Tensor renormalization of three-dimensional Potts model

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**Abstract:** We study the $q$-state Potts models on a cubic lattice in the thermodynamic limit using tensor renormalization group transformations with the triad approximation. By computing the thermodynamic potentials, we locate the first-order phase transitions for $10 < q \leq 20$ which has not been explored using any method. We also examine the efficiency of the triad approximation method in obtaining the fixed-point tensor and comment on how this can be improved.
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### SECTION 1

**Introduction**

The motivation of this work is to examine some recent developments in the tensor renormalization group method referred to as the ‘triad’ method. We find that this method is reasonably precise in computing the potentials and critical temperatures for a range of models, including the $q$-state Potts model in three dimensions. However, this method most likely misses the correct fixed-point tensor. In order to reach this conclusion, we use an observable defined in Ref. [1] and show that this method cannot accurately compute this either for the Ising model or for the $q$-state Potts model in three dimensions when we go sufficiently close to criticality for some fixed and finite bond dimension. Therefore, while this is a promising method to study statistical systems in higher dimensions, admittedly, much work remains to be done to generate a more precise scheme.

The framework of renormalization group (or rather ‘semi-group’) is probably the most important advance in the last fifty years and has taught us the correct way to think about quantum field theories. One of the most exciting areas of research in the past fifteen years is the development that we can use tensors to effectively carry out the renormalization group (RG) procedure through some well-defined transformations numerically. In his famous paper
on the solution of Kondo problem, Wilson emphasized and clearly pointed out that this feature (which was called the ‘fourth aspect’ in his paper) of studying renormalization group theory on digital computers was the most exciting. In the last five decades with improved computing resources and the possibility of quantum computers in the future, this is even more exciting than Wilson had envisaged. This approach has taught us valuable things about entanglement, holography, phase transitions in statistical models while much more still remains to be understood. The numerical method introduced by Wilson for the solution of the impurity problem was not applicable to a wider class of one-dimensional models. The numerical RG program was stagnant until 1992, when White showed that by using the density matrices and making reasonable assumptions, it was possible to study the one-dimensional systems much more efficiently than any previous methods. The next development in the real-space renormalization group came when it was proposed that one can use multi-index objects called tensors to carry out RG transformations for gapped systems. The idea of tensor renormalization group (TRG) started with the seminal work of Levin and Nave in 2007 [2] and was later improved by a new method called ‘second renormalization group’ (SRG) introduced in Ref. [3] which took the effect of the tensor environment into account to carry out a well-defined renormalization group flow. However, both TRG and SRG were shown to be inefficient at the critical point. This gave rise to the idea of another well-known algorithm known as tensor network renormalization (TNR) [4] which works better than both TRG and SRG for gapless systems and the convergence in the bond dimension is exponential rather than polynomial. Though all these methods work reasonably well for two-dimensional classical models, the extension to three or more dimensions is not straightforward. In this pursuit, a new approach called higher-order TRG (HOTRG) was introduced in Ref. [5]. However, the memory cost of this method scale rather poorly with dimensions as $D^{4d-2}$ and becomes unmanageable (unless one has access to supercomputers with such memory) quickly. To deal with this problem, a few years ago, a new approximate method called ‘triad TRG’ (TTRG) was introduced. This method is basically the application of the ‘divide and conquer’ rule applied to HOTRG. The triad RG significantly cuts down the memory requirements and computation time since a higher rank tensor is never explicitly made and offers a fairly acceptable level of accuracy by running on small machines especially in three and four dimensions. However, this method is certainly not as robust as HOTRG and the real effectiveness of this method and comparison to HOTRG in higher dimensions remains a topic of discussion. For a recent review on tensor networks, we refer the interested reader to Ref. [6] and to Ref. [7] for an extended review of real-space renormalization in statistical mechanics over the past five decades. In this paper, we will focus on the triad method applied to the three-dimensional spin system especially the $q$-state Potts model and see how far we can go. This is a continuation of a long program of research where tensor networks have been applied extensively to spin systems and gauge theories in two and three dimensions [8–13]. Most of the tensor network studies of three-dimensional spin models are restricted to Ising model, however, there was a study of $q = 3$ Potts model in Ref. [9] and very recently we studied the $O(2)$ model using tensor methods in Ref. [12].
The model we study in this paper was first defined\textsuperscript{1} by Renfrey Potts in 1951 and describes a generalization of the Ising model. This is now known as \( q \)-state Potts model based on the local Hilbert space dimension of the individual spin. In fact, there was a previous study of models of this type already around 1943 when the \( q = 4 \) model was considered by Askhin-Teller (a model now known by their name). For a detailed review of Potts model, its history, and various exact solutions in different dimensions, we refer the interested reader to Ref. [15]. Though the model seems relatively straightforward, for the three-dimensional classical \( q \)-state Potts model, we do not even have an understanding of how the critical temperatures depend on \( q \). Note that this is at least well-known on square lattice even though full solution does not exist for free energy for generic temperature with \( q \geq 3 \) [14]. In two dimensions, by mapping to Ice-type models, this was computed to be: \( T_c = 1/\ln(1 + \sqrt{q}) \). Though this reduces to Onsager result for \( q = 2 \) (up to a multiplicative factor) and has been checked by Baxter and Hintermann for \( q \geq 4 \), a rigorous proof still lacks for \( q = 3 \), see Ref. [15] for details. In three dimensions, the determination of the critical temperature has to be done through numerical methods and even though a large volume of work has been done and numerical results are available up to \( q = 10 \), there is no work beyond this with any method! This is surprising for a model which was introduced more than 70 years ago. In this work, we aim to fill this gap by computing critical temperatures on cubic lattice for \( 10 < q \leq 20 \) using tensor network methods with the triad method developed in Ref. [16].

