Phase diagram of the Bose-Hubbard model on complex networks

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Abstract – Critical phenomena can show unusual phase diagrams when defined in complex network topologies. The case of classical phase transitions such as the classical Ising model and the percolation transition has been studied extensively in the last decade. Here we show that the phase diagram of the Bose-Hubbard model, an exclusively quantum mechanical phase transition, also changes significantly when defined on random scale-free networks. We present a mean-field calculation of the model in annealed networks and we show that when the second moment of the average degree diverges, the Mott-insulator phase disappears in the thermodynamic limit. Moreover we study the model on quenched networks and we show that the Mott-insulator phase disappears in the thermodynamic limit as long as the maximal eigenvalue of the adjacency matrix diverges. Finally we study the phase diagram of the model on Apollonian scale-free networks that can be embedded in 2 dimensions showing the extension of the results also to this case.

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Introduction. – Recently great attention [1,2] has been addressed to critical phenomena unfolding on complex networks. In this context it has been observed that the topology of the networks might significantly change the phase diagram of dynamical processes. For example when networks have a scale-free degree distribution $P(k) \sim k^{-\lambda}$ and the second moment $\langle k^2 \rangle$ diverges with the network size, i.e., $\lambda \in (2,3]$, the Ising model [3–6], the percolation phase transition [7,8] and the epidemic spreading dynamics on annealed networks [9] are strongly affected. Moreover, the spectral properties of the networks drive the epidemic spreading on quenched networks [10,11], the synchronization stability [12,13], the critical behavior of $O(N)$ models [14,15] and the critical fluctuations of an Ising model on spatial scale-free networks [16]. Quantum critical phenomena also might depend on the topology of the underlying lattice as has been shown for Bose-Einstein condensation in heterogeneous networks [17]. Although large attention has been devoted to classical critical phenomena on scale-free networks, the behavior of quantum critical phenomena on scale-free networks has just started to be investigated. In particular the Anderson localization [18,19] was studied in complex networks showing that by modulating the clustering coefficient of the network one might induce localization transition in scale-free networks. Moreover, attention has been addressed to quantum processes on Apollonian networks [20,21], which provide an example of scale-free networks embedded in two dimensions. The quantum processes investigated are the Hubbard model [22], the free-electron gas within the tight-binding model [23], and the topology-induced Bose-Einstein condensation in Apollonian networks [24]. The study of quantum phase transitions on these networks has attracted attention particularly in recent years motivated by the creation of a new self-similar macromolecule — a nanometer-scale Sierpinski hexagonal gasket [25]. Recently [26] it has been shown that the random transverse Ising model is strongly affected by a scale-free network topology of the underlying networks on which it is defined and in particular by the second moment of the degree distribution $\langle k^2 \rangle$. Indeed the critical temperature for the onset of the disordered phase is infinite if this second moment diverges and the network is scale free with power-law exponent $\lambda \leq 3$.

In this paper we investigate a critical process with no classical equivalent, the Bose-Hubbard model on
In this paper we show by mean-field approximations that the phase diagram of the model defined on an annealed network depends on the second moment of the degree distribution \( k^2 \). In particular, by the mean-field approximation, we found both for annealed and quenched networks that for scale-free networks with \( \lambda \leq 3 \) the Mott-insulator phase reduces with increasing network size, disappearing in the thermodynamic limit. Moreover, we observe differences between the model defined on a quenched network and an annealed network. In fact it is sufficient for a quenched random network to have diverging maximum degree in order to reduce the Mott-insulator phase to zero in the thermodynamic limit. This demonstrates that complex networks might strongly perturb the phase diagram of quantum phase transitions.

The paper is structured as follows: In the second section we give the solution of the Bose-Hubbard model in annealed complex networks within the mean-field approximation. In the third section we study numerically the phase diagram of the Bose-Hubbard model on quenched scale-free networks in the mean-field approximation and also on Apollonian networks. Finally we give the concluding remarks.

Mean-field solution of the Bose-Hubbard model on annealed complex networks. – An annealed network evolves dynamically on the same time scale as the dynamical process occurring on it. During this process, links are created and annihilated but the expected degree of each node remains the same. Solving dynamical models in annealed networks is usually straightforward. We are nevertheless in general not guaranteed that the phase diagram of the dynamical model on annealed scale-free networks will capture the essence of the dynamical model on quenched networks. Our strategy here will be first to study the Bose-Hubbard model in the annealed approximation and then to study the model on quenched networks to validate the main conclusions of the paper.

