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1989 J. Phys.: Condens. Matter 1 2017

(http://iopscience.iop.org/0953-8984/1/11/009)

J. Phys.: Condens. Matter 1 (1989) 2017–2023. Printed in the UK

A self-consistent approximation method for the Lyapunov exponents in the Anderson localisation problem

K M Slevin
Blackett Laboratory, Imperial College, London SW7 2BZ, UK

Received 27 April 1988, in final form 3 October 1988

Abstract. We develop a self-consistent approximation for the Lyapunov exponents of a product of random matrices using a weak-disorder expansion. We compare our results with those of published simulations.

1. Introduction

Lyapunov exponents are widely used in studying the electronic properties of disordered systems. They are of relevance to studying such physical quantities as the conductance, density of states, magnetisation and free energy. Numerical simulation methods [1, 2] for calculating exponents have produced important results concerning the scaling theory of localisation [3] and the distribution of Lyapunov exponents [4].

In one dimension, analytic methods [5, 6] and weak-disorder expansions [7–9] allow easy calculation of the Lyapunov exponents for this case and have proved very useful in understanding electron localisation in one dimension. In two and three dimensions the problem is more difficult. In [10, 11] an explicit expression for the sum of the positive Lyapunov exponents was obtained, whereas in [12] a weak-disorder expansion for the Lyapunov exponents of a product of random matrices describing a multi-channel system was developed. However, applied to the two-dimensional localisation problem, the expansion is not valid for energies inside the bands of the averaged system.

In this paper, we show how to use a weak-disorder expansion to calculate the exponents at all energies. The basic idea is to use a basis of decaying waves, rather than the standard plane waves, to describe a localised state. We then make the decay lengths of our basis consistent with the exponents estimated from the weak-disorder expansion. This gives us a self-consistent approximation for the Lyapunov exponents.

2. Weak-disorder expansion

In this section, we develop a weak-disorder expansion for the Lyapunov exponents of a product of random matrices $\mathbf{T}_L$ where

$$\mathbf{T}_L = \prod_{n=1}^{L} (\mathbf{A} + \mu \mathbf{B}_n). \tag{1}$$

0953-8984/89/112017 + 07 $02.50

Matrix $\mathbf{A}$ is a fixed diagonal matrix with the form

$$A_{ij} = w_i \delta_{ij} \tag{2}$$

where $|w_i| \neq |w_j|$ if $i \neq j$. Matrix $\mathbf{B}_n$ is a random matrix. In the limit that L tends to infinity a limiting matrix Γ exists [13] where

$$\Gamma = \lim_{L\to\infty} (\mathbf{T}_L^* \mathbf{T}_L)^{1/2L}. \tag{3}$$

The Lyapunov exponents are defined as the logarithms of the eigenvalues of the matrix Γ. So, if n_i is the ith eigenvalue of $\mathbf{T}_L$ and τ_i is the ith Lyapunov exponent, then

$$\tau_i = \lim_{L\to\infty} (1/L) \operatorname{Re}(\log n_i). \tag{4}$$

We can expand the product in (1) as series in powers of μ:

$$\mathbf{T}_L = \mathbf{A}^L + \mu\mathbf{C} + \mu^2\mathbf{D} + \mathrm{O}(\mu^3) \tag{5}$$

where

$$\mathbf{C} = \sum_{n=1}^{L} \mathbf{A}^{L-n}\mathbf{B}_n\mathbf{A}^{n-1} \tag{6}$$

$$\mathbf{D} = \sum_{n>m} \mathbf{A}^{L-n}\mathbf{B}_n\mathbf{A}^{n-m-1}\mathbf{B}_m\mathbf{A}^{m-1} \tag{7}$$

using standard perturbation theory we obtain the ith eigenvalue n_i of $\mathbf{T}_L$ as

$$n_i = w_i^L + \mu C_{ii} + \mu^2 D_{ii} + \mu^2 \sum_{j\neq i} \frac{C_{ij}C_{ji}}{w_i^L - w_j^L} + \mathrm{O}(\mu^3). \tag{8}$$

