Quantum percolation in power-law diluted chains

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Abstract

We investigate the quantum percolation problem in a diluted chain with long-range hopping amplitudes. Each bond is activated with probability \( p(r) = p_1/r^\alpha \), where \( r \) is the distance between two sites and \( \alpha \) characterizes the range of the interactions. The average participation ratio of all eigenstates is used as a measure of the wave-functions localization length. We found that, above a quantum percolation threshold \( p_1^{(q)} \), true extended states appears for \( \alpha < 1.5 \). In the regime of \( 1.5 < \alpha < 2.0 \) there is no trully extended states even in the presence of a spanning cluster. Instead, a phase of critical wave-functions sets up.

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The quantum percolation phenomenon has been extensively investigated during the last decade. Besides its own challenging theoretical aspects, quantum percolation has also an appealing technological interest due to its possible relevance for the underlying mechanism leading to high-$T_c$ superconductivity as well as to its potential application for the development of nano-structure devices [1–4]. In these systems, the one-electron eigenstates on a site or bond diluted lattice can exhibit a localization/delocalization transition as a function of the disorder strength in a close relation to the Anderson transition [5]. At low dimensions $d \leq 2$ the eigenstates are believed to be localized for any degree of disorder even in the presence of spanning clusters of connected sites.

Several approaches have been employed for studying the nature of one-electron eigenstates in diluted lattices. The most usual numerical algorithms put forward Green’s function, renormalization group, transfer matrix or diagonalization techniques, or a combination of these, to explicitly compute some relevant quantities such as the wave-function localization length, reflection and transmission coefficients, conductance and spectral statistics [1,6–10]. The results obtained from numerical works on finite lattices have to be extrapolated by exploring the finite size scaling hypothesis to get the true thermodynamic behavior. In spite of all efforts made to fully understand all features related to the quantum percolation phenomenon, some relevant points are still open to debate. In 3D lattices, estimates from different techniques of the critical exponent $\nu$ describing the divergence of the localization length are still quite scattered and often differ from that expected for the Anderson model [6–9]. However, recent energy level statistics analysis have reported results supporting that quantum percolation indeed belongs to the Anderson transition universality class [10]. In 2D the present picture is also not firmly settled. Although all states are believed to be localized according to Anderson-like scaling arguments, some studies have reported signatures of a localization-delocalization transition [11–13].

In the present work, we introduce a simple but rather non-trivial model which exhibits a quantum percolation transition in one-dimension. We consider a bond diluted tight-binding Hamiltonian with long-range hopping amplitudes which are activated with probability $p(r_{ij}) = p_1/r_{ij}^\alpha$, where $r_{ij}$ is the distance between sites $i$ and $j$. Models with long-range interactions [14–17] as well as with long-range correlated disorder [18,19] have already been used in the context of the Anderson transition. In these models a localization/delocalization transition have been identified even at low-dimensions.

In the classical counterpart of the long-range diluted model, a percolating cluster emerges above a critical value $p_1(c)$ provided that $\alpha \leq 2$ [20,21]. For $\alpha \leq 1$, a percolating cluster is always present for any finite $p_1$. At $\alpha = 2$ the critical concentration is finite and its value was recently conjectured to be $p_1(c) = 0.703...$ [21,22]. This later particular case has attracted much interest once it depicts an intermediate phase with slowly decaying correlations [23]. In the range $1.5 < \alpha < 2$, the critical exponents of the Ising version of this model are non-trivial and change continuously with $\alpha$ [24]. For $1.0 < \alpha < 1.5$, the transition is characterized by classical mean-field exponents [25,26]. Here, we will show some results from exact diagonalization combined with finite size scaling for the average participation ratio of all one-electron eigenstates of the diluted long-range tight-binding model. These indicate that this model has also a rich phenomenology concerning the quantum percolation transition.

