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Localization of electronic states in 2D disordered systems

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Abstract. Results of numerical investigations of the Anderson model of localization are reported. Using the transfer matrix method and finite size scaling, the localization lengths of electronic states in 2D systems with energetic disorder are determined on honeycomb, square, and triangular lattices. While the actual values of the localization length at a particular disorder differ for the different coordination numbers, complete localization is found in all cases. This result is in agreement with the scaling hypothesis, but in contrast to recent claims.

1. Introduction

The question, whether electronic states in disordered systems are localized for any disorder yielding an insulating behaviour, or whether a mobility edge can be defined by a critical disorder below which extended states allow metallic transport through an infinite sample, has been a central issue of the investigations of disordered systems since the original formulation of the problem by Anderson (1958).

For one-dimensional (1D) systems the following statements can be proven in a mathematically rigorous way (Ishii 1973, Erdös and Herndon 1982, Fröhlich *et al* 1985): even for an arbitrarily small but finite strength of the disorder all states are localized irrespective of their energy. The DC conductivity vanishes in the limit of vanishing temperature. For a finite system the conductance decreases exponentially and the resistance increases exponentially with increasing length of the system.

In 2D and 3D systems, on the other hand, no mathematically rigorous theory of localization exists. Only in the asymptotic regions of large disorder or large energies in the band tails can the appearance of localized states be proven. A general proof for the existence of localized and/or extended states or for the existence of a disorder-induced metal–insulator transition is not available. Early numerical investigations (Licciardello and Thouless 1975, 1978, Weaire and Srivastava 1977, Stein and Krey 1980, 1981) gave values for a critical disorder corresponding to the metal–insulator transition in 2D as well as 3D, but these calculations were suffering from the very limited system size that could be treated in those days.

Substantial progress was made when the problem was formulated in terms of the renormalization group (Wegner 1976) leading to the one-parameter scaling hypothesis of localization (Abrahams *et al* 1979). Accepting the main supposition that the assumed scaling properties of the system close to a possible phase transition can be described by only one scaling variable and employing the quantitative results of the weak localization

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theory for the quantum corrections to the metallic conductivity (Bergmann 1984) together with the assumption of continuity for the logarithmic derivative of the conductance it can be argued that a metal–insulator transition can only exist in 3D systems, while in 2D systems (at least without electron–electron interactions and without magnetic field) all quantum states of an infinitely large, disordered sample are localized even for a vanishingly small but finite disorder.

The scaling hypothesis was convincingly corroborated by a numerical method (MacKinnon and Kramer 1981) employing a recursive technique in connection with a real-space renormalization procedure. This approach allowed the determination of the metal–insulator transition in 3D and also showed the localization of electronic states in 2D for very small disorder. Numerous subsequent applications of this approach for larger and larger systems, for different distributions of the random site energies, for various energies throughout the whole band including the band edges, and with improved accuracy have corroborated these findings (for a recent overview, see: Kramer *et al* 1990), although some doubts have been cast on the universality of the scaling theory (Schreiber 1991).

All these calculations were performed on square or simple cubic lattices. This gave rise to an interesting speculation (Srivastava 1989) whether a metal–insulator transition might occur in a 2D lattice which has the same coordination number as the simple cubic lattice, namely six nearest neighbours. This would not necessarily be in contradiction to the above mentioned conclusions from the scaling hypothesis, because the quantum interference could yield different correction terms to the conductivity for different connectivities. The speculation was based on the argument, that the localization problem in a real lattice can be mapped onto the localization problem in a Cayley tree lattice in which the non-contributing branches are trimmed off (Srivastava 1989). Using an exact method for calculating the connectivity constant for the hierarchy of closed self-avoiding random walks, which are pertinent to the localization problem in the given lattice, the critical disorder and the mobility edge were derived for different lattices. The calculations for 2D lattices revealed the surprise that a mobility edge seems to exist for the triangular lattice (but not for the honeycomb lattice), while the square lattice is a borderline case (Srivastava 1989).

In the present paper we report large-scale computations on these three lattices using the recursive technique of MacKinnon and Kramer (1983). We demonstrate that finite-size scaling is possible in all cases. The high accuracy of our data unambiguously shows that all states are localized even for the smallest disorder considered. Doubts have arisen about the universality of the one-parameter scaling hypothesis (Kravtsov and Lerner 1984). Therefore it is interesting to note that a simultaneous scaling of all data for the different lattices is possible.

