

LOCALIZATION OF ELECTRONS IN LOOPLESS FRACTALS

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We study the localization of electrons in loopless random fractal structures modelled by Bethe lattices (Cayley trees) at the percolation threshold. We determine electronic wavefunctions ψ within the tight-binding approximation. We find that, for fixed energy E , the way $\langle\psi(\ell)\rangle$ decays with increasing topological distance ℓ from the localization center depends on both the type of average performed and the number N of configurations taken into the average. Our numerical results suggest that there exists a crossover length $\ell_{\times}(N)$ which increases logarithmically with N , determining two regimes for ψ . For $\ell < \ell_{\times}(N)$, $\langle\psi(\ell)\rangle$ does not depend on N displaying 'stretched' exponential decay. For $\ell > \ell_{\times}(N)$, $\langle\psi(\ell)\rangle$ does depend on N , and displays 'superlocalized' decay which becomes simply exponential for $\ell \rightarrow \infty$. Analytical arguments are presented to understand this complex localization behavior.

1 Introduction

Percolation has become the standard model for disordered structures commonly observed in natural sciences^{1,2}, with many applications in engineering and applied sciences³. At the percolation threshold, the incipient infinite cluster has a statistical self-similar structure. Below spatial dimensions $d = 6$, the cluster displays loops and dangling ends on all length scales. Above $d = 6$ loops are absent on large length scales and the cluster develops a tree-like structure asymptotically. Such loopless fractal structures can be modelled by random Bethe lattices¹⁻⁴ (also denoted as Cayley trees), having a fractal dimension $d_f = 4$.

The study of localization of one-electron wavefunctions in percolation systems (known as quantum percolation (QP)) was initiated in the early 70's⁵, and since then has attracted a great deal of attention. Of particular interest is the localization-delocalization transition, which occurs above the percolation threshold p_c ^{6,7}, and the question whether QP⁸ belongs to the same universality class as the Anderson model in three dimensions⁹.

Another interesting and not yet completely understood problem regards the question how the localized wavefunctions decay in space. Despite of the large amount of work devoted to this problem, the localization behavior of wavefunctions¹⁰⁻¹³, even at p_c , is still far from being clarified.

Recent work on the related problem of how the probability distribution of random walks, $P(r, t)$, decays on fractal structures¹⁴, has clearly shown that

$P(r, t)$ depends crucially on the type of average performed and explicitly on the number of configurations taken into the average. In the light of these recent theoretical results, it has become clear that a more detailed study is required for understanding localization of electrons on random fractals properly. The aim of this work is to initiate such a program by considering the simplest, yet non trivial model of a random fractal, i.e. a loopless fractal structure. We have therefore studied QP on Cayley trees at criticality.

The paper is organized as follows. We start in Sec. 2 by discussing Cayley trees at criticality and the lattice Hamiltonian employed for describing one-electron wavefunctions. The numerical procedure for solving the corresponding tight-binding equation is discussed in detail in Sec. 3. In Sec. 4 we introduce the averaging procedure employed in this work and present the numerical results for the localization of the wavefunctions as a function of the topological distance from the localization center on the tree. In Sec. 5, finally, we present theoretical arguments for describing the localization behavior quantitatively.

2 Cayley trees and the tight-binding equation

Consider a Bethe lattice of coordination number $z \geq 3$ and unit lattice spacing (see Fig. 1). In such a lattice, two arbitrary sites are connected by just a single path, since loops are absent in the structure. The length of the path connecting the two sites is called the topological or chemical distance¹⁵, and is denoted by ℓ . Taken a given site as the origin, the number M of sites situated up to a chemical distance ℓ from the origin grows as $[z(z-1)^\ell - 2]/(z-2)$. Clearly, such a cluster grows indefinitely with ℓ and can be embedded only in a space of infinite dimensionality ($d \rightarrow \infty$) (for reviews see Refs. 1-3).

