Matrix product representation of gauge invariant states in a $Z_2$ lattice gauge theory

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Abstract: The Gauss law needs to be imposed on quantum states to guarantee gauge invariance when one studies gauge theory in hamiltonian formalism. In this work, we propose an efficient variational method based on the matrix product ansatz for a $Z_2$ lattice gauge theory on a spatial ladder chain. Gauge invariant low-lying states are identified by evaluating expectation values of the Gauss law operator after numerical diagonalization of the gauge hamiltonian.

Keywords: Renormalization Group, Lattice Gauge Field Theory, Gauge Symmetry
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 \cite{1, 2, 3, 4, 5}. In this paper, we apply the matrix product ansatz to a $Z_2$ Hamiltonian lattice gauge theory on a spatial ladder lattice based on the previous work in a U(1) lattice gauge theory \cite{6}.

The matrix product ansatz \cite{7} is a variational method that originates in DMRG (density matrix renormalization group) \cite{8, 9, 10}. 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 \cite{1, 2, 3}. DMRG is also useful for diagonalization of transfer matrices in two-dimensional classical statistical systems \cite{11}. DMRG has been extended to two-dimensional quantum systems \cite{12, 13} and can work for bosonic degrees of freedom \cite{14}. Since DMRG is a variational method based on diagonalization of Hamiltonian and transfer matrices, it is free from the sign problem. Actually, DMRG has been successful in accurate study of $\theta$-vacuum in the

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\footnote{By “$d$-dimensional”, we mean $(1 + d)$-dimensional spacetime.}
massive Schwinger model [18]. There is an old prediction by S. Coleman that quarks decon- 
fine at $\theta = \pi$ [19]. However, the model has not been analyzed accurately with the Monte 
Carlo method because the topological terms give complex action in the Euclidean theory.

The matrix product ansatz is a result of large simplification of trial wavefunction based 
on the knowledge established in the past DMRG studies. Therefore, the ansatz takes over 
the good points of DMRG. Besides, the matrix product ansatz has advantage to DMRG 
because the former can treat periodic one-dimensional systems accurately [21]. Recent 
interesting progress of the matrix product ansatz is its application to non-equilibrium 
quanta physics and quantum information theory [21]. The matrix product ansatz is a 
promising approach to further refinement and extension of the past DMRG studies.

In general, calculation of expectation values of hamiltonian becomes difficult exponen-
tially as the system size increases. If the matrix product ansatz is introduced, the energy 
function has a simple matrix product form, which can be evaluated easily using a computer if the matrix size is small. It is expected that exponentially difficult problems are reduced into small tractable ones by the matrix product ansatz. Actually, the ansatz has 
been successful in giving accurate results in many one-dimensional quantum systems, where 
calculation errors can be controlled systematically. We can say that the matrix product 
ansatz is a first-principle variational method.

Lattice gauge hamiltonian is obtained by choosing temporal gauge in partition function 
of Euclidean lattice gauge theory [22]. In hamiltonian formalism, gauge invariance needs 
to be maintained explicitly by imposing the Gauss law on the Hilbert space. It is a 
hard task to construct gauge-singlet variational space for general gauge group [23]. 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. [3]. 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.

In hamiltonian lattice gauge theory, the dimension of spatial lattice needs to be two or 
larger because the plaquette operator is a two-dimensional object. In this paper, we study 
a $Z_2$ lattice gauge theory on a spatial ladder chain for simplicity. The length of the chain 
needs to be sufficiently long for the matrix product ansatz to work well. The ladder chain 
is squashed into a chain because one-dimensional structure needs to be found in order to 
use the matrix product ansatz.

In the previous work [3], we have studied one- and two-dimensional $S = 1/2$ Heisenberg 
models and a U(1) lattice gauge theory on a ladder chain using the matrix product ansatz 
in a similar way, where energy function is minimized using the Powell method. When the
number of parameters is very large, such naive minimization is not useful because it takes long time to reach the bottom of the energy function. In this work, we use a diagonalization method introduced in ref. [20] to obtain sufficient accuracy.

