Gauge-free cluster variational method by maximal messages and moment matching

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We present a new implementation of the Cluster Variational Method (CVM) as a message passing algorithm. The kind of message passing algorithms used for CVM, usually named Generalized Belief Propagation, are a generalization of the Belief Propagation algorithm in the same way that CVM is a generalization of the Bethe approximation for estimating the partition function. However, the connection between fixed points of GBP and the extremal points of the CVM free-energy is usually not a one-to-one correspondence, because of the existence of a gauge transformation involving the GBP messages.

Our contribution is twofold. Firstly we propose a new way of defining messages (fields) in a generic CVM approximation, such that messages arrive on a given region from all its ancestors, and not only from its direct parents, as in the standard Parent-to-Child GBP. We call this approach maximal messages. Secondly we focus on the case of binary variables, re-interpreting the messages as fields enforcing the consistency between the moments of the local (marginal) probability distributions. We provide a precise rule to enforce all consistencies, avoiding any redundancy, that would otherwise lead to a gauge transformation on the messages. This moment matching method is gauge free, i.e. it guarantees that the resulting GBP is not gauge invariant.

We apply our maximal messages and moment matching GBP to obtain an analytical expression for the critical temperature of the Ising model in general dimensions at the level of plaquette-CVM. The values obtained outperform Bethe estimates, and are comparable with loop corrected Belief Propagation equations. The method allows for a straightforward generalization to disordered systems.

I. INTRODUCTION

The Ising ferromagnet is one of the most studied and celebrated models in Statistical Physics. Although it lacks a proper analytical solution in three dimensions, it is globally well understood [1]. However, the addition of disorder to this model generates a more complex scenario. Roughly speaking, the low temperature phase of the disordered model is not composed any more by two equivalent ordered phases as in the pure ferromagnetic model, but by many disordered phases with a complex structure. Techniques like the replica trick [2] and the cavity method [3, 4] opened the door to the analytical treatment of the disordered variants of this and similar models in fully connected or in locally tree-like random graphs [5].

However, finite dimensional systems remain a challenging problem regarding the analytical solutions. Only recently [6–11] has been realized that a proper generalization of the Bethe approximation, known with the name of Cluster Variational Method (CVM), could be a good
starting point for a systematic treatment of these kind of disordered problems. The main task is
to translate the (approximate) free energy saddle
point conditions in a set of message passing
equations, that can be solved efficiently even on
large systems.

The interest in this kind of approximations is
not only theoretical, but it comes also from many
applications. For example, in image processing
[12–15], it is important to improve the quality
of the reconstruction algorithms, and message
passing derived from CVM approximations has
proved to be a good candidate in this direction
[16]. Error correction and LDPC codes is an-
other example of applications where GBP has
been studied [17], including the idea of fixing
the gauge [18].

Most of previous works on cluster variational
method and replica method, relied on the
so called Parent-to-Child message passing [6],
which consists of an extension of the belief propa-
gation for the Bethe approximation to more in-
volved region graph approximations of the free
energy. It has been shown that the Parent-
to-Child message passing is redundant [18, 19],
since it introduces more “cavity” fields (mes-
sages) than actually needed, producing a sort
of gauge invariance in the solution. According
to our experience, this invariance is not a big
problem in the implementation of message
passing algorithms on a given finite dimensional
instance, but it certainly is a waist of compu-
tational resources, since more parameters need
to be implemented. In [21], however, authors
reports the gauge invariance as causing conver-
gence problems. In any case this gauge invari-
ance may obscure the connection between the
average case prediction of the CVM equations
derived for a disordered model and the solution
of message passing equations in single instances
of the model [8]. To alleviate this problem we
propose a general procedure to generate Gauge
Free Generalized Belief Propagation (GFGBP)
algorithm starting from a Cluster Variational
Method approximation.

The procedure developed consists of the fol-
lowing steps:

1. definition of maximal messages, in

2. definition of moment matching fields
in place of parent-to-child messages

The first is just another possible choice of mes-
sages that is quite general. The latter is a change
of perspective in the interpretation of messages
as Lagrange multipliers forcing marginalizations,
to fields forcing consistency of moments in the
beliefs distributions. This allows a systematic
construction of gauge free message passing for
any model with binary variables.

In [18, 19] authors developed a way to remove
the redundancy in the GBP equations by re-
moving the redundant messages. Our approach
diffs from theirs in that they keep with the
Parent-to-Child approach of [6] and propose to
fix the gauge by removing some messages com-
pletely from the belief expression of given regions
in order to avoid loops in the region graph rep-
resentation. We, instead, propose a larger set of
messages, but with properly reduced degrees of
freedom.

We will apply the gauge free approach to
the computation of critical temperatures in the
plaquette-CVM approximation in Ising model in
general dimensions, obtaining analytical expres-
sions that improve over Bethe. The high dimen-
sion expansion of the critical temperature is cor-
rect until the third order term, as is the loop cal-
culus of Ref. [22]. We also test the procedure in
single instance implementation of message pass-
ing in Ising model. The more complicated (and
interesting) disordered models, are left for future
work.

The paper is organized as follows. Sec. II in-
troduces CVM and message passing algorithm in
general terms, while Sec. III explains the maxi-
mal messages (MM) and the moment matching
(MM) approaches; finally in Sec. IV we apply
the MM-MM CVM (or 4M-CVM in short) algo-

rithm to the calculation of the critical tempera-
ture in Ising models of general dimensions at the
plaquette level. For the sake of readability, we
defer to the appendices the technical proofs.
II. CLUSTER VARIATIONAL METHOD

The kind of problems we are dealing with are those statistical mechanics problems that require the computation of the properties of a large set of binary variables \( x_i \in \{1, -1\} \), whose joint probability distribution

\[
P(x) = \frac{1}{Z} \exp(-\beta H(x))
\]

depends on a Hamiltonian \( H(x) \) that can be written as the sum of local terms

\[
H(x) = \sum_a E_a(x_a),
\]

where every interaction “\( a \)” with energy \( E_a(x_a) \) involves a small subset of variables \( x_a \). This also includes the case of Bayesian networks, and therefore of many interesting inference problems.

Computations of the statistical properties of each variable \( x_i \) or groups of them, face the numerical difficulty of tracing over an exponential number of configurations when marginalizing over the remaining variables, and in general approximations are required. In the case of mean field, Bethe, and region graph approximations (see [23]), the underlying idea is to factorize the full probability distribution \( P(x) \) into many smaller distributions containing a non extensive number of variables that we will refer to as regions.

The CVM [6, 24] starts from a set of maximal regions \( R_0 \) (basic clusters), where no region is subset of another, and constructs a hierarchy of regions over which the approximation is defined. We will require that each degree of freedom \( x_i \) and also all interactions \( E_a(x_a) \) are present in at least one of these regions. Then we extend \( R_0 \) with the closure under the intersection operation as explained next.

From \( R_0 \), we define recursively the set of intersections \( R_k \) as

\[
R_k = \{ r = r_{k-1} \cap r'_{k-1} | r_{k-1}, r'_{k-1} \in R_{k-1} \}
\]

The whole group of regions is \( R = R_0 \cup R_1 \cup R_2 \ldots \). Actually, in the CVM construction, the same regions might appear more than once, and in different levels of intersections. Regardless this degeneracy, the relevant set is \( R \), the collection of all regions obtained. Of utmost importance for later proves is that \( R \) is a closed set under intersections and a partially ordered set, in which the subset relation defines the partial order, and \( R_0 \) is the set of maximal regions.

Since the system Hamiltonian is given by sums of local interactions between subsets of variables, we will consider that every time that the set of variables \( x_a \) are part of a given region \( x_a \subset r \), then the interaction “\( a \)” itself is part of it, allowing us to define the energy of the region as:

\[
E_r(x_r) = \sum_{a \in r} E_a(x_a)
\]

Since all interactions are at least part of one maximal region \( r_0 \in R_0 \), we can write the Hamiltonian of the system as a sum over regions:

\[
H = \sum_{r \in R} c_r E_r(x_r)
\]

where the counting numbers \( c_r \) guarantee that every interaction is counted exactly once [6]:

\[
c_{\alpha} = 1 - \sum_{r \in A_{\alpha}} c_r.
\]

The set \( A_{\alpha} \) stand for the set of all ancestors of region \( \alpha \), this is all super-regions of region \( \alpha \)

\[
A_{\alpha} = \{ r \in R | \alpha \subset r \}.
\]

Before going further in detail, let us visualize an example of the regions generated by the CVM construction. Consider a 3-dimensional spin model, with spins living in the nodes of a 3D-square lattice. In the cubic approximation, maximal regions are taken as the basic cubic cell of the lattice, with all its eight degrees of freedom at the cube’s vertex. As a representative part of the full system, diagrams in figure 1 show all the regions containing the central spin \( s_1 \) (depicted as the central point in the rightmost diagram). Notice that the intersections of the cubic regions in the leftmost diagram produce the square plaquette regions in the center diagram, with a spin at every angle of the squares. And the intersection of those plaquettes result in the rod (edges with two spins) regions in the rightmost diagram, which intersect only in the central spin.
 FIG. 1. Example of regions surrounding the central spin $s_1$ in the cube approximation for the 3D square lattice model. Left: the 8 cubic regions $Q_1, \ldots, Q_8$. Center: the 12 faces (plaquettes) $P_1, \ldots, P_{12}$ shared by the maximal cubic regions. Right: the 6 vertex shared by the plaquettes and the central spin. The cube $Q_1$ is highlighted for later use.

