Gauges, Loops, and Polynomials for Partition Functions of Graphical Models

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(Dated: April 2, 2019)

Graphical models (GM) represent multivariate and generally not normalized probability distributions. Computing the normalization factor, called the partition function (PF), is the main inference challenge relevant to multiple statistical and optimization applications. The problem is \#P-hard that is of an exponential complexity with respect to the number of variables. In this manuscript, aimed at approximating the PF, we consider Multi-Graph Models (MGMs) where binary variables and multivariable factors are associated with edges and nodes, respectively, of an undirected multi-graph. We suggest a new methodology for analysis and computations that combines the Gauge Function (GF) technique from [21, 22] with the technique developed in [34] and [5, 67] based on the recent progress in the field of real stable polynomials. We show that the GF, representing a single-out term in a finite sum expression for the PF which achieves extremum at the so-called Belief-Propagation (BP) gauge, has a natural polynomial representation in terms of gauges/variables associated with edges of the multi-graph. Moreover, GF can be used to recover the PF through a sequence of transformations allowing appealing algebraic and graphical interpretations. Algebraically, one step in the sequence consists in the application of a differential operator over gauges associated with an edge. Graphically, the sequence is interpreted as a repetitive elimination/contraction of edges resulting in MGMs on decreasing in size (number of edges) graphs with the same PF as in the original MGM. Even though the complexity of computing factors in the sequence of derived MGMs and respective GFs grow exponentially with the number of eliminated edges, polynomials associated with the new factors remain bi-stable if the original factors have this property. Moreover, we show that BP estimations in the sequence do not decrease, each low-bounding the PF.

I. INTRODUCTION

Graphical models (GM) are ubiquitous in natural and engineering sciences where one needs to represent a multivariate distribution function with a structure that is expressed in terms of graphical, statistical or deterministic, relations between the variables [29, 41, 51–53, 56, 59, 76]. Focusing on the so-called Normal Factor Graph (NFG) representation [28], where binary variables and factors that express relations between the variables are associated with edges and nodes of the graph, respectively, we are interested in resolving the problem of statistical inference, which entails computing the weighted sum over allowed states. Exact evaluation of the sum, called the partition function (PF), is known to be \#P-hard [38, 69, 71], that is, of complexity which likely requires an exponential number of steps. Subsequently, deterministic and stochastic approximations were made. In this manuscript, we concentrate primarily on the former. (Stochastic methods for the PF estimations are reviewed in [37, 71]. See also some related discussions in [43] and below.)

The inference problem can also be stated as an optimization. The variational approach to PF dates back to Gibbs [31], and possibly earlier. Similar considerations are known in statistics under the name of Kullback–Leibler divergence [44]. The resulting optimization stated in terms of beliefs (i.e., proxies for probabilities of states) is convex but not tractable because of the exponential number of states (and respectively beliefs). Developing relaxations, and more generally approximations, for the Gibbs–Kullback–Leibler (GKL) variational formulation is the primary research to which this manuscript is contributing.

Theoretical efforts in the field of deterministic estimations of PFs have focused on devising (a) lower and/or upper bounds for GMs of a special type and (b) fully polynomial deterministic algorithmic schemes (FPDAS) for even more restrictive classes of GMs. (See Section VII for an extensive discussion of the low bounds and related subjects. Section VIII for a brief discussion on unification of these ideas with FPDAS.)

Provable lower bounds for PFs are known for perfect matching (PM) problems over bipartite graphs [34, 35], independent set problems [10, 65, 79], and Ising models of attractive (log-supermodular) [48, 61, 68] and general

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generalizing both. Our approach consists of the following steps (see also Fig. (1) presenting a diagram of relations for a more general case of the so-called bi-stable (BS) polynomials over arbitrary graphs. The last term in the sequence). In a related paper, [5] a polynomial version of the GM statement of [67] was proven resulting in the statement that BP (the zero term in the sequence) provides a lower bound for the partition function each application of the edge-local differential operator ensures that the respective PF estimate does not decrease, thus in [67] that if all polynomials associated with nodes of the GM are real stable (RS) and the graph is bi-partite, then we refer to BP as a fixed point (possibly one of many) of the BFE, assuming that it can be found efficiently [61]. We will also generalize the notion of fixed points to the cases when the minimum of the BFE may be achieved at a plaquet/side of the belief polytope over which the BFE is defined (not necessarily within the interior of the polytope).

Heuristic success as well as results claiming exactness of BP for some special optimization problems over loopy graphs (e.g., finding maximum weight perfect matching over bipartite graphs [10]) have stimulated the design of a number of methods relating results of BP to exact results. These methods include gauge transformation (GT) and loop calculus (LC) of [21, 22], the spanning tree approach of [79], the cumulant expansion approach of [80], the graph cover approach of [74], and most recently the real stable polynomial (RSP) approach of [5, 34, 67]. The first and last approaches are most relevant to this manuscript.

The GT–LC method of [21, 22] suggests an exact construct exploring invariance of PF with respect to special transformations of factors, called gauges, also related to the so-called re-parametrizations of [77] and holographic transformations of [70]. It was shown that BP corresponds to a special choice of gauges, which then leads to expressing the PF in terms of the so-called generalized loops, where each generalized loop contribution is stated explicitly in terms of the underlying BP solution. The GT–LC approach was utilized (1) to prove that BP provides a lower bound for attractive Ising models with some additional technical constraints in [81] (it was then shown in [61, 62] through the use of the graph cover approach of [74] that the additional constraints are insignificant); (2) to prove that BP is exact asymptotically for an ensemble of independent set problems [15]; (3) to relate matching models, Fermion models of statistical physics with loop and determinant considerations [18, 19]; (4) to approximate PF in planar GM [23, 32]; (5) to apply LC to permanent (PF of perfect matching model over bipartite graph) [78], to provide a proof that is alternative to the original [34] for the fact that BP results in a lower bound for permanent, and then construct a sequence of fractional-BP approximations for permanents [24]; (6) to build a fully polynomial randomized approximation scheme (FPRAS) for a subclass of planar GMs [1] by sampling LS; and (7) to construct a provable lower bound for PF in the case when BP fails to provide such guarantees [2] by finding an optimal non-BP gauge that certifies that all terms in the LS are positive.

The RSP approach to the PF, first developed for permanents in [34] and then generalized to binary GM over (normal) bipartite graphs with submodular factors in [5, 67], is built on the recent progress in the RSP theory [12, 13]. The essence of the approach is in representing the BFE as a polynomial optimization and then showing that the PF is a result of a sequential application of edge-local differential operators to the BFE, BP estimate of PF. It was shown in [67] that if all polynomials associated with nodes of the GM are real stable (RS) and the graph is bi-partite, then each application of the edge-local differential operator ensures that the respective PF estimate does not decrease, thus resulting in the statement that BP (the zero term in the sequence) provides a lower bound for the partition function (the last term in the sequence). In a related paper, [5] a polynomial version of the GM statement of [67] was proven for a more general case of the so-called bi-stable (BS) polynomials over arbitrary graphs.

A. Contributions of this manuscript

We complement the RSP approach of [5, 34, 67] by merging it with the GT approach of [21, 22], and thus in a sense generalizing both. Our approach consists of the following steps (see also Fig. (1) presenting a diagram of relations between the manuscript’s steps and concepts):

- Generalize Variational Bethe Free Energy approach (from the case of normal graphical models) to the Multi-Graphical Models. Show that solution of any Soft MGM is attained strictly within a polytope of parameters – so-called Belief Polytope – describing the solution. All further results reported in the paper (unless specified
otherwise) apply strictly speaking only to MGMs which are soft – even though some of the factors may be infinitesimally small. (Section II).

- Restate the GT expression for PF from [21, 22] as a series of polynomials in variables/gauges. Single out a term from the series, which we call the Gauge Function, relate stationary points of the GF, so-called BP-gauges and show that the minimum of the BFE is achieved at the maximal BP-gauge. (Section III).

- Introduce a sequence of MGMs, where each new member is a result of an edge contraction (graphically) or summation over respective edge variables (algebraically). Build BP polynomial (principal polynomial evaluated at the optimal BP gauge) for each MGM in the sequence such that the last term is the PF (constant) corresponding to the fully contracted graph. Introduce BP-optimal gauge for each MGM and show that BP-optimal estimation stays exact in the process of contraction of a normal edge, however, it becomes approximate respective contraction of a self-edge. (Section IV.)

