Exactly solvable model with two conductor-insulator transitions driven by impurities

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We present an exact analysis of two conductor-insulator transitions in the random graph model. The average connectivity is related to the concentration of impurities. The adjacency matrix of a large random graph is used as a hopping Hamiltonian. Its spectrum has a delta peak at zero energy. Our analysis is based on an explicit expression for the height of this peak, and a detailed description of the localized eigenvectors and of their contribution to the peak. Starting from the low connectivity (high impurity density) regime, one encounters an insulator-conductor transition for average connectivity $1.421529 \cdots$ and a conductor-insulator transition for average connectivity $3.154985 \cdots$. We explain the spectral singularity at average connectivity $e = 2.718281 \cdots$ and relate it to another enumerative problem in random graph theory, the minimal vertex cover problem.

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Random graphs have motivated a lot of work both in mathematics and in physics. In the random graph model, $N$ points numbered $1, 2, \cdots, N$ are used as vertices. A pair of (distinct) vertices $\{i, j\}$ is connected by an edge with probability $p$ and the edges are independent. The adjacency matrix of the graph is the symmetric matrix $H$ with matrix element $H_{i,j} = 1$ if vertices $i$ and $j$ are connected by an edge and zero otherwise. The average connectivity (i.e. average number of neighbors of a given vertex) is $\alpha = pN$.

An interesting asymptotic regime emerges when $\alpha$ is kept fixed as $N$ goes to infinity. The connectivity serves as a parameter, and several phase transitions can be observed.

According to the seminal papers on the subject [1], for $\alpha < 1$ all connected components are finite, and only trees contribute to the extensive (i.e. proportional to $N$) quantities but for $\alpha > 1$, a finite fraction of the points lies in a single connected component, the giant component. So there is a second order (classical) percolation transition at $\alpha = 1$.

The adjacency matrix $H$ can be used as a Hamiltonian that describes hopping of electrons from one site to another if the two are connected by an edge. A large average connectivity means small concentration of impurities and vice-versa.

The spectrum of $H$ is relevant to many problems in physics and has been investigated by many authors. It contains an infinity of delta peaks for any $\alpha$ and also a continuous component for large enough $\alpha$. It has been argued [2] that for $\alpha \approx 1.4$, a quantum percolation transition occurs. This means that the structure of eigenvectors changes: below this value, all eigenvectors are localized, but above, some eigenvectors occupy a finite fraction of the system. It is believed [3] that the continuous component in the spectrum appears at the same threshold. Also an anomaly in the spectrum near the energy 0 for $\alpha \approx 2.7$ has been noticed in [2].

The main results presented in this letter are an analytical expression for $z(\alpha)$, the average height of the delta peak at zero energy in the spectrum of $H$ in the thermodynamic limit, and the identification of the corresponding eigenvectors, leading to precise predictions for two quantum percolation transitions in this model: a delocalization (insulator-conductor) transition at $\alpha_d = 1.421529 \cdots$ and a relocation (conductor-insulator) transition [4] at $\alpha_r = 3.154985 \cdots$. Surprisingly, $z(\alpha)$ is analytic at the classical and quantum percolation transitions and non-analytic only at $\alpha = e$.

The random graph model displays some mean field $D = \infty$ features because the neighbors of a site are chosen with equal probability among all the other points, with the consequence that loops are large. This is in strong contrast with real materials where some underlying geometry (e.g. a lattice) restricts the possible neighbors of a point, even before impurities destroy bonds. But once the random graph is chosen, each point has $\alpha$ neighbors on average so it interacts effectively with only a finite number of points, and this is far from mean field. In the conducting phase, the delocalized states live on the giant component, whose effective average connectivity varies between $2.092917 \cdots$ and $3.312453 \cdots$. Values of this order can be achieved in real two or three dimensional disordered systems, and this suggests that analogous insulator-conductor-insulator transitions might be observed in real materials. Indeed, the random graph model gives a rich phase diagram with a single parameter, and some real systems should exhibit at least the same complexity. On the other hand, we do not expect that the precise values of $\alpha_d$ and $\alpha_r$ will appear in real materials. Whether the critical exponents we obtain (which look very much like mean field exponents) remain valid above some upper critical dimension, and whether this covers some physical situation is still unclear.

The explicit formulæ below will involve five functions which are analytic for real positive $\alpha$ except maybe at three special values. These functions are generating func-
tions related to the enumeration of various types of trees. In particular, they all have the same small $\alpha$ expansion. We start with a short description of these functions.

