Mobility edge and level statistics of random tight-binding Hamiltonians

Fabio Siringo and Giovanni Piccitto

Dipartimento di Fisica e Unità INFM dell'Università di Catania, Corso Italia 57, I 95129 Catania, Italy

Abstract. The energy level spacing distribution of a tight-binding Hamiltonian is monitored across the mobility edge for a fixed disorder strength. Any mixing of extended and localized levels is avoided in the configurational averages, thus approaching the critical point very closely and with high energy resolution. By finite-size scaling the method is shown to provide a very accurate estimate of the mobility edge and of the critical exponent for a cubic lattice with Lorentzian distributed diagonal disorder. Since no averaging in wide energy windows is required, the method appears as a powerful tool for locating the mobility edges in more complex models of real physical systems.

The metal–insulator (MI) transition in disordered systems is still attracting considerable interest with special regard to the critical universal properties [1, 2]. Even in the absence of any interaction, the lack of a full analytical treatment for $d = 3$ has given rise to a very slow convergent process [3–6] for the numerical evaluations, generally based on finite-size scaling [7]. An alternative to the standard transfer matrix method [8] has been recently given by the energy level statistics method (ELSM) [9, 10] which has reached the status of a very reliable tool, yielding accurate predictions for the transition points and critical properties. Localized and delocalized levels have been shown [9, 10] to follow different universal spacing distributions $P(s)$ in the thermodynamic limit. Precisely, in the metallic regime the overlapping states follow the general Wigner–Dyson random-matrix theory [11], and the distribution of the distances between successive levels is well described by the Wigner surmise

$$P_W(s) = \frac{\pi}{2} s \exp\left(-\frac{\pi}{4} s^2\right) \tag{1}$$

which is characterized by the typical level repulsion since $P(0) = 0$. Here s is the level distance in units of the average local level spacing $\Delta E = 1/[ND(E)]$ where N is the total number of states and $D(E)$ is the averaged density of states (DoS) normalized to 1. On the other hand for localized levels the lack of overlap determines a different statistical behaviour described by the Poisson distribution

$$P_P(s) = e^{-s} \tag{2}$$

where level repulsion is absent. For finite systems an intermediate regime shows up in the crossover region, and the corresponding critical ensemble has been recently characterized and shown to be described by a third universal distribution [12–14]. Then, in order

to extrapolate towards the thermodynamic limit, finite-size scaling has been extensively used, allowed by the numerical calculation of any one-parameter scaling function which characterizes the distribution $P(s)$ along the crossover [4, 13]. The critical ensemble which determines the critical properties has been recently shown to be universal and even insensitive to the changes of symmetry determined by a field [15] or spin–orbit coupling [16], or to changes in the nature of the disorder [17]. Thus the method seems to be of practical interest for determining the critical properties of more realistic phenomenological models.

However, although large clusters have been recently considered up to 28^3 sites [6], some shortcomings can be found in the generally accepted ELSM procedure. (i) In order to improve the statistical analysis a wide energy band is usually considered, thus averaging over a dishomogeneous class of levels. In fact, at the critical point, the mixing of extended and localized levels cannot be ruled out even for the most favourable case of a box distribution which yields quite a wide interval of homogeneously extended states at the band centre. As a consequence the critical point cannot be reached with good accuracy. (ii) Only a box distribution for the diagonal matrix levels is well suited for such an approach, since for a generic peaked distribution the use of a wide band would be unacceptable. Thus any realistic calculation, based on a phenomenological model, is ruled out. (iii) The scaling function is usually evaluated for discrete fixed values of the disorder strength parameter W, and the critical point is then recovered by interpolation. Since any new value of W requires a new average over the configurations, a very small step for W around the critical point becomes prohibitive. (iv) No information is obtained about the trajectory of the mobility edge versus W below the critical point, unless the statistics is determined in very small energy ranges.