- Observe that the Bi-Stability (BS) of polynomials correspondent to factors of the original MGM results in the BS of each factor in each MGM of the aforementioned contraction sequence. Show that the variational BP solution (correspondent to the minimum of the respective BFE) for each next MGM in the sequence is larger or equal to BP if all factors in the original MGM correspond to BS polynomials. A direct corollary of this construction is the desired statement that the BP optimal estimation for the PF of the original MGM low bounds the exact PF. (Section V.)

We present in Section II for the purpose of setting terminology and self-consistency of the presentation, introductory material for the BFE approach. For the LC approach of [21, 22], we present introductory material in Appendix A. Section VIII is reserved for discussions of the results and the path forward.

II. PRELIMINARIES

We consider multi-graph generalization of [21, 22]. Following terminology of [50], we may also call it binary Factor- Multi-Graph Model (MGM): variables are associated with edges, and factor functions (or simply factors) are associated with nodes of the undirected multi-graph, \( G = (V, E) \), thus allowing multi-edges between two different nodes and multiple self-edges associated with a single node, where \( V \) and \( E \) are the sets of nodes and edges, respectively. The main reason for dealing with multi-graphs is that certain geometrical graph transformations, namely edge contraction, introduced in Section VII turn simple graphs (no multiple edges, no self-edges) into multi-graphs.
FIG. 2. Multi-Factor Graphical Model notations for undirected (left sub-figure) and directed (middle and right sub-figures) edges are illustrated. \( V = \{a, b\} \), \( E = \{\alpha, \beta, \gamma, \delta, \theta\} \) and \( E_d = \{\alpha_d, \beta_d, \gamma_d, \delta_d, \theta_d\} \) are the sets of nodes, set of undirected edges and set of directed edges, respectively, where \( \bar{\cdot} \) is the notation used to denote the directed edge \( \cdots \) reversal, thus \( \bar{d} \equiv d \). \( \varepsilon(a) = \{\alpha, \beta, \gamma, \delta, \theta\} \) and \( \varepsilon(b) = \{\gamma, \delta, \theta\} \) and \( \varepsilon_d(a) = \{\alpha_d, \beta_d, \gamma_d, \delta_d, \theta_d\} \), \( \varepsilon_d(b) = \{\gamma_d, \delta_d, \theta_d\} \) describe functions, \( \varepsilon(\cdots) : V \to E \) and \( \varepsilon_d(\cdots) : V \to E_d \), mapping a node to the set of directed and undirected edges, respectively, of the multi-graph shown in the figure. \( u(e) : E_d \to E \) describes function mapping directed edges into respective undirected edges; \( u(\alpha_d) = u(\bar{d}) = \alpha \). \( v(\alpha) : E \to V^2 \) describes function mapping an undirected edge to its end nodes.

It is also useful to introduce an oriented version of the undirected multi-graph, i.e., a multi-graph, equipped with orientation. We will then denote \( E_d \) the set of directed edges including the original orientation and its reverse. \( \varepsilon_d(a) \), \( v(\alpha) \) and \( u(\alpha_d) \) will denote, respectively, the set of directed edges associated with the node \( a \), two nodes associated with the undirected edge, \( \alpha \), and undirected edge, \( \alpha \), associated with the directed edge \( \alpha_d \). Also, and abusing notations a bit, \( \alpha_d \) may denote the primary oriented edge for previously introduced undirected edge \( \alpha \); \( \alpha_d \in \varepsilon_d(a) \) denotes a variable directed edge picked from the \( \varepsilon_d(a) \) set. See Fig. 2 for clarifying example.

**Definition II.1** ((Multi-) Graph model). MGM describes factorization for the probability of a binary-component vector, \( \sigma = (\sigma_a = 0, 1) | a \in E \) \( \in \{0, 1\}^{|E|} \), consistent with the (multi)-graph:

\[
p(\sigma) \doteq \frac{f(\sigma)}{Z}, \quad f(\sigma) \doteq \prod_{a \in V} f_a(\sigma_a), \quad Z \doteq \sum_{\sigma} f(\sigma).
\]

Here \( \sigma_a \) is a sub-vector of \( \sigma \) built from all components of the latter containing node \( a \), i.e., \( \sigma_a \in \Sigma_a = \{0, 1\}^{\varepsilon_d(a)} \).

Notice that the PF, \( Z \), defined in Eq. (1) as a summation over all configurations, \( \sigma \), allows a recast in terms of the following exact variational principle.

**Theorem II.2** (Gibbs-Kullback-Leibler (GKL) Variational Reformulation for PF, in the spirit of [31, 44]). The PF, \( Z \), defined in Eq. (1) can be computed through the following optimization

\[
- \log Z = \min_{b} \sum_{\sigma \in \{0, 1\}^{|E|}} b(\sigma) \log \left( \prod_{a \in V} f_a(\sigma_a) \right) \bigg| \forall \sigma : b(\sigma) \geq 0, \sum_{\sigma} b(\sigma) = 1,
\]

where \( b = (b(\sigma) \forall \sigma \in \{0, 1\}^{|E|}) \), and \( b(\sigma) \) are beliefs (i.e., proxies for probabilities) of the state \( \sigma \).

The optimization (2) is convex but not practical because the number of states (and number of respective beliefs) is exponential in the system size (number of edges).

**Theorem II.3** (Exact Maximum Likelihood (ML) as a Linear Programming (LP)). The ML versions of Eqs. (1,2) are

\[
E \doteq - \min_{\sigma} \log f(\sigma) = - \min_{b} \sum_{\sigma} b(\sigma) \sum_{a \in V} \log f_a(\sigma_a) \bigg| \forall \sigma : b(\sigma) \geq 0, \sum_{\sigma} b(\sigma) = 1.
\]

Notice that the formulation on the right of Eq. (3) is an LP over (exponentially many) belief variables.
A. Variational Belief Propagation

Belief propagation (BP) is a popular and practical tool that approximates original beliefs via marginal beliefs according to the following dynamic programming (DP) expression \[51–53, 59, 76\], which gets the following form when stated for the MGM model \[4\]

\[
\mathbb{E}(\sigma) \approx \prod_{a \in E} b_a(\sigma_a) \prod_{a \in \mathcal{V}} \beta_a(1 - \beta_a), \quad \text{s.t.} \quad \forall a \in \mathcal{V}, \forall \sigma_a \in \Sigma_a^{(0)}: \ b_a(\sigma_a) \geq \sum_{\sigma_{\setminus a}} \mathbb{E}(\sigma);
\]

\[
\forall a \in \mathcal{E}: \ \beta_a = \sum_{\sigma_a, \setminus a} \mathbb{E}(\sigma);
\]

which would be exact for a tree-graph (no loops in GM). Reducing description from the exponential in size vector of original beliefs to the linear in the size of the graph (assuming that node degree in the MGM is \(O(1)\)) vector of marginal beliefs

\[
b = (b_a(\sigma_a) | \forall a \in \mathcal{V}, \sigma_a \in \Sigma_a), \quad \beta = (\beta_a | \forall a \in \mathcal{E}).
\]

considered over the following marginal polytope

\[
\Pi \equiv \left\{ (b, \beta) \in [0,1]^{\Sigma} \times [0,1]^\mathcal{E} \mid \forall a \in \mathcal{V}, \forall \sigma_a \in \Sigma_a: \sum_{s \in \Sigma_a} b_a(s) = 1; \forall a \in \mathcal{E}, \forall \sigma_d \in \mathcal{E}_d(a): \sum_{s \in \Sigma_a} b_a(s) = \beta_{\sigma_d(a)} \right\}.
\]

and substituting Eq. (4) into Eq. (2), one arrives at the following optimization.

Definition II.4 (BFE and Variational Belief Propagation (VBP) approximation for the PF, by analogy with \[83\]. VBP estimation for the PF, \(Z^{(vbp)}\), is defined according to

\[
F^{(vbp)}(b, \beta) = -\log Z^{(vbp)} = \min_{(b, \beta) \in \Pi} F^{(bp)}(b, \beta),
\]

\[
F^{(bp)}(b, \beta) \equiv E^{(bp)}(b) - S^{(bp)}(b, \beta),
\]

\[
E^{(bp)}(b) \equiv -\sum_{a \in \mathcal{V}} \sum_{\sigma_a \in \Sigma_a} b_a(\sigma_a) \log f_a(\sigma_a),
\]

\[
S^{(bp)}(b, \beta) \equiv \sum_{a \in \mathcal{V}} \sum_{\sigma_a \in \Sigma_a} b_a(\sigma_a) \log b_a(\sigma_a) - \sum_{a \in \mathcal{E}} (\beta_{\sigma_d(a)} \log \beta_{\sigma_d(a)} + (1 - \beta_{\sigma_d(a)}) \log (1 - \beta_{\sigma_d(a)})),
\]

where \(F^{(vbp)}\) is the Variational Bethe Free Energy (VBFE), \(F^{(bp)}(b, \beta), E^{(bp)}(b)\) and \(S^{(bp)}(b, \beta)\) are the Bethe Free Energy (BFE), Bethe Entropy (BE) and Bethe Self Energy (BSE) functions of marginal beliefs.

