Organization in complex brain networks: energy distributions and phase shift

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The Hamiltonian function of a network, derived from the intrinsic distributions of nodes and edges, magnified by resolution parameter has information on the distribution of energy in the network. In brain networks, the Hamiltonian function follows hierarchical features reflecting a power-law behavior which can be a signature of self-organization. Further, the transition of three distinct phases driven by resolution parameter is observed which could correspond to various important brain states. This resolution parameter could thus reflect a key parameter that controls and balances the energy distribution in the brain network.

Keywords: Constant Potts model; Hamiltonian function; Resolution parameter; Self-organization; Transition of phase.

Brain is a complex universe of neurons in which its functional and structural network properties have diverse features, such as, small worldness (minimizing wiring costs) [1], significant emergence of modules (local signal processing and propagation) [2], and a distribution of rich club of key hubs (crucial for global signal integration) [3]. These properties indicate that a brain has structurally and functionally defined modules with short-ranged characteristics, where perturbations are localized, and then these local signals are propagated due to long-ranged interaction driven by rich club of key hubs. Moreover, weak interaction among these functional modules is essential for efficient information processing with minimum energy cost [4], and the dynamics and stabilization of the wiring/rewiring provide the basis for the adaptive nature of the brain network [6]. The modules are also arranged in a hierarchical manner with bunch of interacting key hubs exhibiting system level organization of the brain network, and through which a local information is distributed globally [5]. Further, the key hubs in the brain network are important for information integration and thus for performing complex cognitive functions, because these hubs are multifunctional, capable of long range information processing, and dynamically complex in nature [7]. However, still debatable open question is on how the energy management, distributions, and minimization happen among the interacting units (neurons or clusters of neurons) of a brain.

Study of a complex networks within the framework of Potts model was done in order to extract patterns and properties of the networks [13], and the formalism has been used as a powerful method for finding communities specially in hierarchical networks [14]. The simplified version of the Potts model, constant Potts model (CPM), in which Hamiltonian operator of the network is constructed from the evolved nodes and edges in the network, can be used to characterize various properties of the network. In this work, we used CPM in order to study properties of complex brain networks specially focusing on energy distributions in the network. Since brain networks follow hierarchical features [2, 8, 9], we apply the formalism to brain networks of *C. elegans*, cat, and macaque monkey [8], and studied how energy is distributed in the brain networks.

Properties of Hamiltonian function in complex brain networks

The energy stored in a complex system represented by a complex network may be interpreted as the energy spent in the distribution and organization of interacting edges (wiring/rewiring of edges), with specified weights and directions, among the constituting nodes in the network. Hierarchical networks, which have the features of system level organization [10], involve the emergence of modules/communities which are also interacting in a certain fashion [11]. Each module/community has its own organization, consisting of cross-talking sub-modules/sub-communities in the next level of organization, which is less affected by sub-modules/sub-communities of other remaining modules/communities (Fig. 1). Similarly, the sub-modules/sub-communities will have their organization of sub-sub-modules/sub-communities at the next further level, and so on. This system level organization of modules/communities at various levels amounts to the complexity in the network organization.

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The modules/communities are relatively more densely connected groups of nodes, which could reflect different functions and cross-talk within the network. Here, we focus on the energy stored in a complex network at various levels of organization, and the way of using the stored energy in the network in organizing the network within the formalism of CPM [14]. Consider a network given by a graph, G = G(E, V), with sets of constituting nodes $V = \{k\}, k = 1, 2, ..., n$, and edges $E = \{e_{ij}\}, \forall i, j \in n$. The distribution of edges among the nodes is given by adjacency matrix $A_{ij}, \forall i, j \in n$, such that $A_{ij} = 1$ if ith and jth nodes are connected, otherwise zero. The Potts model [12] can be used to analyze properties of complex network [13], and its simplified form, known as CPM, is used as a technique to detect communities in complex network [14]. For an undirected and unweighted network, the total number of edges in the network is $L = \sum_{ij} A_{ij}$, where A is $n \times n$ matrix. The Hamiltonian of this network within the CPM formalism [13–16] is given

$$H(c,\gamma) = -\sum_{i,j} (A_{ij} - \gamma) \,\delta(c_i, c_j) \tag{1}$$

where c_i and c_j are ith and jth communities of the network, and γ is the resolution parameter of the network. Now rearranging equation (1), the Hamiltonian can be written as