2. Calculation of the transmission probability through a quasi-1D system

Our investigation is based on the Anderson (1958) Hamiltonian which is commonly used for numerical studies of the localization problem. In site representation the Hamiltonian

$$H = \sum_{n} |n\rangle \varepsilon_n \langle n| + \sum_{n,m}^{NN} |n\rangle V \langle m| \tag{1}$$

describes a regular lattice in the tight-binding approximation with nearest neighbour

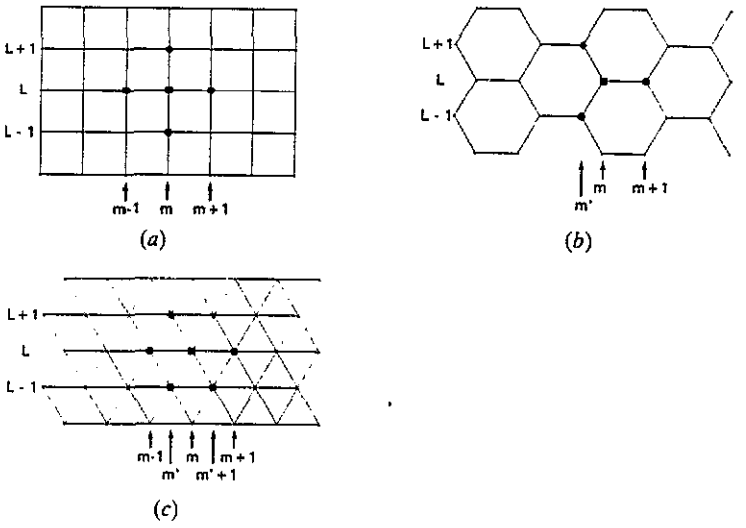

Figure 1. Sections of two-dimensional lattices with (*a*) square; (*b*) honeycomb; and (*c*) triangular structure. The *m*th site of the *L*th layer is marked by a square, its neighbours in the same and the preceding layer by circles, a neighbouring site in the next layer is marked by a diamond, a second neighbouring site in the next layer is marked by a triangle.

transfer only and random potential energies ε_n which are independently chosen according to a box distribution of width W. As usual we define an energy scale by setting $V = 1$.

For the following investigation we employ the transfer matrix technique to calculate the localization length of electronic states in very long quasi-1D systems with small cross-section M and very long length L, which are then used to reach 2D systems by means of a finite-size scaling procedure. Although this approach (MacKinnon and Kramer 1981, Pichard and Sarma 1981) is now a standard one, we sketch it here because the application to the triangular lattice is not straightforward.

The Schrödinger equation corresponding to the Hamiltonian in (1) can be written as an initial-value problem

$$A(L+1) = (E\mathbf{1} - H_M(L))A(L) - A(L-1). \tag{2}$$

Here $H_M(L)$ comprises the Hamiltonian matrix elements on the Lth layer and $A(L)$ describes M linearly independent wave-functions at the M sites within the Lth layer. In a 1D system this means that $H_M(L) = H_1(L) = \varepsilon_L$ and $A(L)$ are scalars yielding the wave-function $|\psi\rangle = \Sigma_L A(L)|L\rangle$.

Considering a 2D square lattice as depicted in figure 1(*a*), $H_M(L)$ reads

$$H_M(L) = \begin{pmatrix} \varepsilon_1 & 1 & & & & 1 \\ 1 & \varepsilon_2 & 1 & & & \\ & \ddots & \ddots & \ddots & & \\ & & 1 & \varepsilon_m & 1 & \\ & & & \ddots & \ddots & \\ 1 & & & & 1 & \varepsilon_M \end{pmatrix} \tag{3}$$

(Only the non-zero elements in rows $1, 2, m, M$ are indicated, an additional index L for the potential energies is omitted for clarity.) Here the off-diagonal elements describe the bonds between the M sites within the Lth layer, employing a periodic boundary condition. The $A(L)$ are now $M \times M$ matrices which contain the expansion coefficients of M wave-functions at the M sites within the Lth layer, and 1 in (2) now denotes the $M \times M$ unity matrix.

