On the Super-exponential Quantum Speedup of Equivariant Quantum Machine Learning Algorithms with SU(d) Symmetry

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We introduce a framework of the equivariant convolutional quantum algorithms which is tailored for a number of machine-learning tasks on physical systems with arbitrary SU(d) symmetries. It allows us to enhance a natural model of quantum computation – permutational quantum computing (PQC) [Quantum Inf. Comput., 10, 470–497 (2010)] – and define a more powerful model: PQC+. While PQC was shown to be efficiently classically simulatable, we exhibit a problem which can be efficiently solved on PQC+ machine, whereas the best known classical algorithm runs in $O(n!n^2)$ time, thus providing strong evidence against PQC+ being classically simulatable. We further discuss practical quantum machine learning algorithms which can be carried out in the paradigm of PQC+.

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Introduction–Symmetry plays a fundamental role in modern physics. Symmetry considerations have also emerged as crucial in several areas of quantum computing, such as covariant quantum optimization algorithms and covariant quantum error correcting codes, to name a few. One of the most fundamental continuous symmetries is SU(2), and covariant quantum optimization algorithms potentially imply quantum advantage over classical algorithms.

Many challenging physical problems, such as finding the ground state of quantum many-body Hamiltonians, exhibit a natural global continuous symmetry, which is exploited for example in $S_n$-equivariant convolutional quantum alternating ansatz$^*$ ($S_n$-CQA) [2] to find the ground state of 2D frustrated magnets. One might ask if such algorithms potentially imply quantum advantage over conventional classical optimization methods such as tensor networks or quantum neural states (NQS). On the other hand, quantum advantage has been established on the random circuit sampling [3]; are we capable of achieving the same in the presence of SU(d) symmetry? Elegantly, the celebrated Schur-Weyl duality implies that any global SU(d) symmetric problem in qudit quantum circuits can be described using the representation theory of the symmetric group $S_n$. More precisely, any SU(d)-symmetric Hamiltonian can be expressed as an element of the symmetric group algebra $\mathbb{C}[S_n]$. Jordan’s permutational quantum computing (PQC) [4] provides an initial framework towards investigating quantum advantage in the presence of global SU(d) symmetry using $S_n$ representation theory. Permutational Quantum Computing (PQC) takes inspiration from Topological Quantum Computing (TQC) and the Penrose spin network model [5]. In particular, the permutational quantum polynomial time (PQP) complexity class is conjectured to capture classically intractable by approximating matrix elements of representation of symmetric group $S_n$. However, it is shown to be classically tractable in qubits recently [6, 7]. Theoretically, Ref.[8] shows that SU(d)-symmetric unitary ensemble that satisfies two-design could achieve near-optimal quantum error-correcting capability to its fundamental limit from approximate Eastin-Knill theorem. However, a no-go theorem which forbids 2-local Hamiltonians to generate SU(2)-symmetric quantum circuit and form SU(d) two-design have been proven in [9–11]. Ignoring phases factors, $S_n$-CQA proposed in [2] remedy the problem by 4-local Hamiltonians.

In this paper we systematically investigate the question of quantum advantage in the presence of global SU(d) symmetry by generalizing the framework of PQC, for which we call PQC+. At its core, we generalize the complexity class PQP to permutation quantum polynomial time plus (PQP+) incorporating a much broader class of SU(d)-symmetric quantum algorithms. Instead of approximating matrix elements of $S_n$, irreducible representations by polynomial time quantum circuits, PQP+ approximates the matrix elements of the time evolution of SU(d)-symmetric $k$-local Hamiltonian. These matrix elements are often called the $S_n$ Fourier coefficients. Best known classical algorithm to compute such coefficients take $O(n!n^2)$ time [12, 13]. Our main result is to show that quantum circuits are capable of approximating the matrix element of any $k$-local SU(d)-symmetric Hamiltonian in polynomial time $O\left(tCk^n n^k \log(tCk^n n^k/\epsilon) \right)$, where $n$ is the number of qudits and error $\epsilon$. Therefore, a super-exponential quan-
Symmetry or more generally equivariance is among one of the key properties of classical CNNs, which roughly states that if the input to the neural network is shifted, then its activations translate accordingly. Equivariance is one of the main reasons behind the unreasonable success of convolution neural networks (CNNs). CNNs are translational equivariant; however, it is difficult to define a similar notion in discrete, spin-based quantum computation. On the contrary we argue, in quantum circuits, translational equivariance takes the natural form of permutation equivariance, whose variational ans"atze are in PQP+, thus offering a generic super-exponential speedup. Furthermore, in quantum circuits under the Schur-Weyl duality this permutation equivariance is naturally inherited from global SU(d) symmetry. Thus, quantum algorithms with permutation equivariance are natural candidates to solve physical problems in presence of global SU(d) symmetry.

