Group theory on quantum Boltzmann machine

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Abstract

Group theory is extremely successful in characterizing the symmetries in quantum systems, which greatly simplifies and unifies our treatments of quantum systems. Here we introduce the concept of the symmetry for a quantum Boltzmann machine and develop a group theory to describe the symmetry. This symmetry implies not only that all the target states related with the symmetry transformations are equivalent, but also that for a given target state all the optimal solutions related with the symmetry transformations that keeps the target state invariant are equivalent. For the Boltzmann machines built on qubits, we propose a systematic procedure to construct the group, and develop a numerical algorithm to verify the completeness of our construction.

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I. INTRODUCTION

Quantum Boltzmann machine is one of the major machine learning models in quantum machine learning [1–3]. A quantum Boltzmann machine is a quantum system with a specific type of Hamiltonians with variable parameters, and it is controlled to approximate a target quantum state as well as possible via tuning these parameters [4–7]. The target quantum state is a “quantum data”, which may contain quantum characteristics such as quantum coherence or entanglement that cannot be simulated classically. In particular, a quantum Boltzmann machine is proposed to be implemented in a D-Wave anneal device, which makes it possible to be trained by experimental samplings [6, 8].

Symmetry plays a predominant role in quantum physics, where it is successively described by group theory [9–11]. However, group theory has rarely been introduced to study quantum Boltzmann machine. Recently we have found one example where symmetry can be used in a specific quantum Boltzmann machine [5]. Here we aim to extend our case study [5] to a group theory suitable for any quantum Boltzmann machine. First we will clarify the concept of the symmetry for a quantum Boltzmann machine, and introduce the symmetry group of a quantum Boltzmann machine to describe the symmetry. Then we answer what the symmetry implies for a quantum Boltzmann machine.

Furthermore, we focus on how to construct the symmetry group for a general quantum Boltzmann machine. We obtain a systematic procedure to construct the symmetry group of a quantum Boltzmann machine, and develop a numerical algorithm to show the completeness of our construction.

II. DEFINITION OF QUANTUM BOLTZMANN MACHINE

A quantum Boltzmann machine is composed by a bipartite quantum system, where one subsystem is called visible, and the other is called hidden [4]. The type of Hamiltonian of the bipartite quantum system is

\[ H(a) = -a \cdot O, \]    

where \( a \) is the vector of variable real parameters, and \( O \) is the vector of linearly independent Hermitian operators with zero trace. The quantum state of the bipartite quantum system
is the Boltzmann thermal equilibrium state [5]

$$\rho(a) = \frac{e^{-H(a)}}{\text{Tr}(e^{-H(a)})} = \frac{e^{a \cdot O}}{\text{Tr}(e^{a \cdot O})}.$$  \hspace{1cm} (2)

Then the reduced state of the visible subsystem is

$$\sigma(a) = \text{Tr}_h(\rho(a)),$$  \hspace{1cm} (3)

where $\text{Tr}_h$ denotes the trace over the hidden subsystem.

The task of the quantum Boltzmann machine is to make the quantum state of the visible subsystem $\sigma(a)$ approximate a given target state $\sigma_*$ as well as possible by adjusting the parameters $a$ in the Hamiltonian. More precisely, the aim of the quantum Boltzmann machine is to minimize

$$S_m(\sigma_*) = \min_a S(\sigma_*|\sigma(a)),$$  \hspace{1cm} (4)

where the quantum relative entropy is defined as

$$S(\sigma|\sigma') = \text{Tr}_v(\sigma(\ln \sigma - \ln \sigma')).$$  \hspace{1cm} (5)

Here the quantum relative entropy is used as a measure of the degree of approximation of one quantum state with another [12, 13].

From the above definition of quantum Boltzmann machine, we learn that a quantum Boltzmann machine is specified by a set of operators $\mathcal{O} = \{O_i\}$, where $\{O_i\}$ are linearly independent Hermitian operators. Then the set of the Hamiltonians in Eq. (1) constructs a real linear space $\mathcal{L}(\mathcal{O})$. Two quantum Boltzmann machines are of the same type if and only if they have the same $\mathcal{L}(\mathcal{O})$. For a Boltzmann machine with $\mathcal{L}(\mathcal{O})$, all the representable states are given by Eqs. (2)(3) denoted as $\mathcal{S}(\mathcal{O})$.

For convenience, we assume that any operator $O_i \in \mathcal{O}$ has a product structure for the visible part and the hidden part, i.e. $O_i = O_i^{v} \otimes O_i^{h}$, where $O_i^{v}$ and $O_i^{h}$ are the Hermitian operators acting on the Hilbert space of the visible subsystem $\mathcal{H}_v$ and that of the hidden subsystem $\mathcal{H}_h$ respectively. Then we divide the set $\mathcal{O}$ into three parts as follows:

$$\mathcal{O} = \mathcal{O}_v \cup \mathcal{O}_h \cup \mathcal{O}_c,$$  \hspace{1cm} (6)

where

$$\mathcal{O}_v = \{O_i \in \mathcal{O} : O_i^{v} \neq 1^v, O_i^{h} = 1^h\},$$  \hspace{1cm} (7)

$$\mathcal{O}_h = \{O_i \in \mathcal{O} : O_i^{v} = 1^v, O_i^{h} \neq 1^h\},$$  \hspace{1cm} (8)

$$\mathcal{O}_c = \{O_i \in \mathcal{O} : O_i^{v} \neq 1^v, O_i^{h} \neq 1^h\}.$$  \hspace{1cm} (9)
with $1^v$ and $1^h$ being the identity operators of the Hilbert spaces $\mathcal{H}_v$ and $\mathcal{H}_h$ respectively. The real linear spaces of Hamiltonians with bases from $\mathcal{O}_v$, $\mathcal{O}_h$, and $\mathcal{O}_c$ are denoted as $\mathcal{L}(\mathcal{O}_h)$, $\mathcal{L}(\mathcal{O}_h)$, and $\mathcal{L}(\mathcal{O}_c)$ respectively. The linear space $\mathcal{L}(\mathcal{O})$ is the direct sum of the linear subspaces $\mathcal{L}(\mathcal{O}_v)$, $\mathcal{L}(\mathcal{O}_h)$, and $\mathcal{L}(\mathcal{O}_c)$. Physically, a Hamiltonian in the composite system can be naturally distinguished as the sum of the free Hamiltonian of the visible subsystem, the free Hamiltonian of the hidden subsystem, and the coupling term between them.

