Bethe Approximation for Self-Interacting Lattice Trees

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Abstract

In this paper we develop a Bethe approximation, based on the cluster variation method, which is apt to study lattice models of branched polymers. We show that the method is extremely accurate in cases where exact results are known as, for instance, in the enumeration of spanning trees. Moreover, the expressions we obtain for the asymptotic number of spanning trees and lattice trees on a graph coincide with analogous expressions derived through different approaches. We study the phase diagram of lattice trees with nearest-neighbour attraction and branching energies. We find a collapse transition at a tricritical $\theta$ point, which separates an expanded phase from a compact phase. We compare our results for the $\theta$ transition in two and three dimensions with available numerical estimates.

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The statistical properties of polymers have been one of the great challenges of statistical physics in the last decades \cite{1,2}. A great understanding has been gained for the case of linear polymers, thanks to the simple but instructive description in terms of self-avoiding walks (SAWs) on a lattice, which is in turn amenable to many different treatments, ranging from Monte Carlo simulations to exact enumerations, from mapping to the $O(n = 0)$ spin model to field theoretical formulations \cite{3}. Less is known about the behaviour of branched polymers (BPs). In lattice statistical mechanics BPs can be efficiently modelled by lattice animals \cite{4}, i.e. by connected clusters of bonds. Analogously to linear polymers, BPs in solution can display a dense and a diluted phase, depending on temperature and quality of the solvent. The collapse transition occurs at the so called $\theta$ point \cite{5} and in recent years has attracted a lot of attention, both for linear \cite{6} and branched polymers \cite{7}.

Recently, a variational approach based on the cluster variation method (CVM) has been introduced for linear polymers \cite{7}, giving results in good agreement with the best numerical simulations in many situations: dense polymers (i.e. Hamiltonian Walks), diluted and self-interacting ones. The CVM \cite{8,9} is a closed form approximation, which finds wide applications in accurate investigations of the phase diagram of lattice spin systems \cite{10}. It is based on the minimisation of a variational free energy which is obtained by truncating
the lattice cumulant expansion of the entropy \[9\]. The largest clusters considered in the expansion determine the “order” of the approximation and are named maximal clusters. For example, standard mean-field and Bethe approximations are recovered by considering as maximal clusters respectively single sites and nearest-neighbours pairs. Most of the present knowledge about the phase behaviour of BPs has been gained through numerical approaches such as Monte Carlo simulations, exact enumerations or transfer matrix techniques (for an exception see, e.g., ref. \[11\]). The possibility to extend to BPs the CVM scheme becomes therefore extremely appealing.

In the present paper we introduce a CVM based variational approximation for lattice trees (LTs), that is lattice animals containing no closed loops. We show that the method performs very well when compared to situations where exact results are known as, for instance, in the case of the enumeration of spanning trees on a lattice. We then use it to explore the phase behaviour of LTs with branching energies and nearest-neighbour attractive interaction between non bonded monomers, in different energy and temperature regimes.

Let us make first a rather important technical remark about our method. Being self-avoiding, LTs face strong non-local constraints on the lattice (neighbouring sites can be occupied by monomers that are extremely far apart on the tree). This is a serious problem when dealing with local approximations such as the CVM. In order to partially overcome this difficulty, we have introduced an intrinsic direction on each edge of a lattice tree, which can be visualised with an arrow. Each occupied site of the lattice is therefore characterised by a certain number of incoming edges (input edges) and by a certain number of outgoing edges (output edges). To ensure that the tree does not form loops we have required that (i) sites with no outputs occur with probability 0 in the thermodynamic limit and (ii) all other occupied sites have exactly one and only one output. It is important to underline that conditions (i) and (ii) uniquely determine the orientation of the arrows on a given LT, so that the descriptions in terms of oriented LTs and non oriented LTs are equivalent. The advantage for our purposes is that we are able in this way to exclude configurations with an inner loop (which is a kind of long range constraint) by means of a local variable (the orientation of the arrow on each occupied bond).

