LBL-29329
Preprint

Lawrence Berkeley Laboratory
UNIVERSITY OF CALIFORNIA

Submitted to Journal of Physics A

Localisation and Spectral Statistics in a Banded Random Matrix Ensemble

M. Wilkinson, M. Feingold, and D.M. Leitner

July 1990

LOAN COPY
Circulates
for 2 weeks
Bldg. 50 Library.
Copy 2
LBL-29329

Prepared for the U.S. Department of Energy under Contract Number DE-AC03-76SF00098.

DISCLAIMER

This document was prepared as an account of work sponsored by the United States Government. While this document is believed to contain correct information, neither the United States Government nor any agency thereof, nor the Regents of the University of California, nor any of their employees, makes any warranty, express or implied, or assumes any legal responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by its trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or the Regents of the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof or the Regents of the University of California.

LBL-29329

Localisation and Spectral Statistics in a Banded Random Matrix Ensemble

Michael Wilkinson

Department of Physics and Applied Physics,
John Anderson Building, University of Strathclyde
Glasgow, G4 ONG, Scotland, U.K.

Mario Feingold*

Lawrence Berkeley Laboratory and Department of Physics
University of California
Berkeley, CA 94720, USA

David M. Leitner

Department of Chemistry
Brown University
Providence, RI 02912, USA

This work was supported by the Director, Office of Energy Research, Office of High Energy and Nuclear Physics, Division of Nuclear Physics of the U.S. Department of Energy under Contract DE-AC03-76SF00098.

*Address after October 1, 1990: Cavendish Laboratory, Mandingley Road, Cambridge, CB3 OHE, U.K.

LOCALISATION AND SPECTRAL STATISTICS IN A BANDED RANDOM MATRIX ENSEMBLE

Michael Wilkinson

Department of Physics and Applied Physics,
John Anderson Building, University of Strathclyde,
Glasgow, G4 0NG, Scotland, U.K.

Mario Feingold*

Lawrence Berkeley Laboratory and Department of Physics
University of California,
Berkeley, CA 94720, U.S.A.

David M. Leitner

Department of Chemistry,
Brown University,
Providence, RI 02912, U.S.A.

ABSTRACT

We give a scaling analysis for the localisation of the eigenvectors of a banded random matrix ensemble, in which the diagonal matrix elements increase along the diagonal. We relate the results to a transition in the spectral statistics which is observed as a parameter is varied, and discuss the relevance of this model to the quantum mechanics of chaotic Hamiltonian systems.

* Address after 1st October 1990: Cavendish Laboratory, Madingley Road, Cambridge, CB3 0HE, U.K.

1. Introduction

It is by now well established that random matrix ensembles can provide a useful statistical model for the fine detail in the spectrum of quantum systems which have a chaotic classical limit: in particular the gaussian orthogonal ensemble (GOE) (Porter, 1965) provides an excellent model for systems with real matrix elements (Bohigas, Giannoni and Schmidt, 1984). Theoretical arguments (Berry, 1977) suggest that the eigenfunctions of these systems can be modelled by a gaussian random function with a known autocorrelation function, and numerical experiments support the view that this picture is essentially correct (Sebr, 1990), although there are additional features which correlate with short period classical orbits (Heller, 1984). If the eigenfunctions are quasi-random, then so are the matrix elements of any operator which uses these states as a basis: this hypothesis is obviously very important in modelling the dynamical response of chaotic quantum systems. In this paper we test the consistency of the idea that the matrix elements can be modelled by a random matrix: we set up a random matrix model which mimics the matrix elements of a chaotic Hamiltonian $\hat{H}=\hat{H}_0+\hat{H}_1$, expressed in the basis formed by the eigenstates of another chaotic Hamiltonian $\hat{H}_0$. If modelling the matrix by random variables is justified, we expect the spectral statistics of our random matrix model to be of GOE type, in agreement with known results. We find that this is not always the case, and conclude that assumptions about the randomness of the matrix elements, while they are a very useful approximation, should be used with caution.

