From closed to open 1D Anderson model: Transport versus spectral statistics

S. Sorathia,[1] F.M. Izrailev,[1,2,*] V.G. Zelevinsky,[2] and G.L. Celardo[3]

[1]Instituto de Física, Universidad Autónoma de Puebla - Apartado Postal J-48, Puebla, Pue., 72570, México
[2]NSCL and Dept. of Physics and Astronomy, Michigan State University - East Lansing, Michigan 48824-1321, USA
[3]Dipartimento di Matematica e Fisica, Università Cattolica,
via Musei 41, 25121, Brescia, and I.N.F.N., Sezione di Pavia, Italy

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We show that the transport properties of a one-dimensional Anderson model of finite size with weak disorder can be effectively expressed in terms of the repulsion parameter $0 \leq \beta \leq \infty$ in the level spacing distribution of eigenvalues of the corresponding closed system. This result stems from the detailed numerical analysis demonstrating that the normalized localization length of eigenstates is nothing but the parameter β. We give the analytical expressions for the mean transmission coefficient $\langle T \rangle$ and its variance $\mathrm{Var}(T)$, as well as for $\langle \ln T \rangle$ for *any* value of β and degree κ of coupling to continuum. The numerical data fully correspond to the analytical predictions.

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Introduction. In spite of a remarkable progress in understanding statistical properties of quantum systems, either deterministic or disordered, one of the important problems still waits for the detailed analysis. The specific question is: to what extent one can predict scattering properties of a complex *open* system, if we know global properties of eigenstates and energy spectra of the corresponding *closed* system? This problem was solved for a specific case of closed systems with maximal chaotic properties described by fully random matrices. A proper mathematical tool in these studies is based on effective non-Hermitian Hamiltonians of a certain structure [1], and many analytical results have been obtained, see, for example, [2–4]. The key point in this method is that the scattering matrix of an open system is expressed in terms of eigenvalues and eigenfunctions of the related closed system along with their decay amplitudes.

A much more difficult problem emerges if the closed system is not fully chaotic being characterized by an additional parameter related to the degree of chaos. Recently, this problem was analyzed numerically in Refs. [5] where the global characteristics of scattering or signal transmission through a system have been studied in dependence on two control parameters, the degree of internal chaos and the strength of coupling to continuum. In particular, it was found that, independently of the degree of chaos, the increasing continuum coupling leads the system from the quasistable regime of isolated narrow resonances to the "super-radiant" regime of overlapping resonances coexisting with long-lived compound states. However, the specific features of this evolution may critically depend on the degree of chaos and therefore the observation of the signal transmission provides important information on regular or chaotic character of intrinsic dynamics.

The above studies have been performed with the use of random matrices (canonical Gaussian ensembles or two-body random interactions). Some statistical assumptions may be questionable in application to realistic physical systems. Below we study the 1D Anderson model, paying main attention to the relation between the scattering properties of an open model and those of eigenstates and spectral statistics of the closed model. We discover unexpected effects that give a new insight to the problem of scattering through finite disordered systems.

The model. The tight-binding Anderson model is often used to describe electron propagation in random media. In the 1D case the corresponding Hamiltonian with diagonal disorder takes the standard form,

$$H_{mn} = \epsilon_n \, \delta_{mn} - \nu(\delta_{m,n+1} + \delta_{m,n-1}). \qquad (1)$$

Here ν is the hopping amplitude connecting the nearest sites (in what follows we set $\nu = 1$); the site energies ϵ_n are assumed to be uniformly distributed in the interval $-W/2$ to $W/2$ giving rise to the disorder variance $\sigma^2 = W^2/12$. Our interest is in the transmission properties through the samples of <u>finite size</u> N with the arbitrary *coupling amplitudes* $\sqrt{\gamma^L}$ and $\sqrt{\gamma^R}$ connecting the left and right edges with attached semi-infinite *ideal* leads (in which $\epsilon_n = 0$). In the case of zero disorder open tight-binding models have been studied in Refs. [6, 7]. As for non-zero disorder, so far, the main interest was related to the statistics and distributions of resonances for one open channel [8, 9]; the relation of the resonances to the transport properties was studied in [10].