A. Variational approach and message passing

Next we reproduce the approach by Zhou et al [19] on the derivation of message passing equations, instead of that of Yedidia [6]. We prefer the former because it is somehow more direct in the choice of the belief equations, saving the time of passing through Lagrange multipliers.

It starts by noting that, in accordance with eq. (2), the exact partition function of a system can be written as:

$$Z(\beta) \equiv \sum_{x} \exp(-\beta H(x)) = \sum_{x} \prod_{r \in R} \left[ \exp(-\beta E_r(x)) \right]^{c_r}$$

A set of non zero test functions $\{m_z(x_z)\}$ can be multiplied and divided in the right hand side, such that they cancel out. We will call these test functions, messages. Let us define $\partial z \subset R$ the set of regions in which the message $m_z(x_z)$ appears, and let $D_r$ be the set of messages entering region $r$, then

$$Z(\beta) = \sum_{x} \prod_{r \in R} \left[ \exp(-\beta E_r(x_r)) \prod_{z \in D_r} m_z(x_z) \right]^{c_r}$$

will still be the same partition function (independently of the values of the messages) if:

$$\forall z \sum_{r \in \partial z} c_r = 0 \quad (4)$$

We can write an approximation to the free energy of the model in terms of the local beliefs

$$b(x_r) = \frac{1}{z_r} \exp(-\beta E_r(x_r)) \prod_{z \in D_r} m_z(x_z) \quad (5)$$

with local partition functions

$$z_r = \sum_{x_r} \exp(-\beta E_r(x_r)) \prod_{z \in D_r} m_z(x_z).$$

The free energy of the model $F = -kT \log Z(\beta)$ can be rewritten as:

$$F = -kT \sum_{r \in R} c_r \log z_r - kT \log \left[ \sum_{z} \prod_{r \in R} b_r(x_r)^{c_r} \right]$$

$$= F_R + \Delta F$$

This expression is still exact (independently of the value of the message functions). We will regard the first term $F_R[\{m\}]$ as a variational approximate to the real free energy. The rationale for this goes as follows. It can be shown (and will be) that the minimization of the first term is equivalent to imposing local consistency between marginals of the beliefs functions (those
appearing in the second term). Once the beliefs are locally consistent it can be shown that the correct joint probability distribution of the model \( P(\mathbf{x}) \) can be written in a factorized form as \( \prod_{x \in R} b_r(\mathbf{z})^{x_r} \) as far as the underlaying graph is a tree, therefore \( \Delta F = -KT \log 1 = 0 \). This proves, \textit{en passant}, that the approximation is exact for the case of tree topologies. A rigorous justification of the approximation is absent, but in \[10\] authors relate \( \Delta F \) to the sum of correction contributions in the loop expansion of the free energy. In the general case, i.e. loopy graphs, working with locally consistent beliefs that follow from the extremization of the first term, does not guarantees that the factorized measure \( \prod_{x \in R} b_r(\mathbf{z})^{x_r} \) is properly normalized, therefore at the fixed point \( \Delta F \neq 0 \) generally. Nevertheless, in all the situations where is meaningful to use message passing algorithms, we expect the corrections due to loops to be small, and for this very reason, also \( \Delta F \ll F_R \).

As a consequence of the variational treatment, we now need to solve the set of equations

\[
\frac{\partial F_R(\{m\})}{\partial m_z} = 0 \ \forall z. \tag{6}
\]

The precise form of the resulting equations, and what exactly are they enforcing depends on the choice made for the messages and how do they appear in the belief equations. Next we explain one possible choice that we retain as the natural one and we will call maximal message passing.

### III. GAUGE-FREE 4M-CVM: MAXIMAL MESSAGES AND MOMENT MATCHING

Previously \[6,18,21\] the set of messages have been defined using the so called Parent-to-Child (P-t-C) approach. This means that messages \( m_{\alpha \rightarrow \gamma}(\mathbf{z}) \) are indexed by two regions labels, the father one \( \alpha \) and the child one \( \gamma \). We will say that a region \( \alpha \) is father of \( \gamma \), if \( \alpha \supset \gamma \) and no region in \( R \) is a subset of \( \alpha \) and a superset of \( \gamma \). In P-t-C no messages are considered from grandparents or higher ancestors.

While this approach is very systematic, it has the problem of introducing too many degrees of freedom in the test functions. As already mentioned this may not have major consequences (besides efficiency) in physical observables measured on a given instance, but introduces a gauge invariance that might be problematic in the comparison with the typical behavior of message passing equations in the average case scenario \[8,20\]. The reason is that in population dynamics one assumes messages arriving on a given region from different ancestors to be mostly uncorrelated: there are situations where this approximation is physically valid (e.g. when correlations are not too strong and regions are large enough), however the gauge invariance implies messages can freely change under the gauge transformation and this introduces undesirable correlations among the messages. For this reason a scheme free from the gauge invariance is very welcome.

We propose a top-down approach, that we call \textit{maximal message} passing, in which messages to region \( r \) flow from all its ancestors \( p \supset r \). We prefer the maximal messages, among other possibilities because it will allow us later to construct a gauge free system of message passing equations.

**Definition 1.** Maximal messages are defined by the set of message functions used, and by how these functions participate in each regions belief, as follows:

- every region \( r \in R \) receives messages from all its ancestors \( p \in A_r \). Messages are functions of the degrees of freedom in \( r \): \( m_{p \rightarrow r}(\mathbf{z}_r) \).
- message \( m_{p \rightarrow r}(\mathbf{z}_r) \) will appear in the region partition function \( z_r \) (i.e. equation (5)) of region \( r \), iff \( r \cap p = \gamma \).

The first point asserts that there are as many message functions as pairs of comparable regions in the CVM construction, and therefore the messages are labeled by these two regions as \( m_{p \rightarrow r}(\mathbf{z}_r) \) where \( r \subset p \). The term \textit{maximal messages} comes since there are messages to every region from all its ancestors, not only the frist direct parents as in parent to child. The second point defines \( D_r \), the set of messages \( m_{p \rightarrow r}(\mathbf{z}_r) \).
that appear multiplicatively in the belief expression (or the partition function) of a certain region \( r \), as

\[
D_r = \{ p, \gamma \in R | p \notin r, p \cap r = \gamma \neq \emptyset \}.
\]

Put together, we have an expression for the beliefs at any region given by:

\[
b(x_r) = \frac{1}{z_r} e^{-\beta E_r(x_r)} \prod_{p, \gamma \in D_r} m_{p \rightarrow \gamma}(x_r) \quad (7)
\]

As a consequence also of the second point in the definition, any given message \( m_{p \rightarrow r} \) is present in the belief equations of all regions whose intersection with \( p \) is exactly \( r \):

\[
\partial m_{p \rightarrow r} = \{ r' \in R | r' \cap p = r \}
\]

In order for this prescription to be valid, we have to show that it satisfies \( 4 \).

To keep with our previous 3D example, let us consider the case of the message \( m_{Q_1 \rightarrow s_1}(s_1) \), going from the cube \( Q_1 \) (dark) to the central spin \( s_1 \), as shown in Fig. 2. Then the set of regions \( \partial m_{Q_1 \rightarrow s_1} \) on whose beliefs the message \( m_{Q_1 \rightarrow s_1}(s_1) \) appear are those whose intersection with \( Q_1 \) is exactly \( s_1 \), as represented in the diagram (Fig. 2).

1. Properties of maximal messages

**Theorem 1.** Equation \( 7 \) defines a valid GBP approximation on any set of regions \( R \) defined by the cluster variational method.

This theorem is proved in the appendix A based on the fact that the cluster variational method defines a partially ordered set, and some properties relating the ancestors of a region and the set of equations in which messages to that region participates.