Now, by starting from the origin, let us occupy the lattice sites with probability $p < 1$ and let the sites which are not connected to the origin remain empty (see Fig. 1). The sites connected to the origin define a cluster. It is easy to show that an infinite cluster, spanning the whole lattice, occurs above a 'percolation' threshold $p_c = 1/(z-1)$, that is also called the critical concentration. Exactly at p_c , the number of cluster sites of this loopless 'incipient' infinite cluster grows as $M \sim \ell^{d_\ell}$, where $d_\ell = 2$ is the fractal dimension in topological space^{2,15}.

Next we consider the simplest model for electronic wavefunctions based on the tight-binding (TB) approximation. We assume that occupied sites represent atoms of the same type, in which a single atomic orbital is available. The matrix elements of the lattice Hamiltonian H between atomic orbitals at different sites i and j , $\langle i | H | j \rangle = t_{i,j}$, are different from zero only when the two sites are nearest-neighbors in ℓ -space, i.e. when the chemical distance between

them is $\Delta\ell = 1$ (see Fig. 1)^a. In this case we have $t_{i,j} = -V$, and $V = 1$ determines the unit of energy. Without loss of generality, we also assume that the diagonal matrix elements $\langle i|H|i\rangle$ are zero, and that the overlaps of atomic orbitals at different sites i and j vanish, i.e. $\langle i|j\rangle = 0$. In such a case the orbitals $|i\rangle$ are referred to as Wannier orbitals.

By expanding the electronic wavefunction of the cluster, $|\psi\rangle$, in terms of Wannier orbitals, $|\psi\rangle = \sum_i \psi_i |i\rangle$, the Schrödinger equation $H|\psi\rangle = E|\psi\rangle$ leads to the tight-binding equation for the coefficients ψ_i

$$-\sum_{\delta} \psi_{i+\delta} = E \psi_i \quad (1)$$

where the sum is over all nearest-neighbor sites $i + \delta$ of site i . The coefficients ψ_i are usually referred to as the wavefunction itself, and can be normalized according to $\sum_i |\psi_i|^2 = 1$.

3 Numerical procedure for solving the tight-binding equation

Next we discuss the procedure employed for solving Eq. 1. For illustration, we consider the cluster shown in Fig. 1 with a maximum chemical distance $\ell_{\max} = 3$ from the origin. In analogy to the solution of a TB equation for the Anderson model in one dimension¹⁶, we solve Eq. 1 iteratively. We start by assigning arbitrarily the value $\psi_i = 1$ to all sites i at the last chemical shell $\ell = \ell_{\max}$ (sites 8, 9 and 10 in Fig. 1), and by assuming a starting value for the energy E .

In the second step, we calculate ψ at the sites with chemical distance $\ell = \ell_{\max} - 1 = 2$ (here sites 4, 5, 6 and 7). Since the sites 4 and 7 are not connected to sites with $\ell = \ell_{\max}$, i.e. they are at dangling ends, the value $\psi_i = 1$ is also assigned to them. For the sites at $\ell_{\max} - 1$ which are connected to sites at ℓ_{\max} (here sites 5 and 6), we employ Eq. 1 with the assumed value for E . To obtain ψ_5 , we apply Eq. 1 to the sites $i = 8$ and 9, $-\psi_5 = E \psi_8$ and $-\psi_5 = E \psi_9$, respectively, both yielding the unique result $\psi_5 = -E$. For the site 6, we obtain immediately $\psi_6 = -E$.

In the third step, we consider the sites at $\ell = \ell_{\max} - 2 = 1$ (here sites 1, 2 and 3). Since the site 2 is at a dangling end, we take $\psi_2 = 1$. Consider next the site 1. From the equation $-\psi_1 = E \psi_4$ we find $\psi_1 = -E$, while from $-\psi_1 - \psi_8 - \psi_9 = E \psi_5$ we get $\psi_1 = E^2 - 2$. To obtain a unique value of ψ_1 one must multiply all previous values of ψ_i , corresponding to one of the

^aNote that in our model, the actual distance in r -space between two sites is neither defined nor required. This corresponds to assuming that chemical bonds are 'confined' along the 'backbone' of the tree structure.

