Loop Calculus in Statistical Physics and Information Science

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Considering a discrete and finite statistical model of a general position we introduce an exact expression for the partition function in terms of a finite series. The leading term in the series is the Bethe-Peierls (Belief Propagation)-BP contribution, the rest are expressed as loop-contributions on the factor graph and calculated directly using the BP solution. The series unveils a small parameter that often makes the BP approximation so successful. An integral representation for the series interprets the BP expression as a saddle-point. Applications of the loop calculus in statistical physics and information science are discussed.

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Discrete statistical models, the Ising model being the most famous example, play a prominent role in theoretical and mathematical physics. They are typically defined on a lattice, and major efforts in the field focused primarily on the case of the infinite lattice size. Similar statistical models emerge in information science. However, the most interesting questions there are related to graphs that are very different from a regular lattice. Moreover it is often important to consider large but finite graphs. Statistical models on graphs with long loops are of particular interest in the fields of error-correction and combinatorial optimization. These graphs are tree-like locally.

A theoretical approach pioneered by Bethe [1] and Peierls [2] (see also [3]), who suggested to analyze statistical models on perfect trees, has largely remained a useful analytical control the Bethe-Peierls approximation gives remarkably accurate results, often out-performing standard mean-field results. The ad-hoc approach was also re-stated in a variational form [4, 5]. Except for two recent papers [6, 7] that will be discussed later in the letter, no systematic attempts to construct a regular theory with a well-defined small parameter and Bethe-Peierls as its leading approximation have been reported.

A similar tree-based approach in information science has been developed by Gallager [8, 9] in the context of error-correcting theory. Gallager introduced so called Low-Density-Parity-Check (LDPC) codes, defined on locally tree-like Tanner graphs. The problem of ideal decoding, i.e. restoring the most probable pre-image out of the exponentially large pool of candidates, is identical to solving a statistical model on the graph [8]. An approximate yet efficient decoding Belief-Propagation algorithm introduced by Gallager constitutes an iterative solution of the Bethe-Peierls equations derived as if the statistical problem was defined on a tree that locally represents with the Tanner graph. We utilize this abbreviation coincidence to call Bethe-Peierls and Belief-Propagation equations by the same acronym – BP. Recent resurgence of interest to LDPC codes [10], as well as proliferation of the BP approach to other areas of information and computer science, e.g. artificial intelligence [11] and combinatorial optimization [12], where interesting statistical models on graphs with long loops are also involved, posed the following questions. Why does BP perform so well on graphs with loops? What is the hidden small parameter that ensures exceptional performance of BP? How can we systematically correct BP? This letter provides systematic answers to all these questions.

The letter is organized as follows. We start introducing notations for a generic statistical model. We next state our main result: a decomposition of the partition function as a finite series. The BP expression for the model represents the first term in the series. All other terms correspond to closed undirected and possibly branching yet not terminating at a node paths/diagrams on the factor-graph. The simplest diagram is a single loop. An individual contribution is the product of the “propagator” terms along the path and the product of “vertices” that correspond to branching points. The propagators and the vertices are expressed explicitly in terms of simple correlation functions calculated within the BP approximation. We proceed with discussing a small parameter that allows to state BP as the bare approximation and loop terms (understanding loops in generalized sense with allowed branching) as corrections to BP. Further, we briefly describe a derivation of the loop expansion via an integral representation. We also show how BP emerges as a saddle-point in the integral representation. We conclude with clarifying the relation of this work to other recent advances in the subject, and discussing possible applications and generalizations of the approach.