Without disorder, the spectrum of the closed chain consists of Bloch waves with the nodes at the ends and energies inside the band $|E| \leq 2$. In the limit $N \to \infty$ and for weak disorder, $\sigma^2 \ll 1$, all eigenstates are exponentially localized with the characteristic length $l_\infty(E)$ given by the Thouless relation [11],

$$l_\infty(E) = 8\sigma^{-2}(1 - E^2/4). \qquad (2)$$

This expression is valid everywhere apart from the vicinity of the band edges, $|E| = 2$, and band center, $E = 0$.

Level repulsion in a closed model. To quantify the degree of chaos in the finite samples with no continuum couplings, $\gamma^L = \gamma^R = 0$, we employ the well known results of random matrix theory (RMT). The maximal chaos in deterministic quantum models with chaotic behavior in its classical counterpart is characterized by the Wigner-Dyson (WD) distribution $P(s)$ of normalized spacings s between the nearest energy levels. In the opposite case of integrable classical counterparts the level spacing distribution is typically close to the Poisson distribution. Therefore, one can take the distribution $P(s)$ as a measure of chaos in the closed Anderson model.

For zero disorder, the energy spectrum near the band center, $\epsilon_n = 0$, is equidistant, so that $P(s) \to \delta(s-1)$, the eigenstates are extended and regular. In the limit of strong disorder, all eigenstates are effectively localized on the scale of the sample size $N \gg 1$, thus resulting in the Poisson distribution. In between these limits, for $l_\infty \approx N$, one can expect that the eigenstates are *both* extended and "chaotic". By the last term we mean that the components of eigenstates are uncorrelated, with the distribution close to the Gaussian. In this region $P(s)$ is expected to be close to the WD-distribution. Thus, when passing from zero to strong disorder, the repulsion parameter β in $P(s)$ changes from $\beta = \infty$ to $\beta = 0$ with $\beta \approx 1$ in the intermediate case.

In order to describe the evolution of $P(s)$ in a large range of the values of β, we use, instead of the Brody interpolation [12], the expression suggested in Ref. [13],

$$P_\beta(s) = B_1 z^\beta (1 + B_2 \beta z)^{f(\beta)} e^{\left[-\frac{1}{4}\beta z^2 - \left(1-\frac{\beta}{2}\right)z\right]}, \qquad (3)$$

where $f(\beta) = \beta^{-1} 2^\beta \left(1 - \frac{\beta}{2}\right) - 0.16874$. Here $z = \pi s/2$ and the parameters B_1 and B_2 are determined by the normalization conditions, $\int_0^\infty P_\beta(s) ds = \int_0^\infty s P_\beta(s) ds = 1$. The function $f(\beta)$ is constructed in such a way that for the values $\beta = 1; 2; 4$, corresponding to the Gaussian ensembles of random matrices of a given symmetry (orthogonal, unitary and symplectic, respectively) it is close to the expressions for $P(s)$ obtained in the RMT for those ensembles [12]. As shown in Ref. [14], for these values of β, the dependence (3) is more accurate (in a whole range of s) than the WD surmise typically used in the literature. Note that for $\beta = 0$ Eq. (3) coincides with the Poisson distribution, and for $\beta = \infty$ it reproduces the delta-function. With Eq. (3) we performed a numerical study by changing the degree of disorder for a closed chain in a large range of the control parameter $x = l_\infty / N$ with l_∞ defined by Eq. (2), see examples in Fig. 1.

Our conclusion is that Eq. (3) gives an amazingly good correspondence (supported by the χ^2 criteria) with the numerical data in a very large range of x. It should be noted that Eq. (3) was obtained in Refs. [13, 14] by using the analytical expressions by Dyson [15] derived for the classical model of two-dimensional charged particles on a ring with the temperature $1/\beta$. For specific values of the inverse temperature $\beta = 1, 2, 4$ the partition function giving the probability to find the particles at specific positions on the ring in this *Coulomb gas model* is the same as for the canonical Gaussian ensembles. Therefore, one can make an unexpected conclusion that the distribution $P(s)$ for the Anderson model on a finite scale N can be described by the Dyson Coulomb gas model for which s is the distance between the nearest particles on a ring.

