Optimal location of sources in transportation networks

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Abstract. We consider the problem of optimizing the locations of source nodes in transportation networks. A reduction of the fraction of surplus nodes induces a glassy transition. In contrast to most constraint satisfaction problems involving discrete variables, our problem involves continuous variables which lead to cavity fields in the form of functions. The one-step replica symmetry breaking (1RSB) solution involves solving a stable distribution of functionals, which is in general infeasible. In this paper, we obtain small closed sets of functional cavity fields and demonstrate how functional recursions are converted to simple recursions of probabilities which make the 1RSB solution feasible. The physical results in the replica symmetric (RS) and the 1RSB frameworks are thus derived and the stabilities of the RS and 1RSB solutions are examined.

Keywords: cavity and replica method, disordered systems (theory), communication, supply and information networks

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1. Introduction

Constraint satisfaction problems (CSPs), which are highly relevant to many applications such as electronic circuit design and frequency assignment in cellular mobile networks, have been studied in the fields of applied mathematics, computer science and engineering. Despite their usefulness, many CSPs are NP-complete problems [1] associated with algorithmic hardness. It is thus important to understand the physical origin of their hardness and map out the easy and hard regimes for typical instances. Physicists approach the problem by making an analogy between CSPs and spin glasses [2, 3]. Objective functions are mapped to spin glass Hamiltonians, enabling the analysis of CSPs using
statistical physical techniques. Successful examples are found in the $K$-satisfiability problem [4], graph coloring [5], and vertex cover [6]–[8]. They suggest a rich physical picture of CSPs corresponding to the glassy phase in spin glasses.

In this paper we study a problem having a wide range of applications and sharing the characteristics of CSPs. Specifically, we consider the optimal locations of source nodes in transportation networks. Transportation networks consist of nodes with either a surplus or a deficiency of resources, and an important problem is to distribute them so as to achieve a networkwide satisfaction with a minimum transportation cost [9]–[11]. This problem is important in load balancing in computer networks [12] and network flow of commodities [13]. Progress has been made in generalizing the message-passing technique of discrete variables to the passing of cavity energy functions in terms of the continuous current variables [9]–[11].

Subsequent work considered networks in which shortages are allowed but a cost penalty is imposed [14]. This models applications such as communications networks where shortages are detrimental to the performance of the nodes. Their effects were modeled by step-like shortage costs. This high nonlinearity gives rise to unique behavior and a physical picture absent in the previous models. When the shortage cost is comparable to the transportation cost, the total cost may be optimized either by saving the transportation cost feeding a poor node while sacrificing the satisfaction of the node, or by saving the shortage cost while spending more on the transportation cost. The picture is reminiscent of the learning of noisy examples in perceptrons, where the field distribution of the examples consists of the bands corresponding to the learned and sacrificed examples [15]–[18]. As a result, frustration arises from competition for resources among connected nodes. Numerous metastable states emerge, leading to typical glassy behavior.

The problem of optimal source location in this paper addresses an even more general and practically relevant issue in network design and optimization. Compared with [14] where some nodes remain unsatisfied in the optimized state, this paper moves one step forward and considers the situation in which the location of the source nodes can also be optimized, and all nodes are satisfied. The source location problem has wide applications in the design of optimized transportation networks. For example, the optimal locations of access points in wireless networks can be determined by balancing the signaling cost of the access points and the power and bandwidth limitations of the channels linking the mobile subscribers (which can be expressed as the transportation cost).

As demonstrated in [9]–[11], the resource allocation problem involves passing messages of continuous variables. When the cost function includes nonlinear terms, the messages generally become extremely complicated. However, as will be described in this paper, there are phases where the space of continuous messages can be replaced by small closed sets of cavity energy functions, and their recursions can be converted to simple recursions of probabilities. In the context of the source location problem, this takes place when the consumer nodes form small clusters surrounded by source nodes. When the ratio of the installation cost of the source nodes and the transportation cost changes, regimes with different maximum cluster sizes are observed, resembling the Devil’s staircase observed in the circle map and other dynamical systems [26]. We will show that the use of small closed sets of cavity energy functions is particularly successful in the singlet regime where the consumer nodes are isolated (clusters of size 1) and, when the cost ratio is commensurate, in the doublet regime where the consumer nodes can be paired or isolated.

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Figure 1. (a), (b) The RFIM of two spins and four fixed boundary spins. Symbols: filled (unfilled) circles—up (down) spins, arrows—direction of random fields of magnitude $h$, thick segments—frustrated couplings of magnitude $J$. When $h/J$ increases from below 2 to above, pattern (a) changes to (b) to form a cluster demarcated by a domain wall of frustrated couplings. (c), (d) The optimal source location problem defined by equation (2) with two nodes and four fixed boundary nodes, and $\Lambda_i = -1$ for all $i$. Symbols: filled (unfilled) circles—consumer (source) nodes, arrows—current flows. When $u^{-1}$ decreases from above $\sqrt{2}$ to below, pattern (c) changes to (d) to form a cluster demarcated by a ‘domain wall’ of inward current flow.

In fact, clusters formed via similar energetic considerations have been found to play an important role in disordered systems such as the random field Ising model (RFIM) [19], as illustrated in figure 1. Indeed, domain sizes in the RFIM are determined by the interplay between the random field energy and the domain wall energy, giving rise to the so-called Griffiths singularities and cascades of phase transitions [20, 21]. Analogously, cluster sizes in the source location problem are determined by the balance between the installation cost of the source nodes and the transportation costs.

Another class of problems that exhibits similar cluster behaviors is the lattice glass models [22]–[24]. In the lattice glass models, each site of a network can be occupied or empty, but the number of nearest neighbors cannot exceed a maximum. Analogously, the energetics of cluster formation in the source location problem implies that two neighboring consumer nodes have effective repulsions, since their contiguity prevents them from drawing resources from more neighboring source nodes. However, the present model is richer in behavior, since the cluster energy depends on the current distribution in non-trivial ways, rather than merely counting the number of neighbors. When the particle density in a lattice glass increases, configurations of clusters are formed, causing the system to undergo dynamical freezing transitions preceding the ideal glass transition. Similar transitions will be reported in the source location problem.

The vertex cover problem [6, 8], one of the NP-complete problems in computational complexity theory [1] that attracted recent attention from physicists, also shares similar cluster behaviors. Drawing the analogy of assigning guards in a museum [6], each site of a network can be covered or uncovered, but none of the links can have both vertices
uncovered. Hence the uncovered nodes form a configuration with an effective repulsion among them. Indeed, an equivalent configuration of consumer nodes can be found in the singlet regime of the source location problem, since for neighboring consumer nodes, each has one less link through which to draw resources from the neighboring source nodes. When the average connectivity of the network increases, we will show that it undergoes a glassy transition analogous to that in the vertex cover problem.

The origin of these interesting phenomena can be traced to the presence of frustrations, which refer to the conflicts between competing interaction energies in the system [25]. This connects our problem with a broad class of network CSPs in which frustrations are inherent. When the system consists of numerous states, the replica symmetry breaking (RSB) solution is applicable, but the distribution of the cavity energy functions is in general infeasible to solve. Nevertheless, with the small closed set of cavity energy functions introduced in this paper, the one-step RSB (1RSB) solution becomes computationally feasible. The physical results based on the replica symmetric (RS) ansatz and the 1RSB configurational entropy are thus derived.

The paper is organized as follows. We introduce our problem in section 2, presenting simulation results of the optimal behaviors. In section 3, we discuss the general RS formalism and derive the piecewise quadratic ansatz of the cavity energy functions. In section 4, we obtain a small closed set of cavity energy functions in the singlet regime and demonstrate how functional recursions are converted to recursions of probabilities. The average energy, the fraction of soft nodes and the RS–RSB phase diagram are derived. In section 6, we apply the small closed set of cavity fields to the 1RSB formalism and obtain results for the configurational entropy. The conclusion is given in section 7. In the appendix, we describe how the small closed set of cavity energy functions can be applied to the doublet regime in the commensurate case, and the corresponding RS and 1RSB results are derived.

2. The model

2.1. Model formulation

We consider a network of \( N \) nodes, labeled \( i = 1, \ldots, N \). Each node \( i \) is connected randomly to a set \( \mathcal{L}_i \) of \( K \) neighbors. Each node \( i \) has capacity \( \Lambda_i \); nodes with positive and negative values of \( \Lambda_i \) correspond to surplus and deficient nodes respectively. The capacities \( \Lambda_i \) are randomly drawn from a distribution of \( \rho(\Lambda_i) \). With network applications in mind, we consider a bimodal distribution in which \( \Lambda_i = A \) (\( \gg 1 \)) with probability \( \phi_s \geq 0 \) and \( \Lambda_i = -1 \) with probability \( \phi_d \equiv 1 - \phi_s \). Naturally, the surplus nodes serve as source nodes providing resources to the consumer nodes. However, to minimize cost functions that include transportation costs, it is often desirable to convert some deficient nodes into source nodes as well. Hence in general, the task is to optimally locate these extra source nodes so as to minimize the total cost function. The relevant glossary used in this paper is summarized in table 1.

We first consider the minimization of the cost function in [14], whose optimization variables are the currents \( y_{ij} \equiv -y_{ji} \) of real values from node \( j \) to node \( i \),

\[
E = \frac{w^2}{2} \sum_i \Theta(-\xi_i) + \sum_{(ij)} \frac{y_{ij}^2}{2}. \tag{1}
\]
Table 1. A summary of glossary used in this paper.

| Λ_i | Before optimization | ξ_i | After optimization |
|-----|---------------------|-----|--------------------|
| ≥0  | Surplus node        | ≥0  | Source node        |
| <0  | Deficient node      | <0^a| Consumer node      |

^a The deficient nodes with ξ_i < 0 after optimization are converted to source nodes.

ξ_i ≡ Λ_i + \sum_{j\in\mathcal{L}_i} y_{ij} is the final resource of node i, and Θ(x) = 1 when x > 0, and 0 otherwise. The link connecting nodes i and j is denoted as (ij). The first term corresponds to the unsatisfaction cost imposed on nodes with negative final resource. The second term is the transportation cost. This cost function models load balancing situations in which insufficient provision of resources to a deficient node produces detrimental effects on it (irrespective of the magnitude of the insufficiency).

The key to applying the cost function in equation (1) to optimize the location of source nodes is to note that once the final resource of a deficient node is negative, the unsatisfaction cost remains the same even when its resources are maximally drawn by other nodes of the network. Hence the deficient node effectively becomes a resource provider. Reference [14] contains many such examples. If we consider the coefficient \(\frac{u^2}{2}\) to be the installation cost of a source node, then we can solve the optimal source location problem by first minimizing the cost function in equation (1), then identifying the deficient nodes whose final resources are negative, and converting them to source nodes.

Formally, in the optimal source location problem, we introduce the state variables \(s_i = \pm 1\) for deficient nodes when node i is a consumer or a source node respectively. The cost function is then

\[
E = \frac{u^2}{4} \sum_{i \in \mathcal{N}_D} (1 - s_i) + \sum_{(ij)} \frac{y_{ij}^2}{2},
\]

subject to \(\xi_i \geq 0\) for \(s_i = 1\). No constraints are imposed on nodes with \(s_i = -1\), since an arbitrary amount of resource can be provided when they are converted to source nodes. \(\mathcal{N}_D\) is the set of deficient nodes.

To check the equivalence between the cost functions in equations (1) and (2), we can easily see that when \(s_i = 1\), the installation (or unsatisfaction) cost vanishes in both cost functions. When \(s_i = -1\), we only have to consider the case \(\xi_i < 0\), and the installation (or unsatisfaction) cost is \(\frac{u^2}{2}\) in both cost functions. This is because when \(\xi_i \geq 0\), we can set \(s_i = 1\) to minimize the total cost.

Note that the cost function of the optimal source location problem is identical to that in [14], but the interpretation is far more relevant to network applications. All previous results on networks with nodes of negative capacity can be directly mapped to networks whose unsatisfied nodes are replaced by source nodes. For example, the single-sat regime studied in [14] corresponds to the case where each consumer node is surrounded by source nodes, since the installation cost is low compared with the transportation cost. When
the installation cost is gradually raised, resource provision is achieved with fewer source nodes, but optimization requires the consumer nodes to be located in clusters surrounded by source nodes, forming the clusters observed in [14].