If we expand the logarithm of (8), substitute for matrices $\mathbf{C}$ and $\mathbf{D}$ and take the limit as $L \to \infty$, we obtain

$$\tau_i = \operatorname{Re}\left(\log w_i + \mu \frac{\langle B_{ii}\rangle}{w_i} - \frac{\mu^2\langle B_{ii}^2\rangle}{2w_i^2} - \sum_{|w_j|>|w_i|} \frac{\mu^2\langle B_{ij}B_{ji}\rangle}{w_i w_j} \right) \tag{9}$$

where averages are calculated as

$$\langle B_{ij}B_{rs}\rangle = \frac{1}{L}\sum_{n=1}^{L} B_{n,ij}B_{n,rs} \tag{10}$$

With L tending to infinity. Here we are only able to take the limit as L tends to infinity to obtain (9) if the modulus of the ith eigenvalue of $\mathbf{A}$ is different from the modulus all other eigenvalues of $\mathbf{A}$. This is the origin of the previously stated condition on the eigenvalues of $\mathbf{A}$.

It should be noted that the first- and second-order terms in (5) may not be the largest corrections to $\mathbf{T}_L$, when μ is non zero, for large L. The application of perturbation theory, to obtain (8), may therefore seem inappropriate. However, what we are interested in is the small-μ expansion of the logarithms of the eigenvalues $\mathbf{T}_L$, and the first- and second-order terms are the largest corrections to these.

If we set $\langle\mathbf{B}\rangle = 0$ and re-order $\mathbf{A}$ so that $|w_i| > |w_j|$ if $i < j$, then (10) is equivalent to the result obtained in [12] by a different method.

3. Application of the expansion

We consider a two-dimensional bar of width M atoms. We write the wavefunction for the bar as a linear combination of atomic orbitals

$$\varphi(\boldsymbol{r}) = \sum_{n,m} a_{n,m}\varphi_{n,m}(\boldsymbol{r} - \boldsymbol{R}_{n,m}) \tag{11}$$

where $n = 1, L$ and $m = 1, M$ and $\boldsymbol{R}_{n,m}$ is the position vector of the (n, m) lattice site.

We use a tight-binding Hamiltonian with nearest-neighbour hopping only:

$$(E - E_{n,m})a_{n,m} - V\beta(a_{n,m-1} + a_{n,m+1}) - V(a_{n-1,m} + a_{n+1,m}) = 0. \tag{12}$$

Here E is the Fermi energy, $E_{n,m}$ is the site energy of the atom at the (n, m) lattice site and V is the hopping integral to nearest neighbours along the chain and βV the hopping integral to nearest neighbours across the chain. We can write this in transfer matrix form as

$$\boldsymbol{u}_{n+1} = \mathbf{M}_n \boldsymbol{u}_n \tag{13}$$

where $\boldsymbol{u}_n^{\mathrm{T}} = (a_{n,1}, \ldots, a_{n,M}, a_{n-1,1}, \ldots, a_{n-1,M})$ and $\mathbf{M}_n$ is a $2M \times 2M$ matrix of the form

$$\mathbf{M}_n = \begin{bmatrix} \mathbf{H}_n & -\mathbf{I} \\ \mathbf{I} & 0 \end{bmatrix} \tag{14}$$

where $\mathbf{H}_n$ is an $M \times M$ matrix given by

$$[\mathbf{H}_n]_{i,j} = (E - E_{n,i})\delta_{i,j}/V - \beta\delta_{i,j\pm 1}. \tag{15}$$

It is usual to use units where $V = 1$ and to measure energies in units of the hopping integral V. We assume that the site energies $E_{n,m}$ are independent, identically distributed random variables and we choose the zero of energy so that the average is zero.

We impose fixed boundary conditions ($a_{n,M+1} = a_{n,0} = 0$) and define a $2M \times 2M$ matrix $\mathbf{Q}$ by

$$\mathbf{Q}^{-1} = \begin{bmatrix} \boldsymbol{x}_q & \boldsymbol{x}_q \\ w_{-q}\boldsymbol{x}_q & w_q\boldsymbol{x}_q \end{bmatrix} \tag{16}$$

where $\boldsymbol{x}_q$ are column vectors with $1 \leqslant q \leqslant M$ and $[\boldsymbol{x}_q]_j = \sin(k_q j)$ and