Figure 1: A Cayley tree of $\ell_{\max} = 3$ chemical shells for the concentration $p = 11/18$ of occupied sites. The black circles denote the occupied cluster sites and the grey circles the empty sites. White circles, occurring at $\ell = 3$, remain empty since they are disconnected from the origin. The continuous lines represent chemical bonds connecting occupied sites on adjacent chemical shells only. The dashed lines are shown as a guide to the eye. The occupied sites are numbered sequentially for convenience (see text).

branches ending at the site 1, by an appropriate factor f . This operation is called the renormalization of a branch, and f the renormalization factor. A branch renormalization is permissible because of the linear form of Eq. 1, and the fact that the starting values of ψ_i at $\ell = \ell_{\max}$ can be adjusted in order to satisfy Eq. 1. For example, by multiplying ψ_5 , ψ_8 and ψ_9 by the factor $f = -E/(E^2 - 2)$, one recovers the unique value $\psi_1 = -E$. Note that one can alternatively multiply ψ_4 by $f = -(E^2 - 2)/E$, yielding an equivalent solution for ψ . Similarly, for the site 3 we find the two different values $E^2 - 1$ and $-E$, and consistency is achieved by multiplying, e.g. ψ_6 and ψ_{10} by $f = -E/(E^2 - 1)$.

In the fourth step, we use Eq. 1 for the sites $i = 1, 2$ and 3 to calculate ψ_0 at the origin. Each equation yields, in general, a different value for ψ_0 . We then determine, for two of the three branches ending at the site 0, the corresponding renormalization factors required to obtain a single value for ψ_0 . In this way, we have obtained an initial set of values for ψ on the cluster.

The equation for $i = 0$ (in the present example $-\psi_1 - \psi_2 - \psi_3 = E\psi_0$), which has not been considered yet, will only be satisfied if ψ is an eigenfunction, or equivalently, if E is an eigenvalue of Eq. 1. Thus, the whole procedure must be repeated from the beginning with a different value of E , until the equation for ψ_0 is satisfied within the required accuracy.

In practice, the problem reduces to searching a zero of the function $\Delta\psi = \psi_1 + \psi_2 + \psi_3 + E\psi_0$, which is achieved when the relative error $|\Delta\psi|/\psi_{\max} < \epsilon$, where $\psi_{\max} = \max|\psi_0, \psi_1, \psi_2, \psi_3|$. In our calculations we used $\epsilon = 10^{-10}$. Finally, ψ_i is normalized over all clusters sites. Throughout the whole paper we considered energies around $E = 1.7$, thus avoiding the special values $E = 0$, $E = \pm 1$ and $E = \pm\sqrt{2}$, where strong degeneracies occur⁵.

4 Types of averages and numerical results

Once a solution of Eq. 1 has been found, we proceed in the following way. First, the site where $|\psi|$ attains its maximum value is identified and taken as the new origin of the lattice. This site is referred to as the localization center (LC). The chemical distances of all cluster sites are recalculated from the LC.

To study the decay of ψ as a function of ℓ , we consider the normalized probability density $\Psi(\ell)$ at chemical shell ℓ defined as

$$\Psi(\ell) = \frac{1}{N_\ell} \sum_{i=1}^{N_\ell} \frac{|\psi_i(\ell)|^2}{|\psi_0|^2} \quad (2)$$

where $\psi_i(\ell)$ denotes the wavefunction on the i th site at the chemical distance ℓ from the LC, and N_ℓ is the total number of sites at the ℓ th shell. Note that $\Psi(0) = 1$.