III. SYMMETRY IN QUANTUM BOLTZMANN MACHINE

What is the symmetry for a quantum Boltzmann machine? Obviously, the concept of the symmetry for a quantum Boltzmann machine is different from that for a given quantum system. For a given quantum system, its Hamiltonian is fixed, and the symmetric group is composed by the unitary transformations that keeps the Hamiltonian invariant $[14] [15]$. For a quantum Boltzmann machine, the Hamiltonian may be any one in the set of the real linear space $\mathcal{L}(\mathcal{O})$. Thus we need to generalize the concept of symmetry for a given Hamiltonian. In particular, to define the concept of the symmetry for a quantum Boltzmann machine, the different roles played by the visible part and the hidden part of the quantum Boltzmann machine must be taken into account. Thus we introduce the symmetry of a quantum Boltzmann machine as follows.

For the quantum Boltzmann machine with the Hamiltonian given by Eq. (1), we define its symmetry operation by the unitary transformation $U_v \otimes U_h$ satisfying $\forall H(a) \in \mathcal{L}(\mathcal{O})$

$$U_v \otimes U_h H(a) U_v^\dagger \otimes U_h^\dagger = H(a') \in \mathcal{L}(\mathcal{O}).$$

(10)

All the symmetric unitary transformations form a group $G(\mathcal{O})$, which is called the symmetry group of the quantum Boltzmann machine specified by $\mathcal{O}$. In particular, the inverse of $U_v \otimes U_h \in G(\mathcal{O})$ transforms $H(a')$ back to $H(a)$, which implies that the map from $H(a)$ to $H(a')$ is bijective. Further more, Eq. (10) gives

$$U_v \otimes U_h \rho(a) U_v^\dagger \otimes U_h^\dagger = \rho(a'),$$

(11)

where $\rho(a)$ is defined by Eq. (2).

For any symmetry unitary transformation $U_v \otimes U_h \in G(\mathcal{O})$ and any target state $\sigma_*$, the transformed target state $U_v \sigma_* U_v^\dagger$ will be approximated by the Boltzmann machine as well.
as the original target state $\sigma_*$, more precisely,
\[ S_m(U_v\sigma_*U_v^\dagger) = S_m(\sigma_*), \tag{12} \]
where $S_m(\sigma_*)$ is defined by Eq. (4). We prove Eq. (12) as follows:
\[
S_m(\sigma_*) = \min_a S(\sigma_\ast | \sigma(a))
= \min_a S(U_v\sigma_*U_v^\dagger | U_v\sigma(a)U_v^\dagger)
= \min_a S(U_v\sigma_*U_v^\dagger | U_v \text{Tr}_h \rho(a)U_v^\dagger)
= \min_a S(U_v\sigma_*U_v^\dagger | \text{Tr}_h(U_v \otimes U_h \rho(a)U_v^\dagger \otimes U_h^\dagger))
= \min_{a'} S(U_v\sigma_*U_v^\dagger | \text{Tr}_h(\rho(a')))
= S_m(U_v\sigma_*U_v^\dagger), \tag{13}
\]
where the fact that the quantum relative entropy is invariant under unitary transformation \[12, 16\] is used on the second line, and Eq. (11) is used on the fifth line. Eq. (12) shows that all the target states related by the symmetry transformation $U_v$ of a quantum Boltzmann machine are equivalent to the quantum Boltzmann machine.

Further more, we study the effect of the symmetry of quantum Boltzmann machine on the possible solutions of parameters for a given target state. Let us denote
\[
A = \arg \min_a S(\sigma_\ast | \sigma(a)), \tag{14}
\]
where the argmin of a function with some arguments outputs the set of the arguments where the function takes its minimum. If some $a_\ast \in A$, then $\forall U_v \otimes U_h \in G(\mathcal{O})$ satisfying $U_v\sigma_*U_v^\dagger = \sigma_*$, we have
\[
U_v \otimes U_h H(a_\ast)U_v^\dagger \otimes U_h^\dagger = H(a'_\ast). \tag{15}
\]
Thus we prove that $a'_\ast \in A$ as follows:
\[
S(\sigma_\ast | \sigma(a_\ast)) = S(U_v\sigma_*U_v^\dagger | \text{Tr}_h(U_v \otimes U_h \rho(a_\ast)U_v^\dagger \otimes U_h^\dagger))
= S(\sigma_\ast | \sigma(a'_\ast)). \tag{16}
\]
Roughly speaking, the symmetry of quantum Boltzmann machine implies the degeneracy of the optimal solutions for a given target state.
Let us analyze the structure of the group $G(O)$. When the Hamiltonian $H(a)$ in Eq. (10) is the free term of the visible subsystem, i.e. $H(a) \in \mathcal{L}(O_v)$, Eq. (10) becomes

$$U_v H(a) U_v^\dagger = H(a').$$

(17)

All the unitary transformations satisfying the above equation construct a group, denoted as $G(O_v)$. Similarly, we can introduce the group of the hidden subsystem, denoted as $G(O_h)$. Then we can construct a product group of $G(O_v)$ and $G(O_h)$, which contains $G(O)$ as a subgroup. In fact, we can construct $G(O)$ by

$$G(O) = \{ U_v \otimes U_h \in G(O_v) \otimes G(O_h) : U_v \otimes U_h O U_v^\dagger \otimes U_h^\dagger \in \mathcal{L}(O_c), \forall O \in \mathcal{L}(O_c) \}. \quad \quad \quad (18)$$

In particular, when a quantum Boltzmann machine without the hidden subsystem, the group $G(O)$ is the group $G(O_v)$. Furthermore, Eq. (18) suggests that, to construct the symmetry group $G(O)$ we can always construct the subgroups $G(O_v)$ and $G(O_h)$ and then check the connect condition shown in Eq. (18).

