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LETTER TO THE EDITOR

Multifractal quantum evolution at a mobility edge

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Abstract. We describe the time evolution of a quantum wavepacket at the Anderson metal–insulator transition using a quasirandom model as an example of a system with a mobility edge. It is demonstrated that the dynamical wavefunction is multifractal characterized by a continuous set of generalized spectral dimensions $\mu(q)$ and we find its $\alpha - f(\alpha)$ spectra. We also define and calculate an infinite hierarchy of diffusion exponents $\gamma(q)$ corresponding to all the displacement moments $\langle |r(t)|^q \rangle$ describing the quantum evolution. A slow subdiffusive decay for the 'staying at the origin probability' $\langle P(t) \rangle$ averaged over all initial sites is obtained at the mobility edge.

The understanding of the dynamical properties of systems which exhibit an Anderson delocalization–localization transition [1] is a very difficult problem which still remains open [2]. The general question of dynamics is best exemplified by considering the time evolution properties of a quantum wavepacket left to evolve in a lattice. In periodic systems unlimited ballistic motion with a constant velocity is expected while for strongly disordered systems absence of quantum diffusion may occur due to localization [3, 4]. In the presence of weak disorder a quantum coherence diffusive regime exists [2] corresponding to timescales intermediate between the elastic scattering time τ and a localization time τ_{loc}. An immediate question which arises concerns the nature of quantum evolution in systems near the critical point of the Anderson transition where one might expect a kind of diffusion to exist. In the present letter we propose a quantitative formalism based on multifractals [5] to describe scaling for all the moments of the important dynamical measures at the transition. Our findings suggest the absence of global scaling as normally expected for ordinary diffusion [6].

Firstly, we formulate the problem of critical localization dynamics as a quantum evolution process in a chain with a quasiperiodic cosine modulation of the potential which mimics the real three-dimensional (3D) problem [1]. It obeys the simple space (n) and time (t) equation

$$\mathrm{i}\frac{\mathrm{d}\psi_n(t)}{\mathrm{d}t} = \epsilon_n \psi_n(t) + V\psi_{n-1}(t) + V\psi_{n+1}(t) \qquad (1)$$

where the site energies are $\epsilon_n = \lambda \cos(2\pi\sigma n)$, the hopping matrix elements between the n and $n \pm 1$ sites are $V = 1$ and σ is an irrational number, such as the inverse golden mean $(\sqrt{5} - 1)/2$, usually approximated by truncating its continued fraction representation.

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The static version of the above equation has been studied many times before [7] and is known to display an Anderson localization–delocalization transition occuring at $\lambda = 2$ [8]. When $\lambda < 2$ for all states and for almost every σ solutions of (1) are believed to be extended. Similarly for $\lambda > 2$ they are known to be localized with an inverse localization length proportional to $\log \lambda$ [8]. Precisely at the transition point $\lambda = 2$ the density of states is a Cantor-set-like singularly continuous object [9] and the wavefunction is a curious intermediate between extended and localized states [10]. The critical spectra show exponents lying in the range [0.42, 0.55] with a density support leading to $D_0 = \frac{1}{2}$ [9]. The critical wavefunctions are measures which fluctuate on all scales and have also been shown to display multifractal properties [10]. One may expect that the static properties will, somehow, be reflected in the corresponding dynamics, which is the concern of the present study.