The most basic generating function for tree enumeration is the Lambert function $W(\alpha)$, which is analytic on the real positive axis and satisfies a fixed point equation,

$$W = \alpha e^{-W}. \tag{1}$$

This implies that $W = -\sum_{n \geq 1} (-\alpha)^n \frac{n^{n-1}}{n!}$, and $n^{n-1}$ is the number of labeled rooted trees on $n$ vertices.

However, as a fixed point, $W$ is unstable for $\alpha > e = \exp(1)$, and there is a stable periodic orbit of length 2. This leads us to introduce the real functions $A(\alpha)$ and $B(\alpha)$ solving the symmetric system

$$A = \alpha e^{-B}, \quad B = \alpha e^{-A}. \tag{2}$$

and satisfying the condition that $A < B$ for $\alpha > e$. For $0 \leq \alpha \leq e$, there is only one solution to the system (so no condition is needed in this range of $\alpha$’s), namely $A(\alpha) = B(\alpha) = W(\alpha)$. Thus $e$ is a special value where a branch point occurs. We shall see later that $A$ and $B$ can also be viewed as generating functions for certain bicolored trees, with $-\alpha$ as weight for vertices of one color and $-\alpha e^{-\alpha}$ for vertices of the other color. This interpretation is relevant at large $\alpha$.

We shall need one more function, $A^*(\alpha)$ which is the smallest solution of the equation

$$A^* = Ae^{\alpha(e^{A^*} - A - 1)}. \tag{3}$$

Clearly $A^* = A$ is a solution, but in general not the smallest. The $\alpha$’s for which the solutions of (3) exhibit a branch point are such that $\alpha = 1$ which leads to

$$2\log \alpha = \alpha e^{-1/\alpha}. \tag{4}$$

This equation has two solutions, $\alpha_d = 1.421529 \cdots$, and $\alpha_r = 3.154985 \cdots$. In fact, $\alpha_d$ is the solution of the simpler equation $2\alpha \log \alpha = 1$. In the interval $[\alpha_d, \alpha_r]$, $A^* < A$, but outside this interval $A^* = A$. The function $A^*$, which coincides with $A$ for large and small $\alpha$, and thus shares the same combinatorial interpretations in these regimes, appears in this discussion via the explicit evaluation of the sum (12).

Replacing $A$’s by $B$’s in (3) leads to another function $B^*(\alpha)$. The functions $W$, $A$, $B$, $A^*$ and $B^*$ are plotted in Fig. 1.

We now argue that $z(\alpha)$, the height of the delta peak at the eigenvalue zero in the spectrum of an infinite random adjacency matrix, is given by the explicit formula

$$z(\alpha) = -1 + \frac{A + B + AB}{\alpha}. \tag{5}$$

What we have proved rigorously is that (3) is true for $\alpha \leq e$ and that the r.h.s of (5) is an upper bound for $z(\alpha)$ for $\alpha > e$. Here is the idea. Let $Z(G)$ denote the number of zero eigenvalues of the adjacency matrix of the graph $G$. Suppose $G$ has a vertex $v$ with exactly one neighbor, say $v'$ (so $v$ is a leaf of $G$). Leaf removal consists in removing from $G$ the vertices $v$ and $v'$ and all edges that meet those two vertices, leading to a new graph $G'$. In [3] it is shown that $Z(G) = Z(G')$. Iteration of leaf removal leads to a graph with consists of say $I$ isolated points and a subgraph $C$ (called the core of $G$) without leaves or isolated points. Then $Z(G) = I + Z(C)$. In [3] it is proved that if $G$ is a random graph of size $N$ and average connectivity $\alpha$, the size of $C$ is $o(N)$ if $\alpha$ is not isolated and only if $\alpha \leq e$ and that $I/N = -1 + \frac{A + B + AB}{\alpha} + o(1)$ for large $N$. But almost by definition, $Z(G)/N = z(\alpha) + o(1)$, and this completes the proof.

Then $z(\alpha)$ is singular at $\alpha = e$. It coincides with the analytic function

$$z_{an}(\alpha) = -1 + \frac{2W + W^2}{\alpha} \tag{6}$$

for $\alpha \leq e$ but $z(\alpha) > z_{an}(\alpha)$ for $\alpha > e$.

We believe that (6) is true as an equality even for $\alpha > e$ for two reasons. First, the Monte Carlo simulations in Fig. 2 are in perfect agreement with (6) for all $\alpha$’s. Second, from combinatorial arguments [4,5], one can show that $z(\alpha)$ can be expressed formally as

$$z(\alpha) = \sum_{T} \frac{1}{\text{Aut}(T)} (-\alpha)^{E(T)}, \tag{7}$$

where the sum over $T$ is over isomorphism classes of bicolored (say brown and green) trees with at least one green vertex, $\text{Aut}(T)$ is the size of the automorphism group of $T$ and $E(T)$ the number of edges of $T$. In fact, (7) is an identity of analytic functions for $\alpha \leq 1/e$. For larger $\alpha$’s,
the sum in (11) is divergent, but a natural partial resum-

mation turns it into a convergent expression as follows.