IV. QUANTUM BOLTZMANN MACHINE COMPOSED BY QUBITS

A. Notation for multi-qubit systems

Usually a quantum Boltzmann machine is built on $n$ qubits, where the visible part contains $n_v$ qubits, and the hidden part contains the other $n_h$ ($n_h = n - n_v$) qubits. Let $Z_2 = \{0, 1\}$, which is an Abelian group under $\oplus$, the addition modulo 2. Let $\gamma = (\alpha, \beta) \in D$, where $D = Z_2 \otimes Z_2$. Let

$$\gamma = (\gamma_1; \gamma_2; \cdots; \gamma_n) = (\alpha_1, \beta_1; \alpha_2, \beta_2; \cdots; \alpha_n, \beta_n) \in D^n.$$ 

The set of the $n$-qubit Pauli operators $\mathcal{P}_n$ is defined by

$$\mathcal{P}_n = \{ \sigma_\gamma \equiv \sigma_{\gamma_1} \otimes \sigma_{\gamma_2} \otimes \cdots \otimes \sigma_{\gamma_n} \} \quad \quad \quad (19)$$

with

$$\sigma_\gamma = \sigma_{\alpha \beta} = i^{\alpha_1 \beta_1} \sigma_x^{\alpha_2} \sigma_z^{\beta_2}, \quad \quad \quad (20)$$

where $\sigma_x$ and $\sigma_z$ are the Pauli operators [17]. Note that the set $\mathcal{P}_n$ is a group up to a phase factor $\{\pm 1, \pm i\}$, which is called the $n$-qubit Pauli group [16]. The advantage of the above
notation lies in the unified multiplication rule:

\[ \sigma_\gamma \sigma_{\gamma'} = i^{\omega(\gamma, \gamma') - \nu(\gamma, \gamma')} \sigma_{\gamma \oplus \gamma'} \]  

(21)

with

\[ \omega(\gamma, \gamma') = (\alpha + \alpha')(\beta + \beta') - (\alpha \oplus \alpha')(\beta \oplus \beta'), \]  

(22)

\[ \nu(\gamma, \gamma') = \alpha \beta' - \alpha' \beta. \]  

(23)

We observe that \( \omega(\gamma, \gamma') = \omega(\gamma', \gamma) \) and \( \nu(\gamma, \gamma') = -\nu(\gamma', \gamma) \). In addition, the multiplication rule implies

\[ \sigma_\gamma^2 = 1, \]  

(24)

\[ \sigma_\gamma \sigma_{\gamma'} = (-1)^{\nu(\gamma, \gamma')} \sigma_{\gamma'} \sigma_{\gamma}. \]  

(25)

In the \( n \)-qubit case, the multiplication rule becomes

\[ \sigma_\gamma \sigma_{\gamma'} = i^{\omega(\gamma, \gamma') - \nu(\gamma, \gamma')} \sigma_{\gamma \oplus \gamma'}, \]  

(26)

where

\[ \omega(\gamma, \gamma') = \sum_i \omega(\gamma_i, \gamma'_i), \]  

(27)

\[ \nu(\gamma, \gamma') = \sum_i \nu(\gamma_i, \gamma'_i). \]  

(28)

And we also have

\[ \sigma_\gamma^2 = 1, \]  

(29)

\[ \sigma_\gamma \sigma_{\gamma'} = (-1)^{\nu(\gamma, \gamma')} \sigma_{\gamma'} \sigma_{\gamma}. \]  

(30)

Since the elements in \( \mathcal{P}_n \) are Hermitian and linear independent, all the Hermitian operators can be expanded uniquely with them as a basis, which form a real vector space

\[ \mathcal{L}_n = \left\{ \sum_\gamma a_\gamma \sigma_\gamma, \gamma \in D^n, a_\gamma \in \mathbb{R} \right\}. \]  

(31)
B. Basic equations for the symmetry group of quantum Boltzmann machine

The type of the quantum Boltzmann machine $\mathcal{O}$ is given by a subset of $\mathcal{P}_n$, which is specified by a subset of $D^n$ denoted by $D^n(\mathcal{O})$. The Hamiltonian space of the quantum Boltzmann machine

$$\mathcal{L}(\mathcal{O}) = \left\{ \sum_{\gamma} b_\gamma \sigma_\gamma ; \gamma \in D^n(\mathcal{O}), b_\gamma \in \mathbb{R} \right\}. \quad (32)$$

Similarly we can obtain its subspaces $\mathcal{L}(\mathcal{O}_v)$ and $\mathcal{L}(\mathcal{O}_h)$.

Now we start to construct the subgroup $G(\mathcal{O}_v)$. Following Eq. (17), $\forall \gamma \in D(\mathcal{O}_v)$ and $\forall U \in G(\mathcal{O}_v)$ we have

$$U \sigma_\gamma U^\dagger = \sum_{\gamma' \in D(\mathcal{O}_v)} U_{\gamma \gamma'} \sigma_{\gamma'}, \quad (33)$$

where

$$U_{\gamma \gamma'} = \frac{1}{2^{n_v}} \text{Tr}(U \sigma_\gamma U^\dagger \sigma_{\gamma'}). \quad (34)$$

Note that $\{U_{\gamma \gamma'}\}$ are real, and they satisfy

$$\sum_{\gamma' \in D(\mathcal{O}_v)} U^2_{\gamma \gamma'} = \sum_{\gamma \in D(\mathcal{O}_v)} U^2_{\gamma \gamma'} = 1, \quad (35)$$

which implies that $\{U^2_{\gamma \gamma'}\}$ is a double stochastic matrix [18, 19]. According to the Birkhoff’s theorem [18], the set of all $n_v \times n_v$ doubly stochastic matrices is a convex set whose extreme points are permutation matrices.

According to Eq. (26), we define the generator $D_a(\mathcal{O}_v)$ of $D(\mathcal{O}_v)$ under the addition modulo 2 as a subset of $D(\mathcal{O}_v)$ such that $\forall \gamma \in D(\mathcal{O}_v)$ there exists a unique decomposition

$$\gamma = \oplus_{\gamma' \in D_a(\mathcal{O}_v)} \gamma', \quad (36)$$

which implies that

$$\sigma_\gamma = c_\gamma \oplus_{\gamma' \in D_a(\mathcal{O}_v)} \sigma_{\gamma'} \quad (37)$$

with $c_\gamma \in \{\pm 1, \pm i\}$.