To formulate an algorithm, we introduce the constraints $s_i \xi_i \geq 0$ for each deficient node. These constraints are not applied to surplus nodes as they are always satisfied. Introducing Lagrange multipliers $\mu_i$ for the resource constraint, we minimize the Lagrangian

$$L = \frac{u^2}{4} \sum_{i \in \Lambda_D} (1 - s_i) + \sum_{i \in \Lambda_D} \mu_i s_i \xi_i + \sum_{(ij)} \frac{y_{ij}^2}{2}$$

(3)

with the Kühn–Tucker conditions $\mu_i s_i \xi_i = 0$ and $\mu_i \leq 0$. Optimizing $L$ with respect to $y_{ij}$, one obtains $y_{ij} = \mu_j s_j - \mu_i s_i$ and $\mu_i = \min[0, (\Lambda_i + \sum_{j \in \mathcal{L}_i} \mu_j s_j )/s_i]$. Given a particular set of $\{s_i\}$, we iterate these equations to find the corresponding set of $\{\mu_i\}$. The set of optimal $\{s_i\}$ is found by an approach similar to the GSAT algorithm [31], by comparing the Lagrangian in equation (3) for each choice of $\{s_i\}$. In each step of this algorithm, a cluster of $N_{\text{flip}}$ nodes is randomly selected. The network energies involving the different configurations of this cluster are compared, and the cluster configuration is updated to the one that yields the lowest network energy [14].

2.2. Major simulation results

As shown in figure 2 for $K = 3$, two phases can be identified: (1) the all-source phase for $u^{-1} \geq \sqrt{3}$, in which all nodes are assigned as source nodes due to the very high

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Figure 2. Simulation results of average energy per node and the fraction of network nodes acting as source nodes. Parameters: $K = 3$, $\phi_d = 0.9$, $N = 100$, $N_{\text{flip}} = 4$, 100 samples and 1000 flips. New clusters formed on increasing $u^{-1}$ are sketched at the top, with filled and unfilled circles representing consumer and source nodes respectively.
Figure 3. Clusters of (a) source nodes, (b) singly consuming nodes, (c) doubly consuming nodes, and (d) triply consuming nodes.

transportation cost; (2) the partial-source phase for $0 < u^{-1} < \sqrt{3}$, in which only some nodes are assigned as source nodes. (In [14] we also identified a phase transition at $u^{-1} = 0$ to an all-consumer phase.)

The fraction of source nodes is a discontinuous function of $u^{-1}$, showing abrupt jumps at threshold values of $u^{-1}$. The step size of the curve decreases as $u^{-1}$ increases, and gradually becomes unresolvable in the numerical experiments. This resembles the Devil’s staircase observed in the circle map and other dynamical systems [26]. These threshold values of $u^{-1}$ mark the positions at which certain configurations of the source and consumer nodes become energetically stable. Similar features are observed in the RFIM due to the formation of ferromagnetic clusters resultant from the competition between the strengths of couplings and random fields [20, 21]. Except for a shift of the average energy per node, these features are qualitatively similar to the simulation results of [14] which correspond to the case $\phi_d = 1$, if the latter is reinterpreted from the perspective of the source location problem.

Measuring the average maximum cluster size of the consumer nodes in the samples, we observe abrupt jumps of the cluster size at the same threshold values. This indicates that new kinds of clusters are formed at each jump, as sketched at the top of figure 2. The observed threshold values can be calculated by considering the energies of consumer clusters surrounded by source nodes as shown in figure 3, obtained by the minimization of equation (1). By comparing the energy of different configurations, we have

$$E_0 \geq E_1 \quad \text{singlet},$$
$$E_0 + E_1 \geq E_2 \quad \text{doublet},$$
$$E_0 + 2E_1 \geq E_3 \quad \text{triplet},$$

resulting in the threshold values in figure 2. These results agree with those obtained through the cavity approach in section 3. We call the regime $\sqrt{3/2} < u^{-1} < \sqrt{3}$ with isolated consumer nodes the singlet regime, and $\sqrt{21/25} < u^{-1} < \sqrt{3/2}$ the doublet regime. The isolated nodes are referred to as singly consuming, while the paired consumer nodes are doubly consuming.
3. The replica symmetric ansatz

3.1. The RS recursion at the zero-temperature limit

We apply the cavity method [2, 3] assuming that the network has a locally tree-like structure. We denote as \( E_j(y_j) \) the energy of the tree terminated at node \( j \) in the absence of its ancestor node \( i \), when a current \( y_j \) is drawn from \( j \) to its ancestor. Relabeling the descendents of \( j \) as \( k = 1, \ldots, K - 1 \), \( E_j(y_j) \) is expressed as

\[
E_j(y_j) = \mathcal{H}(E_{k=1}, \ldots, E_{K-1}; \Lambda_j, y_j).
\]

(5)

The functional \( \mathcal{H} \) is given by

\[
\mathcal{H}(E_1, \ldots, E_{K-1}; \Lambda_j, y_j) \equiv \min_{\{y_k\}} \left[ \sum_{k \in L_j \setminus \{i\}} E_k(y_k) + \frac{u^2}{2} \Theta \left( -\Lambda_j - \sum_{k \in L_j \setminus \{i\}} y_k + y_j \right) + \frac{y_j^2}{2} \right].
\]

(6)

In the absence of node \( i \), there is no supply or demand of resources through the cavity and the last term \( y_j^2/2 \) should be absent. However, the presence of the extra term results in a clear interpretation of \( E_j \), as we will see in the following sections. Care has to be taken when dealing with the change of the cavity energy, where \( y_j \) is taken to be zero to eliminate the effect of the extra transportation cost on the dangling bond.

We note that \( E_j \) is an extensive quantity that depends on size of the tree. To formulate a recursion of an intensive energy, we write \( E_j(y_j) \) as a sum of two terms,

\[
E_j(y_j) = E^V_j(y_j) + E_j(0).
\]

(7)

We call \( E^V_j(y_j) \) the cavity energy functions which correspond to the cavity fields in the language of the cavity approach, and represent the energy variation from \( E_j(0) \), as \( y_j \) varies. In this case, \( E^V_j(0) = 0 \). \( E_j(0) \) corresponds to the energy of the tree when no current is drawn from the vertex. We further define the energy change \( \Delta E_j \) due to the addition of a vertex,

\[
\Delta E_j = E_j(0) - \sum_{k \in L_j \setminus \{i\}} E_k(0),
\]

(8)

which simplifies equation (5) to

\[
E^V_j(y_j) = \mathcal{H}(E^V_{k=1}, \ldots, E^V_{K-1}; \Lambda_j, y_j) - \Delta E_j
\]

(9)

where

\[
\Delta E_j = \mathcal{H}(E^V_1, \ldots, E^V_{K-1}; \Lambda_j, 0).
\]

(10)

We have thus separated the energy contribution due to the addition of a new vertex from the energy variation due to the changes in the current drawn from the tree.

The distribution \( \mathcal{P}[E^V] \) of \( E^V \) over the vertices of the tree is given by the solution of

\[
\mathcal{P}[E^V_j] = \int d\Lambda_j \prod_{k=1}^{K-1} \int dE^V_k \mathcal{P}[E^V_k] \delta[E^V_j - \mathcal{H}(E^V_1, \ldots, E^V_{K-1}; \Lambda_j, y_j) + \Delta E(E^V_1, \ldots, E^V_{K-1}; \Lambda_j)].
\]

(11)
To elucidate the physical behavior of the system, we consider a node fed by \( K \) trees forming a Bethe lattice. For instance, we consider the average energy per node. The change in energy due to the additional node \( i \) is given by

\[
\Delta E_{\text{node}} = \mathcal{H}(E_V^1, \ldots, E_V^K; \Lambda_j, 0).
\]  

Similarly, we can consider a link bridging two trees forming a Bethe lattice. The energy change due to the addition of a link between nodes \( L \) and \( R \) is given by

\[
\Delta E_{\text{link}}(E_V^L, E_V^R) = \min_y \left[ E_V^L(y) + E_V^R(-y) - \frac{y^2}{2} \right].
\]

Denoting as \( \langle \cdots \rangle \) the average over the capacities, the average energy per node is given by

\[
\langle \Delta E \rangle = \langle \Delta E_{\text{node}} \rangle - K^2 \langle \Delta E_{\text{link}} \rangle.
\]

3.2. The piecewise quadratic solution

Due to the quadratic form of the transportation cost assumed in equation (1), we propose that the cavity energy functions are continuous and piecewise quadratic, namely,

\[
E^V_k(y_k) = \min_{n_k} \left[ f^k_{n_k}(y_k) \right]
\]

where \( n_k = 0, 1, 2, \ldots \). Indeed, the recursive nature of the quadratic cavity energy functions has been fully employed in deriving the message-passing approach in [9,10]. We note in passing that a similar recursive structure was used in the Gaussian Belief Propagation algorithm [27] and applied to processing continuous signals such as those in CDMA multiuser detection [28]. As a step forward, the ansatz in equation (15) further captures the multi-valley features in \( E^V_k(y_k) \), which is crucial in formulating the cavity messages for the present model.

We call \( f^k_{n_k} \) the \( n_k \)th composite function of \( E_k(y_k) \). For \( n_k > 0 \), \( f^k_{n_k}(y_k) \) is a quadratic function of the form

\[
f^k_{n_k}(y_k) = a^k_{n_k}(y_k - \tilde{y}^k_{n_k})^2 + d^k_{n_k}
\]

whereas for \( n_k = 0 \), it takes the form

\[
f^k_0(y_k) = \frac{y_k^2}{2} + c_k + \frac{u^2}{2} \Theta(y_k - \alpha_k).
\]

The form of \( f_0 \) is relevant when node \( k \) is a source node. Though \( f_0 \) is discontinuous, we will show that the resulting \( E^V_k(y_k) \) is continuous since the discontinuity at \( y_k = \alpha_k \) is masked by other quadratic functions. An example of a cavity energy function \( E^V_k(y_k) \) composed of three composite functions is shown in figure 4.

We denote the \( f^k_{n_k} \) with the minimum \( d^k_{n_k} \) among all composite functions in \( E^V_k \) as \( f^k_{n_k^*} \), i.e.,

\[
n_k^* = \arg\min_{n_k} d^k_{n_k}.
\]

\( n_k^* \) is particularly relevant when we evaluate the energy of the system in the case where the ancestor node of \( k \) is a source node. In this case, the resource of the ancestor can be...
Figure 4. An example of $E^V_k(y)$ composed of three quadratic functions $f^k_{n_k}(y)$ labeled by $n_k = 0, 1, 2$. Each composite function is characterized by its minimum position $\tilde{y}^k_{n_k}$, minimum value $d^k_{n_k}$, and curvature $a^k_{n_k}$.

Table 2. The table of cavity composite functions $f_n(y) = (\tilde{y}_n, a_n)$ from $n = 0$ to 2.

| $n$ | $\tilde{y}_n$ | $a_n$ |
|-----|----------------|------|
| 0   | 0              | 1    |
| 1   | $-K^{-1}$      | $\frac{1}{2(K-1)^2}$ |
| 2   | $-(K-1)^{-1}$  | $\frac{K^2-1}{2(K-1)^2}$ |

freely drawn by node $k$ without any consequences to other parts of the network, and the optimal current $y_k$ takes the value $\tilde{y}^k_{n_k}$.

As will be shown in the next subsection, only a few composite functions are relevant in the singlet and the doublet regimes. Each composite function has its fixed values of $\tilde{y}^k_{n_k}$ and $a^k_{n_k}$ independent of $k$, but the constant term is $k$ dependent. Thus, the functional form of $E^V_k(y_k)$ is effectively parameterized by the constant terms $d^k_{n_k}$ of the composite functions, as given by

$$E^V_k(y_k) = (d^k_0, d^k_1, d^k_2, \ldots).$$  \hfill (19)

The relevant composite functions in the singlet and doublet regimes are shown in Table 2.