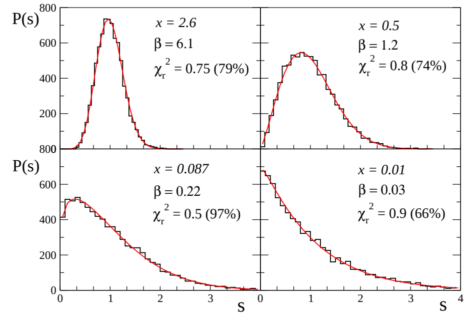

FIG. 1: Examples of $P(s)$ for $0.02 < |E| < 0.2$ (excluding the energies very close to 0), with $N = 1000$. The data are obtained for 120 disorder realizations with the χ^2-fit to Eq. (3) for $r = 40$ bins. Confidence levels are given in parenthesis.

Localization length vs. repulsion parameter. Now we can establish the relation between x and β. It is qualitatively clear that they express the same phenomenon of gradual transformation of standing waves into localized states. All the data are summarized in Fig. 2. We see a precise *linear dependence* between x and β in a whole range of x values independently of the chosen energy range. The fit of the data as $\beta = Ax + C$ gives the slope $A = 2.3 \pm 0.1$ with C essentially zero. This result, obtained carefully with the use of χ^2 statistical criteria, shows that the repulsion parameter β is nothing but the properly normalized localization length l_∞,

$$\beta \approx 2.34 \frac{l_\infty}{N}. \qquad (4)$$

The factor 2.34 in Eq. (4) can be attributed to the fluctuations of components of eigenstates.

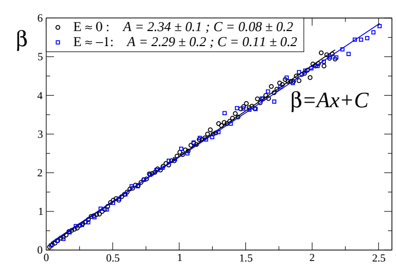

FIG. 2: Repulsion parameter β versus $x = l_\infty/N$ for $E \approx 0$, (circles), and $E \approx -1$ (squares), see details in Fig. 1.

The localization length l_∞ can be defined due to the Shannon entropy, $S = -\sum_{n=1}^N w_n \ln w_n$ with $w_n = \psi_n^2$. For completely random states with the Gaussian distribution of ψ_n one gets, $S = \ln(N/2.07)$. Thus, it is convenient to introduce the normalized *entropic localization length*, $d_N = 2.07\,N \exp\langle S\rangle$, where $\langle ...\rangle$ represent an ensemble average. With this definition we have $d_N = N$ for fully chaotic eigenfunctions occupying N sites. Our numerical data show that the onset of strong chaos occurs when $d_N \approx 2.1 l_\infty$ [16] which is equivalent to $\beta \approx d_N/N \approx 1$. Therefore, one arrives at the same result through an analysis of the spectrum as through the eigenstates.

Open model: Non-Hermitian Hamiltonian. The scattering properties of open systems can be formulated [1] with the effective non-Hermitian Hamiltonian [6, 8, 10, 16], where $\mathcal{D}(E) = E/2 - (i/2)\sqrt{4-E^2}$,

$$\mathcal{H}_{mn}(E) = H_{mn} + \mathcal{D}(E)(\gamma^L \delta_{n,1}\delta_{m,1} + \gamma^R \delta_{n,N}\delta_{m,n}). \quad (5)$$