$$H(L_c, N_c, \gamma) = -\sum_{c} [L_c - \gamma N_c]$$
(2)

where L_c is the total number of internal edges in community c, and $N_c = n_c \times n_c$, with n_c is the total number of nodes in the community c. Complex natural networks are generally self-organized [17, 18], and have various levels of organization, with self-similar democratic constitution at each level of organization [19], down to the fundamental level where basic organizational units are motifs [20]. C. elegans' neuronal network, consisting of N=277 nodes, is one such type which have hierarchical organization of communities/sub-communities at various levels of organization (Fig. 1), and similar nature of topological organization was obtained in cat (N = 52) and macaque monkey (N = 71)brain networks also [8]. If such a network is defined by G(L, N), then network at level-2 is organized by a set of m communities defined by a set of sub-graphs $\{G_i^{[2]}\}$, i=1,2,...,m constructed from level-1, i.e., the whole network. Since the networks at level-1 and level-2 represent the same set of nodes but with different network organization, we have $G^{[1]} = G_1^{[2]} \cup G_2^{[2]} \cup \dots G_m^{[2]} \cup I^{[2]}$, where $I^{[2]}$ is the set of isolated nodes and their degrees. Hamiltonian at level-1 is given by, $H^{[1]} = -\left(L^{[1]} - \gamma N^{[1]}\right)$ with $L^{[1]} = \sum_{ij} A_{ij}^{[1]}$ and $N^{[1]} = n \times n$. Now, the Hamiltonian of the network at level-2 is given by $H^{[2]} = -\sum_{c_1=1}^{m_{c_0}^{[2]}} H_{c_1}^{[2]}$, where c_1 th Hamiltonian at level-2 is $H_{c_1}^{[2]} = L_{c_1}^{[2]} - \gamma N_{c_1}^{[2]}$ with $L_{c_1}^{[2]} = \sum_{ij} \left(A_{c_1}^{[2]} \right)_{ij}$, and $N_{c_1}^{[2]} = n_{c_1} \times n_{c_1}$. Similarly, organization of sub-communities in level-3 is constructed from the respective communities in level-2. Therefore, Hamiltonian of the network at level-3 can be derived as $H^{[3]} = -\sum_{c_1=1}^{m_{c_0}^{[2]}} \sum_{c_2=1}^{m_{c_1}^{[3]}} H_{c_1c_2}^{[3]}$, where Hamiltonian of c_2 th sub-community at level-3 derived from the c_1 th community at level-2 is $H_{c_1c_2}^{[3]} = L_{c_1c_2}^{[3]} - \gamma N_{c_1c_2}^{[3]}$ with $L_{c_1c_2}^{[3]} = \sum_{ij} \left(A_{c_1c_2}^{[3]}\right)_{ij}$, and $N_{c_1c_2}^{[3]} = n_{c_1c_2} \times n_{c_1c_2}$. Hence, the Hamiltonian of the complete network $H^{[1]}$ can be derived from the Hamiltonians at the lower levels (i.e., level-2, level-3,...,level-U) and is given by

$$H^{[U]} = -\sum_{c_1=1}^{m_{c_0}^{[2]}} \sum_{c_2=1}^{m_{c_1}^{[3]}} \sum_{c_3=1}^{m_{c_2}^{[4]}} \cdots \sum_{c_{U-1}=1}^{m_{c_{U-2}}^{[U]}} H_{c_1 c_2 \dots c_{U-1}}^{[U]}; \quad H_{c_1 c_2 \dots c_{U-1}}^{[U]} = L_{c_1 c_2 \dots c_{U-1}}^{[U]} - \gamma N_{c_1 c_2 \dots c_{U-1}}^{[U]}$$

$$(3)$$

Here, $m_{c_0}^{[2]}$, $m_{c_1}^{[3]}$, ..., $m_{c_{U-2}}^{[U]}$ are numbers of communities at levels level-2, level-3,...,level-U, respectively. The sizes of the communities reduce as one goes from level-1 to level-U, and this size reduction of communities with levels persists until the communities are reduced to motifs, which are building blocks of the network. Some communities have short histories of existence, and some have long histories. Nodes in communities having long histories generally have the tendency to regulate the network.