We consider the ensemble of uncorrelated networks in which we assign to each node a hidden variable \( \theta_i \) from a distribution \( p(\theta) \) indicating the expected number of neighbors of a node. We consider the ensemble of networks for which the probability to draw a link between node \( i \) and \( j \) is given by \( p_{ij} \),

\[
p_{ij} = P(\tau_{ij} = 1) = \frac{\theta_i \theta_j}{\langle \theta \rangle N}.
\]

In this ensemble the degree \( k_i \) of a node \( i \) is a Poisson random variable with expected degree \( \overline{k_i} = \theta_i \). Therefore we will have

\[
\langle \theta \rangle = \overline{k},
\]

\[
\langle \theta^2 \rangle = \frac{\overline{k(k-1)}}{N},
\]

where \( \langle \ldots \rangle \) indicates the average over the \( N \) nodes of the network and the overline in eqs. (3) indicates the average over the ensemble of the networks. We assume that the
expected degree distribution of the network ensemble is given by
\[ p(\theta) = N\theta^{-\lambda}e^{-\theta/\xi}, \]
where \( N \) is a normalization constant and \( \xi \) is an exponential cut-off in the expected degree distribution.

In order to study the Bose-Hubbard model on annealed complex networks we consider the fully connected Hamiltonian given by
\[ H = \sum_i \frac{U}{2} n_i(n_i - 1) - \mu n_i - t \sum_{i,j} p_{ij} a_i^\dagger a_j^\dagger, \]
where, in order to account for the dynamical nature of the annealed graph, we have substituted the adjacency matrix element \( p_{ij} \) in \( H \) given by eq. (1) with the matrix element \( p_{ij} \) given by eq. (2). Moreover, we perform the mean-field approximation to the Bose-Hubbard model introduced in [39] by taking
\[ a_i a_j^\dagger \simeq \langle a_i a_j^\dagger \rangle - \langle a_i \rangle \langle a_j^\dagger \rangle \]
\[ \simeq \psi_i a_j^\dagger + a_i \psi_j - \psi_i \psi_j, \]
where \( \psi_i = \langle a_i \rangle = \langle a_i^\dagger \rangle \). The Hamiltonian is then decomposed in single-site terms
\[ H = \sum_i H_i + \langle \theta \rangle N \tau t \gamma^2 \]
with \( H_i \) given by
\[ H_i = \frac{U}{2} n_i(n_i - 1) - \mu n_i - t \theta_i \gamma (a_i + a_i^\dagger) \]
and with \( \gamma \) indicating the order parameter of the superfluid phase, defined as
\[ \gamma = \frac{1}{\langle \theta \rangle N} \sum_i \theta_i \psi_i. \]

In this mean-field picture the Hamiltonian therefore decouples in single-site (-node) Hamiltonians \( H_i \) depending on the mean-field order parameter \( \gamma \). We can therefore write the single-site (-node) Hamiltonian as an unperturbed Hamiltonian plus an interaction depending on the parameter \( \gamma \), i.e.,
\[ H_i = H_i^{(0)} + \gamma \theta_i V_i \]
with
\[ H_i^{(0)} = \frac{U}{2} n_i(n_i - 1) - \mu n_i, \]
\[ V_i = t(a_i + a_i^\dagger). \]

The ground-state energy \( E_i^{(0)}(n) = E_i^{(0)}(n^*) \) with \( E_i^{(0)}(n^*) = 0 \) if \( \mu < 0 \) and \( E_i^{(0)}(n^*) = -\mu n^* + \frac{1}{2} U n^*(n^* - 1) \) if \( \mu \in (U(n^* - 1), U n^*) \). The second-order correction to the energy is given by \( E_i^{(2)} \)
\[ E_i^{(2)}(n^*) = \gamma^2 \theta_i^2 \sum_{n \neq n^*} \frac{|\langle n| V |n^* \rangle|^2}{E_i^{(0)}(n^*) - E_i^{(0)}(n)} \]
\[ = \gamma^2 \theta_i^2 \left( \frac{n^*}{U(n^* - 1) - \mu} + \frac{n^* + 1}{\mu - U n^*} \right). \]
Therefore, the energy spectrum \( E \) is given by the eigenvalues of the Hamiltonian \( H \), i.e.,
\[ E = \text{const} + m^2 \gamma^2 \]
with
\[ \frac{m^2}{\theta(t) N} = 1 + \frac{t \langle \theta^2 \rangle}{\langle \theta \rangle} \left( \frac{n^*}{U(n^* - 1) - \mu} + \frac{n^* + 1}{\mu - U n^*} \right). \]
The phase transition between a Mott-insulator phase where \( \gamma = 0 \) and a superfluid phase where \( \gamma > 0 \) occurs when \( m = 0 \). Therefore, the phase diagram at \( T = 0 \) is given by
\[ t_c(U, \mu, T = 0) = U \langle \theta \rangle \left( \frac{\mu(U - n^* + 1)}{\mu(U + 1)} \right) \]
with \( \mu / U \in [n^* - 1, n^*] \). The difference with respect to the mean-field phase diagram for regular lattices is that \( t_c \), the critical hopping rate, depends on the second moment of the expected degree distribution, i.e., \( \langle \theta^2 \rangle = (k(k - 1)) \).