Another interesting study in the past for these models is the determination of the critical \( q \) where the order of the phase transition changes and is referred to as \( q_c \). This was determined to be \( q_c = 4 \) [14], and \( q_c = 2.35(5) \) [17] for two and three-dimensional models respectively. For \( q \leq q_c \), we have continuous (second-order) phase transition which is the case for the Ising model in both two and three dimensions while for \( q > q_c \) it is first-order. However, it is known that even for \( q = 3 \) in three dimensions, it is still only weakly first-order. Our results confirm this behavior based on the observation that we cannot fit to the first-order ansatz well. The strength of the first-order transitions, measured by their latent heat, increases with \( q \) and our result corroborates this behavior.

The outline of the paper is as follows. In Sec. 2, we introduce the model and write down the tensor formulation in terms of triads. Then in Sec. 3, we start by checking some old results for \( q = 3 \) obtained using HOTRG about eight years ago and for \( q = 10 \) obtained using Monte Carlo methods. Then we present new results for \( 10 < q \leq 20 \). This is summarized in Fig. 1. We end the paper with a brief summary and future directions by mentioning how the triad approximation still needs to be improved to accurately compute critical exponents in Sec. 4. It is clear from our work that though it fairly accurately computes potentials and can locate the critical temperatures, it does not capture the correct fixed-point tensor behaviour around the critical points.

\textsuperscript{1}As noted in Ref. [14], Potts actually defined two separate models. The first was the \( \mathbb{Z}_N \) model and assumed that at each site of a lattice there was a two-dimensional vector that could point in one of the \( N \) equally spaced directions where the vectors interact with an energy proportional to their dot product. The second was the model which was defined on any graph and with edges joining pair of sites.
Figure 1. The critical temperature for $q$-state Potts model in three dimensions calculated using Monte Carlo methods. However, even after seventy years since this model was introduced, nothing is known for $q > 10$. The main purpose of this paper is to fill this gap. The results we obtain are given in Table 1. It remains an open problem to find an expression for $T_c(q)$ for this model.