This paper is organized as follows. In section 2, hamiltonian lattice formulation of the $Z_2$ lattice gauge theory is briefly reviewed. In section 3, the matrix product ansatz is introduced and applied to a $Z_2$ lattice gauge hamiltonian. In the original construction, the matrix product states is assumed to have translational invariance. In this work, that condition is not imposed on variational space before diagonalization of the gauge hamiltonian. In section 4, numerical results are given. Section 5 is devoted to summary.

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

We are going to introduce the $Z_2$ lattice gauge theory, which was invented by F. Wegner [24]. As seen in the literature, the simplicity of the model is useful for testing a new idea [25, 26]. The model cannot have non-vanishing magnetization because local gauge symmetry cannot break spontaneously, which is known as the Elitzur’s theorem [27]. However, the model can have nontrivial phases depending on dimensionality.

We are interested in quantum hamiltonian of the model. Statistical mechanics and quantum hamiltonian are connected through the transfer matrix formalism. In the $Z_2$ lattice gauge theory, quantum hamiltonian is obtained by choosing temporal gauge in the partition function [28]

$$H = -\sum_{n,i} \sigma_x(n, i) - \lambda \sum_{n,i,j} P(n, i, j), \quad (2.1)$$

where $\sigma_x$ and $\sigma_z$ are spin operators

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

and $P$ is a plaquette operator

$$P(n, i, j) \equiv \sigma_z(n, i)\sigma_z(n + i, j)\sigma_z(n + i + j, -i)\sigma_z(n + j, -i). \quad (2.2)$$

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 $|\pm\rangle_{n,i}$, which are eigenstates of the spin operator $\sigma_z(n, i)$

$$\sigma_z(n, i)|\pm\rangle_{n,i} = \pm|\pm\rangle_{n,i}.$$

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

$$G(n) = \prod_{\pm i} \sigma_x(n, i). \quad (2.3)$$

We have

$$G^{-1}(n)\sigma_x(m, i)G(n) = \sigma_x(m, i),$$
$$G^{-1}(n)\sigma_z(n, i)G(n) = -\sigma_z(n, i),$$
$$G^{-1}(n)\sigma_z(m, i)G(n) = \sigma_z(m, i),$$
where the last formula applies only if the link \((m, i)\) is not contained in \(G(n)\). The operator \(G(n)\) defines local gauge transformation

\[
G(n)^{-1}HG(n) = H. \tag{2.4}
\]

In order for physical quantities to be gauge invariant, quantum states need to be invariant under gauge transformation

\[
G(n)|\Psi\rangle = |\Psi\rangle. \tag{2.5}
\]

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. When a state \(|\Psi\rangle\) satisfies the Gauss law \((2.3)\), magnetization vanishes because a relation \(\langle\Psi|\sigma_z(n)|\Psi\rangle = -\langle\Psi|\sigma_z(n)|\Psi\rangle\) holds.

3. Matrix product ansatz on a ladder lattice

We are going to introduce the matrix product ansatz, which is a variational method inspired from density matrix renormalization group (DMRG). DMRG is a variational method that can reproduces very accurate results in one-dimensional quantum systems \([8, 9, 17]\). In DMRG, wavefunction is represented as a product of orthogonal matrices because basis states are rotated for optimization with orthogonal matrices that diagonalize density matrices. The success of DMRG allows us to parametrize wavefunction as a product of finite-dimensional matrices from the beginning. This simplification of wavefunction is called the matrix product ansatz \([7]\). Although DMRG has slow convergence in one-dimensional quantum systems with periodic boundary conditions, the matrix product ansatz gives much better accuracy \([20]\).