Any bicolored tree can be obtained from a bicolored tree
with only green leaves and by appending brown leaves at the

green vertices, so we can explicitly sum over all brown

leaves in the sum over bicolored trees. This yields an

identity valid at small \( \alpha \):

\[
z(\alpha) = \sum_{n \geq 1} \frac{\alpha^{n-1}e^{-n\alpha}}{n!} S_{n-1}(-n\alpha),
\]

where the Stirling polynomials \( S_n \) are defined by:

\[
e^{x(e^t-1)} = \sum_{n \geq 0} S_n(x) \frac{t^n}{n!}.
\]

The sum in (11) converges to the r.h.s. of (3) for all \( \alpha \)'s,
giving further evidence for the validity of (3).

The appearance of bicolored trees with only green

leaves is no hazard. Consider the following pattern: a

subgraph of the random graph which is a finite tree
and which is such that one of its two bicolorings has only

green leaves and the green vertices share no edges with
the complement of \( T \) in the random graph. One can show
that the frequency of apparition of a maximal (that is,
not contained in a larger tree with the same properties)
such tree in the random graph is

\[
\frac{1}{\text{Aut}(T)} B^{V_a(T)} \alpha^{V_G(T)-1} e^{-V_G(T) \alpha},
\]

and that exactly \( V_G(T) - V_B(T) \) eigenvectors with eigen-

value 0 of the adjacency matrix of the random graph are

localized on \( T \) (in fact, they are even localized on the

green vertices of \( T ) \). The sum

\[
z_{\text{loc}}(\alpha) = \sum_T \frac{V_G(T) - V_B(T)}{\text{Aut}(T)} B^{V_a(T)} \alpha^{V_G(T)-1} e^{-V_G(T) \alpha}
\]

of these non-negative contributions gives a lower bound
for \( z(\alpha) \). Note the striking similarity between the sums
defining \( z(\alpha) \) and \( z_{\text{loc}}(\alpha) \). Explicitly,

\[
z_{\text{loc}}(\alpha) = -\frac{Be^A}{\alpha} + \frac{A^* + B + A^* B}{\alpha},
\]

and one checks that

\[
z_{\text{loc}}(\alpha) = z(\alpha) \quad \text{for } 0 \leq \alpha \leq \alpha_d \text{ and } \alpha \geq \alpha_r,
z_{\text{loc}}(\alpha) < z(\alpha) \quad \text{for } \alpha_d < \alpha < \alpha_r.
\]

This is our second important result: for \( 0 \leq \alpha \leq \alpha_d \) and \( \alpha \geq \alpha_r \),

all the (extensive) contributions to the kernel of random adjacency matrices come from vectors

localized on finite bicolored trees, with green leaves only,
attached to the rest of the random graph only by brown

vertices. However, this is not true for \( \alpha_d < \alpha < \alpha_r \),

where \( z_{\text{loc}}(\alpha) < z(\alpha) \).

Moreover, at the “critical” values \( \alpha_d \) and \( \alpha_r \),

the distribution of \( V_B(T) \), \( V_G(T) \), or even \( V_G(T) - V_B(T) \)

becomes large: the second moment diverges. For example,

\[
\langle V_G(T) - V_B(T) \rangle = \frac{1 + 2\alpha_d - \alpha_d^3}{\alpha_d^2 - \alpha_d^2} = 1.139353 \cdots
\]
at connectivity \( \alpha = \alpha_d \) but

\[
\langle (V_G(T) - V_B(T))^2 \rangle \sim \frac{\alpha_d^5 - \alpha_d^4 - 3\alpha_d^3 + 3\alpha_d^2 + 3\alpha_d + 1}{(2\alpha_d^3 - \alpha_d^2 - \alpha_d^2)(\alpha_d - \alpha)}
\]

when \( \alpha \) approaches \( \alpha_d \) from below. The presence of unbound-

ed fluctuations indicates that infinitely extended

objects are responsible for the difference between \( z_{\text{loc}}(\alpha) \) and \( z(\alpha) \) in the range \( \alpha_d < \alpha < \alpha_r \). Thus we infer that at

zero energy, the eigenvectors of the hopping Hamiltonian

exhibit a delocalization (insulator-conductor) transition
at \( \alpha_d \) and a relocation (conductor-insulator) transition
at \( \alpha_r \). The prediction of delocalization at \( \alpha_d \) is in

numercial agreement with Monte-Carlo simulations [3].