SECTION 2
Formulation and Observables

2.1 $q$-state Potts model

We consider the $q$-state Potts model with the Hamiltonian given by:

$$H = -J \sum_{\langle ij \rangle} \delta(\sigma_i, \sigma_j), \quad (2.1)$$

where $J$ is the coupling which we set equal to one, $\sigma_i = 1, \cdots, q$ and $\langle ij \rangle$ are the nearest neighbours on a cubic lattice. The partition function is given by:

$$Z = \sum_{\{\sigma_i\}} \prod_{\langle ij \rangle} \exp \left[ \beta \delta(\sigma_i, \sigma_j) \right], \quad (2.2)$$

where $\beta$ is the inverse temperature. The tensor network approach is the representation of the path integral or partition function of a classical statistical system by a trace over some network. This can be schematically written as:

$$Z = \int D\phi \ e^{-S} = \sum_{\{\phi_i\}} \prod_{\phi_i} T_{\phi_i \phi_j \phi_k \phi_m \phi_n} \cdot \quad (2.3)$$

We can express this partition function as a tensor trace of network as:

$$Z = t \text{Tr} \left( \bigotimes T_{ijklmn} \right). \quad (2.4)$$
It is well-known that the exact evaluation of (2.4) is not possible and hence the goal is to approximate it to the best of our resources. The choice of different $T_{ijklmn}$ corresponds to different Lagrangian/partition function. This tensor description also gives rise to a renormalization group flow of tensor such that if we do it fairly accurately we obtain the correct fixed-point. However, complete removal of the short-distance correlations is difficult to achieve in practice and has so far not been worked out accurately in greater than two dimensions.

2.2 Tensor description of the model

We noted in the preceding subsection that the method of tensor networks approximates the partition function of a system as a tensor trace of some complicated network. In order to obtain this, we start by expressing the initial rank-six tensor in terms of triads and coarse-grain the system several times to reach the thermodynamic limit. There are several ways of constructing the initial tensor for this model [18, 19] and they are all equivalent. We use the simplest one which starts with the Boltzmann weight represented by a $q \times q$ real symmetric matrix $W$ defined as:

$$W_{ij} = \begin{cases} e^{\beta} & \text{if } i = j \\ 1 & \text{otherwise} \end{cases}.$$  \hfill (2.5)

To construct the four initial triads, we perform the factorization as below:

$$W = SDS^T = QQ^T, \quad \text{Cholesky}$$  \hfill (2.6)

and the triads as:

$$
\begin{align*}
A_{xya} &= Q_{ax}Q_{ay} \\
B_{azb} &= Q_{ab}Q_{az} \\
C_{bz'c} &= Q_{bc}Q_{bz'} \\
D_{cy'x'} &= Q_{cy'}Q_{cx'}.
\end{align*}$$  \hfill (2.7)

The local tensor is defined in the usual way: $T_{xx'y'y'zz'} = A_{xya}B_{azb}C_{bz'c}D_{cy'x'}$. In fact, for the Potts model, we never need to explicitly construct $T$ at any stage. We also note that while the fundamental initial tensor $T$ is unique for a given model, the triads can be different based on the way we have chosen to decompose the tensor. The optimum choice of triads for more complicated models remains an open problem.

2.3 Thermodynamic potentials using tensors

The tensor network coarse-graining procedure provides an accurate evaluation of the partition function. Using this, we can compute the free energy, internal energy, and their derivatives. In order to accurately compute the critical temperature corresponding to the first-order phase transitions, we compute the internal energy by doing a finite-difference of the logarithm of
Figure 2. We outline the main steps of the triad method starting with the triads constructed from the Boltzmann weights. At the end of step (a), we have $2d - 2$ triads for a $d$-dimensional system. In the step (b1), we combine four copies of each triad only keeping four $x$ legs and contracting over all others. Similarly, in the step (b2) which is not shown, we combine them to keep four $y$ legs. The dashed color lines show the contraction along a particular direction. In step (c1), we fuse these four indices into two to get a matrix and perform SVD to get the projector $U$. Similarly, step (b2) followed by (c2) will give the projector $V$. Once we have $U, V$, we can take two copies of four triads and combine them with projectors as shown in step (d). In the next step, we can get the transformed triad after performing contractions where the order $x, y, z$ is changed to $z, x, y$. This means that we have effectively carried out the blocking in the plane orthogonal to $z$-direction. We perform the steps (a-e) two more times to do blocking along two other planes and this constitutes one full step with lattice volume increasing by eight times.
partition function and then fit the data using a four-parameter sigmoidal ansatz to determine
the critical temperature. The free energy density is computed as follows:

\[ f = -\frac{T}{V} \ln Z, \]  