Thus the independent relations in Eq. (33) are given by $\forall \gamma \in D_a(\mathcal{O}_v)$

$$U \sigma_\gamma U^\dagger = \sum_{\gamma' \in D(\mathcal{O}_v)} U_{\gamma \gamma'} \sigma_{\gamma'}. \quad (38)$$
Applying $U$ to Eq. (29) gives $\forall \gamma \in D_a(O_v)$,

\[
(U\sigma_\gamma U^\dagger)^2 = \sum_{\gamma'',\gamma''' \in D(O_v)} U_{\gamma''\gamma''} U_{\gamma'''\gamma'''} \sigma_{\gamma''} \sigma_{\gamma'''}
\]

\[
= \sum_{\gamma'' \in D(O_v)} U_{\gamma''\gamma''}^2 + \sum_{\gamma'' \not\in D(O_v)} U_{\gamma''\gamma''} U_{\gamma'''\gamma'''} \sigma_{\gamma''} \sigma_{\gamma'''}
\]

\[
= \sum_{\gamma'' \in D(O_v)} U_{\gamma''\gamma''}^2 + \sum_{\gamma'' \not\in D(O_v)} U_{\gamma''\gamma''} U_{\gamma'''\gamma'''} \epsilon(\gamma'',\gamma''') \cdot \epsilon(\gamma'',\gamma''') \cdot \epsilon(\gamma'',\gamma''') = 1.
\]

Thus we find $\forall \gamma' \in D^{n_v}$ and $\forall \gamma \in D_a(O_v)$,

\[
\sum_{\gamma'' \in D(O_v)} U_{\gamma''\gamma''}^2 = 1,
\]

\[
\sum_{\gamma'' \not\in D(O_v)} U_{\gamma''\gamma''} U_{\gamma'''\gamma'''} \epsilon(\gamma'',\gamma''') \cdot \epsilon(\gamma'',\gamma''') \cdot \epsilon(\gamma'',\gamma''') = 0.
\]

Similarly, applying $U$ to Eq. (30), we find $\forall \gamma' \in D^{n_v}$ and $\forall \gamma \not\in D_a(O_v)$,

\[
\sum_{\gamma'' \not\in D(O_v)} \left( U_{\gamma''\gamma''} U_{\gamma'''\gamma'''} - (-1)^{\epsilon(\gamma',\gamma')} U_{\gamma''\gamma''} U_{\gamma'''\gamma'''} \right) \epsilon(\gamma'',\gamma''') \cdot \epsilon(\gamma'',\gamma''') \cdot \epsilon(\gamma'',\gamma''') = 0.
\]

Following Eq. (37), $\forall \gamma \in D(O_v)$ and $\gamma \not\in D_a(O_v)$, we require

\[
U\sigma_\gamma U^\dagger = c_\gamma \otimes \gamma' \ U\sigma_\gamma U^\dagger = c_\gamma \otimes \gamma' \ \sum_{\gamma''} U_{\gamma''\gamma''} \sigma_{\gamma''} \in L(O_v).
\]

For example, if the decomposition of $\sigma_\gamma$ contains two terms $\sigma_{\gamma_1}$ and $\sigma_{\gamma_2}$, then Eq. (43) becomes

\[
U\sigma_\gamma U^\dagger = c_\gamma \sum_{\gamma''_1,\gamma''_2} U_{\gamma''_1\gamma''_1} U_{\gamma''_2\gamma''_2} \sigma_{\gamma''_1} \sigma_{\gamma''_2}
\]

\[
= c_\gamma \sum_{\gamma''_1,\gamma''_2} U_{\gamma''_1\gamma''_1} U_{\gamma''_2\gamma''_2} \epsilon(\gamma''_1,\gamma''_2 - \epsilon(\gamma''_1,\gamma''_2) \sigma_{\gamma''_1} \otimes \gamma''_2 \in L(O_v),
\]

which implies that $\forall \gamma' \not\in D(O_v)$,

\[
\sum_{\gamma''_1,\gamma''_2} U_{\gamma''_1\gamma''_1} U_{\gamma''_2\gamma''_2} \epsilon(\gamma''_1,\gamma''_2 - \epsilon(\gamma''_1,\gamma''_2) \delta_{\gamma''_1,\gamma''_2} = 0.
\]

Now we concludes that Eqs. (40)(41)(42)(45) construct the basic equations for the coefficients $\{U_{\gamma\gamma'}, \gamma \in D_a(O_v), \gamma' \in D(O_v)\}$. Actually, our basic equations ensure that the
transformation $U$ is unitary, and that the set $\mathcal{O}_v$ can be generated with the new generator with the same rule as the original. Thus, in principle, all the elements in the group $G(\mathcal{O}_v)$ can be determined by solving these basic equations.

C. The continuous and the discrete subgroups of quantum Bolztmann machine

Since the basic equations for the symmetry group $G(\mathcal{O}_v)$ for the Boltzmann machine is difficult to solve directly, we will find the analytical results on the symmetry group in this subsection. We note that the elements in the group $G(\mathcal{O}_v)$ may be divided into two classes, the continuous part $G_c(\mathcal{O}_v)$ and the discrete part $G_d(\mathcal{O}_v)$.

Now we focus on the continuous subgroup $G_c(\mathcal{O}_v)$. First, the one-parameter subgroup \[14\] of $G(\mathcal{O}_v)$ may be written as

$$U(a) = e^{iaK} \tag{46}$$

with

$$K = \sum_{\gamma \in D_{nv}} b_{\gamma} \sigma_{\gamma}. \tag{47}$$

Then $\forall \gamma' \in G(\mathcal{O}_v)$, we have

$$[K, \sigma_{\gamma'}]$$

$$= \left[ \sum_{\gamma \in D_{nv}} b_{\gamma} \sigma_{\gamma}, \sigma_{\gamma'} \right]$$

$$= \sum_{\gamma \in D_{nv}} b_{\gamma} [\sigma_{\gamma}, \sigma_{\gamma'}]$$

$$= \sum_{\gamma \in D_{nv}} b_{\gamma} (1 - (-1)^{\nu(\gamma, \gamma')}\iota^\nu(\gamma, \gamma') - \nu(\gamma, \gamma') \sigma_{\gamma \oplus \gamma'}) \in \mathcal{L}(\mathcal{O}_v), \tag{48}$$

which implies that if $\gamma \oplus \gamma' \notin D(\mathcal{O}_v)$, then

$$b_{\gamma} (1 - (-1)^{\nu(\gamma, \gamma')}) = 0. \tag{49}$$

In other words, $b_{\gamma} \neq 0$ if and only if $\forall \gamma' \in D(\mathcal{O}_v)$

$$\gamma \oplus \gamma' \in D(\mathcal{O}_v) \tag{50}$$

or

$$[\sigma_{\gamma}, \sigma_{\gamma'}] = 0, \tag{51}$$
which is equivalent to
\[ \nu(\gamma, \gamma') \equiv 0 \pmod{2}. \] (52)

Let us denote the set of \( \gamma \) that satisfies Eq. (50) or Eq. (52) for any \( \gamma' \in D(O_v) \) as \( D_c \). Then \( U(\{a_\gamma\}) = e^{i \sum_{\gamma \in D_c} a_{\gamma} \sigma_{\gamma}} \) is the continuous subgroup of \( G(O_v) \), which is denoted as \( G_c(O_v) \).