This exact expression is valid for any disorder ϵ_n, continuum coupling γ^L, γ^R, and energy E. Near the center of the band (the general case of any energy, $-2 < E < 2$, is studied in Ref. [16]) it can be written as

$$\mathcal{H}_{mn}(E) = H_{mn} - \frac{i}{2} W_{mn}, \quad W_{mn} = 2\pi \sum_{c=L,R} A^c_m(0) A^c_n(0), \quad (6)$$

where $W(E)$ is defined by the coupling amplitudes,

$$A^{L,R}_n(E) = (\gamma^{L,R}/\pi)^{1/2}[1 - E^2/4]^{1/4}(\delta^{(L)}_{n,1} + \delta^{(R)}_{n,N}). \quad (7)$$

Here H_{mn} from Eq. (1) describes the internal dynamics, while the non-Hermitian part $W(E)$ is factorized in terms of the coupling amplitudes $A^c_n(E)$ between the internal states $|n\rangle$ and open decay channels labeled by $c = L, R$.

The non-Hermitian Hamiltonian (6) allows us to construct the scattering matrix S in the space of channels,

$$S = \frac{1 - i\pi K}{1 + i\pi K}, \quad (8)$$

where the reaction matrix K is defined as

$$K^{ab}(E) = \sum_j \frac{\tilde{A}^a_j \tilde{A}^b_j}{E - E_j}; \quad \tilde{A}^c_j = \sum_m A^c_m \psi_m(E_j), \quad (9)$$

and $\psi_m(E_j)$ is the m-component of the eigenstate $|j\rangle$ of the closed Hermitian Hamiltonian (1).

In the case of weak disorder, $\sigma^2 \ll 1$, the strength of coupling to the leads is characterized by the coupling parameter, $\kappa^c = 2\pi\gamma^c/ND$, calculated via the average scattering matrix. For this definition the channel transmission coefficient $\tau^c = 1 - |\langle S^{cc}\rangle|^2$ is maximal for *perfect coupling* when $\kappa^c = 1$. Here D is the mean level spacing at the center of the energy band in a closed chain, $\kappa^c = 0$. Below we consider the equiprobable coupling, $\gamma^c \equiv \gamma$, $\kappa^c \equiv \kappa$. The average scattering matrix can be written in the form $\langle S^{cc}\rangle = (1-\kappa)/(1+\kappa)$ and vanishes for perfect coupling. In all numerical simulations we take $N = 1000$ sites and combine an ensemble average over a large number of realizations with a spectral average over 1000 energies across an energy window $|E| < 0.2$.

Transport characteristics. It is known (see, for example, [17]) that, for continuous weak random potentials in 1D geometry, all transport characteristics for finite samples of length N depend on the ratio $N/L_\infty(E)$. Here L_∞ is the back-scattering length of scattering states that can be associated with the localization length l_∞ of eigenstates in infinite samples. This is the core of the *single parameter scaling* (SPS) [18]. Unlike the models with continuous potentials, the SPS is questionable for the tight-binding model (1). It is shown that at least at the band center, $E = 0$, the SPS fails [19]).

Below we demonstrate that the main results obtained for 1D disordered models can be also applied to the Anderson model provided the energy E is not very close to band center. For example, in the case of perfect coupling, the average transmission coefficient and its second moment ($q = 1$ and 2, respectively) are given by [17]

$$\langle T^q\rangle = \sqrt{\frac{2x^3}{\pi}} \exp\left(-\frac{1}{2x}\right) \int_0^\infty f_q(z) \exp\left(-\frac{z^2 x}{2}\right) dz;$$

$$f_1(z) = \frac{z^2}{\cosh z}; \qquad f_2(z) = \frac{2z^2 + z\sinh 2z}{4\cosh^3 z}, \quad (10)$$

which together define the variance of the transmission, $\mathrm{Var}(T) \equiv \langle T^2\rangle - \langle T\rangle^2$. Here $x = l_\infty/N$ with l_∞ defined by Eq. (2), and $\langle ...\rangle$ stands for the ensemble average. A simpler relation emerges for the self-averaged logarithm, $\langle \ln T\rangle = -2N/l_\infty$. Quite often, this expression serves as the definition of the localization length l_∞. Our numerical data for $\langle T\rangle, \langle T^2\rangle, \mathrm{Var}(T)$ and $\langle \ln T\rangle$ manifest excellent correspondence with Eqs. (10).