Extremal values of \( F_{CVM} \) are obtained by enforcing eq. \( 6 \). Since all messages appear linearly, differentiating is equivalent to remove the messages from the equations in which they are present. In order to obtain a nicer presentation we can solve instead

\[
m_{r_0 \rightarrow \gamma}(x_r) \partial F_R[m] \frac{\partial F_R[m]}{\partial m_{r_0 \rightarrow \gamma}} = 0
\]

which generates the following set of equations:

\[
\sum_{r \in \partial m_{r_0 \rightarrow \gamma}} c_r \sum_{x_{\gamma \setminus x}} b_r(x_r) = 0
\]

Notice that, as a consequence of equation \( 4 \), a particular solution to this equation is found when each belief involved has the same marginal over the degrees of freedom \( x_{\gamma \setminus x} \). Since beliefs are usually interpreted as approximations of the marginals of the joint probability distribution \( \Pi \), we would require them to be consistent with one another. It is assuring to see that the consistency indeed is a solution of the extremal equations. In appendix B we proof the following

**Theorem 2.** The extremal points of the approximated variational free energy \( F_R[m] \) are found at consistent beliefs:

\[
\forall r \in R \ \forall p \in A_r \ b_r(x_r) = \sum_{x_{\gamma \setminus x}} b_p(x_p) \quad (8)
\]

From these equations we can write message passing update rules in different ways. Unfortunately maximal message passing do not solves automatically the gauge invariance in the messages. Just as in P-t-C case, the introduced messages do not define the beliefs in an unique way, and many possible messages values may represent the same beliefs. Besides its non optimality as a representation, and probably derived efficiency/convergence problems, this invariance might be problematic for average case predictions, for instance the prediction of critical temperatures in disordered systems.

Another relevant property of maximal message passing, is that it is hierarchical.

**Theorem 3.** Let there be two CVM approximations for a given model. If one of the approximations is contained in the other, meaning that all regions in one are present in the other

\[
R_{CVM1} \subset R_{CVM2}
\]

then the beliefs in the smaller approximation (the less precise one) are obtained from the larger approximation, by just setting to 1 all messages not common to both.
FIG. 2. Regions on whose beliefs the message $m_{Q_1 \to s_1}(s_1)$ from the cubic region $Q_1$ to the central spin $s_1$ appears. On the leftmost diagram, $Q_1$ is still represented to help guiding the eye, but it does not belong to $\partial m_{Q_1 \to s_1}$. The cube opposing $Q_1$, the three palquettes and the three edges and $s_1$ itself, they all intersect with $Q_1$ only at $s_1$, and therefore are in $\partial m_{Q_1 \to s_1}$.

The proof is immediate since the definition of $D_r$ implies that $D^1_r \subset D^2_r$.

As a consequence, if one wants to recover the Bethe approximation from, e.g., the plaquette approximation, we only needs to disregard (setting to 1) the plaquette-to-link and plaquette-to-spin messages in the belief and messages passing equations. This property is also valid in the case of gauge free maximal messages that we explain next. We recall, however, that two different approximations have different counting numbers, and therefore the free energy of the smallest approximation is not obtained by setting to zero the terms of the larger.

A. Moment matching is gauge free

The general way to create a message passing that is also gauge free starts from recognizing that the relevant quantities to match are not necessarily the belief as in eq. (8) but their moments. Next we present the case of Ising variables $s_i = \pm 1$. A more general presentation, regarding for instance Potts variables, is left for future work.

Let’s go back to the messages. It has been shown in the context of P-t-C message passing [18, 20] that when the region graph contains loops, i.e. when from a bigger region there are two paths to get to a smaller region in the region graph, then the messages are not uniquely determined. In other words, since marginalization is transitive, forcing $b_p \to b_{r_1} \to b_{r_0}$ and $b_p \to b_{r_2} \to b_{r_0}$ is redundant. The marginalization $b_{r_2} \to b_{r_0}$, for instance, automatically follows from the first chain of marginalizations and $b_p \to b_{r_2}$. In other words, interpreting the messages as Lagrange multipliers [2], the introduction of a multiplier to force $b_{r_2} \to b_{r_0}$ is unnecessary, and therefore, the set of multipliers is not uniquely determined.

A workaround to this problem has been given previously [18, 20] where authors have identified a link between gauge invariance and loops in the region graph representation. At the end, it all amounts to discovering which are the redundant messages, and remove them from the representation, or set them to an arbitrary value, fixing the gauge [18, 19, 21]. In many case, although the final objective is clear (destroying the loops), there are many different ways to achieve it, and each one has selected his own way. Next we explain how to construct gauge-free message passing algorithms from scratch, not by destroying loops, but by restricting degrees of freedom in the messages. We specify a precise and unique way to do so.

So far, maximal messages were introduced in full generality. Now we will reduce their degrees
of freedom as long as they keep ensuring the consistent marginalization of neighbor regions. Proceeding in this way, we do not affect the overall minimization of the CVM free energy.

We will now change perspective and interpret messages not as arbitrary functions enforcing beliefs consistency, but rather as a set of fields enforcing the agreement between the moments in the beliefs. For instance a message to a 2-spin regions, can be rewritten as

\[ m_{p \rightarrow 1,2}(s_1, s_2) = e^{s_1 s_2 U_{p \rightarrow 1,2} + s_1 u_{p \rightarrow 1} + s_2 u_{p \rightarrow 2}}. \]  

(9)

The four values of function \( m(s_1, s_2) \) are encoded into the 3 parameters \( U, u_1, u_2 \) since messages are insensitive to any normalization factor, a consequence of property in eq. (4). Let us assume that the fields \( u_{p \rightarrow 1}, u_{p \rightarrow 2} \) fix the correct firsts moments between the beliefs at region \( p \) and at the two-spin region \((1,2)\), while \( U \) determines the correlation. In such case, since all parents of region \((1,2)\) are sending messages to it, all those parents will have a first and second moments on variables \( s_1 \) and \( s_2 \) that are consistent to that of the belief at \((1,2)\) and therfore are consistent among them. This also means that given two ancestors of \((1,2)\), lets say \( g, p \in A_{(1,2)} \) such that \( g \in A_p \), the messages from \( g \) to \( p \) do not require fields of the type \( u_1, u_2 \) and \( U_{1,2} \) any longer.

An example is handy. Take for instance the 2D square lattice, a small fraction of which is represented here

and the square plaquette-CVM approximation. Regions are the plaquettes, the links and the spins (variables \( s_i = \pm 1 \)) in the system. Any single spin receives messages of the form

\[ m_{r \rightarrow i} = e^{u_{r \rightarrow i} s_i}. \]

from the four links and the four plaquettes it belongs to. In the diagram, only the fields coming from one plaquette and two links are shown:

This ensures that the first moment of the beliefs in the plaquettes and the links are consistent with the first moment of the belief at spin \( i \),

\[ \langle s_i \rangle = \sum s_i b_i(s_i). \]

Therefore, when plaquettes are sending messages to links (double arrows in diagram), they no longer need a multiplier (field) \( u_{p \rightarrow i} \), and the message will only force the correlation

\[ m_{p \rightarrow (ij)}(s_i, s_j) = e^{U_{p \rightarrow ij} s_i s_j}. \]

In such a way, even though the region graph have loops, the moments are not fixed redundantly, and the message passing is gauge-free.

In general, a message \( m_{p \rightarrow r}(s_r) \) has \( 2^{|r|} - 1 \) degrees of freedom, where \(|r|\) is the number of binary variables (spins) in region \( r \). There are also \( 2^{|r|} - 1 \) non null subsets of \( r \), and therefore the same number of moments to describe a distribution over \(|r|\) variables. The reduction of the degrees of freedom in the messages follow the rule:

**Definition 2** (Moment matching). Message \( m_{p \rightarrow r}(s_r) \) contains a field \( U_q \) enforcing the correlation among variables in \( q \subseteq r \) as

\[ m_{p \rightarrow r}(s_r) = e^{\cdots + U_q \cdot \prod_{s_i} s_i + \cdots} \]

if and only if \( r \) is the smallest region among all those containing the variables in \( q \).

The smallest region containing \( q \) is uniquely determined in the CVM construction thanks to the following properties: (i) the partial order defined by inclusion relations and (ii) the closure of the set of CVM regions under intersections of sets (the proof is easy and left to the reader).

Extreme values of the approximated free energy \( F_{CVM} \) can now be obtained by differentiating directly with respect to the fields \( U_q \) that define the messages:

\[ \frac{\partial F_{CVM}(\{U\})}{\partial U_q} = 0 \]
which generates the following set of equations:

\[ \sum_{r \in \partial m_{\gamma}} c_r \left( \prod_{i \in q} s_i \right) b_r = 0 \]

and

\[ \langle \cdots \rangle_{b_r} = \sum_{\mathcal{A}} \cdots b_r(s_r) \]

Obviously, a particular solution is found when all distributions share the same moments over common degrees of freedom, since equation (4) holds. In such case, all beliefs are also consistent with inner regions. It remains to show that this is in fact the only solution, which is the argument of the following

**Theorem 4.** Maximal messages with moment matching fields ensures the consistency of beliefs.

The previous theorem states that the moment matching fields are enough to guarantee consistency. The next one completes our task by stating that indeed we need all of these fields to do so.

**Theorem 5.** Maximal messages with moment matching fields is gauge free.

Both theorems are proved in appendix C.