$$E - E_c^q - 2\beta\cos(k_q) = 2\cos(\varphi_q) \tag{17}$$

with $k_q = \pi q/(M + 1)$, $w_q = \exp(\mathrm{i}\varphi_q)$ and $w_{-q} = \exp(-\mathrm{i}\varphi_q)$. For the moment we regard the φ_p as variable parameters and $\mathbf{Q}$ as a function of these. We similarity transform the transfer matrix and define matrices $\mathbf{A}$ and $\mathbf{B}$ by

$$\mathbf{A} + \mu\mathbf{B}_n = \mathbf{Q}\mathbf{M}_n\mathbf{Q}^{-1} \tag{18}$$

where $\mathbf{A}$ is a diagonal matrix of form

$$A_{p,q} = w_q\delta_{p,q} \qquad 1 \leqslant p, q \leqslant 2M \tag{19}$$

with

$$w_{q+M} = w_{-q} \qquad 1 \leqslant q \leqslant M. \tag{20}$$

Matrix $\mathbf{B}$ is given by

$$\mu\mathbf{B}_n = \begin{bmatrix} \mathbf{C}_{n,1} & \mathbf{C}_{n,1} \\ \mathbf{C}_{n,2} & \mathbf{C}_{n,2} \end{bmatrix} \tag{21}$$

where the sub-matrices $\mathbf{C}$ are the $M \times M$ matrices given below:

$$[\mathbf{C}_{n,1}]_{p,q} = -w_p\alpha_p(\Omega_{p,q}^n - E_c^q\delta_{p,q}) \tag{22}$$

$$[\mathbf{C}_{n,2}]_{p,q} = -w_{-p}\alpha_{p+M}(\Omega^n_{p,q} - E^q_c\delta_{p,q}) \tag{23}$$

and where

$$\alpha_q = 1/2\mathrm{i}\sin(\varphi_q) \qquad 1 \leqslant q \leqslant M \tag{24}$$

$$\alpha_{q+M} = -\alpha_q \qquad 1 \leqslant q \leqslant M \tag{25}$$

and finally

$$\Omega^n_{p,q} = \frac{2}{(M+1)}\sum_{j=1}^{M} E_{n,j}\sin(k_p j)\sin(k_q j) \tag{26}$$

with $1 \leqslant p, q \leqslant M$.

Provided that we choose the φ_p parameters such that the set of values $\{\mathrm{Re}(\mathrm{i}\varphi_p); i = 1, \ldots, M\}$ are all distinct (equivalent to the moduli of the eigenvalues of $\mathbf{A}$ all being distinct), we may apply the expansion developed in § 2. Doing so and noting that we can immediately re-sum all terms at all orders which do not depend on the disorder, we obtain

$$\tau_p = \mathrm{Re}\left(\mathrm{i}\theta_p - \alpha_p^2 g_{pp}\frac{\langle E^2\rangle}{2} - \sum_{|w_q|>|w_p|}\alpha_p\alpha_q g_{pq}\langle E^2\rangle\right) \tag{27}$$

where

$$g_{pq} = \frac{4}{(M+1)^2}\sum_{j=1}^{M}\sin^2(k_p j)\sin^2(k_q j) \tag{28}$$

and

$$2\cos(\theta_p) = E - 2\beta\cos(k_p) \tag{29}$$

and $\langle E^2\rangle$ is the variance of the site energies.

In previous work on weak-disorder expansions [12], it has been usual to use a basis of travelling waves. Inside an energy band this means that at least two of the eigenvalues of $\mathbf{A}$ have the same modulus. For example, for at least one q, $|w_q| = |w_{q+M}| = 1$. Here, by using a basis of decaying waves, we are able to break this degeneracy, $|w_q| = 1/|w_{q+M}| \neq 1$, and so we are able to apply the expansion. The price that we pay is that we must now justify a choice of φ_p parameters. In § 4, we do this using a self-consistency argument.