Given the general expression for the expected degree distribution of complex networks considered in this paper, eq. (4), including the exponential cut-off \( \xi \), the Mott-insulator phase disappears as \( \xi \to \infty \) if \( \lambda > 3 \) and remains finite instead if \( \lambda > 3 \) and \( \xi \to \infty \). Therefore, as \( \langle \theta^2 \rangle / \langle \theta \rangle \) diverges, i.e., as \( \xi \to \infty \) while \( \lambda \to 1 \), we have that the Mott-insulator phase shrinks and finally disappears for large network sizes. Also, it can be seen that the critical indices will deviate from the mean-field values and they can be found by applying the heterogeneous mean-field techniques [6] developed for the classical phase transition.

At finite temperature we cannot properly speak about a Mott-insulator phase but we have still a phase diagram between a normal phase and the superfluid phase. The local order parameter is given by the thermal average of the creation and annihilation operators, i.e.,
\[ \psi_i = \frac{\text{Tr}_a e^{-\beta H_i}}{\text{Tr}_a e^{-\beta H_i}}. \]

Using the same steps as in [29] we can prove that the critical line for the Mott-insulator superfluid phase is given by
\[ t_c(U, \mu, \beta) = \frac{\langle \theta \rangle}{\langle \theta^2 \rangle} \sum_{r=0}^{\infty} e^{\beta[r U - (U/2)(r - 1)]} Q_r(U, \mu)^{3\beta[r U - (U/2)(r - 1)]}; \]
where
\[ Q_r(U, \mu) = \frac{\mu + U}{(\mu - U)r(U(r - 1) - \mu)}. \]
Therefore the phase diagram at finite temperature is also affected by the topology of the network and significantly changes when \( \langle \theta^2 \rangle \) diverges.
Phase diagram of the Bose-Hubbard phase transition on quenched complex networks. – We now discuss the phase diagram of the Bose-Hubbard model on quenched networks. In particular we focus on the base diagram at $T = 0$. The Hamiltonian we consider is the hopping term as a perturbation. At the first order of the perturbation theory we get that

$$\psi_1 = \frac{t}{U} F(\mu, U) \sum_j \tau_{ij} \psi_j,$$

where

$$F(\mu, U) = \frac{\mu + U}{|\mu - \mu^* U|} \frac{[U(n^* - 1) - \mu]}{[U(n^* - 1) - \mu]}.$$

and the superfluid phase where $\psi_i = 0$ and the superfluid phase where $\psi_i > 0 \ \forall i$. The mean-field Hamiltonian $H^{MF}$ is then parametrized by the self-consistent parameters $\psi_1$ and reads

$$H^{MF} = \sum_i \left[ \frac{U}{2} n_i (n_i - 1) - \mu n_i - t \sum_j \tau_{ij} (a_i a_j^\dagger) \right] + t \sum_i \sum_j \tau_{ij} \psi_i \psi_j.$$

Following [30] we consider the hopping term as a perturbation. At the first order of the perturbation theory we get that

$$\psi_1 = \frac{t}{U} F(\mu, U) \sum_j \tau_{ij} \psi_j,$$

where

$$F(\mu, U) = \frac{\mu + U}{|\mu - \mu^* U|} \frac{[U(n^* - 1) - \mu]}{[U(n^* - 1) - \mu]}.$$

