Exactly solvable tight-binding model on two scale-free networks with identical degree distribution

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Abstract – We study ideal Bose gas upon two scale-free structures $G^1$ and $G^2$ with identical degree distribution. Energy spectra belonging to tight-binding Hamiltonian are exactly solved and the related spectral dimensions of $G^1$ and $G^2$ are obtained as $d_{s1} = 2$ and $d_{s2} = 2\ln 4/\ln 3$. We show that Bose-Einstein condensation only takes place upon $G^2$ instead of $G^1$. The topology and thermodynamical property of the two structures are proven to be totally different.

Introduction. – Understanding the spectral structure of Hamiltonians is of key importance in the study of Bose-Einstein condensation (BEC). The underlying dimensionality of a spectrum determines the occurrence of BEC in most cases. It is well known that for ideal and uniform (homogeneous) Bose gases, only the energy spectra related to three or higher dimensions allow Bose-Einstein phase transition [1]. For confined (inhomogeneous) Bose gases, it was shown that the presence of traps allows BEC to take place in lower dimension though [2,3]. Obviously, the structure and magnitude of the present traps have large influence on the spectral structure for quantum gases, and alter the phase transition phenomena as well. To further show how the structure of traps influences the thermodynamic behaviors of confined quantum gases, several types of weakly coupled discrete traps were investigated in the past decade with the help of network theory [4–10]. For these Bose gases confined by traps with network-like structure, the displayed BEC is topology induced. For example, BEC on star-shaped and wheel-shaped network depends on the number of star-arms and wheel spokes [4,6]. The type of Bose-Einstein transition gone through upon diamond hierarchical lattices was also shown to be fully determined by a structural parameter of the lattice-like trap [7]. Moreover, a fractal-like energy spectrum was found in Bose gas confined by Apollonian network-shaped traps, which shows self-similarity at the same time [10]. As we can see, the topology of different kinds of traps, usually embedded in a $n$-dimensional Euclidean space, is a key issue to studying condensation of inhomogeneously confined Bose gas. However, no theory can give a satisfactory explanation as to how the structures of trap distributions interact with the spectral structure and determine the BEC phenomenon. It is also unclear what topological invariant can decide the occurrence of BEC or the type of phase transition. To fill this gap, we pay our attention to traps with scale-free topology. We will determine whether the scale-free characteristic of weakly coupled traps can govern the BEC.

The term “scale-free” mentioned before is used to describe a network with a power-law degree distribution. In recent decades, dynamics of inhomogeneously coupled systems with a scale-free topology have been studied extensively since lots of real-world networks were verified to inherit the same nature [8,9,11–24]. The Hamiltonian defined by coupling between adjacent vertices is used to describe the time evolution of such systems, related to many observable phenomena [10,25–27]. The entailed dynamics are highly dependent on the network topology, as the BEC we focus on in this paper. Among all the topological features of networks, the degree distribution is one of the most important characteristics.

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Many networks with a scale-free degree distribution have fractal-like properties, due to the self-similarity underlying their topological structure [28–31]. It was also reported that scale-free characteristics control the critical phenomena of many physical processes [15, 20–22]. Moreover, some works suggested that scale-free characteristics cannot determine phase transitions related to cooperative behaviors and epidemic spreadsings [23, 24]. Nevertheless we will show that BEC upon weakly coupled traps belongs to the latter.

In this paper, we introduce two scale-free networks sharing the same degree distribution. We apply the tight-binding Hamiltonian to describe weakly coupled traps [4–10]. We solve the fractal-like spectra exactly for the latter.

**Construction.** The two considered scale-free networks are iteratively constructed in two different patterns [34] (see fig. 1). The first few iterations are shown in fig. 2. We label them as $G_1^t$ and $G_2^t$, respectively, according to the pattern (1 or 2) and iterations ($t \in N$) they undergo. $G_1^t$ and $G_2^t$ denote the networks after infinitely many iterations ($t \rightarrow \infty$).

