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Exact generalized Lyapounov exponents for one-dimensional disordered tight binding models

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Abstract. A conceptually simple procedure is given for computing the moments of the distribution of states of one-dimensional disordered tight binding models, from which generalized Lyapounov exponents are defined.

1. Introduction

Since the early work by Anderson [1] disordered tight binding models have been the subject of extensive analytical and numerical study, with important results for the low temperature transport properties of disordered materials [2] and, recently, for quantum chaos [3], where 'dynamical localization' may occur.

For one-dimensional models with random potential, it has been shown by Borland [4] and Mott and Twose [5] that eigenstates are always exponentially localized, no matter how small the disorder is. The natural quantities to investigate are therefore the Lyapounov exponent γ_0 and its generalizations γ_{2k} [6]. If $\{u_i\}$ are the components of a solution of energy E, they can be defined as follows

$$\gamma_0(E) = \lim_{n\to\infty} \frac{1}{n}\langle \log|u_n|\rangle \qquad \gamma_{2k}(E) = \lim_{n\to\infty} \frac{1}{2kn}\log\langle u_n^{2k}\rangle \tag{1}$$

where the average is taken over different realizations of the random potential. In the low disorder limit $\gamma_0(E)$ is affected by a complicated energy dependence due to resonances [7–9] at values $E = 2\cos(p/q\pi)$. For the generalized exponents γ_{2k}, resonances appear gradually, in increasing number as k increases.

An efficient way to compute the Lyapounov exponent γ_0 is by means of a transfer matrix, which explicitly constructs the solution of the tight binding equation, given the initial condition. The generalized exponents have been studied extensively in several papers by Pendry and others since 1982, in a systematic approach based on the symmetric group. The method involved the construction of a generalized transfer matrix by means of direct products of the transfer matrix, followed by a reduction of the matrix size. This generalized transfer matrix produces the average values of the required power of the quantity under consideration. In place of the components of states, Pendry investigated the closely related amplitudes of the transmission coefficient of the chain (for a list of references, consult [10]). The same approach, at the lowest level, may be found in the paper by Ishii [11].

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If the limit of infinite size is not taken in (1), and one refers to an ensemble of samples of N sites, the inverse of the exponents define lengths which obey scaling relationships. Calling ξ_N the inverse of γ_0 for N sites, Pichard [12] has investigated the scaling ansatz

$$\xi_N/N = f(\xi_\infty/N).$$

This relationship in one dimension is equivalent to the scaling of conductance in the more general analysis of Thouless [13] and Abrahams *et al* [14].

A different approach is based on the definition of an 'information length' [15], suited to samples which are not long enough for the average exponential tail to show up and which are less sensitive to fluctuations. It probes the bulk properties of eigenstates, rather than the tails, and has a remarkable scaling behaviour [16]. More generally one may describe the eigenstates through their fractal exponents [17, 18]. The fractal structure was first explored by Aoki [19], Sokoulis and Economou [20], and recent computations by Schreiber and Grussbach [21] on very long samples have firmly established the multifractal character of one-dimensional eigenstates for low disorder.

The aim of this paper is to provide a very simple method for computing the moments of the distribution of components of states $\langle u_n^k \rangle$ for any length n of the samples. They are related to the eigenvalues of matrices of a peculiar structure and size $k+1$. For $k = 2, 4$ it is easy to derive some exact results. In the limit of small disorder the phenomenon of resonances is easily explained together with the log-normal distribution of components, for large n. I start with a short account of known facts that will be useful in the discussion.

2. The transfer matrix approach

A one-dimensional tight binding model is described by a tridiagonal Hamiltonian with a random potential. The eigenvalue equation is

$$(Hu)_n = u_{n+1} + u_{n-1} + V_n u_n = E u_n. \tag{2}$$

The numbers $\{V_n\}$, which specify the potential, are independent random numbers distributed with the same density $P(V)$, with finite moments

$$V_k = \int P(V) V^k \, \mathrm{d}V. \tag{3}$$

For simplicity I take the odd moments to be zero, although this is not essential. The most investigated example is the Anderson model, with $P(V)$ non-zero in $[-W/2, +W/2]$, where it takes the constant value $1/W$.

The boundary conditions are $u_0 = 0$ and $u_1 = 1$: with this choice all components u_n are proportional to u_1 with coefficients which depend on the random numbers V_k, with $k < n$.