**IV. PLAQUETTE-CVM FOR ISING 2D**

Let us start by a simple case. Ising ferromagnet, in the absence of external fields are defined by the Hamiltonian

\[ \mathcal{H}(s) = -J \sum_{\langle i,j \rangle} s_i s_j \]

where \( \langle i,j \rangle \) defines nearby spins, and is given by the topology in which the system is embedded, and the degrees of freedom are \( s_i = \pm 1 \). The interaction constant \( J \) is normally set to \( J = 1 \).

Though the 2D case of this model has been exactly solved [25], we still can try our approximation on it, before moving to the unsolved higher dimensions. The first approximation beyond mean field and Bethe, is the one containing all square plaquettes (the basic cell) as maximal regions. The cluster variation method then prescribe a free energy in terms of Plaquettes, Links and Spins regions [20], with counting numbers \( c_P = 1, c_L = -1, c_i = 1 \) respectively.

The gauge free 4M-CVM is then written in terms of messages going from plaquettes to the links and spins interior to it. Beliefs are defined as follows

\[ b_P(s_P) = \frac{1}{z_P} e^{-\beta E_3(s_P)} \prod_{L' \supset P} \prod_{P' \supset L} m_{P' \rightarrow L}(s, s') \prod_{s \in P} \prod_{P' \cap P = s} m_{P' \rightarrow s}(s) \prod_{L \in P} m_L \rightarrow s = L \cap P(s) \prod_{L' \supset P} m_{L' \rightarrow s = L \cap P}(s) \]  

(10)

\[ b_L(s, s') = \frac{1}{z_L} e^{-\beta E_2(s, s')} \prod_{P \supset L} \prod_{P' \supset L} m_{P' \rightarrow s}(s) \prod_{s \in L} \prod_{P' \cap L = s} m_{P' \rightarrow s = L \cap P}(s) \prod_{L' \supset L} m_{L' \rightarrow s = L \cap L}(s) \]  

(11)

\[ b_s(s) = \frac{1}{z_s} e^{-\beta E_1(s)} \prod_{L \supset s} \prod_{P \supset s} m_{P \rightarrow s}(s) \prod_{L' \supset s} m_{L' \rightarrow s}(s) \]  

(12)

Graphically, the beliefs of each region are given by

where double arrows represent messages to links \( m_{P \rightarrow L}(s, s') \), oblique arrows messages from plaquettes to spins \( m_{P \rightarrow s}(s) \) and remaining arrows messages from links to spins \( m_{L \rightarrow s}(s) \). Colors have been added (online version) to help identify each arrow with its corresponding term.
1. Message passing

Message passing equations can be obtained in two different but equivalent ways:

- Old way: by imposing the consistency among beliefs, in this case some of the following:
  \[ b_L(s_1, s_2) = \sum_{s_3, s_4} b_P(s_1, s_2, s_3, s_4) \]
  \[ b_s(s_1) = \sum_{s_2, s_3, s_4} b_P(s_1, s_2, s_3, s_4) \]
  \[ b_s(s_1) = \sum_{s_2} b_L(s_1, s_2) \]

- New way: by imposing consistency among the moments of the distributions:
  \[ \sum_{s_1, s_2} s_1 s_2 b_L(s_1, s_2) = \sum_{s_1, s_2, s_3, s_4} s_1 s_2 b_P(s_1, s_2, s_3, s_4) \]
  \[ \sum_{s_1} s_1 b_s(s_1) = \sum_{s_1, s_2, s_3, s_4} s_1 b_P(s_1, s_2, s_3, s_4) \]
  \[ \sum_{s_1} s_1 b(s_1) = \sum_{s_2} s_1 b_L(s_1, s_2) \]

Furthermore, as can be easily checked not all three equations in the old way are independent: the third equation is consequence of the first two. This is the very reason why we reduced the amount of fields. In the new way there is only three values being fixed, and they are all independent. Both ways, however, produce the same update equations (message passing) independently of whether the messages has been reduced to be gauge fixed, or are in full generality.

For instance, forcing any link belief \( b_L(s_1, s_2) \) to marginalize onto one of its spins results in the following equation:

\[
\sum_{s_2} e^{\beta J s_1 s_2} m_{P_1 \rightarrow L}(s_1, s_2) m_{P_2 \rightarrow L}(s_1, s_2) m_{P_3 \rightarrow s_2}(s_2) \prod_{L' \supseteq s_3 \atop L' \neq L} m_{L' \rightarrow s_2}(s_2) \propto m_{L \rightarrow s_1}(s_1) \prod_{P \supset L} m_{P \rightarrow s_1}(s_1) \tag{13}
\]

where we put a sign of proportionality \( \propto \) instead of equality since messages are undefined by a multiplicative constant. These equations can be derived graphically using the representations of the beliefs and messages introduced above. The rules are quite simple. Interactions are represented by the rods, degrees of freedom by the circles, and messages by the arrows. If an interaction or a message appears in both sides of the equations, can be cancel out. The degrees of freedom over which the marginalization is carried appear as full black circles. For instance, equation (13) is represented as in figure 3.

\[ \begin{array}{c}
\begin{array}{c}
\bigcirc \\
\bigcirc
\end{array}
\end{array} \]

FIG. 3. Consistency equation between link beliefs and spin beliefs. Mathematically it corresponds to the first two equations in (15) for \( d = 2 \).

The plaquette to link marginalization produces consistency relation between messages as shown in figure 4.

\[ \begin{array}{c}
\begin{array}{c}
\bigcirc
\end{array}
\end{array} \]

FIG. 4. Consistency equation between plaquette beliefs and link beliefs. Mathematically it corresponds to the first two equations in (15) for \( d = 2 \).

As can be seen, in either cases (link to spin and plaquette to spin) the messages in the right hand side do not appear isolated. Consistency equations force the product of messages. We could have used plaquette to spin marginalization as well, and the situation still would be similar. In such cases, it is left to the programmer to
decide which iterative updating rule she wishes to implement to solve the consistency equations in a message passing way. She could, for instance, use the link to spin equation to update both plaquette to spin messages in a symmetric way, and then use the plaquette to spin equation to update the plaquette to link message. Let us emphasize that this freedom on the implementation of message passing equations remains even when the gauge is fixed, just as any fixed point equation can be written in infinite many ways. The gauge fixed property refers to the unicity of fields values at a given fixed point, not to the strategies to find them.

If messages are considered in full generality, then we have a redundant description

\[
\begin{align*}
    m_{P\rightarrow L}(s_1, s_2) &= e^{U_{P\rightarrow L}s_1s_2 + u_{P\rightarrow 1}s_1 + u_{P\rightarrow 2}s_2} \\
    m_{L\rightarrow 1}(s_1) &= e^{u_{L\rightarrow 1}s_1} \\
    m_{L\rightarrow 2}(s_2) &= e^{u_{L\rightarrow 2}s_2}
\end{align*}
\]

leading to a gauge invariance transformation involving \( u \) messages [20]. On the contrary, using the gauge-free moment matching prescription previously defined in Def. 2 messages are

\[
\begin{align*}
    m_{P\rightarrow L}(s_1, s_2) &= e^{U_{P\rightarrow L}s_1s_2} \\
    m_{P\rightarrow 1}(s_1) &= e^{u_{P\rightarrow 1}s_1} \\
    m_{L\rightarrow 1}(s_1) &= e^{u_{L\rightarrow 1}s_1}
\end{align*}
\]

Details of the update equations and an example on 2D single instance is given next.

A. 2D Single instance implementation

The self consistent message passing equations can be written as

\[
\begin{align*}
    \hat{u}_L &= \frac{1}{2} \log (K(1)/K(-1)) - u_{P_a} - u_{P_b} \\
    \hat{u}_P &= \frac{1}{4} \log \left( \frac{K(1,1)K(1,-1)}{K(-1,1)K(-1,-1)} \right) - u_L \\
    \hat{U} &= \frac{1}{4} \log \left( \frac{K(1,1)K(1,-1)}{K(-1,1)K(-1,-1)} \right) \quad (14)
\end{align*}
\]

The \( K(\cdot) \) terms are partial traces over the spins in the plaquette and link, given by:

\[
\begin{align*}
    K(s_1) &= \sum_{s_2} e^{(\beta J_{12} + U_1 + U_2)s_1s_2 + (u_{P_1} + u_{P_2} + u_{L_1} + u_{L_2} + u_{L_3})s_2} \\
    K(s_1, s_2) &= \sum_{s_3, s_4} \exp \left[ s_2 s_3 (\beta J_{23} + U_{23}) + s_1 s_4 (\beta J_{14} + U_{14}) + s_3 s_4 (\beta J_{34} + U_{34}) + (u_{P_4} + u_{L_1} + u_{L_2} + u_{L_3}) s_4 + (u_{P_3} + u_{L_1} + u_{L_2} + u_{L_3}) s_3 \right]
\end{align*}
\]

in correspondence with the fields in the left hand sides of diagrams 3 and 4.