3.3. The recursion of $E^V$

Using the piecewise quadratic ansatz in equation (15), the recursion of $E^V$ in equation (9) becomes

$$E^V_j(y_j) = \min_{\{n_k\}} H(f^1_{n_1}, \ldots, f^{K-1}_{n_{K-1}}; \Lambda_j, y_j) - \min_{\{n_k\}} \Delta E_j(f^1_{n_1}, \ldots, f^{K-1}_{n_{K-1}}; \Lambda_j).$$  \hfill (20)

We first consider the recursions for a deficient node $j$. Suppose the node is assigned as a source node, i.e., $\Lambda_j + \sum_{k \in \mathcal{L} \setminus \{i\}} y_k - y_j < 0$. In this case,

$$H(f^1_{n_1}, \ldots, f^{K-1}_{n_{K-1}}; \Lambda_j, y_j)|_{\Lambda_j + \sum_{k \in \mathcal{L} \setminus \{i\}} y_k - y_j < 0}$$

$$= \frac{y_j^2}{2} + u^2 \Theta(y_j - \Lambda_j - \sum_{k \in \mathcal{L} \setminus \{i\}} \tilde{y}^k_{n_k}) + \sum_{k \in \mathcal{L} \setminus \{i\}} d^k_{n_k},$$  \hfill (21)
which is exactly the form of \( f_0 \) in equation (17). The combination \( \{ n_k^* \} \) of composite function minimizes the last term in equation (21). Subject to a vertical shift by \( \Delta E_j \), equation (21) is taken to be \( f_0' \) in equation (17) characterized by

\[
d_0' = \frac{u^2}{2} + \sum_{k \in L_j \setminus \{i\}} d_{n_k^*}^k - \Delta E_j
\]

and

\[
\alpha_j = \Lambda_j + \sum_{k \in L_j \setminus \{i\}} \tilde{y}_{n_k^*}^k.
\]

For the moment, we ignore the possibility that combinations other than \( \{ n_k^* \} \) may result in further discontinuity in \( f_0' \), as we will show that composite functions \( f_n \) with \( n > 0 \) eliminate the effect of the discontinuities.

Next we suppose the node remains as a consumer node. In this case, \( \Lambda_j + \sum_{k \in L_j \setminus \{i\}} y_k - y_j = 0 \), and \( \min_{\{n_k\}} H(f_{n_1}^{K-1}; \Lambda_j, y_j) \) is computed subject to this equality constraint,

\[
H(f_{n_1}^{K-1}; \Lambda_j, y_j) | \Lambda_j + \sum_{k \in L_j \setminus \{i\}} y_k - y_j = 0
= A_{\{n_k\}} | (y_j - \tilde{Y}_{\{n_k\}})^2 + D_{\{n_k\}} + \sum_{k \in L_j \setminus \{i\}} d_{n_k}^k
\]

where

\[
A_{\{n_k\}} = \frac{1}{2} \left[ 1 + \frac{1}{\sum_{k \in L_j \setminus \{i\}} \left( 2a_{n_k}^k \right)^{-1}} \right],
\]

\[
\tilde{Y}_{\{n_k\}} = \frac{\Lambda_j + \sum_{k \in L_j \setminus \{i\}} \tilde{y}_{n_k}^k}{\sum_{k \in L_j \setminus \{i\}} \left( 2a_{n_k}^k \right)^{-1}},
\]

\[
D_{\{n_k\}} = \frac{(\Lambda_j + \sum_{k \in L_j \setminus \{i\}} \tilde{y}_{n_k}^k)^2}{2 \left[ 1 + \sum_{k \in L_j \setminus \{i\}} \left( 2a_{n_k}^k \right)^{-1} \right]},
\]

and the optimal currents drawn from the descendents are

\[
y_{k, \{n_k\}}^* = \frac{y_j - \Lambda_j - \sum_{l \in L_j \setminus \{i\}} \tilde{y}_{n_l}^l}{\sum_{l \in L_j \setminus \{i\}} \left( 2a_{n_l}^l \right)^{-1}} + \tilde{y}_k.
\]

Next, we consider the recursions for a source node \( j \). In this case, the cavity energy function consists of the composite function with \( n_j = 0 \) only, with

\[
d_0^j = \sum_{k \in L_j \setminus \{i\}} d_{n_k^*}^k - \Delta E_j.
\]

Table 3 summarizes the combinations \( \{ n_k \} \) which lead to the composite functions \( n_j = 1, 2 \) in table 2, enabling us to analyze the singlet and doublet regimes. We represent these relations of \( \{ n_k \} \) with \( n_j \) by the mapping \( \mathcal{M} \). As an illustration, the relations in table 3 can be expressed as

\[
\mathcal{M}(0, \ldots, 0) = 1, \quad \mathcal{M}(1, 0, \ldots, 0) = 2.
\]
considering the patterns of optimal currents around node $j$ intersects $f$, corresponds to a resource providing state (see figure 3(a)).

Remarkably, the functional recursion of $E^V$ in equation (9) is now simplified to a recursion of the constant terms in equations (22) and (29).

The physical interpretation of the composite functions $n_j = 0, 1, 2$ is revealed by considering the patterns of optimal currents around node $j$. For $n_j = 0$, no resources are drawn from the ancestor, i.e., $\tilde{y}_0 = 0$. Moreover, the optimal currents drawn from the descendents are $\tilde{y}_{n_1}^*$, which are non-positive according to table 3. This shows that $n_j = 0$ corresponds to a resource providing state (see figure 3(a)).

For $n_j = 1$, currents of $K^{-1}$ are drawn from the ancestor and all descendents, i.e., $y_{j-1}^* = \cdots = y_{K-1}^* = K^{-1}$, as shown in table 3. Hence $n_j = 1$ corresponds to the singly consuming state. (See figure 3(b).)

For $n_j = 2$, currents of $(K - 1)^{-1}$ are drawn from the ancestor and $K - 2$ descendents, leaving the link to the remaining descendent idle. This corresponds to the doubly consuming state (see figure 3(c)). Nodes with $n_j > 1$ correspond to other modes of resource consumption.

We return to verifying that $E^V$ is continuous piecewise quadratic, despite the discontinuity of $f_0$ in equation (17). This can be done by substituting $y_j = \alpha_j$ in equation (23) into the composite function equation (24) characterized by $A_{\{n_k\}}$, $Y_{\{n_k\}}$ and $D_{\{n_k\}}$ in equation (25). The result shows that $H = \alpha_j^2/2 + \sum_{k \in L_j \setminus \{i\}} a_{n_k}^k$. Hence it intersects $f_0$ at the lower end of the discontinuity. As shown in figure 5, the discontinuity is masked.

We finally derive a simplified expression of $\Delta E_j$ from equation (10). Since $H(f_{n_1}^1, \ldots, f_{n_K-1}^1, \Lambda_j, 0)$ is already obtained in equations (21) and (24) with $y_j = 0$,

$$\Delta E_j = \min_{\{n_k\}} \left( A_{\{n_k\}} Y_{\{n_k\}}^2 + D_{\{n_k\}} + \sum_{k \in L_j \setminus \{i\}} a_{n_k}^k \right) \frac{u^2}{2} \Theta(-\Lambda_j) + \sum_{k \in L_j \setminus \{i\}} a_{n_k}^k.$$

Table 3. Combinations $\{n_k\}$ from descendents that lead to the composite functions $n_j = 1, 2$ given by table 2. Permutations of $(n_1, n_2, \ldots, n_{K-1})$ result in the same $n_j$.

| $\{n_k\} = (n_1, n_2, \ldots, n_{K-1})$ | $\tilde{Y}_{\{n_k\}} = \tilde{y}_{n_j}$ | $A_{\{n_k\}} = a_{n_j}$ | $D_{\{n_k\}} = D_{n_j}$ | $(y_1^*, y_2^*, \ldots, y_{n_j-1}^*)$ | $n_j$ |
|--------------------------------------|-----------------------------------|----------------|-----------------|---------------------------------|--------|
| $(0, 0, \ldots, 0)$                 | $-\frac{1}{K}$                   | $\frac{K}{2(K-1)}$ | $\frac{1}{2K}$ | $(\frac{1}{K}, \frac{1}{K}, \ldots, \frac{1}{K})$ | 1      |
| $(1, 0, \ldots, 0)$                 | $-\frac{1}{K-1}$                 | $\frac{K^2-1}{2(K^2-K-1)}$ | $\frac{(K+1)}{2(K-1)}$ | $(0, \frac{1}{K-1}, \ldots, \frac{1}{K-1})$ | 2      |

The constant term $d_{n_j}^j$ is taken to be the minimum constant term in all combinations of $f_{n_k}^k$ with $M(\{n_k\}) = n_j$, yielding

$$d_{n_j}^j = \min_{\{n_k\}|n_j=M(\{n_k\})} \left[ D_{\{n_k\}} + \sum_{k \in L_j \setminus \{i\}} a_{n_k}^k \right] - \Delta E_j.$$

Table 3.
4. Closed sets of cavity energy functions: the intense simplifications

4.1. The intense simplification

In this subsection, we consider networks with no surplus nodes ($\phi_s = 0$). In the singlet regime, the energetically stable configurations consist of only the source nodes and singly consuming nodes. Hence we consider $E^V$ with only $f_0$ and $f_1$ as composite functions. $E^V$ is thus given by

$$E^V_k(y_k) = (d^k_0, d^k_1),$$

as a simplification of equation (19). Composite functions with $n_k \geq 2$ have $d^k_{n_k} > d^k_{n_k+1}$ in this regime, and their corresponding configurations are not stable. The recursion relations of $d_0$ and $d_1$ in equations (22) and (29) are simplified to

$$d^j_0 = \frac{u^2}{2} + \sum_{k \in L_j \setminus \{i\}} \min(d^k_0, d^k_1) - \Delta E_j,$$  \hspace{1cm} (32)

$$d^j_1 = \frac{1}{2K} \sum_{k \in L_j \setminus \{i\}} d^k_0 - \Delta E_j,$$  \hspace{1cm} (33)

where

$$\Delta E_j = \min \left[ \frac{u^2}{2} + \sum_{k \in L_j \setminus \{i\}} \min(d^k_0, d^k_1), \frac{1}{2(K-1)} + \sum_{k \in L_j \setminus \{i\}} d^k_0 \right].$$  \hspace{1cm} (34)

To determine the pattern of current flow, it is sufficient to consider the recursion of $\epsilon_j \equiv d^j_1 - d^j_0$, given by

$$\epsilon_j = -\gamma - \sum_{k \in L_j \setminus \{i\}} \min(0, \epsilon_k),$$  \hspace{1cm} (35)

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Figure 6. The closed set of $E_k(y)$ at $K = 3$ and $u^{-1} = 5/3$, corresponding to (a) the $c$ state $E^V_c$, (b) the $b$ state $E^V_b$ and (c) the $s$ state $E^V_s$.

Table 4. The recursion relations given by equation (35). The column $\Delta E_j$ is valid for $u^{-1} \geq \sqrt{K-1}$ in the singlet regime; a constant $(K-1)[u^2/2 - 1/2(K-1)]$ has to be added to $\Delta E_j$ for $u^{-1} < \sqrt{K-1}$ in the singlet regime.

| Descendent states | $\Delta E_j$ | $\mathcal{E}_j$ | Vertex state |
|-------------------|--------------|----------------|-------------|
| $(S,\ldots,S)$   | $u^2/2 - \gamma$ | $-\gamma$ | $c$ $C$ |
| $(C,S,\ldots,S)$ | $u^2/2 - \gamma$ | $0$ | $b$ $S$ |
| $(C,C,S,\ldots,S)$ | $u^2/2 - 2\gamma$ | $\gamma$ | $s$ $S$ |
| $(C,\ldots,C)$   | $u^2/2 - (K-1)\gamma$ | $(K-2)\gamma$ | $s$ $S$ |

where

$$\gamma \equiv \frac{u^2}{2} - \frac{1}{2K}. \quad (36)$$

The simple recursion leads to a closed set of $K$ cavity energy functions

$$E^V_q(y) = (d_0^q, d_0^q + q\gamma) \quad \text{with} \quad q = -1, 0, \ldots, K-2. \quad (37)$$

These functions are classified as consuming for $q = -1$, bistable for $q = 0$, and resource providing for $q = 1, \ldots, K-2$. Their absolute minima are located at $y = -K^{-1}$, both $y = 0$ and $y = -K^{-1}$, and $y = 0$ respectively. We call their states the $c$ state, $b$ state and $s$ state respectively; examples for the case of $K = 3$ are shown in figure 6. The $b$ state behaves in the same way as the $s$ state in the recursion relation, but physically they correspond to different cavity states. The differentiation between $b$ and $s$ states is required only when the entropy of the ground state is calculated. For most other purposes, grouping $b$ and $s$ states together further simplifies the analyses. We thus denote the $b$ and $s$ states as the $S$ state, and the $c$ state as the $C$ state in subsequent analyses. Their recursion relations are summarized in table 4. (The source state ($s$ state) in this paper should not be confused with the satisfied state (also denoted as the $s$ state) in [14]. In fact, the $s$, $u$, $b$ states in [14] have the same cavity energy functions as the $c$, $s$, $b$ states in this paper respectively.)
The recursion relation in table 4 can be summarized by the symbolic equations

\[ S + \cdots + S \rightarrow C. \quad (38a) \]

all other combinations \( \rightarrow S. \quad (38b) \)

To calculate the average energy per node, we can apply the same simplification to \( \Delta E_{\text{node}} \) and \( \Delta E_{\text{link}} \) in equations (12) and (13) respectively. We denote the full states of a node as \( C, B \) and \( S \), respectively representing the consuming, bistable and resource providing states. They are obtained symbolically via

\[ S + \cdots + S \rightarrow C \quad (39a) \]

\[ C + S + \cdots + S \rightarrow B \quad (39b) \]

all other combinations \( \rightarrow S. \quad (39c) \)

The energy changes are

\[ \Delta E_{\text{node}} = \frac{u^2}{2} + \min \left[ -\gamma, \sum_{j=1}^{K} \min(0, \epsilon_j) \right], \quad (40) \]

\[ \Delta E_{\text{link}} = \min(0, \epsilon_L, \epsilon_R). \quad (41) \]

These expressions are valid for \( u^{-1} \geq \sqrt{K-1} \) in the singlet regime; \( N_c[u^2/2 - 1/2(K-1)] \) has to be added to the expressions for \( u^{-1} < \sqrt{K-1} \) in the singlet regime, where \( N_c \) is the number of vertices in the \( C \) state.