The application of this recursion to a honeycomb lattice is straightforward. The different connectivity as illustrated in figure 1(*b*) is reflected in the matrices

$$H_M(L) = \begin{pmatrix} \varepsilon_1 & 1 & & & & \\ 1 & \varepsilon_2 & & & & \\ & & \ddots & & & \\ & & & \varepsilon_m & 1 & \\ & & & & \ddots & \\ & & & & 1 & \varepsilon_M \end{pmatrix}$$

$$H_M(L+1) = \begin{pmatrix} \varepsilon_1 & & & & & 1 \\ & \varepsilon_2 & 1 & & & \\ & & \ddots & & & \\ & & 1 & \varepsilon_{m'} & & \\ & & & & \ddots & \\ 1 & & & & & \varepsilon_M \end{pmatrix}. \tag{4}$$

for the even and odd layers, respectively, with m and m' odd. Obviously, this construction is restricted to an even number of sites per layer due to the periodic boundary condition.

The simplicity of the recursion relation in (2) can be attributed to the lattice structures: if the $(L+1)$th layer is added to the sample of L layers, every new site is connected to the old sample by only one bond in the square as well as in the honeycomb lattice. The amplitudes of the wave-functions at the new site (denoted by a diamond in figure 1) can be derived by applying the Hamiltonian in (1) to the wave-functions on the appropriate site m in the Lth layer (marked by a square in figure 1), i.e. by evaluating $H|m\rangle$. Except for the new (diamond) site, only the sites (indicated by circles) at which the amplitudes are already known are involved, because the transfer term of the Hamiltonian is restricted to nearest neighbours.

A discrepant situation arises in the triangular lattice as depicted in figure 1(*c*). If one applies the Hamiltonian to the wave-functions on the mth site of the Lth layer in order to determine the amplitudes at the m'th site in the $(L+1)$th layer, one has also to consider the, as yet unknown, amplitudes at the $(m'+1)$th site of the new layer (marked by a triangle). The respective recursion relation now reads

$$\mathbf{I}(L+1)A(L+1) = (E\mathbf{1} - H_M(L))A(L) - \mathbf{I}(L-1)A(L-1) \tag{5}$$

where $H_M(L)$ coincides with the matrix in (3) and the operator $\mathbf{I}$ is given by the matrices

$$\mathbf{I}(L+1)=\mathbf{I}(L-1)=\begin{pmatrix} 1 & 1 & & & & \\ & 1 & 1 & & & \\ & & \ddots & & & \\ & & & 1 & 1 & \\ & & & & \ddots & \\ 1 & & & & & 1 \end{pmatrix},$$

$$\mathbf{I}(L)=\begin{pmatrix} 1 & & & & & 1 \\ 1 & 1 & & & & \\ & \ddots & & & & \\ & & 1 & 1 & & \\ & & & & \ddots & \\ & & & & 1 & 1 \end{pmatrix} \tag{6}$$

(6) for odd and even layers, respectively. Multiplying (5) by $\mathbf{I}^{-1}$ again yields a simple recursion relation, but only for odd values of M because otherwise the matrices $\mathbf{I}$ are singular and cannot be inverted.

For all lattices the recursion can be expressed by means of a transfer matrix

$$t_L=\begin{pmatrix} \mathbf{I}^{-1}E-\mathbf{I}^{-1}H_M(L) & -\mathbf{1} \\ \mathbf{1} & 0 \end{pmatrix} \tag{7}$$

where $\mathbf{I}$ is given by (6) for the triangular lattice and by the unity matrix $\mathbf{1}$ for the square and the honeycomb lattice. With these transfer matrices the evaluation of the wavefunctions along a strip of width M and length L can be determined in the following way:

$$\begin{pmatrix} A(L+1) \\ A(L) \end{pmatrix}=t_L\begin{pmatrix} A(L) \\ A(L-1) \end{pmatrix}=T_L\begin{pmatrix} A(1) \\ A(0) \end{pmatrix} \qquad T_L=\prod_{l=1}^{L} t_l \tag{8}$$

The product matrix T_L diverges exponentially with increasing L, but a limiting matrix

$$\mathbf{T}=\lim_{L\to\infty}(T_L T_L^{\dagger})^{1/2L} \tag{9}$$

exists according to the theorem of Oseledec (1968). As the product matrix $\mathbf{T}$ is symplectic, its eigenvalues appear pairwise and can be written as $\exp(\tau_i)$ and $\exp(-\tau_i)$. The τ_i and $-\tau_i$ are the Lyapunov characteristic exponents which characterize how the initial states 'drift apart' exponentially. The inverse values reflect the different characteristic length scales. The largest length (i.e. the inverse of the smallest Lyapunov exponent) describes the weakest possible decay of the transmission probability for a state at the given energy. This length is commonly associated with the localization length, implicitly assuming that the electronic states are exponentially localized. We shall denote this length by λ_M. In the limit of large L this length as well as the other Lyapunov exponents can be computed (Pichard and Sarma 1981, MacKinnon and Kramer 1983) from the exponential decay of the norm of the orthogonalized column vectors of $A(L)$.