Theorem 1. In hierarchical networks having systems level organizations, the fluctuations in the number of nodes in going from one level of organization to the other $(\Delta N^{[k+1]}) = N^{[k]} - N^{[k+1]}$ satisfy the conditions:

- (a) $|\Delta N^{[k+1\to k]}| \ge 0$, (b) $|\Delta N^{[k+1\to 1]}| \ge 0$, (c) $|\Delta N^{[k+1\to 1]}| \ge 0$, (d) $|\Delta N^{[k+1\to 1]}| \ge |\Delta N^{[k+1\to k]}|$.

Proof. Equation (1) allows us to connect the size of the network at level-1 to the size of the network at level-2, which

is the sum of sizes of individual modules and isolated nodes at level-2, given by

$$N^{[1]} = \sum_{c_1=1}^{m_{c_0}^{[2]}} N_{c_1}^{[2]} + S^{[2]} = N^{[2]} + S^{[2]}$$

$$\tag{4}$$

where $m_{c_0}^{[2]}$ is the number of modules at level-2. $N_{c_1}^{[2]}$ is the size of the c_1 th module at level-2. $S^{[2]}$ is the total number of isolated nodes at level-2 of the network. The fluctuations in the number of nodes in retreating from level-2 to level-1 is given by $|\Delta N^{[2\to 1]}| = N^{[1]} - N^{[2]} \ge 0$ for $S^{[2]} \ge 0$. The condition $|\Delta N^{[k+1\to k]}| = 0$ satisfies only when $S^{[2]} = 0$, i.e., all the nodes at level-1 are distributed to modules at level-2.

Proceeding in the same way, the number of nodes at level-k can be derived from the level-(k+1) expression using Equations (1) and (3):

$$N^{[1]} = \sum_{c_{1}=1}^{m_{c_{0}}^{[2]}} \sum_{m_{c_{1}}^{[3]}} \cdots \sum_{c_{k-1}=1}^{m_{c_{k-2}}^{[k]}} N_{c_{1}c_{2}...c_{k-1}}^{[k]}$$

$$N^{[k]}_{c_{1}c_{2}...c_{k-1}} = \sum_{c_{k}=1}^{m_{c_{k-1}}^{[k+1]}} N_{c_{1}c_{2}...c_{k}}^{[k+1]} + S^{[k+1]}; \quad S^{[k+1]} = \sum_{c_{1}=1}^{m_{c_{0}}^{[2]}} \sum_{c_{2}=1}^{m_{c_{1}}^{[3]}} \cdots \sum_{c_{k-1}=1}^{m_{c_{k-2}}^{[k]}} S^{[k+1]}_{c_{1}c_{2}...c_{k-1}}$$

$$(5)$$

where $m_{c_{k-1}}^{[k+1]}$ is the number of sub-modules at $level{-}(k+1)$ constructed from c_k th module at $level{-}k$. $N_{c_1c_2...c_k}^{[k+1]}$ is the size of the c_k th sub-module at $level{-}(k+1)$ derived from c_{k-1} th module at $level{-}k$. If $\Delta N^{k+1 \to 1}$ is considered, then the sum over all nodes in modules/sub-modules and isolated nodes starting from level-(k+1) to level-1 should be added. However, if $\Delta N^{k+1\to k}$ is to be calculated then sum over all nodes in sub-modules and isolated nodes at level-(k+1)have to be done. This can be done by removing the sum indices c_1 to c_{k-1} in Equation (5). The results are:

$$\Delta N^{[k+1\to 1]} = \sum_{c_1=1}^{m_{c_0}^{[2]}} \sum_{c_2=1}^{m_{c_1}^{[3]}} \cdots \sum_{c_{k-1}=1}^{m_{c_{k-2}}^{[k]}} S_{c_1 c_2 \dots c_{k-1}}^{[k+1]}$$

$$(6)$$

$$\Delta N^{[k+1\to k]} = S^{[k+1]} \tag{7}$$

Then, it is trivial to prove that $|\Delta N^{[k+1\to k]}| = N^{[k]} - N^{[k+1]} = S^{[k+1]} \ge 0$ from Equation (7). Similarly, it can also be shown that $|\Delta N^{[k+1\to 1]}| \ge 0$ from Equation (6). It is also trivial from Equations (6) and (7) that $|\Delta N^{[k+1\to 1]}| \ge |\Delta N^{[k+1\to 1]}|$. They are equal only when all the nodes in each level are totally distributed among the modules/sub-modules in the other level such that there are no isolated nodes.