It is worth noting that (2) has the same recursive structure as the expansion of the determinant of a tridiagonal matrix. In this case, if H_n is the $n \times n$ matrix with structure

$$H_n = \begin{bmatrix} V_n & 1 & & \\ 1 & & & \\ & & & H_{n-1} \end{bmatrix} \tag{4}$$

and if $D_n(E) = \det(E - H_n)$, we have the expansion formula

$$D_n(E) = (E - V_n)D_{n-1}(E) - D_{n-2}(E) \tag{5}$$

and the identification $u_{n+1}(E) = u_1 D_n(E) = u_1 \prod_{i=1}^{n}(E - E_i)$.

The boundary condition $u_{N+1}(E) = 0$ clearly becomes the equation for the eigenvalues of H_N, the Hamiltonian for the finite sample of N sites. However, if no restriction on the size of N is imposed, and one considers H_∞ on the half-line, it is straightforward to derive the Thouless formula [22]

$$\gamma_0(E) = \lim_{N\to\infty} \frac{1}{N} \log|u_{N+1}| = \int \mathrm{d}E'\, \rho(E') \log|E - E'| \tag{6}$$

which relates the Lyapounov exponent to the spectral density $\rho(E)$ of H_∞.

An efficient technique with which to evaluate the Lyapounov exponents numerically is by means of transfer matrices [23]. The recursive relationship (2) can be translated into a powerful multiplicative procedure by introducing 2×2 transfer matrices:

$$\begin{pmatrix} u_{n+1} \\ u_n \end{pmatrix} = \begin{bmatrix} E - V_n & -1 \\ 1 & 0 \end{bmatrix} \begin{pmatrix} u_n \\ u_{n-1} \end{pmatrix}. \tag{7}$$

Iterating the process, one ends up with a product matrix that propagates the initial condition (u_1, u_0) to any site. This matrix has determinant one and eigenvalues which approach $\exp[\pm n\gamma_0(E)]$ asymptotically, as a consequence of a theorem by Fustemberg on the product of random matrices [24]. The large eigenvalue, for a given value E, describes the exponential growth in n of $|u_n|$. To observe the exponential decay, characteristic of eigenstates, the knowledge of an energy eigenvalue E is required with exponential precision, to avoid the rapid growth that would follow from rounding errors. In fact, by computer, one usually explores the expanding domain of the 'transfer map' $(u_n, u_{n-1}) \to (u_{n+1}, u_n)$.

The matrix elements of the transfer matrix connecting both ends of the disordered chain allow the transmission coefficient to be computed, as well as the Lyapounov exponent. The transmission coefficient can be related to measurable quantities such as the resistance via Landauer's formula [25]. The connection can be made simpler with a change of basis, as shown by Pichard [12]; the same basis is used in Pendry's papers.

3. The free chain

The free model ($V_n = 0$) is useful for the explanation of the rational anomalies of γ_0 and to perform a kind of perturbation theory with small disorder. Equation (2) without disorder is easily solved by plane waves:

$$u_n^{(0)} = \sin(\omega n)/\sin\omega \qquad E = 2\cos\omega. \tag{8}$$

A special case is given by the 'band-edge' $|E| = 2$, for which the solutions are $u_n^{(0)} = n$ and $u_n^{(0)} = (-1)^n n$, respectively for $\omega = 0, \pi$.

For a finite sample of length N, the condition $u_{N+1} = 0$ implies $\omega = k\pi/(N+1)$, $k = 1, \ldots, N$.

For future reference, it is useful to note the following binomial expansion of (8):

$$(u_n^{(0)})^{2k} = \frac{1}{(4\sin^2\omega)^k} \sum_{r=0}^{2k} \binom{2k}{r} (-1)^{k-r} x_r^n \qquad x_r = \mathrm{e}^{2\mathrm{i}\omega(k-r)} \tag{9}$$

which will have a parallel for averages $\langle u_n^{2k} \rangle$ in the presence of disorder, the phases x_r being replaced by quantities which may have a modulus larger than one. Note also that only in the case of rational values of ω will there be more than one phase equal to one, for a given power $2k$.

In the next section I will compute the average values of u_n^k in the presence of disorder at a given value of the energy E and given site n.