The degree of a vertex is defined as the number of its adjacent vertices. For both patterns of iteration, the degree of any vertex is doubled after one iteration. Thus, $G_1^t$ and $G_2^t$ have the same degree distribution $P(k)$, that is the probability distribution of the degrees of vertices over the whole network. After some algebra, we obtained several common characteristics of the two structures. The total number of edges is $E_t = 4^t$ for both $G_1^t$ and $G_2^t$ and the total number of vertices is $N_t = \frac{4}{3}(4^t + 2)$. Their degree distributions simultaneously obey $P(k) \sim k^{-3}$ when $t \rightarrow \infty$.

The power-law behavior of $P(k)$ indicates that $G_1^t$ and $G_2^t$ are both scale-free networks. But $G_1^t$ and $G_2^t$ are clustered differently. Let $L$ denote the typical distance (length of the shortest path) between two randomly chosen nodes of a network. For $G_2^t$,

$$L \sim \log N_t \sim t$$

holds for large $t$. This means $G_2^t$ is a small-world network [35] with a high clustering coefficient [34], while $G_1^t$ is not since its average shortest path length grows faster than $\log N_t$.

Evidently, the degree distribution does not determine all the global property of a scale-free network. More information is encoded in the pattern in which the local vertices are organized.

**Tight-binding bosons on inhomogeneous structures.**

**Tight-binding Hamiltonian.** Let us label the vertices of any connected graph $G = (\mathcal{V}, \mathcal{E})$ ($\mathcal{V}$ is the set of vertices and $\mathcal{E}$ the set of edges) from 1 to $N$. Let us label the edge connecting vertex $i$ and $j$ by $e_{ij}$. Suppose $G$ corresponds to a network of weakly coupled traps, where vertices denote traps, and edges represent coupling. Following the tight-binding model defined in [10], which is also a simplified LCAO model [36], the Hamiltonian for non-interacting bosons on $G$ is

$$H = \sum_{k \in \mathcal{V}} \epsilon_k |k\rangle \langle k| + \sum_{i,j \in \mathcal{V}} h_{ij} |i\rangle \langle j|,$$  

where $|k\rangle$ is the orbit of localized boson at vertex $k$ and $\epsilon_k$ the on-site ground energy. We ignore all excited states. $h_{ij}$ is the hopping amplitude between trap (vertex) $i$ and $j$. Here we only consider the overlaps of localized states corresponding to adjacent vertices. So $h_{ij} = 0$ if vertex $i$ is not linked to vertex $j$. Suppose the on-site energy is uniform among all sites, we put $\epsilon_k = 0$ in eq. (2) without loss of generality.

Let us first introduce some algebra tools for formulating our model.
The adjacency matrix $A$ is used to describe the connection among vertices of graph $\mathcal{G}$:

$$A_{ij} = \begin{cases} 1, & e_{ij} \in E, \\ 0, & e_{ij} \notin E. \end{cases} \quad (3)$$

The degree matrix $D$ of $\mathcal{G}$ is diagonal, given as $D = \text{diag}(d_1, d_2, \ldots, d_N)$, where $d_k$ is the degree of vertex $k$.

The transition matrix $M$ of the same graph is defined as $M = D^{-\frac{1}{2}}A$, which can be normalized as $P = D^{-\frac{1}{2}}MD^{-\frac{1}{2}} = D^{-\frac{1}{2}}AD^{-\frac{1}{2}}$. The element at row $i$ and column $j$ of $P$ is thus $P_{ij} = \frac{1}{\sqrt{d_id_j}}$.

For homogeneous systems such as Bravais lattices, the hopping amplitude is usually taken as $h_{ij} = \xi A_{ij}$, where $\xi$ is constant. In the case of scale-free structures, we assume $h_{ij} = \xi P_{ij}$ to avoid divergence difficulty.

Further, we introduce the reduced Hamiltonian $\mathcal{H} = \frac{1}{\xi}H$. Then, eq. (2) can be rephrased as

$$\mathcal{H} = \sum_{i,j \in V} \frac{1}{\sqrt{d_id_j}}|i\rangle \langle j|. \quad (4)$$

**Complete energy spectra.** Below we will solve the energy spectrum of $\mathcal{H}$ for $\mathcal{G}^1$ and $\mathcal{G}^2$ by exact matrix renormalization. Similar derivation of spectrum for other renormalizable structures can be found at [37,38].

Let $D_{1,t}$ and $A_{1,t}$ denote the degree matrix and adjacency matrix of $\mathcal{G}_{1}^{t} (i = 1, 2)$.