We exploit the quasirandom model of (1) at the critical point, by numerical simulation, viewed as an initial value problem with $\psi_n(t=0) = \delta_{n,n_0}$ and $n_0 = 0$. The quantity of interest for the quantum evolution is $\psi_n(t)$ which can be found either via the computed eigenvectors $C^{(j)}$ and the eigenvalues E_j of the corresponding Hamiltonian matrix $\mathcal{H}$ by

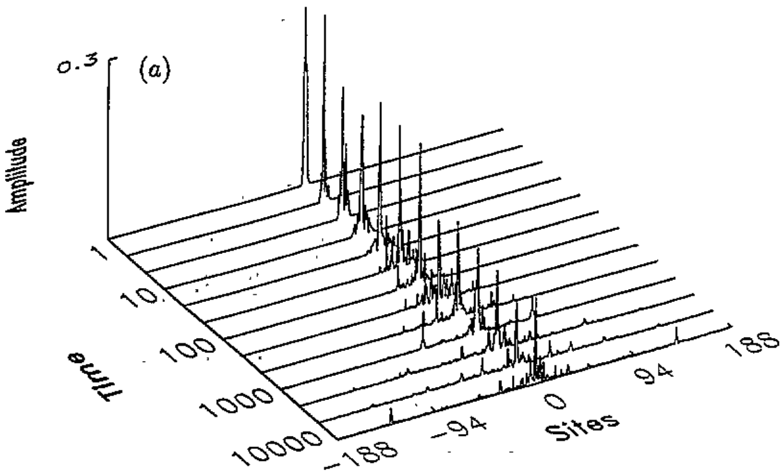
$$\psi_n(t) = \langle n|\exp(-\mathrm{i}\mathcal{H}t)|n_0\rangle \geqslant \sum_j C_n^{(j)} C_{n_0}^{(j)*} \exp(-\mathrm{i}E_j t) \tag{2}$$

or by integrating directly (1) using a finite-time-step Runge–Kutta method [11]. In fact, we have tried both methods, which gave similar results in all the cases we examined. In figure 1(*a*) we illustrate the theme of the letter by showing our results for the wavepacket dynamics at the critical point of the Anderson metal–insulator transition. We view in a space–time(n–t) plot the normalized absolute value $|\psi_n(t)|^2$, which is the probability for finding the electron on lattice site n at time t. Since the model is deterministic it is sufficient to achieve convergence of the numerical results as our system size increases. The converged data shown in the figure were obtained for the longest chain length ($N = 17\,711$) which is a Fibonacci number by using $\frac{10\,946}{17\,711}$ as a rational approximant of σ. We ensure that the wavepacket does not reach the ends of the chain so that we can study unlimited time evolution. In figure 1(*b*) the variety of scales for $|\psi_n(t)|^2$ at two different times can be clearly seen in the chosen log scale for the squared amplitude. The spatial multifractal fluctuations are shown to increase with time and eventually to dominate the dynamics.

In order to understand the unusual critical dynamics displayed in figure 1 we propose a picture based on determining a set of generalized spectral dimensions $\mu(q)$ with $q \in [-\infty, +\infty]$ for the time-dependent amplitude $|\psi_n(t)|^2$ viewing it as a multifractal measure in time. In analogy with the static eigenvectors [12], we introduce the asymptotic (as $t \to \infty$) scaling of the participation moments

$$P_q(t) = \sum_{n=-N/2}^{N/2} |\psi_n(t)|^{2q} \propto t^{(1-q)\mu(q)/2}\,. \tag{3}$$

In our picture the capacity dimension $\mu(0)$ describes the evolution of the support L of the wavefunction versus time and we find ordinary diffusive critical evolution of L with $\mu(0) = 1$. We expect that D_0 is related to $\mu(0)$ via $2D_0 = \mu(0)$, where $D_0 = \frac{1}{2}$ is the fractal dimension for the spectral support of the density of states [9]. The information dimension $\mu(1)$ can also be computed by studying the the time evolution of the entropy function $S(t) = -\sum |\psi_n(t)|^2 \log(|\psi_n(t)|^2)$, which asymptotically becomes proportional to $[\mu(1)/2]\log(t)$. The correlation dimension $\mu(2)$ concerns the evolution of the time-dependent participation ratio $P_2(t) = \sum |\psi_n(t)|^4$, etc. In the ballistic limit ($\lambda = 0$), (1)