We emphasize the significance of the new complexity class PQP+ by showing the ans"atze multiplication has a natural interpretation as $S_n$-equivariant convolution. This observation, we argue, leads to a direct connection to classical equivariant neural networks on so-called Fourier space activation [14–16]. It has been recognized that by constructing neural networks that operate in the basis of irreducible representations (so-called Fourier space neural networks), it is easy to implement group equivariant convolution because it simply reduces to matrix multiplication [14]. Following [15, 16], given a compact group $G$, it is tempting to implement $G$-equivariant convolutions in the quantum circuits, where the equivariance property is given in the corresponding group algebra $L^2(G, \ast)$ equipped with convolution operator $\ast$. For $f_1, f_2 \in \mathbb{C}[G]$, we integrate by the Haar measure $\mu_G$:

$$ (f_1 \ast f_2)(\sigma) \equiv \int_G f_1(\tau)f_2(\tau^{-1}\sigma)d\mu_G, $$

where the equivariance is defined with respect to the left action $L_\eta$ on $\mathbb{C}[G]$:

$$ L_\eta(f_1 \ast f_2)(\sigma) = (L_\eta f_1 \ast f_2)(\sigma) = (f_1 \ast f_2)(\eta^{-1}\sigma). $$

On the other hand any representation $(\pi_G, V)$ can be extended to the group algebra by defining $\tilde{\pi}_G(f) = \int_G f(g)\pi(g)d\mu_G$, which is a homomorphism with respect to the convolution: $\tilde{\pi}_G(f_1 \ast f_2) = \tilde{\pi}_G(f_1)\tilde{\pi}_G(f_2)$ [17] (RHS is a matrix product). Therefore, the so-called equivariance property is just the associativity of $\tilde{\pi}_G$ on the representation space or Fourier space in the sense that $\tilde{\pi}_G(f)$ encodes Fourier coefficients of $f$ [15, 16]. In what follows, this perspective will be applied to $S_n$ representation in the context of a recently studied computational model. In quantum circuits, there is a preferred representation to consider for $(\pi, S_n)$: the permutation representation. In which case, the representation $\pi$ takes meaning of permuting qudits, thus can be implemented in $O(n^2)$ many SWAP operators [4]. To this reason, $S_n$-equivariant quantum circuits are natural Fourier space, with the ans"atze essentially decomposed of polynomially bounded SWAP gates (Theorem 1), –in the case of qubits, in polynomially bounded Pauli gates (Corollary 1)–offering super-exponential quantum speed-up.

Schur-Weyl Duality– Let us first remark on the necessary mathematical concept from representation theory, the Schur-Weyl duality, to introduce PQP+ with its super-exponential speed-up. Let $V$ be a $d$-dimensional complex Hilbert space with orthonormal basis $\{e_1, \ldots, e_d\}$. The tensor product space $V^{\otimes n}$ admits two natural representations: the tensor product representation $\pi_{SU(d)}$ of $SU(d)$ acting as

$$ \pi_{SU(d)}(g)(e_{i_1} \otimes \cdots \otimes e_{i_n}) := g \cdot e_{i_1} \otimes \cdots \otimes e_{i_n}, $$

where $g \cdot e_{i_k}$ is the fundamental representation of $SU(d)$, and permutation representation $\pi_{S_n}$ of $S_n$ acting as

$$ \pi_{S_n}(\sigma)(e_{i_1} \otimes \cdots \otimes e_{i_n}) := e_{i_{\sigma^{-1}(1)}} \otimes \cdots \otimes e_{i_{\sigma^{-1}(n)}}. $$

Physically, $V^{\otimes n}$ is though as the Hilbert space of $n$ qudits with $SU(d)$ acting on these qudits. One the other, $S_n$ action permutes qudits which provides the very first feeling on the notion of PQC. The so-called Schur-Weyl duality reveals the relationship of these two kinds of group representations on the same Hilbert space.