The implementation of the message passing is carried by randomly selecting a plaquette (or link) and updating their fields as prescribed by equations (14). In 2D Ising model we obtain the expected results (see Fig. 5). Above the approximation critical temperature (not exact) \( T_c = 1/\beta_c \simeq 2.43 \) all fields acting on single spins are zero \( u_{L\rightarrow i} = u_{P\rightarrow i} = 0 \), and the system is in a paramagnetic phase with zero global magnetization. In this range, the only non zero field is the correlation field \( U_{P\rightarrow L} \) (a detailed studied of this phase is in [26]). Below \( T_c \), the system is in a ferromagnetic phase, with non zero fields over spins and local as well as global magnetization.
Next we show how to generalize this method to compute the critical temperature of the Ising model in general dimension, under the plaquette-CVM approximation.

B. Critical temperature for Ising d-dimensional

Let us focus on the case of the plaquette CVM approximation in the general d-dimensional Ising model on the hypercubic lattice. This case includes the model of the previous section.

We will show how to obtain analytic expression for the critical temperature of the ferromagnetic model in this approximation at all dimensions, and furthermore, we will show that the asymptotic behavior is correctly until the third order in $1/d$, therefore being equivalent to the loop corrections of [22].

The plaquette approximation is the one that uses plaquettes as the biggest regions. In such case, the counting numbers of the plaquettes are always $c_P = 1$. Every link belongs to $2(d-1)$ plaquettes, and therefore its counting number is $c_L = 1 - 2(d-1)$. Every spin belongs to $2d$ links and $2d(d-1)$ plaquettes and have counting number $c_s = 1 - 2d(d-1) - 2d[1 - 2(d-1)] = 1 - 2d(2 - d)$. Beliefs, therefore, have the following schematic representation, where, as usual, double arrows are messages from plaquette to link, oblique arrows from plaquette to spin and remaining (vertical and horizontal) arrows are from links to spins.

For clarity, only one type of message of each type is represented in each region together with the number of such messages that enter in the belief equation of that region. However, the reader should keep in mind that, for instance, there are $2d(d-1) - 4d + 5$ plaquette-to-spin fields entering at very corner of the represented plaquette.

In general, consistency equations for messages keep the same structure represented graphically in the previous section, but only the amount of messages entering every region changes. Exploiting the isotropy of the model, we can look for fixed points in which all messages are the same. In other words, we will assume that all link to spin messages are characterized by a unique field $u_L$, while plaquette to link messages by the field $U$ and plaquette to spin messages by $u_P$.

Graphically, the updating equations for the messages have the following representation:
its side, have the same multiplicity that is represented for its equivalent by a reflection along the horizontal axis.

Let us define

\[ K(s_1) = \sum_{s_2} e^{(\beta J + (2(d-1)U))s_1 s_2 + (2(d-1)^2 u_P + (2d-1)u_L)s_2} \]

\[ K(s_1, s_2) = \sum_{s_3, s_4} \exp \{ s_2 s_3 (\beta J + (2d-3)U) + s_1 s_4 (\beta J + (2d-3)U) + s_3 s_4 (\beta J + (2d-3)U) + ((2d(d-1) - 4d + 5)u_P + (2d - 2)u_L)s_4 + ((2d(d-1) - 4d + 5)u_P + (2d - 2)u_L)s_3 \} \]

In terms of this, the self consistent equations can be written as

\[ U = \hat{U}(\beta, J, u_L, U, u_P) \]
\[ = \frac{1}{4} \log \left( \frac{K(1,1)K(-1,-1)}{K(1,-1)K(-1,1)} \right) \]

\[ u_P = \hat{u}_P(\beta, J, u_L, U, u_P) \]
\[ = \frac{1}{2d-3} \left[ \frac{1}{4} \log \left( \frac{K(1,1)K(1,-1)}{K(-1,1)K(-1,-1)} \right) - u_L \right] \]

\[ u_L = \hat{u}_L(\beta, J, u_L, U, u_P) \]
\[ = \frac{1}{2} \log(K(1)/K(-1)) - 2(d-1)u_P . \]

The solution to this set of equations is to be found numerically in general. A simpler case is that of the high temperatures, in which we suppose a paramagnetic phase characterized by \( u_L = u_P = 0 \) and \( U \neq 0 \). In such case the equation \( U = \hat{U} \) becomes the simpler

\[ U = \arctanh \left( \left[ \tanh \left( (2d-3)U + \beta J \right) \right]^3 \right) . \]

This corresponds to the case treated in [26].

Moreover the paramagnetic solution is the starting point to obtain the critical temperature of the system as the instability of the paramagnetic solution. Taking

\[ \mathbb{K}(\beta) = \begin{pmatrix}
1 - \frac{\partial \hat{\alpha}_L}{\partial u_L} & \frac{\partial \hat{\alpha}_P}{\partial u_P} \\
\frac{\partial \hat{\alpha}_P}{\partial u_L} & 1 - \frac{\partial \hat{\alpha}_L}{\partial u_P}
\end{pmatrix} \] \[ \text{at } u_L = 0, U = \hat{U}, u_P = 0 \]

a continuous instability appears at the point in which \( \mathbb{K}(\beta) \) is singular, and therefore the critical temperature is defined as

\[ \det \mathbb{K}(\beta_c) = 0 . \]

Note that this is not fully analytical at this point, since the numerical solution of (16) is still needed. However, after some transformations we obtain an analytic expression for the critical temperature at all dimensions \( d > 2 \):

\[ \beta_{\text{CVM}} = \frac{1}{2} \log \left( \frac{(d-2)}{d} \right)^{d-2} \left( \frac{2d-1}{2d-3} \right)^{2d-3} . \]

In the \( d = 2 \) case, the solution is also analytical but given by

\[ \beta_{\text{CVM}}(d = 2) = \frac{1}{2} \log \left( \frac{5 + \sqrt{17}}{4} \right) . \]

This prediction can be compared with known results. In table [4] we show the best estimate of the true \( \beta_c \) on a regular hypercubic lattice with \( 2 \leq d \leq 6 \), together with the estimate from plaquette CVM, that from the Bethe approximation, where \( \beta_{\text{Bethe}} = \arctanh[(2d-1)^{-1}] \), and the one from Bethe with loop corrections due to Rizzo and Montanari [22]. In the latter approximation the critical temperature can be computed only if \( d > 2 \).

In the large \( d \) limit, the plaquette-CVM critical temperature is correct up to the second order in the \( 1/d \) expansion, exactly as the loop corrected Bethe approximation [22]

\[ \frac{1}{2d \beta_{\text{CVM}}} = \frac{\text{Bethe}}{1 - \frac{1}{2d}} \left( 1 - \frac{1}{3d^2} \right) - \frac{5}{12d^3} + \ldots \]

while the standard Bethe approximation is correct only up to the \( O(1/d) \) term.
TABLE I. Inverse critical temperatures of the Ising model on a regular hypercubic lattice in $d$ dimensions. In the second column we report the best estimate for the true $\beta_c$, while the other columns contain the inverse critical temperatures in 3 different mean field approximations: the plaquette CVM discussed in this work, the loop corrected Bethe of Ref. [22], that can be computed only for $d > 2$, and the standard Bethe approximation.

| $d$ | true $\beta_c$ (exact) | plaquette CVM | loop corr Bethe | Bethe |
|-----|------------------------|----------------|-----------------|-------|
| 2   | 0.440687               | 0.412258       | —               | 0.346574 |
| 3   | 0.221654(6)           | 0.216932       | 0.238520        | 0.202733 |
| 4   | 0.14966(3)            | 0.148033       | 0.151650        | 0.143841 |
| 5   | 0.11388(3)            | 0.113362       | 0.114356        | 0.111572 |
| 6   | —                      | 0.092088       | 0.092446        | 0.091161 |

We find this result very interesting, because it improves over the Bethe approximation by one order of magnitude in the $1/d$ expansion, while still providing a very accurate critical temperature at $d = 2$. On the contrary the loop corrected Bethe approximation is divergent in $d = 2$, and this makes the present 4M-CVM much more useful for the study of low dimensional systems.

V. CONCLUSIONS

We have shown how to create gauge-free message passing implementations of the cluster variational approximations for general models of spin-like variables. To do so we presented a new way of introducing the messages in the CVM that differs from standard parent-to-child messages in that messages are sent to a region from all its ancestors, and not only by its direct parents. While previous attempts to fix the gauge invariance in GBP equations [18, 19, 21] relied on the idea of removing some selected messages from the equations, our approach increases the number of such messages, but with a restriction on their degrees of freedom.

This systematic restriction of messages degrees of freedom automatically produces gauge-free variational approximations, such that there is a one-to-one correspondence between free energy minima, and the values of the fields that define the messages. Furthermore, we put emphasis in a new interpretation of the fields involved in the message passing as imposing consistency between moments of the local distributions (beliefs) rather than the usual interpretation of messages forcing consistent beliefs marginalization. We called the resulting method, maximal messages with moment matching (4M-CVM).

