Survey Propagation as local equilibrium equations

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It has been shown experimentally that a decimation algorithm based on Survey Propagation (SP) equations allows to solve efficiently some combinatorial problems over random graphs. We show that these equations can be derived as sum-product equations for the computation of marginals in an extended space where the variables are allowed to take an additional value \(\ast\) when they are not forced by the combinatorial constraints. An appropriate “local equilibrium condition” cost/energy function is introduced and its entropy is shown to coincide with the expected logarithm of the number of clusters of solutions as computed by SP. These results may help to clarify the geometrical notion of clusters assumed by SP for the random K-SAT or random graph coloring (where it is conjectured to be exact) and helps to explain which kind of clustering operation or approximation is enforced in general/small sized models in which it is known to be inexact.

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I. INTRODUCTION

Recent developments in statistical physics of disordered systems have shown a remarkable convergence of themes with other disciplines such as computer science (e.g. combinatorial optimization \([1]\)), information theory (e.g. error correcting codes \([2]\)) and discrete mathematics (e.g. random structures \([3, 4, 5]\)). While the study of a typical static measure characterizing the slow dynamics of both physical and algorithmic processes is the unifying issue in out-of-equilibrium problems, the study of the geometrical structure of ground states of spin-glass-like energy functions \(E\) is central to the understanding of the onset of computational complexity in random combinatorial problems. The combinatorial problem of satisfying a given set of constraints is viewed in the physics framework as the problem of minimizing \(E\) and “ground state configurations”, “solutions” or “satisfying assignments” should be understood as synonymous.

Important in an attempt of providing a complete theory of random combinatorial problems is the notion of pure states, or clusters of configurations, on which the probability measure over optimal configurations is assumed to concentrate. Recently, a new class of algorithms has been proposed \([8, 9, 10]\) that have shown surprising capabilities in dealing with the (exponential) proliferation of clusters of metastable states and therefore in solving random instances of combinatorial problems which are difficult to solve for local search heuristics. Such algorithms are based on the so called Survey Propagation (SP) equations in which indeed a decomposition of the ground states probability distribution – the Gibbs measure – into an exponential number of clusters is assumed from the beginning. The SP equations can be viewed as zero temperature cavity equations \([20]\) formulated for single instances at a level equivalent to the one-step of replica symmetry breaking (1-RSB) scenario \([27]\).

The SP algorithm consists in a message-passing technique which is closely related to another message-passing method – known as sum-product or Belief Propagation (BP) \([11, 12]\) algorithm – which have shown amazing performance for solving the decoding problem \([13]\) in error correcting codes based on sparse graph encodings \([14, 15, 16, 17, 18, 19]\).

The aim of this study is to discuss the precise (finite size) structure of the SP equations, linking them to the BP formalism. This is a well defined mathematical issue, independent on the physical origin of the equations. Due to the algorithmic relevance of both BP and SP for coding theory and combinatorial optimization, it is a basic question to understand what these equations are doing for a finite number of variables \(N\) since this is the regime in which they are used.

As we shall see, the SP “algorithmic” equations at finite \(N\) are performing a very specific clustering operation over the solution space. Moreover, the number of such clusters in the Bethe approximation will be shown to coincide with the prediction of the cavity theory.
These results will be obtained by showing that the SP equations are the BP equations for a modified combinatorial problem. By this mapping we clarify how the hypothesis making BP exact (that is, uncorrelation of distant variables) translate onto a condition of uncorrelation of "frozen" variables belonging to different clusters: SP produces a collapse of the internal structure of clusters and eliminates correlations among the unfrozen parts.

We shall present the results in the case of the K-SAT problem even though the method could be applied to any discrete combinatorial model defined over locally tree-like graphs. The results concerning the cluster entropy will be compared with the prediction of the 1-RSB cavity analysis for random K-SAT.

The line of reasoning of the paper consists in showing that the SP equations can be re-derived as sum-product or BP equations – i.e. simple replica symmetric (RS) cavity equations – over an extended configuration space. The definition of this space consists in associating to each binary variable a new extra value "∗" which will correspond to the possibility that the variable is not forced to take one of the binary values \{-1, +1\} in a given solution [28]. We will introduce a local equilibrium condition (LEC) cost-energy function \(\hat{E}\) derived from \(E\), acting over the extended space, together with a (technical) duality transformation needed to preserve the locality of the interactions for implementing properly the BP equations. The following two statements will hold:

1. **Marginals given by the BP equations derived from \(\hat{E}\) coincide with the marginals given by SP on the original problem.**

2. **Bethe approximation to the entropy of \(\hat{E}\) in the enlarged space as computed by BP coincides with the logarithm of the number of clusters of solutions – the so called “complexity” – predicted by SP on the original problem.**

The proof of (I) will be achieved by finding a direct connection between quantities (“messages”) propagated by the two algorithms at each iteration step. We recall that the Bethe approximation to the entropy is exact over trees without and with boundary conditions, i.e. with leaf variables taking given values.

The possibility of interpreting SP as appropriate BP equations may have consequences for their rigorous probabilistic analysis, through a proper application/generalization of the known methods for the analysis of convergence of BP like equations over random graphs (as it has already been done for problems like the random matching [3]). Some preliminary exact numerical results that we give in the concluding section are in support of this possibility.

Throughout the paper we heavily rely on the notations of refs. [9, 10] for what concerns the SP equations.

### II. SURVEY PROPAGATION, BELIEF PROPAGATION AND K-SAT

SP and BP (or sum-product) are examples of message-passing procedures. In BP the unknowns which are evaluated by iteration are the marginals over the solution space of the variables characterizing the combinatorial problem (e.g. binary “spin” variables). According to the physical interpretation, the quantities that are evaluated by SP are the probability distributions of local fields over the set of clusters. That is, while BP performs a “white” average over solutions, SP takes care of cluster to cluster fluctuations, telling us which is the probability of picking up a cluster at random and finding a given variable completely biased (frozen) in a certain direction – that is forced to take the same value within the cluster – or unfrozen.

In both SP or BP one assumes to know the marginals of all variables in the temporary absence of one of them and then writes the marginal probability induced on this “cavity” variable in absence of another third variable interacting with it (i.e. the so called Bethe lattice approximation for the problem). These relations define a closed set of equations for such cavity marginals that can be solved iteratively (this fact is known as message-passing technique). The equations become exact if the cavity variables acting as inputs are uncorrelated. They are conjectured to be an asymptotically exact approximation over some random locally tree-like structures [2].