For $i = 1$, by proper permutation of rows and columns, $D_{1,t}$ and $A_{1,t}$ read

$$D_{1,t} = \begin{pmatrix} 2I & 0 \\ 0 & 2D_{1,t-1} \end{pmatrix}, \quad (5)$$

$$A_{1,t} = \begin{pmatrix} 0 & J^T \\ J & 0 \end{pmatrix}. \quad (6)$$

where $I$ is the identity matrix of order $\Delta_t = N_t - N_{t-1}$. And the $N_{t-1} \times \Delta_t$ matrix $J$ represents the adjacency among new vertices and the old ones. The hopping matrix (i.e., the normalized transition matrix of $\mathcal{G}_{1}^{t}$) is

$$P_{1,t} = D_{1,t}^{-\frac{1}{2}} A_{1,t} D_{1,t-1}^{-\frac{1}{2}} = \begin{pmatrix} 0 & \frac{1}{2} J^T D_{1,t-1}^{-\frac{1}{2}} \\ \frac{1}{2} D_{1,t-1}^{-\frac{1}{2}} J & 0 \end{pmatrix}. \quad (7)$$

The characteristic polynomial of $P_{1,t}^{T}$ is thus

$$\det(\lambda - P_{1,t}) = \lambda^{N_{t-1} - N_{t-1}} \det(\lambda - \frac{1}{4\lambda} D_{1,t-1}^{-\frac{1}{2}} J J^T D_{1,t-1}^{\frac{1}{2}}), \quad (8)$$

using the identity

$$\det \begin{pmatrix} A & B \\ C & D \end{pmatrix} = \det A \cdot \det(D - CA^{-1}B). \quad (9)$$

Let $j_{mn}$ denote the $(m,n)$-entry of $J$. The symmetric matrix $J J^T$ is represented by

$$(J J^T)_{mn} = \sum_{t} j_{ml}j_{nt}. \quad (10)$$

For $m = n$, $(J J^T)_{mn}$ is exactly the degree of node $m$ in $\mathcal{G}_{1}^{t}$, i.e., twice its degree in $\mathcal{G}_{1}^{t-1}$. For $m \neq n$, $(J J^T)_{mn}$ is 2 if node $m$ and node $n$ is previously adjacent in $\mathcal{G}_{1}^{t-1}$, otherwise 0.

Hence one obtains

$$J J^T = 2D_{1,t-1} + 2A_{1,t-1}, \quad (11)$$

which leads to

$$\det(\lambda - P_{1,t}) = \frac{1}{2} \xi^{N_{t-1} - 2N_{t-1}} \det((2\lambda^2 - 1) - P_{1,t-1}). \quad (12)$$

The recursive relation in eq. (12) indicates if $\lambda$ is an eigenvalue of $P_{1,t}$, then $R_1(\lambda) = (2\lambda^2 - 1)$ is an eigenvalue of $P_{1,t-1}$ with the same degeneracy unless $\lambda = 0$. Conversely, for any eigenvalue $\eta$ of $P_{1,t-1}$, the inverse of $R_1$ gives its two descendents with the same degeneracy as $\eta$, unless $\eta = -1$ (notice $R_1(-1) = 0$). Hence the degeneracy of the exceptional eigenvalue 0 should be $\frac{2 - \xi^2}{2}$ to ensure the spectrum of $P_{1,t-1}$ is complete.

Subsequently, the spectrum of $P_{1,t}$, denoted by $\sigma_{1,t}$, can be analytically determined from the initial spectrum $\sigma_{1,1} = \{\cos 0, \cos \frac{\pi}{2}, \cos \frac{\pi}{2}, \cos \pi\}$, given as

$$\sigma_{1,t} = \{E_t\} = \bigcup_{0 \leq k \leq 2^t} \left\{ \cos \frac{k\pi}{2^t} \right\}. \quad (13)$$

The symmetry of $\sigma_{1,t}$ with respect to 0 is obvious and the lowest energy is always $E_0 = -1$.

The integrated density of states (IDOS) $f(\varepsilon)$ is defined to be the number of states between $E_0$ and $E_0 + \varepsilon$ ($0 \leq \varepsilon \leq 2$) divided by the total number of states.