We further notice that Eq. (7) may be restated as a polynomial optimization \[67\]. To derive the polynomial representation one, first, rewrites Eq. (7) as

\[
\log Z^{(vbp)} = \max_{\beta \in [0,1]^\mathcal{E}} \left( S^{(bp-r)}(\beta) - E^{(bp-r)}(\beta) \right),
\]

\[
S^{(bp-r)}(\beta) \equiv \sum_{a \in \mathcal{E}} (\beta_{\sigma_d(a)} \log \beta_{\sigma_d(a)} + (1 - \beta_{\sigma_d(a)}) \log (1 - \beta_{\sigma_d(a)})),
\]

\[
E^{(bp-r)}(\beta) \equiv \min_{b \in \Pi_r(\beta)} \sum_{a \in \mathcal{V}} \sum_{\sigma_a \in \Sigma_a} b_a(\sigma_a) \log \frac{b_a(\sigma_a)}{f_a(\sigma_a)}
\]

\[
\Pi_r(\beta) \equiv \left\{ b \in [0,1]^{\Sigma} \mid \forall a \in \mathcal{V}, \forall \sigma_d \in \mathcal{E}_d(a): \sum_{s \in \Sigma_a} b_a(s) = 1; \forall a \in \mathcal{E}, \forall \sigma_d \in \mathcal{E}_d(a): \sum_{s \in \Sigma_a} b_a(s) = \beta_{\sigma_d(a)} \right\}.
\]

where \(S^{(bp-r)}(\beta)\) and \(E^{(bp-r)}(\beta)\) are the reduced BP entropy and the reduced BP self-energy functions, respectively, dependent only on the vector of edge probabilities, \(\beta\). Applying strong duality to the reduced BP self-energy one derives

\[
E^{(bp-r)}(\beta) = \sup_{a \in \mathcal{E}_d} \left( \sum_{a \in \mathcal{E}} \beta_{\sigma_d(a)} \log (x_{\sigma_d(a)}) - \sum_{a \in \mathcal{V}} \log (h_a(x_a)) \right),
\]

\[
h_a(x_a) \equiv \sum_{s \in \Sigma_a} f_a(s) \prod_{a \in \mathcal{E}_d(a)} x_{\sigma_d(a)}^s,
\]
where, \( x = (x_\alpha > 0 | \alpha \in \mathcal{E}_d) \in \mathbb{R}^{|\mathcal{E}_d|}_+ \) and \( x_\alpha = (x_\alpha > 0 | e_d(a) \in \mathbb{R}^{|e_d(a)|}_+) \). The \( \log(x_\alpha) \) components, with \( \alpha \in \mathcal{E}_d \) were introduced as Lagrangian multipliers (dual variables) for the belief consistency conditions in Eq. (9). Combining Eqs. (8, 11, 12, 15), one arrives at the following statement.

**Theorem II.5** (Polynomial Max-Min Representation for VBP, multi-graph version of Theorem 3.1 of [67]). VBP, defined Eqs. (7, 8), can also be stated as the following max-min optimization:

\[
Z^{(vbp)} = \sup_{\beta \in [0,1]^{|\mathcal{E}_d|}} \min_{x \in \mathbb{R}^{|\mathcal{E}_d|}_+} \mathcal{L}(\beta, x),
\]

\[
\mathcal{L}(\beta, x) = \left( \prod_{\alpha \in \mathcal{E}} \beta^{|h_\alpha|}(1 - \beta) \right) \prod_{a \in V} \frac{h_a(x_a)}{x_a^{\beta h_a(a)}}.
\]

**B. LP–BP Relaxation for Maximum Likelihood**

**Definition II.6** (Linear programming–belief propagation (LP–BP) approximation). LP–BP approximation for ML optimization is

\[
E^{(lp-bp)} = \min_{(b, \beta) \in P_B} \left( \sum_{a \in V} \sum_{\sigma_a \in \Sigma_a} b_a(\sigma_a) \log f_a(\sigma_a) \right).
\]

Notice that LP–BP is tractable, and it can be considered both as the “entropy-free” version of the optimization and also as a relaxation of the exact LP formulation and therefore results in the following statement.

**Theorem II.7** (Lower bounding by LP–BP (see for example [39, 66, 76] and references therein)). LP–BP lower bounds exact self-energy. \( E^{(lp-bp)} \leq E \).

Note that the same LP–BP is known under the name of “Basic Linear Programming Relaxation” in the community analyzing Constraint Satisfaction Problems. See, e.g. [42] and references therein.

**C. Variational Belief Propagation in the Soft Model**

**Definition II.8** (Soft MGM). If \( \forall a \in V, \forall \sigma_a \in \Sigma_a : f_a(\sigma_a) > 0 \), the MGM is called soft.

**Theorem II.9** (VBP of Soft MGM – in the spirit of Proposition 6 of [83]). Minimum in Eq. (7) is achieved within the interior of \( \Pi \) in the case of soft MGM.

**Proof.** The theorem is proved in three steps: first, one shows that the minimum in Eq. (7) cannot be achieved at \( \beta \) such that at one edge, \( \alpha \) (at least one edge), \( \beta_\alpha \) is exactly zero or one; (b) given (a) one checks explicitly that when all factors are soft (and thus no terms in the multi-linear polynomials \( h_a \) are zero) the minimum over \( x \) in Eq. (17) is achieved at a finite \( x \in \mathbb{R}^{|\mathcal{E}_d|}_+ \); finally, given that the Lagrangian multipliers, \( x \), for the edge and node belief consistency are all finite, the minimum in Eq. (7) can only be achieved at \( \forall a \in V, \forall \sigma_a \in \Sigma_a : b_a(\sigma_a) \in [0; 1] \).

Therefore, only the first step is left to be proven. We present here only a sketch of the proof. Assume that \( \exists \alpha \in \mathcal{E} \) such that the minimum in Eq. (7) is achieved at \( \beta_\alpha = 0 \). Our strategy consists in showing that one can find a direction from the point on the polytope boundary towards interior along which \( -\log Z(b) \) will decrease, thus arriving at a contradiction. Indeed, when \( \beta_\alpha = \epsilon > 0 \) with \( \epsilon \to 0 \), one derives that according to the belief consistency relations, i.e. equality relations between beliefs embedded in the definition of the polytope \( \Pi \), all \( b_a(\sigma_a) = O(\epsilon) \) where \( \forall a \in v(\alpha), \sigma_a \) is consistent with \( \sigma_\alpha = 1 \). Moreover, one may redistribute the \( O(\epsilon) \) perturbations over these \( b_a(\sigma_a) \) such that \( \beta_\gamma \), where \( \gamma \neq \alpha \), do not depend on the \( \epsilon \)-perturbation at all. On the other hand, \( \epsilon \)-corrections to \( -\log Z(b) \) are \( O(\epsilon \log \epsilon) \). The corrections originate from the entropy contributions associated with \( O(\epsilon) \) beliefs of two types — associated with \( \beta_\alpha \) and associated with the respective \( h_a(\sigma_a) \). Accurate counting of the contributions results in the overall \( \epsilon \log \epsilon \) correction to \( -\log Z(b) \), where \( 2\epsilon \log \epsilon \) term comes from the two \( b_a(\sigma_a) = O(\epsilon) \) contributions and one \( -\epsilon \log \epsilon \) term comes from the single \( \beta_\alpha \) contribution. The resulting, \( \epsilon \log \epsilon \), is negative and it decreases with increase in \( \epsilon \), thus leading to the contradiction. Similar consideration, now with, \( \beta_\alpha = 1 - \epsilon \), where \( \epsilon > 0, \epsilon \to 0 \), results in the statement that at the optimum \( \beta_\alpha \) cannot be equal to unity. \( \square \)
Note that solution of Eq. (7) can be on the boundary of the II polytope if the MGM is hard. See [40, 78] for discussion of special hard cases, e.g., of the perfect matching problem, where solution is achieved at the boundary of II.