The \(K\)-satisfiability problem (K-SAT) is easily stated: Given \(N\) Boolean variables each of which can be assigned the value True (1) or False (-1), and \(M\) clauses between them, is there a 'SAT-assignment', i.e. an assignment of the Boolean variables which satisfies all constraints? A clause takes the form of an ‘OR’ function of \(K\) variables in the ensemble (or their negations). A SAT formula in conjunctive normal form over \(N\) Boolean variables \(\{\sigma_i = \pm 1\}\) can be written as

\[
\mathcal{F} = \prod_{a \in A} C_a
\]

where

\[
C_a = 1 - E_a, \quad E_a \equiv \prod_{i \in a} \delta(J_{a,i}, \sigma_i)
\]
where \( \delta(x, y) \) is the Kronecker function (also written as \( \delta_{x,y} \) in the rest of the paper) and \( \{ C_a \} \) are the clauses encoded by the parameters \( J_{a,i} \) as follows: \( J_{a,i} = \pm 1 \) if respectively \( \pm \sigma_i \) appears in clause \( a \) (in Boolean notation we would have \( J_{a,i} = -1 \) (resp. \(+1\)) if the Boolean variable \( x_i \) (resp. \(-x_i\)) appears in clause \( a \)). We call \( E_a \) the “energy” of a clause. The symbol \( i \in a \) will denote the set of variables participating in clause \( a \). Additionally it will be useful to use the symbol \( a \in i \) to denote the set of clauses depending on variable \( i \). The clause size \( |\{i : i \in a\}| \) will be denoted by \( n_a \) (\( n_a \equiv K \) for K-SAT), and the variable connectivity \( |\{a : a \in i\}| \) will be denoted by \( n_i \).

The satisfiability problem consists in determining the existence of an assignment to the Boolean variables which satisfies all clauses at the same time, that is such that \( \mathcal{F} = 1 \). We may write the energy function which counts the number of violated clauses as \( E = \sum_a E_a \) so that the satisfiability problem becomes finding the zero energy ground states of \( E \). The random version of K-SAT corresponds to the case in which the variables appearing in each clause are chosen uniformly at random, and negated with probability \( \frac{1}{2} \). For the sake of simplicity, hereafter we concentrate mostly on the 3-SAT case.

The energy function \( E \) of a random 3-SAT formula is a spin glass model defined over a locally tree-like graph that can be studied with the techniques of statistical physics of random systems, namely the replica and cavity methods.

Numerical experiments have shown that a decimation algorithm based on SP equations allows to find satisfying assignments of critically constrained random 3-SAT instances – that is random formulas with \( \alpha = M/N \) just below a critical ratio \( \alpha_c \approx 4.267 \) where formulas are conjectured to become unsatisfiable with high probability – with a computational cost roughly scaling as \( N \log N \) while the other known algorithms typically take times that are exponential in \( N \). According to the cavity – or SP – analysis, in such hard region (more precisely for \( \alpha \in [4.15, 4.267] \) there is a genuine one step RSB phase, in which the space of solution decomposes into an exponential number of clusters and where metastable states are even more numerous.

As discussed in great detail in ref. 21, one crucial feature that comes out from the SP analysis is the distinction between frozen and unfrozen variables within the different clusters and we shall introduce a formalism which naturally incorporates such phenomenon (see also refs. 22).

We want to represent the condition for a variable of being not forced to take any specific value in a given ground state (unfrozen) and to this end we consider configuration space of 3-value variables \( s_i \in \{-1,*,1\} \) instead of \( \sigma_i \in \{-1,1\} \).

We observe that \( C_a \) as defined in Eq. (2) can be evaluated also in extended variables: it behaves as if variables with the * value could be chosen to the best of \(-1\) or \(1\) and thus satisfy the clause. This gives the name “joker state” to the value *. For a configuration \( s^{(i,x)} \) such that \( s_i^{(i,x)} = x \) and \( s_j^{(i,x)} = s_j \) for \( j \neq i \) call

\[
C^{i,x}_a(s) = C_a(s^{(i,x)})
\]

and introduce the constrain over \( \{-1,*,1\}^n \) configurations given by

\[
V_i = \delta_{s_i,*} \prod_{a \in I} C^{a,-1}_a C^{a,1}_a + \sum_{\sigma=\pm 1} \delta_{s_i, \sigma} \prod_{a \in I} C^{a,\sigma}_a \left( 1 - \prod_{a \in I} C^{a,-\sigma}_a \right)
\]

The LEC formula derived from \( \mathcal{F} \) will be defined as

\[
\mathcal{G} = \prod_i V_i.
\]

Note that \( V_i \) depends only on \( (s_j)_{j \in a, a \in i} \) and therefore preserves the “locality” of the structure, if any, of the original formula. A solution of the LEC problem is a configuration \( s = (s_i)_{i \in I} \in \{-1,*,1\}^n \) such that \( \mathcal{G}(s) = 1 \). As a particular case, a solution \( \mathcal{G}(s) = 1 \) such that \( s_i \in \{\pm 1\} \) is also a solution of \( \mathcal{F} \).

To fix ideas it might be useful to compare the LEC cost-energy function with the original 3-SAT one. To this end we adopt the so-called factor graph representation 22: Given a formula \( \mathcal{F} \), we define its associated factor graph as a bipartite undirected graph \( G = (V; E) \), having two types of nodes, and edges only between nodes of different type: (i) Variable nodes, each one labeled by a variable index in \( I = \{1,\ldots,N\} \) and (ii) Function nodes, each one labeled by a clause index \( a \in A \) (\(|A| = M\)). An edge \((a, i)\) will belong to the graph if and only if \( a \in i \) or equivalently \( i \in a \). For instance, the factor graph representation of the random 3-SAT problem consists in a bipartite graph with \( N \) variable nodes having a Poisson random connectivity of mean \( 3\alpha \) and \( M \) function nodes with energy \( E_a \) of uniform connectivity 3 (a portion is shown in part (a) of Fig. 1). The extended LEC spin glass energy function reads:

\[
\hat{E} = \sum_{a=1}^M \hat{E}_a + \sum_{i=1}^N A_i
\]
where now $\hat{E}_a = 1 - C_a$ is evaluated in the extended configuration space and

$$A_i = \delta_{s_i,\star} \left( 1 - \delta_{E_i^{-1},E_i^1} \right) + \sum_{\sigma = \pm 1} \delta_{s_i,\sigma} \theta \left( E_i^\sigma - E_i^{-\sigma} \right)$$

(7)

with $E_i^\sigma = \sum_{a \in i} (1 - C_i^{a,\sigma})$ and $\theta(x) = 1$ if $x > 0$ and 0 otherwise. The factor graph of the LEC has $N$ additional function nodes (the $A_i$ terms enforcing the joker condition) that extend over the second neighbors (inset (b) in Fig. 1).

