive scattering. This model is a variant of the renowned Kicked Rotator; it exhibits classical chaotic diffusion and quantum mechanical localization. The scattering matrix can be numerically computed with a good accuracy , so that the transmission coefficient can be determined and its dependence on various parameters analyzed. It turns out that this quantum model possesses the three characteristic regimes of disordered conductors, i.e. the ballistic, ohmic and localized regimes. We note in passing that the existence of the 'ohmic' regime provides an illustration of how a typical result of nonequilibrium statistical mechanics such as the inverse dependence of the transmission coefficient on the length stems from the quantum mechanics of a 'small' quantum system, in spite of the well-known absence of chaos in quantum dynamics.

2. Our classical model is a dynamical system on the cylinder parametrized by the variables n, θ, $-\infty < n < +\infty$, $0 \leq \theta < 2\pi$. The discrete time dynamics is defined by :

$$\begin{aligned} \bar{n} &= n + k \sin\theta \\ \bar{\theta} &= \theta + \tau\bar{n} \quad for \quad n_0 \leq n \leq n_0 + L \\ \bar{\theta} &= \theta \quad elsewhere \end{aligned} \tag{1}$$

Inside the finite cylindrical slab defined by $n_0 \leq n \leq n_0 + L$ ("interaction region"), the map (1) is just the Standard Map with parameters k and τ. For $k\tau >> 1$ the corresponding dynamics is strongly chaotic and diffusion in the variable n occurs according to the Fokker-Planck equation :

$$\frac{\partial f}{\partial t}(n,t) = \frac{D}{2}\frac{\partial^2 f}{\partial n^2}(n,t) \tag{2}$$

where t is time (number of iterates of the map) and the diffusion coefficient D is given by :

$$D = \beta D_0 \equiv \beta\frac{k^2}{2} \tag{3}$$

with β a numerical coefficient[6] that depends on $K = k\tau$; D_0 is the so called quasi-linear diffusion coefficient.

Outside the interaction region, the free motion is uniform in n and takes place along straight lines (generatrices) $\theta = const.$

A simple statistical description of the classical scattering process can be obtained from the Fokker-Planck equation (2), by supplementing it with boundary conditions at $n = n_0$ and $n = n_0 + L$. For this it is necessary that $k\tau >> 1$ and that $L >> k$; these conditions define the classical diffusive regime because they ensure that orbits dwell a long time inside the interaction region and that they experience a large number of almost uncorrelated kicks.

The appropriate boundary conditions are given by the balance of outgoing and incoming fluxes at the left and the right boundaries; outgoing fluxes can be estimated from f and its derivative f' and one gets[8]

$$-\frac{\bar{D}}{4}f'(n_0) = -\frac{k}{\pi}f(n_0) + \Phi_L^{(i)}$$

$$-\frac{\bar{D}}{4}f'(n_0+L) = -\frac{k}{\pi}f(n_0) - \Phi_R^{(i)} \tag{4}$$

where $\bar{D} = (2\beta - 1)D_0$ and $\Phi^{(i)}_{L,R}$ are the incoming fluxes from the left and the right respectively. The boundary value problem (2)(4) can be solved, and the solution can be used to express the outgoing fluxes $\Phi^{(o)}_{L,R}$ as functions of the incoming fluxes $\Phi^{(i)}_{L,R}$; in this way a "kinetic" solution of the scattering problem is obtained[8]. In particular, if $\Phi^{(i)}_{L,R}$ are constant in time , one gets

$$\Phi_R^{(o)} = \eta\Phi_L^{(i)} \tag{5}$$

with the transmission coefficient η given by :

$$\eta = \frac{\pi D}{\pi\bar{D} + 2kL} \tag{6}$$

The chaotic transport is characterized by this law (at large $L \gg k$). We call this transport "Ohmic" on account of the inverse dependence of η on L.

