

# Gauge invariance in a $\mathbb{Z}_2$ hamiltonian lattice gauge theory

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We propose an efficient variational method for  $Z_2$  lattice gauge theory based on the matrix product ansatz. The method is applied to ladder and square lattices. The Gauss law needs to be imposed on quantum states to guarantee gauge invariance when one studies gauge theory in hamiltonian formalism. On the ladder lattice, we identify gauge invariant low-lying states by evaluating expectation values of the Gauss law operator after numerical diagonalization of the gauge hamiltonian. On the square lattice, the second order phase transition is well reproduced.

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# 1. Introduction

The importance of the first-principle study in quantum chromodynamics is increasing largely because RHIC experiment has started and LHC is also coming. For precise description of high-energy heavy ion collisions, gauge theory needs to be studied at finite temperature and density in a systematic way. Ideally, we should also have a methodology for tracing time-evolution of quantum states based on the Schrödinger equation because heavy ion collisions should be treated as non-equilibrium evolving systems rather than static. Lattice gauge theory is the most useful method for studying the quark-gluon systems at zero and finite temperature. However, Monte Carlo integration does not work for lattice gauge theory with large chemical potential because of the severe sign problem. It would be worthwhile to pursue a systematic variational approach to gauge theory. In the previous works, the matrix product ansatz has been applied to hamiltonian lattice gauge theory on a spatial ladder lattice [1, 2].

The matrix product ansatz [3] is a simplified version of DMRG (density matrix renormalization group) [4, 5]. DMRG has been developed as the method that gives the most accurate results for spin and fermion chain models such as one-dimensional quantum Heisenberg and Hubbard models at zero and finite temperature [7]. <sup>1</sup> DMRG is also useful for diagonalization of transfer matrices in two-dimensional classical statistical systems [8]. DMRG has been extended to two-dimensional quantum systems [9] and can work for bosonic degrees of freedom [5].

Lattice gauge hamiltonian is obtained by choosing temporal gauge in partition function of Euclidean lattice gauge theory. In hamiltonian formalism, gauge invariance needs to be maintained explicitly by imposing the Gauss law on the Hilbert space. On the other hand, Euclidean lattice gauge theory can keep gauge invariance manifestly by construction. This is one of the reasons why hamiltonian version of lattice gauge theory is not popular. In addition, no systematic methods had been known for diagonalization of gauge hamiltonian before the matrix product ansatz was applied to lattice gauge theory in ref. [1]. If trial wavefunction is constrained directly with the Gauss law, the advantage of the matrix product ansatz is completely spoiled because calculation of energy function becomes impossible in a practical sense. If the hamiltonian is diagonalized without the Gauss law, all possible states are obtained including gauge variant states. However, it must be possible to extract gauge invariant states because all eigenstates of the hamiltonian can be classified using generators of the considered gauge group. Therefore, if the matrix product ansatz is used, we better start from the whole Hilbert space and then identify gauge invariant states using the Gauss law operator after all calculations.

# 2. Quantum hamiltonian in the $Z_2$ lattice gauge theory

We are interested in quantum hamiltonian of the  $Z_2$  lattice gauge theory. Statistical mechanics and quantum hamiltonian are connected through the transfer matrix formalism. The quantum hamiltonian is obtained by choosing temporal gauge in the partition function [10]

$$H = -\sum_{n,i} \sigma_{x}(n,i) - \lambda \sum_{n,i,j} P(n,i,j), \qquad (2.1)$$

<sup>&</sup>lt;sup>1</sup>By "d-dimensional", we mean (1+d)-dimensional spacetime.

where  $\sigma_x$  and  $\sigma_z$  are Pauli matrices and P is a plaquette operator. In eq. (2.1), the first and second summations are taken on the spatial lattice for all possible link and plaquette operators, respectively. In general, arbitrary states can be represented as a superposition of products of  $|\pm\rangle_{n,i}$ , where  $\sigma_z(n,i)|\pm\rangle_{n,i}=\pm|\pm\rangle_{n,i}$ .

Let us introduce time-independent operators G(n), each of which flips spins on all the links emerging from a site n

$$G(n) = \prod_{i} \sigma_{x}(n, i). \tag{2.2}$$

The operator G(n) defines local gauge transformation  $G(n)^{-1}HG(n) = H$ . In order for physical quantities to be gauge invariant, quantum states need to be invariant under gauge transformation

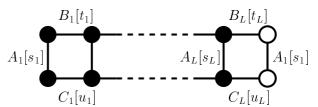
$$G(n)|\Psi\rangle = |\Psi\rangle.$$
 (2.3)

We need to impose the Gauss law (2.3) on the wavefunction to keep gauge invariance. Otherwise, unphysical states may be obtained because gauge invariance is not guaranteed.