Schur-Weyl duality is widely used in quantum computing [18], quantum information theory and high energy physics. In particular, in Quantum Chromodynamics it was used to decompose the $n$-fold tensor product of $SU(3)$ representations. In that context, standard Young tableaux are referred to as Weyl-tableaux and labeled by the three iso-spin numbers $(u, d, s)$. The underlying
Young diagrams containing three rows $\lambda = (\lambda_1, \lambda_2, \lambda_3)$ are used to denote an SU(3) irreducible representation (irrep). On the other hand, $S_n$ irreps can also be denoted by Young diagrams and that is actually the origin of using Young diagrams. Schur-Weyl duality says that irreps of both SU($d$) and $S_n$ are dual in the following sense and denoted by the same Young diagrams.

**Theorem** (Schur-Weyl Duality). For all Young diagrams $\mu, \lambda$ of size $n$ with at most $d$ rows, $\pi_{SU(d)}$ and $\pi_{S_n}$ can be decomposed as

$$ \pi_{SU(d)} \cong \bigoplus_{\mu} W_\mu \otimes 1_{m_{SU(d),\mu}}, \quad \pi_{S_n} \cong \bigoplus_{\lambda} 1_{m_{S_n,\lambda}} \otimes S_\lambda,$$

where $W_\mu$ denotes an SU($d$)-irrep, $S_\lambda$ denotes the dual $S_n$-irrep and $m_{SU(d),\mu}, m_{S_n,\lambda}$ are multiplicities. With respect to the same Young diagram, $\dim W_\lambda = m_{S_n,\lambda}$ and $\dim S_\lambda = m_{SU(d),\lambda}$ (see for example, Fig.2 (a) and (b)).

![Fig. 2](image.png)

**Fig. 2:** (a) is the decomposition of $(\mathbb{C}^2)^n$ with respect to SU(2) while (b) is for $S_6$ by Schur-Weyl duality.

A unitary transformation which transforms common matrix representations of SU($d$) into irrep matrix blocks like Fig.2 (a) as above is called a Schur transform $U_{\text{Sch}}$. The transformed basis is called a Schur basis. By Schur-Weyl duality, $U_{\text{Sch}}$ with reordered columns and rows would transform $S_n$ permutation matrices into irrep matrix blocks like Fig.2 (b). We mainly focus on the $S_n$ irrep blocks in this work. We call the reordered Schur basis, which reveals $S_n$ irreps, Young-Yamanouchi basis or briefly Young basis in the following context. For more details about Schur-Weyl duality and $S_n$-representation theory, we recommend [17, 19, 20] for more details.

**PQP+ and Super-Exponential Speed-up**—In the original setting of PQC, we first prepare an appropriate Young basis vector $|v\rangle = U_{\text{Sch}}|x\rangle$ for some $x \in \{0,1\}^n$. The quantum Schur transform $U_{\text{Sch}}$ can be efficiently compiled even for qudits with gate complexity $\text{Poly}(n, \log d, \log(1/\epsilon))$ [21–23]. Then we measure the matrix elements: $\langle u | \pi(\sigma) | v \rangle$. Using $O(n^2)$ SWAP gates, Jordan argues that these measurements form the permutational quantum polynomial (PQP) class [4]. Capable of computing the matrix elements of the $S_n$-irreps in polynomial time was conjectured to capture the non-classical aspects of quantum computing. One inspiration of this conjecture is the scaling behavior of dimensions of irreps decomposed from $V^\otimes n$ by Schur-Weyl duality. Given a Young diagram $\lambda$ with no more than $d$ rows,

$$ \dim W_\lambda = \prod_{1 \leq i < j \leq d} \frac{\lambda_i - \lambda_j - i - j}{i - j}, \quad \dim S_\lambda = \frac{n!}{\prod_{i \in \lambda} h_{i,j}},$$