![Figure 1: A spatial chain with lattice size \(L\). The open circles indicate periodicity. The site variables are dynamical. The same set of matrices \(A[s]\) is assigned to all the sites.](image)

In the original construction, the matrix product state is parametrized as follows \([7]\):

\[
|\Psi\rangle = \text{tr} \left( \prod_{n=1}^{L} \sum_{s_n} A[s_n]|s_n\rangle \right), \tag{3.1}
\]

where \(|\{s_n\}\rangle\) is a complete set of basis states for the \(n\)-th site (see figure \([1]\)). Hamiltonian needs to have periodicity for consistency with the trace operation in the variational state. As a result, energy becomes a function of the matrices \(A[s]\). The minimum of the energy function corresponds to the ground state. We are going to apply the ansatz to a \(Z_2\) gauge theory and see its compatibility with gauge symmetry.

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 2). We assume periodicity in the horizontal direction on the ladder for later convenience. In figure 2, periodicity is denoted with the open circles.

Figure 2: 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.

In the free case \( \lambda = 0 \), the hamiltonian (2.1) can be diagonalized analytically. The vacuum state is given by

\[
|\text{vac}\rangle = \prod_{n,i} \frac{1}{\sqrt{2}} (|+\rangle_{n,i} + |-\rangle_{n,i}).
\] (3.2)

Vacuum expectation values of the hamiltonian and plaquette operators are \( \langle H \rangle / L = -3 \) and \( \langle P \rangle = 0 \), respectively. In this case, one-dimensional matrices are sufficient to represent the vacuum state (3.2)

\[
A[+] = A[-] = \frac{1}{\sqrt{2}}.
\] (3.3)

When the coupling constant is very large \( \lambda \to \infty \), the first term of the hamiltonian (2.1) can be neglected. As a result, the hamiltonian has a diagonal form. The vacuum state is given by

\[
|\text{vac}\rangle = \frac{1}{\sqrt{2^{2L+1}}} \sum_{m=0}^{2L} G^{(m)} \prod_{n,i} |\pm\rangle_{n,i},
\] (3.4)

where the operator \( G^{(m)} \) represents a summation of all possible products that are composed of \( m \) pieces of different Gauss-law operators \( G \). The operator \( G^{(m)} \) has \( 2L C_m \) terms \( (G^{(0)} \equiv 1) \). In eq. (3.4), the two definitions are identical. Then, we have \( \langle H \rangle / L \to -\lambda \) and \( \langle P \rangle \to 1 \) in the limit \( \lambda \to \infty \). The states (3.2) and (3.4) are both gauge invariant, \( G^{(n)}|\text{vac}\rangle = |\text{vac}\rangle \).

The \( \mathbb{Z}_2 \) 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 parametrization of wavefunction (see figure 3). The index \( n \) represents the \( n \)-th square on the ladder chain and runs from 1 to \( L \). The dimension of the matrices is \( M \). Then, our matrix product state is

\[
|\Psi\rangle = \text{tr} \left( \prod_{n=1}^{L} \sum_{s_n=\pm} \sum_{t_n=\pm} \sum_{u_n=\pm} A_n[s_n]B_n[t_n]C_n[u_n] |s_n\rangle_n |t_n\rangle_n |u_n\rangle_n \right),
\] (3.5)

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 \( \sigma_z \) as before. In this
expression, the variables $s$, $t$, and $u$ are used instead of the index $i$ 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. [7], we have

$$
\sum_{j=1}^{M} \sum_{s=\pm}(X_n[s])_{ij}(X_n[s])_{i'j'} = \delta_{i'i'}, \quad \text{(3.6)}
$$

$$
\sum_{i=1}^{M} \sum_{s=\pm}(X_n[s])_{ij}(X_n[s])_{ij'} = \delta_{jj'}, \quad \text{(3.7)}
$$

where $X$ stands for $A, B,$ and $C$. If these conditions are not imposed, norm of the matrix product state (3.5) may becomes very small, which results in numerical instability.