Consider the matrix elements of $\hat{H}=\hat{H}_0+\hat{H}_1$ in the basis formed by the (energy ordered) eigenstates $|i\rangle, |j\rangle..$ of $\hat{H}_0$: $\langle i|\hat{H}|j\rangle=E_i\delta_{ij}+\langle i|\hat{H}_1|j\rangle$, where E_i are eigenvalues of $\hat{H}_0$. These matrix elements are small if $|E_i-E_j|\gg\hbar/\tau$, where τ is a classical timescale characterising the autocorrelation of H_1 under the dynamics of H_0 (Feingold and Peres, 1986, Wilkinson 1987). We can model this matrix using a random matrix ensemble with the following properties: the matrix elements are independently gaussian distributed, so that the ensemble is defined by giving the mean and variance of the distributions of the matrix elements H_{ij} :

$$\langle H_{ij} \rangle = \alpha\, i\, \delta_{ij}$$

$$\langle (H_{ij} - \langle H_{ij} \rangle)^2 \rangle = \begin{cases} 1 + \delta_{ij} & |i-j| < b \\ 0 & |i-j| \geq b \end{cases} \qquad (1.1)$$

i.e the matrix is banded, with 2b-1 elements in each row, and with the mean of the diagonal matrix elements increasing along the diagonal. The parameters α and b are related to the density of states ρ of H_0 and typical size σ of the matrix elements of H_1 by $b=\rho\hbar/\tau$, $\alpha=1/\rho\sigma$. The dimension $\mathcal{N}$ of the matrix is assumed to be very large, and to eliminate end effects it will become clear that $\mathcal{N}$ should satisfy $\mathcal{N} \gg b^2$. We discuss the spectral statistics of this model, which undergo a transition from GOE to Poisson statistics as a parameter is varied. This transition depends on the fact that the eigenvectors of the matrix exhibit Anderson localisation, and most of the technical content of this paper is concerned with estimating the localisation length. The method used to estimate the localisation length is an adaptation of an argument used by Chirikov, Izraelev and Shepelyansky (1981) for a unitary operator : we believe that it may be useful for both analytical and numerical studies of other localisation problems involving hermitean operators. We note that a very similar random matrix ensemble was studied by Wigner (1955), whose analysis was confined to a study of the density of states. A more detailed discussion of the spectral statistics of our model and its semiclassical significance will be published elsewhere (Feingold, Leitner and Wilkinson, 1990).

2. Spectral Statistics of the Model

First we consider the special case in which $\alpha=0$, where the model is already well understood. When $b=\mathcal{N}$, the model becomes the gaussian orthogonal ensemble (GOE), and exhibits level repulsion: in particular the level spacing distribution P(S) is very similar to the Wigner distribution (Porter, 1965). On the other hand when $b \ll \mathcal{N}$ our model is a banded random matrix, and a generalisation (Johnson and Kunz, 1983) of the Furstenberg theorem (Ishii, 1973) implies that the eigenvectors are localised, with some characteristic localisation length L. When

$L \ll N$, this implies that level repulsion does not affect the level spacing distribution P(S), because eigenfunctions localised in regions separated by more than a localisation length would not experience level repulsion. In this case it is clear that P(S) must be a Poisson distribution (Molcanov, 1981). When $L \simeq N$ there is a crossover between Poisson and Wigner statistics, which has been characterised in a finite-size scaling picture by Casati, Molinari and Izraelev (1990).

Now consider what happens when α is non-zero. An eigenvector $\underline{\phi}_i$ which is localised so that its dominant contributions are around the ith element will have an energy E_i which is close to the value of the ith diagonal matrix element, with mean value αi. The difference between E_i and αi can be estimated by regarding the eigenvectors as quasirandom, so that the off-diagonal terms contribute incoherently, hence