The quantum percolation problem in a bond diluted chain with non-random long-range
hopping amplitudes can be represented by a one-electron tight-binding Hamiltonian with a single orbital per site. In the atomic orbital wave-function basis \{\ket{n}\}, it is expressed as

\[
\mathcal{H} = \sum_n \epsilon_n \ket{n}\bra{n} + t \sum_{n \neq m} h(r = |n - m|) \ket{n}\bra{m},
\]

where the sum extends over the \(L\) sites of a chain with open boundaries. Hereafter, we will use energy units such that the hopping amplitude \(t = 1\). To avoid degeneracies during the numerical diagonalization procedure, the orbital energies \(\epsilon_n\) will be considered to have a very weak disorder being uniformly distributed in the interval \([-W, W]\) with \(W = 0.0005\).

\(h(r)\) are binary distributed following

\[
P[h(r)] = p(r)\delta[h(r) - 1] + [1 - p(r)]\delta[h(r)],
\]

with power-law decaying probabilities \(p(r) = p_1/r^\alpha\), where the probability of a first-neighbors bond being activated \(p_1 \leq 1\) and \(\alpha\) governs the long-range character of the interactions. Note that even in the case of \(p_1 = 1\) disorder is present through the dilution of further neighbors bonds and the wave-functions may become localized if these probabilities decay fast enough. On the other hand, for slowly decaying probabilities, the high connectivity of the chain may stabilize extended states.

In what follows we diagonalize the Hamiltonian (1) in finite chains of size up to \(L = 1,600\) to obtain all normalized one-electron eigenfunctions \(\Psi^{(k)} = \sum_n \psi^{(k)}_n \ket{n}\). Distinct realizations of the disorder were implemented such that for each chain size we computed 32,000 eigenfunctions. The localized/delocalized nature of the wave-functions is characterized by the behavior of the participation ratio \(P^{(k)} = 1/\sum_n [\psi^{(k)}_n]^4\). For exponentially localized states, the participation ratio gives an estimate for the localization length \(\xi\). For truly extended states it scales as \(L\). At the localization/delocalization transition it depicts a power-law growth \(P \propto L^{\tau_2}\) with \(\tau_2 < 1\) due to the power-law tails and the multifractal character of the critical wave-functions [27–30].

The density of states for this model can be directly measured from the distribution of energy eigenvalues. Typical integrated density of states (IDOS) are shown in figure 1 as obtained from a lattice of \(L = 1600\) and \(\alpha = 1.25\). For \(p_1 = 0.1\) there is no spanning cluster [21]. The density of states gaps and the delta-function singularities reflect the chain’s finite clusters structure. All wave-functions are then localized within the finite clusters. In the opposite situation of high bond concentration \((p_1 = 0.9)\), previous Monte Carlo simulations [21] have shown that a spanning cluster is present. In this situation, the density of state turns out to be gapless.

In order to investigate the possible existence of delocalized states in the regime where a spanning cluster is present, we computed the average participation ratio of the wave-functions with energy between \(E\) and \(E + \Delta E\) as a function of \(E\) for distinct chain sizes. The interval \(\Delta E\) was chosen to be much smaller than the band width but large enough to contain many states. Figure 2a shows the result corresponding to localized states when only finite clusters are present \((p_1 = 0.1, \alpha = 1.25)\). The participation ratio is \(L\)-independent as expected. For the same value of \(\alpha\) but with a higher concentration \(p_1 = 0.9\), we obtained the participation ratio to scale as \(P(E) \propto L\) within the entire band. This corroborates our preliminary idea that the presence of long-range bonds with slow-decaying probabilities favors the emergence of delocalized states.

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To locate the critical concentration $p_1^{(q)}$ above which extended states appear, we computed the average participation ratio of all eigenstates within the band $P = \langle P^{(k)} \rangle_k$ as a function of the first neighbors concentration $p_1$. The results for $\alpha = 1.25$ are shown in figure 3. It clearly depicts a transition from localized to delocalized states with the critical quantum percolation threshold being roughly $p_1^{(q)} = 0.25(3)$. This value is above, although relatively close to, a recent Monte Carlo estimate for the classical percolation threshold $p_1^{(c)}$ such that the general trend $p_1^{(q)} > p_1^{(c)}$ seems also to hold for the present model. However, the error bars on both estimates of $p_1^{(c)}$ and $p_1^{(q)}$ are still large to firmly state this trend. Within the range $1.0 < \alpha < 1.5$, the above picture remains with the critical concentration monotonically increasing with $\alpha$.