where the second one is called hook length formula with $h_{i,j}$ denoting the number of boxes including the $(i, j)$ box in $\lambda$ plus all those on the RHS of $(i, j)$ and below $(i, j)$ [19, 20]. It is easy to check that the dimension of SU($d$) irrep $W_\lambda$ is bounded by a polynomial of $n$. While for $\dim S_\lambda$, depending on $\lambda$, it would scale exponentially. Let us consider a simple example with even number of qubits $n = 2m$ and $d = 2$. Let $\lambda = (m, m)$. Then

$$ \dim S_\lambda = \frac{(2m)!}{(m+1)!m!} = \frac{2^m}{m+1} \prod_{k=1}^{m} \frac{2k-1}{k} < \frac{2^m}{m+1}. $$

Evaluating matrix elements of this size was thought to be difficult for classical algorithm. However, a classical sampling method was later found in [6, 7] for qubits.

In this work, we extend the class of PQP (for which we call PQP+) in the hope to capture some of the non-classical aspects. The motivation comes from by interpolating quantum circuits as natural Fourier spaces. Let us consider a class of problems that can be solved by measuring

$$ \langle u | \tilde{\pi}(f) | v \rangle := \sum_{\sigma \in S_n} c_{\sigma} \langle u | \pi(\sigma) | v \rangle.$$

in polynomial time via Fourier space convolution. In particular, we define PQP+ by the set of polynomially-bounded quantum algorithms able to approximate the matrix elements of the so-called Hamiltonian simulation in qudits:

$$ \exp(-i\tilde{\pi}(f)) = \sum_{n=0} \frac{(-i)^n}{n!} (\tilde{\pi}(f))^n$$

$$ = \sum_{n=0} \frac{(-i)^n}{n!}\tilde{\pi}(f \cdots f). \quad (2)$$

Obviously, $f$ is chosen such that $\tilde{\pi}(f)$ is Hermitian. Note that the Wedderburn theorem implies that Eq.(2) encompasses all unitary $S_n$-Fourier coefficients. If $f$ is supported on $k$-qudits, we can efficiently simulate it using standard Hamiltonian simulation methods. We show the implementation complexity, depending linearly on the time and polynomially on the number of qudits, by one of these methods called Linear Combination of Unitaries (LCU) from [24–26] in the following theorem. Combining with the efficient quantum Schur transform to produce
Young basis vectors, it follows that the $\mathbb{C}[S_n]$ generalization to PQC is able to achieve super-exponential speed-up computing the matrix element of $\mathbb{C}[S_n]$ Fourier coefficients of the following form, where no polynomial-time classical algorithm is found.

**Theorem 1.** Consider a k-local $\mathbb{C}[S_n]$ Hamiltonian $H = \pi(f) = \sum_s c_s \sigma_s$ with Young basis elements $|u\rangle, |v\rangle$ prepared using the efficient high dimensional QST. The quantum circuit of qubits is able to simulate the matrix element $\langle u | \exp(-itH) | v \rangle$ by

$$O\left(tCK^3n^k \frac{\log(tCK^k/\epsilon)}{\log(\log(tCK^k/\epsilon))}\right)$$

**Proof.** We first note a standard result for the symmetric SWAP gates with the constant $C = \max_i |c_i|$. Then we truncate the derangement:

$$D_l = \frac{n!}{(n-l)!} \left( \frac{1}{2}! - \frac{1}{3}! + \cdots + (-1)^{l} \frac{1}{l}! \right).$$

When $H$ is k-local, then it contains at most $D_2 + \cdots + D_k$ different permutations from $S_n$. Since $n!/(12(n-l)!)$ $\leq D_1 \leq n!/(4(n-l)!)$, the number is of order $O(kn^k)$. Let $C = \max_i |c_i|$, then $||c||_1 := \sum_i |c_i| \leq O(Ckn^k)$ where $||c||_1$ is defined in the setting of LCU.