4. Self-consistent procedure

In this section, we explain how the φ_p $(p = 1, M)$ parameters are calculated. A given set of φ_p values corresponds to a basis of decaying waves, the inverse of the pth decay length being $\mathrm{Re}(\mathrm{i}\varphi_p)$. Suppose that we start with some initial set of values for the φ_p parameters and then estimate the Lyapunov exponents by evaluating the perturbation series (27). This gives us a new set of decay lengths. We choose the φ_p values so that these two sets of lengths are identical. From (27) it is clear that, for this choice of φ_p values,

$$\mathrm{i}\varphi_p - \mathrm{i}\theta_p + \alpha_p^2 g_{pp}\frac{\langle E^2\rangle}{2} + \sum_{|w_q|>|w_p|}\alpha_p\alpha_q g_{pq}\langle E^2\rangle = 0 \qquad (p = 1, M). \tag{30}$$

The problem thus becomes to find the zero of M non-linear complex equations in M

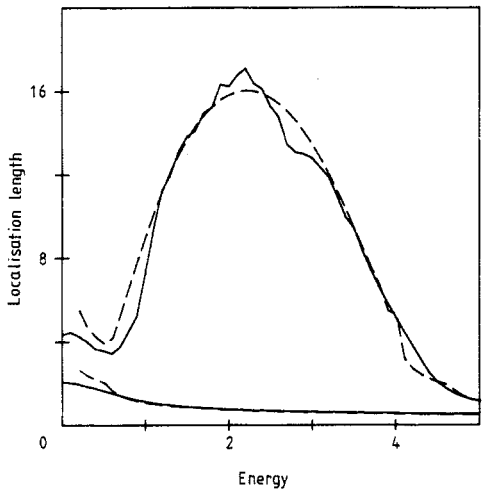

Figure 1. Localisation lengths for a chain width $M = 2$, disorder $W = 2$ and inter-chain coupling $\beta = 2$: ——, simulation; – – –, perturbation theory.

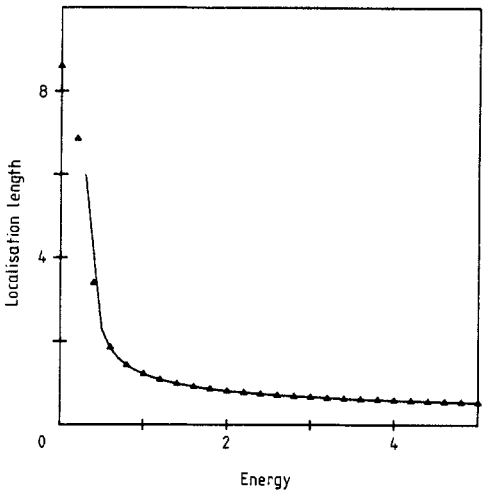

Figure 2. Shortest localisation length for a chain width $M = 5$, disorder $W = 1$ and inter-chain coupling $\beta = 1$: ▲, simulations; ——, perturbation theory.

complex variables. The approximation is made in using a weak-disorder expansion to estimate the Lyapunov exponents.

If we can solve these equations, we identify the pth localisation length l_p as

$$l_p^{-1} = \mathrm{Re}(\mathrm{i}\varphi_p). \tag{31}$$

5. Results and discussion

We applied the above method to the case of a binary alloy, with site energies $\pm W/2$. The zeros are found using the C05NBF routine of the NAG library (which is a general-purpose routine for locating the zero of M non-linear equations in M real variables.) The results were compared with a simulation procedure provided by A Mackinnon.

In figure 1 we show the results for a chain of width two with $\beta = 2$, good agreement is obtained at all energies except near $E = 0$. The cause of the disagreement is probably the low order of the expansion. This can be seen from the fact the expansion for the Lyapunov exponent associated with the eigenvalue of **A** with largest modulus is one dimensional. The term involving inter-channel scattering does not appear. Only if this Lyapunov exponent is also the largest exponent can we obtain a self-consistent solution. It is this which breaks down near $E = 0$. At higher orders the expansion for this exponent is no longer one dimensional. However, as is seen in [12] the expressions are extremely unwieldy.

In figures 2–4, we show results for a five-atom chain $\beta = 1$. Agreement is best for the shortest length and worst for the longest length and becomes worse as we move nearer $E = 0$. In fact, for $E < 3$, it is not possible to obtain a solution for the smallest exponent, while for the largest exponent we can obtain a solution for $E > 0.3$. Again, these difficulties are probably due to the low order of the expansion as in the case of the chain of width two.

For both the width-two and the width-five chains the variation in localisation lengths with energy reflects the choice of a discrete binary alloy distribution for the site energies.