As the matrix A^{-1} can be associated (MacKinnon and Kramer 1983) with the one-electron Green's function describing the probability amplitude for the transition of an

electron between the first and the last layer of the quasi-1D strip, the decay length of the transmission probability can be calculated more directly from the Euclidean norm of A^{-1} in the following way:

$$(L+1)/\lambda_M(L+1) = (L/\lambda_M(L)) - \ln\|A^{-1}(L+1)\|. \tag{10}$$

We have used this procedure for a few parameter combinations to control the validity of our results obtained by means of the transfer matrix method. For the implementation of the algorithms on a modern computer it is important to note that the advantage of the transfer matrix method is that it can be much more effectively vectorized.

It is an essential feature of the Green's function method as well as the transfer matrix method that the statistical accuracy of the determined decay length can be controlled during the recursion. The fluctuations decrease slowly with increasing system size. Therefore, it is possible to extend the length of the systems under consideration until the error falls below a given accuracy which has generally been taken as 1% in the present investigation. A high accuracy is necessary to allow a reasonable subsequent treatment of the data by means of the finite-size scaling technique discussed below. A further improvement is, however, limited by the available computer resources, because the accuracy influences the computation time quadratically. Another problem arises because the smallest positive Lyapunov exponent is, unfortunately, the one most sensitive to a loss of significance due to rounding errors. Therefore, the accuracy of the accumulated transfer matrix has to be carefully controlled, otherwise a fast convergence towards wrong values of λ_M can be observed.

In figure 2 the obtained data for the honeycomb lattice and the triangular lattice are presented. Here we restrict ourselves to the band centre, $E = 0$. For a comparison it should be noted that the number of sites in each layer is 1.5 times larger in the triangular lattice than in the honeycomb lattice for the same width and that all lengths in the present investigation are given in units of the nearest neighbour distance.

It can be clearly seen from figure 2 that λ_M/M decreases with increasing M in all cases except for finite-size effects for the smallest widths. Accordingly, the wave-functions can be considered to be already more or less confined within the strip, i.e. they are localized. It cannot be expected that an increase of the width would change this behaviour. In order to obtain extended states in the infinite 2D systems, the computed decay length λ_M should increase faster than M so that the state would grow more and more with increasing width. This behaviour, which is well known from respective calculations in 3D systems (MacKinnon and Kramer 1983) cannot be found in the present systems. It can therefore be safely concluded that all states are localized in these systems.

This also holds true for the square lattice as determined before (MacKinnon and Kramer 1981, 1983). For the subsequent investigation we have also computed the decay length λ_M for the square lattice, taking into account the following values for the width of the strip: $M = 5$, 10, 15, 20, and 32. Respective values for the honeycomb and the triangular lattice follow from figure 2. Actual values for the disorder parameter W can be found in table 1. This table demonstrates that very large systems are necessary in order to obtain a reasonable accuracy. Although the accuracy of 1% was not reached for the smaller values of the disorder, we believe that our data are good enough to draw the above mentioned conclusions that all states are localized in 2D systems irrespective of the number of nearest neighbours. This belief will be substantiated in the next section by showing that all data can be simultaneously fitted onto a common scaling curve.