In this paper, in order to deal with such difficulties, we propose the first attempt to characterize the transition through a scaling function of the level energy E. Below the critical disorder, a mobility edge separates localized and extended levels in the thermodynamic limit. Thus the spacing distribution $P(s)$ changes discontinuously at the mobility edge from $P_P(s)$ to $P_W(s)$. For a finite system the transition is rounded and a continuous crossover is observed. Any monotonic functional α of $P(s)$ could in principle be employed for characterizing the spacing distribution as a function of the energy E across the transition [4]. According to the one-parameter scaling theory of localization [18] the coherence length of the states is a function of the level energy $\xi(E)$ diverging at the mobility edge E_c as

$$\xi \sim (E - E_c)^{-\nu}. \tag{3}$$

For a finite system, neglecting boundary effects, the functional α depends on E through the only parameter $\xi(E)/L$ where L is the linear dimension of the system. Thus finite-size scaling yields the mobility edge E_c and the critical exponent ν provided that the functional α can be determined as a function of E across the transition, for a fixed disorder strength W. We choose for α the second moment $\alpha = \langle s^2 \rangle$, and directly evaluate such a functional on the level configurations for any E by a new method which avoids both averaging inside a wide window of levels and any fit for the distribution $P(s)$. Apart from statistical fluctuations, we obtain α as a continuous function of E across the mobility edge which can be approached with the desired accuracy within the same set of configurations (only one set of configurations, with a fixed disorder distribution, is required for each value of L). Moreover, we avoid any mixing between localized and extended states in the evaluation of α which now acquires a different value for any different energy.

In order to illustrate the method we consider a standard tight-binding Hamiltonian on a cubic lattice with nearest-neighbour hopping and diagonal disorder described by a peaked

Lorentzian

$$g(\epsilon) = \frac{1}{\pi} \frac{W}{W^2 + \epsilon^2}. \tag{4}$$

The mobility edge is obtained for several values of W, and the critical exponent $\nu = 1.30 \pm 0.05$ is recovered in excellent agreement with previous reports [3, 4, 13, 16]. Note that the field-theoretical argument reported in [3] for the universality of the critical exponent does not hold for the Lorentzian distribution since now the moments are not well defined. Thus the agreement with the estimates obtained for the box and Gaussian distribution [3], and for the binary percolation model [17] should be understood in the framework of a more general theoretical argument.

The Hamiltonian reads

$$\hat{H} = \sum_i \epsilon_i c_i^\dagger c_i + t \sum_{\langle ij \rangle} c_i^\dagger c_j \tag{5}$$

where c_i, $c_i^\dagger$ are annihilation and creation operators for a local state on the cubic lattice site i, and the diagonal level ϵ_i is randomly distributed according to the Lorentzian (4). All energies are reported in units of the nearest-neighbour hopping term t, thus the system is entirely characterized by the width W of the distribution.

The eigenvalues are exactly evaluated for each random configuration of a finite $M \times M \times M$ cubic lattice with $M = 6, 7, 8, 9, 10$. No special boundary conditions have been imposed and a total number of 10^4 configurations have been considered for each lattice size M.

The choice of the second moment $\alpha = \langle s^2 \rangle$ for characterizing the spacing distribution comes from statistical convenience: no fit is required or knowledge of the distribution, since α is computed by direct average over the configurations. Moreover, all the configurations contribute on average, and both the large and small s regions are taken into account. Such a functional has a monotonic behaviour from the Poisson limit value $\alpha = 2$ to the Wigner surmise opposite limit $\alpha = 4/\pi \approx 1.27$, as can be easily checked from equations (1) and (2).

The second moment has already been used for characterizing the spacing distribution $P(s)$ as a function of the strength W of the disorder [13]. In that work a wide energy window was used in order to decrease the statistical fluctuations. Conversely in this work, at the cost of a larger fluctuation of α, we evaluate a basically independent average for each value of E, at a fixed disorder strength. For any energy E, and for each configuration, we find two consecutive eigenvalues E_i, E_{i+1} satisfying $E_i < E < E_{i+1}$. Then the variable $y = (E_{i+1} - E_i)/\Delta E$ is averaged over the N_{conf} random configurations of the system. Note that the average level spacing ΔE is a function of E, and is independently evaluated by the average DoS. Since each couple of consecutive eigenvalues has a probability proportional to y of containing the point E, then the generic moment follows

$$\langle s^n \rangle = \langle y^{n-1} \rangle. \tag{6}$$

From the central limit theorem the statistical fluctuation of α may be estimated as $\Delta \alpha^2 \approx (\langle s^4 \rangle - \langle s^2 \rangle^2)/N_{\text{conf}}$. In the Poisson limit, where the fluctuations are larger, and for $N_{\text{conf}} = 10^4$, we obtain from equation (2) $\Delta \alpha \approx 0.045$ which is slightly more than 2%.