Energy

$$
E = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle}, \quad \text{(3.8)}
$$

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:

$$
\langle \Psi | H | \Psi \rangle = -\sum_{n=1}^{L} \text{tr} \left( (a_n y_n z_n + x_n b_n z_n + x_n y_n c_n) \prod_{m=n+1 \text{ mod } L}^{n-1 \text{ mod } L} w_m + \lambda \alpha_n \beta_n \gamma_n \prod_{m=n+2 \text{ mod } L}^{n-1 \text{ mod } L} w_m \right), \quad \text{(3.9)}
$$

$$
\langle \Psi | \Psi \rangle = \text{tr} \left( \prod_{m=1}^{L} w_m \right), \quad \text{(3.10)}
$$

where

$$
a_n \equiv \sum_{s,s'} (\sigma_x)_{ss'} A_n^*[s] \otimes A_n[s'], \quad b_n \equiv \sum_{t,t'} (\sigma_x)_{tt'} B_n^*[t] \otimes B_n[t'], \quad c_n \equiv \sum_{u,u'} (\sigma_x)_{uu'} C_n^*[u] \otimes C_n[u'],
$$

$$
\alpha_n \equiv \sum_{s,s'} (\sigma_z)_{ss'} A_n^*[s] \otimes A_n[s'], \quad \beta_n \equiv \sum_{t,t'} (\sigma_z)_{tt'} B_n^*[t] \otimes B_n[t'], \quad \gamma_n \equiv \sum_{u,u'} (\sigma_z)_{uu'} C_n^*[u] \otimes C_n[u'],
$$

$$
x_n \equiv \sum_{s} A_n^*[s] \otimes A_n[s], \quad y_n \equiv \sum_{t} B_n^*[t] \otimes B_n[t], \quad z_n \equiv \sum_{u} C_n^*[u] \otimes C_n[u],
$$

$$
w_n \equiv x_n y_n z_n.
$$

The dimension of the matrices on the left hand side is $M^2$. By the outer product symbol $\otimes$, we mean

$$
a_{(i,k),(j,l)} = \sum_{s,s'} \sigma_{ss'} A_{ij}[s] A_{kl}[s'].
$$

The minimum of the energy function (3.8) corresponds to the ground state, which can be obtained based on matrix diagonalization as explained below. We can reduce the minimization problem (3.8) into a generalized eigenvalue problem [20]

$$
v^\dagger \hat{H} v = E v^\dagger N v, \quad \text{(3.11)}
$$
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 equations (3.9) and (3.10) are bilinear of the matrix $A_n[s]$

$$\langle \Psi | \bar{H} | \Psi \rangle = \sum_{i,j,k,l} \sum_{s,t} (A^*_n[s])_{ij} \bar{H}_{(i,j),s,(k,l),t} (A_n[t])_{kl}, \quad (3.12)$$

$$\langle \Psi | \Psi \rangle = \sum_{i,j,k,l} \sum_{s} (A^*_n[s])_{ij} N_{(i,j),s,(k,l),t} (A_n[t])_{kl}, \quad (3.13)$$

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 (3.8) reduces to (3.11).

There is one more trick that needs to be implemented. As explained in equations (3.6) and (3.7), we encounter numerical instability on the right hand side in eq. (3.11) if the above procedure is used as it is. This is because the matrix $N$ may have very small eigenvalues if the matrices $A_n[s]$, $B_n[s]$, and $C_n[s]$ are varied freely. For this reason, we need to impose one of the conditions (3.6) or (3.7) on the matrices.

A matrix can be decomposed into a product of three matrices, which is called singular value decomposition. For example, if we regard a tensor $A[s]$ as a matrix $A_{i,(j,s)} = (A[s])_{ij} = A_{IJ}$, singular value decomposition of $A_{IJ}$ is given by

$$A_{IJ} = \sum_{K=1}^{M} U_{IK} D_K V_{KJ}. \quad (3.14)$$

where $D_K$ are the singular values of the matrix $A_{IJ}$. The matrices $U$ and $V$ are orthonormal

$$\sum_{I=1}^{M} U^*_{IK} U_{IK'} = \delta_{KK'}, \quad \sum_{J=1}^{2M} V^*_{KJ} V_{K'J} = \delta_{KK'}. \quad (3.15)$$