Model. Consider a generic discrete statistical system, with configurations characterized by a set of binary variables: $\sigma_i = \pm 1$, $i = 1, \ldots, n$, which is factorized so that
the probability \( p(\sigma_i) \) to find the system in the state \( \{ \sigma_i \} \) and the partition function \( Z \) are
\[
p(\sigma_i) = Z^{-1} \prod_{\alpha} f_\alpha(\sigma_\alpha), \quad Z = \sum_{\{ \sigma_i \}} \prod_{\alpha} f_\alpha(\sigma_\alpha),
\]
where \( \sigma_\alpha \) represents a subset of \( \sigma_i \) variables, and \( \alpha \) labels one of \( m \) factor-functions \( f_\alpha \) that are all non-negative and finite. Relations between factor functions (checks) and elementary discrete variables (bits), expressed as \( i \in \alpha \) and \( \alpha \ni i \), can be conveniently represented in terms of the system-specific factor graph. If \( i \in \alpha \) we say that the bit and the check are neighbors. An example of the factor graph with \( m = 3 \) corresponding to \( p(\sigma_1, \sigma_2, \sigma_3, \sigma_4) = Z^{-1} f_3(\sigma_3) f_3(\sigma_3) f_3(\sigma_3) \), where \( \sigma_a \equiv (\sigma_1, \sigma_2) \), \( \sigma_b \equiv (\sigma_1, \sigma_2, \sigma_3) \), \( \sigma_c \equiv (\sigma_1, \sigma_3, \sigma_4) \) and \( \alpha = a, b, c \), is shown in Fig. 1.

**Loop series.** The main exact result of the letter is decomposition of the partition function defined by Eq. 1 in a finite series:
\[
Z = Z_0 \left( 1 + \sum_C r(C) \right), \quad r(C) = \prod_{i, \alpha \in C} \mu_\alpha(C) \mu_i(C), \tag{2}
\]
where summation goes over all allowed \( C \) called marked paths or generalized loops. They consist of sets of bits and checks so that each of them has at least two distinct neighbors on the path. For the aforementioned example there are four allowed marked paths (loops) shown in Fig. 1 on the right. In Eqs. 2, \( b_i(\sigma_i) \), \( b_\alpha(\sigma_\alpha) \) and \( Z_0 \) are beliefs (probabilities) defined on bits and checks and partition function, respectively, calculated for the BP solution. A BP solution can be interpreted as an exact solution on an infinite tree built by unwrapping the factor graph. A convenient representation for a BP solution is given in Fig. 1 as a set of beliefs minimizing the Bethe free energy
\[
\mathcal{F} = \sum_{\alpha} b_\alpha(\sigma_\alpha) \ln b_\alpha(\sigma_\alpha) f_\alpha(\sigma_\alpha) \sum_i (k_i - 1) b_i(\sigma_i) \ln b_i(\sigma_i),
\]
under the set of realizability, \( 0 \leq b_i(\sigma_i), b_\alpha(\sigma_\alpha) \leq 1 \), normalization, \( \sum_\sigma b_i(\sigma_i) = \sum_\sigma b_\alpha(\sigma_\alpha) = 1 \), and consistency \( \sum_{\sigma_i} b_i(\sigma_i) = b_i(\sigma_i) \) constraints. Each term associated with a marked path is the product of “vertices” \( \mu_\alpha(C) \) and “propagators”, \( \mu_i(C) \), defined on the checks and bits which belong to the marked path, \( C \). A “vertex” is an irreducible correlation function calculated within BP. It contains products of spins on the marked bits neighboring a common check. The “propagator” is expressed in terms of magnetization at the corresponding bit of \( C \) calculated within BP.

