

Optimality of T -gate for generating magic resource

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Abstract

In the stabilizer formalism of fault-tolerant quantum computation, stabilizer states serve as classical objects, while magic states (non-stabilizer states) are a kind of quantum resource (called magic resource) for promoting stabilizer circuits to universal quantum computation. In this framework, the T -gate is widely used as a non-Clifford gate which generates magic resource from stabilizer states. A natural question arises as whether the T -gate is in some sense optimal for generating magic resource. We address this issue by employing an intuitive and computable quantifier of magic based on characteristic functions (Weyl transforms) of quantum states. We demonstrate that the qubit T -gate, as well as its qutrit extension, the qutrit T -gate, are indeed optimal for generating magic resource among the class of diagonal unitary operators. Moreover, up to Clifford equivalence, the T -gate is essentially the only gate having such an optimal property. This reveals some intrinsic optimal features of the T -gate. We further compare the T -gate with general unitary gates for generating magic resource.

Keywords: stabilizer formalism, Pauli group, Clifford group, quantifiers of magic, T -gate

(Some figures may appear in colour only in the online journal)

1. Introduction

A convenient and popular framework for fault-tolerant quantum computation is the stabilizer formalism with magic state injection [1–22]. The celebrated Gottesman–Knill theorem shows that stabilizer circuits (composed of Clifford unitaries, Pauli measurements, conditioning on measurement outcomes, and classical randomness) can be efficiently simulated by classical computers [1, 8], while universal fault-tolerant quantum computation can be achieved via injection of magic states (non-stabilizer states) or magic-resource-generating gates (e.g. the T -gate) into stabilizer circuits [1–6].

Various protocols for magic state distillation, which generate more refined magic states from coarse ones have been extensively studied [6, 9–11, 14–16, 21]. This is helpful in paving the way for generating magic resource in order to implement quantum computation via the stabilizer formalism and magic resource.

For controlling and manipulating magic resource, it is desirable to quantify the amount of magic (non-stabilizerness) from different perspectives. Many quantifiers of magic have

been introduced in various contexts. For example, the sum negativity (with the associated mana and thauma) uses the negative part of the discrete Wigner functions as an indicator of magic [11, 20, 21]. The stabilizer rank, defined as the minimal number of components in the expansion of a state in terms of stabilizer states, was introduced in [13, 18]. The relative entropy of magic (with the associated max-relative entropy and min-relative entropy of magic), and the robustness of magic, were studied in [11, 15, 17]. Apart from the sum negativity, these quantifiers of magic are in general quite difficult to calculate. The sum negativity is computable, however, it relies heavily on the discrete Wigner functions in odd dimensions, which excludes its direct usage in other dimensions. In particular, the ubiquitous qubit case is excluded. It is desirable to seek easily computable quantifiers of magic applicable to all dimensions and not depending on the discrete Wigner functions [22].

The T -gate plays a crucial role in the Clifford + T gate set, which is approximately universal for fault-tolerant quantum computation [23–35]. The qutrit version of the qubit T -gate is introduced in [10, 23, 27], and shares a variety of

similar properties with the qubit T -gate. The T -count (the number of T -gate used in a circuit) is widely used as a benchmark for the complexity of a circuit [24, 25]. A basic feature of the T -gate lies in that it is a powerful and convenient gate for generating magic states from stabilizer states, and can be fault-tolerantly implemented.

In this context, a natural question arises as how powerful or optimal the T -gate is for generating magic resource. The present work is devoted to addressing this issue. For this purpose, we will employ a quantifier of magic based on characteristic functions (Weyl transforms) of quantum states to assess the power (capability) of quantum gates for generating magic resource. We will demonstrate that both the qubit T -gate and qutrit T -gate are optimal for generating magic resource in the class of diagonal unitary operators, and up to Clifford equivalence, they are essentially the only ones having this optimality.

The remainder of the work is structured as follows. In section 2, as preliminaries, we review some basic aspects of the stabilizer formalism, in which states are classified into stabilizer states and magic states, with the latter regarded as a magic resource serving as quantumness for promoting stabilizer circuits to universal quantum computation. In section 3, we study magic-resource-generating power of quantum gates (i.e. unitary operators) and reveal some optimal features of the T -gate for both qubit and qutrit systems. We employ characteristic functions (which are well-defined on all dimensions) rather than the discrete Wigner functions (which are only well-defined on odd dimensions) to construct a computable quantifier of magic. We consider both the maximal and average scenarios for quantifying magic-resource generating power. Finally, we present a summary and discussion in section 4. The detailed proof of the main result, proposition 2, is presented in the [appendix](#).