Within the CVM scheme, the Bethe approximation is obtained by choosing nearest neighbour (NN) pairs as maximal clusters. For a homogeneous and isotropic model with only single site and NN pair interaction terms, the variational (reduced) free energy density has the form \[9\]

\[
\tilde{f}^{(u)} = \frac{\beta F^{(u)}}{N} = \frac{q}{2} \beta \text{Tr}(\rho_{NN} H_{NN}) + \frac{q}{2} \text{Tr}(\rho_{NN} \ln \rho_{NN}) - (q - 1) \text{Tr}(\rho_{\bullet} \ln \rho_{\bullet}),
\]

where \(q\) is the coordination number of the lattice, \(\beta = 1/k_B T\) \((k_B = 1\) from now on\), \(H_{NN}\) is the contribution of a generic NN pair to the Hamiltonian and \(\rho_{\bullet}\) and \(\rho_{NN}\) are the site and NN pair density matrices, respectively. For classical models the density matrices are diagonal and their diagonal elements are the probability of the corresponding configurations. The free energy must be minimised with respect to the density matrices, which must satisfy the condition of normalisation to 1 and compatibility (that is, \(\rho_{\bullet}\) must be obtainable from \(\rho_{NN}\) by a partial trace).

The first problem we deal with are spanning trees (STs). A ST visits all sites of a lattice and therefore STs can be seen as a special case (a subset) of LTs. In particular,
STs are believed to model compact branched polymers. For the moment we are interested in estimating the total number $N_{ST}$ of STs on a lattice. To leading order, this number should scale with the number of sites $N$ as $N_{ST} \sim \mu_{ST}^N$, where $\mu_{ST}$ is the so called connective constant. As the entropy per site $s_{ST}$ is given by $s_{ST} = \ln \mu_{ST}$ and there is no energy term, it follows that the reduced free energy per site $\tilde{f}_{ST}$ is simply related to the connective constant by $\tilde{f}_{ST} = - \ln \mu_{ST}$. The value of $\mu_{ST}$ for a given graph is a non trivial number, which can anyway be calculated exactly. It is therefore an excellent starting point to test the accuracy of our method.

The configurations of a site and a NN pair are classified according to the number of edges attached to each site and they are reported schematically in fig. 1. In the following we will denote with $s_i$ the probability variable of a site configuration with $i$ occupied edges (e.g. for a square lattice $i$ takes values between 1 and 4) and with $e_{ij}$ the probability variable assigned to a disconnected pair having $i$ edges on one site and $j$ edges on the other site. Similarly we will denote with $\vec{f}_{ij}$ the probability variable of a connected pair with an intrinsic direction from the site with $i$ edges to the site with $j$ edges. The free energy (1) takes then the form

$$\tilde{f}^{(n)}_{ST} = \frac{q}{2} \left\{ \sum_{i,j=1}^{q-1} m_e(i,j) e_{ij} \ln e_{ij} + 2 \sum_{i=0}^{q-1} \sum_{j=1}^{q-1} m_f(i,j) \vec{f}_{ij} \ln \vec{f}_{ij} \right\} - (q-1) \left\{ \sum_{i=1}^{q} m_s(i) s_i \ln s_i \right\}$$

(2)

where $m_s(i)$, $m_e(i,j)$ and $m_f(i,j)$ stand respectively for the multiplicity of site, disconnected pair and connected pair configurations (see fig. 1 for the actual values of $m_s(i)$, $m_e(i,j)$ and $m_f(i,j)$). The factor 2 in front of the contribution from the connected pairs configurations arises from the degeneracy associated with the direction of the arrow. In writing equation (3), moreover, we have implicitly assumed translational invariance in the system, a condition which in the thermodynamic limit is fulfilled. The normalisation and compatibility conditions on the density matrices can be written respectively as

$$\sum_{i,j=0}^{q-1} m_e(i,j) e_{ij} + 2 \sum_{i=0}^{q-1} \sum_{j=1}^{q-1} m_f(i,j) \vec{f}_{ij} = 1$$

(3)

and

$$\sum_{j=1}^{q-1} \binom{q-1}{j} j e_{ij} = s_i, \quad i = 1, \ldots q - 1$$

$$\sum_{j=1}^{q-1} \binom{q-1}{j} j \vec{f}_{i-1,j} = s_i, \quad i = 1, \ldots q$$

$$\sum_{j=0}^{q-1} \binom{q-1}{j} \vec{f}_{j,i-1} = s_i, \quad i = 2, \ldots q.$$

