Localization of non-interacting electrons in thin layered disordered systems

2006 J. Phys.: Condens. Matter 18 7155

(http://iopscience.iop.org/0953-8984/18/31/010)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **18** (2006) 7155–7162 doi:10.1088/0953-8984/18/31/010

Localization of non-interacting electrons in thin layered disordered systems

V Z Cerovski, R K Brojen Singh and M Schreiber

Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz, Germany

Received 19 April 2006
Published 21 July 2006
Online at stacks.iop.org/JPhysCM/18/7155

Abstract

Localization of electronic states in disordered thin layered systems with b layers is studied within the Anderson model of localization using the transfer-matrix method and finite-size scaling of the inverse of the smallest Lyapunov exponent. The results support the one-parameter scaling hypothesis for disorder strengths W studied and $b = 1, \ldots, 6$. The obtained results for the localization length are in quantitative agreement with both the analytical results of the self-consistent theory of localization and the numerical scaling studies of the two-dimensional Anderson model. The localization length near the band centre grows exponentially with b for fixed W but no localization–delocalization transition takes place.

1. Introduction

The one-parameter scaling theory of Abrahams *et al* [1], which predicts that all single-particle electronic states of non-interacting electronic systems in two dimensions (2D) are localized for arbitrarily weak random potential, has attracted much attention in the last 25 years. This subtle effect is understood as being due to the constructive interference between time-reversed paths which increases the probability of returning to the original position leading to universal conductance fluctuations [2, 3] and corrections to conductivity, whose divergence in $d = 2$ explains the absence of diffusion [4–9]. It has also been investigated numerically for different lattice structures, e.g. square, honeycomb and triangular at the band centre ($E = 0$) and away from the band centre in two-dimensional (2D) systems, but no extended states were found for the non-interacting and zero-field case, supporting the scaling hypothesis [10]. There have been more theoretical and experimental investigations to see the validity of the conclusions of scaling theory [5, 11–15], supporting the theory from a variety of numerical, experimental and analytical approaches in the absence of electron–electron interactions, magnetic field and spin–orbit interactions [3–5, 8, 9, 15, 16].

In 3D systems, on the other hand, scaling theory predicts that there exists a second-order continuous phase transition, with a critical disorder above which all the states are localized whereas below it extended states appear at the band centre, separated by mobility edges from the localized states in the rest of the spectrum. This was supported by numerical [8, 9, 17, 18]

and analytical investigations [3, 5], with $d = 2$ being the lower critical dimension of the transition. The question then can be posed of what happens in thin films of finite thickness. When such a small thickness in terms of a few layers is introduced in an infinite 2D electron system, the degrees of freedom of the electron motion will be increased. This thin film can be expected to behave as a 2D system, if the Thouless length L_{Th}, which is the length scale up to which an electron can diffuse without inelastic collisions, is larger than the film thickness b, whereas for usual thin films, $L_{\mathrm{Th}} < b$ [4]. The study of such systems should be important because experiments are always done in thin films of finite thickness, and some experiments [19] which studied electron transport with the variation of film thickness showed a fascinating role of the film thickness in the metal–insulator transition (MIT): the authors observed an MIT in Mo–C films at a certain thickness and found that the characteristic parameters like localization length and dielectric constant grow exponentially with increasing thickness near the transition.

The numerical investigations in 2D and 3D systems played an important role to study the properties of electronic eigenstates in these systems. There have been various numerical methods applied in these systems, e.g. using exact diagonalization of the secular matrices [20], energy-level statistics [21], transfer-matrix method (TMM) [8, 10, 17], studies of the dimensionless conductance [23, 24], etc. The results of these studies support the one-parameter scaling hypothesis.

Recently [25], there was a discrepancy between numerical results obtained using the TMM and an analytical analysis of thin films of finite thickness based on the self-consistent theory [4, 5]. Numerically, an MIT induced by film thickness was found whereas the analytical results showed no metallic phase if the thickness of the film is finite [25]. The discrepancy is rather surprising since previous studies of 2D systems [8–10, 22] showed good agreement between the analytical and numerical results.

