Mobility Edge and Level Statistics
of Random Tight-Binding Hamiltonians

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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.

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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 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 the 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

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

$$P_P(s) = e^{-s}$$  \hspace{1cm} (2)$$

where level repulsion is absent. For finite systems an intermediate regime shows up in the cross-over 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 scaling has been extensively used,
allowed by the numerical calculation of any one-parameter scaling function which characterizes the distribution $P(s)$ along the cross-over[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 even 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 a box distribution which is known to yield a very flat behaviour. 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 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.

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 cross-over is observed. Any monotonic functional \( \alpha \) 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

\[
\xi \sim (E - E_c)^{-\nu}
\]  

(3)

For a finite system, neglecting boundary effects, the functional \( \alpha \) 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 \( \nu \) provided that the functional \( \alpha \) can be determined as a function of \( E \) across the transition, for a fixed disorder strength \( W \). We choose for \( \alpha \) the second moment \( \alpha = \langle s^2 \rangle \), and directly evaluate such 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 \( \alpha \) 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 \( \alpha \) 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

\[
g(\epsilon) = \frac{1}{\pi} \frac{W}{W^2 + \epsilon^2}
\]  

(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]. We notice that the fieldtheoretical argument reported in Ref.[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

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

(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 $\epsilon_i$ 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 $\alpha$ is computed by direct average over the configurations. Moreover all the configurations contribute in the average, and both the large $s$ and small $s$ regions are taken in due account. Such 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 equation
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 the present work, at the cost of a larger fluctuation of \( \alpha \), 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. Notice that the average level spacing \( \Delta E \) 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 \( \alpha \) may be estimated as

\[
\Delta \alpha^2 \approx (\langle s^4 \rangle - \langle s^2 \rangle^2)/N_{conf}. \]

In the Poisson limit, where the fluctuations are larger, and for \( N_{conf} = 10^4 \), we obtain from eq.(2) \( \Delta \alpha \approx 0.045 \) which is slightly more than 2 per cent.

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 \( P(s)ds \) 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 \( E+(s+ds)\Delta E \):

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

(1) and (2).
Dividing by $g(E + s\Delta E) ds$ and differentiating with respect to $s$ we obtain

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

Such 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

$$P(s) = P(0) \exp \left[ -s - \frac{g'}{Ng^2} \left( \frac{1}{2} s^2 - s \right) + 0(1/N^2) \right]$$  \hspace{1cm} (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 a larger and larger system size is required for recovering the Poisson limit $\gamma \to 2$ 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 $g'/(Ng^2) \sim E/(NW)$ and, as we checked by a numerical test, for $N \approx 10^2 - 10^3$, up to $E \approx 7W$ the deviations from the Poisson limit $\alpha = 2$ are negligible as shown in figure 1. In such figure the functional $\alpha$ is compared for $t = 0$ and $t \neq 0$, at a fixed disorder strength.
and sample size. For \( t \neq 0 \) the second moment \( \alpha \) approaches the Wigner limit around the band center, indicating that for such energy range the states are extended. In the band tail \( \alpha \) tends to the Poisson limit, and a cross-over region shows up around \( E = E_c \).

In order to get rid of the statistical fluctuations of \( \alpha \), 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 \( \alpha \), 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 the very accurate determination of the mobility edge \( E_c = 3.8 \pm 0.5 \).

According to the one-parameter scaling hypothesis, linearizing \( \alpha \) around \( E_c \), we obtain

\[
\log L = \nu \log |\alpha'(E_c, L)| + \text{const}
\]  

where the derivative \( \alpha' \) 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 \( \nu \) 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 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 center of the DoS. In such 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 transfer matrix method [5] and standard ELSM[6] reporting 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 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 $W_c = 3.5 \pm 0.1$.

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 out towards the existence of a critical $P(s)$ distribution which is expected to be universal[12-14]. Our estimate for $\alpha_c$ 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 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 fieldtheoretical argument of Ref.[3] which is based on the assumption that the distribution has well defined moments.
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Figure Captions

Fig.1 The second moment $\alpha$ 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 cross-over region shows the position of the mobility edge $E_c = 3.8$ as determined by finite size scaling. The dashed line is the corresponding averaged DoS scaled by an arbitrary factor.

Fig.2 Polynomial fit of the data for $\alpha$ in the cross-over energy range, for $M = 6, 7, 8, 9, 10$ and $W = 2$. At the band center $E \approx 0$ the lower curve corresponds to the largest size.