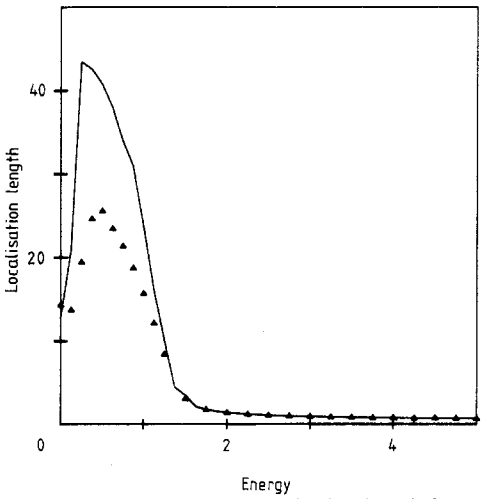

Figure 3. Third-longest localisation length for a chain width $M = 5$, disorder $W = 1$ and inter-chain coupling $\beta = 1$: ▲, simulation; ——, perturbation theory.

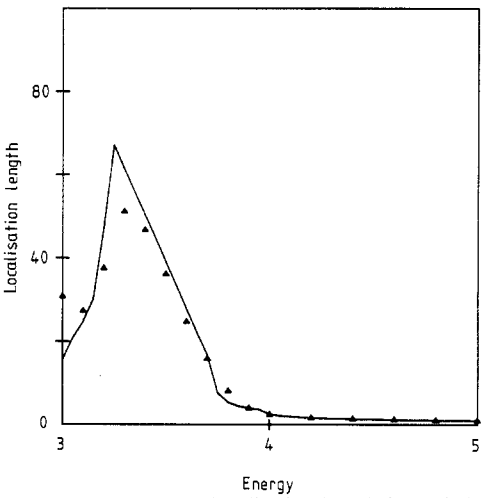

Figure 4. Longest localisation length for a chain width $M = 5$, disorder $W = 1$ and inter-chain coupling $\beta = 1$: ▲, simulation; ——, perturbation theory.

The variation for a smooth distribution of site energies, such as a top-hat distribution, would be considerably more monotonic, the localisation lengths increasing as E tends towards the band centre at $E = 0$.

6. Conclusions

We have developed a self-consistent approximation scheme for the Lyapunov exponents of the Anderson localisation problem. We obtain reasonable agreement with direct simulation except in the cases indicated.

The method developed here is limited to the case of a fixed diagonal matrix **A** whose eigenvalues all have a distinct modulus. The choice of a basis of decaying waves allows the application of the expansion to the normal Anderson model for energies within the band. However, we think that the method will be of limited use in cases where eigenvalues of **A** are actually degenerate and do not just have the same modulus. Some progress has been made here in the work in [14].

Acknowledgments

K Slevin would like to thank the Science and Engineering Research Council for financial support, and E Castaño for useful discussions.

References

[1] MacKinnon A and Kramer B 1983 *Z. Phys.* B **53** 1
[2] Pichard J and Sarma G 1981 *J. Phys. C: Solid State Phys.* **14** L127–32
[3] Abrahams E, Anderson P, Licciardello D and Ramakrishnan T 1979 *Phys. Rev. Lett.* **42** 673
[4] Pichard J and André G 1986 *Europhys. Lett.* **2** 477–86

[5] Pendry J B and Kirkmann P 1984 *J. Phys. C: Solid State Phys.* **17** 4327–44
[6] Slevin K and Pendry J B 1988 *J. Phys. C: Solid State Phys.* **21** 141–9
[7] Kappus M and Wegner F 1981 *Z. Phys.* B **45** 15
[8] Derrida B and Gardner E 1984 *J. Physique* **45** 1283
[9] Lambert C 1984 *Phys. Rev.* B **29** 1091
[10] Pendry J B and Castaño E 1988 *Phys. Rev. Lett.* **60** 20 2093
[11] Pendry J B and Castaño E 1988 *J. Phys. C: Solid State Phys.* **21** 4333
[12] Derrida B, Mecheri K and Pichard J 1987 *J. Physique* **48** 733–40
[13] Oseledec V 1968 *Trans. Moscow Math. Soc.* **19** 197
[14] Zannon N and Derrida B 1988 *J. Stat. Phys.* **50** 509