For homogeneous systems such as a single particle in a 3D cavity, it is well known that $f(\varepsilon) \propto \varepsilon^2$. For inhomogeneous systems also showing power-law behavior $f(\varepsilon) \propto \varepsilon^{d_s/2}$ near the band bottom ($\varepsilon \ll 1$), the exponent $d_s/2$ can be irrational. And $d_s$ is said to be the spectral dimension of a structure related to a certain Hamiltonian [32,33]. It was reported that the spectral dimension is a crucial index categorizing the universality classes of topology-induced Bose-Einstein transitions [7]. Also, it has been proven that the phase transition breaking a continuous symmetry cannot take place on systems with a spectral dimension not greater than 2 [39–42]. The theoretical determination of the spectral dimension is not an easy task. However, by appropriate renormalization, analytical results on spectral dimension are still obtainable for several fractal-like structures [43].

To compute the spectral dimension of our networks, we first pay attention to the IDOS $f(\varepsilon)$ corresponding to $\mathcal{G}^1$. Transforming $R_1$ for expressing the iterative relation for
Hence $f(\varepsilon)$ of the spectrum. Polynomial: and obtain the iterative expression for the characteristic eigenvalues here are $1, -\frac{1}{2},$ and 0. Their degeneracies are $(N_t - 3N_{t-1} + 2)/2, (N_t - 3N_{t-1} + 2)/2$ and $N_{t-1}$, respectively, according to eq. (15). Since $\sigma_{2,t} = \{1, 0, 0, -1\}$, the energy spectrum $\sigma_{2,t}$ of $G^2_t$ is symmetric with respect to zero and the lowest energy is still $E_0 = -1$. For $G^2_t$, when

$$
\det(\lambda - P_{2,t}) = 2^{-N_{t-1}} \cdot (\lambda^2 - \frac{1}{\lambda})^{\frac{N_t - 3N_{t-1}}{2}} \cdot \lambda^{2N_{t-1}} \cdot \det \left( \frac{2\lambda^2 - 1}{\lambda} - P_{2,t-1} \right). 
$$

(15)

Now the iteration is formulated as $R_2(\lambda) = \frac{2\lambda^2 - 1}{\lambda}$. By taking the inverse of $R_2$, we are able to generate the spectrum of any order from the initial one. The exceptional eigenvalues here are $\frac{1}{2}, -\frac{1}{2}$ and 0. Their degeneracies are $(N_t - 3N_{t-1} + 2)/2, (N_t - 3N_{t-1} + 2)/2$ and $N_{t-1}$, respectively, according to eq. (15). Since $\sigma_{2,1} = \{1, 0, 0, -1\}$, the energy spectrum $\sigma_{2,1}$ for $G^1_1$ is symmetric with respect to zero and the lowest energy is still $E_0 = -1$. For $G^2_t$, when

$$
f(\varepsilon) = (1 - f(\tilde{R}_1(\varepsilon))) \lim_{t \to \infty} \frac{N_{t-1}}{N_t}
= \frac{1}{4} f(2 - \tilde{R}_1(\varepsilon))
\approx \frac{1}{4} f(4\varepsilon).
$$

(14)

Hence $f(\varepsilon) \propto \varepsilon^4$ near the origin. The spectral dimension of $G^1$ is thus $d_{s1} = 2$. Figure 3 gives schematic representation of the spectrum.

By the same method, we calculate the spectrum for $G^2_t$ and obtain the iterative expression for the characteristic polynomial:

$$
\det(\lambda - P_{2,t}) = 2^{-N_{t-1}} \cdot (\lambda^2 - \frac{1}{\lambda})^{\frac{N_t - 3N_{t-1}}{2}} \cdot \lambda^{2N_{t-1}} \cdot \det \left( \frac{2\lambda^2 - 1}{\lambda} - P_{2,t-1} \right).
$$

(16)

Since $\sigma_{2,1} = \{1, 0, 0, -1\}$, the energy spectrum $\sigma_{2,1}$ for $G^1_1$ is symmetric with respect to zero and the lowest energy is still $E_0 = -1$. For $G^2_t$, when

$$
f(\varepsilon) = (1 - f(\tilde{R}_1(\varepsilon))) \lim_{t \to \infty} \frac{N_{t-1}}{N_t}
= \frac{1}{4} f(2 - \tilde{R}_1(\varepsilon))
\approx \frac{1}{4} f(4\varepsilon).
$$

(17)

Fig. 5: (Color online) Condensed fraction $f$ as a function of $\tilde{T}$ for $G^1_t$ ($\gamma = 0.2$). The finite-size effect decreases as $t$ increases.