Theorem II.9 guarantees that an infinitesimally weak softening of a hard model (achieved by adding an infinitesimal positive correction to \( f_a(\sigma_a) = 0 \) factors) shifts a solution of the optimization (8) into the interior of the polytope. We will use this softening feature of MGM later in Section IIIB to relate Variation Belief Propagation (VBP) formulations and solutions discussed in this Section to the Gauge Transformation and Belief Propagation Equations we are switching our attention to in the next Section.

III. GAUGE TRANSFORMATION AND BELIEF PROPAGATION EQUATIONS

A. Gauge Transformation

Definition III.1 (GT, [21, 22]). GT is a multi-linear transformation of the GM factors:

\[
\forall a \in V, \ \forall \sigma_a \in \Sigma_a^{(0)} : \ f_a(\sigma_a) \mapsto \tilde{f}_a(\sigma_a|G) = \sum_{\varsigma_a \in \Sigma_a} f_a(\varsigma_a) \prod_{a \in E_d(a)} G_a(\sigma_a, \varsigma_a),
\]

which keeps the PF invariant; that is,

\[
\forall G : \ Z = \sum_{\sigma \in S} \prod_{a \in V} f_a(\sigma_a) = \sum_{\sigma \in S^{(0)}} \prod_{a \in V} \tilde{f}_a(\sigma_a|G) = \sum_{\sigma \in S^{(0)}} z(\sigma|G),
\]

(20)

where \( \varsigma_a \in \Sigma_a^{(0)} = \{0,1\}^E(a) \).

It is straightforward to check that Eq. (20) holds if the following condition is met.

Theorem III.2 (Orthogonality of GT [21, 22]). GT \( 2 \times 2 \) (in the case of a binary alphabet) matrices satisfy

\[
\forall \alpha \in \mathcal{E}, \ G_{\alpha d}^T \cdot \bar{G}_{\bar{\alpha} d} = 1_\alpha,
\]

(21)

where \( \alpha_d \) and \( \bar{\alpha}_d \) mark two directed siblings of \( \alpha \), and the matrices, \( G_{\alpha d} \) and \( \bar{G}_{\bar{\alpha} d} \) are non-singular with real-valued components.

To lift the gauge-constraint (21), one introduces the following explicit representation for \( G \).

Definition III.3 (Polynomial, \( x \)-, Representation of Gauges). We call the following representation for \( G \), polynomial-or \( x \)-representation.

\[
G = (G_{\alpha} | \alpha \in \mathcal{E}) \quad G_{\alpha} = \frac{1}{(x_{\alpha d} \bar{x}_{\bar{\alpha} d})^{1/4} \sqrt{1 + x_{\alpha d} x_{\bar{\alpha} d}}} \left( \begin{array}{c} \sqrt{x_{\alpha d}} \ x_{\alpha d} \sqrt{x_{\bar{\alpha} d}} \\ -\sqrt{x_{\bar{\alpha} d}} \ x_{\alpha d} \sqrt{x_{\alpha d}} \end{array} \right),
\]

(22)

where the vector \( x \) is positive component-wise, i.e., \( x_{\alpha} > 0 \), \( \forall \alpha \in \mathcal{E} \).

A number of remarks are in order.

- \( x \)-representation for \( G \) (22) satisfies Eq. (21) automatically (by construction).
- The trivial, \( G = 1 \), case is recovered in the \((x_{\alpha d} = x_{\bar{\alpha} d}) \rightarrow 0\) limit.
- Emergence of negative components in the matrix (in the lower left corner of the representation of Eq. (22)) is unavoidable in order to ensure validity of Eq. (21).
where

\[ h \]

Definition III.4 (Interior BP-gauge \[21, 22\] for Soft (S) MGM) represented as Eq. (28), is:

\[ \text{Eq. (27), is:} \]

where the Variational Belief Propagation (VBP) estimate for the partition function was defined in Eq. (7).

Corollary III.5 (Soft MGM BP gauge optimality) Theorem II.9. We observe in the next sections that a single out

Given that

A relation between the VBP and BP gauge approaches is established by the following straightforward corollary of

\[ \text{here, we transitioned in our notation from the general gauges } G \text{ to the } x \text{-representation; } x_a \doteq (x_a | \alpha \in \mathcal{E}_d(a)). \]

- \[ z(\sigma|x) \text{ is a polynomial in } x, \text{ up to the factor on the left-hand side of the first raw in Eq. (23) and when stated in terms of } x, \text{ thus explaining the name chosen for the representation.} \]

- \[ Z = \sum_\sigma z(\sigma|x) \text{ is a constant; that is, } x \text{-independent, polynomial in } x. \]

We observe in the next sections that a single out \( \sigma \)-term, say \( \sigma = 0 \) (chosen without loss of generality) and represented as

\[ z(x) \doteq \prod_{a \in V} h_a(x_a) \]

where \( h_a \) is the vertex polynomial, defined in Eq. (16), and \( z(x) \) is a short-cut notation for \( z(0|x) \) that plays a special role in establishing known and new relations. We call \( z(x) \), described by Eq. (27), the Gauge Function (GF) of the MGM \( G \).

B. Belief Propagation Gauges

Definition III.4 (Interior BP-gauge \[21, 22\] for Soft (S) MGM). We call a solution \( x^{(bp)} \in \mathbb{R}_+^{d} \) of the following stationary-point condition for the GF \( (27) \) equations of the S-MGM

\[ \forall a \in V, \forall \alpha \in \mathcal{E}_d(a) : \partial_{x_a} z(x) |_{x = x^{(bp)}} = 0, \]

\[ (28) \]

a BP gauge.

A relation between the VBP and BP gauge approaches is established by the following straightforward corollary of Theorem II.9

Corollary III.5 (Soft MGM BP gauge optimality). In the case of S-MGM there exists a BP-gauge, \( x \), solving Eq. (28)

\[ Z^{(bp)} = z(x), \]

where the Variational Belief Propagation (VBP) estimate for the partition function was defined in Eq. (7).

Given that \( z(x) \) is differentiable in \( x \), BP-equations (28) are well defined. Explicit version of Eq. (28), derived from Eq. (27), is:

\[ \forall a, \forall \alpha_d \in e_d(a) : \sum_{\varsigma_a} f_a(\varsigma_a) \left( \prod_{\beta_d \in e_d(a)} (x_{\beta_d}^{(bp)})^\varsigma_a \right) \left( \frac{x_{\alpha_d}^{(bp)} x_{\alpha_d}^{(bp)}}{1 + x_{\alpha_d}^{(bp)} x_{\alpha_d}^{(bp)}} - \varsigma_a \right) = 0. \]

\[ (29) \]

\[ (30) \]
Theorem III.6 (BP-Solution as the “No Loose Coloring” Condition \[21\ 22\]). The BP Eq. (28), or equivalently Eq. (30) can be restated in terms of the following conditions:

\[
\forall a, \quad \sum_{\alpha_d \in e_d(a)} \sigma_{\alpha_d} = 1: \quad Q_a(x_a; \sigma_a) = 0. \tag{31}
\]

This result follows from the definition of \(Q\) in Eq. (25) or Eq. (26). With regard to the name chosen for the Theorem III.6, it emphasizes that rewriting BP equations in the form of Eq. (31) highlights interpretation of BP in terms of the “edge coloring”. Indeed, Eq. (31) enforces cancellation (exact zero) for all \(z(\sigma|x) = z(\sigma|G)\) terms in the series on the right-hand side of Eq. (20), where at least one node, \(a\), has one of its neighboring edges, say \(\alpha_d \in e_d(a)\), “colored”; that is, it is set to \(\sigma_{\alpha_d} = 1\), whereas all other neighboring edges of the node, \(\beta_d \in e_d(a)\), \(\beta_d \neq \alpha_d\), remain “uncolored”, that is, set to \(\sigma_{\beta_d} = 0\).

