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Generalized belief propagation for the magnetization of the simple cubic Ising model

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Abstract

A new approximation of the cluster variational method is introduced for the three-dimensional Ising model on the simple cubic lattice. The maximal cluster is, as far as we know, the largest ever used in this method. A message-passing algorithm, generalized belief propagation, is used to minimize the variational free energy. Convergence properties and performance of the algorithm are investigated.

The approximation is used to compute the spontaneous magnetization, which is then compared to previous results. Using the present results as the last step in a sequence of three cluster variational approximations, an extrapolation is obtained which captures the leading critical behavior with a good accuracy.

Keywords: Generalized belief propagation; Cluster variational method; Simple cubic Ising model

1. Introduction

A major approximate tool in the equilibrium statistical physics of lattice models is the mean-field theory, together with its many generalizations. These techniques are known to give quite often reliable qualitative results, which makes them very useful in understanding properties of a model like its phase diagram. Due to the limited quantitative accuracy of simple mean-field theory, many generalizations were developed. Since mean-field neglects correlations, typically

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the idea is to include local, but progressively longer range correlations in the treatment, for example by means of cluster expansions where clusters of increasing size can be included.

This line of research started with the Bethe–Peierls approximation [1,2], where nearest-neighbour correlations are taken into account, and the Kramers–Wannier approximation [3,4], including correlations up to a square plaquette. Many generalizations were then proposed, and a particularly successful one was the cluster variational method (CVM), introduced by Kikuchi in 1951 [5] and applied to the Ising model. The largest clusters considered by Kikuchi in this work were a cube of 8 sites for the simple cubic lattice and a tetrahedron of 4 sites for the face centered cubic lattice.

Larger clusters were later considered: in 1967 Kikuchi and Brush [9] introduced the B_{2L} sequence of approximations for the two-dimensional square lattice, whose convergence properties were later studied [10] using maximal clusters up to 13 sites. Kikuchi and Brush also suggested that a similar approach could in principle be carried out in three dimensions, although the computational costs would have been prohibitively large at that time. Their intuition was put on a firmer ground by Schlijper [6–8], who showed that, for translation-invariant models in the thermodynamical limit, there exist sequences of CVM approximations whose free energy converges to the exact one. For a d-dimensional model, the largest clusters to consider grow in $d-1$ dimensions only, as in a transfer matrix approach. In 3 dimensions this idea was used by the present author to develop a CVM approximation for the Ising model on the simple cubic lattice based on an 18-site ($3 \times 3 \times 2$) cluster [11].

The main difficulty encountered in trying to enlarge the basic clusters is the computational cost, which grows exponentially with the cluster size. More precisely the problem can be written as the minimization of a free energy whose number of independent variables increases exponentially with the cluster size. A significant amount of work was then devoted to develop efficient algorithms. The original iterative algorithm proposed by Kikuchi [12–14], the so-called natural iteration method, is not particularly efficient, but in certain cases it is provably convergent [15] to a (maybe local) minimum of the free energy. Faster, provably convergent algorithms were developed more recently [16,17].

A very important step in the direction of speeding up algorithms for the minimization of the CVM free energy has been made in 2001, when it was shown [18] that Belief Propagation (BP) [19], a message-passing algorithm widely used for approximate inference in probabilistic graphical models, is strictly related to the Bethe–Peierls approximation. In particular, it was shown [18] that fixed points of the BP algorithms correspond to stationary points of the Bethe–Peierls variational free energy. This result was later extended by showing that stable fixed points of BP are (possibly local) minima of the Bethe–Peierls variational free energy, though the converse is not necessarily true. This provides us with the fastest, but not always convergent, algorithm for the minimization of the Bethe–Peierls free energy. When convergent, BP outperforms the other algorithms by orders of magnitude (see [10] for a detailed comparison). BP was also extended to an algorithm, named Generalized Belief Propagation (GBP) [18,20], whose fixed points are stationary points of the CVM free energy for any choice of basic clusters. Like BP, GBP is extremely fast but not always convergent.

The purpose of the work described here is twofold: we aim both to test how GBP performs in minimizing a CVM free energy with a very large (32 sites) basic cluster, and to make one more step in the hierarchy of CVM approximations for three-dimensional lattice models. Working on the Ising model on the simple cubic lattice as a paradigmatic example, we follow Schlijper's ideas and enlarge the basic cluster for our CVM approximation in 2 dimensions only, thus choosing a $4 \times 4 \times 2$ cluster (as far as we know, the largest cluster ever considered in CVM). We then use a