With this motivation we address numerically the problem of localization in thin disordered systems of noninteracting electrons using the standard TMM and finite size scaling (FSS) [8, 17] for non-interacting electrons in zero magnetic field as described by the Anderson model of localization (defined below), in systems of considerably larger sizes than in [25], and compare it with the analytical results. To this end we first note that the analytical expression for the localization length ξ from [25] can be expressed as

$$\xi = F\sqrt{\frac{b'}{\sinh b'}}\exp(b'\,C/W^2), \tag{1}$$

where C and F are non-universal constants, W is the disorder strength and b' is the film thickness. The expression is valid for $\lambda_{\mathrm{F}} \ll \ell \ll L < L_{\mathrm{Th}}$ and $\lambda_{\mathrm{F}} \ll b' \ll L$, where λ_{F} is the Fermi wavelength, ℓ the elastic mean-free path, and L the system size. In infinitely thick films ($b' \to \infty$), on the other hand, a crossover from 2D to 3D takes place where one can get both a metallic and an insulating phase depending on the disorder strength.

In section 2, we describe the model and the notations; the TMM and FSS are discussed in section 3; obtained numerical results are presented in section 3 and some conclusions based on our numerical results drawn in section 4.

2. The model

The Hamiltonian we have used for our numerical calculations is the Anderson model of localization given by

$$H = \sum_{r}^{N} \epsilon_r |r\rangle\langle r| - t \sum_{\langle r,r'\rangle}^{N} |r\rangle\langle r'|, \tag{2}$$

where $|r\rangle$ is a tight-binding state at site r. The sites r form a simple cubic lattice with $N = M \times b \times L$ atoms where L is the length, M is the width, and b is the thickness of the lattice, here measured in the number of layers of the system, in units of the distance a between the layers. Since the only relevant microscopic scale in the continuum model that gives equation (1) is ℓ, we compare the length scales of the continuum and Anderson model *via* the relation $b' = \alpha b$, where $\alpha \equiv a/\ell$ is a non-universal number which needs to be taken into account when comparing analytical and numerical results.

We use open boundary conditions along the b (thickness) direction and periodic boundary conditions along the M (width) direction. The on-site potentials ϵ_r are taken to be randomly distributed in the interval $[-W/2, W/2]$; $\langle r, r' \rangle$ denotes that the hopping t is restricted to the nearest neighbours and the energy units are chosen by setting $t = 1$.

We assume that this model describes the thin layered system if $b \ll M$. When b becomes comparable to M at small W, one should expect a crossover from insulating towards metallic behaviour after FSS, and it is therefore important to have b/M as small as possible in order to stay in the limit of finite thickness. We therefore attribute the appearance of the metallic-like behaviour in the numerical simulations of [25] to the large values of b/M used. Indeed, for $b = 6$, for instance, as M was changed from 2 to 15, the cross-section of the bars changed from rectangular to square to rectangular shape, and the scaling analysis for such geometries should not be compared with the analytical results of [25]. Instead, we focus on systems (2) with $M \gg b$. In the case of the thickest system studied here, for example, the scaling analysis is done for $b = 6$ and $M = 23, 33, 47$, and 65, as we discuss in detail below.

3. One-parameter finite size scaling

In the TMM one determines localization properties by a scaling analysis of the Lyapunov exponents (LE) of the transfer matrices of quasi-1D bars.

The largest length scale λ_{Mb} is obtained from the smallest LE, $\lambda_{Mb} \equiv 1/\gamma_{Mb}$. The accuracy of these λ_{Mb} is determined from the variance of the changes of the exponents in the course of the iteration, and the relative error of λ is 1% in our calculations. For $b = 1$ our system is a 2D strip of width M and length $L \gg M$, while for $b = M$ it becomes a 3D bar with square cross-section of $M \times M$ atoms and length L.