(2.8)

which in tensor notation can be computed by using the tensor norm at each step of coarse-
graining. In every coarse-graining step, we normalize the tensor by the maximum element of
that tensor (which we call ‘norm’). We can then calculate the free energy density \( f \) from
these normalization factors as:

\[ f = -\frac{1}{\beta} \left( \sum_{i=1}^{N} \frac{\log(\text{norm}_i)}{2^i} + \frac{\log(Z_N)}{2^N} \right) = -\frac{1}{\beta 2^N} \left( \sum_{i=1}^{N} \log(\text{norm}_i) 2^{N - i} + \log Z_N \right), \]  

(2.9)

where \( Z_N \) is the scalar calculated from the tensor contraction after the last step of coarse-
graining and \( 2^N \) is the lattice volume and \( N \) is the number of times we do coarse-graining (i.e.,
number of times we do step \( (a) \) through step \( (e) \) of Fig. 2). In this paper, we have usually
considered \( N = 24 \). The internal energy density \( E \) is defined as:

\[ E = \frac{T^2}{V} \frac{\partial \ln Z}{\partial T}, \]  

(2.10)

and we compute it by taking the numerical derivative of \( Z \) obtained from tensor contraction.

SECTION 3

Results

3.1 \( q = 3 \) and 10 - Comparison to old results

The \( q = 3 \) case has been well-studied and we use this as a check of our computations. The
extensive explorations of this model have made it clear that this case has a weak first-order
transition and the result obtained from most recent Monte Carlo is \( T_c = 1.81632(6) \). In the
past decade, tensor network methods were only used for \( q = 3 \) Potts model. For this case, it
was found in Ref. [9] that \( T_c = 1.8166(5) \) using the HOTRG method. Using triads, we compute
the location of phase transition to be \( T_c = 1.8175(15) \) as seen in Fig. 3. We found that the
determination of the critical temperature for \( q = 3 \) is harder than that for large \( q \). This can be
seen in Fig. 3 where it is not possible to fit using our ansatz. We attribute this issue to the fact
that for \( q = 3 \), the transition is only weakly first-order. As the transition becomes strongly
first-order with increasing \( q \), tensor approximation method we have used works effectively to
locate the critical temperature. Though the tensor network methods were not used beyond
\( q = 3 \) until this work, the model was well-studied using Monte Carlo starting already in 1970s\(^2\)
up to \( q = 6 \) and we refer the reader to the old literature in Table II of Ref. [15] but the most
recent extensive study of this model was carried out in Ref. [21] for \( 3 \leq q \leq 10 \) where critical
temperatures and thermodynamic observables were computed. The most precise MC result

\( ^2 \text{Ref. [20]}, \) was one of the earliest papers studying \( q = 3 \)
Figure 3. The dependence of $q = 3$ internal energy on bond dimension $D$ and lattice volume. The critical temperature is found to be $T_c = 1.8175(15)$.

i.e., $T_c = 1.816316(33)$ for $q = 3$ was obtained using some new techniques in Ref. [22]. For the $q = 10$ model, the MC result locate $T_c$ to be 1.13446(4) [21]. Our results are in slight disagreement and we obtain $T_c = 1.1328(10)$ and is shown in bottom right panel of Fig. 6. It is not clear whether this is because of the small volume considered for $q = 10$ in Ref. [21] or because of the finite-$D$ effect of our tensor computations. We have found no other work to compare for this case and hence it would be desirable to resolve this in the future.

3.2 $q > 10$ - New results

The previous subsection provides a reasonable check of the procedure we implemented using the triads. In this subsection, we discuss new results for Potts model with $10 < q < 20$. Though this method can be effectively used to explore the large $q$ limit, we have left that for future work. For each $q$, we studied the thermodynamic potentials as shown in Fig. 5 and Fig. 4 respectively. The fit to the internal energy using an ansatz gives a precise determination of the critical temperature. We collect the results for $10 < q \leq 20$ in Table 1. We used the tensor contraction package opt_einsum [23] for this work. In order to obtain the results of this paper we make the notebook available for the reader\(^3\). We find that the computational cost is $O(D^p)$ where we obtained $p = 6.18(8)$ for the $q$-state Potts model with $q = 10$ and 6.04(8) for the cubic lattice Ising model. In our computations, we used the standard SVD and not randomized SVD (RSVD) as was done in the original triad prescription. For lattice volume of $256^3$ with $D = 70$, the computation for a single temperature took about 11 hours while for the same $D$ and volume of $1024^3$, it took about 14 hours on a modern laptop. This