and the superfluid phase where $\psi_i = 0$ is stable as long as

$$\frac{t}{U} F(\mu, U) \Lambda < 1. \quad (21)$$

We observe that in random scale-free networks with degree distribution $p(k) = N k^{-\lambda}$ the maximal eigenvalue $\Lambda$ of the adjacency matrix diverges with a diverging value of the maximal degree of the network $k_{max}$ as $\Lambda \propto \sqrt{k_{max}}$ [48–51]. Therefore, we find that also as long as the maximal degree of the network diverges the Mott-insulator phase disappears in the large network limit, changing the phase diagram of the model significantly with respect to regular networks where the maximal degree of the network remains constant. We have checked these results by performing numerical integration of the mean-field calculations. We have studied the phase diagram of single quenched networks with scale-free degree distribution $p(k) = N k^{-\lambda}$ and different values of the power-law exponent $\lambda$ to see how fast the convergence of the solution to the asymptotic phase diagram is. In the following we will show our finite-size scaling calculations and the resulting effective phase diagram of the Bose-Hubbard model within the mean-field approximation on the quenched network for different values of the number of nodes $N$. In fig. 1 we plot the effective phase diagram for network sizes $N = 100, 1000, 10000$ finding that for $\lambda = 2.2 < 3$ the boundary of the Mott insulating phase decreases with the network size. On the other hand for a typical network with $\lambda = 3.5 > 3$ (see fig. 2) the phase diagram has slower finite-size dependencies. This shows that the annealed approximation for the Bose-Hubbard model on scale-free networks strongly differs from the quenched phase diagram of the model for $\gamma > 3$. In particular we have that the Mott-insulator phase transition on annealed scale-free networks,

Fig. 1: (Color online) Average order parameter for the superfluid phase for scale-free networks with power-law exponent $\lambda = 2.2$ and network sizes $N = 100$ (top), $N = 1000$ (middle) and $N = 10000$ (bottom). As the network size increases, the phase diagram changes monotonically, as predicted by the mean-field treatment in the case $\lambda < 3$. Therefore, there is no Mott-insulator phase in the limit $N \to \infty$.

Fig. 2: (Color online) Average order parameter for the superfluid phase for scale-free networks with power-law exponent $\lambda = 3.5$ and network sizes $N = 100$, $N = 1000$ and $N = 10000$. As the network size increases, the phase diagram has slower finite-size effects with respect to the case $\lambda < 3$. Nevertheless, the maximal eigenvalue increases with network size as $\Lambda \propto \sqrt{k_{max}}$ and, therefore, the Mott-insulator phase disappears in the thermodynamic limit also in this case.
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Fig. 3: (Color online) Left panel: the first 3 generations of the Apolloniangraph. The nodes and links added to construct the 1st (red), 2nd (green) and 3rd (purple) generations are shown. Right panel: the 5th-generation Apollonian network.

Fig. 4: (Color online) Effective phase diagram of the Bose-Hubbard model on Apollonian networks of the 5th, 7th and 9th generation, with network sizes \( N = 124, N = 1096 \) and \( N = 9844 \), respectively. As the network size diverges, the Mott-insulator phase is reduced and it disappears in the limit of an infinite network.

Conclusions. – In conclusion in this paper we have shown that the scale-free network topology of the underlying network strongly affects the phase diagram of the Bose-Hubbard model. By performing mean-field calculations on annealed networks we have shown that the Mott-insulator phase disappears in the large network limit as long as the power-law exponent \( \lambda \) of the degree distribution is \( \lambda \leq 3 \) and the exponential cut-off \( \xi \) of the distribution diverges. We have performed mean-field calculations in annealed networks finding in this approximation the phase diagram of the model both at \( T = 0 \) and at finite temperature. Moreover, the analytical and numerical solutions of the Bose-Hubbard model on quenched networks show that this argument must be corrected in the quenched case and that it is sufficient that the maximal eigenvalue diverges in order to change the phase diagram of the model. Finally we have considered the Bose-Hubbard model on Apollonian networks that are an example of scale-free networks embedded in a two-dimensional space. In short, this work offers a new perspective on the characterization of quantum critical phenomena in annealed and quenched complex networks and shows that the second moment of the degree distribution \( \langle k^2 \rangle \) and the maximal eigenvalue of the adjacency matrix play a crucial role in determining the phase diagram of the Bose-Hubbard model.

REFERENCES

[1] Dorogovtsev S. N., Goltsev A. V. and Mendes J. F. F., Rev. Mod. Phys., 80 (2008) 1275.
[2] Barrat A., Barthelemy M. and Vespignani A., Dynamical Processes on Complex Networks (Cambridge University Press, New York) 2008.
[3] Bianconi G., Phys. Lett. A, 303 (2002) 166.