We check the one-parameter scaling theory by the FSS analysis [8] of the renormalized decay length, $\Lambda_{Mb} = \lambda_{Mb}/M$, for each b individually by expressing it as

$$\Lambda_b(M, W) = f_b\left(\xi_b(W)/M\right), \tag{3}$$

where $\xi_b(W)$ is the scaling parameter which can be identified as the localization length in the insulating regime and the resistivity in the metallic regime of the infinite system [8] and $f_b(x)$ should be, if the one-parameter hypothesis holds, a universal function $f(x)$ independent of b. The scale of ξ is determined from the condition that $f_b(x) = x$ when $x \to 0$ [8], which corresponds to expressing ξ in units of a. The numerical determination of $f_b(x)$ is done by the method based on [8], and the thus obtained scaling functions for different b are compared to check for the universality. If there is an MIT, then Λ_b for given b will have two branches, one which goes to zero as M increases (indicating localization of electronic eigenstates) and the other which diverges as M increases (indicating extended eigenstates).

Figure 1 shows $\Lambda_b(M, W)$ as a function of strip width M for various W, the scaling function $f_b(\xi_b(W)/M)$, as well as the localization length $\xi(W)$ for systems with $b = 2, 3, 4$ layers, and figure 2 shows the same quantities for systems with $b = 5, 6$ layers. Our results for $b = 1$ are not shown since they are in agreement with results obtained before [22]. For larger W values, Λ_{Mb} decreases as the width of the system M increases, indicating localization, while for smaller W values the decrease becomes much weaker.