In the regime of $1.5 < \alpha < 2.0$, our data for the participation ratio exhibit only a slow growth with increasing chain size. In figure 4, we show the results for $\alpha = 1.75$. In this case, we have a transition from localized states to critical states having $P \propto L^{\tau_2}$, with $\tau_2 < 1$ (see inset). Contrary to the classical percolation case, there is no truly extended one-electron states in this regime. The estimated critical concentration separating localized and critical states $p_1^{(q)}(\alpha = 1.75) = 0.60(5)$ is also relatively above the numerical estimate of classical percolation threshold $p_1^{(c)}$. In figure 5, we plot two typical wave-functions representing an extended and a critical state. Notice that the critical wave-function exhibits spikes of many sizes reflecting its multifractal nature.

In summary, we studied the quantum percolation problem in a one-dimensional tight-binding Hamiltonian with diluted long-range hopping amplitudes whose probability of occurrence decay as $p(r) = p_1/r^\alpha$. For the regime of $1.0 < \alpha < 2.0$, a spanning cluster of connected sites emerges above a classical percolation threshold $p_1^{(c)}$ with mean-field like exponents for $\alpha < 1.5$ and non-trivial ones for $\alpha > 1.5$. Using numerical diagonalization on finite lattices and finite size scaling, we found that for $1.0 < \alpha < 1.5$ the one-electron eigenstates exhibit a localization/delocalization transition with increasing first-neighbors bond concentration $p_1$. The quantum critical percolation was found to be above, although relatively close to, the classical threshold. In the regime of $1.5 < \alpha < 2.0$, no truly extended states appears even for $p_1 = 1$. Instead, a phase transition between localized and critical states takes place.

The diagonalization procedure employed in the present work does not allow much larger systems to be investigated within a reasonable computational effort. Therefore, precise estimates of quantum critical thresholds and exponents governing the presently reported transitions require the use of alternative methods that are able to overcome the large corrections to scaling present in this model, specially at the vicinity of the $\alpha = 2$ anomaly. Numerical techniques which are less sensitive to geometrical problems, such as energy levels and multifractal analysis, would provide further relevant insights on these points. Also, analytical approaches along the lines used to investigate the power-law random band Anderson model [14,17] would certainly be valuable. We hope the present report can stimulate further works in these directions.

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REFERENCES

[1] A. Mookerjee, I. Das Gupta and T. Saha, Int. J. Mod. Phys. B 9, 2989 (1995).
[2] J. C. Phillips, Phys. T. Roy. Soc. Lond. A 334, 451 (1991).
[3] V. Dellacasa and R. Feduzzi, Physica C 251, 156 (1995).
[4] Y. Kodama and T. Maekawa, Nanotechnology 10, 217 (1999).
[5] P. W. Anderson, Phys. Rev. 109, 1492 (1958).
[6] K. C. Chang and T. Odagaki, J. Phys. A 20, L1027 (1987).
[7] L. Root, J. D. Bauer and J. L. Skinner, Phys. Rev. B 37, 5518 (1988).
[8] C. M. Soukoulis, Q. Li and G. S. Grest, Phys. Rev. B 45, 7724 (1992).
[9] R. Berkovits and Y. Avishai, Phys. Rev. B 53, 16125 (1996).
[10] A. Kaneko and T. Ohtsuki, J. Phys. Soc. Jpn. 68, 1488 (1999).
[11] Y. Meir, A. Aharony and A. B. Harris, Europhys. Lett. 10, 275 (1989).
[12] Th. Koslowski and W. von Niessen, Phys. Rev. B 42, 10342 (1990).
[13] D. Daboul, I. Chang and A. Aharony, Eur. Phys. J. B 16, 303 (2000).
[14] A. D. Mirlin et al, Phys. Rev. E 54, 3221 (1996).
[15] A. D. Mirlin and F. Evers, Phys. Rev. B 62, 7920 (2000).
[16] D. A. Parshin and H. R. Schober, Phys. Rev. B 57, 10232 (1998).
[17] J. C. Cressoni and M. L. Lyra, Physica A 256, 18 (1998).
[18] F. A. B. F. de Moura and M. L. Lyra, Phys. Rev. Lett. 81, 3735 (1998).
[19] F. M. Izrailev and A. A. Krokhin, Phys. Rev. Lett. 82, 4062 (1999).
[20] L. S. Schulman, J. Phys. A: Math. Gen. 16, L639 (1983).
[21] H. H. A. Rego, L. S. Lucena, L. R. da Silva and C. Tsallis, Physica A 266, 42 (1999).
[22] S. A. Cannas and A. C. N. de Magalhães, J. Phys. A 30, 3345 (1997).
[23] J. Z. Imbrie and C. M. Newman, Commun. Math. Phys. 118, 303 (1988).
[24] M. Barati and A. Ramazani, Phys. Rev. B 62, 12130 (2000).
[25] E. Luijten and H. W. J. Blote, Phys. Rev. B 56, 8945 (1997).
[26] S. A. Cannas, Phys. Rev. B 52, 3034 (1995).
[27] M. Schreiber and H. Grussbach, Phys. Rev. Lett. 67, 607 (1991).
[28] M. Janssen, Phys. Rep. 295, 1 (1998).
[29] V. E. Kravtsov and K. A. Muttalib, Phys. Rev. Lett. 79, 1913 (1997).
[30] S. M. Nishigaki, Phys. Rev. E 59, 2853 (1999).
I. FIGURE CAPTIONS