By inspecting Eq. (5) we notice a first problem, namely that we have lost the locally tree-likeness of the original graph. There are interactions between every (ordered) pair of neighbors variable nodes $i, j \in a$ (in the original graph), and thus for instance every such pair shares two constraints $V_i, V_j$ (making an effective 2-loop). This introduces an obvious problem for implementing BP over this combinatorial problem, and moreover would make difficult to compare both algorithms, as the underlying geometry is now different. Fortunately, there is an easy (but unfortunately notationally somewhat involved) way out. We will group together neighbor variables, effectively performing a sort of duality transformation over the graph. We describe the procedure explicitly below (Note that this is a particularly simple case of a Kikuchi or “generalized belief propagation”-type approximation [26]).

We will define: (i.) $M$ multi state variables each one corresponding to a tuple $t_a = \{t_a^{(i)}\}_{i \in a} (t_a^{(i)} \in \{-1, \star, 1\})$ and “centered” on $a$ clauses and have (uniform) connectivity $n_a$ (c) in Fig. 1, and (ii.) $N$ function nodes $\chi_{i \in a}^{dbp}$ having Poisson connectivity, depending on $T_i \equiv \{t_a\}_{a \in i}$ and enforcing both the joker state condition as well as identifying the values of the single variables $t_a^{(i)}$ shared by different tuples $a \in i$ (d) in Fig. 1. An explicit expression of $\chi_{i \in a}^{dbp}(T_i)$ (conf. Eq. (4)) is

$$\chi_{i \in a}^{dbp} = \sum_{\{s_i\}} \left( \prod_{a \in i} \delta_{s_i^{(i)},s_i} \right) \left( \delta_{s_i,\star} \prod_{a \in i} C_{a}^{s_i,1} + \sum_{\sigma = \pm 1} \delta_{s_i,\sigma} \prod_{a \in i} C_{a}^{s_i,\sigma} \right) \left( 1 - \prod_{a \in i} C_{a}^{s_i,-\sigma} \right)$$

(8)

We shall refer to the BP equations over the dual graph as Dual BP (DBP).

III. SP EQUATIONS AS BP EQUATIONS OVER THE DUAL GRAPH

Basic SP and DBP iterations can be thought of as transformations in the space of probability distributions of the signs $h_i = \{-1, 0, 1\}$ of the effective fields acting on the single spin variables and of the tuples $t_a = \{-1, \star, 1\}^{n_a}$ in the dual graph. In the cavity notation the quantities that are iterated refer to a graph in which a given node and all its neighbor nodes are temporarily eliminated (see Fig. 1(a) and (d)) and all quantities are labeled by oriented
indices of the type $a \to i$ or $i \to a$ where the node on the right of the arrow is the one eliminated. Therefore the equations describe a local transformation of some input probability distributions into an output distribution in which a characteristic function $\chi$ eliminates contributions from those combinations of input and output fields or variables that violate some kind of local constraints (it is worth noticing that these cavity equations are closely related to the iterative local equations of the so called Objective Method of combinatorial probability). Explicitly we have:

**DBP equations:**

$$P_{a \to i}^{dbp} (t_a) \propto \sum_{\{t_b\} j \in a \setminus i} \prod_{j \in b} C_b \cdot \prod_{j \in b \setminus a} P_{b \to j}^{dbp} (t_b)$$  \hspace{1cm} (9)

**SP equations:**

$$P_{j \to a}^{sp} (t_j) \propto \sum_{\{h_k\}} \chi_{j \to a}^{sp} (h_j, \{h_k\}) \prod_{b \in j \setminus a} \prod_{k \in b \setminus j} P_{k \to b}^{sp} (h_k)$$  \hspace{1cm} (10)

where

$$\chi_{j \to a}^{sp} = \delta_{h_j, \sigma} \prod_{b \in j \setminus a} C_b^{ij -1} + \sum_{\sigma=\pm 1} \delta_{h_j, \sigma} \prod_{b \in j \setminus a} C_b^{ij \sigma} \left(1 - \prod_{b \in j \setminus a} C_b^{ij -\sigma}\right)$$  \hspace{1cm} (11)

$C_b$ clauses are here evaluated in $\{(h_k)_{k \in b \setminus j}, h_j\}$.

In order to show the connection between the above equations it is convenient to introduce an auxiliary transformation $\tau$ of a similar type:

**$\tau$ transformation:**

$$P_{a \to i}^{\tau} (t_a) \propto \sum_{\{h_j\}} \prod_{j \in a \setminus i} \chi_{j \to a}^{\tau} (t_a, h_j) P_{j \to a} (h_j)$$  \hspace{1cm} (12)

and

$$\chi_{j \to a}^{\tau} = \sum_{\sigma=\pm 1} C_a \delta_{h_j, \sigma} \delta_{i, \sigma^*} + \delta_{h_j, \sigma^*} \left[ \delta_{i, \sigma^*} C_a^{ij -1} + \sum_{\sigma=\pm 1} \delta_{i, \sigma^*} C_a^{ij \sigma} (1 - C_a^{ij -\sigma}) \right]$$  \hspace{1cm} (13)

$C_a$ terms are evaluated here in $t_a$.

We will drop now the argument dependence of the measures $P_{j \to a}^{sp}$, $P_{a \to i}^{dbp}$ and $P_{j \to a}^{\tau}$ and make instead explicit the dependence on the input probability measures $\{P_{k \to b}\}$, $\{P_{b \to j}\}$, $\{P_{j \to a}\}$ respectively.