Let us divide the Hamiltonian evolution $\exp(-itH)$ into $M$ steps $\exp(-i\Delta tH)$. We set $M = tCK^k$ so that $\Delta t||c||_1 = t||c||/M = O(1)$. This is a crucial step to validate the so-called oblivious amplitude amplification in LCU (see [24–26] and SM for more details). Then we truncate the Taylor series of each product term to order $K$:

$$\| \exp(-i\Delta tH) - \sum_{m=0}^{K-1} \frac{(-i\Delta tH)^m}{m!} \| = \frac{\Delta t\|H\|_1^1 K}{K!} \leq \epsilon.$$  

In order to bound the total error by $\epsilon$, each product term should be simulated within error $\epsilon = \epsilon/M$. Using $(m/\epsilon)^m \leq m!$, the above inequality holds when $K = O(\log(\log(||c||_1)) \geq \log(1/\epsilon)$. Note that $||H||$ means operator norm here and should not be confused with $||c||_1$. However, by definition,

$$||H|| = \max_{||\psi||=1} \|H|\psi\| = \sum_i |c_i| \max_{||\psi||=1} \|\sigma_i |\psi\|. $$

As $\sigma_i$ are unitary, $||H||$ is upper bounded by $||c||_1$. Thus $\Delta t\|H\| = O(1)$, we can further relax the condition to require $K \log K \geq \log(1/\epsilon)$. Let $K' := \frac{\log 1/\epsilon}{\log \log 1/\epsilon}$. Then

$$K' \log K' \geq \log \frac{1}{\epsilon} - \log \frac{\log 1/\epsilon}{\log \log 1/\epsilon} \approx \log \frac{1}{\epsilon}$$

for small $\epsilon$. Setting $K = K'$ this bound also recovers the result from [25]. Since the time evolution also contains $M$ steps and since any k-local permutation $\sigma_i$ can be written in $O(k^2)$ geometrically local SWAPs, the total circuit complexity is:

$$O\left(k^2 MK = O\left(tCK^3n^k \frac{\log(tCK^k/\epsilon)}{\log(\log(tCK^k/\epsilon))}\right)\right).$$

which finishes the proof.

Note that in our work we assume that qudit SWAP gates are easy to implement with constant overhead. We can thus disregard the polynomially-scaling constant on $k$ in the approximation and write the total circuit complexity $O(tn^k \log(tn^k/\epsilon)/\log(\log(tn^k/\epsilon))$. Theorem 1 establishes a generic quantum super-exponential speed-up. We also present a practically relevant quantum super-exponential speed-up for qubits using the following beautiful identity:

$$\pi((i,j)) = 2\tilde{S}_i \cdot \tilde{S}_j + \frac{1}{2}I, \quad (3)$$

where $\tilde{S}_i$ is further expanded as the half of standard Pauli operators $\{X,Y,Z\}$. For example, consider $f = \{12\} + \{23\} + \{34\} + \{41\}$. Therefore under $\pi$,

$$H_P = \pi(f) = 2(\tilde{S}_1 \cdot \tilde{S}_2 + \tilde{S}_2 \cdot \tilde{S}_3 + \tilde{S}_3 \cdot \tilde{S}_4 + \tilde{S}_4 \cdot \tilde{S}_1 + I),$$

where $H_P$ is simply the 1D Heisenberg chain with a periodic boundary condition of 4 spins. Eq. (3) was first discovered by Heisenberg himself [27, 28] (an elementary proof can be found in SM) and more recently noted by [29] in analyzing the ground state property of 1-D Heisenberg chain using symmetry adapted VQE. This identity also supports the numerical simulation on 2-D Heisenberg model in one related work of us [2].

**Corollary 1.** With the above assumption, but exclusively on a qubits system, the matrix element $\langle u | \exp(-itH) | v \rangle$ can be simulated by a quantum circuit with

$$O\left(tL(k)n^k \frac{\log(tL(k)n^k/\epsilon)}{\log(\log(tL(k)n^k/\epsilon))}\right)$$

$k$-local Pauli operators with the constant $L(k) = 2^{k-1}C$.