We proceed next by averaging $\Psi(\ell)$ over N configurations. Denoting by $\Psi^{(k)}(\ell)$ the value of $\Psi(\ell)$ for the k th configuration, we define its mean value as

$$\langle \Psi(\ell) \rangle_N = \frac{1}{N} \sum_{k=1}^N \Psi^{(k)}(\ell).$$

Similarly as for the probability density $P(r, t)$ of random walks on random fractals¹⁴, we find that the decay of $\langle \Psi(\ell) \rangle_N$ as a function of ℓ depends strongly on N .

Since we are interested in the typical behavior of $\langle \Psi(\ell) \rangle_N$, we average the function $\ln \langle \Psi(\ell) \rangle_N$ over several sets of N configurations. This average just smooths out the fluctuations of $\langle \Psi(\ell) \rangle_N$ among the different sets of N configurations. Thus, we define our N -dependent average as

$$\bar{\Psi}_N(\ell) = \exp \langle \ln \langle \Psi(\ell) \rangle_N \rangle \quad (3)$$

which describes the typical behavior of $\langle \Psi(\ell) \rangle_N$. We notice that for $N = 1$, Eq. 3 yields the 'typical' average¹⁴, $\bar{\Psi}_{\text{typ}}(\ell) = \exp \langle \ln \Psi(\ell) \rangle$, and for $N \rightarrow \infty$ the 'annealed' average¹⁴, $\bar{\Psi}_{\text{ann}}(\ell) = \langle \Psi(\ell) \rangle_\infty$.

Figure 2: The decay of $\bar{\Psi}_N(\ell)$ versus $\ell/\lambda_\ell(N=1)$ for $E = 1.7 \pm 0.1$, $N_T = 2^{17}$, and $N = 1, 2, 4, 8, \dots, N_T$. Cayley trees of $\ell_{\max} = 1200$ shells were considered. Here, the value $\lambda_\ell(N=1) = 3.4$ is used. Actually, the plot has been obtained from the values $-\log_{10}[-\log_{10} \bar{\Psi}_N(\ell)]$, while the scale on the y -axis shows the values of $\bar{\Psi}_N(\ell)$ directly. The ticks refer to the powers 10^{-n} with $n = 2, 3, \dots, 9$ on the upper-half of the axis and $n = 20, 30, \dots, 90$ on the lower half of it. The straight line drawn below the numerical results has a slope $v = 1$ and is shown for illustration.

Figure 3: The effective localization exponent v as a function of $\ell/\lambda_\ell(N=1)$, for $N=1$ (triangles), $N=2^5$ (circles), $N=2^{10}$ (squares) and $N=2^{15}$ (stars).

Numerical results for $\bar{\Psi}_N(\ell)$ are shown in Fig. 2, where we have considered a total number of $N_T = 2^{17}$ configurations. Thus, for $N=1$ we have N_T different sets to perform the average of the function $\ln\langle\Psi(\ell)\rangle_N$, for $N=2$ we have $N_T/2$ sets, etc. We find that $\bar{\Psi}_N(\ell)$ becomes independent of N for ℓ below a crossover length $\ell_\times(N)$, while for $\ell > \ell_\times(N)$ it depends on N . The results suggest a decay of the form

$$\bar{\Psi}_N(\ell) = \exp[-(\ell/\lambda_\ell)^v] \quad (4)$$

where the effective localization exponent v , as well as the localization length λ_ℓ , depend on both ℓ and N .

To describe the decay of $\bar{\Psi}_N(\ell)$ (Eq. 4) quantitatively, we have calculated v from the local slopes of the curves shown in Fig. 2. The results for v are reported in Fig. 3. They show that $v < 1$ for $\ell < \ell_\times(N)$, i.e. $\bar{\Psi}_N(\ell)$ displays stretched exponential decay ('sublocalization') in the small ℓ regime. For $\ell > \ell_\times(N)$, we find that $v > 1$ corresponding to a faster than exponential decay ('superlocalization') in the large ℓ regime. The value $v = 1$ describing a simple exponential decay is reached only asymptotically for $\ell \rightarrow \infty$. Note, however, that $\bar{\Psi}_1(\ell) = \bar{\Psi}_{\text{typ}}(\ell)$ shows simple exponential decay already for relatively small values of ℓ . The results for $N > 1$ are quite surprising since they are in