It is instructive recovering the Poisson limit for $t = 0$, and for a generic distribution $g(\epsilon)$. Since the Hamiltonian is diagonal, the DoS is directly given by the distribution g for the diagonal level. At a fixed energy E the average spacing is $\Delta E = 1/[Ng(E)]$ where the total number of states is $N = M^3$. Following an argument first considered by Hertz [19],

the probability $P(s)\,\mathrm{d}s$ must be equal to the probability that no levels exist between E and $E+s\Delta E$ times the probability that a level does exist between $E+s\Delta E$ and $E+(s+\mathrm{d}s)\Delta E$:

$$P(s)\,\mathrm{d}s = \left[1 - \int_0^s P(s')\,\mathrm{d}s'\right] N\Delta E g(E + s\Delta E)\,\mathrm{d}s. \tag{7}$$

Dividing by $g(E + s\Delta E)\,\mathrm{d}s$ and differentiating with respect to s we obtain

$$\frac{P'(s)}{P(s)} = -\frac{1}{g(E)}\left[g(E + s\Delta E) - \frac{g'(E + s\Delta E)}{Ng(E + s\Delta E)}\right]. \tag{8}$$

Such an equation may be directly integrated, yielding a different distribution $P(s)$ for each value of E. In the very special case of a box distribution the function g is constant and the Poisson distribution is recovered for any E. In general, assuming N large, we may expand the right-hand side of equation (8) in powers of $s\Delta E$, then integrating

$$P(s) = P(0)\exp\left[-s - \frac{g'}{Ng^2}\left(\frac{1}{2}s^2 - s\right) + \mathrm{O}(1/N^2)\right]. \tag{9}$$

Thus, for large N, the distribution $P(s)$ tends to the Poisson universal limit at any E, and for any distribution g. However, the convergence is not uniform, since it is controlled by the parameter $g'/(Ng^2)$ which is strongly energy dependent and diverging in the limit $E \to \infty$ for any regular normalized distribution. In other words, deep in the tail of the DoS an increasingly large system size is required for recovering the Poisson limit $\alpha \to 2$ as the energy E increases. Strong deviations from the limit distribution are then expected in the tails, where the size required for the convergence could be prohibitive for any numerical calculation. Once more we show the importance of avoiding level mixing inside a wide energy window, since not all the levels are generally described by the same spacing distribution even in the case of strong localization ($t = 0$). The convergence towards the Poisson limit must be checked as a function of E before undertaking any serious calculation, in order to fix a bound to the accessible range of energy for a given system size. For the Lorentzian (4) $g'/(Ng^2) \sim E/(NW)$ and, as we checked by a numerical test, for $N \approx 10^3$, up to $E \approx 7W$ the deviations from the Poisson limit $\alpha = 2$ are negligible as shown in figure 1. However, we must stress that whenever the ratio E/W increases a larger cluster size is required in order to reach the Poisson limit. A progressively worse accuracy is expected when exploring the band tails (E large) or in the limit $W \to 0$, where the present method would require prohibitive values of N.

In figure 1 the functional α is compared for $t = 0$ and $t \neq 0$, at a fixed disorder strength and sample size. For $t \neq 0$ the second moment α approaches the Wigner limit around the band centre, indicating that for such an energy range the states are extended. In the band tail α tends to the Poisson limit, and a crossover region shows up around $E = E_c$.