The decomposition $A = U'V$, where $U' = UD$ is a square matrix, is the key of the trick. Consider a part of the matrix product wavefunction

$$C[u]A[s] = C'[u]A'[s], \quad (3.16)$$

where $(A'[s])_{ij} = V_{i,(j,s)}$ and $C'[u] = C[u]U'$. If the decomposition (3.14) is accurate, the both representations give the same result. Based on this trick, the eigenvalue problem (3.11) is solved successively for all the sets of the matrices starting from the right end in figure 3

$$C_L[u_L] \rightarrow B_L[t_L] \rightarrow A_L[s_L] \rightarrow \cdots \rightarrow C_1[u_1] \rightarrow B_1[t_1] \rightarrow A_1[s_1], \quad (3.17)$$

which we call sweep. In one sweep process, eq. (3.11) is solved $3L$ times. If this sweep process is repeated several times, energy of low-lying states converges to some value. Calculation error can be controlled systematically by increasing the matrix dimension $M$. See Appendix A for generation of initial matrices.
4. Numerical results

The matrix product ansatz assumes large lattice. Our lattice size $L = 500$ is sufficiently large. We solve the generalized eigenvalue problem (3.11) using LAPACK [30]. For steady states, real matrices are sufficient for parameterizing the matrix product state (3.5). 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.

\[
\begin{array}{ccccccc}
  M & E_0/L & E_1/L & E_2/L & E_3/L & E_4/L & E_5/L \\
  \lambda = 0.1 \\
  2 & -3.001 & -2.997 & -2.997 & -2.997 & -2.993 & -2.993 \\
  3 & -3.001 & -2.997 & -2.997 & -2.997 & -2.994 & -2.993 \\
  4 & -3.001 & -2.997 & -2.997 & -2.997 & -2.995 & & \\
  \lambda = 1 \\
  2 & -3.124 & -3.121 & -3.121 & -3.118 & -3.114 & -3.112 \\
  3 & -3.124 & -3.121 & -3.121 & -3.118 & -3.114 & -3.112 \\
  4 & -3.124 & -3.121 & -3.121 & -3.118 & -3.114 & -3.112 \\
  \lambda = 10 \\
  2 & -10.27 & -10.27 & -10.27 & -10.27 & -10.23 & -10.23 \\
  3 & -10.27 & -10.27 & -10.27 & -10.27 & -10.26 & -10.23 \\
  4 & -10.27 & -10.27 & -10.27 & -10.27 & -10.26 & -10.23 \\
\end{array}
\]

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 $M$.

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 [6][7]. 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 2. 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 3 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) $E_1$, (c) $E_2$, and (d) $E_3$. In figures 3 (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 3 (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
Figure 3: 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.

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 $M = 4$.

According to the Elizur’s theorem, gauge variant operators have vanishing expectation values. We have checked that expectation values of single spin operators $\sigma_z(n)$ vanish for the gauge invariant states in accuracy of ten digits or higher when $M = 4$. We also have checked that the gauge variant states have vanishing expectation values of $\sigma_z(n)$ in the same accuracy. These statements apply to the low-lying states shown in table 1.

In this way, we can classify the obtained states into gauge invariant states and others.
Figure 4: Vacuum energy density $E_0/L$ is plotted as a function of the coupling constant $\lambda$ with lattice size $L = 500$. The circles are the calculated values, which are consistent with the exact ones given in sec. 3.

In order to see how spatial distribution look like, we evaluate expectation values of the plaquette operator for the vacuum and the excited states. Figure 5 plots expectation values of the plaquette as functions of the spatial lattice coordinate $n$ for the gauge invariant low-lying states (a) $E_0$, (b) $E_3$, and (c) $E_5$ in the case of $\lambda = 10$. As expected, the vacuum state $E_0$ has complete uniformity. On the other hand, the excited states $E_3$ and $E_5$ have lumps around $n = 500$. The higher excited states have similar lumps around the boundary.