4. The first and the second moment

The average value of a function $f(V_1, \ldots, V_n)$ is defined in the obvious way:

$$\langle f \rangle = \int \mathrm{d}V_1 \ldots \mathrm{d}V_n \, P(V_1) \ldots P(V_n) f(V_1, \ldots, V_n). \tag{10}$$

It is crucial to note the fact that u_k depends only on the variables $V_1, \ldots, V_{k-1}$. The method of computing the average values $\langle u_n^k \rangle$ is then simply stated: take the power k of equation (2) and average; some averages factorize, for the above remark; for the other terms build new recurrence relations based on (2). Finally, translate these relationships into matrix form, to obtain the generalized matrix $T^{(k)}(E, W)$, where the energy E and the disorder strength W are given.

The first moment is obtained by directly averaging equation (2)

$$\langle u_{n+1} \rangle = E\langle u_n \rangle - \langle u_{n-1} \rangle \tag{11}$$

with a solution that coincides with the free solution (8)

$$\langle u_n(E) \rangle = u_n^{(0)}(E). \tag{12}$$

More interesting is the next moment. By squaring (2) and averaging one obtains

$$\langle u_{n+1}^2 \rangle = \langle (E - V_n)^2 \rangle \langle u_n^2 \rangle - 2\langle E - V_n \rangle \langle u_n u_{n-1} \rangle + \langle u_{n-1}^2 \rangle. \tag{13a}$$

For the cross term we obtain a useful relationship by multiplying (2) by u_n and averaging:

$$\langle u_{n+1} u_n \rangle = \langle E - V_n \rangle \langle u_n^2 \rangle - \langle u_n u_{n-1} \rangle. \tag{13b}$$

One may now compute the averages $\langle (E-V)^2 \rangle = E^2 + V_2$ etc, but it is more useful to keep the symbolic notation for some time. The two equations (13a) and (13b) can be put in matrix form

$$\begin{pmatrix} \langle u_{n+1}^2 \rangle \\ \langle u_{n+1} u_n \rangle \\ \langle u_n^2 \rangle \end{pmatrix} = \begin{bmatrix} \langle (E-V)^2 \rangle & -2\langle (E-V) \rangle & 1 \\ \langle (E-V) \rangle & -1 & 0 \\ 1 & 0 & 0 \end{bmatrix} \begin{pmatrix} \langle u_n^2 \rangle \\ \langle u_n u_{n-1} \rangle \\ \langle u_{n-1}^2 \rangle \end{pmatrix} \tag{14}$$

where now the 3×3 transfer matrix $T^{(2)}$ is independent of the position n and may be therefore taken to any power to construct the second moment for any site n starting from the initial state $(1,0,0)$. The basic knowledge that is needed is the eigenvalues, which solve a cubic equation

$$x^3 - x^2(E^2 - 1 + V_2) + x(E^2 - 1 - V_2) - 1 = 0. \tag{15}$$

The solution $\langle u_n^2 \rangle$ takes therefore the form

$$\langle u_n^2 \rangle = a_1 x_1^n + a_2 x_2^n + a_3 x_3^n. \tag{16}$$

It is easy to check that the cubic equation always has a single root greater than one, which determines the diverging behaviour of $\langle u_n^2 \rangle$ with increasing n.

The coefficients a_i may be found either from the similarity transformation which diagonalizes the transfer matrix, built with the left and right eigenvectors, or through the initial conditions $\langle u_0^2 \rangle = 0$, $\langle u_1^2 \rangle = 1$, $\langle u_2^2 \rangle = E^2 + V_2$. Taking into account equation (15) one finds

$$a_i = \frac{1 + x_i}{3x_i^2 - 2x_i(E^2 - 1 + V_2) + (E^2 - 1 - V_2)}. \tag{17}$$

Some special cases of the cubic equation (15) are particularly simple.

For the centre of the spectrum $E = 0$, putting $V_2 = 2 \sinh \alpha$ one calculates the roots

$$x_1 = -1 \qquad x_{2,3} = \tfrac{1}{2}[V_2 \pm \sqrt{V_2^2 + 4}] = \pm e^{\pm\alpha} \tag{18a}$$

with solution

$$\langle u_n^2 \rangle = \frac{e^{n\alpha} - (-1)^n e^{-n\alpha}}{\cosh \alpha}. \tag{18b}$$

When the disorder V_2 is large compared with E^2, one is essentially in this case.