Numerical iterations of equation (35) starting from random \( \epsilon_k \) show that the closed set of \( E^V \) is stable. The closed set corresponds to the integer cavity fields in the language of the cavity approach. Another example of a closed set of \( E^V \) is found in the doublet regime as described in the appendix.

We return to discussing the range of the singlet regime. From equation (35), it becomes apparent that when \( \gamma < 0 \), we would have \( \epsilon_j \) always positive, implying that the singly consuming state is always unstable. Hence a necessary condition of the singlet regime is \( \gamma \geq 0 \), or \( u^{-1} < \sqrt{K} \).

Similarly, in the doublet regime, we obtain the recursion relations

\[ d_1^i - d_0^i = -\gamma - \sum_{k \in L \setminus \{i\}} \min(0, d_1^k - d_0^k, d_1^k - d_0^k), \quad (42) \]

\[ d_2^i - d_0^i = -\kappa + \min_{(k)}(d_1^k - d_0^k) - \sum_{k \in L \setminus \{i\}} \min(0, d_1^k - d_0^k, d_1^k - d_0^k), \quad (43) \]

where

\[ \kappa \equiv \frac{u^2}{2} - \frac{K + 1}{2K(K-1)}. \quad (44) \]

Consider the difference \( d_2^i - d_1^i = -\kappa + \min_{(k)}(d_1^k - d_0^k) + \gamma \). In the singlet regime described by equation (35), \( d_2^i - d_1^i \) is always positive only if \( \kappa < 0 \), implying that
$u^{-1} > \sqrt{K(K-1)/(K+1)}$. Combining the two results, the range of the singlet regime is $\sqrt{K(K-1)/(K+1)} < u^{-1} < \sqrt{K}$, agreeing with the result reported in figure 2.

It is convenient to represent the recursion relations in the probabilistic framework of the BP algorithm [29]. We denote as $\psi^j_i \rightarrow c$ the probability that node $j$ is in the $C$ state, in the absence of the ancestor node $i$. The probability that node $j$ is in the $S$ state in the absence of $i$ is described as $\psi^j_i \rightarrow s$. We call $\psi^j_i \rightarrow c$ and $\psi^j_i \rightarrow s$ the cavity probabilities. In this framework, equation (38a) in the singlet regime can be written as

$$\psi^j_i \rightarrow c = \prod_{k \in \mathcal{L} \setminus \{i\}} (1 - \psi^k_c \rightarrow j - \gamma),$$

and $\psi^j_i \rightarrow s + \psi^j_i \rightarrow s = 1$. Note that the recursion relation (5) with the functional form of $E^V$ is now represented by a recursion of a single scalar $\psi^j_i \rightarrow c$, greatly simplifying the analysis. This framework will be useful in establishing a connection with the RSB ansatz.

### 4.2. Networks with surplus nodes

In this subsection, we consider networks with surplus nodes ($\phi_s > 0$) in the singlet regime. The recursion relations of the deficient nodes follow those in table 4, whereas the $E^V$ of the surplus nodes are always in the $s$ state. The symbolic equations equation (38a) are thus extended to

$$S + \cdots + S^{\Lambda = -1} \rightarrow C,$$

all other combinations $\Lambda = -1 S$, (46b)

all combinations $\Lambda = A S$. (46c)

The recursion of $\psi^j_i \rightarrow c$ is given by

$$\psi^j_i \rightarrow c = \delta_{\Lambda_j = -1} \prod_{k \in \mathcal{L} \setminus \{i\}} (1 - \psi^k_c \rightarrow j - \gamma),$$

and $\psi^j_i \rightarrow s + \psi^j_i \rightarrow s = 1$. (47)

| Descendent states | $\Lambda = -1$ | $\Lambda = A$ |
|-------------------|---------------|---------------|
| $(S,\ldots,S)$    | $\frac{\Lambda^{2}}{2} - \gamma$ | $0$ | $S$ |
| $(C,S,\ldots,S)$  | $\frac{\Lambda^{2}}{2} - \gamma$ | $-\gamma$ | $S$ |
| $(C,C,S,\ldots,S)$| $\frac{\Lambda^{2}}{2} - 2\gamma$ | $-2\gamma$ | $S$ |
| ...               | ...           | ...           | ... |
| $(C,\ldots,C)$    | $\frac{\Lambda^{2}}{2} - K\gamma$ | $-K\gamma$ | $S$ |

$\sqrt{K(K-1)/(K+1)} < u^{-1} < \sqrt{K}$.
The full energy change is given by

\[ \Delta E^i_{\text{node}} = \begin{cases} \frac{u^2}{2} + \min \left[ -\gamma, \sum_{j \in L_i} \min(0, \epsilon^i_j) \right], & \Lambda_i = -1 \\ \sum_{j \in L_i} \min(0, \epsilon^i_j), & \Lambda_i = A \end{cases} \quad (48) \]

and \( \Delta E_{\text{link}} \) is still given by equation (40). For deficient nodes, the optimized state is either consuming, bistable, or resource providing. Surplus nodes are fixed as source nodes. \( \Delta E_{\text{node}} \) and the full states of node \( i \) are shown in table 5 with the corresponding combination of descendent states. The full states of the node \( i \) are thus described by the probabilities \( \psi^i_C, \psi^i_B \) and \( \psi^i_S \) given by

\[ \psi^i_C = \delta_{A_{i,-1}} \prod_{j \in L_i} (1 - \psi^i_j), \]

\[ \psi^i_B = \delta_{A_{i,-1}} \sum_{j \in L_i} \psi^i_j \prod_{k \in L_j \setminus \{i\}} (1 - \psi^i_k), \quad (49) \]

with \( \psi^i_C + \psi^i_B + \psi^i_S = 1 \).

We derive the fraction of nodes with different full states by assuming independence between descendent branches of a tree. From equation (45), the average probability \( \langle \psi_c \rangle \) of a node in the cavity \( C \) state is thus given by

\[ \langle \psi_c \rangle = \phi_d [1 - \langle \psi_c \rangle]^{K-1}, \quad (50) \]

where \( \langle \cdot \rangle \) represents averaging over nodes. Iteration of equation (45) on Cayley trees reveals that \( \langle \psi_c \rangle \) does not approach the stable fixed point of equation (50) when \( \phi_d \) is high. At \( \phi_d = 1 \), a period-2 solution of \( \langle \psi_c \rangle = 0 \) and 1 emerges. Physically, this corresponds to alternating layers of consumer and source nodes on Cayley trees. This happens in similar problems such as that of the Bethe glass [23] and is referred to as the modulation mode. On real networks, nodes are randomly connected, rendering whole layers of consumer and source nodes highly unlikely. The period-2 situations are suppressed, making a fixed point solution of equation (50) possible in random networks. The fractions of nodes with full states \( C, B \) and \( S \) are thus given by

\[ f_C = \phi_d (1 - \langle \psi_c \rangle)^K, \quad f_B = K \phi_d \langle \psi_c \rangle (1 - \langle \psi_c \rangle)^{K-1}, \quad (51) \]

with \( f_C + f_B + f_S = 1 \). We leave the discussion of their physical interpretation to section 5.1.

5. The average energy

We evaluate the average energy by considering the energy change due to the addition of new nodes and links. Summarizing table 5, \( \langle \Delta E_{\text{node}} \rangle \) becomes

\[ \langle \Delta E_{\text{node}} \rangle = \phi_d \left[ \frac{u^2}{2} - (1 - \langle \psi_c \rangle)^{K \gamma} \right] - K \langle \psi_c \rangle \gamma. \quad (52) \]

Similarly, \( \langle \Delta E_{\text{link}} \rangle \) is given in table 6 by

\[ \langle \Delta E_{\text{link}} \rangle = -\gamma [2 \langle \psi_c \rangle - \langle \psi_c \rangle^2]. \quad (53) \]
Figure 7. The average fraction of source nodes in simulations with $K = 3$, $N = 100$, 500 and 3000 N steps with $N_{\text{flip}} = 4$, as compared with the $f_{s}^{\text{RS}}$ obtained from the RS ansatz, $f_{s}(x_{s})$ and $f_{s}(x_{d})$ obtained from the 1RSB ansatz. Inset: $f_{s}^{\text{RS}}$ for different values of $K$. The circles indicate the values of $\phi_{d}$ above which the RS assumption is not stable.

Table 6. $\Delta E_{\text{link}}$ as given by equation (13).

| Vertex states | $\Delta E_{\text{link}}$ |
|---------------|--------------------------|
| $(S, S)$      | 0                        |
| $(C, S)$      | $-\gamma$                |
| $(C, C)$      | $-\gamma$                |

After some algebra, equations (14), (50), (52) and (53) lead to

$$E_{\text{RS}} = \langle \Delta E \rangle = \phi_{d} \frac{u^{2}}{2} - \left[ \langle \psi_{c} \rangle + \left( \frac{K}{2} - 1 \right) \langle \psi_{c} \rangle^{2} \right] \gamma. \quad (54)$$

When a deficient node changes from a source to a consumer, the energy of the node reduces by $\gamma$ from $u^{2}/2$. We thus identify the coefficient of $\gamma$ in equation (54) as the fraction of consumer nodes. The fraction $f_{s}^{\text{RS}}$ of source nodes is then given by

$$f_{s}^{\text{RS}} = 1 - \langle \psi_{c} \rangle - \left( \frac{K}{2} - 1 \right) \langle \psi_{c} \rangle^{2}. \quad (55)$$

Note that $f_{s}$ is distinguished from $f_{S}$, since $f_{s} = f_{S} + f_{B}/2$, i.e., $f_{s}$ also counts those bistable nodes that become source nodes in the network configuration. Through the linear relationship $\langle \mathcal{E} \rangle = u^{2}/2 - f_{c}\gamma = 1/(2K) + f_{s}\gamma$, we consider $f_{s}$ as a measure of the average energy $\langle \mathcal{E} \rangle$.

The inset of figure 7 shows the fraction of source nodes as a function of $\phi_{d}$ derived from equations (50) and (55). For all connectivities $K$, $f_{s}^{\text{RS}}$ decreases with $\phi_{d}$. A higher
connectivity leads to an increase in $f_{s}^{RS}$ since more nodes are required to convert to source nodes to satisfy the demand of a consumer node.

Figure 7 shows the difference between $f_{s}^{RS}$ and $f_{s}^{sim}$ obtained from numerical simulations, in which the energy of real instances is minimized by the GSAT algorithm as described in section 2.2. The differences between $f_{s}^{RS}$ and $f_{s}^{sim}$ are roughly zero when $\phi_{d}$ is below some critical value. Above the critical value, $f_{s}^{RS}$ is significantly lower than $f_{s}^{sim}$. Hence the energy $E_{RS}$ is lower than the simulated energy. This discrepancy is related to the instability of the RS ansatz, which will be discussed below.