$$|E_i - \alpha i| = O(\sqrt{b}) \tag{2.1}$$

Note that this estimate is consistent with the Wigner semicircle law (Porter, 1965) for the density of states of the GOE. States which are separated by a distance of the order of the localisation length are expected to exhibit level repulsion if they have nearly equal energies, but states separated by many localisation lengths cannot experience level repulsion. If α is sufficiently large, (2) shows that two states separated by more than a localisation length are very unlikely to have similar energies, so that all pairs of states of similar energy exhibit level repulsion, implying that the level spacing distribution is of the Wigner type. The condition for this is:

$$\gamma = \frac{\alpha L}{\sqrt{b}} \gg 1 \tag{2.2}$$

When $\gamma \ll 1$ on the other hand, states separated by several localisation lengths can have similar energies, and we expect a transition to Poisson statistics as $\gamma \to 0$. In order to characterise this transition in the spectral statistics we must compute the localisation length L as a function of α and b.

3. Estimates of the Localisation Length

To estimate the localisation length L, we proceed as follows. We consider a vector $\underline{v}_0$ with one non-zero element:

$$(\underline{v}_0)_i = \delta_{i0} \tag{3.1}$$

This vector can be written as a linear combination of eigenvectors $\underline{\phi}_j$ of the matrix $\tilde{H}$:

$$\underline{v}_0 = \sum_j a_j \underline{\phi}_j \tag{3.2}$$

If the localisation length is L, then we expect that approximately L of the amplitudes a_j are significant, and that most of the others are extremely small. Consider what happens when we multiply $\underline{v}_0$ by $\tilde{H}$ N times:

$$\underline{v}_N = \tilde{H}^N \underline{v}_0 = \sum_j a_j E_j^N \underline{\phi}_j \tag{3.3}$$

When N is large, the sum is dominated by values of j for which $|E_j|$ is largest. For simplicity, let us assume that all but L of the a_j vanish: in this case, after a large number of multiplications the vector $\underline{v}_N$ is approximately equal to a multiple of $\underline{\phi}_{max}$, the eigenvector corresponding to the the largest eigenvalue $|E_{max}|$. The number of multiplications required for $\underline{\phi}_{max}$ to become dominant is

$$N^* \simeq E_{max}/(|E_{max}|-|E_{next}|) \simeq E_{max}\rho \tag{3.4}$$

where E_{next} is the next largest of the L contributing eigenvalues and ρ is the density of states for these L states. Since the distribution of eigenvalues is symmetric about E=0, the density of states is:

$$\rho \simeq L/|E_{max}|. \tag{3.5}$$

The vector $\underline{v}_N$ therefore becomes essentially a multiple of $\underline{\phi}_{max}$ when $N \gg N^* \simeq L$.

We can characterise the vector $\underline{v}_N$ conveniently by considering the standard deviation S(N) of the distribution of

its elements $(\underline{v}_N)_i$:

$$S^2(N) = \frac{B_N}{A_N} = \sum_i i^2 \, (\underline{v}_N)_i^2 \Big/ \sum_i (\underline{v}_N)_i^2 \qquad (3.6)$$

The spread S of the vector $\underline{v}_N$ increases until $N \simeq N^*$, when S(N) saturates at a value

$$S(N^*) \simeq L \simeq N^* \qquad (3.7)$$

The second approximate equality follows from (3.4) and (3.5). The strategy for calculating the localisation length is to compute S(N) using an alternative method which ignores the possibility of localisation, and to solve (3.7) using this expression for S(N). Taking account of the fact that some of the neglected coefficients a_j will correspond to eigenvalues with magnitude greater than E_{max}, we see that S(N) continues to increase logarithmically after the break point N^* instead of saturating, but this does not affect the equation (3.7) for the localisation length.