The connection between $DBP$ and $SP$ can be written as follows:

$$P_{a \to i}^{dbp} (\{P_{k \to b}\}) = P_{a \to i}^{sp} (\{P_{j \to a}\})$$  \hspace{1cm} (14)

where both sides of the (functional) equality in turn depend on some arbitrary set of probability distributions $\{P_k(h_k)\}$ where $k \in b \setminus j$ for $b \in j \setminus a$ and finally $j \in a \setminus i$. In short,

$$P^{dbp} \circ P^{\tau} \equiv P^{\tau} \circ P^{sp}$$  \hspace{1cm} (15)

In order to check the validity of the above identity we observe that a direct inspection of the composition shows that it is true if for every $j \in a \setminus i$ the following condition among the characteristic functions holds:

$$\sum_{\{h_j\}} \chi_{j \to a} \chi_{j \to a}^{sp} = \sum_{\{t_b\}} \chi_{j \to a}^{dp} \prod_{b \in j \setminus a} \prod_{k \in b \setminus j} \chi_{k \to b}$$  \hspace{1cm} (16)

In appendix we display the proof that this identity holds and, as a consequence, that also identity Eq. (16) is valid. Eq. (16) in turn implies that

$$(P^{dbp})^{(k)} \circ P^{\tau} \equiv P^{\tau} \circ (P^{sp})^{(k)}$$  \hspace{1cm} (17)
where the \((k)\) exponent means composition. This in turn implies that we have a direct step-by-step connection between the elementary quantities used in the DBP equations and those used in the SP equations: convergence is obtained simultaneously and Eq. (15) holds for the respective fixed points. It is straightforward to compute from the DBP equations the marginals \(P_i^{dbp}(s_i)\) of the single variables as a marginalization of \(P_a^{dbp}(t_a)\) for some \(a \in i\) with respect to all other variables in the clause, (on a fixed point, it doesn’t matter which \(a \in i\) one chooses). One finds that the marginals predicted by DBP are in one to one correspondence with the local fields given by SP, that is \(P_i^{dbp}(s_i = -1, *, 1)\) coincides respectively with \(P_i^{sp}(H_i = -1, 0, 1)\) (see refs. [10, 11]).

A. Clustering and whitening

The marginals over \(\{1, *, -1\}^N\) given by SP/DBP acquire a computational/physical significance once we interpret what solutions of combinatorial problem defined by Eq. (5) mean in term of clusters (or groups) of solutions of the original problem defined by Eq. (1). We will first define the Hamming distance between configurations \(s, t \in \{1, *, -1\}^n\), \(H(s, t) = |\{i : s_i \neq t_i\}|\) and an ordering relation over \(\{-1, *, 1\}\) configurations: if \(s, t \in \{1, *, -1\}^n\) we say that \(s \leq t\) iff \(t_i \neq s_i\) implies that \(t_i = *\). For instance, \((0, 1) \leq (0, *)\) and \((1, 1, 1) \leq (1, *, *)\) but \((0, 1) \not\leq (1, *)\).

We will say that a configuration \(s \in \{\pm 1\}^n\) is contained in \(t \in \{\pm 1\}^t\) if \(s \leq t\). In this sense, “clustering” would mean, starting with some set \(S \subset \{\pm 1\}^n\) of solutions of the original combinatorial problem, to find some set \(T \subset \{1, *, -1\}^t\) such that every \(s \in S\) is contained in some \(t \in T\). Of course, one would like to do so in some maximal way, but satisfying some kind of separation between different clusters.

One trivial observation about the set \(G = 1\) is that solutions are by force separated, in the sense that \(H(s, t) > 1\) if \(G(s) = G(t) = 1\) and \(s \neq t\). To prove this, suppose that \(H(s, t) = 1\). If their difference comes because \(s_i = \pm 1\) and \(t_i = *\) then by force one of \(V_i(t)\) or \(V_i(s)\) is clearly violated. If on the contrary, it comes because \(s_i = 1\) and \(t_i = -1\) or viceversa, then by force both of \(V_i(t)\) and \(V_i(s)\) are violated and the only possible “correct” value for \(s_i\) is *.

A more important observation is that every solution of \(\mathcal{F} = 1\) is contained in a solution of \(G = 1\) with the minimal number of *s, and that solution can be easily found. Take a solution \(x \in \mathcal{F} = 1\), and suppose that \(G = 0\). Choose a \(V_i\) such that \(V_i = 0\). It can be easily seen that by replacing \(x_i\) by *s, then \(V_i\) becomes 1. Then we pick another violated constrain and repeat the process, until \(G = 1\). We will call the resulting configuration \(w(x)\) (this procedure has been already used under the name of whitening in the context of graph coloring by G. Parisi in [22]). It is easy to prove that the result of this procedure does not depend on the order in which you pick variables violating nodes \(V_i\) (the proof being that any violated \(V_i\) will continue to be violated in the procedure, exactly until we switch \(x_i\) to *), and so \(w(x)\) is uniquely defined. Note that two configurations \(x, y\) at Hamming distance \(H(x, y) = 1\) will have \(w(x) = w(y)\) and so every solution in a fixed connected component of the solution space will end up inside the same “cluster”. An example of the whitening procedure for some set of solutions is depicted in Figure [4]. An interesting point of view is that if one tries to build from scratch a Hamiltonian to describe the behaviour of the outcomes of the whitening procedure of some SAT formula, Eq. (15) comes naturally.

The reader should note however that the presented definition of clustering is far from perfect in the worst case: there is a number of systematic errors produced by the whitening. For instance, in Figure [4] we can see one cluster claiming an uncorrectly large volume. And there is of course also another problem: unfortunately, there is no warranty that the sole solutions of \(G = 1\) are the ones of the whitening, and in fact small counter-examples can be easily constructed. Numerical work is being done to ascertain a quantification of these two types of errors ([32]).

IV. ENTROPY AND COMPLEXITY

The equivalence between the DBP marginals and the SP local field probability distributions has the direct consequence that the Bethe approximation to the entropy on the dual graph, \(S^{dbp}\), coincides with the logarithm of the
number of clusters of solutions predicted by SP, the so called complexity $\Sigma$.