5.1. The soft nodes in the ground states

Nodes with the full state $B$ are bistable, between the consumer and source states. Figure 8 shows an example with two central nodes in the $B$ state. Using table 4, the cavity energy functions passed among them are worked out. In particular, $E_{b}^{V}$ is sent from the bistable nodes to all its resource providing neighbors, implying that a zero current or a current of $-K^{-1}$ would have no effect on the optimized energy. Hence, the central pairs correspond to the soft nodes which can be a consumer or a source node in different degenerate configurations. These degenerate configurations are connected in the configuration space, since transitions among them only involve the flipping of states of the soft nodes [30]. In other words, using the notions of $S$, $C$ and $B$ states, the single cluster is described by a unique set of $S$, $C$ and $B$ labels for each node. On the other hand, if the network enters the RSB phase, the configuration space is dominated by numerous clusters, each with its
own set of $S$, $C$ and $B$ states of the nodes. Transitions among the clusters involve flipping the hard (non-soft) nodes as well. In this section, we discuss the RS case.

The fraction of soft nodes is given by the fraction of nodes with full state $B$. From equation (51), we have

$$f_{\text{RS soft}} = f_B = K \phi_d \langle \psi_c \rangle (1 - \langle \psi_c \rangle)^{K-1}.$$  

(56)

On the other hand, the hard nodes are either consumer or source nodes in all degenerate states. They correspond to nodes in the backbone in a vertex cover [6]–[8]. Surplus nodes are certainly in the source backbone. Deficient nodes can be found either in the consumer or the source backbone. From table 5, the fraction of nodes in the consumer backbone is given in equation (51) by the probability of finding a node with full state $C$, namely,

$$f_{\text{RS con-bone}} = f_C = \phi_d (1 - \langle \psi_c \rangle)^K.$$  

(57)

Remarkably, it can be shown easily that $f_{\text{RS soft}}/2 + f_{\text{RS con-bone}} = 1 - f_{\text{RS}}$ which implies that exactly half of the soft nodes are consumers.

The fraction of soft nodes relative to the fraction of deficient nodes obtained from equation (56) is shown in the inset of figure 9. When the fraction $\phi_d$ of deficient nodes increases from 0, the fraction increases until it reaches a maximum value at $\langle \psi_c \rangle = K^{-1}$ and $\phi_d = K^{K-2}/(K - 1)^{K-1}$. When $\phi_d$ is small, most deficient nodes are surrounded by surplus nodes and hence are found in the consumer backbone, leading to a small fraction of soft nodes. When $\phi_d$ increases, the probability of finding contiguous deficient nodes increases, which leads to an increase in $f_{\text{RS}}$.

The fraction of soft nodes in simulations is compared with $f_{\text{RS}}$ in figure 9. In simulations, we use an algorithm similar to the GSAT [31] to lower the energy of the

Figure 9. The average fraction of soft nodes in simulations of $K = 3$ and 3000 $N$ steps with $N_{\text{flip}} = 4$, as compared with $f_{\text{RS}}$. Inset: $f_{\text{RS}}/\phi_d$ for different values of $K$. The circles indicate the values of $\phi_d$ above which the RS assumption is not stable.
system until it becomes steady. Then we allow further cluster flips and identify the nodes which can be flipped with no change in global energy, such as the example in figures 8(b) and (c). Like in figure 7, the simulation results have an excellent agreement with the RS result when \( \phi_d \) is below the value at the peak of \( f_{\text{soft}}^{\text{RS}}/\phi_d \). Above this critical value, the fraction of soft nodes in simulations is less than the RS prediction, which will be shown to be due to RS instability.

Algorithmically, a high fraction of soft nodes leads to an unfavorable consequence. After the convergence of BP on real instances, nodes with the \( B \) state are bistable and a further determination of the final optimal configuration is required for the resulting sub-graph of \( B \) nodes. A random assignment of \( B \) nodes to either consuming or resource providing does not generally result in an optimal configuration. When \( \phi_d \) is low, the sub-graphs of \( B \) nodes are disconnected and the assignment is easy. When \( \phi_d \) is high, the sub-graphs of \( B \) nodes are connected and the assignment is more difficult.

5.2. The instability of the RS ansatz

The discrepancy between the simulation results and the predicted average energy \( E_{\text{RS}} \) and \( f_{\text{soft}}^{\text{RS}} \) suggests that the RS ansatz is unstable at high \( \phi_d \). In the RS formalism, a single ground state is assumed. We thus examine the stability of this assumption against the picture of multiple ground states, by relaxing the constraints of \( \psi_j^{\eta_j} = 0, 1 \). In other words, \( 0 \leq \psi_j^{\eta_j} \leq 1 \). To study the stability of the integer ansatz of \( \psi_j^{\eta_j} \), we define the variables

\[
\eta_c^{\eta_j} = \delta_{\eta_j,1}, \quad \eta_s^{\eta_j} = \delta_{\eta_j,1} \quad \text{and} \quad \eta_g^{\eta_j} = 1 - \eta_c^{\eta_j} - \eta_s^{\eta_j}.
\]

Thus, the recursion rule (45) is extended to include non-integer values of \( \psi_j^{\eta_j} \). \( \eta_g^{\eta_j} = 1 \) corresponds to the onset of non-zero probabilities over the range of \( 0 < \psi_j^{\eta_j} < 1 \), indicating the occurrence of glassy behavior with node \( j \) having a probabilistic distribution of \( C \) and \( S \) states in the stable states of the configuration space. Hence the RS solution is stable only if \( \eta_g^{\eta_j} = 0 \) for all \( j \rightarrow i \) is a stable fixed point.

We thus formulate the recursion relations of \( \eta_c^{\eta_j}, \eta_s^{\eta_j} \) and \( \eta_g^{\eta_j} \) by considering table 4, namely,

\[
\eta_c^{\eta_j} = \delta_{\Lambda_j,-1} \prod_{k=1}^{K-1} \eta_s^{k-j}.
\]

\[
\eta_s^{\eta_j} = \delta_{\Lambda_j,A} + \delta_{\Lambda_j,-1} \left[ 1 - \prod_{k=1}^{K-1} (\eta_s^{k-j} + \eta_g^{k-j}) \right]
\]

\[
\eta_g^{\eta_j} = \delta_{\Lambda_j,-1} \left[ \prod_{k=1}^{K-1} (\eta_s^{k-j} + \eta_g^{k-j}) - \prod_{k=1}^{K-1} \eta_s^{k-j} \right].
\]

Denoting the site averages of \( \eta_c^{\eta_j}, \eta_s^{\eta_j} \) and \( \eta_g^{\eta_j} \) as \( \langle \eta_c \rangle, \langle \eta_s \rangle \) and \( \langle \eta_g \rangle \) respectively, we obtain their stable fixed points by solving

\[
\langle \eta_c \rangle = \phi_d \langle \eta_s \rangle^{K-1}
\]

\[
\langle \eta_s \rangle = 1 - \phi_d \langle \eta_s \rangle + \langle \eta_g \rangle)^{K-1}
\]

\[
\langle \eta_g \rangle = \phi_d \langle \eta_s \rangle^{K-1} - \langle \eta_s \rangle^{K-1}.
\]

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Figure 10. (a) The stable solution of equation (60) for $K = 3$. The symbols represent the simulated fraction of non-converging BP messages. (b) The dependence of the variance $\sigma^2_{j \rightarrow i}$ on $\phi_d$. The dotted lines indicate the corresponding values of $\phi_d^{AT}$.

For all $\phi_d$, $\langle \eta_g \rangle = 0$ is a trivial solution of the last line of equation (60), and the above recursions reduce to the RS recursions (45). By introducing a small perturbation $\delta \eta_g^{k \rightarrow j}$ to $\eta_g^{k \rightarrow j} = 0$, we obtain the corresponding $\delta \eta_g^{j \rightarrow i}$. The solution of $\langle \eta_g \rangle = 0$ is stable under the perturbation if

$$\left| \frac{\langle \delta \eta_g^{i \rightarrow j} \rangle}{\langle \delta \eta_g^{k \rightarrow j} \rangle} \right| = (K - 1)\phi_d \langle \eta_s \rangle^{K - 2} \leq 1. \quad (61)$$

Alternatively, the stability of the RS solution can be studied by considering the propagation of fluctuations $\langle (\delta \psi_s^{k \rightarrow j})^2 \rangle$ under the recursion relation equation (45) [34]. This leads to the Almeida–Thouless (AT) stability condition,

$$\frac{\langle (\delta \psi_s^{j \rightarrow i})^2 \rangle}{\langle (\delta \psi_s^{k \rightarrow j})^2 \rangle} = (K - 1)\phi_d \langle (\psi_s)^2 \rangle^{K - 2} \leq 1. \quad (62)$$

In the RS regime, $\langle (\psi_s)^2 \rangle = \langle \eta_s \rangle$ since $\psi_s^{j \rightarrow i} = 0$ or 1. The AT stability condition is thus equivalent to equation (61).

The stable solution of $\langle \eta_c \rangle$, $\langle \eta_s \rangle$ and $\langle \eta_g \rangle$ for $K = 3$ is shown in figure 10(a). The RS solution becomes unstable when $\phi_d > 0.75$ for $K = 3$. This critical value agrees with those found in the simulation of the average energy and the fraction of soft nodes. For general values of $K$, simple algebra leads to the AT line

$$\phi_d^{AT} = \frac{K^{K - 2}}{(K - 1)^{K - 1}} \quad (63)$$

which separates the RS and the RSB phases in the space as shown in the inset of figure 11. From equations (50), (56) and (62), it can be shown that $\langle \psi_s \rangle = f_{\text{soft}}^{\text{RS}} = K^{-1}$ on the AT line.

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Figure 11. Sketch of the Poissonian subnetwork of deficient nodes in the large connectivity limit with only a fraction $O(K^{-1})$ of deficient nodes (squares) and the rest being surplus nodes (circles). Filled and unfilled symbols represent consumer or source states respectively. Inset: the RS and RSB phases in the $K-\phi_d$ space.

In the large $K$ limit, $\phi_d^{AT}$ approaches $e/K$. This result has an interesting connection with the vertex cover problem. Considering the covered set as the set of source nodes, all links involving surplus nodes are covered. The remaining links are those among the deficient nodes. These deficient nodes have at least one neighbor that is a deficient node. Hence from table 5, their surplus node neighbors do not affect the states of the deficient nodes. Rather, their states are determined by the states of their deficient node neighbors. Thus, the problem of minimizing the covered set size reduces to one that minimizes the subset size of covered nodes in the subnetwork of deficient nodes as sketched in figure 11. In the large $K$ limit, this subnetwork has a Poissonian connectivity distribution with a mean $K\phi_d$. The result $K\phi_d^{AT} = e$ agrees with the point of RS instability derived in [6,7].

Comparisons between the simulation results and the RS analytical results from figures 7 and 9 have yielded evidence of an AT transition in real instances at $\phi_d = \phi_d^{AT}$. Here we provide two more supporting numerical experiments. In the first experiment, we consider the BP algorithm initialized with $\psi^{j\rightarrow i} = 0, 1$ for all $j \rightarrow i$. As shown in figure 10(a), effectively all messages converge to their steady states in the RS regime. However, a significant fraction of messages fluctuate between 0 and 1 when $\phi_d$ rises above $\phi_d^{AT}$, indicating the breakdown of the RS ansatz. This leads to the non-convergence of the BP algorithm on real instances. As shown in figure 10(a), the fraction of non-converging BP messages has an excellent agreement with the theoretical values of $\langle \eta_L \rangle$. Consequently, improved algorithms are needed for ground state searching. Algorithmically, decimation procedures, such as those used in the survey propagation (SP) algorithm [4], are required. We have tested the BP algorithm with decimation and obtained results with simulated energy lower than for those from the GSAT algorithm, which will be reported elsewhere.

In the second experiment, we consider numerical iterations of equation (45) using population dynamics [9,10]. We start with different sets of initial values of $\psi^{j\rightarrow i} = 0, 1$, each set following the same sequence of random connections among the nodes. When the dynamics reaches the steady state, we measure the variance $\sigma_{\psi_{j\rightarrow i}}^2 = (\overline{\psi_{j\rightarrow i}})^2 - (\overline{\psi_{j\rightarrow i}})^2$, where the overline denotes the average over random initial conditions. $\sigma_{j\rightarrow i} \approx 0$ implies
that the cavity state of node $j$ is independent of the boundary condition of the tree represented by the population dynamics, and is always frozen in either $S$ or $C$ states. $\sigma_{j\rightarrow i} > 0$ implies that the cavity state of node $j$ is dependent on the boundary conditions and shows a long range correlation. The numerical results of $\sigma_{j\rightarrow i}$ averaged over nodes are shown in figure 10(b) for $K = 3, 4, 5$. In the figure $\langle \sigma_{j\rightarrow i} \rangle > 0$ when $\phi_d > \phi_d^{AT}$ with almost no dependence on the number of iterations in the population dynamics.