The spread S(N) can be estimated by considering the multiplication of $\underline{v}_0$ by a string of N *different* realisations of the random matrix ensemble, $\tilde{H}_1 \ldots \tilde{H}_N$:

$$\underline{v}_N' = \tilde{H}_N \, \tilde{H}_{N-1} \ldots \tilde{H}_2 \, \tilde{H}_1 \, \underline{v}_0 \qquad (3.8)$$

We can easily compute S(N) for the vector $\underline{v}_N'$ since all the random variables involved are independent. The spread of the vector $\underline{v}_N$ would be expected to be similar to that of $\underline{v}_N'$ until the localisation effects become apparent when $N \simeq N^*$, when the spread of $\underline{v}_N'$ continues to increase instead of saturating. Because the matrix elements of the $\tilde{H}_n$ are random variables, we can regard the elements of the vectors $\underline{v}_n'$ as random variables, with second moment Y_i^n :

$$Y_i^n = \langle (\underline{v}_n')_i^2 \rangle, \qquad (3.9)$$

where $\langle \quad \rangle$ denotes an average over the random matrix ensemble. The matrix elements satisfy

$$(\underline{v}'_{n+1})_i = \sum_j (\tilde{H}_n)_{ij} \, (\underline{v}'_n)_j \tag{3.10}$$

so that the Y_i^n satisfy the recursion relation

$$Y_i^{n+1} = \sum_{j=-b}^{b} (1 + \delta_{ij}) \, Y_j^n + \alpha^2 \, i^2 \, Y_i^n \tag{3.11}$$

We consider the case in which b is large. In this case we can represent the Y_i^n by a function $Y_n(x)$, and approximate the sum in (3.11) by an integral:

$$Y_{n+1}(x) = \int_{x-b}^{x+b} dx' \, Y_n(x') + \alpha^2 \, x^2 \, Y_n(x) \tag{3.12}$$

$$= \int_{-\infty}^{\infty} dx \;\; \chi_b(x-x') \, Y_n(x') + \alpha^2 \, x^2 \, Y_n(x)$$

where $\chi_b(x)$ is a characteristic function on an interval of width 2b. The sum, A_N and second and fourth moments, B_N, C_N of the variances are given by (c.f. (3.6)):

$$A_N = \int_{-\infty}^{\infty} dx \, Y_N(x) \;, \quad B_N = \int_{-\infty}^{\infty} dx \, x^2 \, Y_N(x) \;, \quad C_N = \int_{-\infty}^{\infty} dx \, x^4 \, Y_N(x)$$

(3.13)

We can use (3.13) to write down recurrence relations for the A_N and B_N : performing the x integral in (3.12) and substituting (3.13) gives the following results.

$$A_{N+1} = 2 \, b \, A_N + \alpha^2 \, B_N \tag{3.14}$$

$$B_{N+1} = 2 \, b \, B_N + \frac{2}{3} \, b^3 \, A_N + \alpha^2 \, C_N \tag{3.15}$$

We can get a single equation for S(N) if we approximate the fourth moment using the square of the second moment:

$$C_N \simeq B_N^2 \, / \, A_N \tag{3.16}$$

Combining (3.14)-(3.16) leads to a simple recursion relation for the spread S(N) of the vector, defined by (3.6):

$$S^2(N+1) = \frac{B_{N+1}}{A_{N+1}} = S^2(N) + \frac{\frac{1}{3}b^2}{1 + (\alpha^2 S^2(N)/2b)} \qquad (3.17)$$

The asymptotic solutions of these two equations are easily obtained. When N is small, $S^2(N)$ grows linearly: $S^2(N) \simeq Nb^2/3$. This linear growth continues until a crossover point $N_{cr} \simeq (\alpha^2 b)^{-1}$. For $N \gg N_{cr}$ the spread S(N) increases as the fourth root of N: ignoring those numerical factors which have ceased to be meaningful, we have

$$S(N) \simeq (N\, b^2/3)^{1/2} \quad , \quad N \ll N_{cr} = (\alpha^2\, b)^{-1} \qquad (3.18)$$

$$S(N) \simeq (N\, b^3/\alpha^2)^{1/4} \quad , \quad N \gg N_{cr} \qquad (3.19)$$

We now have all the information required to solve the equation for the localisation length, (3.7). There are two asymptotic regimes, depending on whether N^* is large or small compared to N_{cr}. First consider the case in which α is very small, so that N_{cr} is large and the diagonal terms have no effect on the localisation length: equating (3.7) and (3.18) gives $L \simeq b^2$, and the condition $N^* \ll N_{cr}$ can be expressed in the form $x \ll 1$, where $x = \alpha b^{3/2}$. When α is large enough that the diagonal elements affect the growth of S(N) before saturation is reached, equating (3.7) and (3.19) gives $L \simeq b\alpha^{-2/3}$. These results can be summarised as follows:

$$L = b^2\, f(x) \quad , \qquad x = \alpha\, b^{3/2},$$

$$f(0) = C_0 \quad , \qquad f(x) \xrightarrow[x \to \infty]{} C_1\, x^{-2/3} \qquad (3.20)$$

where C_0 and C_1 are constants.