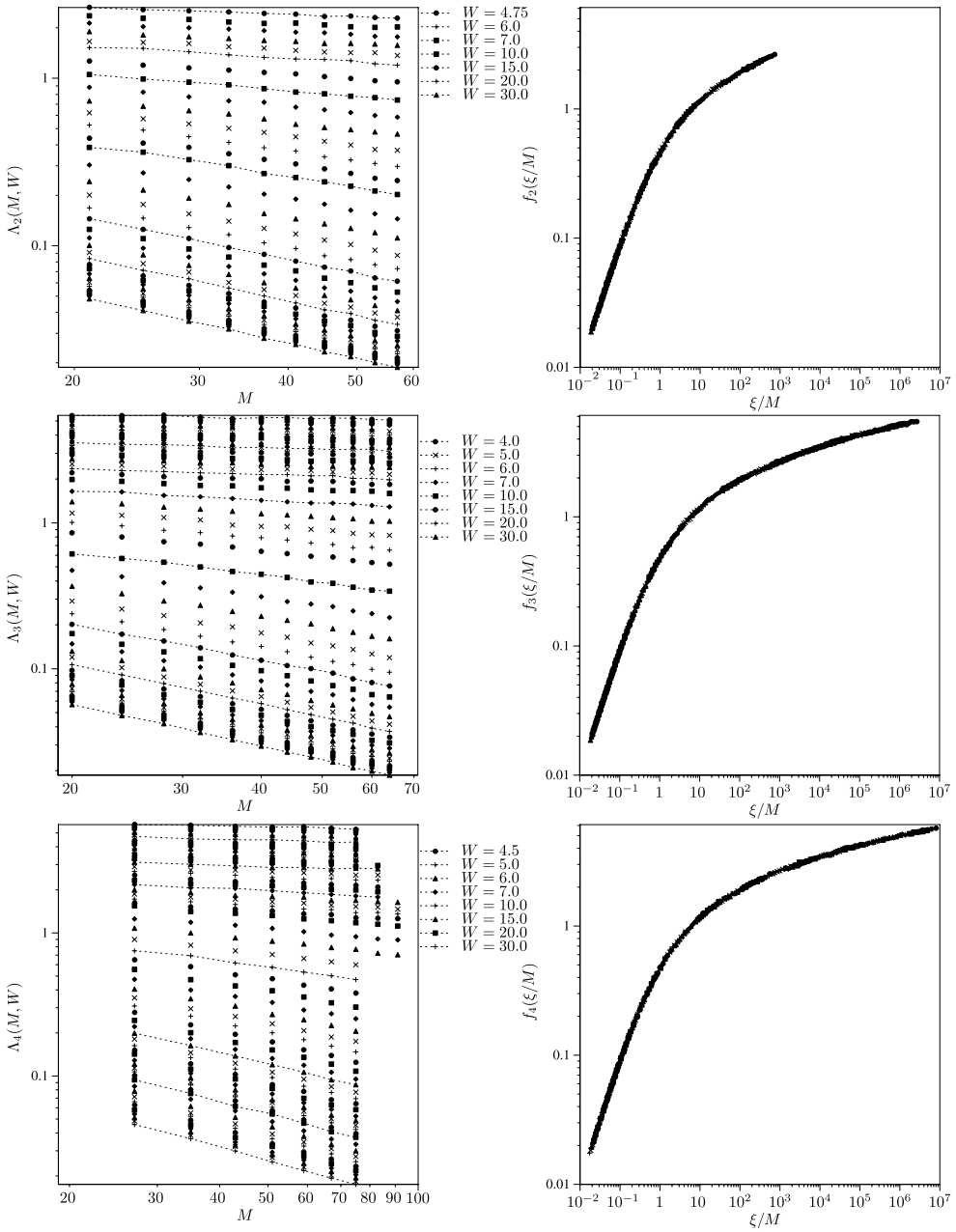

Figure 1. Plot of the renormalized decay length $\Lambda_b(M, W)$ (left panels), scaling function f_b (right panels) for systems of width M and $b = 2, 3, 4$ layers, from top to bottom. Dotted lines connect points for W values indicated in the corresponding legend.

In addition to the results presented in figures 1 and 2, we have calculated Λ_b for W values as small as $2, 2, 4, 4, 4$ for $b = 2, 3, 4, 5, 6$, respectively, but no metallic behaviour was found. Instead, the $\Lambda_b(M)$ become approximately constant for smaller W values, which is in qualitative agreement with 2D being the lower critical dimension of the localization–delocalization transition.