Solutions of the BP Eq. (30) (or Eq. (31)) also allow a transparent interpretation in terms of the edge-consistent (but graph-globally not consistent) probability distributions. Expressions for the node- and edge- marginal probabilities evaluated at a BP gauge are

\[
P^{(bp)}_a(s_a) \equiv \frac{f_a(s_a) \prod_{\alpha_d \in e_d(a)} G^{(bp)}_{\alpha_d}(0, s_{\alpha_d})}{\sum_{s_a} f_a(s_a) \prod_{\alpha_d \in e_d(a)} G^{(bp)}_{\alpha_d}(0, s_{\alpha_d})} = \frac{f_a(s_a) \prod_{\alpha_d \in e_d(a)} (x_{\alpha_d}^{(bp)})^{s_{\alpha_d}}}{\sum_{s_a} f_a(s_a) \prod_{\alpha_d \in e_d(a)} (x_{\alpha_d}^{(bp)})^{s_{\alpha_d}}} = \sum_{s_a} P^{(bp)}_{a,s_a}(s_a) = \sum_{s_a} P^{(bp)}_{a,s_a}(s_a). \tag{32}
\]

Edge-consistency of the marginal beliefs means

\[
\forall a, \quad \forall \alpha_d \in e_d(a), \quad \forall s_{\alpha_d} = \{0, 1\} : 
\]

\[
P^{(bp)}_{a,s_{\alpha_d}} = \frac{f_a(s_a) \prod_{\beta_d \in e_d(a)} (x_{\beta_d}^{(bp)})^{s_{\beta_d}}}{\sum_{s_a} f_a(s_a) \prod_{\gamma_d \in e_d(a)} (x_{\gamma_d}^{(bp)})^{s_{\gamma_d}}} = \sum_{s_a} P^{(bp)}_{a,s_a}(s_a). \tag{34}
\]

Multiplying Eq. (34) on \(s_{\alpha_d}\) and summing it up over \(s_{\alpha_d} = 0, 1\), one arrives at the already introduced system of BP Eqs. (30). We will also denote, for consistency with earlier notations introduced in Section ??,

\[
\forall \alpha \in \mathcal{E} : \beta^{(bp)}(\alpha) \equiv P^{(bp)}(1), \quad \beta^{(bp)}(\alpha) \equiv \left(\beta^{(bp)}(\alpha) \mid \alpha \in \mathcal{E}\right). \tag{35}
\]

Notice that, consistently with the Corollary III.5, an S-MGM may have multiple (more than one) BP-gauges solving Eqs. (28).

IV. ELIMINATION OF EDGES

Assume some ordering of the graph edges,

\[
m = 1, \ldots, |\mathcal{E}| : \alpha^{(1)}, \ldots, \alpha^{(|\mathcal{E}|)} \tag{36}
\]

and consider summing up over (i.e., eliminating) edges in the expression for the PF one-by-one according to this order, therefore naturally arriving at the sequence of graphs, \(G^{(0)} = (\mathcal{V}^{(0)}, \mathcal{E}^{(0)}), \ldots, G^{(|\mathcal{E}|)} = (\mathcal{V}^{(|\mathcal{E}|)}, \mathcal{E}^{(|\mathcal{E}|)})\) such that \(\forall m = 1, \ldots, |\mathcal{E}| : \mathcal{E}^{(m)} \subseteq \mathcal{E}^{(m-1)} \setminus \alpha^{(m)}\). Each next graph in the sequence has one less number of edges and the same or one less number of nodes than its predecessor, see Fig. 3 for illustration. (If the number of nodes at elementary step of the sequence decreases by one, then one of the two merged nodes, chosen arbitrarily is removed from the resulting/new set of nodes.) Then we define a sequence of MGMs, on the sequence of graphs just defined, as follows

\[
m = 0 : \quad \sigma^{(0)}(\alpha) = \sigma, \quad p^{(0)}(\sigma^{(0)}) = p(\sigma),
\]

\[
\forall m = 1, \ldots, |\mathcal{E}| : \quad \sigma^{(m)} = \sigma^{(m-1)} \setminus \sigma_{\alpha^{(m)}}, \quad p^{(m)}(\sigma^{(m)}) \equiv \frac{f^{(m)}(\sigma^{(m)})}{Z}, \quad f^{(m)}(\sigma^{(m)}) \equiv \prod_{\alpha \in \mathcal{V}^{(m)}} f^{(m)}_{\alpha}(\sigma^{(m)}),
\]

\[
\forall a \in \mathcal{V}^{(m)}, a \notin v(\alpha^{(m)}) : \quad f^{(m)}_a(\sigma^{(m)}) \equiv f^{(m-1)}_{a}(\sigma_{\alpha^{(m)}}),
\]

\[
\forall a \in \mathcal{V}^{(m)}, v(\alpha^{(m)}), \mathcal{V}^{(m-1)} : \quad f^{(m)}_a(\sigma^{(m)}) \equiv \sum_{\sigma_{\alpha^{(m)}} : b \in v(\alpha^{(m)})} f^{(m-1)}_{b}(\sigma_{b^{(m-1)}}). \tag{37}
\]
FIG. 3. Graph transformation via elimination of edges is demonstrated through a sequence of sub-figures (from left to right, top to bottom). Each step results in elimination of an edge. Eliminations of edges of two types are possible: (1) elimination of an edge connecting two nodes, e.g., as seen eliminating edges $\rho, \mu, \eta$ and $\delta$ in the first four steps in the sequence, and (2) elimination of self-edges, as seen eliminating edges $\delta, \gamma, \beta, \alpha$.

where $v(\alpha^{(m)})$ is defined as a set of nodes in $V^{(m-1)}$ associated with the edge $\alpha^{(m)}$ (there may be one or two of these depending on if the edge is a self-edge or edge linking two distinct nodes). Notice also that the elimination procedure just introduced is such that the node picked in the last condition (last line) in Eq. (37) is defined uniquely.

In the following, we state a number of remarks about the elimination sequence.

- Notice that by construction, the PF stays the same for all the MGMs in the sequence. The following relations elucidate this point, $m = 1, \cdots, |E|$

\[
Z = \sum_{\sigma} f(\sigma) = \sum_{\sigma^{(1)}} \cdots \sum_{\sigma^{(|E|)}} \prod_{a \in V} f_a(\sigma_a) = \sum_{\sigma^{(1)}} \cdots \sum_{\sigma^{(|E|)}} \prod_{a \in V} f_a(\sigma_a) = \sum_{\sigma^{(m)}} f^{(m)}(\sigma^{(m)}). \tag{38}
\]

- As illustrated in Fig. (3), the elimination procedure may lead to double-, triple-, and in general multiple-edges connecting the same nodes, and it may also result in self-edges, even if the original graph is a normal/simple graph. In fact, this observation explains why we choose to work in this manuscript with the general MGMs.

- Even though we are free to choose any edge-elimination sequence, it is reasonable to eliminate, first, all normal edges (having two distinct nodes associated with the edge), as in the illustrative example of Fig. (3). This results in a “bouquet” (of self-edges) graph containing a single node and multiple self-edges. Notice that if the original graph is a tree the resulting bouquet graph contains no self-edges, and then in this case the elimination sequence is completed. It is straightforward to check that the number of self-edges in the bouquet is invariant of the the normal portion of the edge elimination procedure, i.e. it does not depend on the order of the normal edge eliminations. Moreover this number is exactly equal to the number of edge cuts one needs to apply to the original graph to turn it into a tree. In the following (and unless specify otherwise) we will be assuming that the normal edges are eliminated in the elimination sequence first. Significance of the bouquet graph for our procedure will become clear in the following when we analyze application of the BP procedure to MGMs from the sequence.

- Obviously the exact elimination \cite{37} is not practical because the factor degree and most importantly the complexity of computing the factors grow exponentially with $m$.

- A number of approximate elimination schemes was introduced in the past to bypass the hardness of the exact computations of $Z$. Of these approximations the mini-bucket elimination schemes \cite{3, 4, 25, 49} are arguably the most popular and also related to the gauge GT and BP subjects. See Section \ref{VIII} for additional discussions.

- Even though the sequence of MGMs is not tractable, it is still of a theoretical interest (e.g., in relation to analyzing the class of MGMs where one can derive tractable bounds on GF, to analyze an intermediate MGM in the sequence from the perspective of the GT and BP). This approach is explored in the following section.
V. FROM GAUGE FUNCTION, $z(x)$, TO PARTITION FUNCTION, $Z$

**Theorem V.1** (“Differentiate+marginize”). Exact PF, $Z$, of the GM can be recovered from the GF, $z(x)$, defined in Eq. (27), via application of the following mixed-derivative operator:

$$m = 0: \quad x^{(0)} = x, \quad Z^{(0)}(x) = z(x),$$
$$m = 1, \cdots, |\mathcal{E}|: \quad x^{(m)} = x^{(m-1)} \setminus \{x^{(m)}_{\alpha_d}, x_{\bar{\alpha}_d}\},$$

$$Z^{(m)}(x^{(m)}) \doteq \left(1 + \partial x^{(m)}_{\alpha_d} \partial x^{(m)}_{\bar{\alpha}_d}\right) \left((1 + x^{(m)}_{\alpha_d}x^{(m)}_{\bar{\alpha}_d})Z^{(m-1)}\right)|_{x^{(m)}_{\alpha_d}=x^{(m)}_{\bar{\alpha}_d}=0},$$

$$m = |\mathcal{E}|: \quad x^{(|\mathcal{E}|)} = \emptyset, \quad Z^{(|\mathcal{E}|)} = Z,$$

where ordering of edges according to Eq. (36) is assumed.