6. The one-step replica symmetry breaking ansatz

6.1. The 1RSB formalism

In the RSB formalism, the network behavior is explained by the dominance of numerous states in the configuration space, instead of a single ground state in the RS formalism. Here, we consider the 1RSB ansatz [32, 33] where the density of states with energy $\epsilon = \mathcal{E}/N$ per node is assumed to have the form $\mathcal{N}_N(\epsilon) = \exp[\mathcal{N}\Sigma(\epsilon)]$ for a network of $N$ nodes and total energy $\mathcal{E}$. $\Sigma(\epsilon)$ is called the complexity or configurational entropy. For small changes in the average energy, we can write $\Sigma(\epsilon) = x(\epsilon - \epsilon^R)$ where $\epsilon^R$ is the reference energy. This assumption leads to a recursion for the cavity probability functional $P_j[\mathcal{E}^V]$:

$$
P_j[\mathcal{E}^V(y_j)] = \frac{1}{\Xi} \prod_{k \in \mathcal{L}\setminus\{i\}} \left( \int \mathcal{D}\mathcal{E}^V_k(y_k) P_k[\mathcal{E}^V_k(y_k)] \right) 
\times \prod_{y_j} \left( \delta[\mathcal{E}^V_j(y_j)] - \mathcal{H}(\mathcal{E}^V_1, \ldots, \mathcal{E}^V_{K-1}; \Lambda_j, y_j) + \Delta\mathcal{E}_j(\mathcal{E}^V_1, \ldots, \mathcal{E}^V_{K-1}; \Lambda_j) \right) 
\times \exp[-x\Delta\mathcal{E}_j(\mathcal{E}^V_1, \ldots, \mathcal{E}^V_{K-1}; \Lambda_j)]$$

where $\Xi$ is the normalization constant. We now define the right-hand side of equation (64) to be $\mathcal{H}_P$ and the recursion can be represented by $P_j[\mathcal{E}^V] = \mathcal{H}_P(P_{k=1}, \ldots, P_{c-1}, \mathcal{E}^V_j; \Lambda_j, x)$. Solving the recursion in equation (64) using population dynamics is equivalent to solving for a stable functional distribution $Q$ in

$$
Q[P_j] = \int d\Lambda_j \rho(\Lambda_j) \prod_{k=1}^{K-1} \int \mathcal{D}P_k Q[P_k] 
\times \prod_{\mathcal{E}^V_j} \delta\{P_j[\mathcal{E}^V] - \mathcal{H}_P(P_{k=1}, \ldots, P_{c-1}, \mathcal{E}^V_j; \Lambda_j, x)\},
$$

which is analogous to the RS case of solving for $\mathcal{P}[\mathcal{E}^V]$ in equation (11). Note that the RS recursions in equation (9) correspond to the recursions of the cavity energy functions $\mathcal{E}^V$ yielding a solution of the functional $\mathcal{P}[\mathcal{E}^V]$, while the 1RSB recursions in equation (64) correspond to recursions of the functional probability $P[\mathcal{E}^V]$ yielding a solution of the probability functional $Q[P]$.

To analyze the physical properties of the network, we write the partition function when the $K$ cavity probability functional feeds a central node:

$$
\Xi_{\text{node}} = \prod_{j \in \mathcal{L}_c} \left( \int \mathcal{D}\mathcal{E}^V_j P_j[\mathcal{E}^V_j] \right) \exp[-x\Delta\mathcal{E}_{\text{Node}}(\mathcal{E}^V_1, \ldots, \mathcal{E}^V_K; \Lambda_i)]
$$

$$
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$$

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with $\Delta \mathcal{E}_{\text{node}}$ given by equation (12). Similarly, the partition function obtained by bridging two trees with a link is

$$
\Xi_{\text{link}} = \int D\mathcal{E}_L D\mathcal{E}_R P_L[E^V_L] P_R[E^V_R] \exp[-x\Delta \mathcal{E}_{\text{link}}(E^V_L, E^V_R)].
$$

(67)

The average configuration free energy is given by

$$
\Phi(x) = -\frac{1}{x} \left( \langle \ln \Xi_{\text{node}} \rangle - \frac{K}{2} \langle \ln \Xi_{\text{link}} \rangle \right).
$$

(68)

The averages $\langle \cdots \rangle$ are taken over $\Lambda_i$ and $P_j$ from the distribution $Q[P_j]$. $\Phi$ is related to the complexity $\Sigma$ and the average energy $e$ by

$$
x \Phi = e - \Sigma, \quad \Sigma = x^2 \frac{\partial \Phi}{\partial x}, \quad e = \frac{\partial (x \Phi)}{\partial x}.
$$

(69) \quad (70) \quad (71)

While solving for $P[E^V]$ in equation (64) is in general difficult, simple solutions can be obtained if a closed set of countably many $E^V$ is sufficient for describing the recursions of $E^V$. The singlet regime in which the $C$ and $S$ states form a closed set is a good example. We emphasize, however, that the techniques are generally applicable to regions beyond the singlet regime where closed sets of $E^V$ are found, such as the commensurate point in the doublet regime discussed in the appendix.

6.2. The 1RSB solution

In the singlet regime there are only two representative states, $C$ and $S$ states; we parameterize $P[E^V]$ as

$$
P_j[E^V_j] = \psi^{j\rightarrow i}_c \delta(E^V_j - E^V_c) + \psi^{j\rightarrow i}_s \delta(E^V_j - E^V_s).
$$

(72)

Using table 4 to obtain $\Delta E$ for different combinations of $C$ and $S$ states, equation (64) can be simplified to

$$
\begin{align*}
\psi^{j\rightarrow i}_c &= \delta_{\Lambda_{j\rightarrow i}} e^{-xu^2/2} \frac{1}{Z^{j\rightarrow i}} \prod_{k \in \mathcal{L}_j \setminus \{i\}} \psi^{k\rightarrow j}_s, \\
\psi^{j\rightarrow i}_s &= \delta_{\Lambda_{j\rightarrow i}} e^{-xu^2/2} \frac{1}{Z^{j\rightarrow i}} \left[ \prod_{k \in \mathcal{L}_j \setminus \{i\}} (\psi^{k\rightarrow j}_c e^{\gamma} + \psi^{k\rightarrow j}_s) - \prod_{k \in \mathcal{L}_j \setminus \{i\}} \psi^{k\rightarrow j}_s \right] + \delta_{\Lambda_{j\rightarrow A}}, \\
Z^{j\rightarrow i} &= e^{-xu^2/2} \prod_{k \in \mathcal{L}_j \setminus \{i\}} (\psi^{k\rightarrow j}_c e^{\gamma} + \psi^{k\rightarrow j}_s).
\end{align*}
$$

(73)
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Figure 12. (a) The stable solution of \(Q(\psi_c)\) obtained by solving equation (65) in the singlet regime using equation (73) with \(K = 3\) and \(x = 0\). (b) The stable solution of \(Q(\psi_c)\) with \(K = 3\) and \(\phi_d = 1\).

The above recursions of \(\psi^{j \rightarrow i}_c\) are gross simplifications of the recursions of the functional probabilities in equation (64). These equations can be solved by population dynamics involving a pool of values of \(\psi^{j \rightarrow i}_c\) with \(0 \leq \psi^{j \rightarrow i}_c \leq 1\). Alternatively, the solution to the 1RSB recursion can be found by directly solving for the distribution \(Q(\psi_c)\) in equation (65) which is isomorphic to \(Q[P]\) in equation (65).

The stable solution of \(Q(\psi_c)\) for \(K = 3\) and \(x = 0\) is shown in figure 12(a). When \(\phi_d \leq \phi^\text{AT}_d\), there are no fractional components of \(\psi_c\), and \(Q(\psi_c) = \langle \psi_c \rangle \delta(\psi_c - 1) + (1 - \langle \psi_c \rangle)\delta(\psi_c)\). When \(\phi_d > \phi^\text{AT}_d\), non-zero components of \(0 < \psi_c < 1\) exist. This agrees with the result in section 5.2 that in this regime, the RS solution is an unstable solution of equation (65). When \(\phi_d = 1\), there is no disorder in the capacities. All vertices are identical and \(Q(\psi_c) = \delta(\psi_c - \langle \psi_c \rangle)\) where \(\langle \psi_c \rangle\) is given by the RS equation (50). This means that among the different states of the system, all vertices are equally likely to be in the \(C\) state with probability \(\langle \psi_c \rangle\). The stable solutions of \(Q(\psi_c)\) are dependent on \(x\) via the factor \(x\gamma\). For the case of \(\phi_d = 1\), the dependence of \(Q(\psi_c)\) on \(x\) is shown in figure 12(b). The position of the delta peak at \(\langle \psi_c \rangle = (1 - \langle \psi_c \rangle)^{K-1}/((e^{\gamma\gamma} - 1)\langle \psi_c \rangle + 1)^{K-1}\) shifts to left from \(x\gamma = 0\) to \(x\gamma = x^{(l)}\gamma = 1.92\). For \(x > x^{(l)}\) in figure 12(b), \(Q(\psi_c)\) becomes a continuous distribution, indicating the instability of the 1RSB ansatz to be discussed in section 6.3.

With the stable solution of \(Q(\psi_c)\), we derive the complexity \(\Sigma(e)\) in the singlet regime. Obtaining \(\Delta E_{\text{node}}\) in table 5, we write the partition function \(\Xi_{\text{node}}\) in equation (66) as

\[
\Xi_{\text{node}} = \delta_{\Lambda_{j,-1}} \left[ \prod_{j \in L_i} (\psi^{j \rightarrow i}_c e^{\gamma} + \psi^{j \rightarrow i}_s) + (e^{\gamma} - 1) \prod_{j \in L_i} \psi^{j \rightarrow i}_s \right] e^{-xu^2/2} \\
+ \delta_{\Lambda_{j,A}} \left[ \prod_{j \in L_i} (\psi^{j \rightarrow i}_c e^{\gamma} + \psi^{j \rightarrow i}_s) \right] e^{-xu^2/2}.
\]

(74)

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Figure 13. The 1RSB complexity $\Sigma(e)$ obtained by numerically solving for $Q(\psi_c)$ with $K = 3$ and $\phi_d = 0.94, 0.96, 0.98, 1$. Inset: $\Sigma(e)$ for $K = 3$ and $\phi_d = 1$ obtained from the ansatz $Q(\psi_c) = \delta(\psi_c - \langle \psi_c \rangle)$. It approaches the modulation limit at $f_s = 0.5$ as $x \to \infty$. Symbols are spaced at intervals of 0.9 in $x^\gamma$.

With $\Delta E_{\text{link}}$ from table 6, we write $\Xi_{\text{link}}$ as

$$
\Xi_{\text{link}} = \psi_{L}^{S \to R} \psi_{L}^{R \to L} + (\psi_{s}^{L \to R} \psi_{c}^{L \to R} + \psi_{c}^{L \to R} \psi_{R}^{L \to R}) e^{x^\gamma} + \psi_{c}^{L \to R} \psi_{R}^{L \to R} e^{x^\gamma}.
$$

The configurational free energy $\Phi$ is given by equation (68) with $\psi_{j \to i}$ averaged over $Q(\psi_c)$. The complexity $\Sigma(e)$ obtained is shown in figure 13. Again, $e$ is expressed in terms of the fraction of source nodes through the relation $f_s = (e - 1/2K)/\gamma$.

Generally, we identify three segments on the complexity curve: (i) the unphysical segment (the dotted segment with $\Sigma \geq 0$), (ii) the physical segment (the solid segment with $\Sigma \geq 0$), and (iii) the highly unlikely segment (the dotted segment with $\Sigma < 0$). The physical segment of $\Sigma$ is related to the number $N$ of metastable states with energy $e$. We denote the values of $x$ when $\Sigma = 0$ and $\Sigma$ is maximum as $x_s$ and $x_d$ respectively. $e(x_s)$ corresponds to the lowest energy among the states with non-vanishing complexity, which is considered as the ground state in the picture of 1RSB. $e(x_d)$ corresponds to the energy of the states with the highest complexity, which are believed to be the states where search algorithms get trapped, giving rise to dynamical transitions. However, recent work on the coloring problem shows that the efficacy of the BP algorithm is not affected by the dynamical transition [30]. We leave this issue for future studies.