Theorem 2. The variations in the number of edges as we move from one level of organization to the other $(\Delta L^{[k+1\to k]} = L^{[k]} - L^{[k+1]})$ because of wiring or rewiring among the modules satisfy the following conditions:

- (a) $|\Delta L^{[k+1\to k]}| > 0$, (b) $|\Delta L^{[k+1\to 1]}| > 0$, (c) $|\Delta L^{[k+1\to 1]}| > |\Delta L^{[k+1\to k]}|$.

Proof. The total number of edges at *level-1* and *level-2* can be related by using Equation (1), as given below:

$$L^{[1]} = \sum_{c_1=1}^{m_{c_0}^{[2]}} \left[L_{c_1}^{[2]} + \sum_{\substack{c_1'=1, \\ c_1 \neq c_1'}}^{m_{c_0}^{[2]}} \delta(\sigma_{c_1}^{[2]}, \sigma_{c_1'}^{[2]}) \right] + \sum_{i_1=1}^{s_{i_0}^{[2]}} D_{i_1}^{[2]}$$

$$(8)$$

where $L_{c_1}^{[2]}$ is the number of edges in the c_1 th module at level-2, constructed from the network at level-1. $\delta(\sigma_{c_1}^{[2]}, \sigma_{c_1'}^{[2]})$ is delta function which is equal to one if modules $\sigma_c^{[2]}$ and $\sigma_{c'}^{[2]}$ are connected, otherwise zero. $\epsilon_{c_1c'_1}^{[2]}$ is the number of inter-edges between the connected c_1 th and c'_1 modules. $D_{i_1}^{[2]}$ is the degree of ith isolated node at level-2, and $s_{i_0}^{[2]}$ is the number of isolated nodes in the network at level-2. Since the first term is $L^{[2]}$, we have

$$\Delta L^{[2\to1]} = \sum_{\substack{c_1, c_1'=1, \\ c_1 \neq c_1'}}^{m_{c_0}^{[2]}} \epsilon_{c_1 c_1'}^{[2]} \delta(\sigma_{c_1}^{[2]}, \sigma_{c_1'}^{[2]}) + \sum_{i_1=1}^{s_{i_0}^{[2]}} D_{i_1}^{[2]}$$

$$(9)$$

The second term could be zero if the nodes at level-1 network are exactly distributed among the modules at level-2. The number of inter-edges among the connected sub-modules at level-2 cannot be zero. Hence, $|\Delta L^{[2\to 1]}| > 0$.

Similarly, following the same process, we can generalize and arrive at the expressions for $L^{[1]}$ constructed from the network organization at any level-(k+1), and $L^{[k]}$ constructed from neighboring level of organization level-(k+1). The respective expressions are

$$L^{[1]} = \sum_{\substack{c_1, c'_1 = 1, c_2, c'_2 = 1, \\ c_1 \neq c'_1 \ c_2 \neq c'_2}}^{m_{c_1}^{[3]}} \cdots \sum_{\substack{c_{k-1}, c'_{k-1} = 1, \\ c_{k-1} \neq c'_{k-1}}}^{m_{c_{k-2}}^{[k]}} L^{[k]}_{c_1 c_2 \dots c_{k-1}}$$

$$L^{[k]}_{c_1 c_2 \dots c_{k-1}} = \sum_{\substack{c_{k-1} = 1, \\ c'_1 c'_2 \dots c'_{k-1}}}^{m_{c_{k-1}}^{[k+1]}} \left[L^{[k+1]}_{c_1 c_2 \dots c_k} + \sum_{\substack{c'_k = 1 \\ c'_1 c'_2 \dots c'_k}}^{m_{c_{k-1}}^{[k+1]}} \epsilon^{[k+1]}_{c_1 c'_2 \dots c'_k} \delta(\sigma_{c_1 c_2 \dots c_k}, \sigma_{c'_1 c'_2 \dots c'_k}) \right] + \sum_{i_k = 1}^{s_{i_{k-1}}^{[k+1]}} D^{[k+1]}_{i_1 i_2 \dots i_k}$$

$$D^{[k+1]}_{i_1 i_2 \dots i_k} = \sum_{i_1 = 1}^{s_{i_1}^{[2]}} \sum_{i_2 = 1}^{s_{i_1}^{[3]}} \cdots \sum_{i_{k-1} = 1}^{s_{i_{k-2}}^{[k]}} D^{[k]}_{i_1 i_2 \dots i_{k-1}}$$