On general grounds the Bethe approximation to the entropy of a problem is exact if correlations among cavity variables can be neglected (i.e. the global joint probability distribution takes a factorized form). This is certainly true over tree graphs and it is conjectured to be true in some cases for locally tree-like random graphs in the limit of large size (one informal explanation is that distance between cavity variables diverges with probability tending to one). Factorization of marginal probabilities over our dual factor graph amounts at writing $P(\{t_a\}) = \prod_{i \in I} P_{i}^{dbp}(T_i) \prod_{a \in A} [P_{a}^{dbp}(t_a)]^{1-n_a}$ where $P_{i}^{dbp}(T_i)$ is the joint probability distribution of the triples connected to node $i$ ($T_i \equiv \{t_b\}_{b \in i}$) and $P_{a}^{dbp}(t_a)$ is the single triple marginal. Under this condition the entropy reads

$$S = - \sum_i \sum_{\{T_i\}} P_{i}^{dbp}(T_i) \log P_{i}^{dbp}(T_i) + \sum_{a} (n_a - 1) \sum_{\{t_a\}} P_{a}^{dbp}(t_a) \log P_{a}^{dbp}(t_a). \quad (18)$$

Showing $S = \Sigma$ is a straightforward calculation that we report in the appendix. It requires to express the entropy in terms of the cavity fields given by SP exploiting both Eq. (15) and the fixed point conditions. One finds

$$S = \sum_{i} \log c_{i} - \sum_{a} (n_a - 1) \log c_{a} - \sum_{i} \sum_{a \in i} \log D_{a \rightarrow i} \quad (19)$$

where the three normalization constants are defined by

$$c_{i} = \sum_{\{T_i\}} \prod_{a \in i} P_{a \rightarrow i}(t_a) \chi_i(T_i) \quad (20)$$

$$c_{a} = \sum_{t_a} \sum_{\{h_j\}} \prod_{j \in a} P_{j \rightarrow a}(h_j) \chi_{j \rightarrow a}^\tau(h_j, t_a) \quad (21)$$

$$D_{a \rightarrow i} = \sum_{t_a} \sum_{\{h_j\}} \prod_{j \in a \setminus i} P_{j \rightarrow a}(h_j) \chi_{j \rightarrow a}^\tau(h_j, t_a) \quad (22)$$

These constants are not independent and the explicit expressions of the first two are sufficient for writing $S$ in terms of SP quantities:

$$c_{a} = \sum_{\{h_j\}} \prod_{j \in a} P_{j \rightarrow a}(h_j) \sum_{\{t_a\}} \prod_{j \in a} \chi_{j \rightarrow a}^\tau(h_j, t_a) \quad (23)$$

$$= 1 - \sum_{\{h_j\}} \prod_{j \in a} P_{j \rightarrow a}(h_j) \left( 1 - \sum_{\{t_a\}} \prod_{j \in a} \chi_{j \rightarrow a}^\tau(h_j, t_a) \right) \quad (24)$$

$$= 1 - \prod_{j \in a} P_{j \rightarrow a}(J_{a, j}) \quad (25)$$

$$= 1 - \prod_{j \in a} \left( \frac{\Pi_{j \rightarrow a}^\tau}{\Pi_{j \rightarrow a}^0 + \Pi_{j \rightarrow a}^\tau + \Pi_{j \rightarrow a}^\nu} \right) \quad (26)$$

where we have borrowed the notation of Eq. (18) in [10]. For computing $c_i$ we first notice that

$$P_{a \rightarrow i}(t_a) = D_{a \rightarrow i} \sum_{\{h_j\}_{j \in a \setminus i}} \chi_{j \rightarrow a}^\tau(t_a, h_j) \prod_{j \in a \setminus i} P_{j \rightarrow a}(h_j) \quad (27)$$
so that Eq. (20) reads

\[ c_i = \prod_{a \in i} D_{a \rightarrow i} \sum_{\{H_i\}} \chi_i (T_i) \prod_a \prod_{j \in a \setminus i} \chi^c_j (t_a, h_j) P_{j \rightarrow a} (h_j) \]

\[ = \prod_{a \in i} D_{a \rightarrow i} \sum_{\{H_i\}} \chi^c_i (H_i) \prod_a \prod_{j \in a \setminus i} P_{j \rightarrow a} (h_j) \]

\[ = \prod_{a \in i} D_{a \rightarrow i} \left( \hat{\Pi}^+_i + \hat{\Pi}^0_i + \hat{\Pi}^-_i \right) \]  

in the notations of Eq. (21) in [10]. Finally, plugging these expressions into Eq. (19) and calling

\[ w_i = \hat{\Pi}^+_i + \hat{\Pi}^0_i + \hat{\Pi}^-_i \]

\[ x_{i \rightarrow a} = \Pi^+_j + \Pi^0_j + \Pi^-_j \]

\[ y_{i \rightarrow a} = \Pi^a_j \]  

we get from Eq. (19)

\[ S = \sum_i \log w_i - (n_a - 1) \sum_a \log \left( 1 - \prod_{j \in a} \frac{y_{i \rightarrow a}}{x_{i \rightarrow a}} \right) \]  

(30)

In this expression, \( w_i \) represents the probability the local field acting on the spin variable \( i \) does not produce a contradiction and \( 1 - \frac{w_{i \rightarrow a}}{x_{i \rightarrow a}} \) is the probability that the cavity fields satisfy clause \( a \).

We recall that the expression of the SP complexity \( \Sigma \) defined in Eq. (25-27) in [10] is

\[ \Sigma = \sum_i (1 - n_i) \log w_i + \sum_a \log \left( \prod_{i \in a} x_{i \rightarrow a} - \prod_{i \in a} y_{i \rightarrow a} \right) \]

\[ = \sum_i \log w_i - \sum_a \sum_{i \in a} \log w_i + \sum_a \log \left( \prod_{i \in a} x_{i \rightarrow a} - \prod_{i \in a} y_{i \rightarrow a} \right) \]  

(31)

Despite their different look, it turns out that Eq. (30) and Eq. (31) are identical if evaluated in a fixed point of the SP equations. Their difference

\[ \Sigma - S = \sum_a \left\{ - \sum_{i \in a} \log w_i + n_a \log \left( 1 - \prod_{i \in a} \frac{y_{i \rightarrow a}}{x_{i \rightarrow a}} \right) - \sum_{i \in a} \log x_{i \rightarrow a} \right\} \]  