2. Preliminaries: stabilizer states and magic states

In this section, we review the basic features of the stabilizer formalism, which plays an important role in quantum error correction and fault-tolerant quantum computation [1–9, 11–22]. The Pauli group (discrete Heisenberg-Weyl group) and the Clifford group are basic ingredients for constructing stabilizer circuits, which can be efficiently simulated by classical means, while non-Clifford gates such as the T -gate are necessary for universal quantum computation.

We first recall the Pauli group, which will play a crucial role in this work. For a d -dimensional quantum system \mathbb{C}^d with computational basis $\{|j\rangle: j \in \mathbb{Z}_d\}$, we may regard $\mathbb{Z}_d = \{0, 1, \dots, d-1\}$ (the ring of integers modulo d) as a discrete configuration space of this system, and identify $L^2(\mathbb{Z}_d)$ (the set of complex functions on \mathbb{Z}_d) with \mathbb{C}^d , regarded naturally as a finite-dimensional Hilbert space. In this space, two fundamental unitary operators [36]

$$X = \sum_{k=0}^{d-1} |k+1\rangle\langle k|, \quad Z = \sum_{k=0}^{d-1} \omega^k |k\rangle\langle k|, \quad \omega = e^{2\pi i/d},$$

emerge naturally and serve as building blocks for finite-dimensional quantum mechanics. Clearly,

$$X|k\rangle = |k+1\rangle, \quad Z|k\rangle = \omega^k |k\rangle, \quad k \in \mathbb{Z}_d.$$

The arithmetic is modular d , and thus $|d\rangle = |0\rangle$. Associated with these two basic operators, the discrete Heisenberg-Weyl operators are defined as

$$D_{k,l} = \tau^{kl} X^k Z^l, \quad k, l \in \mathbb{Z},$$

where $\tau = -e^{\pi i/d} = -\sqrt{\omega}$. Here we emphasize that $D_{k,l}$ are well defined for all $k, l \in \mathbb{Z}$, though we will mainly consider $k, l \in \mathbb{Z}_d$. We call $(k, l) \in \mathbb{Z}_d \times \mathbb{Z}_d$ (discrete phase-space) a phase-space point. The discrete Heisenberg-Weyl operators constitute a projective representation of the translation groups $\mathbb{Z}_d \times \mathbb{Z}_d$ and $\mathbb{Z} \times \mathbb{Z}$, and satisfy

$$D_{k,l} D_{s,t} = \tau^{ls-kt} D_{k+s, l+t}, \quad k, l, s, t \in \mathbb{Z}. \quad (1)$$

Moreover,

$$\text{tr}(D_{k,l} D_{s,t}^\dagger) = d \delta_{k,s} \delta_{l,t}, \quad k, l, s, t \in \mathbb{Z}_d,$$

and $\{\frac{1}{\sqrt{d}} D_{k,l}: k, l \in \mathbb{Z}_d\}$ constitutes an orthonormal basis for the d^2 -dimensional operator space $L(\mathbb{C}^d)$, the set of all operators on \mathbb{C}^d equipped with the Hilbert-Schmidt inner product $\langle A|B \rangle = \text{tr}(A^\dagger B)$.

For the convenience of our approach, we take the Pauli group (discrete Heisenberg-Weyl group) as

$$\mathcal{P}_d = \{\tau^j D_{k,l}: j \in \mathbb{Z}_{2d}, k, l \in \mathbb{Z}_d\}.$$

In particular, $\mathcal{P}_2 = \{c1, c\sigma_x, c\sigma_y, c\sigma_z: c = \pm 1, \pm i\}$, with $\sigma_x, \sigma_y, \sigma_z$ being the standard Pauli operators. The Clifford group

$$\mathcal{C}_d = \{V \in \mathcal{U}_d: V \mathcal{P}_d V^\dagger = \mathcal{P}_d\}$$

is the normalizer (natural symmetry group) of \mathcal{P}_d in the full unitary group \mathcal{U}_d on \mathbb{C}^d . This group plays an instrumental role in the stabilizer quantum computation.