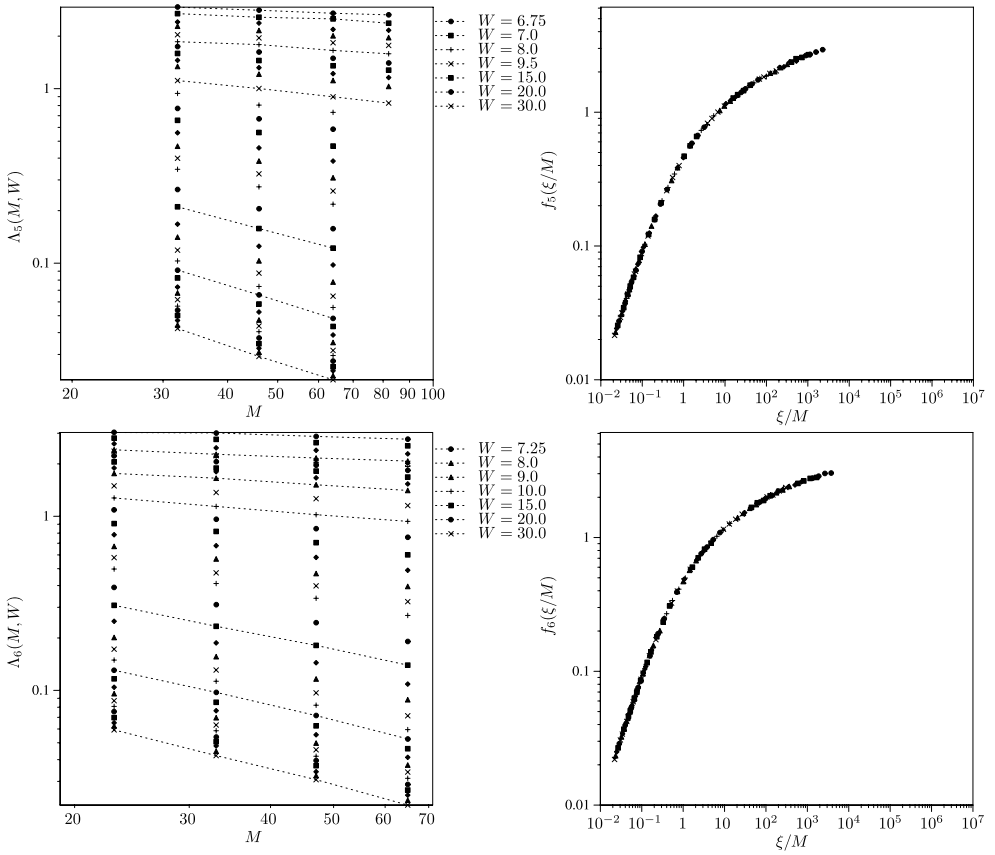

Figure 2. The same as figure 1, for $b = 5$ and 6 layers, respectively.

To see the dependence of the scaling function f_b on b, we first plot all the obtained results for f_b in figures 1 and 2 using the same range on the axes for easier comparison, and then show all of the obtained f_b together in figure 3, without any rescaling or shifting of individual curves, including the curve for $b = 1$. The figure shows that f_b does not depend on b, therefore supporting the universality of the scaling function $f(x)$. Since it has only one branch corresponding to the localized states it is also in agreement with the one-parameter scaling hypothesis for disorder strengths $W \geqslant 4.75, 4.0, 4.5, 6.75, 7.25$ for $b = 2, 3, 4, 5, 6$, respectively. For $b = 1$, one parameter-scaling was found [8, 22] to hold for $W > 2$, and the previously obtained [8] scaling function $f(x)$ for the 2D system agrees within error bars with the $f(x)$ obtained here for $b \geqslant 1$, furthermore supporting the universality of the result.

To compare the dependence of the localization lengths on W to the analytical result (1), we fit the obtained $\xi_b(W)$ to the form

$$\xi_b(W) = A_b \exp\left(\frac{C_b}{W^2}\right), \tag{4}$$

as shown in the left panel of figure 4. The upper and lower right panels of the same figure show, respectively, the dependence of C_b and $F_b \equiv A_b\sqrt{\sinh b/b}$ on the number of layers b. The upper right panel of the figure also contains the mean least-squares linear fit of C_b, which gives $C_b = C\,b + C_0$, $C = 99 \pm 4$, $C_0 = 10 \pm 15$. The obtained value $C_0 \approx 0$ is an

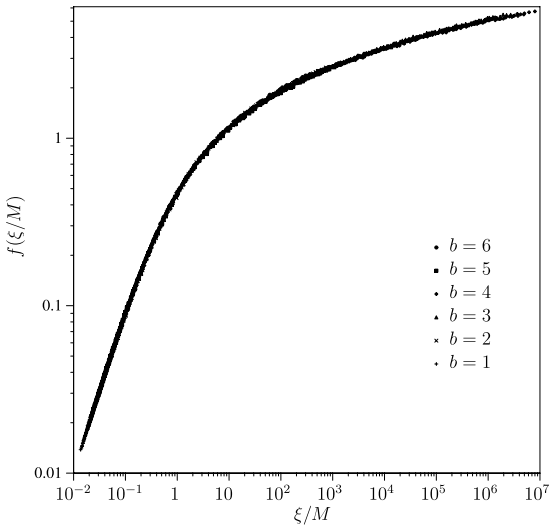

Figure 3. Plot of the scaling functions $f_b(\xi/M)$ for $b = 1, 2, \ldots, 6$ from figures 1 and 2.