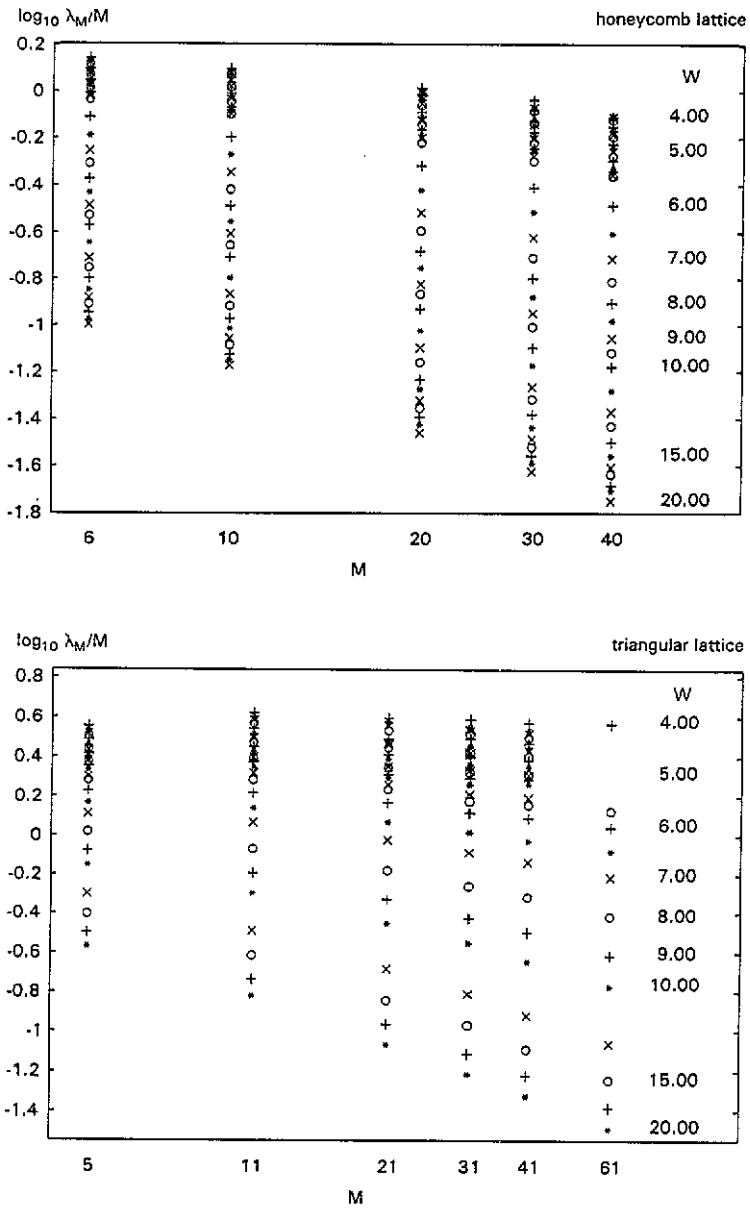

Figure 2. Doubly logarithmic plot of the renormalized exponential decay length λ_M/M of the transmission coefficient versus the width M of the strip in the band centre ($E = 0$) for several values of disorder W of the box distribution of random site energies on (*a*) the honeycomb lattice; and (*b*) the triangular lattice. All values of W are compiled in table 1.

3. Finite size scaling

In order to describe the transmission properties of a system with infinite width it is necessary to extrapolate the computed data of λ_M with respect to M. This cannot be performed in a straightforward manner, because the raw data cover only a relatively

Table 1. Decay lengths ξ of the transmission probability through a honeycomb, square and triangular lattice determined by a finite-size scaling procedure for different values of the disorder W. The length L which was necessary to obtain the raw data with the required accuracy of 1% in the recursive procedure for the largest width M of the quasi-1D strip is also given. The prefix '>' indicates that this accuracy could not be obtained up to the given recursion length. In those cases the decay lengths given are determined with an accuracy better than 1.2%†, 1.7%‡, 2.2%§, 2.7%‖. Values in italics indicate that the largest width M used for that disorder was 41 only.