(32)

is zero since in the fixed point every term inside the curly brackets vanishes: using Eq. (17) in [10] we have that \( \eta_{a \rightarrow i} = \prod_{j \in a \setminus i} \frac{y_{j \rightarrow a}}{x_{j \rightarrow a}} \), i.e. \( \prod_{j \in a} \frac{y_{j \rightarrow a}}{x_{j \rightarrow a}} = \eta_{a \rightarrow i} \frac{y_{i \rightarrow a}}{x_{i \rightarrow a}} \) for every \( i \in a \) and hence

\[ n_a \log \left( 1 - \prod_{j \in a} \frac{y_{j \rightarrow a}}{x_{j \rightarrow a}} \right) = \sum_{j \in a} \log \left( 1 - \eta_{a \rightarrow i} \frac{y_{i \rightarrow a}}{x_{i \rightarrow a}} \right) \]  

(33)

A simple calculation shows that \( w_i = x_{i \rightarrow a} - \eta_{a \rightarrow i} y_{a \rightarrow i} \) for every \( a \in i \) and therefore we get \( \Sigma = S \) as desired.

### V. DISCUSSION AND CONCLUSIONS

In this work we have shown by elementary means that the SP equations can be interpreted and derived as sum-product equations for the marginals over a modified combinatorial problem. An important consequence of this fact is a clarification of the hypothesis behind the algorithm. It is to be expected that the essential hypothesis making sum-product to work is the uncorrelation of the marginals of distant (or cavity) variables. Under the shown mapping, this directly implies that the hypothesis behind SP (and in a way, of its definition of clusters) is the uncorrelation of the frozen part of distant variables, that is the uncorrelation between different clusters.

Under this light one can think of the SP procedure of obtaining \( \hat{E} \) from \( E \) as a way of collapsing the internal structure of pure states: the resulting problem \( \mathcal{G} \) has many pure states but with zero internal entropy. Note that this
is a completely different limit case with respect to the “one pure state” in which BP (more precisely DBP) is shown to work correctly and to predict an accurate entropy (which we remind is the complexity of the original $E$).

As far as the connection between solutions of the modified problem and the original one is concerned, things are particularly simple over tree factor graphs (see also [10] for results concerning propagation of messages): Indeed, for any fixed boundary condition (i.e. an assignment for the leaf variables), there is at most one solution with $\hat{E} = 0$, and it is easy to prove (see appendix [C]) that all solutions of $\hat{E} = 0$ correspond to the same connected component of the solution space (i.e. every two solutions can be joined by a path of solutions in which successive configurations in the path differ by exactly one spin flip).

The situation on loopy graphs (corresponding for instance to random formulae) is obviously more complicated. A coherent interpretation would be that not only the recursive DBP/SP equations themselves are accurate in a probabilistic sense (i.e. when the factorization of the corresponding input joint probability is sound) to compute the statistics of the ground states of $\hat{E}$, but also that the exactness of the interpretation of the ground states of $\hat{E}$ in terms of clustering of the ground states of $E$ relies on this hypothesis being true.

To this extent we mention that exact enumerations on a large number (thousands) of small random 3-sat formulas (up to $N = 100$) showed that all the zero energy configurations of $\hat{E}$ which are stable under SP iterations can be extended to real solution of the original problem. Spurious ground states (i.e. configurations that are not extensible to real solutions) do exist with a non negligible probability for small $N$, however they turn out to be always unstable fixed points of SP , that is unsat configurations which are irrelevant for the SP marginals [32]. While such a result was expected to hold for tree-like graphs, it is somewhat surprising to observe it numerically on small, loopy, random factor graphs. The robustness of such result calls for a finite extended to real solution of the original problem. Spurious ground states (i.e. configurations that are not extensible over tree factor graphs (see also [10] for results concerning propagation of messages): Indeed, for

$\chi_{j \rightarrow a}^{\bar{a}} = \delta_{t_{a}^{(j)} \sigma} \prod_{b \in j \setminus a} C_{b} \left( 1 - \prod_{b \in j \setminus a} C_{b}^{j, -\sigma} \right)$

(A1)

If $h_{j} = \bar{a}$ then

$\chi_{j \rightarrow a}^{\bar{a}} = \delta_{t_{a}^{(j)} \sigma} C_{a}^{j, -\sigma} + \sum_{\sigma = \pm 1} \delta_{t_{a}^{(j)} \sigma} C_{a}^{j, \sigma} \left( 1 - C_{a}^{j, \sigma} \right)$

(A2)

Summing up both products and regrouping the LHS of Eq. (10) reads:

$\sum_{\sigma = \pm 1} \delta_{t_{a}^{(j)} \sigma} C_{b}^{j, \sigma} \left( 1 - \prod_{b \in j} C_{b}^{j, -\sigma} \right) + \delta_{t_{a}^{(j)} \sigma} C_{b}^{j, -\sigma}$

(A3)

where $C_{b}$ for $b \in j \setminus a$ is evaluated here in $\left( \{ h_{k} \}_{k \in b \setminus j}, t_{a}^{(j)} \right)$ and $C_{a}$ is evaluated in $t_{a}$.

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APPENDIX A: PROOF OF EQUIVALENCE

For the LHS of Eq. (10) we have:

If $h_{j} = \sigma \in \{ \pm 1 \}$ then

If $h_{j} = \bar{a}$ then

$\chi_{j \rightarrow a}^{\bar{a}} = \delta_{t_{a}^{(j)} \sigma} \prod_{b \in j \setminus a} C_{b} \left( 1 - \prod_{b \in j \setminus a} C_{b}^{j, -\sigma} \right)$

(A1)

$\chi_{j \rightarrow a}^{\bar{a}} = \delta_{t_{a}^{(j)} \sigma} C_{a}^{j, -\sigma} + \sum_{\sigma = \pm 1} \delta_{t_{a}^{(j)} \sigma} C_{a}^{j, \sigma} \left( 1 - C_{a}^{j, \sigma} \right)$

(A2)

$\sum_{\sigma = \pm 1} \delta_{t_{a}^{(j)} \sigma} C_{b}^{j, \sigma} \left( 1 - \prod_{b \in j} C_{b}^{j, -\sigma} \right) + \delta_{t_{a}^{(j)} \sigma} C_{b}^{j, -\sigma}$