(4)

Conditions (3) assures that single site and pair probability variables are defined consistently, so that by summing over all allowed configurations of one site of a pair, one should recover the probability $s_i$ associated to a single site configuration. Our problem is then to find the minimum of the CVM free energy $\tilde{f}^{(n)}_{ST}$ subject to the above constraints. In general this problem can be easily dealt with numerically with the help of an algorithm named numerical iteration method [12]. In this special case of spanning trees enumeration however one can
first guess on the basis of numerical results and then verify by direct substitution that the
solution takes the analytical form
\[ s_i = \frac{(q - 2)^{q-i}}{q(q - 1)^{q-1}}, \quad e_{ij} = \frac{q}{q - 2}s_is_j, \quad \tilde{f}_{ij} = s_{i+1}s_{j+1}, \]
which gives for the reduced free energy
\[ \tilde{f}^{(B)}_{ST} = \frac{(q - 2)\ln[q(q - 2)] - 2(q - 1)\ln(q - 1)}{2} \tag{5} \]
from which one can derive the connective constant
\[ \mu^{(B)}_{ST} = \exp(-\tilde{f}^{(B)}_{ST}). \]

It is interesting to remark that the same result for the reduced free energy (5) can be
obtained by exploiting the well-known relation between STs and the Q-state Potts model
\[ [13].\] Indeed by applying the same approximation scheme to the Potts model and then taking
the \( Q \to 0 \) limit of the reduced free energy density calculated in
\[ \beta = \ln(1 + Q^\alpha), \]
where \( \beta \) denotes the Potts coupling divided by \( k_BT \) and \( 0 < \alpha < 1 \), one recovers expression (5).

Actually, the exact number of STs on a \( d \)-dimensional hypercubic lattice can be computed
exactly \[ [14].\] The entropy is the logarithm of this number and, in the thermodynamic limit
\( N \to \infty \), the entropy per site is
\[ s_{ST} = \frac{1}{(2\pi)^d} \int_0^{2\pi} dk_1... \int_0^{2\pi} dk_d \ln \left( \frac{2d - 2}{\sum_{i=1}^{d} \cos(k_i)} \right) \tag{6} \]
The large \( d \) expansion of (6) is
\[ s_{ST} = \ln(2d) - \frac{1}{4d} - \frac{3}{8d^2} + o\left(\frac{1}{d^3}\right) \tag{7} \]
Expanding (6) for large \( q \) we get
\[ s^{(B)}_{ST} = \ln q - \frac{1}{2q} - \frac{1}{2q^2} + o\left(\frac{1}{q^3}\right) \tag{8} \]
With \( q = 2d \) the first three terms (the logarithm, the vanishing constant and the first power
of \( 1/d \)) coincide.

In fig. 2 we show a comparison between \( s^{(B)}_{ST} \) and the exact result \( s_{ST} \), which indicates
that the accuracy of the approximation is rather good. This check is of utmost importance.
Indeed, the CVM is an approximation on the entropy estimate of the system. Having an
extremely good approximation of the entropy gives confidence in more complicated situations
where energies are introduced into the model. The probability \( p_i \) that a randomly chosen
site is connected to \( i \) nearest-neighbour sites can also be calculated exactly for STs on the
square lattice \[ [15].\] The result is
\[ p_1 \approx 0.29454, \quad p_2 \approx 0.44699, \quad p_3 \approx 0.22239 \quad \text{and} \quad p_4 \approx 0.03608, \]
which agree quite well with the values we obtain within our approximation \( (p_i = m_s(i)s_i) \),
i.e. \( p_1 \approx 0.29630, \quad p_2 \approx 0.44444, \quad p_3 \approx 0.22222 \quad \text{and} \quad p_4 \approx 0.03704. \)