The approach includes the Bethe approximation as the starting point, and improves it when larger regions are taken in consideration. We showed that the method produces sensible analytical results for the plaquette approximation of the critical temperature of the Ising ferromagnet in general dimensions, that correctly accounts for the next leading order in the high dimensional expansions, just as the more complicated loop calculus does [22].

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Appendix A: Maximal GBP is always valid

We will prove that independently of the regions chosen as maximal, the introduction of multiplicative messages from maximal regions to their children, as explained in the main text, generates a valid GBP.

Valid means that equations \([\text{I}]\) is satisfied. First of all, let us prove that \([\text{I}]\) satisfies equation \([\text{II}]\). Without loss of generality, let us focus on a given region \(r_0 \in R\) and one of its children \(\alpha \subset r_0\). The message \(m_{r_0 \rightarrow \alpha}(\mathcal{X}_0)\) appears in the beliefs equations of all regions \(r\) such that \(r_0 \cap r = \alpha\), which defines:

\[
B_{r_0,\alpha} \equiv \partial m_{r_0 \rightarrow \alpha} = \{r' \in R | r' \cap r = \alpha\}
\]

An example of \(B_{r_0,\alpha}\) are the regions (except \(Q_1\)) appearing in the diagrams of Fig. 2.

The property we need to prove is (restating eq. \([\text{I}]\))

**Proposition 1.**

\[
\forall r_0 \in R_0 \forall_{\alpha \in R_0} \sum_{r' \in B_{r_0,\alpha}} c_{r'} = 0 \quad (A1)
\]

This property is similar to the one defining the counting numbers eq. \([\text{3}]\), but not the same. We will show the validity of \((A1)\) from that of the eq. \((3)\). Let us start by re-stating eq. \((3)\) as

\[
\sum_{r \in A_{\alpha}} c_r = 1. \quad (A2)
\]

where we have defined \(A_{\alpha}\) the extended set of ancestors of any region \(\alpha\) to include \(\alpha\) itself

\[
A_{\alpha} \equiv A_{\alpha} \cup \{\alpha\}
\]

The set \(B_{r_0,\alpha} \subset A_{\alpha}\). Furthermore, we can write:

\[
A_{\alpha} = B_{r_0,\alpha} + B_{r_0,\alpha}'
\]

where the sets in the right hand side are disjoint, and
Definition 3. $\bar{B}^o_{r_0,\alpha}$

$$B^o_{r_0,\alpha} = \{ r \in R | r \cap r_0 > \alpha \}$$

is the set of all ancestors of $\alpha$ such that their intersection with $r_0$ is larger than $\alpha$.

The part $\bar{B}^o_{r_0,\alpha}$ contains the ancestors of $\alpha$ in whose beliefs the message $m_{r_0} \to \alpha$ does not appear, and it will never be an empty set, since it includes at least $r_0$ and its ancestry. In figure 2 $\bar{B}^o_{r_0,\alpha}$ is exactly the absent part with respect to Fig. 1 including also $Q_1$.

From now on we will use relational operators $>,<,\geq,\leq$ freely, since the hierarchy established by the inclusion of sets in the regions defines a partially ordered set. In this sense, $\alpha < \beta$ means that $\alpha \subset \beta$ and $\alpha \neq \beta$.

Since the sets $B_{r_0,\alpha}, \bar{B}^o_{r_0,\alpha}$ are disjoint, the sum (A2) can be split among them becoming

$$\sum_{r \in B^o_{r_0,\alpha}} c_r + \sum_{r \in \bar{B}^o_{r_0,\alpha}} c_r = 1. \quad (A3)$$

If $B^o_{r_0,\alpha} = A^o_{r_0}$, then proposition 1 is proved, since the second sum will equal 1. Otherwise, the validity of the maximal messages (eq. (A1)) falls from proving that in the most general case

$$\sum_{r \in \bar{B}^o_{r_0,\alpha}} c_r = 1, \quad (A4)$$

as we will through the rest of the appendix.

Let us see some properties of the set $\bar{B}^o_{r_0,\alpha}$.

Form now on, all greek letters $\alpha, \beta, \gamma \ldots$ refer to regions in $\bar{B}^o_{r_0,\alpha}$.

Lemma 1. $\bar{B}^o_{r_0,\alpha}$ is a finite partially ordered set.

Proof. Since $\bar{B}^o_{r_0,\alpha} \subset R$, it is finite. Furthermore, the set of all regions $R$ itself is a partially ordered set, defined by the inclusion relation $r_1 < r_2 \iff r_1 \subset r_2 \land r_1 \neq r_2$.

From now on we will use the terminology of partially ordered sets. For instance, we will say that region $r_2$ covers $r_1$ if $r_2 > r_1$ and there is no $z$ such that $r_2 > z > r_1$.

Lemma 2. $\bar{B}^o_{r_0,\alpha}$ is closed under intersection with $r_0$.

Proof. The set of regions generated by the cluster variational method is closed under intersections in general. Let $\gamma \in \bar{B}^o_{r_0,\alpha}$, then $\gamma > \alpha$ and $\gamma \cap r_0 = \eta > \alpha$. Then, trivially, $\eta \cap r_0 = \eta > \alpha$ which guarantees that $\eta \in \bar{B}^o_{r_0,\alpha}$.

Since $\eta < r_0$, the following corollaries follows.

Corollary 1. All $\beta_i \in \bar{B}^o_{r_0,\alpha}$ such that $\beta_i$ covers $\alpha$ inside $\bar{B}^o_{r_0,\alpha}$, are subsets of $r_0$ ($\beta_i < r_0$).

Corollary 2.

$$B = \{ \beta_i \in \bar{B}^o_{r_0,\alpha} | \beta_i \text{ covers } \alpha \text{ in } \bar{B}^o_{r_0,\alpha} \}$$

is the set of minimal elements in $\bar{B}^o_{r_0,\alpha}$.

Lemma 3. If $\gamma \in \bar{B}^o_{r_0,\alpha}$ then $A^o_{\gamma} \subset B^o_{r_0,\alpha}$.

Proof.

$$\forall \eta \in A^o_{\gamma} \eta \cap r_0 \geq \gamma > \alpha \Rightarrow \eta \in \bar{B}^o_{r_0,\alpha}$$

As a consequence the entire $\bar{B}^o_{r_0,\alpha}$ is generated by the ancestry of members of $B$, this is:

Lemma 4.

$$\bar{B}^o_{r_0,\alpha} = \bigcup_{\beta_i \in B} A^o_{\beta_i}$$

We have written $\bar{B}^o_{r_0,\alpha}$ in terms of the set of ancestors of some minimal elements $\beta_1, \beta_2 \ldots$. We emphasize that all such ancestries are not empty, which is the case of all minimal elements $\beta_1, \beta_2 \ldots$ since they all share $r_0$, there exists an element in $\gamma \in \bar{B}^o_{r_0,\alpha}$, such that $A^o_{\gamma} = A^o_{\beta_1} \cap A^o_{\beta_2} \ldots$. Let us formalize and generalize this idea.

Let us use the definition of least upper bound $\phi = \text{lub}(\gamma, \eta)$ as the smallest element in $\bar{B}^o_{r_0,\alpha}$ that is both $\phi \geq \gamma$ and $\phi \geq \eta$. By minimum we mean that every other $z$ that shares both properties, happens to be $z > \eta$. In finite posets,
If the intersection of ancestries is not null, we end up with a unique value \( \eta \) such that \( A^\theta \) includes that of both \( \theta \) and \( \gamma \). In this representation, all regions containing one central spin \( s_1 \) are depicted. Central spin \( s_1 = \alpha \) is surrounded by eight maximal cubic regions \( Q_1, \ldots, Q_8 \). We represent the partially ordered set defined by the inclusion relations among the ancestors of \( s_1 \). Arrows point in the Parent-to-Child direction.

Bottom figures are the eight cubes, next level are all the square plaquettes that intersect among these cubes, the third layer is made of the six links containing spin \( s_1 \). We consider \( Q_1 = r_0 \) to be the region sending message to spin \( s_1 \). Shapes correspond to the position in the ancestry of \( s_1 \) with respect to the message \( m_{Q_1, s_1} \). All circular regions represent elements of \( B_{r_0, \alpha} \), and therefore their intersection with \( Q_1 \) is exactly \( s_1 \) (represented also in Fig. 2 except for \( Q_1 \)). Angular regions are those in \( B_{r_0, \alpha} \) (the absent part of Fig. 2 including \( Q_1 \)).