Exact expressions for the spin correlation functions can be obtained by differentiating Eq. 2 with respect to the proper factor functions. In the tree case (no loops) only the unity term in the r.h.s. of Eq. 2 survives. In the general case Eq. 2 provides a clear criterion of the BP approximation validity: The sum over the loops in the r.h.s. of Eq. 2 should be small compared to one. The number of terms in the loop series increases exponentially with the number of bits. Therefore, Eq. 2 becomes useful for selecting a smaller than exponential number of leading contributions. In a large system the leading contribution comes from paths where the number of degree two connectivity nodes substantially exceeds the number of branching nodes, i.e. the ones with higher connectivity degree. According to Eq. 2 the contribution of a long path is given by the ratio of the along-the-path product of the irreducible nearest-neighbor spin correlation functions \( \mu_{ij} \) to the along-the-path product of the local bit contributions, \( 1/(1 - m_i^2) \). All are calculated within BP. Therefore, the small parameter in the theory is \( \varepsilon = \prod_{(i,j) \in C} \mu_{ij} / \prod_{i \in C} (1 - m_i^2) \). If \( \varepsilon \) is much smaller than one for all the marked paths the BP approximation is valid. The leading correction to the BP result is given by the marked path with the largest \( \varepsilon \), which is typically represented by the shortest single loop on the factor graph.

**Integral representation.** A function of a set of \( k \) scalar binary variables, \( \sigma_a = \pm 1, a = 1, \cdots, k \), which is a constant if all the \( \sigma_a \) are equal and zero otherwise, can be represented as a contour integral
\[
\int_\Gamma \prod_a d\chi_a \exp \left( \sum_a \chi_a \sigma_a \right) \cosh \left( (k - 1)^{-1} \sum_a \chi_a \right)^{1-k},
\]
defined in the complex domain of \( k \) auxiliary variables, \( \chi_a \). The cycle \( \Gamma \) constitutes a cartesian product of \( k \) contours in the complex plane each connecting points \( z_a \) and \( z_a + 2\pi i (k - 1) \). The result of integration does not depend on the choice of the reference points \( z_a \). We introduce a product of the integral formula replicas, one per each bit with more than one check neighbor. This formal trick decouples the bit spin variables \( \sigma_i \) from the check spin variables \( \sigma_\alpha \) at the cost of additional integrations, one per any edge of the factor graph connected to a bit with the connectivity degree of two or higher.
This results in an integral representation for the partition function defined by Eq. (1):

$$Z \sim \int \left( \prod_i \prod_{\alpha} d\chi_{i\alpha} \right) \prod_i \cosh \left( \frac{1}{k_i - 1} \sum_{\alpha \geq i} \chi_{i\alpha} \right) \left( 1 - k_i \right) \times \prod_{\alpha} \left( \sum_{\sigma_i} \left( f_{\sigma}(\sigma_i) \exp \left( \sum_{i \in \alpha} \chi_{i\alpha} \right) \right) \right), \quad (3)$$

where $k_i$ is $i$'s bit connectivity degree. Before manipulating the integral explicitly we comment on its approximate saddle-point evaluation. First of all, the equations for the stationary points $\chi^{(sp)}$ of the integrand in Eq. (3) turn out to be exactly equivalent to the BP equations, so that, $b_{\alpha}(\sigma_{\alpha}) \sim f_{\sigma}(\sigma_{\alpha}) \exp(\sum_{i \in \alpha} \sigma_i \chi^{(sp)}_{i\alpha})$, where $b_{\alpha}(\sigma_{\alpha})$ are the beliefs that minimize the Bethe free energy, $\mathcal{F}$. It is also possible to show that all Gaussian corrections (Jacobian contribution) are only of a “loop” type, i.e. they disappear on a tree. The way how other than loop corrections cancel out in this perturbative analysis suggests that there may be a way of explicit resummation in all orders. Below we demonstrate that this what happens.

To that end we note that the integrand in Eq. (3) is a product of a contribution local in bits [the upper line in Eq. (3)] and the local in checks counterpart [the second line in Eq. (3)]. The idea is to keep the local in bits contribution as is, while decomposing the check contribution into a finite sum and evaluating the resulting integrals explicitly. It is also important to account for the saddle-point solution (shift) as well as to incorporate some part of the check term, local both in bits and checks, into the bit term. This is achieved as follows. First, we make a linear change of variables in Eq. (3), $\chi_{i\alpha} = \chi^{(sp)}_{i\alpha} + \zeta_{i\alpha}$. Second, we multiple and divide the bit and check terms in Eq. (3), respectively, by the term, $\prod_i \prod_{\alpha \geq i} \sum_{\sigma_i} \exp(\sigma_i \zeta_{i\alpha}) f_{\sigma}(\sigma_{\alpha}) \exp(\sum_{j \in \alpha} \sigma_j \chi^{(sp)}_{j\alpha})$. Finally, we decompose the combined check contribution in a finite series to arrive at