(A3)

where $C_{b}$ for $b \in j \setminus a$ is evaluated here in $\left( \{ h_{k} \}_{k \in b \setminus j}, t_{a}^{(j)} \right)$ and $C_{a}$ is evaluated in $t_{a}$.
For the RHS of Eq. (16) we first note that as the $\chi^{dbp}_j$ term includes $\prod_{a \in J} \delta_{t_a^{(j)}, s_j}$ we will simply replace all occurrences of $t_b^{(j)}$ and $s_j$ variables by $t_a^{(j)}$ and drop the outer sum and the product term itself. For instance, the sum over $\{t_b\}_{b \in J}$ thus reduces to a sum over $\{t_a^{(j)}\}_{k \in b \setminus J, j \in a \setminus j}$. Let’s evaluate the RHS of Eq. (16) on the three possible values of $t_a^{(j)}$:

If $t_a^{(j)} = \ast$ then by Eq. (13) $\chi^{dbp}_j = \prod_{b \in J} C_a^{j_1} C_b^{j_2}$. Moreover, just by looking at its definition Eq. (13), one finds that $\chi^{dbp}_j$ of Eq. (16) becomes

$$C_a^{j_1} C_b^{j_2} \prod_{b \in J \setminus a} \left( \sum_{k \in b \setminus J} \chi^{dbp}_{k \rightarrow b} \right) - C_a^{j_1} \prod_{b \in J \setminus a} \left( \sum_{k \in b \setminus J} C_b^{j_2} \chi^{dbp}_{k \rightarrow b} \right).$$

which is exactly the term in Eq. (A5) corresponding to $t_a^{(j)} = \ast$ (remember that $C_b$ clauses here are evaluated in $t_b$).

If $t_a^{(j)} = \sigma \in \{\pm 1\}$ then it is convenient to break $\chi^{dbp}_j$ in two addenda:

$$\prod_{b \in J} C_b - \prod_{b \in J} C_b C_b^{j_2} \sigma,$$

so that the RHS of Eq. (16) becomes

$$C_a \prod_{b \in J \setminus a} \left( \sum_{k \in b \setminus J} \chi^{dbp}_{k \rightarrow b} \right) - C_a \prod_{b \in J \setminus a} \left( \sum_{k \in b \setminus J} C_b C_b^{j_2} \sigma \chi^{dbp}_{k \rightarrow b} \right).$$

Finally, both sums can be computed explicitly and the result is again exactly the corresponding term in Eq. (A5).

This ends the proof of the identity Eq. (16).

**APPENDIX B: COMPUTATION OF THE ENTROPY**

For simplicity of notation, in what follows we write $P_a(t_a)$, $P_{a \rightarrow i}(t_a)$, $P_i(T_i)$ and $\chi_i(T_i)$ in place of $P^{dbp}_a(t_a)$, $P^{dbp}_{a \rightarrow i}(t_a)$, $P^{dbp}_i(T_i)$ and $\chi^{dbp}_i(T_i)$ respectively and $P_{i \rightarrow a}(h_i)$ in place of $P^{sp}_{i \rightarrow a}(h_i)$.

To compute the entropy (B1) we first need

$$P_a(t_a) = e^{-1} \prod_{\{h_i\} \in a} P_{i \rightarrow a}(h_i) \prod_{i \in a} \chi^{dbp}_{i \rightarrow a}(t_a, h_i),$$

$$= e^{-1} \prod_{i \in a} \sum_{\{h_i\}} P_{i \rightarrow a}(h_i) \chi^{dbp}_{i \rightarrow a}(t_a, h_i).$$

Thus calling

$$f_{a \rightarrow i} = \sum_{\{h_i\}} P_{i \rightarrow a}(h_i) \chi^{dbp}_{i \rightarrow a}(t_a, h_i)$$

we have that

$$\sum_{\{t_a\}} P_a(t_a) \log P_a(t_a) = -e^{-1} \log c_a + \sum_{\{t_a\}} P_a(t_a) \sum_{i \in a} \log f_{a \rightarrow i},$$

$$= -e^{-1} \log c_a + \sum_{i \in a} \sum_{\{t_a\}} P_a(t_a) \log f_{a \rightarrow i}.$$ 

(B2)

Writing $\omega_{a \rightarrow i} = \sum_{\{t_a\}} P_a(t_a) \log f_{a \rightarrow i}$ we get

$$\sum_a \sum_{i \in a} (n_a - 1) \sum \omega_{a \rightarrow i} = \sum_i \sum_{a \in i} \sum_j \omega_{a \rightarrow j}$$
\[
\begin{align*}
&= \sum_{i} \sum_{a \in i} \sum_{j \in a \setminus \{i\}} P_a(t_a) \log f_{a \rightarrow j} \\
&= \sum_{i} \sum_{a \in i} \sum_{j \in a \setminus \{i\}} P_a(t_a) \prod_{j \in a \setminus i} \log f_{a \rightarrow j} \\
&= \sum_{i} \sum_{a \in i} \sum_{j \in a \setminus i} P_i(T_i) \prod_{j \in a \setminus i} \log f_{a \rightarrow j} \\
&= \sum_{i} \sum_{a \in i} \sum_{j \in a \setminus i} P_i(T_i) \log \prod_{j \in a \setminus i} f_{a \rightarrow j}
\end{align*}
\]

The term inside the logarithm above reads
\[
\prod_{j \in a \setminus i} f_{a \rightarrow j} = \sum_{\{h_j\} \in a \setminus i} \chi_{j \rightarrow a}^{p_h}(t_a, h_j) \prod_{j \in a \setminus i} P_j \rightarrow a(h_j) = \frac{1}{D_{a \rightarrow i}} P_{a \rightarrow i}(t_a)
\]

where \(D_{a \rightarrow i}\) is an appropriate normalization constant. Going back to Eq. \((B3)\), we have

\[
\sum_{a} (n_a - 1) \sum_{i \in a} \omega_{a \rightarrow i} = - \sum_{i} \sum_{a \in i} \log D_{a \rightarrow i} + \sum_{i} \sum_{a \in i} \sum_{\{T_i\}} P_{i}(T_i) \log P_{a \rightarrow i}(t_a)
\]