For non-perfect coupling we derived the following formula for $\langle \ln T\rangle$ which is valid for any coupling κ,

$$\langle \ln T\rangle = -\frac{2N}{l_\infty} + 2\ln\left[\frac{4\kappa}{(1+\kappa)^2}\right]. \quad (11)$$

Our data nicely correspond to this expression for $0.05 \le \kappa \le 10$ and $0.2 \le \beta \le 22$ with β defined by Eq. (4); $\beta = 1$ marks the strongest chaos in a closed system.

Another quantity of theoretical and experimental interest is the *reflectivity factor* F,

$$F = \frac{\langle R\rangle - \langle S^{cc}\rangle^2}{\langle T\rangle} \quad \text{with} \quad c = L, R, \quad (12)$$

where R and T are the reflection and transmission coefficients, respectively, and the term $\langle S^{cc}\rangle^2$ takes into account *direct scattering* emerging for a non-perfect coupling [5]. For perfect coupling, $\kappa = 1$, we have $\langle S^{cc}\rangle = 0$, and Eq. (12) with $R = 1 - T$ can be written explicitly with the use of Eq. (10). For non-perfect coupling, $\kappa \ne 1$, we found an approximate relation,

$$F = a_0(e^{a_1/\beta} - 1) + \frac{(1-\kappa)^2}{(1+\kappa)^2}, \quad (13)$$

that gives quite a good description of the data for $a_0 = 2.8$, $a_1 = 1.4$, see Fig. 3. For $\beta \to \infty$ the expression $F = (1-\kappa)^2/(1+\kappa)^2$ can be confirmed analytically. Our data demonstrate that the reflectivity factor strongly depends on the degree of internal disorder. It is remarkable that regardless of the coupling there is a sharp change in the value F at $\beta \approx 1$ corresponding to the onset of strong "chaos" in the closed system. Thus, measuring experimentally F one can observe the transition from extended to localized states on the scale of the sample size N.

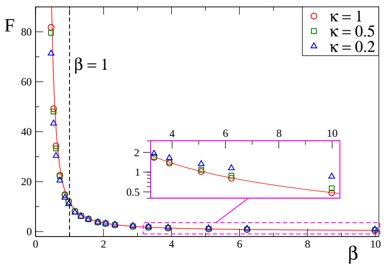

FIG. 3: Reflectivity factor versus the parameter $\beta = 2.34 l_\infty/N$ for $N = 1000$ and different couplings. Each symbol is obtained by an average over 1000 disorder realizations. The inset shows a closer view of the indicated section with a logarithmic scale on the vertical axis.

Conclusion. We studied the transport properties of the 1D Anderson model in dependence on the degree of internal chaos and strength of coupling to continuum. We found that the level spacing distribution $P(s)$ for a closed model of finite size N is well described by the phenomenological expression (3) in which the repulsion parameter β changes from $\beta = 0$ to $\beta = \infty$. This expression is originated from the two-dimensional Coulomb gas model with the temperature $1/\beta$, and gives the distribution of spacings between nearest charged particles moving on a ring. This fact may be used for further analytical studies of the spectrum statistics in the finite Anderson model.

In the closed model we established the linear relation between the repulsion parameter β and normalized localization length, l_∞/N, of the eigenfunctions. Thus, the repulsion parameter β reflects the transformation of the wave functions from localized states to extended standing waves. In a narrow region with $\beta \sim 1$ the properties of the model can be adequately described by the RMT.

Opening the system at the ends we used the effective non-Hermitian Hamiltonian to study the transport properties of the model. We demonstrated that the average transmission coefficient and its variance entirely depend on the parameter β for a given strength of continuum coupling. Finally, the reflectivity factor (the ratio of average fluctuative reflection to average transmission) is shown to be a universal function of the same parameter. We conclude that the transmission properties of the Anderson model provide a reliable tool for getting information on the degree of randomness and spectrum statistics in the closed system.

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* Electronic address: felix.izrailev@gmail.com

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