$$Z \sim \int \prod_i d\zeta_{i\alpha} \prod_i P_i \left( \zeta; \chi^{(sp)} \right) \prod_{\alpha} V_{\alpha} \left( \zeta; \chi^{(sp)} \right), \quad (4)$$

where

$$P_i \equiv \prod_{\alpha \geq i} \left( \cosh \zeta_{i\alpha} + m_i \sinh \zeta_{i\alpha} \right) \left( \cosh \left( \sum_{\alpha \geq i} \left( \chi^{(sp)}_{i\alpha} + \zeta_{i\alpha} \right) / (k_i - 1) \right) \right)^{k_i - 1},$$

$$V_{\alpha} \equiv \sum_{\sigma_{\alpha}} \exp \left( \sum_{i \in \alpha} \sigma_i \chi^{(sp)}_{i\alpha} \right) \prod_i \left( 1 + \frac{(\sigma_i - m_i) \tanh \zeta_{i\alpha}}{1 + m_i \tanh \zeta_{i\alpha}} \right).$$

Expanding the product in the $V_{\alpha}$ term into a sum of individual contributions, picking up one of the contributions for any $\alpha$ and integrating over $\zeta$-fields one derives the corresponding term in Eq. (4). One finds that the first term in the series, $Z_0$, corresponds to BP itself. This accomplishes a brief derivation of Eq. (4). Details, together with an alternative derivation of Eq. (2) bypassing integral representation, will be published elsewhere [12].

**Discussions of the derivation.** The diagrammatic technique we have developed is of a special kind. Its major peculiarity is the non-Gaussian form of the $P$-term in Eq. (4). This is reminiscent of the Vaks-Larkin-Pikin technique [14] developed for non-perturbative corrections to the ferromagnetic ground state in magnets. The reference is not precise as it only means to emphasize a vague structural relation of our method to the one introduced in the classical paper [14] where the “propagator”-P-term was also non-Gaussian.

The transformation from Eq. (3) to Eq. (4) involves two important steps: (i) shift of the integration variables, (ii) dividing and multiplying adjacent bit and check terms, respectively, by the same local object. One might ask: What is so special about the particular choices we made for the shift and the multiplication factor? Additionally, what kind of result would one expect for other choices? Our argument in favor of the specific choice made above was based on the expectation of getting the BP solution as a saddle-point and also extending the correct Gaussian structure encountered around the BP solution to the “non-Gaussian” expansion. The consequence of this “right” choice was complete cancellation of the tree-like structures among the marked paths: A marked path associated with a diagram is not allowed to terminate at a node without forming a loop. These “forbidden” tree corrections would appear for any other choice for either of the two steps. We can reverse the logic and instead of making the two choices rather require that the resulting technique gives no “forbidden” tree corrections. This interprets the BP as the “right” shift of the integration variables. Finally, we emphasize that the integral representation utilized to derive Eq. (4) is not unique. Thus, it can actually be replaced by, in essence simpler, Fourier transformation to a set of discrete variables (in contrast with continuous $\chi$-variables) defined on the edges of the factor graph. If this completely discrete-variables approach is chosen there are still two points of selections (of the type discussed above) at our disposal to get the desired – closed loops only – structure.