	Honeycomb lattice		Square lattice		Triangular lattice	
W	$L(M=40)$	ξ	$L(M=32)$	ξ	$L(M=61)$	ξ
2.5			>400 000	326 977.3§		
2.7			>400 000	109 097.3‡		
3.0			>400 000	26 943.8‡		
3.3			>400 000	7804.9‡		
3.6			>400 000	2911.4†		
4.0	>450 000	258.4†	>300 000	1027.7‡	>420 000	486 631.5‖
4.1	513 750	235.1			*>420 000*	*279 999.1§*
4.2	532 220	223.8			*>360 000*	*197 516.2§*
4.3	495 840	198.7			*>360 000*	*121 294.9§*
4.4	>450 000	188.5†			*>360 000*	*87 292.3§*
4.5	>450 000	166.6†	>300 000	380.0†	*>360 000*	*47 071.6§*
4.6	438 380	145.8			*>360 000*	*33 686.5§*
4.7	431 540	133.7			*>360 000*	*23 479.8§*
4.8	397 000	115.3			*>360 000*	*17 910.9§*
4.9	386 370	103.8			*>360 000*	*11 168.7§*
5.0	>300 000	94.2†	269 400	171.0	*>360 000*	*6953.3§*
5.1	355 560	83.0			*>360 000*	*5860.4‡*
5.2	353 200	75.4			*>360 000*	*4545.0‡*
5.3	316 310	67.3			*>360 000*	*3155.9‡*
5.4	288 050	61.4				
5.5	287 070	55.2	211 950	88.0	*>360 000*	*1991.8‡*
5.7					>360 000	1246.1‡
6.0	214 210	34.0	166 250	51.3	>360 000	699.1‡
6.5	157 410	22.0	136 890	32.8	>360 000	291.0‡
7.0	>100 000	15.2†	100 900	22.3	>360 000	130.9†
7.5	90 330	11.1	83 810	16.7		
8.0	73 040	8.6	72 440	12.5	258 714	46.9
8.5	61 270	6.8				
9.0	51 640	5.5			163 818	22.9
9.5	43 890	4.7				
10.0	35 810	4.0	38840	5.9	110 556	13.8
11.0	28 380	3.1				
12.0	22 390	2.5				
12.5			20120	3.2	51 000	6.0
13.0	17 950	2.1				
14.0	15 400	1.8				
15.0	14 690	1.6	12040	2.2	31 236	3.7
16.0	11 880	1.4				
17.0	10 960	1.3				
17.5			9920	1.6	20 880	2.6
18.0	9690	1.1				
19.0	8710	1.1				
20.0	7790	1.0	7710	1.3	16 560	2.0

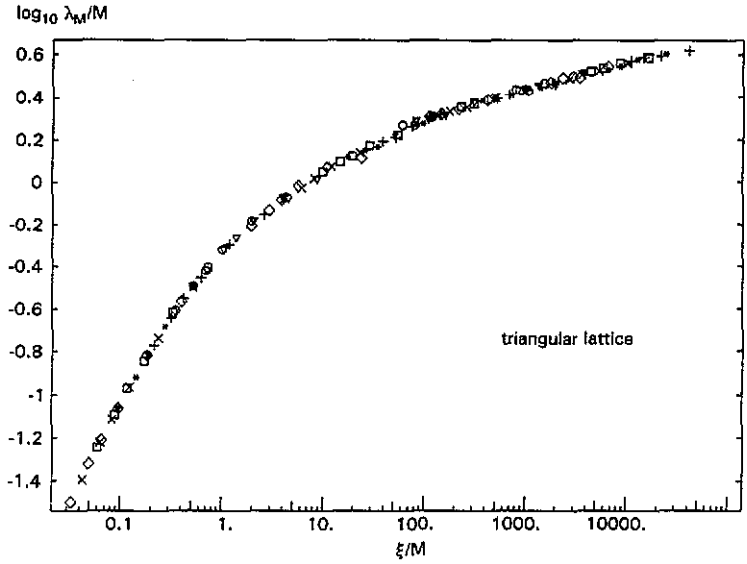

Figure 3. Scaling function for the triangular lattice. All raw data of figure 2(*b*) (except those values for $M = 5$ which show drastic finite size effects) are scaled onto a common curve f by changing the scale of M^{-1} via fitting parameters $\xi(W)$.

small interval of M-values. It is, however, possible to gain further knowledge about the behaviour of the data for $M \to \infty$ if one assumes that a suitable scaling variable Λ exists, which can be expressed as a function of the system size M and some scaling parameter ξ, which comprises the dependence on the disorder W and the energy E

$$\Lambda = f(\xi/M) \qquad \xi = \xi(W, E). \tag{11}$$

This assumption corresponds to the *ansatz* of the scaling theory of localization, in which the conductance itself is taken as the relevant scaling parameter.

Whether or not the raw data obtained in the last section fulfil the scaling relation (11) can be quantitatively verified by attempting a mean least squares fit of the data onto a common curve by suitably adjusting the scale of M (or equivalently of $1/M$) by the parameter ξ for each parameter combination of E and W. It is demonstrated in figure 3 that the attempt of finding a common functional relationship $f(\xi/M)$ has been successful within the accuracy of our raw data.

The claim of universality of the scaling hypothesis (Abrahams *et al* 1979) has been questioned (Kravtsov and Lerner 1984, Schreiber 1991). In the present context it is possible to test whether at least a universal scaling behaviour can be observed for the different lattice structures under consideration. Figure 4 demonstrates that all raw data for the square, for the honeycomb, and for the triangular lattice at the band centre can be fitted onto a common curve.