We find that \( G_c(O_v) \) is an invariant group of \( G(O_v) \), which is proved as follows: \( \forall V \in G(O_v) \), we have
\[
V U(\{a_\gamma\}) V^\dagger = e^{i \sum_{\gamma \in D_c} a_{\gamma} V^{\sigma_\gamma} V^\dagger} \in G_c(O_v)
= U(\{a_{\gamma}'\}).
\] (53)

Thus we conclude that the group \( G(O_v) \) is a product of the continuous subgroup \( G_c(O_v) \) and some discrete subgroup \( G_d(O_v) \), i.e., \( G(O_v) = G_c(O_v) \otimes G_d(O_v) \). In other words, any element in \( G(O_v) \) can be written as \( U = U(\{a_\gamma\}) W \) with \( W \in G_d(O_v) \).

Now we focus on constructing the discrete subgroup \( G_d(O_v) \). A direct method is as follows. We numerically solve the set of basic equations (40)(41)(42)(45) with random initial conditions to obtain a random element in \( G(O_v) \). Combining with the known \( G_c(O_v) \), we will obtain a random element in \( G_d(O_v) \). Repeat the above procedure until all the elements in \( G_d(O_v) \) be found. However, this method only works when the number of the qubit in the system is small (less than 5 qubits).

To obtain the discrete group \( G_d(O_v) \) in the systems with more qubits, we make the assumption that \( G_d(O_v) \) is a subgroup of the Clifford group \([20, 21]\) of \( n_v \) qubits, where the Clifford group is defined as all the unitary transformations that map one element to another in \( P_{n_v} \) up to the sign \( \pm \). This assumption is numerically supported for the lower dimensional system by the method given in the previous paragraph.

Under the above assumption, Eqs. (40)(41) in the basic equations are satisfied automatically. Eqs. (42) ensures the commutation relations between different elements in the generator of the set \( O_v \) invariant after transformations. Since the commutation relation between any two elements in the Pauli group is either commutative or anti-commutative, we can describe these relations by a graph, where an vertex denotes an element in the Pauli group, and an edge between two nodes denotes the two elements in the Pauli group are anti-commutative. In the language of graph \([22]\), the commutation relations among the elements in the generator of the set \( O_v \) can be described as a graph, and a graph is transformed to another isomorphic graph under the unitary transformation in the group \( G_d(O_v) \) \([23–25]\).
Eqs. (45) ensures the set $\mathcal{O}_v$ can be generated with the new generator with the same rule as original.

So far we are ready to present a general procedure to determine the symmetry group of a quantum Boltzmann machine $\mathcal{O}$:

1. Give $D(\mathcal{O})$, and classify it into $D(\mathcal{O}_v)$, $D(\mathcal{O}_h)$, and $D(\mathcal{O}_c)$.

2. Calculate the subgroup $G(\mathcal{O}_v)$.
   
   (a) Calculate the continuous subgroup $G_c(\mathcal{O}_v)$ by Eqs. (50)-(52).
   
   (b) Calculate the discrete subgroup $G_d(\mathcal{O}_v)$.
       
       First, calculate the commutation relations $\nu(\gamma_i, \gamma_j) \mod 2$ in $D(\mathcal{O}_v)$ and associate it with a graph. Second, select one generator $D_a(\mathcal{O}_v)$ and obtain its graph. Find all the other generator $D_{a,k}(\mathcal{O}_v)$ with the isomorphic graph. Third, find all the generators in $D_{a,k}(\mathcal{O}_v)$ such that all the elements in $D(\mathcal{O}_v)$ can be generated from $D_{a,k}(\mathcal{O}_v)$ with the same rule as from $D_a(\mathcal{O}_v)$. Then any map from $D_a(\mathcal{O}_v)$ to $D_{a,k}(\mathcal{O}_v)$ defines an element in $G_d(\mathcal{O}_v)$.

3. Calculate the subgroup $G(\mathcal{O}_h)$ Similarly.

4. Determine the group $G(\mathcal{O})$ by checking the connect condition in Eq. (18).

D. Examples of constructing the symmetry group of quantum Boltzmann machine

Let us demonstrate the above procedure with the quantum Boltzmann machine with the Hamiltonian:

$$H_I = a_1 \sigma_x^{(1)} + a_2 \sigma_z^{(1)} + a_3 \sigma_x^{(2)} + a_4 \sigma_z^{(2)} + a_5 \sigma_z^{(1)} \otimes \sigma_z^{(2)}.$$  

Then the set

$$D(\mathcal{O}_I) = \{ \gamma_1 = (1, 0; 0, 0), \gamma_2 = (0, 1; 0, 0), \gamma_3 = (0, 0; 1, 0), \gamma_4 = (0, 0; 0, 1), \gamma_5 = (0, 1; 0, 1) \}.$$  

The commutation relations, which are characterized by the matrix $\nu(\gamma_i, \gamma_j) \mod 2$, can be described by the graph in Fig. 1. To obtain the continuous subgroup $G_c(\mathcal{O}_I)$, we need to solve Eqs. (50)-(52). We find that there is only one solution, $\gamma = (0, 0; 0, 0)$, which means that $G_c(\mathcal{O}_I) = I$.  