3. The quantization of the model is straghtforwardly achieved. The quantum discrete-time dynamics is defined by the unitary propagator:

$$\hat{U} = \hat{T}\hat{U}_0 \tag{7}$$

with $\hat{U}_0 = e^{ik\cos\theta}$,($\hbar = 1$) and

$$\hat{T} = \sum_{n=n_0}^{n_0+L} e^{-in^2\tau/2}|n><n| + (\sum_{n<n_0} + \sum_{n>n_0+L})|n><n| \tag{8}$$

where $|n>$ are the eigenstates of the quantized momentum $\hat{n}$. In the n-representation, the model describes the propagation of waves on the 1-d discrete lattice with sites labelled by the integer eigenvalues n of $\hat{n}$.

The free dynamics is defined by $\hat{U}_0$ and the "interaction" $\hat{T}$ is effective only inside the finite "scatterer" $n_0 \leq n \leq n_0 + L$. Quasi-energy eigenstates $|u^\lambda>$ are defined by the eigenvalue equation :

$$\hat{U}|u^\lambda> = e^{i\lambda}|u^\lambda> \tag{9}$$

Unperturbed quasi-energy eigenstates in the n-representation have the form of plane waves :

$$u_0^{\lambda,\alpha}(n) = (2\pi)^{-1/2}e^{-in\theta_\alpha} \tag{10}$$

where θ_α are the roots of the equation :

$$\lambda = k\cos\theta \qquad (mod 2\pi) \tag{11}$$

For any quasi-energy λ there are $N_\lambda \simeq 2k/\pi$ such roots, that define the "quasi-energy" shell at quasi-energy λ.

As is well known from the theory of the Quantum Kicked Rotator[7] the phase factors $e^{-in^2\tau/2}$ in eqn (8) have generically a pseudo-random character that can be held responsible for the onset of localization. Qualitatively, our quantum model describes a 1-d lattice dynamics, with free waves (10) impinging on a finite "disordered" scatterer, whence they are partly reflected and partly transmitted. This model therefore bears some resemblance to well-known tight-binding models used in the theory of mesoscopic fluctuations; but we wish to emphasize that unlike those models, the present one has a well defined classical limit, and this fact allows for a direct comparison of quantum and classical transport properties.

A complete description of the quantum scattering process is provided by the Scattering Matrix $S_{\alpha\beta}(\lambda)$, that determines the asymptotics of quasi-energy eigenfunctions (9) at large distance from the scatterer, in the form:

$$u^{\lambda}(n) \sim \sum_{\alpha=1}^{N_\lambda} a_\alpha(\lambda) u_{0,in}^{\lambda,\alpha}(n) +$$

$$+ \sum_{\alpha,\beta=1}^{N_\lambda} |\nu_\alpha|^{1/2} |\nu_\beta|^{-1/2} S_{\alpha\beta}(\lambda) a_\beta(\lambda) u_{0,out}^{\lambda,\beta}(n) \tag{12}$$

where $|\nu_\alpha| = 1/|\sin(\theta_\alpha)|$ is the density of states, $a_\alpha(\lambda)$ are arbitrary complex amplitudes, and the suffix *in* (resp. *out*) of a free plane wave means that that particular wave does actually appear in the sum only if, in the considered region (either far to the left or far to the right) it is incoming (resp. outgoing).

In order to compute the Scattering Matrix we adapted some standard methods of Scattering Theory to the case of discrete-time dynamics . Our method is summarized by the following eqs[8] :

$$S_{\alpha\beta}(\lambda) = \delta_{\alpha\beta} - |\nu_\alpha|^{1/2} |\nu_\beta|^{1/2} 2\pi < (\hat{T} - 1) u_0^{\lambda\alpha} | u_+^{\lambda\beta} > \tag{13}$$

$$\left[1 - e^{i\lambda} \hat{G}_+(\lambda)(\hat{T}^\dagger - 1)\right] u_+^{\lambda\alpha} = u_0^{\lambda\alpha} \tag{14}$$

$$\hat{G}_+(\lambda) = \lim_{\epsilon \to 0^+} \left(\hat{U}_0 - e^{i\lambda+\epsilon}\right)^{-1} \tag{15}$$

Since eqn (13) requires the values of u_+ only at sites inside the scatterer, the Lippman-Schwinger equation (14) actually calls for inverting a matrix of rank L+1.