Figure 4: The crossover length $\ell_{\times}(N)/\lambda_{\ell}(N=1)$ versus N in a semi-logarithmic plot. It has been obtained from the values of $\ell/\lambda_{\ell}(N=1)$ for which $v=1$ in Fig. 3. The straight line is the best fit with the form $\ell_{\times}(N) = c_1 \ln N + c_2$, where $c_1 = 16. \pm 3.$ and $c_2 = 36. \pm 5.$

contrast to the simple exponential decay usually assumed on random fractals in chemical space^{10–13}.

To see how the crossover length $\ell_{\times}(N)$ increases with N , we have plotted $\ell_{\times}(N)$ versus $\log N$ (see Fig. 4). The straight line indicates a simple logarithmic dependence of $\ell_{\times}(N)$ on N . Such logarithmic behavior is typical of random fractals¹⁴.

5 Discussion of the results

The key for understanding the non-standard behavior of $\bar{\Psi}_N(\ell)$ is to look at the distribution function for the single values $\psi_i(\ell)$, entering the definition of $\Psi(\ell)$ in Eq. 2. Typical examples of the distribution are shown in Fig. 5. We find that $\psi_i(\ell)$ is approximately log-normally distributed

$$P(x) = \frac{A}{\sqrt{\pi\sigma\ell/\lambda_0}} \exp \left[-\frac{(x - \ell/\lambda_0)^2}{(\sigma\ell/\lambda_0)} \right] \quad (5)$$

where $x = \ln(|\psi_0|^2/|\psi_i(\ell)|^2) \geq 0$. Thus, $P(x)$ is normalized according to $\int_0^{\infty} P(x) dx = 1$, yielding $A = 2/[1 + \text{erf}(\ell/\sigma\lambda_0)]$, where $\text{erf}(x)$ is the error function.

Figure 5: Distribution of $|\psi_i(\ell)|^2/|\psi_0|^2$ for fixed chemical shell ℓ : (a) $\ell = 32$, (b) $\ell = 128$, and (c) $\ell = 1024$. The continuous lines represent Gaussian fits to the numerical data according to Eq. 5; 10^4 configurations were considered to calculate the distributions.

As is apparent from Fig. 5, the parameters $\sigma = 5.5$ and $\lambda_0 = 3.2$ (which actually depend weakly on E) describe the distributions quite well for sufficiently large ℓ . Some discrepancies occur near the upper tails of the distributions ($x \rightarrow \infty$), but these are not relevant for the following discussion.

Next, we describe how to derive the N and ℓ dependences of $\bar{\Psi}_N(\ell)$ from the probability distribution $P(x)$, Eq. 5. To make contact with the quantity $\bar{\Psi}_N(\ell)$, we first note that for a given ℓ , relatively large values of $|\psi_i(\ell)|^2$ (i.e. small x) become extremely unlikely for large ℓ (see Fig. 5). In the case of a finite number of configurations, however, $P(x)$ jumps abruptly from a minimum value P_{\min} at a cut-off value x_c , to zero for $x < x_c$. For N configurations, the mean value of P_{\min} is given by $\bar{P}_{\min} = 1/\bar{N}$, where $\bar{N} = N N_\ell$, and $N_\ell = \ell^{d_\ell - 1} = \ell$ represents the mean number of sites at distance ℓ from the LC. As a result, only values of x larger than the lower cut-off x_c contribute to the average $\bar{\Psi}_N(\ell)$.