The obtained solutions have periodicity because the plaquette distributions are continuous around the boundary. The position of the lumps can be moved without changing energy in the sweep process as explained in figure 3. Figure 6 plots vacuum expectation values of the plaquette operator as a function of the coupling constant $\lambda$. For small and large $\lambda$, the tendency of energy and plaquette is consistent with the exact values given in section 3.

5. Summary

We have extracted gauge invariant physical states in a $Z_2$ hamiltonian lattice gauge theory on a spatial ladder chain. The calculations are based on the matrix product ansatz, which gives sufficiently convergent energy and wavefunction for low-lying states. In the future studies, similar calculations should be tested in higher dimensional lattice gauge theory including supersymmetric cases [31]. The proposed method will be useful especially for non-perturbative analysis of vacuum structure at the amplitude level.

Acknowledgments

The author would like to thank T. Nishino for useful communications. The numerical calculations were carried on the RIKEN RSCC system. This work has been partially supported by RIKEN BNL.
Figure 5: Vacuum expectation values of the plaquette operator are plotted for the gauge invariant states (a) $E_0$, (b) $E_3$, and (c) $E_5$ with $\lambda = 10$ and $L = 500$. The excited states (b) and (c) have non-uniformity around the boundary $n = 500$.

A. Generation of initial matrices

Before starting sweep process, we need to prepare initial values of matrices for the variational state (3.5). As explained in section 3, the matrices need to satisfy one of the orthogonality conditions (3.6) or (3.7) for numerical stability. The algorithm shown below is also useful for minimization of energy function with the Powell method [6].

Let us consider real matrices $A[s]$ that satisfy the following normalization condition

$$\sum_{j=1}^{M} \sum_{s=1}^{K} A[s]_{ij} A[s]_{i'j'} = \delta_{ii'}, \quad (A.1)$$

where $M$ is the dimension of the matrices $A[s]$ and $K$ is the degrees of freedom of each site or link. To parametrize the matrices $A[s]$, we introduce $KM$-dimensional vectors $v^{(n)}$

$$v^{(n)} = (v_1^{(n)}, \ldots, v_{KM-n+1}^{(n)}, 0, \ldots, 0), \quad n = 1, \ldots, M. \quad (A.2)$$

These vectors are linearly independent and can be orthonormalized using the Gram-
Figure 6: Vacuum expectation value of the plaquette operator is plotted as a function of the coupling constant $\lambda$ with lattice size $L=500$. The circles are the calculated values, which are consistent with the exact ones given in sec. 3.

Schmidt method

$$a^{(1)} = \frac{v^{(1)}}{|v^{(1)}|}$$  \hspace{1cm} (A.3)

$$b^{(k+1)} = v^{(k+1)} - \sum_{n=1}^{k} \langle v^{(k+1)} , a^{(n)} \rangle a^{(n)}$$  \hspace{1cm} (A.4)

$$a^{(k+1)} = \frac{b^{(k+1)}}{|b^{(k+1)}|}$$  \hspace{1cm} (A.5)

where $k = 1, \ldots, M - 1$ and the brackets represent inner product. The orthonormalized vectors $a^{(n)}$ are used to parametrize the matrices $A[s]_{ij} = A_{i,(j,s)}$

$$A_{i,(j,s)} = \begin{pmatrix} a^{(1)} \\ \vdots \\ a^{(M)} \end{pmatrix} ,$$  \hspace{1cm} (A.6)

which satisfy the conditions (A.1). When eq. (A.1) is satisfied, the number of independent degrees of freedom associated with the matrices $A[s]$ is given by

$$KM^2 - \frac{M(M + 1)}{2} ,$$  \hspace{1cm} (A.7)

which is equal to that of the vectors $v^{(n)}$

$$\sum_{n=0}^{M-1} (KM - n) - M .$$  \hspace{1cm} (A.8)

In eq. (A.8), the first term counts the number of the parameters $v_i^{(n)}$ and the second term comes from the normalization conditions (A.3) and (A.5).
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