Since the set \( B_{r_0, \alpha} \) is written as the union of ancestries of the minimal sets \( \beta_1, \beta_2, \ldots \) (see lemma [1]), then from the previous lemma and the fact that all ancestries of the minimal elements share at least \( r_0 \) and its ancestry, it follows that

\[
\exists \eta \in B_{r_0, \alpha} \cap A^\beta \text{ such that } A^\eta = A_{\gamma_1} \cap A_{\gamma_2}
\]

**Lemma 5 (The intersection of ancestries).** Let \( \gamma_1, \gamma_2 \in B_{r_0, \alpha} \) with a non null intersection of their ancestors \( A^\alpha_{\gamma_1} \cap A^\alpha_{\gamma_2} \neq \emptyset \) then,

\[
\exists \eta = \text{lub}(\gamma_1, \gamma_2) \in B_{r_0, \alpha}
\]

Proof. If the intersection of ancestries is not null, then it has at least one element, let us say \( \theta \). Since \( \gamma_1, \gamma_2 \leq \theta \), then all ancestors of \( \theta \) are also comparable and above \( \gamma_1 \) and \( \gamma_2 \). In other words, \( \theta \in A^\alpha_{\gamma_1} \cap A^\alpha_{\gamma_2} \Rightarrow A^\eta_{\gamma_1} \subset A^\alpha_{\gamma_1} \cap A^\alpha_{\gamma_2} \). Let us suppose that \( A^\alpha_{\gamma_1} \cap A^\alpha_{\gamma_2} \) is the union of more than one ancestries of many incomparable \( \theta_i \)’s. This cannot be the case, since the intersection of any two \( \theta_1 \) and \( \theta_2 \) produces a lower \( \theta \), that is again in \( A^\alpha_{\gamma_1} \cap A^\alpha_{\gamma_2} \) and whose ancestry includes that of both \( \theta_1 \) and \( \theta_2 \). Repeating this procedure, we end up with a unique value \( \eta \), such that \( A^\eta_{\gamma_1} = A^\alpha_{\gamma_1} \cap A^\alpha_{\gamma_2} \). The fact that \( \eta = \text{lub}(\gamma_1, \gamma_2) \) is trivial.

Now, using the inclusion exclusion principle, we can write

\[
\sum_{r \in B_{r_0, \alpha}} c_r = \sum_{\beta \in B} \sum_{\gamma \in A^\beta_\gamma} c_\gamma - \sum_{\beta_1, \beta_2 \in B} \sum_{\gamma \in A^\beta_{\beta_1} \cap A^\beta_{\beta_2}} c_\gamma + \sum_{\beta_1, \beta_2, \beta_3 \in B} \sum_{\gamma \in A^\beta_{\beta_1} \cap A^\beta_{\beta_2} \cap A^\beta_{\beta_3}} c_\gamma - \cdots
\]

where every second sumatory is itself of the form

\[
\sum_{r \in A^\beta_\gamma} c_r = 1
\]
by the previous corollary. So, if the set \( \bar{B}_{r_0,\alpha} \) is generated by the ancestries of \( K \) minimal elements \( \beta_i \), then

\[
\sum_{r \in \bar{B}_{r_0,\alpha}} c_r = \left( \binom{K}{1} \right) - \left( \binom{K}{2} \right) + \left( \binom{K}{3} \right) - \\
\ldots + (-1)^{K+1} \binom{K}{K} = 1 + (1 - 1)^K = 1
\]

which concludes the proof of (A1) and from it that of (A4). \( \blacksquare \)

To help visualize a little bit the rather complicated algebra of sets, we depict in Fig. 6 the Hasse diagram and the sets \( \bar{B}_{r_0,\alpha} \) and \( B_{r_0,\alpha} \) for the Cube-CVM approximation for the 3D square lattice spin model. In particular the case of the message going from the cubic region \( Q_1 \) to the central spin region \( s_1 \) is shown.

**Appendix B: Marginalization of beliefs**

Extremization of the variational free energy with respect to the message functions result in the following equation

\[
\sum_{r \in \partial m_{r_0 \to \gamma}} c_r \sum_{x_0 \mid x_0} b_r(x_0) = 0 \quad (B1)
\]

for each message \( m_{r_0 \to \gamma} \).

In this appendix we show that the only solution for such set of equations are beliefs satisfying

\[
\forall p \in A_r \ b_r(x_r) = \sum_{x_0 \mid x_0} b_{r_0}(x_0) \quad (B2)
\]

We will prove this in an inductive manner, assuming that starting from the maximal regions onto a certain level, all regions marginalize and from this assumption, we will show that the next level also correctly marginalize.

**Induction: base case**

Let \( r_0 \) be a region whose ancestry \( A_{r_0} \) consists only on maximal regions. Then the intersection of members of any two members of \( A_{r_0} \) cannot be smaller than \( r_0 \) since by definition \( r \in A_{r_0} \Rightarrow r_0 \subset r \), but the intersection cannot be larger than \( r_0 \), since in such case \( \gamma = r_1 \cap r_2 \supset r_0 \) would be an ancestor of \( r_0 \) that is not a maximal region. So, any two elements of \( A_{r_0} \) intersect exactly at \( r_0 \).

Given the definition of the set of regions in whose belief a given message is present

\[
\partial m_{p \to r} = \{ r^p | r^p \cap p = r \}
\]

the previous result implies that any message \( m_{r_1 \to r_0}(x_0) \) from a parent \( r_1 \) of \( r_0 \) appears in the belief of all the other parents except \( r_1 \) itself and including \( r_0 \). Mathematically:

\[
\forall r \in A_{r_0} \partial m_{r_0 \to r} = \{ r_0 \} \cup A_{r_0} \setminus \{ r \} = A_{r_0} \setminus \{ r \}
\]

Let there be \( |A_{r_0}| = K \) parents to \( r_0 \). We have \( K \) equations of the type (B1)

\[
\forall i \in [1,2,\ldots,K] \sum_{r \in A_{r_0} \setminus \{ r_i \}} c_r \sum_{x_0 \mid x_0} b_r(x_0) = 0
\]

Except for \( c_{r_0} = 1 - K \), all other counting numbers are \( c_r = 1 \). Furthermore, we can add the missing sumand in each case, to obtain, for each \( i \in [1,2,\ldots,K] \)

\[
(1 - K)b_0(x_0) + \sum_{r \in A_{r_0} \setminus \{ x_0 \}} b_r(x_0) = \sum_{x_0 \mid x_0} b_{r_i}(x_0)
\]

Now, the left hand side is independent of \( i \), and therefore all righthand sides have to be equal for every \( i \). This proves that the parents are consistent among each other on their belief at region \( r_0 \). To show that they agree with \( b_0(x_0) \), we now use the fact that they agree to write

\[
(1 - K)b_0(x_0) + K \sum_{x_0 \mid x_0} b_{r_i}(x_0) = \sum_{x_0 \mid x_0} b_{r_i}(x_0)
\]

which concludes the induction base case with

\[
\forall i \in [1,\ldots,K] \ b_0(x_0) = \sum_{x_0 \mid x_0} b_{r_i}(x_0).
\]

as desired.

**Induction: inductive step**

Focus on a given region \( r_0 \), and consider its ancestry \( A_{r_0} \). In a partial order, the ancestry of a given element is always generated by the
union of ancestries of all elements covering it (see the previous appendix for the definition of the cover). Let there be \( K \) such elements \( r_i \) covering \( r_0 \), then
\[
A_{r_0} = \bigcup_{1 \leq i \leq K} A^o_{r_i}
\]
The induction step assumes that all ancestors \( p \in A_{r_i} \) of \( r_i \) are consistent with \( r_i \), in the sense of \((B2)\), and will then prove that \( r_i \) has also to be consistent with \( r_0 \). Since consistency between any \( p \in A_{r_i} \) and \( r_i \) and between \( r_i \) and \( r_0 \) is given, transitivity implies consistency between \( r_0 \) and \( p \), and generalizing, with all the ancestry \( A_{r_0} \) of \( r_0 \), concluding the induction step.

The tricky part is to show that consistency of the cover elements \( r_i \) with their ancestry \( A_{r_i} \) implies consistency of \( r_i \) with \( r_0 \). In order to do so let us start by the following

**Lemma 6** (Intersection of ancestries). If the set \( \{r_1, \ldots, r_K\} \) covers the element \( r_0 \), then for any two distincts \( k_1 \) and \( k_2 \) in \([1, \ldots, K]\), if there exists \( p \in A_{r_{k_1}} \) such that \( \gamma = p \cap r_{k_2} > r_0 \), then \( \gamma = r_{k_2} \).

In other words, any element \( p \in A_{r_0} \) such that the intersection \( p \cap r_i \) with one of the covers \( r_i \) is larger than \( r_0 \), is itself an ancestor of that cover \( p \in A^o_{r_i} \).