**Proof.** We first note a simple fact that any $\sigma \in S_n$ can be expanded as a product of cycles, e.g., $(123) = (12)(23) \in S_3$. By assumption, $\sigma_i$ is $k$-local and hence can be expanded by at most $k - 1$ transpositions $\tau_{i,j} = (ij, i_{j+1})$. These transpositions may not be geometrically local, but by Eq.(3) one can compile them as a product of Pauli gates. Then $\sigma_i$ equals

$$\prod_{j=1}^{k-1} \tau_{i,j} = \prod_{j=0}^{k-1} (2\tilde{S}_{i,j} \cdot \tilde{S}_{i_{j+1}} + \frac{1}{2}I)$$

$$= \sum_{j=0}^{k-1} \frac{1}{2^{2k-1-2j}} (\tilde{S}_{i,j} \cdot \tilde{S}_{i_{j+1}}) \ldots \cdot (\tilde{S}_{i_{k-1}} \cdot \tilde{S}_{i_k}) \cdot \tilde{S}_i \cdot \tilde{S}_j \ldots \cdot \tilde{S}_{i_k}.$$

for small $\epsilon$. Setting $K = K'$ this bound also recovers the result from [25]. Since the time evolution also contains $M$ steps and since any k-local permutation $\sigma_i$ can be written in $O(k^2)$ geometrically local SWAPs, the total circuit complexity is:

$$O\left(k^2 MK = O\left(tCK^3n^k \frac{\log(tCK^k/\epsilon)}{\log(\log(tCK^k/\epsilon))}\right)\right).$$

which finishes the proof.
The operator norm of $\hat{S}_{ij} \cdot \hat{S}_{i,j+1}$ can be seen directly from Eq. (3) as $\frac{3}{4}$. Because we are going to expand $H$ by Pauli operators and then apply LCU, we should recompute $|c|_1$ used in Theorem 1. As a first step, the sum of absolute values of coefficients of each $\sigma_i$ is bounded by

$$\sum_{j=0}^{k-1} 2^{k-1-2j} \left( \frac{3}{4} \right)^{j-1} \left( \frac{k-1}{j} \right) = 2^{k-1},$$

where the last step uses binomial theorem. Then $|c|_1$ is bounded by $n^k L(k)$ as $H$ contains at most $O(n^k)$ $k$-local permutations. Substituting this into Theorem 1, we complete the proof.

A more involved derivation using Pauli gates in Theorem 1 in the form of unitary coupled clusters suggests a potentially hardware-friendly implementation on quantum computers [30].

Our results strongly suggest that the PQP+ class is able to capture some non-classical aspects of quantum computation in the qudit case. The above form of $C[S_n]$ Hamiltonian simulation by Eq. (3) encompasses a large class of physically relevant problems, such as the Heisenberg spin model. Naturally, multiplication of $C[S_n]$ Hamiltonian operators correspond to $C[S_n]$ convolution, which leads to further useful applications of machine learning and optimization tasks. In the related work [2], we focus on utilizing the quantum super-exponential speed-up to address quantum machine learning tasks by designing alternating variational $S_n$ equivariant convolution ansätze. From this point of view, PQP+ may be interpreted as the natural complexity class for quantum $S_n$-Fourier space activation for quantum machine learning and optimization tasks.

Discussion—The significance of studying PQC originally stems from imitating the behavior of anyons by a quantum computer. The so-called braided group $B_n$ which determines the symmetry of these systems are relegated to its elementary counterpart: the symmetric group $S_n$ [4, 31]. Even though, studying matrix element from $d$-symmetric Hayden-Preskill experiment for $S_n$-invariant quantum circuits is proved false in [9] for $S_n$-invariant quantum circuit when $d \geq 3$. Subsequently, we proved in the related work in [2] that the 4-local ensemble of $S(d)$-symmetric unitaries CQA($p$) is strictly universal on any one of the irreducible subspace, at large limit of $p$ or a long time (towards the end of adiabatic evolution). It then follows that CQA($p$) is a $S(d)$-symmetric $k$ design for all $k$ with some sufficiently large $p$. Furthermore, by Theorem 1, CQA($p$) can be simulated efficiently in polynomial time for $p$ scales polynomially with $n$ the number of qudits. PQP+ manifestly contains any random unitaries coming from CQA($p$) such that $p$ is bounded in polynomial of the number of qudits, for which generic super-exponential quantum speed-up is always achieved. Would random unitaries from CQA($p$) form SU($d$)-symmetric $k$ design, for $p$ grow at most polynomial in the number of qudits? Answering this question would give a physically concrete model for which near optimal quantum error correction can be achieved to the leading order of the limit set forth by the approximate Eastin-Knill theorem. In addition, it relates to recent works on linear growth of circuit complexity of random unitaries [33–35], in the presence of global SU($d$) symmetry. Furthermore, it relates by nature to SU($d$)-symmetric Hayden-Preskill experiment for which scrambling of U(1)-charged information [1] is replaced by generalized SU($d$)-charged information. We leave it for our upcoming work and future directions.