**Comments, Conclusions and Path Forward.** We expect that BP equations may have multiple solutions for the model with loops. This expectation naturally follows from the notion of the infinite covering graph, as different BP solutions correspond to different ways to spontaneously break symmetry on the infinite structure. This different BP solutions will generate loop series that are different term by term but give the same result for the sum. Finding the “optimal” BP solution with the smallest $\varepsilon$, characterizing loop correction to the BP solution, is important for applications. A solution related to the absolute minimum of the Bethe free energy would be a natural candidate. However, one cannot guarantee...
that the absolute minimum, as opposed to other local minima of $F$ is always “optimal” for arbitrary $f_\alpha$.

Another remark concerns possible generalizations. In [13] we describe a vertex model generalizing [11]. (The model is also a certain generalization of the celebrated six- and eight-vertex models of Baxter [3].) Spin variables in the vertex model reside on the graph edges, rather than on the nodes, while the factors that generalize $f_\alpha$ belong to the nodes. The vertex model obeys a high symmetry: it contains a set of transformations of the factor functions that keep the full probability $p(\sigma)$ of any state the same. The loop series for the vertex model, similar to Eq. (2), turns out to be term-by-term invariant with respect to the symmetry transformations, whereas the “propagators” and “vertices” that contribute to any particular marked path will be different. This invariance allows to interpret BP equations as a way to parameterize the gauge-invariant (with respect to the symmetry) loop series. Stated differently, all BP solutions that represent the same loop expansion are gauge-equivalent.

Let us now comment on two recent relevant papers [6, 7]. Montanari and Rizzo [6] considered the Ising model (pair-wise interactions between the bits) on a graph with loops. They derived a set of exact equations that connect the correlation functions. This system of equations is underdefined, however if irreducible (what the authors called connected) correlations are neglected the BP result is restored. This feature was used in [6] to generate a perturbative expansion to derive corrections to BP with respect to the irreducible correlations. Structurally the perturbative approach of [6] is consistent with our results: The loop expansion of Eq. (2) is a series in $\mu_\alpha(C)$, i.e. irreducible correlations functions discussed in [6]. Parisi and Slanina [7] extended the approach of Efetov [17] to the Ising model on a lattice by introducing an integral representation. Very much like in the case of the integral representation discussed above, the saddle-point for the integral representation of [7] becomes BP. Similarity between our approach and the one of [7] also extends to the analysis of the leading corrections to the saddle-point. The authors of [7] find that the diagrams that account for fluctuations around the BP saddle-point reproduce the lattice topology, i.e. the loop structure. However, there are also very important differences in these two approaches. Our series do not contain any formal divergences (e.g. no zero modes appear in the Gaussian approximation around the BP saddle-point). Moreover, our result sums up into the finite series [7]. On the contrary, the authors of [7] encounter divergences in their representation (e.g. for the original partition function) even though this potentially very dangerous (as lacking analytical control) divergence cancels out from the leading order correction to the magnetization. Accounting for corrections in all orders within the technique of [7] does not look feasible.

We conclude with a discussion of possible applications and generalizations. We see a major utility for Eq. (2) in its direct application to the models without short loops. In this case Eq. (2) constitutes an efficient tool for improving BP through accounting for the shortest loop corrections first and then moving gradually (up to the point when complexity is still feasible) to account for longer and longer loops. Another application of Eq. (2) is direct use of $\epsilon$ as a test parameter for the BP approximation validity: If the shortest loop corrections to BP are not small one should either look for another solution of BP (hoping that the loop correction will be small within the corresponding loop series) or conclude that no feasible BP solution, resulting in a small $\epsilon$, can be used as a valid approximation. There is also a strong generalization potential here. If a problem is multi-scale with both short and long loops present in the factor graph, a development of a synthetic approach combining Generalized Belief Propagation approach of [3] (that is efficient in accounting for local correlations) and a corresponding version of Eq. (2) can be beneficial. Finally, our approach can be also useful for analysis of standard (for statistical physics and field theory) lattice problems. A particularly interesting direction will be to use Eq. (2) for introducing a new form of resummation of different scales. This can be applied for analysis of the lattice models at the critical point where correlations are long-range.

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