$\varepsilon$ is small, the invariance of $f(\varepsilon)$ requires

$$
f(\varepsilon) = f(2\varepsilon - 1 - \frac{1}{\varepsilon - 1}) \lim_{t \to \infty} \frac{N_{t-1}}{N_t}
\approx \frac{1}{4} f(3\varepsilon).
$$

(18)

Thus,

$$
f(\varepsilon) \propto \varepsilon^2
$$

near the band bottom and the spectral dimension is

$$
d_{s2} = \frac{2\ln 4}{\ln 3} = 2.524.
$$

(19)

The IDOS for a finite-size network is shown in fig 4. So far, the spectra related to the two networks have shown unique fractal-like structures, which will lead to different behaviors of tight-binding particles.

**Different cryogenic behaviors of Bose gas.** In this section we investigate the cryogenic behaviors of non-interacting Bose gas on $G^1$ and $G^2$ and check whether Bose-Einstein condensation will take place.

Suppose there are $N_p$ bosons on the structures. The particle density is defined as $\gamma = \frac{N_p}{N_t}$. To approach the thermodynamic limit, we fix $\gamma$ and let $t \to \infty$. Bose-Einstein statistics gives the expected number of bosons in state $i$:

$$
n_i = \frac{1}{z^{1-i}e^{\beta \mu} - 1},
$$

(20)

where $\beta = \frac{1}{k_B T}$ and the fugacity $z = e^{\beta (\mu - \xi E_0)}$. $\mu$ is the chemical potential,

$$
n_{i0} = \frac{1}{z^{-1} - 1}
$$

is the number of condensed particles and $f = \frac{n_0}{\gamma N_t}$ the condensed fraction.

The normalization condition requires

$$
\sum_i n_i = \gamma N_t.
$$

(21)
Transforming eq. (21) into integral, one obtains

$$\int_0^2 \frac{\rho(\varepsilon)}{z^{-1} e^{\beta z} - 1} \, dz = \gamma, \quad (22)$$

where $\rho(\cdot)$ is the state density and $\varepsilon$ the relative energy.

Let $T$ = $k_b T_c$ be the dimensionless critical temperature. Substitute $\xi \beta$ with $\beta = 1/T$. Equation (22) is rewritten as

$$\int_0^2 \frac{\rho(\varepsilon)}{z^{-1} e^{\beta z} - 1} \, dz = \gamma. \quad (23)$$

Below the critical temperature where the Bose-Einstein phase-transition occurs, $z$ is always 1. In fig. 5 we present the relation between the condensed fraction and the dimensionless temperature with finite-size effects. There is no sign of first-order phase transition, which is proved analytically as follows.

Suppose $G^1$ allows the occurrence of BEC transition in thermodynamic limit. The uncondensed fraction of bosons at the (dimensionless) critical temperature $T_{c_1}$ is

$$f_u = \frac{1}{\gamma} \lim_{\varepsilon \to 0} \int_{\varepsilon_1}^{\varepsilon_2} \frac{\rho(\varepsilon)}{e^{\beta_{c_1} \varepsilon} - 1} \, d\varepsilon > \frac{1}{\gamma} \int_{\varepsilon_1}^{\varepsilon_2} \frac{\rho(\varepsilon)}{e^{\beta_{c_1} \varepsilon} - 1} \, d\varepsilon, \quad (24)$$

where $\beta_{c_1} = 1/T_{c_1}$, $\varepsilon_1 < \varepsilon_2 \ll 1$.