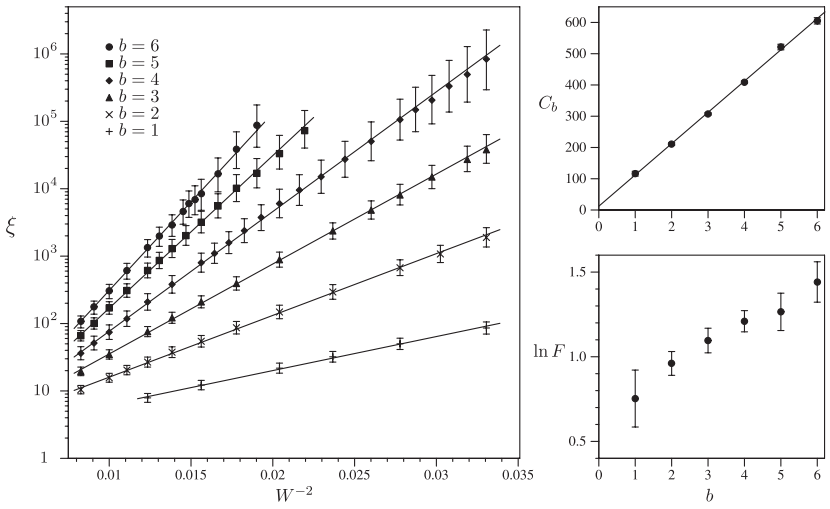

Figure 4. Left panel: dependence of the localization length ξ_b on W^{-2}. Straight lines are fits to the expression $\xi_b(W) = A_b \exp(C_b/W^2)$. The rightmost point for each b value corresponds to the W of the topmost curve of the corresponding panel in figures 1 and 2. Right panels: dependence of the fitting parameters on the thickness b.

additional check that the numerical results are in agreement with equation (1) as far as the W^{-2} dependence in the exponent is concerned.

The obtained values of $\ln F$ depend on b, which seems to be in contradiction with equation (1) but can be explained by taking into the account the scale factor α, and figure 5 shows $\ln F$, where $F \equiv A_b\sqrt{\sinh \alpha b/\alpha b}$ for $\alpha = 0.73$, when $\ln F$ becomes approximately constant, and $\alpha = 0.73 \pm 0.13$, where the error bar is estimated from the range of α values for which the values of $\ln F$ for different b remain within error bars among themselves. This result can be interpreted as that the effective ℓ of the lattice model (2) in the range of W studied is of the order of 1.4 ± 0.2 lattice constants.

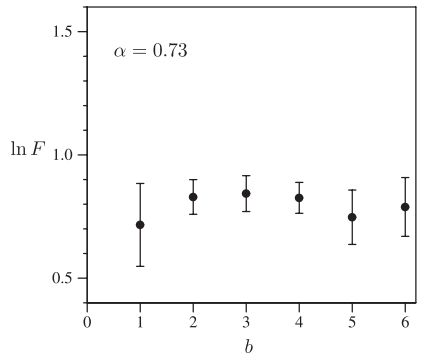

Figure 5. Dependence of $\ln F$ on b for $\alpha = 0.73$.

As an additional check of the validity of the above results we notice that the obtained value of C is in agreement with the value $C \approx 100$ obtained in the numerical studies of the 2D Anderson model [8, 22], i.e. for $b = 1$, even though the method by which we determine C relies essentially on the study of systems with $b > 1$.

Finally, we have done one more check of the results obtained so far, by nonlinear fitting of results presented in the left panel of figure 4 to equation (1). The obtained values of the fitting parameters, with $\chi^2 = 58.3$, $C = 94 \pm 3$, $\alpha = 0.64 \pm 0.13$, and $\ln F = 0.41 \pm 0.16$, are consistent with the parameters discussed above.

4. Conclusions

Thin quasi-1D bars with rectangular cross section of $M \times b$ and length $L \gg M$ atoms were studied using the TMM and FSS of the inverse of the smallest Lyapunov exponent, for $b = 1, 2, 3, 4, 5, 6$ and $M \gg b$. The obtained localization lengths were found to be in a quantitative agreement with the analytical results. Despite the exponential increase of the localization length as the thickness increases, we find no signs of extended states for the disorder strengths studied, in agreement with the one-parameter scaling hypothesis.

Acknowledgments

One of us (BKRS) would like to thank Professor Deepak Kumar for valuable discussions.