$$(10)$$

where $L_{c_1c_2...c_{k-1}}^{[k]}$ is the number of edges of c_{k-1} th sub-sub-module at level-k constructed from c_{k-2} th sub-module $c_1c_2...c_{k-1}$

at level-(k-1), starting from c_1 th module at level-2. From Equation (10) we know that the total number of edges at level-(k+1) can be constructed from the edges at level-k. Then removing the running indices up to c_{k-1} in Equation (10), we get the fluctuations in edges when there is a change from level-(k+1) to level-k or vice versa. Then, the variations in edges due to changes from one level of organization to the other are given by

$$\Delta L^{[k+1\to k]} = \sum_{\substack{c_k c'_k = 1 \\ c_k \neq c'_k}}^{m^{[k+1]}_{c_{k-1}}} \epsilon^{[k+1]}_{c_k c'_k} \delta(\sigma_{c_k}, \sigma_{c'_k}) + \sum_{i_k = 1}^{s^{[k+1]}_{i_k = 1}} D^{[k+1]}_{i_k}$$

$$(11)$$

$$\Delta L^{[k+1\to1]} = \sum_{\substack{c_1,c_1'=1, c_2,c_2'=1, \\ c_1\neq c_1'}}^{m_{c_0}^{[2]}} \sum_{\substack{c_k,c_k'=1, \\ c_1\neq c_1'}}^{m_{c_1}^{[3]}} \cdots \sum_{\substack{c_k,c_k'=1, \\ c_k\neq c_k'}}^{m_{c_{k-1}}^{[k+1]}} \delta(\sigma_{c_1c_2...c_k}, \sigma_{c_1'c_2'...c_k'}) + \sum_{i_1=1}^{s_{i_0}^{[2]}} \sum_{i_2=1}}^{s_{i_1}^{[3]}} \cdots \sum_{i_k=1}^{s_{i_{k+1}}^{[k+1]}} D_{i_1i_2...i_k}^{[k+1]}$$

$$(12)$$

The second terms in Equations (11) and (12) are larger than zero if isolated nodes are involved when one crosses from one level of organization to another, otherwise the term equals to zero. However, the first terms in these equations are always greater than zero. This means the organization of a larger network at a particular level from a smaller network at another level needs significant number of edges for rewiring them to achieve the self-organization at that level. Hence, $\Delta E^{[k+1\to k]} > 0$ and $\Delta E^{[k+1\to 1]} > 0$. Further, it is trivial that $\Delta E^{[k+1\to 1]} > \Delta E^{[k+1\to k]}$.

Theorem 3. The shift in the Hamiltonian of a complex network due to change of levels of organization satisfies $|\Delta H| > 0$.

Proof. Equations (3), (6), (7), (11), and (12) allow us to write the expression for shift in Hamiltonian due to change in the levels of organization as

$$|\Delta H^{[2\to 1]}| = |\Delta L^{[2\to 1]} - \gamma \Delta N^{[2\to 1]}| \tag{13}$$

$$|\Delta H^{[k+1\to k]}| = |\Delta L^{[k+1\to k]} - \gamma \Delta N^{[k+1\to k]}| \tag{14}$$

$$|\Delta H^{[k+1\to 1]}| = |\Delta L^{[k+1\to 1]} - \gamma \Delta N^{[k+1\to 1]}| \tag{15}$$

Since $|\Delta L^{[2 \to 1]}| > 0$, $|L^{[k+1 \to k]}| > 0$, $|L^{[k+1 \to 1]}| > 0$ $|N^{[2 \to 1]}| \ge 0$, $|\Delta N^{[k+1 \to k]}| \ge 0$, and $|\Delta N^{[k+1 \to 1]}| \ge 0$, we can straightforwardly prove that $|\Delta H^{[2 \to 1]}| > 0$. Further, it can also be proven that $|\Delta H^{[k+1 \to k]}| > 0$ and $|\Delta H^{[k+1 \to 1]}| > 0$. Also, there is a competition between the two terms $\Delta L^{[k+1 \to k]}$ and $\Delta N^{[k+1 \to k]}$ magnified by resolution parameter γ . From Equations (6) and (12), we can further prove that $|\Delta H^{[k+1 \to 1]}| > |\Delta H^{[k+1 \to k]}|$.