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CONTENTS

I. More facts about Schur-Weyl duality and $S_n$ representation

II. Linear Combination of Unitaries

References

I. MORE FACTS ABOUT SCHUR-WEYL DUALITY AND $S_n$ REPRESENTATION

Lemma I.1. Any local part $\hat{S}_i \cdot \hat{S}_j$ constituting a Heisenberg Hamiltonian $H = \sum_{i,j} J_{ij} \hat{S}_i \cdot \hat{S}_j$ can be written as

$$\hat{S}_i \cdot \hat{S}_j = \frac{1}{2}(ij) - \frac{1}{4}I.$$

Proof. Let us consider $\hat{S}_1 \cdot \hat{S}_2$. Expanded by definition,

$$\hat{S}_1 \cdot \hat{S}_2 = \frac{1}{2}(J_{12}^2 - J_1^2 - J_2^2),$$

where for now the subscripts on $J^2$ denotes all sites $J^2$ acting on. Under total spin basis, it is easy to see that

$$J_{12}^2 - J_1^2 - J_2^2 = \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} - \frac{3}{4}I - \frac{3}{4}I = \begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{3}{2} \end{pmatrix}.$$

While

$$(12) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}.$$

Therefore,

$$\hat{S}_1 \cdot \hat{S}_2 = \frac{1}{2}(J_{12}^2 - J_1^2 - J_2^2) = \frac{1}{2}((12) - \frac{1}{2}I).$$

This argument holds for any $i, j$, hence the proof follows. \qed

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Theorem I.2. Let $\langle \pi_{SU(d)} \rangle$ be the collection of all matrices on $V^\otimes n$ generated by $\pi_{SU(d)}$ (i.e., taking both linear spans and matrix products) and let $\langle \pi_{S_n} \rangle$ be defined similarly. Note that $\langle \pi_{S_n} \rangle$ is just the representation of $\mathbb{C}[S_n]$. Let $M$ be an arbitrary matrix of $V^\otimes n$. If it commutes with $\langle \pi_{SU(d)} \rangle$, then $M \in \langle \pi_{S_n} \rangle$. If it commutes with $\langle \pi_{S_n} \rangle$, then $M \in \langle \pi_{SU(d)} \rangle$.

This theorem is proved by the so-called double commutant theorem, details can be found in [1].

Theorem I.3 (Wedderburn Theorem). Given any $S_n$-irrep $S^\lambda$, let $\text{End}(S^\lambda)$ denote the collection of linear transformation of $S^\lambda$. With respect to any basis, e.g., the Young basis, $\text{End}(S^\lambda)$ is simply the collection of all $\dim S^\lambda \times \dim S^\lambda$ matrices. As a vector space, the group algebra $\mathbb{C}[S_n]$ is isomorphic with the direct sum of $\text{End}(S^\lambda)$:

$$
\mathbb{C}[S_n] \cong \bigoplus_{\lambda \vdash n} \text{End}(S^\lambda).
$$

We emphasize that being different from decomposing $V^\otimes n$ by $SU(d) - S_n$ duality, all kinds of Young diagrams $\lambda$, standing for inequivalent $S_n$-irreps, appears once and only once in the above direct sum decomposing $\mathbb{C}[S_n]$. In any case, restricting to each $\lambda$, $\pi_{\mathbb{C}[S_n]}$ produces all $\dim S^\lambda \times \dim S^\lambda$ matrices and hence any matrix commuting with $\pi_{\mathbb{C}[S_n]}$ should be a scalar.