References

[1] Abrahams E, Anderson P W, Licciardello D C and Ramakrishnan T V 1979 *Phys. Rev. Lett.* **42** 673
[2] Altshuler B L, Lee P A and Webb R A (ed) 1991 *Mesoscopic Phenomena in Solids* (Amsterdam: North-Holland)
[3] Lee P A and Stone A D 1985 *Phys. Rev. Lett.* **55** 1622
McKane A J and Stone M 1981 *Ann. Phys.* **131** 36
[4] Lee P A and Ramakrishnan T V 1985 *Rev. Mod. Phys.* **57** 287
[5] Vollhardt D and Wölfle P 1980 *Phys. Rev. Lett.* **45** 842
Vollhardt D and Wölfle P 1980 *Phys. Rev.* B **22** 4666
Hanke W and Kopaev Yu V (ed) 1992 *Electronic Phase Transitions* (Amsterdam: Elsevier Science) p 1
[6] Bergmann G 1984 *Phys. Rep.* **107** 1
[7] Chakravarty S and Schmid A 1986 *Phys. Rep.* **140** 193
[8] MacKinnon A and Kramer B 1981 *Phys. Rev. Lett.* **47** 1546
MacKinnon A and Kramer B 1983 *Z. Phys.* B **53** 1

[9] Kramer B and MacKinnon A 1993 *Rep. Prog. Phys.* **56** 1469
[10] Schreiber M and Ottomeier M 1992 *J. Phys.: Condens. Matter* **4** 1959
Tit N and Schreiber M 1995 *J. Phys.: Condens. Matter* **7** 5549
[11] Dolan G J and Osheroff D D 1979 *Phys. Rev. Lett.* **43** 721
[12] Bishop D J, Tsui D C and Dynes R C 1980 *Phys. Rev. Lett.* **44** 1153
Bishop D J, Dynes R C and Tsui D C 1982 *Phys. Rev.* B **26** 773
[13] Uren M J, Davies R A and Pepper M 1980 *J. Phys. C: Solid State Phys.* **13** L985
[14] Marković N, Christiansen C and Goldman A M 1998 *Phys. Rev. Lett.* **81** 5217
[15] Abrahams E, Kravchenko S V and Sarachik M P 2001 *Rev. Mod. Phys.* **73** 251
[16] Dobrosavljević V, Abrahams E, Miranda E and Chakravarty S 1997 *Phys. Rev. Lett.* **79** 455
[17] Pichard J L and Sarma G 1981 *J. Phys. C: Solid State Phys.* **14** L127
[18] Slevin K and Ohtsuki T 1999 *Phys. Rev. Lett.* **82** 382
[19] Lee S J, Ketterson J B and Trivedi N 1992 *Phys. Rev.* B **46** 12695
[20] Schreiber M and Grussbach H 1991 *Phys. Rev. Lett.* **67** 607
Schreiber M and Grussbach H 1993 *Fractals* **1** 1037
Grussbach H and Schreiber M 1995 *Phys. Rev.* B **51** R663
[21] Shklovskii B I, Shapiro B, Sears B R, Lambrianides P and Shore H B 1993 *Phys. Rev.* B **47** 11487
Simons B D and Altshuler B L 1993 *Phys. Rev.* B **48** 5422
Hofstetter E and Schreiber M 1994 *Phys. Rev.* B **49** 14726
[22] Zharekeshev Kh, Batch M and Kramer B 1996 *Europhys. Lett.* **34** 589
[23] Shapiro B 1990 *Phys. Rev. Lett.* **65** 1510
Altshuler B L, Kravtsov V E and Lerner I V 1989 *Phys. Lett.* A **134** 488
[24] Slevin K, Markoš P and Ohtsuki T 2001 *Phys. Rev. Lett.* **86** 3594
Slevin K, Markoš P and Ohtsuki T 2003 *Phys. Rev.* B **67** 155106
[25] Brojen Singh R K and Kumar D 2002 *Phys. Rev.* B **66** 75123