In order to get rid of the statistical fluctuations of α, the data around E_c have been fitted by a polynomial. Data for $W = 2$ are shown in figure 2: for different sizes $L = M - 1$ the fitted curves all cross at one point with surprising accuracy; in fact the fit procedure allows an averaging over a large number of fluctuating estimates of α, thus improving the accuracy without spoiling the energy dependence of the curves. The crossing point $E = E_c$ corresponds to the mobility edge of the infinite system. For $W = 2$ averaging over all the crossing points yields a very accurate determination of the mobility edge $E_c = 3.8 \pm 0.05$ despite the small sizes considered in the calculation. The standard error is mainly due to a residual small shift of the mobility edge, and an even more accurate determination of E_c would be achievable by increasing the system size.

According to the one-parameter scaling hypothesis, linearizing α around E_c, we obtain

$$\log L = \nu \log|\alpha'(E_c, L)| + \text{constant} \tag{10}$$
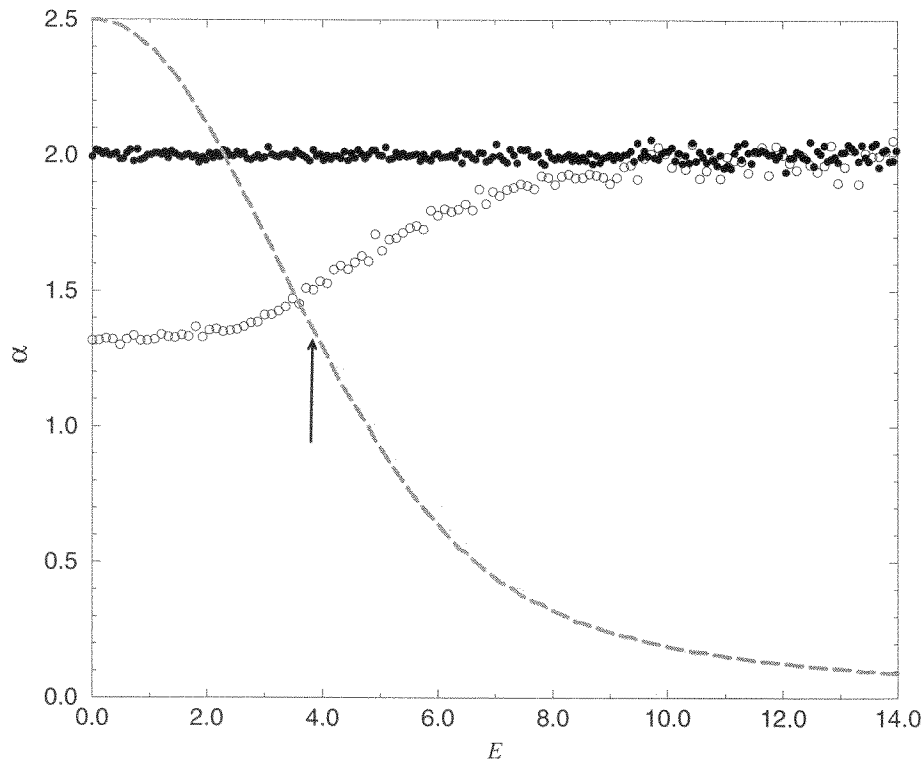
Figure 1. The second moment α versus the energy E inside the band for $t = 0$ (full circles) and $t \neq 0$ (open circles). The disorder strength is fixed at $W = 2$, and the sample size is $M = 10$. All the energies are in units of t. An arrow in the crossover region shows the position of the mobility edge $E_c = 3.8$ as determined by finite-size scaling. The broken curve is the corresponding averaged DoS scaled by an arbitrary factor.