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To study the discrete subgroup $G_d(O_I)$, let the generator of $O_I$ be $D_a(O_v) = \{\gamma_1, \gamma_2, \gamma_3, \gamma_4\}$, whose commutation relations are demonstrated in a graph in Fig. 2. Under the unitary transformation $U \in G_d(O_I)$, the generator $D_a(O_v)$ becomes $D_a(O_v')$ that preserves the commutation relations.

We observe that only $\gamma'_5 = \gamma_5$ the remaining part in the graph in Fig. 1 is isomorphic to the left side of the graph in Fig. 2. Since $\gamma_5 = \gamma_2 \oplus \gamma_4$, correspondingly we have $\gamma'_5 = \gamma'_2 \oplus \gamma'_4$. Thus we have two choices: $\{\gamma'_2 = \gamma_2, \gamma'_4 = \gamma_4\}$ or $\{\gamma'_2 = \gamma_4, \gamma'_4 = \gamma_2\}$. Together with the commutation relations between $D_a(O_v')$, we finally obtain

$$\gamma'_1 = \gamma_1, \gamma'_2 = \gamma_2, \gamma'_3 = \gamma_3, \gamma'_4 = \gamma_4, \gamma'_5 = \gamma_5; \quad (56)$$

or

$$\gamma'_1 = \gamma_3, \gamma'_2 = \gamma_4, \gamma'_3 = \gamma_1, \gamma'_4 = \gamma_2, \gamma'_5 = \gamma_5. \quad (57)$$

Therefore the group $G_d(O_I)$ is

$$G_d(O_I) = S^S_{1,2} \otimes P_{1,2}; \quad (58)$$

where $S^S_{a_1,a_2,\ldots,a_n}$ is the $n$-qubit permutation group containing all possible permutations of the qubits labeled from $a_1$ to $a_n$. Here $S^S_{1,2} = \{I, S_{12}\}$, and $S_{ij}$ is the swap gate between qubit $i$ and qubit $j$. $P_{a_1,a_2,\ldots,a_n}$ are the $n$-qubit Pauli group for the qubits labeled from $a_1$ to $a_n$ the qubits labeled from $a_1$ to $a_n$. 

FIG. 1: A graph showing commutation relations in $O_I$.

FIG. 2: Isomorphism under unitary transformation
Note that the above quantum Boltzmann machine can be extended to its $n$-qubit version, where the Hamiltonian is

$$H_{II} = \sum_{i=1}^{n} (a_{2i-1}\sigma_x^{(i)} + a_{2i}\sigma_z^{(i)}) + \sum_{i<j}^{n} a_{i,j}\sigma_x^{(i)} \otimes \sigma_z^{(j)}$$

(59)

Similarly we find $G_c(O_{II}) = I$, and the discrete subgroup

$$G_d(O_{II}) = S^S_{1,2,...,n} \otimes P_{1,2,...,n}.$$  

(60)

From Eq. (18) we know

$$G(O_{II}) = G_c(O_{II}) \otimes G_d(O_{II}) = G_d(O_{II}).$$

(61)

We now consider the quantum Boltzmann machine with the ZZXX-XZ Hamiltonian:

$$H_{III} = \sum_{i=1}^{n} (a_{2i-1}\sigma_x^{(i)} + a_{2i}\sigma_z^{(i)}) + \sum_{i<j}^{n} (a_{i,j}\sigma_x^{(i)} \otimes \sigma_z^{(j)} + b_{i,j}\sigma_x^{(i)} \otimes \sigma_z^{(j)}) + \sum_{i \neq j}^{n} c_{i,j}\sigma_x^{(i)} \otimes \sigma_z^{(j)}.$$  

(62)

The commutation relations in $O_{III}$ is demonstrated in Fig. 3.

![FIG. 3: A graph showing commutation relations in $O_{III}$ with $n = 2$.](image)

According to Eq. (50)(52), we obtain

$$\sigma_{\gamma_j} = \sigma_y^{(j)}.$$  

(63)

The continuous subgroup is

$$U(\{a_j\}) = e^{i\sum_j a_j\sigma_y^{(j)}}.$$  

(64)

And the discrete subgroup is

$$G_d(O_{III}) = S^H_n \otimes S^S_{1,2,...,n} \otimes P_{1,2,...,n},$$

(65)

where $S^H_n$ is the $n$-qubit permutation group generating by generators $\{I, H_i\}$, and $H_i$ is the permutation between $\sigma_x^{(i)}$ and $\sigma_z^{(i)}$. 

14
Because $S^H_n \subset U(\{a_j\})$, from the uniqueness of group elements and Eq. (18) we know

$$G(O_{III}) = G_c(O_{III}) \otimes G_d(O_{III}) = e^{i \sum_j a_j \sigma_j^{(j)}} \otimes S_{1,2,\ldots,n}^{S} \otimes P_{1,2,\ldots,n}. \quad (66)$$

Finally we study an example of the quantum Boltzmann machine with hidden subsystem, whose Hamiltonian is

$$H_{IV} = H_{IV,v} + H_{IV,h} + H_{IV,w}, \quad (67)$$

where

$$H_{IV,v} = a_1 \sigma_x^{(1)} + a_2 \sigma_z^{(1)} + a_3 \sigma_x^{(2)} + a_4 \sigma_z^{(2)} + a_5 \sigma_x^{(1)} \otimes \sigma_z^{(2)} + a_6 \sigma_z^{(1)} \otimes \sigma_x^{(2)},$$

$$H_{IV,h} = a_7 \sigma_x^{(3)} + a_8 \sigma_z^{(3)} + a_9 \sigma_x^{(4)} + a_{10} \sigma_z^{(4)} + a_{11} \sigma_x^{(3)} \otimes \sigma_z^{(4)} + a_{12} \sigma_z^{(3)} \otimes \sigma_x^{(4)},$$

$$H_{IV,w} = a_{13} \sigma_x^{(1)} \otimes \sigma_z^{(3)} + a_{14} \sigma_z^{(1)} \otimes \sigma_x^{(4)} + a_{15} \sigma_x^{(2)} \otimes \sigma_z^{(3)} + a_{16} \sigma_z^{(2)} \otimes \sigma_x^{(4)}$$

$$+ a_{17} \sigma_x^{(1)} \otimes \sigma_z^{(3)} + a_{18} \sigma_x^{(1)} \otimes \sigma_x^{(4)} + a_{19} \sigma_x^{(2)} \otimes \sigma_z^{(3)} + a_{20} \sigma_z^{(2)} \otimes \sigma_x^{(4)}. \quad (68)$$

The commutation relations for $O_{IV,v}$ and $O_{IV,h}$ are represented by the same graph shown in Fig. 4.