### 3. Matrix product ansatz on a ladder lattice

Since this work is the first application of the matrix product ansatz to  $Z_2$  gauge theory, we would like to consider a simple model. The simplest one is a  $Z_2$  hamiltonian lattice gauge theory on a spatial ladder lattice (see figure 1). We assume periodicity in the horizontal direction on the ladder for later convenience. In figure 1, periodicity is denoted with the open circles.

The  $Z_2$  lattice gauge model has only link variables. In our construction, each link is assigned a different set of matrices  $A_n$ ,  $B_n$ , and  $C_n$  for parameterization of wavefunction (see figure 1). The index n represents the n-th square on the ladder chain and runs from 1 to L. The dimension of the matrices is M. Our matrix product state is give by



**Figure 1:** A spatial ladder chain with lattice size *L*. The open circles indicate periodicity. The link variables are dynamical. Different sets of matrices are assigned to links.

$$|\Psi\rangle = \operatorname{tr}\left(\prod_{n=1}^{L} \sum_{s_n=\pm} \sum_{t_n=\pm} \sum_{u_n=\pm} A_n[s_n] B_n[t_n] C_n[u_n] |s_n\rangle_n |t_n\rangle_n |u_n\rangle_n\right),\tag{3.1}$$

where the matrices are multiplied in ascending order keeping the order of  $A_nB_nC_n$ , and the basis states  $|s\rangle_n$ ,  $|t\rangle_n$ , and  $|u\rangle_n$  are eigenstates of the spin operator  $\sigma_z$ . In this expression, the variables s, t, and u are used to denote the position of the links. The implementation of the matrix product ansatz means that a ladder lattice has been represented as a one-dimensional system with non-nearest neighbor interactions. Gauge invariance of matrix product states will be discussed in the next section.

If we require orthogonality of optimum basis states according to ref. [3], we have

$$\sum_{j=1}^{M} \sum_{s=\pm} (X_n[s])_{ij} (X_n[s])_{i'j} = \delta_{ii'}, \quad \sum_{i=1}^{M} \sum_{s=\pm} (X_n[s])_{ij} (X_n[s])_{ij'} = \delta_{jj'}, \tag{3.2}$$

where X stands for A, B, and C. If these conditions are not imposed, norm of the matrix product state (3.1) may becomes very small, which results in numerical instability.

Energy

$$E = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle},\tag{3.3}$$

is a function of the matrices  $A_n[s]$ ,  $B_n[t]$ , and  $C_n[u]$ . The numerator and denominator can be calculated by evaluating trace of a product of 3L matrices numerically.

The minimum of the energy function (3.3) corresponds to the ground state, which can be obtained based on matrix diagonalization as explained below. We can reduce the minimization problem (3.3) into a generalized eigenvalue problem [6]

$$v^{\dagger} \bar{H} v = E v^{\dagger} N v, \tag{3.4}$$

where  $\bar{H}$  and N are  $2M^2$  by  $2M^2$  matrices. To understand what is going here, let us consider how energy can be minimized by varying  $A_n[s]$  when other matrices are fixed. Note that the hamiltonian and norm matrices are bilinear of the matrix  $A_n[s]$ 

$$\langle \Psi | H | \Psi \rangle = \sum_{i,j,k,l} \sum_{s,t} (A_n^*[s])_{ij} \bar{H}_{(i,j,s),(k,l,t)} (A_n[t])_{kl}, \tag{3.5}$$

$$\langle \Psi | H | \Psi \rangle = \sum_{i,j,k,l} \sum_{s,t} (A_n^*[s])_{ij} \bar{H}_{(i,j,s),(k,l,t)} (A_n[t])_{kl},$$

$$\langle \Psi | \Psi \rangle = \sum_{i,j,k,l} \sum_{s,t} (A_n^*[s])_{ij} N_{(i,j,s),(k,l,t)} (A_n[t])_{kl},$$
(3.5)

where the matrix N is diagonal for the indices s and t. Once these expressions are obtained and the variational parameters  $A_n[s]$  are regarded as a vector v, the minimization problem (3.3) reduces to (3.4).