The derivation above assumes that $N_{cr} \gg 1$ and $N^* \gg 1$, as well as $b \gg 1$. When α is large, the latter condition need not hold: using (3.19) we find that $N_{cr} \simeq 1$ when $\alpha^2 b \simeq 1$. This suggests that deviations from the scaling relation (3.20) will become apparent when $x \gg b$. In the limit of large α the problem can be analysed by treating the off-diagonal elements as a perturbation, but we will not pursue this further.

It is interesting to note that, provided α is small enough

for the scaling relation (3.20) for the localisation length to hold, the paramter γ describing the transition in the spectral statistics is a function of $x=\alpha b^{3/2}$ alone, $\gamma=xf(x)$, so that we have a one parameter scaling theory for the transition.

4. Numerical Experiments

We have performed numerical experiments which verify these predictions, using matrices of dimension $N\simeq 5b^2$, and eliminating states from the highest and lowest 15% of the spectrum to guard against finite-size effects. Figure 1 shows numerical measurements of the entropy localisation length (Casati, Izraelev and Molinari, 1990), for various values of b, plotted to show the scaling function f(x). In the region where $x\gg 1$, the scaling curve is fitted well by a $x^{2/3}$ power law (solid line). The results follow a scaling curve up to a break point, which increases as $b\to\infty$: deviations from the scaling curve are already visible for the b=3 data in figure 1. We estimate $C_0=1.3$, $C_1=2.1$ for the constants in (3.20).

We also investigated the transition from Poisson to Wigner statistics as γ increases by calculating a histogram of the level spacing distribution P(S), and performing a least-squares fit to a Brody distribution (Brody 1973), which interpolates between the Poisson and Wigner distributions as a parameter q is increased from 0 to 1. For these numerical experiments we used a sample of at least 125 matrices of dimension 800 for each point, and the bin size used for computing the histogram was 0.1. The results are shown in figure 2: most of the data lie on a scaling curve, implying that the level spacing distribution is a function of the parameter $\gamma(x)$ only. The deviations from the scaling curve are due to finite-size effects: for large values of b the localisation length can be comparable to the dimension of the matrix and it is not possible to get a Poissonian level spacing distribution, which requires the superposition of many independent spectra. Usually the fit to the Brody distribution was very good as judged by eye (see figure 3), but we do not claim that the fit is statistically significant.

5. Discussion

We have argued that the structure of the matrices of our ensemble mimics that of the matrix encountered when diagonalising one chaotic quantum Hamiltonian in the eigenbasis of another such Hamiltonian. Also, we have shown that the model exhibits a transition in the form of its spectral statistics, rather than displaying the universal GOE statistics observed in chaotic quantum systems. We should therefore consider the reasons why the transitional spectral statistics are not observed in chaotic systems.

One possibility is that γ is always large, so that GOE statistics are expected after all. We can use semiclassical estimates of the density of states ρ and typical size of matrix elements σ, to compute how the transition parameter γ scales as $\hbar\to 0$ (it is only in this limit that the spectrum becomes dense, so that we can compute well-defined statistics). These estimates give $\rho=O(\hbar^{-d})$ and $\sigma=O(\hbar^{(d-1)/2})$ (Wilkinson, 1987, Feingold, Leitner and Piro, 1989), so that $\alpha=O(\hbar^{(d+1)/2})$, $b=O(\hbar^{1-d})$, $x=\alpha b^{3/2}=O(\hbar^{2-d})$, where d is the number of degrees of freedom. It follows that $\gamma(x)\to\infty$ as $\hbar\to 0$, implying GOE statistics, only if $d>2$. In the important case when $d=2$ semiclassical considerations do not constrain γ to be large. We must conclude that the observed GOE statistics are explained by differences between our model and the matrix elements of a semiclassical system.