As a further test, we have considered the case of directed spanning trees (DSTs) in \( d \)
dimensions, where the exact result is known and it is simple. In this case a preferred direction
along a lattice diagonal is chosen and all edges must have a positive component along this
direction. This means that the output at each site is restricted to \( d \) possible directions.
Moreover the output direction in the bulk of the system can be chosen independently one site
from the other, as by construction loops cannot be formed. The number of DSTs is therefore
$\mathcal{N}_{DST} \sim d^N$ (neglecting boundary terms). We have studied DSTs within our framework, selecting among all the single site and pair configurations for STs only those allowed by the directedness constraint (for instance, the number of single site configurations with $i$ edges is $m_s(i) = d \left( \frac{d}{i} \right)$ for DSTs, as compared to $m_s(i) = i \left( \frac{2d}{i} \right)$ for STs). Similarly to the ST case, we have then written a variational free energy from (1). Minimising it numerically (subject to proper constraints), we have indeed verified that the exact result is recovered, i.e. $\mu_{DST}^{(b)} = d$.

In order to test the consistency of the scheme, we have studied the case of spanning trees with energies depending on the number of branchings at each site. To this end we have assigned a reduced energy penalty $E_i$ to each site with $i$ branches. In the limit $E_1 \to \infty$ (and $E_i = 0$ for $i > 1$) tips are not allowed, so that one should recover the case of space filling self-avoiding walk, i.e. Hamiltonian walks (HWs). We have verified that in fact when $E_1 \to \infty$ the only configuration which have a non zero weight are those of a linear polymer. The resulting entropy moreover coincides with that of HWs in the Bethe approximation \[^7\]. Our Bethe approximation suggests a smooth crossover from STs to HWs, with no sign of discontinuity in the free energy. We have also verified, in the case $q = 4$, that the HW limit can be reached by sending simultaneously $E_3$ and $E_4$ to infinity, thus forbidding the occurrence of branchings.

We now turn to the problem of LT collapse. Just as for linear polymers, the collapse transition is driven by an attractive interaction $\beta$ between nearest neighbour contacts\[^6\]. The partition function of the so called $t$-model reads

$$\mathcal{Z}_N = \sum_{c \geq 0} t_N(c) e^{\beta c}$$

(9)

where $t_N(c)$ denotes the number of trees with $N$ sites and $c$ contacts. Introducing a monomer fugacity $z$, the grand canonical partition function reads therefore

$$\mathcal{Z} = \sum_{N=1}^\infty \sum_{c \geq 0} z^N t_N(c) e^{\beta c}$$

(10)

where the first sum is over all possible number of sites in the tree. We then proceed analogously to the ST case and write a pair approximation for the free energy of the system as

$$\tilde{f}_{LT}^{(p)} = -\ln z \sum_{i=1}^q m_s(i) s_i + \frac{q}{2} \beta \sum_{i,j=1}^{q-1} m_e(i,j) e_{ij} +$$

$$\frac{q}{2} \left\{ \sum_{i,j=0}^{q-1} m_e(i,j) e_{ij} \ln e_{ij} + 2 \sum_{i=0}^{q-1} \sum_{j=1}^{q-1} m_f(i,j) \tilde{f}_{ij} \ln \tilde{f}_{ij} \right\} - (q - 1) \left\{ \sum_{i=0}^{q} m_s(i) s_i \ln s_i \right\}$$

(11)

where the symbols $s_i$, $e_{ij}$, $\tilde{f}_{ij}$ have similar meanings as in eq. (2) (note that contrary to eq. (2) the possibility of an empty site must be considered in eq. (11)). The stable phase at

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\[^1\] A contact is defined as a pair of nearest neighbour vertices of the tree which are not linked by an edge.
given $\beta$ and $z$ is obtained by minimising the free energy $\tilde{f}_{LT}$ subject to normalisation and consistency conditions on the probability variables (see previous discussion for STs). In this case it is not possible to express the solution in a simple, analytical form and one has to fully resort to numerical methods, e.g. the natural iteration method [12].