The statement of Theorem V.1 expressed in Eqs. (39, 40, 41) is a direct consequence of the following observation:

$$\left(1 + \partial x^{(m)}_{\alpha_d} \partial x^{(m)}_{\bar{\alpha}_d}\right) \left(x^{(m)}_{\alpha_d}x^{(m)}_{\bar{\alpha}_d}\right)|_{x^{(m)}_{\alpha_d}=x^{(m)}_{\bar{\alpha}_d}=0} = \delta (\varsigma_{\alpha_d}, \varsigma_{\bar{\alpha}_d}),$$

where $\delta (\varsigma_{\alpha_d}, \varsigma_{\bar{\alpha}_d})$ stands for the Kronecker symbol, which returns unity when $\varsigma_{\alpha_d} = \varsigma_{\bar{\alpha}_d}$ and is zero otherwise.

Furthermore, comparing sequence of transformations in the Theorem V.1 with the edge-elimination sequence described in Section IV, one arrives at the following statement.

**Theorem V.2** (Equivalence of the Algebraic (differentiate+marginize) and Graphical (edge elimination) transformations). $Z^{(m)}(x^{(m)})$, defined in Eq. (40), is the Gauge Function introduced in Eq. (27) however applied to the $m$-th GM in the edge-elimination sequence defined in Eq. (37):

$$Z^{(m)}(x^{(m)}) = \prod_{a \in \mathcal{E}^{(m)}} \frac{h^{(m)}(x^{(m)})}{(1 + x^{(m)}_{\alpha_d}x^{(m)}_{\bar{\alpha}_d})},$$

$$h^{(m)}(x^{(m)}) \doteq \prod_{a \in \mathcal{V}^{(m)}} \left(\sum_{\varsigma_{\alpha_d} \in \Sigma^{(m)}} f^{(m)}_{\alpha_d}(\varsigma_{\alpha_d}) \prod_{a \in \mathcal{E}^{(m)}(a)} x^{(m)}_{\alpha_d}\right).$$

The sequence of the graph-algebraic transformations from the GF, $z(x)$, to the PF, $Z$, introduced and discussed in this and preceding sections is the main technical point of this manuscript.

In the next section we relate this sequence, and each step in the sequence of edge eliminations resulting in the mapping, to BP estimations of MGMs in the sequence.

VI. BP-ELIMINATION

Let us take advantage of the rational, in $x$, structure of the GF, $z(x)$, and represent $h(x)$ in Eq. (27), as a generic quadratic function of $x_{\alpha_d}$ and $x_{\bar{\alpha}_d}$, where the edge $\alpha$ of the original graph, $\mathcal{G}$ is selected arbitrarily,

$$h(x) \doteq h^{(0,0)} + h^{(1,0)}x_{\alpha_d} + h^{(0,1)}x_{\bar{\alpha}_d} + h^{(1,1)}x_{\alpha_d}x_{\bar{\alpha}_d},$$

the coefficients of the expansion are non-negative, $\forall i, j = 0, 1, \quad h^{(i,j)} \geq 0$, and also dependent on $x^{(1)} = x \setminus \{x^{\alpha_d}, x^{\bar{\alpha}_d}\}$ (the dependence is dropped here and also in some formulas below to avoid bulky expressions). Substituting Eq. (45) into the BP-equations (28) for the edge $\alpha$, one arrives at a quadratic equations for $x_{\alpha_d}$ and $x_{\bar{\alpha}_d}$, which results in two roots of which only one is physical, i.e. consistent with respective positive marginal probabilities:

$$x_{\alpha_d}^{(\alpha-bp)} = \frac{h^{(1,1)} - h^{(0,0)} + \sqrt{(h^{(1,1)} - h^{(0,0)})^2 + 4h^{(0,1)}h^{(1,0)}}}{2h^{(1,0)}},$$
$$x_{\bar{\alpha}_d}^{(\alpha-bp)} = \frac{h^{(1,1)} - h^{(0,0)} + \sqrt{(h^{(1,1)} - h^{(0,0)})^2 + 4h^{(0,1)}h^{(1,0)}}}{2h^{(0,1)}},$$
The value of \( h(x)/(1 + x_{\alpha_d}x_{\tilde{\alpha}_d}) \) evaluated at the physical \( \alpha\)-BP-gauge is

\[
h(\alpha\text{-bp}) = \frac{h(x)}{1 + x_{\alpha_d}x_{\tilde{\alpha}_d}} \bigg|_{x_{\alpha_d}=x^{(\alpha\text{-bp})}_d, x_{\tilde{\alpha}_d}=x^{(\alpha\text{-bp})}_{\tilde{\alpha}}} = \frac{h(1,1) + h(0,0) + \sqrt{(h(1,1) - h(0,0))^2 + 4h(0,1)h(1,0)}}{2}. \tag{48}
\]

Notice that the expression (45) for \( h \), simplifies when \( \alpha \) is a normal edge (not a self-edge). In this special case \( h \) is a product of two polynomials of the first order over \( x_{\alpha_d} \) and \( x_{\tilde{\alpha}_d} \), respectively, i.e. in this case \( h^{(1,1)}h(0,0) = h^{(0,1)}h(1,0) \). Then Eqs. (46,47) and Eq. (48) transform to

\[
\text{If } \alpha \text{ is a normal edge: } x^{(\alpha\text{-bp})}_d = \frac{h^{(1,1)}}{h^{(1,0)}}, \quad x^{(\alpha\text{-bp})}_{\tilde{\alpha}} = \frac{h^{(1,1)}}{h^{(0,1)}}, \quad h^{(\alpha\text{-bp})} = h(1,1) + h(0,0). \tag{49}
\]

Comparing Eq. (49) with the first step of the exact edge elimination (first step of the mixed derivative application to the PF) described in Section VII, observing that the result is equivalent to the exact elimination, as long as our MGM has a maximal BP gauge, which happens to be interior. Therefore, sequential BP-elimination of edges will be still equivalent to exact elimination, as long as the edge to be eliminated is normal, and the MGM has a maximal BP gauge, which is interior, on each step of the elimination procedure. A formal statement is as follows.

**Theorem VI.1 (BP-to-bouquet).** Elimination of normal edges in MGM via application of the sequential edge-by-edge BP-gauge procedure, resulting in MGM for the bouquet graph, is exact, i.e. it is equivalent to the exact elimination via summation over binary variables associated with the eliminated edges.

Notice that the sequential BP-elimination approach does not generalize to self-edges, because in this case expression (48) for \( h^{(\alpha\text{-bp})} \) returns a fractional function of \( h^{(\nu,\rho)} \), thus resulting in a fractional (not polynomial) function over the remaining gauge variables, \( x \setminus \{x_{\alpha_d}, x_{\tilde{\alpha}_d}\} \). However, the general fractional relations (46,47,48) still result in a number of useful statements.

**Theorem VI.2 (BP-saddle).** Any BP gauge solution of Eq. (28) is a saddle-point of the GF, \( z(x) \), defined in Eq. (27), over any pair of the edge-gauges, \( x_{\alpha_d}, x_{\tilde{\alpha}_d} \).

**Proof.** We only need to discuss here the case of an interior gauge, extending it to the (generic) case of a BP gauge following the logic of Section IIIB. Expanded in the Taylor series over deviations from the BP-gauge, the rational expression, \( h(x)/(1 + x_{\alpha_d}x_{\tilde{\alpha}_d}) \), representing the \( x_{\alpha_d}, x_{\tilde{\alpha}_d} \)-dependent part of \( z(x) \), where \( h(x) \) is from Eq. (45), becomes

\[
h(x) - h^{(\alpha\text{-bp})} - \text{cubic corrections} = d \left( x_{\alpha_d} - x^{(\alpha\text{-bp})}_{\alpha_d} \right) \left( x_{\tilde{\alpha}_d} - x^{(\alpha\text{-bp})}_{\tilde{\alpha}_d} \right)
= \frac{d}{4} \left( x_{\alpha_d} + x_{\tilde{\alpha}_d} - x^{(\alpha\text{-bp})}_{\alpha_d} - x^{(\alpha\text{-bp})}_{\tilde{\alpha}_d} \right)^2 - \left( x_{\alpha_d} - x_{\tilde{\alpha}_d} - x^{(\alpha\text{-bp})}_{\alpha_d} + x^{(\alpha\text{-bp})}_{\tilde{\alpha}_d} \right)^2, \tag{50}
\]

where \( d > 0 \) (we skip presenting here bulky but explicit expression for \( d \)), thus completing the proof.