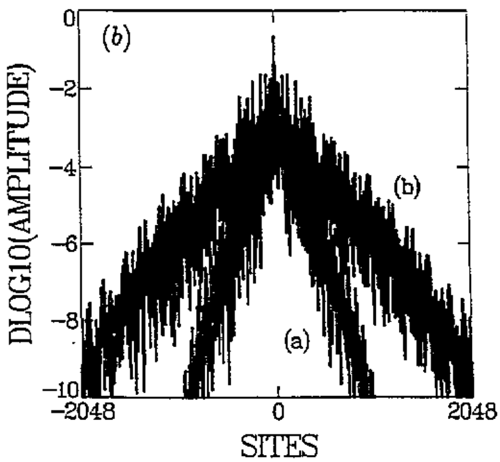
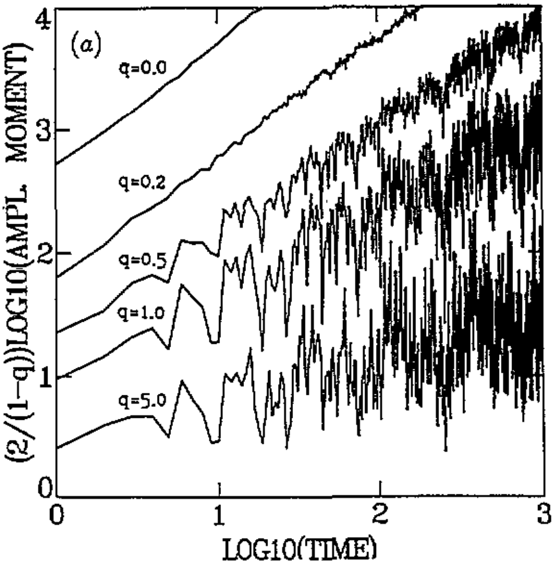


Figure 1. (a) Space–time plot describing the critical evolution of a quantum wavepacket initially placed at a single site $n_0 = 0$, for the model of (1) with $\lambda = 2$. Note that the scale is logarithmic in time and the maximum always remains at the initial site $n_0 = 0$. (b) Two snapshots of the probability amplitude $|\psi_n(t)|^2$ versus space n for times (a) $t = 10\,000$, (b) $t = 60\,000$ on a semi-log scale. Although the evolution could be imagined as resembling a Gaussian, it is shown to be dominated by multifractal spatial fluctuations which increase as t increases.

can be exactly solved exploiting the recursion properties of the Bessel functions, so that $\psi_n(t) = \mathrm{e}^{-\mathrm{i}n\pi/2} J_n(2t)$, where J_n is the nth Bessel function. Then one easily obtains all the asymptotic relations which lead to trivial global scaling $\mu(q) = 2$ and the non-exponential atomistic decay law $|\psi_0(t)|^2 \propto t^{-1}$. In the localized case the evolution ceases and all $\mu(q) = 0$. In figure 2(a) we see how the various critical participation moments evolve with time.

We were able to evaluate the critical exponents $\mu(q)$ in a more efficient manner, by box-counting techniques [5], studying the spatial instead of the time distribution of the wavefunction whose support is L. Using $\mu(0) = 1$ we may use, instead of (3), the fixed-t relation