Computing $\hat{G}_+(\lambda)$ is a crucial point. In order to do that, we had to substitute for the potential $V(\theta) = k\cos(\theta)$ a smooth approximation $2q\arctan(\xi\cos(\theta))$ which yields $k\cos(\theta)$ in the limit $\xi \to 0, q \to \infty, 2\xi q \to k$..

4. In our quantum computations we made a systematic use of "disorder averaging" defined as follows. As remarked above, the scatterer can be assimilated to a "sample" of a disordered solid : the finite string of pseudorandom numbers $T_k = exp(-ik^2\tau/2)$, $n_0 \le k \le n_0 + L$ plays a role similar to that of the random potential in tight-binding models. If n_0 is changed a different string is obtained , which corresponds to a different realization of the (pseudo-) random potential, i.e., to a different sample. Thus averaging over different choices of n_0 is equivalent to averaging over disorder in solid-state models.

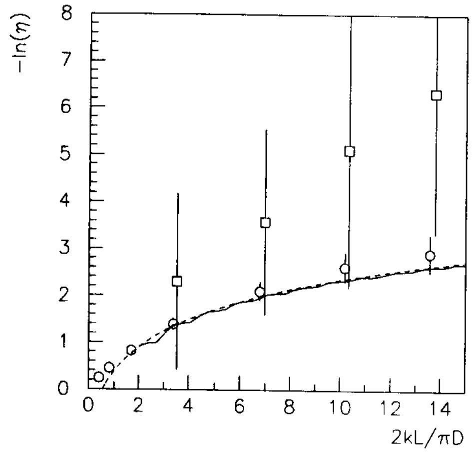

Figure 1

Average logarithm of the inverse transmission coefficient versus the scaled length $2kL/\pi D$ of the sample.Quantum data from averages over $50 - 100$ different samples. Circles: $q = 29, \xi = 1, 2\xi q\tau = 10$. Squares:$q = 29, \xi = 0.1, 2\xi q\tau = 10$. The dashed line is the classical theoretical prediction ,eqn.(11); continuous line, classical numerical.

Our model possesses two characteristic lengths: the localization length ℓ, which in the semiclassical regime ($k \sim 2\xi q >> 1, \tau << 1$) is approximately equal to the classical diffusion coefficient[9], and the mean free paths χ, which is roughly defined by the number of states coupled by the "free" propagator $\hat{U}_0$, so that $\chi \sim k$. The classical transmission coefficient (eqn. (6)) is a function of the scaled length L/χ.

The quantum transmission coefficient is defined as the sum of the squared moduli of all the S-matrix elements for transitions between free states with the same direction of propagation. In Fig.1 we show the logarithm of $1/\eta$ as a function of the scaled length; quantum data are averaged over $50 - 100$ realizations. Classical numerical data are in excellent agreement with the theoretical law (6); quantum data are shown for two different values of k that correspond to localization lengths $\ell = 26$ and $\ell = 880$. The maximum sample length in Fig.1 is L=410. The left-hand part of Fig.1 corresponds to the ballistic regime, where the sample length is less than or on the order of the mean free path. Moving to the right one approaches the localized regime, marked by an exponential decrease of the transmission coefficient and by huge fluctuations. The crossover between the ballistic and the localized regimes occur in the range $k < L < \ell$. Since ℓ is proportional to k^2, this range becomes broader, the larger k (i.e. in the semiclassical region) : in this range the quantum transmission coefficients follows more or less closely the classical "Ohmic" behaviour. We note in passing that our model behaves differently from 1d and quasi-1d models of the Anderson type, where the mean free path is proportional to the localization length. The reason of this difference is that here the number of channels is not fixed but it is proportional to the man free path.