![Graph showing commutation relations](image)

**FIG. 4:** A graph showing commutation relations in $O_{IV,v}$ and $O_{IV,h}$.

To find out the symmetric groups of $H_{IV,v}$ and $H_{IV,h}$, we first need to calculate the continuous subgroups and the discrete subgroups respectively. By solving Eqs. (50)(52), we find that $G_c(O_{IV,v}) = G_c(O_{IV,h}) = I$. By a similar procedure we obtain the discrete subgroups:

$$G_d(O_{IV,v}) = \{I, H_1 H_2, C_{12}, H_1 H_2 \times C_{12}, (H_1 H_2 \times C_{12})^2, (H_1 H_2 \times C_{12})^3\} \times \{I, S_{12}\} \times P_{1,2}, \quad (69)$$

$$G_d(O_{IV,h}) = \{I, H_3 H_4, C_{34}, H_3 H_4 \times C_{34}, (H_3 H_4 \times C_{34})^2, (H_3 H_4 \times C_{34})^3\} \times \{I, S_{34}\} \times P_{3,4}, \quad (70)$$

where $H_i$ is the Hadamard gate for qubit-$i$, $C_{ij}$ is the controlled-NOT with qubit-$i$ as the control qubit and with qubit-$j$ as the target qubit. By acting $G_d(O_{IV,v}) \otimes G_d(O_{IV,h})$ on
we obtain the transformations satisfying Eq. (27):

\[
G(O_{IV}) = \{ I, I_{12} \otimes H_3 H_4, S_{12} \otimes S_{34}, S_{12} \otimes (H_3 H_4 \times S_{34}), H_1 H_2 \otimes I_{34}, \\
H_1 H_2 \otimes H_3 H_4, (H_1 H_2 \times S_{12}) \otimes S_{34}, (H_1 H_2 \times S_{12}) \otimes (H_3 H_4 \times S_{34}) \} \times P_{1,2} \otimes P_{3,4}.
\]

E. Numerical verification

In Section IV B, we give the basic equations for calculating the symmetry group \(G(O)\) of a quantum Boltzmann machine \(O\). And we also present a general procedure to construct the symmetry group \(G(O)\) in Section IV C with the assumption that the discrete subgroup \(G_d(O_v)\) is a subgroup of the Clifford group. Now we numerically calculate the symmetry group \(G(O_v)\) with the basic equations, and attempt to show that the assumption is valid.

The main steps of the numerical algorithm is as follows. First, for a given type of quantum Boltzmann machine, we can obtain the basic equations \(\{ f_i(U) = 0 \}\) from Eqs. (40)(41)(42)(45). Second, we numerically solve these basic equations by the Levenberg–Marquardt (LM) algorithm [26]. The LM algorithm converts the problem of solving equations into a nonlinear least squares problem:

\[
\min_{U} F(U) \quad \text{(72)}
\]

with

\[
F(U) = \frac{1}{2} \sum_{i} |f_i(U)|^2. \quad \text{(73)}
\]

The LM algorithm is a nonlinear optimization between gradient descent and Newton method. Since \(F(U)\) may have many local minima, we often arrive at a local minimum but not a solution of the equations by the algorithm. To ensure a solution is arrived at, we need to check the condition that the limit of \(F(U)\) is zero, which is given numerically by \(F(U^*) \leq 10^{-6}\), where \(U^*\) is the convergent result obtained from the LM algorithm. When our system consists of a small number \(n\) of qubits (here the small number \(n\) is related to numbers of variables and equations, for example, \(n \leq 3\) in the cases of \(H_{II}\) and \(H_{III}\)), we can directly numerically solve the basic equations by the LM algorithm. When our system consists of more qubits (for example, \(n = 4\) in the cases of \(H_{II}\) and \(H_{III}\)), we cannot solve the basic equations directly. We find that when \(\forall \gamma'', \gamma''' \in D(O_v), \exists! \gamma'' \oplus \gamma''' = \gamma_* \in D^{\text{wc}},\) one of
the basic equations, Eq. (41), can be simplified to $U_{\gamma\gamma''}U_{\gamma'\gamma'''} = 0$ ($\forall \gamma \in D_a(\mathcal{O}_v), \forall \gamma'', \gamma''' \in D(\mathcal{O}_v)$ and $\gamma'' < \gamma'''$), which implies that $U_{\gamma\gamma''} = 0$ or $U_{\gamma'\gamma'''} = 0$. So we first solve these equations and get some possible zero solutions. After substituting these zero solutions into the rest of the basic equations, we apply the LM algorithm to solve the simplified basic equations. The process of our numerical solution of the basic equations is shown in the algorithm 1.

The numerical results on the symmetry groups of the quantum Boltzmann machines with Hamiltonian $H_I$, $H_{II}$ with $n = 3, 4$, and $H_{III}$ with $n = 2, 3$ are shown in Table I, II, III respectively. Because every term in our quantum Boltzmann machines is invariant under the operations in their Pauli groups, the Pauli group is the subgroup of the symmetry groups of our quantum Boltzmann machines. Here we thus need to consider only the discrete part of the symmetry groups of our quantum Boltzmann machines beyond the Pauli groups. The case of Hamiltonian $H_I$, $n = 2$, as shown in Table I, we take 500 different initial values to solve the basic equations of the symmetry group. We get $\mathcal{U} = I$ for 38 times, $\mathcal{U} = S_{12}$ for 33 times, and local minima (NOT solutions) for 429 times. Similarly, for the case of Hamiltonian $H_{II}$ with $n = 3$ shown in Table II, we take 50000 different initial values to solve the basic equations, 49931 of which fall to local minima (NOT solutions). All the symmetry operations we obtained are consistent with Eqs. (60) (61). For the case of Hamiltonian $H_{III}$ with $n = 2$, shown in Table III, we take 10000 different initial values to solve the equations, 8855 of which fall to local minima. Furthermore, we get the continuous symmetry 1076 times and the discrete symmetries, which are given in Eqs. (65). In summary, we observe that all the numerical solutions for the symmetry groups have already been obtained in Section IV C, which shows that our procedure given in Section IV C is valid for calculating the symmetry group of a given quantum Boltzmann machine.