where the derivative α' can be evaluated with good accuracy at the critical point by the polynomial fit parameters. Thus the method allows a very close approach to the critical point, while avoiding any mixing between localized and extended states. The critical exponent ν has been determined by a linear fit of equation (10) for $M = 6, 7, 8, 9, 10$ yielding $\nu = 1.35 \pm 0.05$ for $W = 2$ and $\nu = 1.26 \pm 0.05$ for $W = 2.5$. The average value $\nu = 1.30$ is very close to previous estimates obtained by several authors for the box distribution [3, 4, 9, 13], for the Gaussian and binary distributions [3], in the presence of a field [15] or of spin–orbit coupling [16], and even for the off-diagonal binary disorder of a percolation system [17]. All these estimates were found by averaging over a more or less wide energy window of levels at the centre of the DoS. In such a case the monitored transition corresponds to the disappearance of any extended state from the system. For the percolation system the occurrence of a more realistic peaked DoS has forced the authors [17] to focus on narrow windows. A more detailed study of the mobility edge in that system would be achievable by the present method. All these predictions are in slight contrast to recent findings by the transfer matrix method [5] and standard ELSM [6] which report a larger estimate for the critical exponent ($\nu = 1.45$ and $\nu = 1.54$ respectively) which is not confirmed by the present work.

A tentative trajectory for the mobility edge has been recovered by repeating the
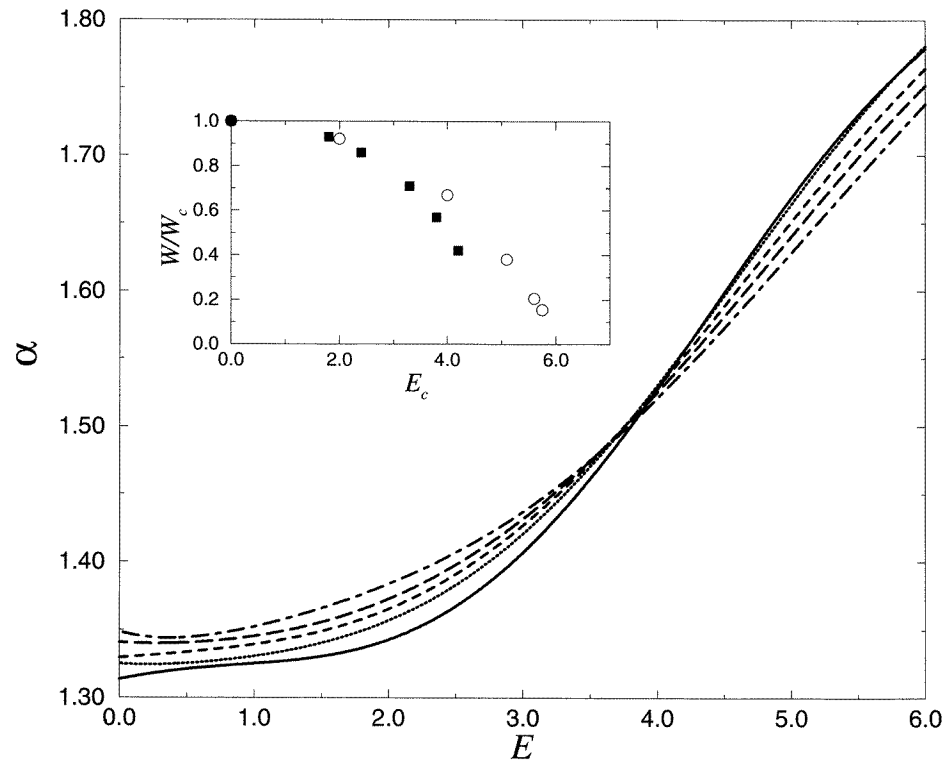
Figure 2. Polynomial fit of the data for α in the crossover energy range, for $M = 6, 7, 8, 9, 10$ and $W = 2$. At the band centre $E \approx 0$ the lower curve corresponds to the largest size. The trajectory of the mobility edge is shown in the inset (squares) and compared with the data reported in [20] (circles).

calculation at different values of W. No crossing occurs for $W > 4$, indicating that the critical point must lie below that value. For $W = 1.5, 2.0, 2.5, 3.0, 3.25$ and 3.5 the mobility edge has been found at the energy $E_c = 4.2, 3.8, 3.3, 2.4, 1.8$ and 0.0 respectively. Thus we may locate the critical disorder at $W_c = 3.5 \pm 0.1$. The trajectory of the mobility edge is shown in the inset of figure 2, and compared with previous data reported by Bulka *et al* [20]. We must observe that any extrapolation of our data towards the $W = 0$ limit does not make any sense since, as previously discussed below equation (9), whenever the ratio E_c/W increases, the cluster size becomes too small to reach the Poisson limit, thus determining a progressive underestimate of the critical edge position E_c. Such a shortcoming is a consequence of the ELSM method by itself when applied to realistic distributions, and could in part be avoided by employing large cluster sizes and approximate diagonalization routines.