It should be noted, however, that an error of 1% corresponds approximately to the size of the symbols of figure 3 and 4. Correspondingly, the inaccuracy of the scaling parameter which controls the horizontal shift of the symbols during the fitting procedure is considerable especially in the rather flat part of the scaling curves. Moreover, as the scaling curve is fixed for large disorder, i.e. for small ξ (MacKinnon and Kramer 1983), higher values of the scaling parameter are more and more influenced by the accumulation

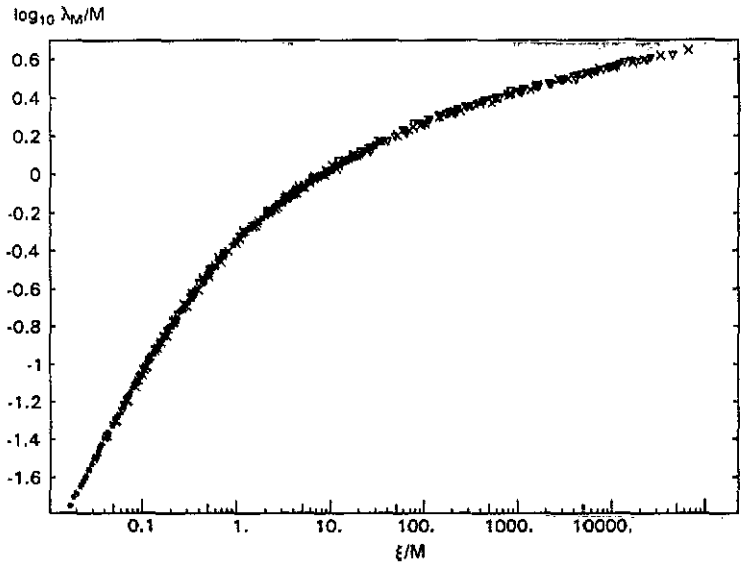

Figure 4. Scaling function obtained by a simultaneous fit of the raw data for the honeycomb lattice (*–see figure 2(*a*)), the triangular lattice (∇–see figure 2(*b*)) as well as respective data for the square lattice (×), for $E = 0$ in each case. The values of W that have been taken into account are compiled in table 1.

of errors. Consequently, we estimate the uncertainty of the largest scaling parameters obtained in this investigation to be at least a factor of 2. Thus, the above mentioned warning is specified; namely, why we consider a high accuracy of the raw data to be necessary in order to obtain reliable conclusions.

The actual dependence of the scaling parameter ξ on the disorder W is displayed in figure 5 for the different lattice structures. Qualitatively, the data agree with the results of previous calculations (MacKinnon and Kramer 1983, Zdetsis *et al* 1985), small quantitative discrepancies can be attributed to the mentioned numerically delicate determination of the scaling curve. The present data should be more reliable because they are based on larger samples than previous investigations.

The dependence of the scaling parameters on the disorder shown in figure 5 is in agreement with the scaling theory of localization. In all cases the decay length ξ increases with decreasing disorder. In the limit $W \to \infty$ the decay length diverges. But there is no sign of a metal–insulator transition, not even for the triangular lattice.

The calculated values of the decay length for the different lattice types are compiled in table 1. In this table it can also be seen that very large systems have to be taken into consideration in order to obtain the scaling parameters for small values of the disorder W.

In order to analyze the divergence of the scaling parameter for small disorder we have studied various functional dependencies. For the triangular lattice a clear dependence

$$\xi \propto e^{3/W^2} \tag{12}$$

could be established which is shown in figure 6. We note that this dependence leads to