A peculiar situation is found at the 'edge of the spectrum' $E = 2$, which is a resonant case. The cubic equation can be written in the form

$$(x - 1)^3 = x(x + 1)V_2 \tag{19a}$$

and for small disorder one finds

$$x_k = 1 + (2V_2)^{1/3} e^{2ik\pi/3} + \cdots \qquad (k = 1,2,3). \tag{19b}$$

The case of zero disorder, whose result we already know (see equation (9)), has eigenvalues $x_1 = 1$, $x_{2,3} = \exp(\pm 2i\omega)$, $(E = 2\cos\omega)$. They are the starting point for a low disorder expansion. The result is

$$x_1 = 1 + \frac{2V_2}{4 - E^2} + \frac{2V_2^2}{(4 - E^2)^2} + \cdots \qquad x_{2,3} = e^{\pm 2i\omega}\left(1 - \frac{V_2}{4 - E^2} + \cdots\right) \tag{20}$$

5. Higher moments

The procedure is easily generalized to higher moments k, which involves transfer matrices of size $k+1$ which have a peculiar structure. For evaluating $\langle u_n^k(E)\rangle$ one defines a column vector with components $\langle u_{n+1}^{k+1-i}u_n^{i-1}\rangle$, $i=1,\ldots,k+1$, and a transfer matrix $T^{(k)}(E,W)$ with rows $r=1,\ldots,k+1$ given by the terms in the binomial expansion of $\langle(E-V-1)^{k+1-r}\rangle$. These matrices have the property of being factorized by the transfer matrix with zero disorder $T^{(k)}(E,0)$ times a lower triangular matrix with only disorder terms and no energy parameter E.

The eigenvalues of the matrix $T^{(2k)}(E,0)$ for the moment of order $2k$ are precisely the $2k+1$ complex numbers x_r of equation (9); one of them is always equal to one. However, the phases equal to one become more numerous for rational values of ω in $E=2\cos\omega$, leading to small disorder corrections which are computed by means of the perturbation theory of degenerate eigenvalues. This is the source of the resonant behaviour that affects the generalized exponents at more and more rational ω values as $2k$ increases.

As an example, let us consider the case $2k=4$. The transfer matrix is

$$T^{(4)}(E,W)=\begin{bmatrix}\langle(E-V)^4\rangle & -4\langle(E-V)^3\rangle & 6\langle(E-V)^2\rangle & -4\langle(E-V)\rangle & 1\\ \langle(E-V)^3\rangle & -3\langle(E-V)^2\rangle & 3\langle(E-V)\rangle & -1 & 0\\ \langle(E-V)^2\rangle & -2\langle(E-V)\rangle & 1 & 0 & 0\\ \langle(E-V)\rangle & -1 & 0 & 0 & 0\\ 1 & 0 & 0 & 0 & 0\end{bmatrix}$$

$$=\begin{bmatrix}E^4 & -4E^3 & 6E^2 & -4E & 1\\ E^3 & -3E^2 & 3E & -1 & 0\\ E^2 & -2E & 1 & 0 & 0\\ E & -1 & 0 & 0 & 0\\ 1 & 0 & 0 & 0 & 0\end{bmatrix}\begin{bmatrix}1 & 0 & 0 & 0 & 0\\ 0 & 1 & 0 & 0 & 0\\ V_2 & 0 & 1 & 0 & 0\\ 0 & 3V_2 & 0 & 1 & 0\\ V_4 & 0 & 6V_2 & 0 & 1\end{bmatrix}. \tag{21}$$

The eigenvalue equation is of fifth order:

$$x^5-A_4x^4+A_3x^3-A_2x^2+A_1x-1=0 \tag{22}$$

where the coefficients are

$$A_4=V_4+3V_2(2E^2-1)+(E^4-3E^2+1)$$
$$A_3=-3V_2V_4+(6V_2^2-V_4)(3E^2-1)+3V_2(E^4-2E^2-1)+(E^2-2)(E^4-3E^2+1)$$
$$A_2=-3V_2V_4+V_4(3E^2-1)+18V_2^3-3V_2(E^4-2E^2-1)+(E^2-2)(E^4-3E^2+1)$$
$$A_1=-V_4+6V_2^2-3V_2(2E^2-1)+(E^4-3E^2+1).$$