The following technical statement, proven through a straightforward algebraic manipulation, introduces another useful feature of Eq. (48).

**Lemma VI.3 (BP- vs exact- reductions).** Consider a generic polynomial, \( h(x) \), representing MGM and stated in the form of expansion (45) over variables \( x_{\alpha_d} \) and \( x_{\tilde{\alpha}_d} \) associated with the edge, \( \alpha \). Then, condition that for all values of the variables remaining after contraction of the edge \( \alpha_d \), the BP-reduced function, defined according to Eq. (48), is less or equal than the exact-reduced function,

\[
\forall x^{(1)} : \quad \frac{h(x)}{1 + x_{\alpha_d}x_{\tilde{\alpha}_d}} \bigg|_{x_{\alpha_d}=x^{(\alpha\text{-bp})}_d, x_{\tilde{\alpha}_d}=x^{(\alpha\text{-bp})}_{\tilde{\alpha}}} \leq h^{(1,1)}(x^{(1)}) + h^{(0,0)}(x^{(1)}), \tag{51}
\]

holds if

\[
\forall x^{(1)} : \quad h^{(0,1)}(x^{(1)})h^{(1,0)}(x^{(1)}) \leq h^{(0,0)}(x^{(1)})h^{(1,1)}(x^{(1)}).
\tag{52}
\]

The following optimization version of the Lemma VI.3 was also introduced (and proven) in [34, 67].

**Lemma VI.4 (BP- vs exact- reductions: variational version).** Given representation (47) of \( h(x) \) as the polynomial in \( x_{\alpha_d}, x_{\tilde{\alpha}_d} \), an arbitrarily chosen marginal belief, \( \beta_\alpha \in [0,1] \), and Eq. (52) satisfied, guarantees that

\[
\forall x^{(1)} : \quad (\beta_\alpha)^{\beta_\alpha} (1 - \beta_\alpha)^{1 - \beta_\alpha} \inf_{x_{\alpha_d}, x_{\tilde{\alpha}_d}} \frac{h(x)}{(x_{\alpha_d}x_{\tilde{\alpha}_d})^{\beta_\alpha}} \leq h^{(1,1)}(x^{(1)}) + h^{(0,0)}(x^{(1)}). \tag{53}
\]
VII. BI-STABILITY AND MONOTONICITY OF BP ELIMINATION

Remarkably the condition (52) was shown to hold generically if $h(x)$ is bi-stable [5], where the stability and bi-stability of a polynomial are defined as follows.

Definition VII.1 (Real Stable (RS) Polynomial and Bi-Stable (BS) Polynomial. See [5]). A nonzero polynomial, $g(x) \in \mathbb{R}[x_1, \cdots, x_N]$, with real coefficients is RS if none of its roots $z = (z_1, \cdots, z_N) \in \mathbb{C}^N$ (i.e., solutions of $g(z) = 0$) satisfies: $\text{Im}(z_i) > 0$ for every $i = 1, \cdots, N$. A polynomial $h(x_{\alpha(1)}, x_{\alpha(2)}; x_{\beta(2)}, \cdots)$ is BS if $h(x_{\alpha(1)}, -x_{\alpha(1)}; x_{\alpha(2)}, -x_{\alpha(2)} \cdots)$ is Real Stable (RS).

Therefore we arrive at the following powerful statement.

Theorem VII.2 (Monotonicity of VBP). Consider an MGM over graph $G$ and with the factors correspondent to a bi-stable polynomial, $h(x)$, build a sequence of MGMs, $m = 0, \cdots, |E|$, starting with the original MGM and getting next MGM in the sequence by contraction of an edge, and denote (according to notations of the preceding Sections), graph, vector of gauge variables, polynomial and VBP estimation for PF evaluated at the $m$-th step of the hierarchy, $G(m), x(m), h(m)(x(m))$ and $Z^{(m;vbp)}$, respectively. Then

1. Each polynomial, $h^{(m)}(x^{(m)})$, in the sequence is bi-stable.

2. Value of the VBP estimation for PF does not decrease with elimination and therefore

$$Z^{(vbp)} = Z^{(0;vbp)} \leq Z^{(1;vbp)} \cdots \leq Z^{(|E|;vbp)} = Z.$$  

Proof. The first step of exact contraction, applied to $h(x)$, consists of applying a differential operator $(1 + \partial_{\alpha_{\beta(1)}} \partial_{\alpha_{\beta(1)}})$, followed by setting both $x_{\alpha(1)}$ and $x_{\beta(1)}$ to zero. The composite operator preserves bi-stability. This follows from a standard argument that involves characterization of linear operators $T$ that preserve real stability of polynomials in terms of their algebraic symbols [12, 13]. The algebraic symbol of the above composite operator is easily computed, and the stability of its symbol is obvious, therefore $h^{(1)}(x^{(1)})$ is bi-stable. Applying the logic sequentially, we conclude that all polynomials in the sequence: $m = 1, \cdots, |E|$, $h^{(m)}(x^{(m)})$ are bi-stable. Statement (1) of the Theorem VII.2 is proven.

Applying Lemma VI.4 to each elimination in the sequence one writes

$$m = 1, \cdots, |E| \quad \forall \beta^{(m-1)} \in [0, 1], \quad \forall x^{(m)}:
$$

$$(\beta^{(m)})^{\beta^{(m-1)}} (1 - \beta^{(m)})^{1-\beta^{(m-1)}} \inf_{x^{(m)}_{\alpha_{\beta} > 0}} \frac{h^{(m-1)}(x^{(m-1)})}{x^{(m)}_{\beta_{\alpha} > 0}} \leq h^{(m)}(x^{(m)}).$$  

Next one multiplies both sides of Eq. (55) on,

$$\prod_{\alpha \in E^{(m)}} (\beta^{(m)}_{\alpha})^{\beta^{(m-1)}_{\alpha} (1 - \beta^{(m-1)}_{\alpha})^{1-\beta^{(m-1)}_{\alpha}}}$$

and observe that $\inf_{x^{(m)}_{\beta > 0}}$ applied to the left hand side of the resulting inequality is less or equal to the $\inf_{x^{(m)}_{\beta > 0}}$ applied to the right hand side of the inequality. Finally, similar application of the $\max_{x^{(m-1)}}$ operation to the two sides of the inequality obtained at the previous step results in the desired Eq. (54). (2) is proven.

Notice that related technical statements and proofs were reported in [5] and [67].

VIII. DISCUSSION AND PATH FORWARD

Inspired by [5, 67], we began this manuscript by generalizing the Bethe Free Energy approach from normal GM to multi-GM. Then we reformulate gauge representation of [21, 22] for computing PF of an MGM in terms of polynomials. According to [21, 22], picking up a Gauge Function, which is a term in the gauge-transformed series, and making it least sensitive to the gauge transformations (looking for stationary point of the GF over gauges) results in the BF gauge and subsequently in the LS expression for the PF, where each term is an explicit functional of the BF gauge. One may say that the algebraic essence of the LS approach is in reconstructing exact PF from its tractable BP approximation by summing the LS terms. The main construct of this manuscript is an alternative map, suggested by
analogy with the polynomial construct of \( [5, 33, 67] \) from the GF to the PF, \( Z \). Now, this is possible via a sequence of differentiation of the GF over gauge variables, each associated with a directed edge of the graph. We show that a differentiation step in the sequence can be interpreted graphically as contraction/elimination of an edge, which results in a new MGM with one less edge and one less node. PF of each MGM in the sequence is exactly equal to PF of the original MGM. (Note in passing that (a) construction is similar to an elementary transformation step in the graph minor theory \[26\]; and (b) even if the original GM is normal, i.e. it contains only normal edges and no self-edges, one eventually arrives advancing in the sequence at an MGM, containing self-edges, therefore justifying discussion of the most general MGM setting.) Evaluating minimum of the BFE, or equivalently specially defined optimum of the respective GF, for each MGM in the sequence we get an optimal BP estimation for each MGM in the sequence. We observe that BP transformation is exact for contraction of a normal edge but approximate for contraction of a self-edge. Then, utilizing the power of the Real Stable Polynomials (RSP) theory \[58, 72, 75\], we showed that (a) all polynomials associated with factors of the contracted MGMs are BS if all polynomials associated with factors of the original MGM are BS; (b) optimal BP estimation for PF of an MGM in the sequence upper bounds optimal BP estimation for PF of the preceding MGM (in the sequence). Corollary of the latter statement is a new proof (also generalization from GM to MGM) that the optimal BP estimation of the original MGM low bounds the exact PF. The original proof was made for the special case of bipartite GM in \[67\], when BS is reduced to RS, while the polynomial version of our results is a particular case of the relation presented in \[5\].