Nature of Hamiltonian shift

Hamiltonian of a complex network is quantified by the contributions from the edges resulted from interactions among

Conclusion

One important quest in understanding variabilities in brain functionalities is how connectivities in complex brain networks get changed in random/non-random way with dynamic behavior [2]. Brain diseases which generally involve short and long range network dysfunctions could be due to the drastic change in the distributions of wiring/rewiring of these connectivities [4, 21]. These distributions of connectivities, in brain networks constructed from functional magnetic resonance imaging, diffusion tensor imaging, electroencephalogram, electrooculogram, etc., may be fundamentally related to energy distributions in brain. We have studied the energy distribution in the brain networks of three species [8] using simple but efficient CPM approach [12–14]. The edge distributions at various levels of organization are found to be different which are reflected in the energy distributions calculated via CPM, and also the Hamiltonian calculated as a function of levels of organization is found to follow power-law or fractal behavior which is a signature of self-organization red in the system. Moreover, the fractal nature of the Hamiltonian function is controlled by a key resolution parameter which balance the dominance of edges over nodes or vice versa. We also observe three different phases driven by this resolution parameter which may correspond to different brain states describing various situations/irregularities in the brain system. However, the existence of these brain states need to be verified experimentally.

Brain states with various phases exhibited are highly dynamic in nature which may depend on various factors. Since energy distributions among the the nodes in various communities and sub-communities could be one of the fundamental working principle in brain networks, studies in this perspective could give important insights of how brain system is organized.

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Author Contributions

SKS, SSS, MZM, and RKB conceptualized the work. SKS, SSS, DH, and MZM did the simulation and preparation of the figures. SKS, SSS, DH, MZM, and RKB wrote the manuscript. All the authors read and approved the manuscript.

Ethics approval and consent to participate Not applicable

Competing Interests

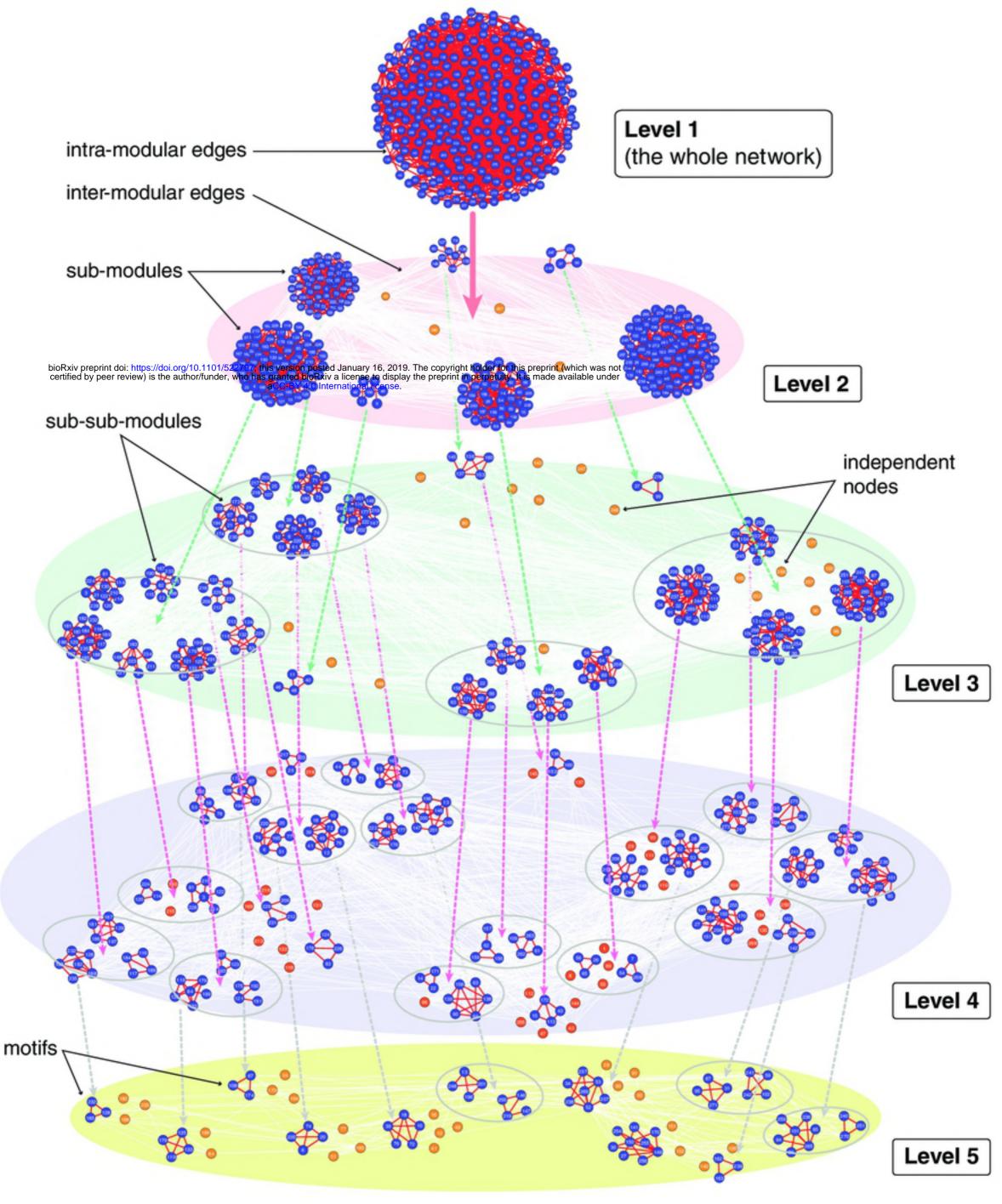
The authors declare that they have no competing interests.