By the approximation $\rho(\varepsilon) \approx k \frac{d(x^2_c)}{d\varepsilon}$, the last integral becomes

$$\frac{1}{\gamma} \int_{\varepsilon_1}^{\varepsilon_2} \frac{\rho(\varepsilon)}{e^{\beta_{c_1} \varepsilon} - 1} \, d\varepsilon \approx \frac{1}{\gamma} \int_{\varepsilon_1}^{\varepsilon_2} \frac{k}{e^{\beta_{c_1} \varepsilon} - 1} \, d\varepsilon = \frac{k}{\gamma} \int_{\varepsilon_1}^{\varepsilon_2} 1 \, d\varepsilon, \quad (25)$$

where $k$ is a positive constant.

Since $\varepsilon_1$ and $\varepsilon_2$ are small, $e^{\beta_{c_1} \varepsilon} \approx 1 + \beta_{c_1} \varepsilon$ holds for $\varepsilon \in [\varepsilon_1, \varepsilon_2]$. It follows that

$$\frac{k}{\gamma} \int_{\varepsilon_1}^{\varepsilon_2} 1 \, d\varepsilon \approx \frac{k}{\gamma \beta_{c_1}} \ln \left( \frac{\varepsilon_2}{\varepsilon_1} \right). \quad (26)$$

Thus,

$$1 \geq f_u > \frac{k}{\gamma \beta_{c_1}} \ln \left( \frac{\varepsilon_2}{\varepsilon_1} \right). \quad (27)$$

$e_2/c_1$ has no finite upper bound. This contradicts eq. (27) when $T_{c_1} > 0$. Hence positive $T_{c_1}$ does not exist for $G^1$. In consequence, Bose-Einstein condensation will not take place at low temperature.

Will the massive bosons behave differently on $G^2$ at low temperature? A schematic representation of the relation between condensed fraction for network $G^2$ and $\bar{T}$ is given in fig. 6. The curves converge quickly, suggesting the transition temperature when the thermodynamic limit is approached. For $\gamma = 0.2$, we obtain the transition temperature $\bar{T}_c \approx 0.107$ and $f \propto |T - T_c|^1$ near the critical point.

By further numerical computation, the dependence of the critical temperature on $\gamma$ and a series of critical exponents can be obtained, which are not the main interest of this study. Related discussions on these can be found at [7,44]. We claim that the BEC in $G^2$ belongs to the universality class of the ideal BEC in networks with spectral dimension $d_s \approx 2.524$.

Moreover, the state $\psi_c$ of the condensate can be determined analytically. Since the hopping amplitude is negative ($\xi < 0$), $\psi_c$ is related to the eigenvector of $P_{2,t}$ with respect to the eigenvalue 1, which is usually called the equilibrium distribution or steady state of random walks depicted by the transition matrix. With finite-size effects ($t$ is finite), $\psi_c$ is expressed as

$$\psi_c = A \sum_i \frac{d_i}{N_t} |i\rangle. \quad (28)$$

$A$ is the normalization constant. The sum is taken over all the vertices.

Equation (28) indicates that the state of the condensate follows the degree distribution though the occurrence of phase transition is determined by more in-depth topology. Not only for $G^2$, this consequence holds true also for all discrete structures with a tight-binding Hamiltonian. If the structure is a random regular graph, the lowest state is simply the unweighted combination of all tight-binding local orbits up to phase difference.

**Conclusion.** – Tight-binding models upon two scale-free networks with identical degree distribution $P(k) \sim k^{-3}$ were investigated.

By renormalization, we iteratively obtained the fractal-like spectra of the two networks and determined their spectral dimensions ($d_{s_1} = 2$, $d_{s_2} = 2 \ln 4/\ln 3$). Suggested by the value of $d_{s_1}$, we analytically proved that BEC would not take place in $G^1$. On the contrary, with the same scale-free degree distribution, the structure of $G^2$ allows the occurrence of the Bose-Einstein phase transition. Moreover, the BEC in $G^2$ belongs to the universality class of the
ideal BEC, related to spectral dimension $d_s = 2 \ln 4 / \ln 3$. We also found the state $\psi_c$ for the condensate, which was determined by the degree distribution of the structure.

The divergent behaviors of the two structures give a good example as to how the topology as well as the thermodynamical property of networks vary regardless of scale-free characteristics. The divergence not merely lies in several critical exponents but also in the occurrence of phase transition. The scale-free characteristics do not always play an important role in dynamical systems governed by equations of the form $dx_i/dt = \sum k_{ij}(x_j - x_i)$, related to diffusion, relaxation, etc.

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