As an important by-product, we have noticed the existence of a universal critical value $\alpha_c = 1.5 \pm 0.03$ for all the considered disorder strengths W, thus pointing toward the existence of a critical $P(s)$ distribution which is expected to be universal [12–15]. Our estimate for α_c is not too far from the previous evaluation $\alpha_c = 1/0.7 = 1.43$ reported by Varga *et al* [13] for a box distribution.

In summary we have shown that the ELSM provides a very accurate way of determining the mobility edge and the critical exponent even for more realistic disorder distributions.

The scaling function has been determined for any energy point E avoiding any mixing of localized and extended states in the configurational average. Moreover, a standard fit procedure allows a very close approach to the critical point with a small statistical error without spoiling the energy dependence of the scaling function. Thus the method provides a powerful tool for detecting the mobility edge in the framework of more complex phenomenological models of real physical systems. As a by-product we have shown that the Lorentz distributed random system belongs to the same universality class of the box and the Gaussian, as is evident from a comparison of the critical exponents. We notice that, in spite of being generally expected, such universality cannot be proved by the weaker field-theoretical argument of [3] which is based on the assumption that the distribution has well-defined moments.

References

[1] Lee P A and Ramakrishnan T V 1985 *Rev. Mod. Phys.* **57** 287
[2] Kramer B and MacKinnon A 1993 *Rep. Prog. Phys.* **56** 1469
[3] Hofstetter E and Schreiber M 1993 *Europhys. Lett* **21** 933
[4] Hofstetter E and Schreiber M 1994 *Phys. Rev.* B **49** 14 726
[5] MacKinnon A 1994 *J. Phys.: Condens. Matter* **6** 2511
[6] Zharekeshev I K and Kramer B 1995 *Phys. Rev.* B **51** 17 239
[7] Binder K 1981 *Phys. Rev. Lett.* **47** 693
[8] MacKinnon A and Kramer B 1981 *Phys. Rev. Lett.* **47** 1546
[9] Shklovskii B I and Shapiro B 1993 *Phys. Rev.* B **47** 11 487
[10] Hofstetter E and Schreiber M 1993 *Phys. Rev.* B **48** 16 979
[11] Wigner E P 1955 *Ann. Math.* **62** 548
     Wigner E P 1957 *Ann. Math.* **65** 203
     Dyson F J 1962 *J. Math. Phys.* **3** 140
     Dyson F J 1962 *J. Math. Phys.* **3** 1199
[12] Kravtsov V E, Lerner I V, Altshuler B L and Aronov A G 1994 *Phys. Rev. Lett.* **72** 888
     Aronov A G, Kravtsov V E and Lerner I 1995 *Phys. Rev. Lett.* **74** 1174
[13] Varga I, Hofstetter E, Schreiber M and Pipek J 1995 *Phys. Rev.* B **52** 7783
[14] Evangelou S N 1994 *Phys. Rev.* B **49** 16 805
[15] Hofstetter E and Schreiber M 1994 *Phys. Rev. Lett.* **73** 3137
[16] Kawarabayashi T, Ohtsuki T, Slevin K and Ono Y 1996 *Phys. Rev. Lett.* **77** 3593
[17] Berkovits R and Avishai Y 1996 *Phys. Rev.* B **53** R16 125
[18] Abrahams E, Anderson P W, Licciardello D C and Ramakrishnan T V 1979 *Phys. Rev. Lett.* **42** 673
[19] Hertz P 1909 *Math. Ann.* **67** 387
[20] Bulka B, Schreiber M and Kramer B 1987 *Z. Phys.* B **66** 21