A stabilizer state is defined as a common eigenstate (with common eigenvalue 1) of a maximal Abelian subgroup of the Clifford group \mathcal{C}_d . In this context, the subgroup is called the stabilizer group of the stabilizer state. The set of (pure) stabilizer states in \mathbb{C}^d is denoted by \mathcal{S}_d , which consists exactly of $|\mathcal{S}_d| = d(d+1)$ elements [7]. In prime power dimensions, any state of the form $V|j\rangle$ is a stabilizer state. Here $|j\rangle \in \mathbb{C}^d$ is any computational basis state and $V \in \mathcal{C}_d$ is any Clifford operator [7, 11]. Convex mixtures (i.e. probabilistic mixtures) of pure stabilizer states are called mixed stabilizer states. Any state (pure or mixed) that cannot be expressed as a convex mixture of pure stabilize states is called a magic state (non-stabilizer state). Any magic state is regarded as magic resource.

The sets of pure stabilizer states in \mathbb{C}^d for $d=2$ and 3 are listed in tables 1 and 2, respectively, which will be needed in the sequel.

For the purpose of studying the power of quantum gates for generating magic resource, we need to quantify magic resource [11, 14–22]. For any quantum state (pure or mixed) ρ on \mathbb{C}^d , we employ the following quantifier

$$M(\rho) = \sum_{k,l \in \mathbb{Z}_d} |\text{tr}(\rho D_{k,l})| \quad (2)$$

Table 1. Qubit stabilizer states and the corresponding stabilizer generators, which stabilize the corresponding states and generate the corresponding maximal Abelian subgroups of \mathcal{P}_2 stabilizing the corresponding states. For example, $\sigma_x|+\rangle = |+\rangle$, and σ_x generates the maximal Abelian subgroup $\{1, \sigma_x\}$ stabilizing the state $|+\rangle$. The three operators σ_x , σ_y and σ_z are the Pauli spin operators (matrices).

Stabilizer state	$ +\rangle$	$ -\rangle$	$ +i\rangle$	$ - i \rangle$	$ 0\rangle$	$ 1\rangle$
Stabilizer generator	σ_x	$-\sigma_x$	σ_y	$-\sigma_y$	σ_z	$-\sigma_z$

Table 2. Qutrit stabilizer states $|\phi_j\rangle$, $j = 1, 2, \dots, 12$, and the corresponding stabilizer generators, which stabilize the corresponding states and generate the corresponding stabilizer groups. For example, $Z|0\rangle = |0\rangle$, and Z generates the corresponding stabilizer group $\{1, Z, Z^\dagger\}$, which is a maximal Abelian subgroup of \mathcal{P}_3 stabilizing the state $|0\rangle$. Noting that $XX^\dagger = ZZ^\dagger = 1$, $X^3 = Z^3 = 1$, $XZ = \omega^{-1}ZX$, $\omega = e^{2\pi i/3}$.

Stabilizer state	Stabilizer generator
$ \phi_1\rangle = 0\rangle$	Z
$ \phi_2\rangle = 1\rangle$	$\omega^{-1}Z$
$ \phi_3\rangle = 2\rangle$	ωZ
$ \phi_4\rangle = (0\rangle + 1\rangle + 2\rangle)/\sqrt{3}$	X
$ \phi_5\rangle = (0\rangle + \omega^{-1} 1\rangle + \omega 2\rangle)/\sqrt{3}$	$\omega^{-1}X$
$ \phi_6\rangle = (0\rangle + \omega 1\rangle + \omega^{-1} 2\rangle)/\sqrt{3}$	ωX
$ \phi_7\rangle = (0\rangle + 1\rangle + \omega 2\rangle)/\sqrt{3}$	XZ
$ \phi_8\rangle = (\omega 0\rangle + 1\rangle + 2\rangle)/\sqrt{3}$	$\omega^{-1}XZ$
$ \phi_9\rangle = (0\rangle + \omega 1\rangle + 2\rangle)/\sqrt{3}$	ωXZ
$ \phi_{10}\rangle = (0\rangle + 1\rangle + \omega^{-1} 2\rangle)/\sqrt{3}$	XZ^\dagger
$ \phi_{11}\rangle = (0\rangle + \omega^{-1} 1\rangle + 2\rangle)/\sqrt{3}$	$\omega^{-1}XZ^\dagger$
$ \phi_{12}\rangle = (\omega^{-1} 0\rangle + 1\rangle + 2\rangle)/\sqrt{3}$	ωXZ^\dagger

introduced in [22], which is easy to compute and has a variety of useful properties:

- $1 \leq M(\rho) \leq 1 + (d-1)\sqrt{d+1}$.
- $M(\rho)$ is invariant under the Clifford operations in the sense that $M(V\rho V^\dagger) = M(\rho)$, $\forall V \in \mathcal{C}_d$.
- $M(\rho)$ is convex in ρ .
- Among all states (pure or mixed), $M(\rho)$ achieves the minimal value 1 if and only if $\rho = \mathbf{1}/d$ is the maximally mixed state. In view of this property, one may prefer to employ $M_0(\rho) = M(\rho) - 1$ as a more appropriate quantifier of magic. However, we will not make this convention.
- Among pure states, $M(|\psi\rangle\langle\psi|)$ achieves the minimal value d if and only if $|\psi\rangle$ is a stabilizer state. Consequently, all pure stabilizer states have the same value of magic (i.e. d). In particular, by the above properties, we have the following simple criterion for non-stabilizerness (magic states): if $M(\rho) > d$, then the state ρ is magic. It should be noticed that this is only a sufficient, but not necessary, condition for a state on \mathbb{C}^d to be magic.

A remarkable feature of $M(\rho)$ is that it achieves the maximal value $1 + (d-1)\sqrt{d+1}$ by any SIC-POVM

fiducial state (assuming its existence, which has been proved in many dimensions) [22]. In particular, it is known that such fiducial states exist in many dimensions, including the cases $d=2, 3$ [37, 38]. Recall that a SIC-POVM (symmetric informationally complete positive operator valued measure) in \mathbb{C}^d is a POVM $\{E_\alpha: \alpha=1, 2, \dots, d^2\}$ (i.e. $E_\alpha \geq 0$, $\sum_{\alpha=1}^{d^2} E_\alpha = \mathbf{1}$) consisting of d^2 rank-one operators with equal trace and equal overlap and spanning the whole state space [37, 38]. It has been shown that SIC-POVMs exist in many dimensions, although the general existence remains an outstanding open problem (Zauner's conjecture) [37–53]. A SIC-POVM fiducial state is a pure state $|f\rangle \in \mathbb{C}^d$ such that its orbit $\{E_{k,l} = \frac{1}{d} D_{k,l}|f\rangle\langle f| D_{k,l}^\dagger: k, l \in \mathbb{Z}_d\}$ under the Pauli group constitutes a SIC-POVM. Fiducial states have been explicitly constructed in many dimensions, and most SIC-POVMs are constructed from fiducial states [37, 38].

For any quantum gate described by a unitary operator U on \mathbb{C}^d , by employing $M(\cdot)$ defined by equation (2) as a quantifier of magic, we introduce the following quantities

$$M_{\max}(U) = \max_{|\psi\rangle \in \mathcal{S}_d} M(U|\psi\rangle),$$

$$M_{\text{ave}}(U) = \frac{1}{|\mathcal{S}_d|} \sum_{|\psi\rangle \in \mathcal{S}_d} M(U|\psi\rangle),$$

which characterize the maximal and average magic-resource-generating powers of U , respectively. Here $|\mathcal{S}_d| = d(d+1)$ is the number of pure stabilizer states in \mathbb{C}^d [7]. We will use these quantities to characterize the T -gate from an optimal perspective.

3. Optimality of T -gate for generating magic-resource

In this section, we evaluate explicitly the magic-resource-generating power of some unitary gates in the qubit ($d=2$) and qutrit ($d=3$) cases. In particular, we illuminate some optimal features of the T -gate: In these low dimensions, the T -gate is optimal for generating magic resource among the class of diagonal unitary gates.

3.1. Qubit T -gate

For a qubit system ($d=2$) with computational basis $\{|0\rangle, |1\rangle\}$, there are six pure stabilizer states [7, 16]

$$|\pm\rangle = \frac{1}{\sqrt{2}}(|0\rangle \pm |1\rangle), \quad |\pm i\rangle = \frac{1}{\sqrt{2}}(|0\rangle \pm i|1\rangle), \quad |0\rangle, |1\rangle,$$

which correspond to the three pairs of antipodal points in the intersection of the three principal axes and the Bloch sphere, and may be partitioned into three mutually unbiased bases $\{|\pm\rangle\}$, $\{|\pm i\rangle\}$, and $\{|0\rangle, |1\rangle\}$ for \mathbb{C}^2 . Geometrically, they constitute the vertex of the stabilizer octahedron inscribed in the qubit Bloch sphere. These states are listed in table 1 together with the corresponding stabilizer generators.