#### 4. Numerical results

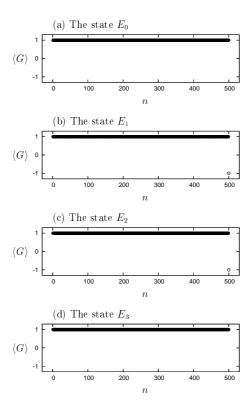
The matrix product ansatz assumes large lattice. Our lattice size L = 500 is sufficiently large. We solve the generalized eigenvalue problem (3.4) using LAPACK. For steady states, real matrices are sufficient for parameterizing the matrix product state (3.1). Convergence of energy needs to be checked for the number of sweeps and the matrix dimension M. Energy density E/L converges in accuracy of five digits or higher after two sweeps when the matrix size M is fixed.

Table 1 shows energy spectra of six low-lying states for three values of the coupling constant:  $\lambda = 0.1, 1$ , and 10. The sweep process has been repeated twice. In this model, convergence of energy is very fast in contrast to Heisenberg chains [1][3]. Small matrix dimension is sufficient for good convergence. Since we have obtained low-lying states without imposing the Gauss law on the variational space, gauge variant states are contained. In table 1, gauge invariant states are denoted with underlines. The other states are gauge variant. As we will see, gauge invariant physical states can be identified by calculating expectation values of the Gauss law operator.

In the ladder chain model, the Gauss law operator G(n) is a product of three  $\sigma_z$  operators (two horizontal and one vertical). We evaluate expectation values of G(n) on the upper lattice sites shown in figure 1. Then, the number of the Gauss law operators to be evaluated is L. Expectation values on the lower sites are same as the upper ones because of reflection symmetry. Figures 2 plots expectation values of the Gauss law operator  $\langle G(n) \rangle$  in the case of  $\lambda = 10$  for the states (a)  $E_0$ , (b)

M	$E_0/L$	$E_1/L$	$E_2/L$	$E_3/L$	$E_4/L$	$E_5/L$
$\lambda = 0.1$						
2	-3.001	-2.997	-2.997	-2.997	-2.993	-2.993
3	-3.001	-2.997	-2.997	-2.997	-2.994	-2.993
4	-3.001	-2.997	-2.997	-2.997	-2.997	-2.995
$\lambda = 1$						
2	-3.124	-3.121	-3.121	-3.118	-3.114	-3.112
3	-3.124	-3.121	-3.121	-3.118	-3.114	-3.112
4	-3.124	-3.121	-3.121	-3.118	-3.114	-3.112
$\lambda = 10$						
2	-10.27	-10.27	-10.27	-10.27	-10.23	-10.23
3	-10.27	-10.27	-10.27	-10.27	-10.26	-10.23
4	-10.27	-10.27	-10.27	-10.27	-10.26	-10.23

**Table 1:** Energy density E/L of six low-lying states is listed for  $\lambda = 0.1, 1$ , and 10 when lattice size is L = 500. Good convergence of energy is obtained with small M.



**Figure 2:** Expectation values of the Gauss law operator is plotted for the four low-lying states (a)  $E_0$ , (b)  $E_1$ , (c)  $E_2$ , and (d)  $E_3$  with  $\lambda = 10$ , L = 500, and M = 4. The circles are the calculated values. The states (a) and (d) are gauge invariant because the Gauss law is satisfied on every lattice sites. On the other hand, the states (b) and (c) are gauge variant because  $\langle G(500) \rangle = -1$ . These statements hold in accuracy of seven digits or higher.

 $E_1$ , (c)  $E_2$ , and (d)  $E_3$ . In figures 2 (a) and (d), the Gauss law G(n)=1 is satisfied uniformly on every lattice sites. Therefore, the obtained states  $E_0$  and  $E_3$  are gauge invariant. On the other hand, in figures 2 (b) and (c), the states  $E_1$  and  $E_2$  are gauge variant because gauge symmetry is definitely broken at the site n=500. The position of this special lattice site depends on where the sweep process ends. The relation  $\langle G(n) \rangle = 1$  or -1 holds for the obtained low-lying states in accuracy of seven digits or higher when M=4. In this way, we can classify the obtained states into gauge invariant states and others.

#### 5. Extension to square lattice

We apply the matrix product ansatz to (2+1)-dimensional  $Z_2$  lattice gauge theory on a square lattice, which has a second order phase transition. It is possible to solve the model in the same way as before without imposing the Gauss law on a variational space. However, we solve the Gauss law analytically to reduce calculation load. As a result, the model is equivalent to the transverse field Ising model. The square lattice is organized into one-dimensional lattice so that the matrix product ansatz can be applied. The non-local interactions can be handled by increasing the dimension of the matrix size. The matrix size used for the calculation is M=30. The obtained value of the critical coupling is  $\lambda_c \sim 3.12$ , which is close to the past numerical results. However, our lattice size L=12 is still small. Further refinement will be given elsewhere.

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