We report the complete phase diagram for $d = 3$ in fig. 3, as a function of $z$ and $\beta$. There are two distinct phases: a zero density phase, where the average number of edges in a tree is finite, and a finite density phase, where instead this number is infinite. These two phases are separated by a transition line $z_c(\beta)$ which could either be first order (corresponding to a finite jump in density) or second order (corresponding to a continuous change in density). The tricritical point where the two lines merge is the $\theta$ point, $\beta_\theta$, i.e. the point where the collapse transition of the LT occurs. The structure of the infinite LT along the line $z_c(\beta)$ is expanded for $\beta < \beta_\theta$ and compact for $\beta > \beta_\theta$. We obtain $\beta_\theta \approx 0.406$ in $d = 2$ and $\beta_\theta \approx 0.224$ in $d = 3$. Recent estimates from extensive Monte Carlo simulations on the collapse of lattice trees [16] yield the values $\beta_\theta = 0.699 \pm 0.052$ and $\beta_\theta = 0.346 \pm 0.017$, respectively in $d = 2$ and $d = 3$.

The phase diagram for LTs appears to be identical to the one for SAWs (see e.g. fig. 2 in [9]), except for a rescaling of the fugacity $z$ by a factor $\left(\frac{q-1}{q-2}\right)^{q-2}$. In particular the numerical values $\beta_\theta$ of the collapse transition of the polymers coincide and, in both cases, $z_c$ does not depend on $\beta$, as long as $\beta < \beta_\theta$. This similarity is an intriguing result for which at the moment we don’t have any plausible explanation. We have also investigated a generalisation of the partition function (9) by including an energy term $E_1$ which penalises configurations with tips. At any given $E_1$ the phase diagram in $\beta$ and $z$ shares similar features with the phase diagram for LTs or SAWs. The difference is just restricted to a scale factor in $z$ which is determined by the value of $E_1$. This means in particular that the value of $\beta_\theta$ does not depend on $E_1$, at least at this level of the approximation. Similarly to the ST case, we have also verified that in the limit $E_1 \to \infty$, where tips are not allowed, the phase diagram of a linear polymer is recovered.

It is interesting to remark that in the special case $\beta = 0$ we numerically obtain for the connective constant of a LT $\mu_{LT} = z_c(0)^{-1}$ a result which agrees with the analytical expression

$$\mu_{LT}^{(b)} = \frac{(q-1)(q-1)}{(q-2)(q-2)}$$

This expression was indeed derived in [17] by studying LTs on a Bethe lattice with coordination number $q$ and specializes to $\mu_{LT}^{(b)} = 6.75$ for $q = 4$ and $\mu_{LT}^{(b)} = 12.21$ for $q = 6$. The most accurate numerical estimates [18] for the connective constant of LTs are $\mu_{LT} \approx 5.14$ for the square lattice and $\mu_{LT} \approx 10.50$ for the cubic lattice.

In summary, we have introduced a novel variational technique to investigate the behaviour of branched polymers. It is based on the cluster variation method with nearest neighbour pairs as maximal clusters. It can therefore be viewed as the natural formulation of the Bethe approximation for these systems and it provides the starting point on which systematic improvements can be made by applying the CVM recipe [8,9] to clusters larger than the NN pair (the first step being the plaquette). Also, it should be possible to deal with
different branched polymer representations, such as weakly and strongly embedded lattice animals.

The method yields exact results in the trivial case of directed spanning trees and extremely accurate ones for the enumeration of spanning trees, where the exact result is still available. Introducing branching energies in the spanning tree problem we have shown that the Hamiltonian walk limit is correctly recovered. Finally, we have studied the collapse transition of branched polymers, obtaining estimates for the $\theta$ point which compare reasonably well with the most accurate simulations.

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FIG. 1. Schematic representation of independent (a) site and (b) pair configurations, in the case of spanning trees. The continuous line represents the spanning tree; $q = 2d$ is the coordination number of the lattice. The configurations drawn in the picture correspond to (a) $s_3$, (b) $c_{2,3}$ and $\vec{f}_{3,2}$.

FIG. 2. Entropy per site as a function of coordination number $q$ in the case of spanning trees. The continuous line corresponds to the Bethe approximation, the circles are exact results.
FIG. 3. Phase diagram of self-interacting lattice trees as a function of $\beta$ and $z$ for $d = 3$. The average number of bonds in a tree is finite (infinite) in region I (II). The continuous (dashed) line is a second (first) order transition. The cross marks the tricritical point ($\beta_\theta \approx 0.224$ and $z_\theta \approx 0.08192$).