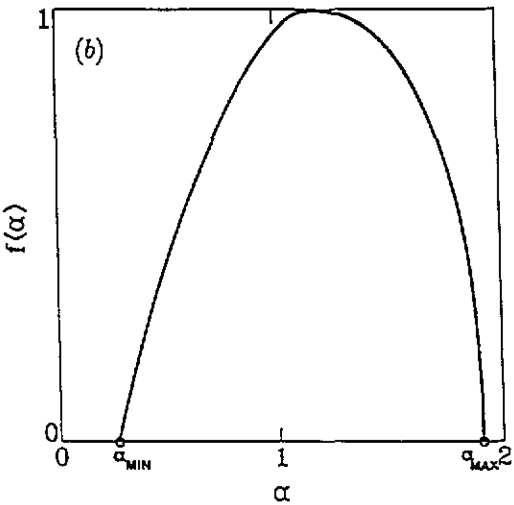


Figure 2. (*a*) Log–log plot of the participation moments $P_q(t)$ versus time t which allows the computation of the generalized exponents $\mu(q)$ via the aymptotic scaling proposed by (3). (*b*) The α–$f(\alpha)$ spectra for the local dimensions $\mu(q)$ found from (5) and (6). We obtain $\alpha_{\min} \approx 0.27$ and $\alpha_{\max} \approx 1.90$ which specify scaling near the centre and near the edge of the spatial $|\psi_n(t)|^2$-distribution, respectively.

$$P_q(L) \propto L^{(1-q)\mu(q)}. \tag{4}$$

In figure 2(*b*) we show the computed singularity strength density function $f(\alpha)$ obtained from the $\mu(q)$ via the Legendre transform [6, 9, 10]

$$\alpha(q) = \frac{\mathrm{d}[(q-1)\mu(q)]}{\mathrm{d}q} \tag{5}$$

$$f(\alpha) = q\alpha(q) - (q-1)\mu(q)\,. \tag{6}$$

The $f(\alpha)$ spectrum takes values in a finite range $[\alpha_{\min}, \alpha_{\max}]$, while $f(\alpha)$ turns out to be a usual single humped function with $\mu(0) = 1$ at its maximum. The exponents $\alpha_{\min} = \mu(+\infty) \simeq 0.27$ and $\alpha_{\max} = \mu(-\infty) \simeq 1.90$ characterize the scaling properties where the measure is most concentrated and most rarefied, respectively. A statistical error for the exponents, which arises in taking the corresponding slopes, is monitored in our calculation by varying the system size until convergence is reached.

However, scaling in the time-dependent displacement moments is more often studied in the context of dynamics [6]. We expect that the multifractal time evolution implied by the previous analysis should also affect these moments. We define, accordingly, the qth moment $R_q(t) = \langle |r(t)|^q \rangle$ of the corresponding spatial probability distribution $|\psi_n(t)|^2$ versus t and asymptotically ($t \to \infty$) we expect the scaling

$$R_q(t) = \langle |r(t)|^q \rangle = \sum_{n=-N/2}^{N/2} |n - n_0|^q |\psi_n(t)|^2 \propto t^{(q/2)\gamma(q)}\,. \tag{7}$$

For example, an estimate of the wavepacket spread in space is usually given by the second moment $R_2(t) = \langle |r(t)|^2 \rangle$ [13], where $\gamma(2) = 1$ for normal diffusion [6]. The set of $\gamma(q)$, for $q \in [-\infty, +\infty]$, are the generalized diffusion exponents and in the case of ballistic motion $\gamma(q) = 2$, for $q > 0$ and $\gamma(q) = -2/q$, for $q < 0$. Our definition of (7) fails for $q = 0$ where the fluctuations grow. We obtain $\gamma(0)$, instead, from a small-q expansion of both sides of (8) via the quantity $\sum \log |n - n_0| |\psi_n(t)|^2 \propto \frac{1}{2}\gamma(0) \log t$; this means that $\gamma(0)$ specifies the logarithmic behaviour of the critical displacement evolution. In figure 3(a) we present our results for the moments $R_q(t)$ versus time t. Although for short enough times the motion starts as ballistic, asymptotically we obtain a set of $\gamma(q)$, $q \in [-\infty, +\infty]$ which are shown in figure 3(b). They lie within the range defined by $\gamma(-\infty)$ approaching zero and $\gamma(+\infty)$ slightly above 1. These limits describe the scaling of the fastest and the slowest motions in the system, respectively.