In the case of zero disorder, the five roots of the equation (22) are

$$e^{\pm 4i\omega}\qquad e^{\pm 2i\omega}\qquad 1. \tag{23}$$

They coincide with the phases x_r in equation (9) for $2k=4$. If we exclude the exceptional cases where more than one root is equal to 1, the leading behaviour for small disorder is given by the perturbation to the single eigenvalue $x_1\simeq 1$. One finds that

$$x_1=1+6V_2/(4-E^2). \tag{24}$$

For the centre of the band, the eigenvalue equation is easily factorized into

$$(x^2 + 3V_2 - 1)[x^3 - x^2(V_4 + 1) + x(V_4 - 1 - 6V_2^2) + 1] = 0 \quad (25a)$$

for which the only root greater than one belongs to the cubic factor; for small disorder

$$x_1 = 1 + \sqrt{3}V_2 + \tfrac{1}{4}(3V_2^2 + V_4) + \cdots. \quad (25b)$$

At the band edge, since for small disorder the equation is

$$(x - 1)^5 = 21x(x - 1)^2(x + 1)V_2 + \cdots \quad (26a)$$

one obtains

$$x_1 = 1 + (42V_2)^{1/3} + \cdots. \quad (26b)$$

The sextic case is extremely laborious to work out by hand. Here I confine myself to a perturbative treatment of the non-degenerate case. The left and right eigenvectors with eigenvalue $x_1 = 1$ of the matrix $T^{(6)}(E, 0)$ are

$$\begin{aligned} L &= (1, -3E, 3 + 3E^2, -E^3 - 6E, 3 + 3E^2, -3E, 1) \\ R &= \left(1, \frac{E}{2}, \frac{E^2 + 1}{5}, \frac{E^3 + 6E}{20}, \frac{E^2 + 1}{5}, \frac{E}{2}, 1\right). \end{aligned} \quad (27)$$

They are not normalized; the L vector is equivalent to the eigenvector of the transposed matrix $T^{(6)t}$. If M is the perturbation matrix at lowest order, $M = T^{(6)}(E, W) - T^{(6)}(E, 0)$ with V_4 and V_6 set to zero, the correction of order V_2 to the eigenvalue $x_1 = 1$ is

$$\delta x_1 = \frac{L^t M R}{L^t R} = 12\frac{V_2}{4 - E^2}. \quad (28)$$

6. Conclusions

For large n, the behaviour of $\langle u_n^{2k} \rangle$ is dominated by the largest eigenvalue x_1 of the generalized transfer matrix $T^{(2k)}$, the other contributions being exponentially smaller. The log of this eigenvalue, divided by $2k$, gives the exponent γ_{2k} of equation (1) precisely. For small disorder we obtained

$$\gamma_2 = \frac{V_2}{4 - E^2} \qquad \gamma_4 = \frac{3}{2}\frac{V_2}{4 - E^2} \qquad \gamma_6 = 2\frac{V_2}{4 - E^2}. \quad (29)$$

These results are consistent with the hypothesis that for large n and small disorder the distribution of the amplitude $s = |u_n|$ is of log-normal type [26]. The broadness of such distribution, increasing with n, is the source of the important physical phenomenon of mesoscopic fluctuations [27, 28]. The same distribution was introduced by Pendry for the resistance in the weak disorder limit [29].

The probability density of a log-normal distribution is

$$p(s) = \sqrt{\frac{\beta}{\pi}} \frac{1}{s} e^{-\beta(\log s - \mu)^2} \qquad s > 0. \tag{30}$$

With this distribution we compute the Lyapounov exponent

$$\gamma_0 = \frac{1}{n}\langle \log s \rangle = \frac{1}{n}\mu \tag{31}$$

and the generalized Lyapounov exponents

$$\gamma_{2k} = \frac{1}{2kn} \log\langle s^{2k} \rangle = \frac{1}{n}\left(\frac{k}{2\beta} + \mu\right). \tag{32}$$

The generalized Lyapounov exponents coincide with the perturbative values (29) provided that the following choice is made for the parameters:

$$\mu = \frac{1}{2\beta} \qquad \frac{1}{\beta} = n\frac{V_2}{4 - E^2}. \tag{33}$$

Moreover, equation (31) gives us the correct small disorder limit for γ_0, which may be checked against the expansion given in [7].

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