The segment of negative complexity corresponds to states with vanishing number in the thermodynamic limit. Its physical meaning is clear in the limit $x \to \infty$, which corresponds to a single state with lowest possible energy, since the reweighting process allows only one state. We show $\Sigma$ in the inset of figure 13 as $x \to \infty$. The result is obtained from the solution of $Q(\psi_c)$ restricted to being the 1RSB solution in the form of $Q(\psi_c) = \delta(\psi_c - \langle \psi_c \rangle)$, i.e. the unstable solution when $x > x^{(I)}$. The complexity curve

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Figure 14. The optimized $f_s$ on real instances as a function of $N$ with $K = 3$, as obtained by the GSAT algorithm (○) and the BP algorithm with decimation (△). The horizontal dashed lines show the analytical results from the RS ansatz, $f_s(x_s)$ and $f_s(x_d)$ in the 1RSB ansatz. Inset: the fraction $f_{\text{dec}}$ of decimated nodes before convergence.

approaches the limit of $\psi_c = 0.5$, which corresponds to the highly unlikely structure of networks with alternating layers of consumer and source nodes.

6.3. Comparison with real instances

Though successful in finding low lying states on real instances, the GSAT algorithm that we described in section 2.2 requires long computation times for large systems. To compare the predictions of RS and 1RSB approximations with real instances, we employ the BP with decimation. As the BP does not converge in the RSB phase, we measure the time average of the fluctuating messages $\psi_j^i$ and evaluate for each node the time average probability of the full $S$ states. The node with the highest $\psi_i^S$ is fixed as resource providing. Only source nodes are decimated, as bistable nodes should be left undecimated, and decimating a consumer node will fix its neighbors simultaneously, which may hinder the convergence of the BP. On repeating the above procedure, the BP messages finally converge and the full states of all nodes are determined.

Figure 14 shows that lower simulated energy can be obtained from the BP with decimation as compared with the GSAT algorithm. The simulated energy approaches the $e(x_d)$ as obtained by the 1RSB ansatz. However, the fraction of decimated nodes before convergence increases with system size as shown in the inset of figure 14. This greatly increases the computational time for large systems if only a single node is decimated at a time. Several nodes can be decimated simultaneously to shorten the computation time, with a tradeoff in energy.

6.4. The instability of the 1RSB formalism

To test the stability of the 1RSB ansatz against further steps of RSB, we consider two kinds of instabilities that lead to the two-step RSB (2RSB) formalism [35]. They are
the so-called type I and type II instabilities, corresponding to the aggregation of states and fragmentation of states respectively, as shown schematically in figure 15. In type I instability, metastable states aggregate in clusters and the 1RSB ansatz is valid in each cluster. The whole state space is composed of clusters and the 2RSB formalism is required to describe the state space structure. In type II instability, some states split to form clusters of states instead of single states. The 1RSB ansatz is valid inside the clusters while the 2RSB ansatz is required to describe the state space structure. It is generally believed that once 1RSB is not stable, the full RSB is required to describe the system, as illustrated by the 1RSB instability found in graph coloring [36] and K-satisfiability problems [37]. Here we focus on the case of $K = 3$ in the 1RSB regime with $\phi_d > \phi_d^{AT}$, following the approach of [36].

6.4.1. Type I instability: aggregation of states. In the 1RSB phase, each vertex $k$ is characterized by the cavity probability functional $P_k[E^V]$. This characterization is much simplified due to the small closed set of states in the singlet regime, rendering it isomorphic to single values of $\psi_c^k$. In the 2RSB formalism, each vertex $k$ is characterized by the probability functional of $P_k$. For the closed set of states in the singlet regime, this characterization is isomorphic to the distribution $Q_k(\psi_c^k)$. In the example illustrated in figure 15, the probability $\psi_c^k = 0.4$ is originally uniform in the state space of the 1RSB phase. When it enters the 2RSB phase, $\psi_c^k$ starts to take diversified values of $\psi_c^k = 0.39, 0.40, 0.41$ in three different clusters of states.
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To examine type I instability, we test for the possible spreading in $\psi_{c}^{j-i}$ by introducing small fluctuations in $\psi_{c}^{k-j}$ of the descendents. We define $T_{k-j}(x)$ to be the derivative

$$
T_{k-j}(x) = \left| \frac{\partial \psi_{c}^{j-i}}{\partial \psi_{c}^{k-j}} \right|_{\text{1RSB}}
$$

from equation (73), which is evaluated at the values of $\psi_{c}^{k-j}$ from the 1RSB solution. The propagation of noise is thus given by

$$
(\delta \psi_{c}^{j-i})^{2} = \sum_{k \in L_{j}\setminus(i)} [T_{k-j}(x)]^{2}(\delta \psi_{c}^{k-j})^{2}.
$$

In the thermodynamic limit, we consider a tree structure with $L$ generations. The noise at the $L$th generation vanishes if $(T_{L-1-L} T_{L-2-L-1} \cdots T_{0-1})^{2} \to 0$ as $L \to \infty$. Hence we measure the quantity

$$
\lambda_{L}^{(i)}(x) = (K-1)^{L}(T_{L-1-L} T_{L-2-L-1} \cdots T_{0-1})^{2},
$$

averaged over the quenched disorder and boundary conditions of the trees. This can be implemented by iterating equation (73) using population dynamics and evaluating the corresponding $\lambda_{L}^{(i)}(x)$ in each iteration. Alternatively, we solve for the distribution $P_{L}[\lambda_{L}^{(i)}, \psi_{c}]$ at layer $L$ by using the recursion relation

$$
P_{L+1}[\lambda_{L+1}^{(i)}, \psi_{c}^{L+1}] = \int d\lambda_{L}^{(i)} \int d\psi_{c}^{L} P_{L}[\lambda_{L}^{(i)}, \psi_{c}^{L}] \prod_{k=2}^{K-1} \int d\psi_{c}^{k} Q(\psi_{c}^{k})
$$

$$
\times \left\{ \phi_{d}[\lambda_{L+1}^{(i)} - (T_{L-L+1})^{2} \lambda_{L}^{(i)}] \delta \left[ \psi_{c}^{L+1} - \frac{e^{-xu^{2}/2}}{Z^{j-i}} \psi_{c}^{L} \prod_{k=2}^{K-1} (1 - \psi_{c}^{k}) \right] 
$$

$$
+ \phi_{c} \lambda_{L+1}^{(i)} \delta(\psi_{c}^{L+1}) \right\}
$$

(79)

with the initial condition

$$
P_{1}[\lambda_{1}^{(i)}, \psi_{c}] \equiv Q(\psi_{c}^{1}) \delta(\lambda_{1}^{(i)} - 1)
$$

(80)

for $L = 1$. We note that the case of $\phi_{d} = 1$ is a special case where no disorder is present and $T_{0-1} = \cdots = T_{L-1-L}$ since $Q(\psi_{c}^{k}) = \delta(\psi_{c}^{k} - \langle \psi_{c}^{k} \rangle)$ for all $k$. Thus for $\phi_{d} = 1$, $\langle \lambda_{1}^{(i)}(x) \rangle \geq 1$ is sufficient to show that the 1RSB solution is unstable at $x$. To evaluate $\langle \lambda_{L}^{(i)}(x) \rangle$ for general values of $\phi_{d} < 1$, solving equation (65) gives more reliable results than population dynamics. This is because for large $L$ and non-vanishing values of $\phi_{s}$, such as those close to $\phi_{s}^{\text{AT}}$, the presence of the factor $\prod_{i=1}^{L} \delta_{\lambda_{i},A}$ in $\lambda_{L}^{(i)}(x)$ requires an extremely large population for a finite fraction of non-zero $\lambda_{L}^{(i)}(x)$ in the pool of population dynamics.

We show $\langle \lambda_{L}^{(i)}(x) \rangle$ as a function of $L$ in figure 16(a) for $\phi_{s} = 0.1$ from $x\gamma = 0$ to 4.5, and define $x^{(i)}$ by

$$
\lim_{L \to \infty} \frac{d \log \langle \lambda_{L}^{(i)}(x) \rangle}{dL} \bigg|_{x=x^{(i)}} = 1.
$$

(81)

From figure 16(a), the 1RSB solution for $\phi_{d} = 0.9$ is stable against type I instability when $x\gamma < x^{(i)}\gamma \approx 3.07$. 

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6.4.2. Type II instability: fragmentation of states. In the 1RSB phase, vertex $k$ is characterized by a cavity energy function $E^V_k$ in each single state. In the 2RSB phase, some 1RSB single states split into different states in which some vertices are characterized by more than one cavity energy function. In the example illustrated in figure 15, a state with $E^V_k = E^V_c$ is fragmented into states with $E^V_k = E^V_s$ and $E^V_k = E^V_s$ on entering the 2RSB phase.

As the cavity energy functions of some vertices are modified during fragmentation, we examine the probability of changes in $E^V_i$ for a node $i$ due to changes in $E^V_j$ among its descendant nodes $j$, the so-called proliferation of bugs [36]. In the singlet regime, we denote $\pi^{k\rightarrow j}_{s\rightarrow c}$ as the joint probability that vertex $k \rightarrow j$ is in the $S$ state in the absence of bugs, and in the $C$ state in the presence of a small number of bugs. From the recursion equation (73), we note that contributions to $\pi^{j\rightarrow i}_{c\rightarrow s}$ come from the case where all descendents of $j$ are in the $S$ state, and one of them changes to the $C$ state in the presence of bugs. Hence

$$\pi^{j\rightarrow i}_{c\rightarrow s} = \delta_{\Lambda_1,-1} \frac{e^{-xu^2/2}}{Z_{j\rightarrow i}} \sum_{k \in L_j \setminus \{i\}} \pi^{k\rightarrow j}_{s\rightarrow c} \prod_{l \in L_j \setminus \{i,k\}} \psi^{j,l}_{s} e^{x\gamma}. \quad (82)$$

Similarly, contributions to $\pi^{j\rightarrow i}_{s\rightarrow c}$ come from the case where only one descendent of $j$ is in the $C$ state which changes to the $S$ state in the presence of bugs. Hence

$$\pi^{j\rightarrow i}_{s\rightarrow c} = \delta_{\Lambda_1,-1} \frac{e^{-xu^2/2}}{Z_{j\rightarrow i}} \sum_{k \in L_j \setminus \{i\}} \pi^{k\rightarrow j}_{s\rightarrow c} \prod_{l \in L_j \setminus \{i,k\}} \psi^{j,l}_{s}. \quad (83)$$
We define the matrix $V_{k \to j}(x)$ to be
\[
V_{k \to j}(x) = \delta_{j,j-1} \left( \prod_{l \in \mathcal{L}_j \setminus \{i,k\}} \psi_{s \to j} \right) e^{-xu_{2}/2} \mathbf{Z}_{j \to i}(0).
\]

The instability of the 1RSB solution against fragmentation of states can be thus examined by considering the maximum eigenvalue of the products of matrices $V$. We measure the quantity
\[
\lambda^{(II)}(L)(x) = (K-1)^{L} \mathcal{I}(V_{L-1}^{-1} V_{L-2}^{-1} \cdots V_0^{-1}),
\]
averaged over quenched disorders, where $\mathcal{I}(\cdots)$ is defined as the maximum eigenvalue of the matrix. The 1RSB solution is stable against the type II instability if $\langle \lambda^{(II)}(L)(x) \rangle \to 0$ as $L \to \infty$. $\langle \lambda^{(II)}(L)(x) \rangle$ can be solved using the population dynamics of equation (73) or by solving for the distribution on $P_L[\lambda^{(II)}(L), \psi^{(L)}_c]$ like for equation (79).

We show $\langle \lambda^{(II)}(L)(x) \rangle$ as a function of $L$ in figure 16(b) for $\phi_d = 0.9$ from $x_{\gamma} = 0$ to 4.5, and define $x^{(II)}$ using an expression similar to equation (81). From figure 16(b), the 1RSB solution for $\phi_d = 0.9$ is stable against type II instability when $x_{\gamma} < x^{(II)} \approx 2.93$.