\(^3\)https://github.com/rgjha/TensorCodes/blob/master/3d/qPotts.ipynb

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Figure 4. We show the free energy density with temperature for $q = 11, 12, 15, 16, 17, 18$. The data is obtained with $D = 70$ on a $256^3$ lattice.

is another advantage of tensor methods: the approach to thermodynamic limit is much faster than in other numerical methods.

### 3.3 Fixed-point analysis

One of the main goals of the tensor renormalization group approach is to obtain the correct fixed-point tensor. This is easier said than done and though it might be possible to achieve this reasonably accurately in two dimensions with the developments over the past decade, the same cannot be said for three dimensions. In order to visualize this fixed-point (FP) tensor more closely in different phases and across a phase transition it was noticed that one
Figure 5. We show the internal energy for $q = 11, 12, 15, 16, 17, 18$ with temperature. The red dashed lines represent the ansatz we used to determine the critical temperature. The data is obtained with $D = 70$ on a $256^3$ lattice.

One of the easiest ways is to compute a specific observable which we have referred to as $X$. This observable is invariant under the change of scale of the tensor i.e., $T \rightarrow \lambda T$. This quantity is computed from a fixed-point tensor as:

$$X = \frac{\langle \text{Tr } T \rangle^2}{\text{Tr}(T \cdot T)}, \quad (3.1)$$

where $T = B_{abj} C_{bjg} D_{gfi} A_{ipa}$ is a $D \times D$ matrix which is a good approximation to the FP tensor. After carrying out a sufficient number of coarse-graining steps, when the initial tensor has presumably flowed to the fixed-point tensor $T^* = T$, this observable would have converged to an integer depending on the phase of the system. In the low-temperature symmetry breaking...
| $q$ | $T_c$       |
|-----|------------|
| 11  | 1.0998(10) |
| 12  | 1.0705(10) |
| 13  | 1.0450(10) |
| 14  | 1.0226(10) |
| 15  | 1.0016(10) |
| 16  | 0.9834(10) |
| 17  | 0.9669(10) |
| 18  | 0.9508(10) |
| 19  | 0.9371(10) |
| 20  | 0.9246(10) |

Table 1. We summarize the results for the critical temperatures obtained in this paper for $10 < q \leq 20$ state Potts model.

phase, the degeneracy is $q$ while for high-temperature ($T > T_c$) it is one. There is also an additional advantage of this - it is a bonafide candidate for determining the critical temperature for the phase transition. Usually, one computes the derivatives of logarithm of partition function or magnetic susceptibility for these determinations, which are usually prone to errors in tensor methods\(^5\), but computing $X$ is straightforward. It was in this manner that the tensor methods were used to compute the critical temperature for $q = 3$ in Ref. [9] on a cubic lattice. However, we find that the tensor approximation method we use in this work is not able to capture this fixed-point tensor very accurately and also the convergence with lattice volume and bond dimensions ($D$) is erratic. It would be interesting to explore this in more detail and to check if $X$ can be reliably computed for $q \geq 4$ Potts model in three dimensions. To explore this issue in more detail using the triad method, we studied the Ising model in the vicinity of the well-known critical temperature known through earlier numerical investigations. The most precise result corresponds to a continuous transition at $T_c = 4.51152469(1)$ for cubic lattice. The RG analysis shows that in the high-temperature phase i.e., $T \gg T_c$, the observable defined in (3.1) must equal 1 and in the low-temperature phase, it should be $q$ i.e., 2 and it should change values at $T = T_c$. The triad method on a $256^3$ lattice shows the change of $X$ happens between $4.5121 \leq T \leq 4.5122$ with $D = 73$ which is different from the numerical result in the literature. This is a sign that the triad method does not correctly capture the FP behaviour with $D = 73$. The existing methods usually compute the free energy at $T = T_c$ and find convergence to some value but since there is no exact result for the three-dimensional Ising model yet, this determination cannot be considered rigorous. Rather, we argue that computing $X$ is better to test their effectiveness around the critical point. In this sense, the convergence

\(^3\)In this work, we use $T$ for both the tensor with six indices and temperature. We hope this distinction is more than obvious from the context.