The method we use for estimating the localisation length is clearly insensitive to many features of the model, provided the matrix elements are independent: for instance it does not matter if the matrix is not strictly banded (the matrix elements only have to decay rapidly away from the diagonal), and it does not matter whether or not their distribution is gaussian. We conclude that the matrix elements of semiclassical systems must be subtly correlated. This is consistent with earlier work in which correlations between matrix elements were used to explain deviations of semiclassical spectra from the GOE model (Wilkinson 1988).

In conclusion, we have investigated the scaling properties of the localisation length in a banded random matrix ensemble, and we have shown that localisation gives rise to a transition

in the spectral statistics of this model, depending on a single scaling parameter. We have commented on the similarity of the matrices to those occuring in the quantum mechanics of chaotic systems, and shown that the results of using a random matrix to model matrix elements of these systems may be misleading.

6. Acknowledgements

We wisk to thank Dr.W.Swiatecki for many useful discussions. DML acknowledges the support of J.D.Doll. This work was supported in part by the Director, Office of Energy Research, Office of High Energy and Nuclear Physics, Division of Nuclear Physics, and Office of Basic Energy Sciences Research, Engineering and Geoscience Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098, and by the U.S. National Science Foundation under Grant No. NSF-PYI-84-51276.

References

Berry,M.V. 1977 J.Phys.A10,2083-2091.

Bohigas,O.,Giannoni,M.J., and Schmidt,C. 1984 Phys.Rev.Lett. 52,1-4.

Brody,T.A., 1973 Nuovo Cimento Lett.7,482.

Casati,G., Molinari,L., and Izraelev,F.M., Phys.Rev.Lett. 64,1852-1855.

Chirikov,B.V., Izraelev,F.M., and Shepelyanski,D.L. 1981 Sov.Sci.Rev.C2,209.

Feingold,M., Leitner,D.M., and Piro,O., 1989, Phys.Rev.A39, 6507.

Feingold,M., Leitner,D.M., and Wilkinson,M. 1990 submitted to Phys.Rev.Lett.

Feingold,M., and Peres,A. 1986 Phys.Rev.A34,591.

Heller,E.J. 1984 Phys.Rev.Lett.53,1515-1519.

Ishii,K. 1973 Prog.Theor.Phys.Suppl.(Japan),53,77.

Johnson,R., and Kunz,H. 1983 J.Phys.C16,3895.

Molcanov,S.A. 1981 Commun.Math.Phys. 78,429-446.

Porter,C.E.(ed.) 1965 'Statistical Theories of Spectra: Fluctuations',New York: Academic.

Sebr,P. 1990 Phys.Rev.Lett.64,1855-1858.

Wigner,E.P. 1955 Ann.Math.62,145.

Wilkinson,M. 1987 J.Phys.A20,2415-2423.

-1988 J.Phys.A21,1173-1190.