The running time for the above calculations is shown in Table IV. Our algorithms are run on 8-core 4.0GHz CPU. With the increase of qubits number, the number of equations increases rapidly. As the increase of equations, more local minima of $F(\mathcal{U})$ appear, and we need to take more initial values to get all the solutions of the basic equations. In the case of $H_{II}, n = 4$, the running time is $1.37 \times 10^6$ seconds in our computer. It implies that it is almost impossible to calculate the symmetry group for a quantum Boltzmann machine with more qubits (e.g. a quantum Boltzmann machine with 10 qubits) in our computer.
Algorithm 1: Numerical solution of symmetric group

**Input:** Given the quantum Boltzmann machine model: number of qubits \( n \), type of Hamiltonian \( H \) (eg. \( H_{II} = \sum_{i=1}^{n} (a_{2i-1} \sigma_x^{(i)} + a_{2i} \sigma_z^{(i)}) + \sum_{i<j} a_{i,j} \sigma_x^{(i)} \otimes \sigma_z^{(j)}) \), \( \gamma \);

**Output:** Transformation matrices \( \mathcal{U} \), as show in Eqs. (34);

1. **Initialize** Random initialization: \( \mathcal{U}_{\gamma \gamma'} \in [-1, 1] \);
2. Obtain the basic equations \( \{f_i(\mathcal{U}) = 0\} \) from Eqs. (40)(41)(42)(45);
3. Solve the basic equations:
   4. if \( n \leq 3 \) then
      5. Solve the equations by the LM algorithm;
   6. end
   7. else
      8. if \( \exists ! \gamma' \oplus \gamma'' = \gamma \ast (\gamma', \gamma'' \in D(O_v)) \) then
         9. Obtain the equations \( \{ \mathcal{U}_{\gamma \gamma'} \mathcal{U}_{\gamma \gamma''} = 0 \} \) from Eq. (41);
         10. for all \( \gamma', \gamma'' \) do
             11. Find all possible zero solutions of \( \{ \mathcal{U}_{\gamma \gamma'} \mathcal{U}_{\gamma \gamma''} = 0 \} \);
             12. end
         13. for all \( \gamma \) do
             14. Find all the combinations of zero solutions \( \{ \mathcal{U}_{\gamma \gamma'}^i \mathcal{U}_{\gamma \gamma''}^i = 0 \} \):
             15. \( C = \{ \mathcal{U}_{\gamma \gamma'}^1, \mathcal{U}_{\gamma \gamma'}^2, \ldots \} \);
             16. end
         17. for batches of \( i \) do
             18. Substitute \( \{ \mathcal{U}_{\gamma \gamma'}^i \mathcal{U}_{\gamma \gamma''}^i = 0 \} \) into the basic equations to get the simplified basic equations;
             19. Solve the simplified basic equations with random initial value:
             20. \( \mathcal{U}_{\gamma \gamma'} \in [-1, 1], \mathcal{U}_{\gamma \gamma'} \notin \{ \mathcal{U}_{\gamma \gamma'}^i \mathcal{U}_{\gamma \gamma''}^i = 0 \} \);
         21. end
    22. return Transformation matrices \( \mathcal{U} \).
TABLE I: The result of solving the basic equations of the symmetry group for $H_I, n = 2$

| Symmetry | $I$ | $S_{12}$ | local minima | Total InitialValue |
|----------|-----|----------|--------------|--------------------|
| Frequency | 38  | 33       | 429          | 500                |

TABLE II: The result of solving the basic equations of the symmetry group for $H_{II}, n = 3$

| Symmetry | $I$ | $S_{132}$ | $S_{213}$ | $S_{231}$ | $S_{312}$ | $S_{321}$ | local minima | Total InitialValue |
|----------|-----|-----------|-----------|-----------|-----------|-----------|--------------|--------------------|
| Frequency | 10  | 10        | 14        | 8         | 12        | 15        | 49931        | 50000              |

V. DISCUSSION AND SUMMARY

In summary, we introduce the concept of the symmetry of a quantum Boltzmann machine, and build a general group theory to describe this symmetry. For any quantum Boltzmann machine composed of multiqubits, we give the basic equations for its symmetry group. Furthermore, we classify the symmetry group into the continuous subgroup and the discrete subgroup, and simplify the basic equations to the isomorphic graphs with the generators and the same rule to generate all other elements. To demonstrate how to apply the method, we analyze the symmetries for four typical quantum Boltzmann machines and obtain their symmetry groups, which is supported by the numerical calculation based on the basic equations.

Our work builds a direct connection between group theory and quantum Boltzmann machine, which answers not only what target states are equivalent to a quantum Boltzmann machine, but also what solutions are equivalent to the quantum Boltzmann machine. We expect that such type of symmetry in a quantum Boltzmann machine can be further extended to study the symmetries in other machine learning models, which can be used to obtain their global symmetric features in simulating physical data.

TABLE III: The result of solving the basic equations of the symmetry group for $H_{III}, n = 2$

| Symmetry | $I$ | $S_{12}$ | $H_1$ | $H_2$ | $H_1H_2$ | $S_{12} \times H_1$ | $S_{12} \times H_2$ | $S_{12} \times H_1H_2$ | $G_c$ | local minima | Total InitialValue |
|----------|-----|----------|-------|-------|----------|-----------------|-----------------|-----------------|-----|--------------|-------------------|
| Frequency | 9   | 6        | 7     | 12    | 11       | 11              | 4               | 9               | 1076| 8855         | 10000              |
TABLE IV: Running time of our algorithm for different quantum Boltzmann machines

|          | Number of Eqs. | Total Initial Value | Running time (s) |
|----------|----------------|---------------------|------------------|
| $H_I, n=2$ | 81             | 500                 | $4.52 \times 10$ |
| $H_{III}, n=2$ | 132          | 10000               | $9.10 \times 10^2$ |
| $H_{II}, n=3$ | 393          | 50000               | $2.18 \times 10^4$ |
| $H_{III}, n=3$ | 1032         | 100000              | $2.08 \times 10^5$ |
| $H_{II}, n=4$ | 1298         | 500000              | $1.37 \times 10^6$ |

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