Our results also enable us to focus on the autocorrelation function or 'staying at the origin' probability $P(t) = |\psi_0(t)|^2$, that the 'particle' will remain on the initial central site $n_0 = 0$ at a time instant t. The power-spectrum of $\psi_0(t)$ measures the fluctuations of the local density of states. Moreover, $P(t)$ is characterized by the exponent $\alpha_{\min}$ since the maximum of the amplitude, at any time, lies at the centre of the wavepacket. Subsequently, taking the appropriate limits from (3), the maximal scaling relation

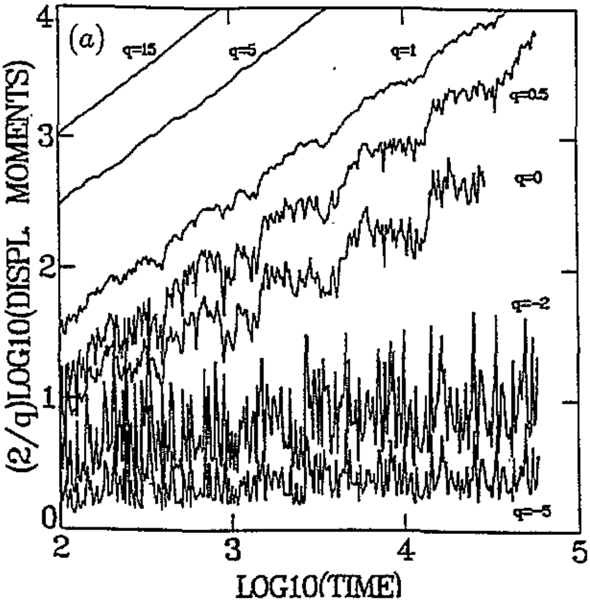
$$P(t) \propto t^{-\mu(\infty)/2} \tag{8}$$

valid only at the critical point, is easily established. $P(t)$ asymptotically goes to zero as $\sim t^{-1}$ in the ballistic case and becomes eventually constant for the localized case. At the critical point we obtain $\mu(\infty) \approx 0.27$, in agreement with previous considerations [14], which imply a very slow decay of correlations at the mobility edge.

We also introduce the 'return probability', averaged over all possible initial states n_0, that is

$$\langle P(t) \rangle = \frac{1}{N} \sum_{n_0} |\psi_{n_0}(t)|^2 \tag{9}$$

for an N-site system with periodic BC. The need for taking $\langle P(t) \rangle$ is that it fluctuates much less than $P(t)$ being related to the total, rather than the local, density of states. $\langle P(t) \rangle$ is



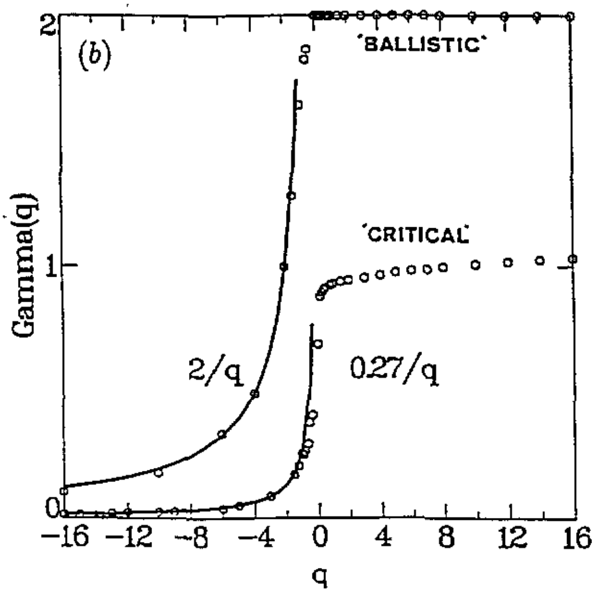


Figure 3. (*a*) Log–log plot of the displacement moments $R_q(t)$, defined by (7), versus t. $R_2(t)$ is the mean square displacement which defines the usual exponent $\gamma(2)$. (*b*) The obtained critical generalized diffusion dimensions $\gamma(q)$ versus q and also with the results for the ballistic case. For negative q the asymptotic forms are also shown. We find $\gamma(0) \approx 0.69$, $\gamma(1) \approx 0.93$ and $\gamma(2) \approx 0.96$. The error bars are of about the sizes of the circles.

shown in figure 4. In the same figure the ballistic case is also demonstrated. The results again show an anomalous slow subdiffusive power law.