The cut-off value x_c can be determined from the condition $P(x_c) = \bar{P}_{\min}$. From Eq. 5 we find

$$x_c = \frac{\ell}{\lambda_0} - \sqrt{\frac{\sigma \ell}{\lambda_0} \ln \left[N \sqrt{\frac{\ell \lambda_0}{\pi \sigma}} \right]}. \quad (6)$$

Taking this lower cut-off into account, the average $\bar{\Psi}_N(\ell)$ can be obtained

Figure 6: Comparison between the numerical data (points) and the theoretical results (continuous lines), for: (a) $N = 2^5$, (b) $N = 2^{10}$ and (c) $N = 2^{15}$.

from the distribution $P(x)$ as

$$\bar{\Psi}_N(\ell) \cong \int_{x_{\min}}^{\infty} dx \exp(-x) P(x) \quad (7)$$

where $x = \ln(|\psi_0|^2/|\psi_i(\ell)|^2)$ and $x_{\min} = \text{Max}(0, x_c)$. Similarly as for $P(r, t)$ ¹⁴, the lower integration limit plays an essential role for determining the behavior of the integral.

For a fixed value of N , a crossover behavior of $\bar{\Psi}_N(\ell)$ is expected as a function of ℓ . For small ℓ , $x_c < 0$ and the lower integration limit sticks at the value $x_{\min} = 0$. In this case, the average $\bar{\Psi}_N(\ell)$ does not depend on N . For large ℓ , however, $x_c(N) > 0$ and $\bar{\Psi}_N(\ell)$ depends explicitly on N .

The crossover length $\ell_{\times}(N)$ at which the N -dependence of $\bar{\Psi}_N(\ell)$ sets in is obtained when $x_c = 0$. From Eq. 6 we find,

$$\ell_{\times}(N) = \frac{\lambda_0 \sigma}{2} [2 \ln N + \ln \ell_{\times}(N) - \ln(\pi \sigma / \lambda_0)]$$

which is an implicit equation for ℓ_{\times} . It can be shown that when $N \gg 1$, ℓ_{\times} is given, to a very good approximation, by the simpler expression

$$\ell_{\times}(N) \cong \lambda_0 \sigma \ln N + \frac{\lambda_0 \sigma}{2} \ln[(\lambda_0^2 / \pi) \ln N] \quad (8)$$

which has the expected logarithmic dependence on N displayed in Fig. 4, since the second term depends weakly on N . Now we discuss the results for $\bar{\Psi}_N(\ell)$ for a fixed value of N .

For $\ell < \ell_\times(N)$, $x_{\min} = 0$, and straightforward integration of Eq. 7 yields,

$$\bar{\Psi}_N(\ell) \cong \frac{A}{2} \exp[(\sigma/4 - 1)\ell/\lambda_0] \left(1 - \operatorname{erf} \left[(\sigma/2 - 1)\sqrt{\ell/\lambda_0\sigma} \right] \right) \quad (9)$$

corresponding to the annealed result since it does not depend on N . For $\ell > \ell_\times(N)$, $x_{\min} = x_c > 0$, and Eq. 7 yields

$$\bar{\Psi}_N(\ell) \cong \frac{1}{2} \exp[(\sigma/4 - 1)\ell/\lambda_0] \left(1 - \operatorname{erf} \left[\sqrt{\frac{\sigma\ell}{4\lambda_0}} - \sqrt{\ln(N\sqrt{\ell\lambda_0/\pi\sigma})} \right] \right) \quad (10)$$

displaying an explicit dependence on the number of configurations N . The typical behavior $\bar{\Psi}_{\text{typ}}(\ell)$ can be obtained from Eq. 10 by setting $N = 1$.

To facilitate the comparison of the present theoretical results with the numerical calculations, we have plotted in Fig. 6 the effective exponents v derived from Eq. 9 and Eq. 10, together with the numerical results. The theory predicts the occurrence of the crossover length $\ell_\times(N)$ correctly, although it yields a sublocalization value of v for $\ell < \ell_\times(N)$ a little smaller than that found numerically. However, the qualitative trend observed in the numerical data is reproduced very well by the present theory.

We expect these results to be relevant for describing the localization of wavefunctions in topological space on more general random fractal structures as well. Such a study is presently under way.

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