It turns out that the same delocalization value was al-

ready found by Harris in [4] in a loopless model of ran-

dom Bethe trees. This is surprising because at \( \alpha_d \),

the random graph has already (many) loops.

Note the analog of (3) for \( z_{\text{loc}}(\alpha) \):

\[
z_{\text{loc}}(\alpha) = \sum_{n \geq 1} \frac{\alpha^{n-1}e^{-n\alpha}}{n!} \frac{n(1+B)S_{n-1}(nB) - S_n(nB)}{n}
\]

Our main results are summarized in Fig. 2.

As noticed before, the expressions for \( z(\alpha) \), \( z_{\text{loc}}(\alpha) \)

and their difference show a singularity at \( \alpha = e \), due
to the fact that the frequency of certain patterns is

non-analytic. It is tempting to relate this singularity to the

flattening of the spectral distribution near the zero
eigenvalue for \( \alpha \simeq 2.7 \) observed in [3]. In fact, a

transition in properties of random graphs at \( \alpha = e \)

has already been observed in a different context, mini-

mal vertex covers [10,11]. A vertex cover of a graph is

a subset of the vertices containing at least one extrem-

ity of every edge of the graph. An analogous concept
is that of an edge disjoint system, i.e. a subset of the edges such that no two edges in the subset have a vertex in common. Given a graph $G$ on $N$ vertices, let $X(G)$ be the minimal size of a vertex cover and $Y(G)$ be the maximal size of an edge disjoint system. It is clear that $X(G) \leq N$ and $2Y(G) \leq N$. Those quantities share a very important property with $Z(G)$, they behave simply under leaf removal: $X(G') = X(G) - 1$, $Y(G') = Y(G) - 1$ whereas $Z(G') = Z(G)$. For general graphs, $X(G) \geq Y(G)$ and $Z(G) \geq N - 2X(G)$. Examples show that $Z(G) - N + 2Y(G)$ can have any sign.

But if $G$ is a random graph with $\alpha \leq e$, leaf removal leaves a core of size $o(N)$ so if $x(\alpha)$, $y(\alpha)$ and $z(\alpha)$ denote the limits of the averages of $X(G)/N$, $Y(G)/N$ and $Z(G)/N$ when $N \to \infty$ we get

$$x(\alpha) = y(\alpha) = \frac{1}{2}(1 - z(\alpha)) \quad \text{for} \quad \alpha \leq e. \quad (18)$$

This is the formula for $x(\alpha)$ when $\alpha \leq e$ obtained by Hartmann and Weigt via a replica symmetric ansatz \cite{10,11}. However, the relation (18) has to break down at some $\alpha > e$, because for large $\alpha$, $z(\alpha)$ is exponentially small in $\alpha$, whereas a rigorous result \cite{12} predicts that

$$x(\alpha) = 1 - \frac{2}{\alpha}(\log \alpha - \log \log \alpha - \log 2 + 1) + o(\frac{1}{\alpha}). \quad (19)$$

Simulations seem to indicate that the simple relation between $x(\alpha)$ and $z(\alpha)$ breaks down at $e$, together with replica symmetry stability. Our interpretation is that the remnant after leaf removal is a complicated graph with a size of order $z_{an}$ which can be described only by a more refined replica asymmetric order parameter.

In this paper, we have given an exact description of the size of the kernel of the hopping Hamiltonian associated to a large random graph and of the structure of the corresponding eigenvectors, leading to predictions of a delocalization and relocalization transition at $\alpha_d$ and $\alpha_r$. We have also explained the singularities affecting all spectral and several combinatorial properties at $\alpha = e$. A surprising fact is that all such properties are regular at the (classical) percolation transition at $\alpha = 1$. Possibilities to extend these results to more realistic models remain to be explored.

\footnotesize
\begin{itemize}
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  \item [4] It is generally believed that the first delocalized states appear at zero-energy. However, the disappearance of delocalized states at zero-energy for $\alpha_r = 3.154985 \cdots$ does not exclude that some exited delocalized states remain above this threshold.
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  \item [7] If $\alpha < 1$, it is obvious that $C = o(N)$, because $G$ is essentially a collection of trees.
  \item [8] A striking feature of Eq. (11) is that despite the maximality condition, it depends only on the most basic features of $T$: the number of green and brown vertices. Each brown vertex gives a weight $B$, which is non-analytic at $e$. So, at $e$, the random graph has a geometric phase transition in that the frequency of certain patterns is non-analytic. This is related to the appearance of a large core at the same threshold.
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\end{itemize}