$x^{(I)}$ and $x^{(II)}$ from $\phi_d = 0.78$ to 1, together with $x_s$ and $x_d$ obtained from the complexity curve, are plotted in figure 16(c) as a function of $\phi_d$. Reliable results for $\phi_d \approx \phi^A_d = 0.75$ are difficult to obtain as the continuous component in $Q(\psi_c)$ becomes extremely small (see, for instance, figure 12) and extremely high precision is required. For $\phi_d$ lower than $\approx0.88$, the 1RSB ansatz is stable in the range of $x^{(II)} < x < x^{(I)}$, corresponding to the shaded region in figure 16(c). Both $x_s$ and $x_d$ are found below the shaded region, indicating the instability of the physical segment of $\Sigma$. The stable range of $x$ lies on the negative segment of $\Sigma$, which implies that states with vanishing probability are stable in the 1RSB ansatz. For $\phi_d$ higher than $\approx0.88$, the shaded region disappears and all complexity curves are unstable. We thus conclude that the 1RSB quantities evaluated at $x_s$ and $x_d$ are unstable. Nevertheless, the agreement with simulation results shows that the 1RSB ansatz is a good approximation of the physical picture of the system.

7. Conclusion

In this paper, we have studied the source location problem on transportation networks. As the formulation involves continuous variables, the cavity fields are represented by the cavity energy functions which satisfy the piecewise quadratic ansatz. The ansatz decomposes the cavity energy functions into composite functions, and effectively parameterizes them using the energy minimum of each composite function.

This enables us to obtain a small closed set of cavity energy functions in the singlet regime, which greatly simplifies the functional RS recursions to simple recursions of probabilities. Physical results such as the average energy and the fraction of soft nodes are obtained and have excellent agreement with simulations when the fraction of deficient nodes is small. We examined the stability of the RS solution and derived the AT line for the transition to the RSB phase. In the high connectivity limit, such results are consistent with the RS instability obtained in the vertex cover problem for Poissonian graphs.
Though the solution of the 1RSB ansatz corresponds to a stable distribution of functionals, which is in general infeasible to solve, the closed sets of cavity energy functions greatly simplify the 1RSB recursions which make the 1RSB solution feasible. We remark that the analysis is applicable to regimes other than the singlet regime of the system, such as the commensurate points of the doublet regime considered in the appendix. In other cases, closed sets with a large number of functions are found and the 1RSB solution may once again become computationally infeasible. We expect the present techniques to be applicable to other problems where closed sets of cavity fields exist.

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Appendix. The doublet regime

A.1. The closed set of cavity energy functions and the simplified RS recursion

Besides the closed set of cavity energy functions \( E^V \) in the singlet regime, a closed set with countable elements of \( E^V \) can also be found in other regimes. In the doublet regime, we find that a small number of functions \( E^V \) spans a closed set at the commensurate points

\[
\gamma = m\kappa, \quad (A.1)
\]

with the rational number \( m \geq 2 \). These commensurate points correspond to the values of

\[
u^{-1} = -\sqrt{\frac{K(K-1)(m-1)}{(m-1)K+m+1}}, \quad (A.2)
\]

at which abrupt jumps in the fraction of source nodes are found in the range \( \sqrt{21/25} < \nu^{-1} < \sqrt{3/2} \) in figure 2 for \( K = 3 \). Each value of rational \( m \) corresponds to a switch of energetic stability from one configuration of consumer nodes to another.

To find the closed set of \( E^V \) in the doublet regime, we only have to consider the composite functions \( f_0, f_1 \) and \( f_2 \). \( E^V_k(y_k) \) is thus denoted as

\[
E^V_k(y_k) = (d_0^k, d_1^k, d_2^k). \quad (A.3)
\]

All other composite functions \( f_{n_k} \) with \( n_k \geq 3 \) have \( d_{n_k}^k > d_{n_k}^k \) and their corresponding configurations are not stable in the doublet regime. We thus consider only the recursions \( M(0, \ldots, 0) = 1 \) and \( M(1, 0, \ldots, 0) = 2 \). As an illustration, we consider the case \( m = 2 \) and \( \phi_d = 1 \) where a closed set of \( E^V \) is shown in figure A.1. The cavity energy change \( \Delta E_j \) from equation (30), and the constant terms \( d_0^j, d_1^j \) and \( d_2^j \) from equations (22) and (29) are simplified to

\[
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\]
The average optimized energy in the RS ansatz is obtained by evaluating the full energy change \( \Delta E \):

\[
\Delta E_j = \frac{n^2}{2} + \sum_{k \in \mathcal{L}_j \setminus \{i\}} \min(0, d^k_1, d^k_2),
\]

\( d^0_0 = 0, \quad d^1_1 = -2\kappa - \sum_{k \in \mathcal{L}_j \setminus \{i\}} \min(0, d^k_1, d^k_2), \quad d^2_2 = -\kappa + \min_{k \in \mathcal{L}_j \setminus \{i\}} d^k_1 - \sum_{k \in \mathcal{L}_j \setminus \{i\}} \min(0, d^k_1, d^k_2), \tag{A.4}
\]

where the zero point of \( E^V \) is set at the minimum values of \( f_0 \) for convenience of analysis. The energy change of \( \Delta E_j \) on adding vertex \( j \) is obtained by comparing the energies of the \( S \) states of the vertex and its descendents, and can be shown to produce the same physical results as the full energetic comparison. From the recursion relations, the full closed set of \( E^V \) is found to be

\[
E^V_a(y) = (0, -2\kappa, (-1 + r)\kappa)
\]

\[
E^V_c(y) = (0, -\kappa, (-1 + r)\kappa)
\]

\[
E^V_d(y) = (0, r\kappa, -1\kappa)
\]

\[
E^V_s(y) = (0, q\kappa, r\kappa) \tag{A.5}
\]

with integers \( q, r \geq 0 \). \( E^V_a \) corresponds to cavity states with a strong preference for being singly consuming; \( E^V_c \), \( E^V_d \) and \( E^V_s \) correspond to cavity states which are respectively singly consuming, doubly consuming and resource providing. They are denoted as the \( a, c, d \) and \( s \) states. Note that the integer \( r \geq 1 \) in equation (A.5) may correspond to the form of \( E^V \) where \( f_1 \) and \( f_2 \) are not relevant (see for instance figures A.1(f) and (g)). For \( K = 3 \), there are two forms of \( E^V_c \) with \( r = 0 \) and \( r \geq 1 \) and four forms of \( E^V_s \) with \((q, r) = (\geq 1, 1), (\geq 1, 0), (0, \geq 1) \) and \((0, 0) \). Hence the closed set of \( E^V \) has eight forms of \( E^V \) as shown in figure A.1.

Next, we consider the disordered case \( \phi_d < 1 \). The recursion relations can be simplified in terms of \( \psi^i_a, \psi^i_c, \psi^i_d \) and \( \psi^i_s \), corresponding to the probabilities for a vertex to be in the \( a, c, d \) and \( s \) states, as given by

\[
\psi^j_{a} = \delta_{\Lambda_j,-1} \prod_{k \in \mathcal{L}_j \setminus \{i\}} \psi^k_{a},
\]

\[
\psi^j_{c} = \delta_{\Lambda_j,-1} \sum_{k \in \mathcal{L}_j \setminus \{i\}} (\psi^k_{c} + \psi^k_{d}) \prod_{l \in \mathcal{L}_j \setminus \{i,k\}} \psi^l_{a}, \tag{A.6}
\]

\[
\psi^j_{d} = \delta_{\Lambda_j,-1} \sum_{k \in \mathcal{L}_j \setminus \{i\}} \psi^k_{d} \prod_{l \in \mathcal{L}_j \setminus \{i,k\}} \psi^l_{a},
\]

and \( \psi^j_{s} = 1 - \psi^j_{a} - \psi^j_{c} - \psi^j_{d} \). In the RS phase, we set \( \psi^j_{a}, \psi^j_{c}, \psi^j_{d}, \psi^j_{s} = 0, 1 \). The average optimized energy in the RS ansatz is obtained by evaluating the full energy change \( \Delta E_{\text{node}} \) and \( \Delta E_{\text{link}} \) resulting from the addition of new nodes and new
Figure A.1. A closed set of cavity energy functions $E_k(y)$ at $K = 3$, $u^{-1} = 1$ in the doublet regime. The forms of $E^V$ correspond to (a) the $a$ state, (b), (c) the $c$ state, (d) the $d$ state and (e)–(h) the $s$ state.

links. The expressions for $\Delta E_{\text{node}}$ and $\Delta E_{\text{link}}$ from equation (8) can be simplified as

$$
\Delta E_{\text{node}} = \delta_{\Lambda_n, -1} \left\{ \frac{u^2}{2} + \min \left[ \sum_{j \in \mathcal{L}_i} \min(0, d_1, d_2), -2\kappa, -\kappa + \min d_1 \right] \right\} 
+ \delta_{\Lambda_n, A} \sum_{j \in \mathcal{L}_i} \min(0, d_1, d_2).
$$

$$
\Delta E_{\text{link}} = \min \left[ 0, d_1^l, d_1^R, \frac{1}{K(K - 1)} + d_1^l + d_1^R, d_2^l, d_2^R \right].
$$

(A.7)

A.2. The instability of the RS ansatz

To obtain the AT line between the RS and the RSB phases, we consider the variations $\delta \psi^{a-j}_k, \delta \psi^{c-j}_k, \delta \psi^{d-j}_k$ and $\delta \psi^{s-j}_k$ in the recursions of probabilities in equation (A.6), with $\delta \psi^{a-j}_k + \delta \psi^{c-j}_k + \delta \psi^{d-j}_k + \delta \psi^{s-j}_k = 0$. Though the $c$ and $d$ states lead to different degeneracies of the full states, the two states play the same role in the recursion relations and lead to the same $\Delta E$, $\Delta E_{\text{node}}$ and $\Delta E_{\text{link}}$. Combining $\psi^{k-j}_c$ and $\psi^{k-j}_d$ in the recursions, the variations $\delta \psi^{a-j}_k, \delta (\psi^{k-j}_c + \psi^{k-j}_d)$ and $\delta \psi^{s-j}_k$ depend only on $\delta \psi^{s-j}_k$ for the descendents. We thus write down the AT condition for the disordered case of the doublet regime,

$$
\frac{\langle (\delta \psi^{s-j}_k)^2 \rangle}{\langle (\delta \psi^{s-j}_k)^2 \rangle} = (K - 1)(K - 2)\phi_d(1 - \langle \psi^{k-j}_s \rangle)\langle \psi^{k-j}_s \rangle K^{-3},
$$

(A.8)
where we have applied the relation $\langle (\psi_{s}^{k-j})^2 \rangle = \langle \psi_{r}^{k-j} \rangle$ in the derivation. Simple algebra leads to the following form for the AT line:

$$
\phi_d^{AT} = \frac{1}{(K-1)(K-2)(1-\langle \psi_s \rangle^{AT})(\langle \psi_s \rangle^{AT})K-3},
$$

$$(A.9)$$

where $\langle \psi_s \rangle^{AT}$ is the average value of $\psi_s$ on the AT line. The $K-\phi_d$ phase diagram is shown in figure A.2(a), which is compared to the phase diagram of the singlet regime in figure 11 inset. The comparison suggests that the RSB phase shrinks when $u^{-1}$ decreases from the singlet regime to the doublet regime.

### A.3. The 1RSB solution

To obtain the 1RSB solution, we follow the approach adopted in the singlet regime and evaluate the partition functions $\Xi_{\text{node}}$ and $\Xi_{\text{link}}$ using the full energy change $E_{\text{node}}$ and $E_{\text{link}}$. We solve the 1RSB solution for the case without disorder (i.e. $\phi_d = 1$) with the 1RSB restriction on the delta functional form of $Q\{P[E^V]\}$, i.e. $Q(\psi_a, \psi_c, \psi_d) = \delta(\psi_a - \langle \psi_a \rangle)\delta(\psi_c - \langle \psi_c \rangle)\delta(\psi_d - \langle \psi_d \rangle)$. The complexity function $\Sigma$ is obtained from the 1RSB solution for $K = 3$, and is shown in figure A.2(b). Compared against the singlet regime, the $\Sigma$ functions in the two cases have similar forms and similar maximum values. The physical segment of the curve is shown by the solid segment. Note that $e = (1 - f_C - f_D)/2 + f_C/6 + f_D/3$ and the fractions $f_C$ and $f_D$ of singly and doubly consuming nodes are not uniquely determined by the energy $e$. The negative segment of the complexity function approaches the limit of $e = 1/3$ as $x \to \infty$, as shown in the inset of figure A.2(b). It corresponds to the lowest possible energy on graphs with special

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structures, which occur with vanishing probability in the thermodynamic limit. \( e = 1/3 \) implies \( 4f_C + 3f_D = 2 \), suggesting the modulation limit of \( f_C = 1/2 \) when \( f_D = 0 \) as in the singlet regime, or the limit of \( f_D = 2/3 \) when \( f_C = 0 \) where two-thirds of nodes are doubly consuming.

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