\(^5\)Though there have been some progress recently with automatic differentiation [24] which reduces a lot of time and makes these computations faster.
of free energy is a red herring for concluding whether correct fixed-point behaviour is obtained in a given tensor network renormalization scheme.

SECTION 4
Discussion and Summary

One of the motivations of this work was to understand how the critical temperature changes with \( q \) for three-dimensional Potts models on a cubic lattice. In two dimensions, the critical temperature for a \( q \)-state model can be obtained analytically, however, no such relation is yet known for the three-dimensional model. We studied the three-dimensional model on a cubic lattice and obtained critical temperatures for different \( q \). Since there are already existing results for \( q \leq 10 \), we focused on the unexplored region: \( q > 10 \). Our results fill an important gap in the literature and further clarifies that the gap i.e., \( T_c(q) - T_c(q-1) \) decreases with \( q \). We find that it is comparatively difficult to resolve the transition for \( q = 3 \) which we attribute to it being weakly first-order which is clear from the variation of internal energy with temperature close to the critical value. For larger \( q \), we find it straightforward to fit a sigmoid-shape ansatz and for all \( q > 3 \) see a strong signal of a first-order transition. To our knowledge, this work is the first known example where tensor renormalization methods have obtained results for a spin model where no other numerical methods have been applied. We envisage that further numerical studies of the Potts model with \( q \geq 10 \) will be done in coming years though one needs to properly control the slowing down close to the first-order critical point which becomes stronger with increasing \( q \). The second issue we addressed in the paper is the reliability of the triad approximation method to obtain the fixed-point tensor. A rigorous study of RG transformations for tensor networks in the vicinity of a critical point is still an open problem. It would be very interesting to compute critical exponents for the three-dimensional Ising model, however, we expect that the local correlations which are not very well-controlled in the triad method would first need to be addressed. There are various prescriptions for removing these but they are not yet practical in three Euclidean dimensions. A refined tensor algorithm with improved fixed-point behaviour and reasonable time complexity would be pathbreaking. It would be interesting to see if the idea of triads can be combined with additional transformations like the ‘disentanglers’ to achieve a proper RG map. We leave these questions and many more for future explorations.

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Appendices

A.1 Convergence of $Z$ and internal energy dependence on $D$ for $q = 10$

In a tensor network computation, it is crucial to understand how the finite bond dimension affects the convergence of the partition function or the free energy. This convergence is a sign of how efficiently the algorithm works in practice. In cases where exact solution is available, we can compute precisely how much it deviates from the expected result. For example, it is well-known that for two-dimensional Ising model, this convergence is slowest around and at the critical temperature. For the $q$-state Potts model, we monitored the convergence for two temperatures below and around $T_c$. Though the convergence is slow for the latter, we find that $D = 70$ is a reasonable bond dimension to obtain reliable results. We show the result in Fig. 6. We also studied the effect of the truncation of singular values at each coarse-graining step ($D$) on observables we compute. To understand this dependence, we studied $D = 40, 50, 60, 70$ for fixed $q = 10$. The results are shown in Fig. 7 where the internal energy is shown for different $D$. We see that there are some fluctuations for small $D$ which improves as we increase $D$ to 70.

A.2 Volume dependence of internal energy for $q = 15$

In the previous subsection, we saw the effect of finite bond dimensions. Here, we see the finite-size effects for a fixed $D = 70$. In order to understand the finite-size effects, we compared the results obtained for different lattice volumes by fixing to $q = 15$. The results obtained from $16^3, 32^3, 256^3, 1024^3$ are shown in Fig. 8. We find that the effects are small and ascer-
tain that results we have obtained on a fixed lattice of $256^3$ can be correctly interpreted as thermodynamic limit.

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Figure 8. The internal energy dependence on lattice volume for $q = 15$ Potts model is shown for fixed $D = 70$ for $16^3$ (triangle), $32^3$ (square), $256^3$ (circle), and $1024^3$ (star) lattice volumes.

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