Figure 1 - The integrated density of states (IDOS) as a function of $E/t$ for a linear chain with $L = 1,600$ sites and $\alpha = 1.25$. A configurational average over 20 realizations of the disorder was employed. For $p_1 = 0.1$, all clusters are finite. The gaps and delta function singularities in the density of states reflect the absence of a spanning cluster. For $p_1 = 0.9$, a spanning cluster is present and the density of states becomes smooth.

Figure 2 - The participation ratio as a function $E/t$ for chains with $\alpha = 1.25$. (a) $p_1 = 0.1$ and linear sizes $L = 800$ (circles) and $1,600$ (triangles): all eigen-functions are exponentially localized and the participation ratio is roughly size independent; (b) $p_1 = 0.9$ and linear sizes $L = 800$ (diamonds) and $1,600$ (squares): all eigenfunctions are extended and the participation ratio scales linearly with $L$.

Figure 3 - The average participation ratio (normalized by the chain’s size) as a function of the first-neighbors concentration $p_1$ and distinct lattice sizes $L = 200$ (circles), 400 (squares), 800 (diamonds) and $1,600$ (triangles) for $\alpha = 1.25$. It shows a clear localization/delocalization transition around $p_1^{(q)} = 0.25(3)$. This behavior is typical for the range $1 < \alpha < 1.5$ with an $\alpha$-dependent critical concentration.

Figure 4 - The average participation ratio as a function of the first-neighbors concentration $p_1$ and distinct lattice sizes $L = 200$ (circles), 400 (squares), 800 (diamonds) and $1,600$ (triangles) for $\alpha = 1.75$. It shows a crossover from a phase of localized states at low concentrations to a phase of weakly delocalized states at high concentrations. Inset: the size dependence of the participation ratio for concentrations $p_1 = 0.2$ (diamonds), 0.6 (triangles) and 1.0 (circles). At high concentrations, a phase of critical states sets up where the participation ratio scales as $P \propto L^{\tau_2}$. For $p_1 = 1$ we obtained $\tau_2 = 0.73(2)$. At the estimated critical concentration $p_1^{(q)} = 0.60$, we found $\tau_2 = 0.38(2)$. This behavior is typical for the range $1.5 < \alpha < 2.0$ with $\alpha$-dependent critical concentration and exponents.

Figure 5 - Representative extended (bottom) and critical (top) wave-functions. These were obtained from a $L = 1,600$ chain, $p_1 = 1.0$, $\alpha = 1.25$ (extended state) and $\alpha = 1.75$ (critical state). The extended state presents a random uniform distribution over all chain. The critical state has spikes of many sizes characterizing its multifractal distribution.
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