The second term in the right-hand side equals

\[
\sum_{i} \sum_{\{T_i\}} P_{i}(T_i) \log \prod_{a \in i} P_{a \rightarrow i}(t_a) = \sum_{i} \sum_{\{T_i\}} P_{i}(T_i) \log \chi_i(T_i) \prod_{a \in i} P_{a \rightarrow i}(t_a)
\]

\[
= \sum_{i} \sum_{\{T_i\}} P_{i}(T_i) \log Q_i(T_i)
\]

\[
= \sum_{i} \sum_{\{T_i\}} P_{i}(T_i) \log P_{i}(T_i) + \sum_{i} \sum_{\{T_i\}} P_{i}(T_i) \log c_i
\]

where in the second step above \(\chi_i(T_i)\) has been artificially multiplied inside the logarithm (we can do it because there is a \(P_i(T_i)\) outside) and \(P_i(T_i) = \frac{1}{c_i} Q_i(T_i)\). Eqs. \((B5), (B6)\) give:

\[
\sum_{a} (n_a - 1) \sum_{i \in a} \omega_{a \rightarrow i} = - \sum_{i} \sum_{a \in i} \log D_{a \rightarrow i} + \sum_{i} \sum_{\{T_i\}} P_{i}(T_i) \log P_{i}(T_i) + \sum_{i} \sum_{\{T_i\}} P_{i}(T_i) \log c_i
\]

Going back to the first expression of the entropy Eq. \((B8)\), and using Eq. \((B2)\) and Eq. \((B7)\) we get:

\[
S = - \sum_{i} \sum_{\{T_i\}} P_{i}(T_i) \log P_{i}(T_i) + \sum_{a} (n_a - 1) \sum_{\{t_a\}} P_{a}(t_a) \log P_{a}(t_a)
\]

\[
= \sum_{i} \log c_i - \sum_{i} \sum_{\{T_i\}} P_{i}(T_i) \log Q_i(T_i) + \sum_{a} (n_a - 1) \sum_{\{t_a\}} P_{a}(t_a) \log P_{a}(t_a)
\]

\[
= \sum_{i} \log c_i - \sum_{a} (n_a - 1) \log c_a - \sum_{i} \sum_{a \in i} \log D_{a \rightarrow i}
\]

where the constants are defined in Eqs. \((20), (22)\).

**APPENDIX C: TREE FACTOR GRAPHS**

The argument turns out to be similar to the one given in an analogous “tutorial” appendix in ref. \([31]\) for the Vertex Cover problem.

We will first build a reference solution \(x\), and then show that every solution of \(E = 0\) is connected to it. \(x\) will be built from the leaves to the root. Suppose the variables are labeled in an ordering that respects distances to the root, such that the first ones are the leaves and the last one is the root. In such an ordering, the parents (resp. child) of \(i\) are neighbors with labels \(j < i\) (resp. \(j > i\)). We will fix \(x_i\) iteratively: once \(x_j\) for \(j < i\) are fixed, all parents of \(j\) are
fixed; then for $x_j$ there are two possibilities: either its parents force it to take a specific value, or they don’t. In the first case we chose $x_j$ to take the forced value; in the second one we chose the value that satisfy the child clause. Now we can show that $x$ is connected with every other solution $s$ (and thus every two solution are connected). It is easy to see that the configurations $y^{(k)}$ defined by $y^{(k)}_j = s_j$ if $j < k$ and $y^{(k)}_j = x_j$ if $j \geq k$ form a path of configurations connecting $x$ and $s$. Clearly $y^{(1)} = x$ and $y^{(n)} = s$. Also they are all solutions, since if $y^{(k)}$ is a solution, then clearly $y^{(k+1)}$ is also a solution: if they are different it is because $y^{(k+1)}$ has been chosen to satisfy the child clause (and it was not forced from parents in $s$ and thus neither in $y^{(k+1)}$).

We can now look for solutions of $\tilde{E}$ on a satisfiable tree (with boundary conditions). Let’s start with a free-boundary tree with 2 and 3-clauses: it is easy to see that the solution with all * assignment has $\tilde{E} = 0$. It is also clearly unique: suppose that there is a solution with some variable set to $\sigma \neq *$. Then there is forcefully one of its neighboring clauses in which the two (or one) remaining variables are fixed in order to not satisfy the clause. Repeating again the argument recursively for one of them, we can get a never-ending path of fixed variables in the tree. But as a trees have no loops, this is a contradiction.

There is also exactly one such solutions for a satisfiable tree with boundary conditions (if we disregard $V_i$ constraints on the variables with assigned boundary values). We will build it explicitly using the so-called unit clause propagation (UCP). The UCP procedure consists in removing (in this case starting from the boundary) every fixed variable by (a) removing all clauses satisfied by the variable and (b) removing the variable from all clauses in which it appears without satisfying the clause. (if the original tree is satisfiable, no 0-clause can appear in this erasure step). Then every possibly appearing 1-clause is taken and its variable fixed in order to satisfy the clause, and the procedure starts again from the beginning until no more 1-clauses show up. The resulting graph is boundary-free and with no 1-clauses.

The promised solution will be built by taking all variables fixed by UCP with their assigned value, and by assigning the value * to the remaining ones. The resulting configuration $\tilde{x}$ has $\tilde{E}(\tilde{x}) = 0$. Clearly the constraints $V_i$ (see Eq. 32) are satisfied by $\tilde{x}$ for all $i$ fixed by UCP (because they are “frozen” by their neighbors). We easily see that this partial assignment is the unique one that can give $\tilde{E} = 0$. Using the fact that the subgraph produced by UCP has no boundary condition and that the unique solution for $\tilde{E} = 0$ on that subgraph is the all-* one, we see that the proposed configuration is indeed the unique solution.

Note also that every solution of $E = 0$ will coincide with $\tilde{x}$ in the −1, 1-assigned variables of the latter, because these variables were fixed by UCP and thus are forced in every satisfying configuration. Moreover, if one takes an index $i$ such that $\tilde{x}_i$ is *, then there is at least one solution of $E(s) = 0$ with $s_i = 1$ (resp. −1): by fixing $s_i$ and applying again UCP one cannot get any contradiction (i.e. a 0-clause) because the subgraph has no loops nor 1-clauses. The remaining graph is still loop-free, and thus trivially satisfiable.

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