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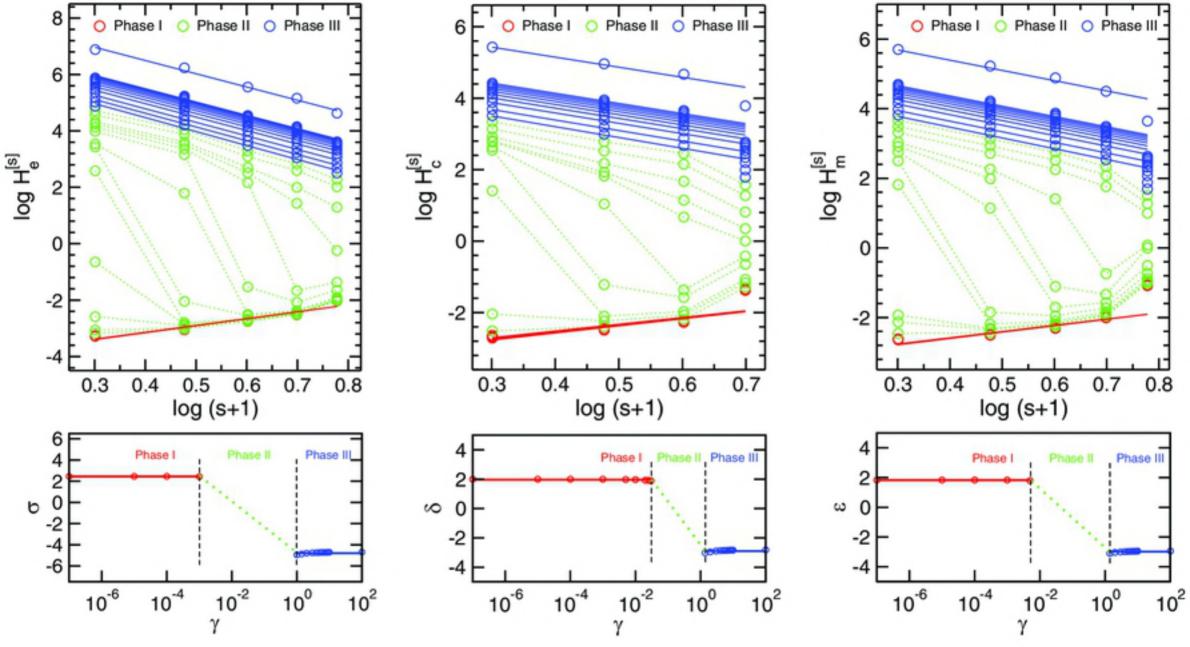
Figure caption:

Figure 1: Hierarchically organized *C. elegans'* neuronal network. Each layer (or level) constitutes a similar set of nodes and edges, but with different distributions describing various organizational hierarchies.

Figure 2 Hamiltonian spectrum of C. elegans (left), cat (middle), and macaque monkey (right) brain networks. Upper plots show the Hamiltonian function H as a function of levels of network organization s in log-log scale. Lower plots represent phase plots as a function of resolution parameter γ .



Figure



Figure