Fluctuations of the S-matrix elements could be easily observed in our model on

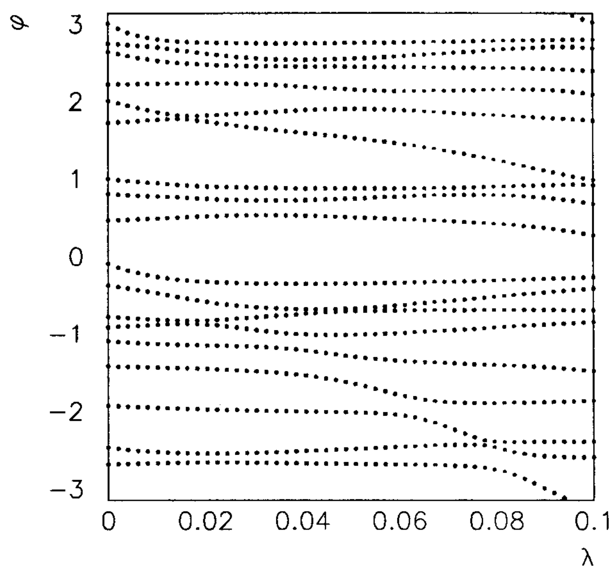

Figure 2

Phase shifts φ versus quasi-energy λ at $q = 15$, $\xi = 1.5, 2\xi q\tau = 10, L = 200$

changing the quasi energy. Fig 2 shows phase shifts versus quasi-energy in a small neighborhood of $\lambda = 0$, of size approximately equal to the correlation length for the same data. Following Ref[5], we computed the correlation function

$$\mathcal{C}_{\alpha\beta}(\omega) = \frac{|C_{\alpha\beta}(\omega)|^2}{|C_{\alpha\beta}(0)|^2} \tag{16}$$

$$C_{\alpha\beta}(\omega) = \overline{S^*_{\alpha\beta}(0) S_{\alpha\beta}(\omega)} \tag{17}$$

where the bar denotes disorder averaging. Typical results are shown in Fig.3. In the ballistic and close to ballistic cases, a Lorentzian fit proved very good over a large interval in ω; in other cases, relevant deviations were found only in the tails; in a minority of cases, deviations of $\mathcal{C}_{\alpha\beta}$ from the Lorentzian form were observed both at small and at large values of ω. The Lorentzian form of $\mathcal{C}_{\alpha\beta}(\omega)$ is consistent with some general predictions relying on semiclassical formulas for the Scattering Matrix[5]. According to that theory, the width of the Lorentzian curve should be approximately equal to the classical rate of exponential decay (inverse time of escape from the scatterer). This expectation was well confirmed in the case of Fig. 3 by a direct numerical computation of classical decay rates[8].

These results indicate that the ballistic regime of our model fits well in the general picture of chaotic Ericson-like fluctuations. More indications in this sense will be provided by the analysis of the Scattering Matrix from the viewpoint of random Matrix Theory, which is now in progress.

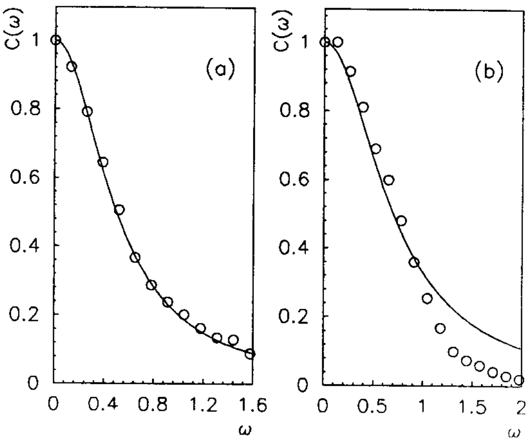

Figure 3

Squared moduli of some normalized quasi-energy autocorrelations of different S-matrix elements averaged over 100 different samples, for $\lambda = 0$ (band center) $2\xi q\tau = 10, \xi = 1.5, q = 15$.
(a):$L = 50$,(b):$L = 28$. Full lines are Lorentz curves of width corresponding to the average correlation length of 6 different $S-$matrix elements.

In conclusion we have described a model for diffusive chaotic scattering that is amenable to numerical simulation both in its classical and in its quantum mechanical version. The results summarized above show that this model displays the essential features of quantum transport in disordered conductors. Being endowed with a well defined chaotic classical limit, it is therefore apt to the investigation of transport fluctuations in the framework of chaotic scattering; we believe that, in spite of its abstract character it can provide some general indications, as it was the case for the Kicked Rotator of which it is a variant.

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