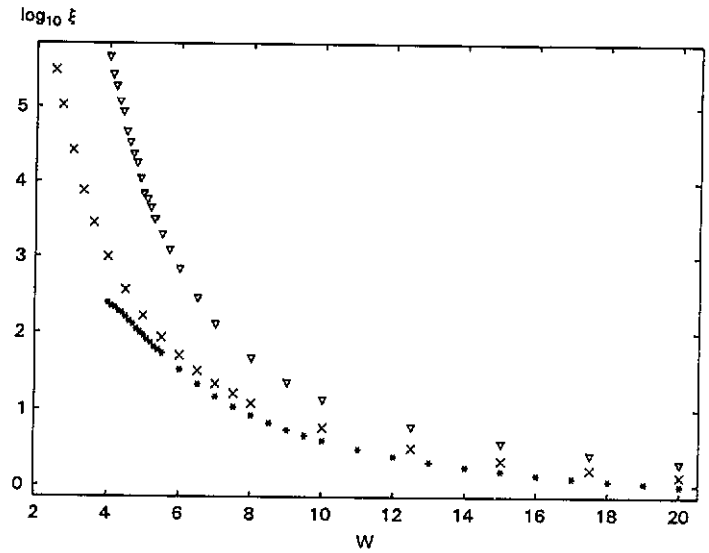

Figure 5. Scaling parameters $\xi(W, E = 0)$ for the honeycomb (*), the square (×), and the triangular lattice (▽) lattice. The data correspond to the curve in figure 4, obtained by simultaneous scaling of all the raw data that have been computed.

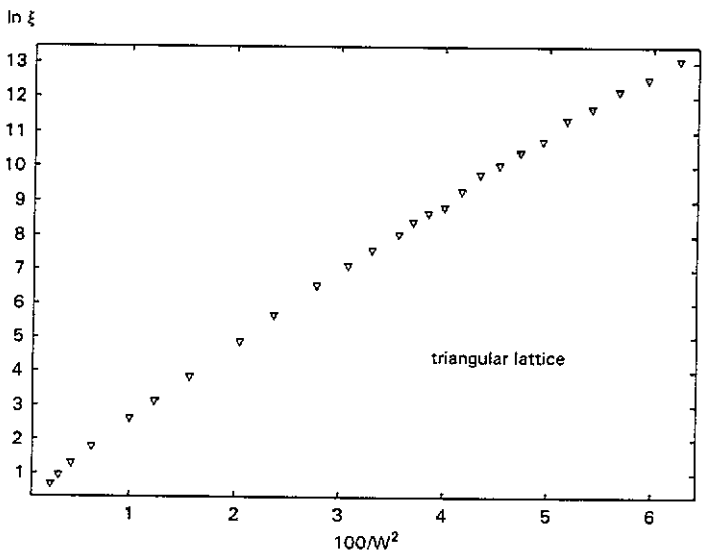

Figure 6. Dependence of the scaling parameter ξ on $1/W^2$ for the triangular lattice.

a divergent decay length ξ only for vanishing disorder W. Accordingly no metal–insulator transition at a finite W can be expected.

For the other lattices a similar dependence with considerably smaller prefactors in the exponent seems to be asymptotically reached, but the presently available data are inconclusive. For the triangular lattice, however, the dependence in figure 6 is obvious

and allows one to extrapolate the obtained values of the decay constant ξ to even lower values of the disorder W.

4. Concluding remarks

We have demonstrated numerically, within the well-defined error bars of the computation, that a one-parameter scaling function can be defined for different two-dimensional lattices in the band centre. The scaling parameter which corresponds to the exponential decay length of the transmission coefficient has been computed for various disorders for the three lattice types. It should be noted that this decay length of the transmission coefficient does not necessarily mean that the wave-function itself is exponentially localized. In view of recent calculations of the (multi)fractal properties of electronic wave-functions in disordered systems (Schreiber and Grussbach 1991) we argue that the fractal behaviour of the wave-function manifests itself in the Lyapunov characteristic exponents. If the essential fractal dimension is small enough, the wave-function will be concentrated on a set with small fractal dimension so that a small Lyapunov exponent results. But this set will be dispersed, accordingly the wave-function will formally extend over the whole system. Correspondingly, the transmission probability decays strongly so that the state appears to be localized. In 2D systems the multifractal behaviour has been demonstrated for small disorder for various values of the energy (Schreiber and Grussbach 1992). Although it is possible to increase the size of the system that could be investigated to as much as 720 000 sites (Grussbach and Schreiber 1992) it is impossible to prove that the multifractal behaviour extends to length scales as large as the decay lengths found in the present investigation for the smallest disorder. Therefore, the possibility cannot be ruled out that the fractal behaviour is characteristic for smaller scales only, so that the decay length obtained here can still be interpreted as a localization length for the electronic wave-function. It will probably be very difficult to clarify this obscurity convincingly.

In contrast, the present investigation has unambiguously shown that the transmission probability decays exponentially for the different 2D lattices irrespective of the coordination number. In conclusion, no metal–insulator transition can be found, not even in the triangular lattice with six nearest neighbours, contradicting recent proposals based on the mapping of the localization problem in the real lattice onto the localization problem in a trimmed Cayley lattice.

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