II. LINEAR COMBINATION OF UNITARIES

Linear Combination of Unitaries (LCU) was proposed in [2–4] and we adapt this as a possible methods for simulating Hamiltonians constructed by elements from $\mathbb{C}[S_n]$. With the awareness of Schur-Weyl duality, these Hamiltonians have direct physics implication: they preserve $SU(d)$ symmetry. A well-known example is the Heisenberg Hamiltonian of magnetism [5, 6]. We provide in the following a brief description of LCU. Practical implementation details with complexity analysis can be found in [2–4].

Suppose we are going to simulate $e^{-itH} |\psi\rangle$ for some state $|\psi\rangle$ with $H = \pi(f)$ for some $f \in \mathbb{C}[S_n]$. As we written in the main text, $e^{-itH}$ would always be expanded by truncated to a certain order $K$. Let us denote the approximate matrix by $M$ and suppose $M = \sum_{j=1}^{m} \alpha_j V_j$ with $V_j$ being unitaries. Note that in our case, $V_j$ are products of permutations $\sigma_{i_1}, ..., \sigma_{i_k} \in S_n$. The coefficients $\alpha_j$ can be set as positive reals, as their complex phase can be absorbed into $V_j$. We denote by $\|\alpha\|_1 = \sum_j |\alpha_j|$ for later use.

Then we need to prepare $|\log_2 m\rangle$ ancilla qudits with respect to which the computational basis is registered as $|j\rangle$ for $j = 0, ..., m$. Let $W$ be a unitary acting on these ancillas such that

$$
W |0\rangle = \frac{1}{\sqrt{\|\alpha\|_1}} \sum_j \sqrt{\alpha_j} |j\rangle.
$$

Assume we can also construct control operators: $|j\rangle \langle j| \otimes V_j$ with $V = \sum_{j=1}^{m} |j\rangle \langle j| \otimes V_j$. Then

$$
(\langle 0| \otimes I) W^{-1} W |0\rangle \langle 0| \otimes V_j = \frac{1}{\|\alpha\|_1} \left( \sum_j \sqrt{\alpha_j} |j\rangle \otimes I \right) \left( \sum_j \sqrt{\alpha_j} |j\rangle \langle j| \right) = \frac{1}{\|\alpha\|_1} M |\psi\rangle,
$$

which gives the state we want to approximate when we measure ancillas with the outcome being $0$. However, the probability to retrieve this outcome is $\|M |\psi\rangle\|^2/\|\alpha\|_1^2$ which may not be large enough. Then we apply oblivious amplitude amplification to amplify it. Roughly speaking, by applying $-URU^{-1}R$ with $R = (I - 2 |0\rangle \langle 0|) \otimes I$ and $U := W^{-1} VW$ to $|0\rangle |\psi\rangle$, the amplitude of the target state will be enlarged. Note that as $M \approx e^{-itH}$ is nearly unitary, $\|M |\psi\rangle\|^2/\|\alpha\|_1^2 \approx 1/\|\alpha\|_1^2$ and $O(1/\|\alpha\|_1^2)$ times amplification will be enough [2–4].

In our case, let $H = \pi(f)$ with $f = \sum c_i \sigma_i$ and $\sigma_i$ being $k$-local. Then

$$
\exp(-i\Delta t H) = \sum_{m=0}^{K} \sum_{i_1,...,i_m} (-i\Delta t)^m_{m!} c_{i_1}...c_{i_m} \sigma_{i_1}...\sigma_{i_m} = \sum_{m=0}^{K} \sum_{i_1,...,i_m} \tilde{c}_{i_1}...\tilde{c}_{i_m} \sigma_{i_1}...\sigma_{i_m} + O(\tilde{c}) = M + O(\tilde{c}),
$$

where $N = O(n^k)$ is the number of all $k$-local permutations. To apply LCU, we need $O(K \log d N)$ qudits. We divide the evolution into small steps with time $\Delta t$ in each step such that

$$
\|\tilde{c}\|_1 = \sum_{k=0}^{K} \sum_{i_1,...,i_m} \tilde{c}_{i_1}...\tilde{c}_{i_m} \leq \sum_{k=0}^{\infty} \left(\frac{-i\Delta t}{m!}\right)^m \sum_{i_1,...,i_m} c_{i_1}...c_{i_m} = e^{\Delta t \|c\|_1} = O(1).
$$
Thus applying the oblivious amplitude amplification by constant times is sufficient to complete the task.

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