**Proof.** It is enough to note that \( \gamma = p \cap r_{k_2} > r_0 \) is necessarily bounded \( r_0 < \gamma \leq r_{k_2} \), but since \( r_{k_2} \) is a cover of \( r_0 \), no such intermediate element can exists, and therefore the only accepted situation is \( \gamma = r_{k_2} \). But this also implies that \( r_{k_2} = p \cap r_{k_2} \) which means that \( p \) is ancestor of \( k_2 \). \( \square \)

**Corollary 4.** The set \( \partial m_{r_i \rightarrow r_0} = \{ p \in A^o_{r_0} | p \cap r_i = r_0 \} \) is given by
\[
\partial m_{r_i \rightarrow r_0} = A^o_{r_0} \setminus A^o_{r_i}
\]
Graphically this means that the only possible situation for the sets \( \partial m_{r_i \rightarrow r_0} \) is the one in the left panel of figure \([7]\) and the situation in the right is forbidden.

Now, for every cover region \( r_i, i \in [1, \ldots, K] \) we will have an equation \((B1)\), that using the previous corollary can be written as
\[
\sum_{r \in A^o_{r_0}} c_r \sum_{x \notin \Xi_0} b_r(x) = \sum_{r \in A^o_{r_i}} c_r \sum_{x \notin \Xi_0} b_r(x), \text{ (B3)}
\]
Now it is quite similar to the base case of the induction. The left hand side does not depend on \( i \in [1, \ldots, K] \), while the right hand does. Therefore any two \( i_1, i_2 \in [1, \ldots, K] \) will be consistent
\[
\sum_{r \in A^o_{i_1}} c_r \sum_{x \notin \Xi_0} b_r(x) = \sum_{r \in A^o_{i_2}} c_r \sum_{x \notin \Xi_0} b_r(x)
\]
Furthermore, using that \( c_{r_i} = 1 - \sum_{r \in A_{r_i}} c_r \) and the consistency of \( r_i \) with its ancestry, the previous equality can be transformed in
\[
\sum_{x \notin \Xi_{i_1}} b_{r_{i_1}}(x) = \sum_{x \notin \Xi_{i_2}} b_{r_{i_2}}(x)
\]
Proceeding in a similar fashion as done in the base case for the induction, we can use the consistency between all different \( r_i \) back in equation \((B3)\) to show that they also have to agree with \( r_0 \)
\[
b_{r_0}(x) = \sum_{x \notin \Xi_i} b_{r_i}(x)
\]
concluding the inductive step. \( \blacksquare \)

**Appendix C: Moment matching fields are gauge free**

Let us prove theorems \([4] \) and \([5] \). They both say that using Maximal Messages with Moment Matching fields guarantees the consistency of beliefs, and is gauge free. We have already shown in the previous appendix \([A] \) that extremization of the CVM free energy with respect to message functions, ensures consistency of the beliefs. However, when using Moment Matching fields, we reduce the degrees of freedom of the message functions, and therefore it is not clear that consistency still holds.

The reduction on the active fields was done seeking a gauge free parametrization of the variational free energy. So we would also like to prove that the solution to the extremization problem gives a unique solution to the fields defining the messages. In other words, that when doing moment matching, we have removed all fields except those necessary to guarantee the consistency between the beliefs.
The proof of the consistency of the beliefs (theorem 4) will be carried in the following way:

1. Show that extremization with respect to moment matching fields on a set of variables \( \prod_{i \in q} s_i \) ensure consistency of the corresponding moments \( \langle \prod_{i \in q} s_i \rangle \) among those beliefs containing that group of variables.

2. Show that all moments are fixed by some field.

3. Conclude by saying that if all moments are equal, distributions have to be consistent.

The proof of the gauge free character (theorem 5) will be carried out simply by showing that, after removing of the undesired fields, there are as many variables (fields) as equations to be solved.

1. **Moment consistency (theorem 4)**

The prescription given by the moment matching definition \( \ref{def:moment_matching} \) says that message \( m_{p \rightarrow r}(s_r) \) counts with a field \( U_q \) forcing the correlation among variables in \( q \subseteq r \) as

\[
m_{p \rightarrow r}(s_r) = e^{\sum_{r \in \partial U_q} c_r \xi_q,r} \prod_{i \in q} s_i + \cdots
\]

if and only if \( r \) is the smallest region containing the subset \( q \). Therefore, for any given set \( q = \{s_{q_1}, \ldots, s_{q_k}\} \) there is a single region \( r_0 \) such that the fields \( U_q^{p \rightarrow r_0} \) appear in the message from its ancestors \( p \in A_{r_0} \). The situation is depicted in figure 8.

When extremizing with respect to the fields \( U \) that parametrize the messages we get equations similar to (B1), but instead of the belief functions, we get the moments corresponding to the field

\[
\forall_{p \in A_{r_0}} \sum_{r \in \partial U_q^{p \rightarrow r}} c_r \xi_q,r = 0 \quad \text{(C1)}
\]

and the expected value is taken with respect of the belief \( b_r(x_r) \) (local distribution) at region \( r \) and \( \partial U_q^{p \rightarrow r} = \partial m_{p \rightarrow r} \) is the set of regions in whose beliefs the message \( m_{p \rightarrow r} \) participates, and therefore so does \( U_q^{p \rightarrow r} \).

We will have as many equations (C1) as ancestors \( r_0 \) have \( K = |A_{r_0}| \), corresponding to derivation with respect to each field (each arrow in figure 8). We will further assume that no counting number is zero, and therefore the set of linear equations (C1) relates all moments \( \xi_{q,r} \) which are \( K + 1 \), including the one obtained at \( r_0 \) itself.

Since we have proven in Appendix A that

\[
\sum_{r \in \partial U_q^{p \rightarrow r}} c_r = 0 \quad \text{(C2)}
\]

a particular solution of the system of equations will always be

\[
\forall_{r \in A_{r_0}} \xi_{q,r} = \xi_{q,r_0}
\]

which is part of what we are trying to prove. We can also write equation (C1) as

\[
\forall_{p \in A_{r_0}} \sum_{r \in \partial U_q^{p \rightarrow r} \setminus r_0} c_r \xi_{q,r} = -c_{r_0} \xi_{q,r_0}
\]
where the right hand side is the same irrespective of who is $p$. Considering only the correlations involved in the left hand side, this system of equation will have only one solution (at fixed $\xi_{q,r_0}$) if the matrix $G_{K \times K}$ made of elements

$$g_{r,p} = \begin{cases} c_r & \text{if } r \in \partial U_q^{p \rightarrow r_0} \\ 0 & \text{otherwise} \end{cases}$$

has non zero determinant.

In order not to make the paper far too long, we ask the reader to prove in each cluster variational method implemented that the set of regions used fulfill this property. Yet, we warn that this property wont be fulfilled any time that some of the following conditions is present:

- There are zero counting numbers, since a column of the matrix will be full of zeros.
- A given message does not appear in any belief equation, since a row will be full of zeros.
- Two or more rows of the matrix are equal, causing a zero determinant.

Without a proof (that seems rather complicated to us), we give the hint that these seems to be the only situations possible, after many random playing with arbitrary clusters approximations. It is not obvious why two or more lines could not be linearly combined into another line, to cause a zero determinant, but some properties of the counting numbers seems to forbid this.

So, we have that under the condition of non-singular matrix $G_{K \times K}$ the set of equations involving the correlation of a given set of spins $q$, force all such correlations to be equal. Now since every set of spins contained in two or more regions is contained in their intersection (which also has to be a region by CVM prescription), then all two regions agree on the moments of every common subset of variables.

We finish the proof by noting that if all regions agree on all correlations of the intersecting variables, they have to be consistent in the sense that the marginal probabilities over these variables should agree.

2. Gauge free (theorem 5)

We note from the previous proof that we have $K$ fields $U_q^{p \rightarrow r_0}$ if there are $K$ ancestor of region $r_0$. Since the consistency of the corresponding correlations $\xi_{q,p}$ is fixed by $K$ equations, we have as many parameters as equations to be satisfied. Furthermore, the consistency among the local distributions $b_r(x_r)$ that contain a given set of variables $q$, can not be forced with less than $K$ equalities, since equalities are transitive and therefore all we need is to conect the set of $K + 1$ regions containing $q$ in a graph with minimal number of edges (each edge meaning an equality) among moments. Among $K + 1$ nodes, the single component graph with minimal edges is the tree, which happens to have $K$ edges. So, as we said, the $K$ fields $U_q^{p \rightarrow r_0}$ are exactly the minimum required amount to enforce all local distribution to agree on the respective moment $\xi_{q,p}$.

This used not to be the case in Parent-to-Child CVM, for instance, as seen in [20], where
the consistency of a single spin magnetization that belonged to four links and four plaquettes in the square plaquette Ising model, appear after the derivation with respect to twelve parameters (field) instead of eight. Therefore there are 12 equations (and 12 parameters) to assign the equality among 8 local distributions, forcing 4 of the equations (and parameters) to be redundant.

So, in this appendix we have proven that maximal messages and moment matching fields generate a set of equations with the following properties:

1. every correlation among a set of variables that belongs to two or more regions is present in some equation;

2. there are as many free parameters as relations required to guarantee consistency;

3. consistent correlations is one solution of the system.