It is also natural to ask whether a similar kind of anomalous diffusion is likely to occur at the mobility edge of the more realistic 3D case, where the eigenfunctions are

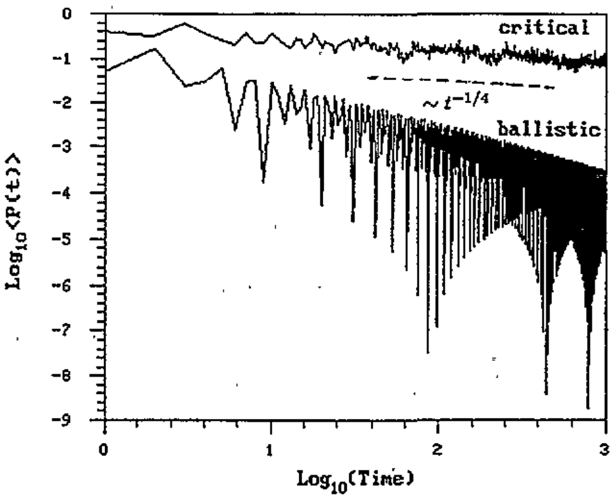


Figure 4. Log–log plots of the averaged overall sites 'return probability' $\langle P(t)\rangle$ (9) with periodic BC. The ballistic and the critical limits are shown with decay laws t^{-1} and $t^{-0.25}$, respectively. It is also worth noticing that the exponents describing the decays of $P(t)$ and $\langle P(t)\rangle$ are not the same.

also multifractals [15, 16]. The inevitable contribution of all the states to the dynamics, via (2), which is not a problem for the quasirandom model, where all the states become simultaneously critical for the 3D Anderson model brings difficulties since the mobility edges are believed to be sharp for a given disorder (e.g. a box distribution of mean zero and width W). However, at the critical value of the disorder $W_c \simeq 16.5$ the large majority of states in the spectrum also become simultaneously critical, as suggested from the W_c versus E mobility edge trajectory phase diagram which displays an almost flat part at $W_c \simeq 16.5$ [17, 18]. Therefore, apart from small-density localized states lying at the band edges, the dynamics at $W = W_c$ should be dominated by critical states even for the 3D Anderson mode. This fact is also confirmed by level statistical studies which turn out at criticality to be independent of the energy band range considered [18].

In the present study using as a guide a quasirandom model which, albeit one-dimensional, shows critical behaviour, we derived novel results for the critical localization dynamics. We summarize our main findings. (i) The different moments of the wavepacket probability amplitude are found to grow with time via a set of independent exponents $\mu(q), q \in [-\infty, +\infty]$, which can be understood within a thermodynamic multifractal description. Moreover, the support L of the wavefunction evolves as $L \propto t^{\mu(0)/2}$, $\mu(0) \approx 1$ and the 'staying at the origin' local probability $P(t)$ decays as $\propto t^{-\mu(\infty)/2}$, $\mu(\infty) \approx 0.27$. (ii) The critical dynamics is also shown to involve a variety of displacement motions which are extracted via a novel set of exponents $\gamma(q)$ by scaling of the corresponding moments. Furthermore, (iii) we conjecture that a similar fractal analysis should apply to the mobility edge of the 3D system. Before we ask for the experimental implications of the complicated critical dynamics found in a variety of related systems, e.g. in describing slow relaxation phenomena in glasses, polymers, or the shape of the NMR resonance lines in small metallic particles, etc, our results call for a better understanding also by exploiting their relationship with statistical energy level correlation and fluctuation studies [18].

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