Synthesis of the two approaches, GM/gauges/BP/loops and RSP, is far from explored by this and preceding \[5, 33, 67\] manuscripts. Therefore, we find it useful to combine in the remainder of this section some remarks, that follow from the manuscript results, with speculations about future research directions.

- **BSP examples**: Linear (degree one) real polynomials, \( a + \sum_i b_i z_i \), with \( a > 0 \) and \( \forall i, b_i > 0 \), correspondent to generic matching (monomer–dimer) models over bi-partite graphs, is the main example of a GM represented by BSPs/RSPs. A non-bi-partite BSP example can be derived from the bi-partite case by contraction of (a number of) edges described in Section \[IV\]. Other known classes of BSPs are also to be explored in GMs. In particular, determinantal polynomials, \( \det(B + \sum_i z_i A_i) \), with positive semi-definite matrices, \( \forall i: A_i > 0 \), and Hermitian matrix \( B \) (all matrices are quadratic of the same dimensionality) is another (and arguably the most popular example in the RSP theory) that may also have interesting relations/consequences for Fermion GM of statistical and quantum physics, see \[18, 19\] and references therein. All statements made in this manuscript (e.g., on the ordering of the PF estimates for the contracted sequence of MGMs) would apply to the special MGM with the underlying BSP structure.

- **Improving BP approximation**: The elimination scheme of Section \[IV\] has a significant approximation potential, both theoretically and empirically. On the theoretical side, one may attempt to seek a more restrictive class of polynomials, for example, models which are BSP locally and not globally in the upper-half planes for each complex variable (associated with a directed edge). Approached from an empirical/algorithic stand point, the elimination can be carried over and then checked post-factum (if it results in an increase or decrease of the PF of the contracted graphs). Given that the complexity of the contracted MGM evaluations will be increasing exponentially with the elimination steps, one may consider approximate methods in the spirit of the mini-bucket elimination schemes \[3, 4, 25, 49\]. Therefore, developing new mini-bucket schemes based on the polynomial stability properties is another promising direction for the future. Besides, it will be important to take advantage of the polynomial structure in creating synthetic practical algorithms mixing BT/GT/LC ideas with random sampling ideas; for example, in the spirit of FPRAS and empirical schemes a-la \[1\], and the mini-bucket elimination schemes a-la \[3, 4\].

- **Efficient computation of BP gauge**: A comment in Section 3.3 of \[67\] suggests that some algorithmic improvements for computing \( Z^{(bp)} \) based on techniques from the theory of stable polynomials are possible. In general, an RS feature of the node polynomials does not guarantee convexity of the BFE, \( 7 \), even though for some special cases and noticeably for the case of perfect matching \[46, 47, 73\], the convexity may be guaranteed. Moreover, an optimal solution of the BFE may be achieved at the boundary of the belief polytope, thus not satisfying the BS Eq. \[30\]. Since results of this manuscript are dependent on the existence of a valid solution of BP Eq. \[30\], it is imperative for future progress to develop RSP theory-based schemes answering the question of existence and discovering solution(s) of BP equations efficiently. It will also be important to generalize the analysis of this manuscript to the case when solution of the BP Eqs. \[30\] is found outside of the feasibility domain (outside of the BP polytope).

- **Higher alphabets and higher-degree polynomials**: Both the gauge transformation and the RSP theory extend, in principle, to the case of higher alphabets and related higher-degree polynomials. The loop tower approach of \[17\] and alternative approach of \[54\] build generalizations of the GT and LS for the case of higher
IX. ACKNOWLEDGEMENTS

MC and YM are grateful to organizers and participants of the EPFL, Bernoulli center, workshops on “Introduction to Partition Functions” in July of 2018 and "Applications of the Partition Functions" in November of 2018, where this work was initiated and where its first version was criticized, respectively. We are particularly indebted to Nisheeth Vishnoi for many discussions and useful explanations, to Peter Csikvari for attracting our attention to inconsistency in our early notes and to Nima Anari explaining to us the notion of bi-stability. We are also thankful to Pascal Vontobel, Vishnoi for many discussions and useful explanations, to Peter Csikvari for attracting our attention to inconsistency in work was initiated and where its first version was criticized, respectively. We are particularly indebted to Nisheeth Vishnoi for many discussions and useful explanations, to Peter Csikvari for attracting our attention to inconsistency in our early notes and to Nima Anari explaining to us the notion of bi-stability. We are also thankful to Pascal Vontobel, Jinwoo Shin, and Marc Lelarge for help with references and useful comments. The work at LANL was carried out under the auspices of the National Nuclear Security Administration of the U.S. Department of Energy under Contract No. DE-AC52-06NA25396. The work was partially supported by DOE/OE/GMLC and LANL/LDRD/CNLS projects.

Appendix A: Loop Series [21, 22] restated in the polynomial form

With gauge $x$ chosen to satisfy the BP Eqs. (28), or equivalently Eqs. (31), of an S-MGM, thus denoted $x^{(bp)}$, consistently with notations introduced in the main part of the manuscript, one derives from Eq. (20) the Loop Series, expression for $Z$:

$$Z = \sum_{\sigma \in \Sigma_{glp}} z(\sigma | x^{(bp)}), \quad (A1)$$

where $\Sigma_{glp}$ stands for the set of $\sigma$ vectors corresponding to the so-called generalized loops (GLs), $\sigma \in \Sigma_{glp}$ iff $\forall a \in V$, $\sum_{\alpha \in e(a)} \sigma_\alpha \neq 1$. Note that an empty set, $\sigma = 0 | E|$ is included in $\Sigma_{glp}$. A GL can also be thought of as a subgraph of $G$, $G^{(\sigma)} = (V^{(\sigma)}, E^{(\sigma)}) \subseteq G$, constructed by coloring edges of the graph (setting respective $\sigma_\alpha$ to unity) according to the following rules: each node neighboring an edge of the GL set contains at least two edges colored, i.e. $V^{(\sigma)}$ $\equiv$ $\{ a \in V | \sum_{\alpha \in e(a)} \sigma_\alpha > 1 \}$ and $E^{(\sigma)}$ $\equiv$ $\{ \alpha \in E | \sigma_\alpha = 1 \}$.

Each GL contribution in Eq. (A1) is expressed via a BP solution as follows:

$$\forall \sigma \in \Sigma_{glp} : \quad z(\sigma | x^{(bp)}) = Z^{(bp)} \prod_{\alpha \in V^{(\sigma)}} \mu^{(bp)}_\alpha \prod_{\alpha \in E^{(\sigma)}} (1 - \beta^{(bp)}_\alpha), \quad (A2)$$

$$\forall a \in V^{(\sigma)} : \quad \mu^{(bp)}_a = \frac{\sum_{\sigma_a} f_a(\sigma_a) \prod_{\alpha \in e^{(\sigma)}(a)} (x^{(bp)}_\alpha)^{\sigma_\alpha} (\varsigma_\alpha - \beta^{(bp)}_\alpha)^{\sigma_\alpha}}{\sum_{\sigma_a} f_a(\sigma_a) \prod_{\alpha \in e^{(\sigma)}(a)} (x^{(bp)}_\alpha)^{\sigma_\alpha}}, \quad (A3)$$
where $Z^{(bp)} = z(x^{(bp)})$ and $e^{(\sigma)}(a)$ marks the set of edges of $E^{(\sigma)}$ associated with the node $a$ of $V^{(\sigma)}$; $\beta^{(bp)}_\alpha$ is the marginal BP belief of observing edge $\alpha$ in the state $\varsigma_\alpha = 1$; and $\mu^{(bp)}_a$ is the following average

$$\forall a \in V^{(\sigma)} : \mu^{(bp)}_a = E^{(bp)} \left[ \prod_{\alpha \in e^{(\sigma)}(a)} (\varsigma_\alpha - \beta^{(bp)}_\alpha) \right] = \sum_{\varsigma_\alpha} P^{(bp)}_a(\varsigma_\alpha) \prod_{\alpha \in e^{(\sigma)}(a)} (\varsigma_\alpha - \beta^{(bp)}_\alpha),$$

over the BP-induced probability distribution, $P^{(bp)}_a$, defined in Eq. (32).
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