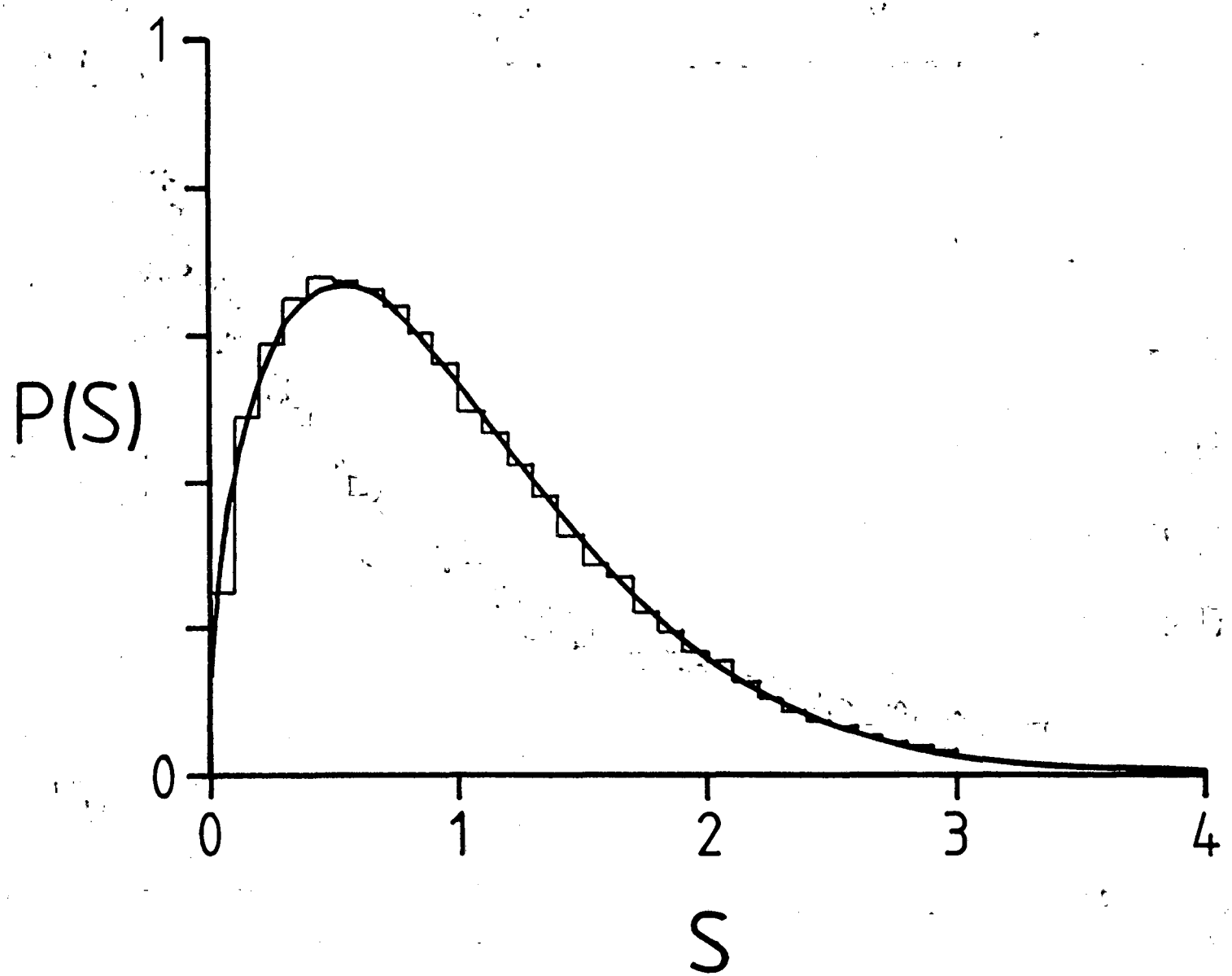
Figure captions

Figure 1 : Plot showing one parameter scaling function for localisation length, defined by $L=b^2f(x)$, $x=\alpha b^{3/2}$: the different styles of point indicate different values of b, and the solid curve is a $x^{-2/3}$ power law, which fits the scaling curve for $x \gg 1$. The points deviate from the scaling relation for large x, but the break point where the deviations begin increases as $b \to \infty$.

Figure 2: The parameter q characterising a fit of the Brody distribution to the level spacing distribution, plotted as a function of the scaling parameter x. Different styles of point indicate different values of b. The deviations at small q and large b are a finite-size effect, and are discussed in the text.

Figure 3: A typical level spacing distribution, showing the fit to a Brody distribution: the data are for b=10, x=2.26, and the fitted value of q is 0.484.

fig.3



LAWRENCE BERKELEY LABORATORY
UNIVERSITY OF CALIFORNIA
INFORMATION RESOURCES DEPARTMENT
BERKELEY, CALIFORNIA 94720