In magic state distillation and gate synthesis, the non-Clifford qubit T -gate [6]

$$\begin{aligned} T_2 &= |0\rangle\langle 0| + e^{i\pi/4}|1\rangle\langle 1| \\ &= e^{i\pi/8}(e^{-i\pi/8}|0\rangle\langle 0| + e^{i\pi/8}|1\rangle\langle 1|) \\ &= \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{pmatrix}, \end{aligned} \quad (3)$$

plays a prominent role and has been widely used as a benchmark for non-stabilizerness of qubit gates. Due to the presence of $\pm\pi/8$ (corresponding to rotation with angle $\pi/8$), this T -gate is also called $\pi/8$ -gate, and if one ignores the overall phase $e^{i\pi/8}$, one also regards $e^{-i\pi/8}|0\rangle\langle 0| + e^{i\pi/8}|1\rangle\langle 1|$ as the $\pi/8$ -gate.

To address the optimality of the qubit gate T_2 defined by equation (3), consider the family of qubit diagonal unitary gates

$$U_\theta = |0\rangle\langle 0| + e^{i\theta}|1\rangle\langle 1| = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\theta} \end{pmatrix}, \quad \theta \in [0, 2\pi), \quad (4)$$

which includes the T -gate $T_2 = U_{\pi/4}$ as a special instance. By simple and direct calculations, we have

$$M(U_\theta|\pm) = M(U_\theta|\pm i) = 1 + |\cos \theta| + |\sin \theta|,$$

$$M(U_\theta|0) = M(U_\theta|1) = 2.$$

Consequently

$$M_{\max}(U_\theta) = 1 + |\cos \theta| + |\sin \theta|,$$

$$M_{\text{ave}}(U_\theta) = \frac{4}{3} + \frac{2}{3}(|\cos \theta| + |\sin \theta|),$$

from which we readily conclude that in the qubit gate set $\{U_\theta: \theta \in [0, 2\pi)\}$ defined by equation (4), the qubit T -gate $T_2 = U_{\pi/4}$ has the maximal magic-resource-generating power in the sense that

$$\max_{\theta} M_{\max}(U_\theta) = M_{\max}(T_2) = 1 + \sqrt{2},$$

$$\max_{\theta} M_{\text{ave}}(U_\theta) = M_{\text{ave}}(T_2) = \frac{1}{3}(4 + 2\sqrt{2}).$$

Due to the Clifford invariance of the quantifier of magic $M(\rho)$, we conclude that the gate VT_2W also achieves the above maximal value of magic-resource-generating power for any Clifford unitaries $V, W \in \mathcal{C}_2$.

Since the qubit T -gate T_2 is optimal for generating magic resource among the diagonal unitary gates, it is natural to ask whether it is optimal in the set of all unitary gates. By properties (a) and (c) of the quantifier of magic $M(\rho)$, we know that for a qubit system ($d=2$),

$$\max_U M(U|0) = 1 + (d-1)\sqrt{d+1} = 1 + \sqrt{3},$$

where the max is taken over \mathcal{U}_2 (all unitary operators on \mathbb{C}^2). Consequently, the maximal magic-resource-generating power among all unitary operators is

$$\max_U M_{\max}(U) = 1 + \sqrt{3}. \quad (5)$$

For example, any unitary operator $U \in \mathcal{U}_2$ satisfying

$$U|0\rangle = \cos \beta|0\rangle + e^{i\pi/4} \sin \beta|1\rangle, \quad \cos(2\beta) = \frac{1}{\sqrt{3}}$$

achieves the above maximal value.

In view of the fact that

$$M_{\max}(T_2) = 1 + \sqrt{2} < 1 + \sqrt{3},$$

we conclude that the qubit T -gate T_2 is not optimal in the whole set of unitary gates. However, by simple preprocessing via rotations

$$R_\gamma = \begin{pmatrix} \cos \frac{\gamma}{2} & -\sin \frac{\gamma}{2} \\ \sin \frac{\gamma}{2} & \cos \frac{\gamma}{2} \end{pmatrix}, \quad \gamma \in [0, 2\pi)$$

the maximal magic-resource-generating power in all unitary gates can be achieved. We summarize the results as follows.

Proposition 1. Among the gate set $\{U_\theta: 0 \leq \theta < 2\pi\}$ of diagonal unitary operators on \mathbb{C}^2 , the qubit T -gate T_2 is optimal for generating magic resource in the sense that

$$\max_{\theta} M_{\max}(U_\theta) = M_{\max}(T_2) = 1 + \sqrt{2}.$$

Among the gate set of all unitary operators on \mathbb{C}^2 , the combination of the qubit T -gate T_2 and the rotation R_{γ^*} is optimal for generating magic resource in the sense that

$$\max_U M_{\max}(U) = M_{\max}(T_2 R_{\gamma^*}) = 1 + \sqrt{3}, \quad (6)$$

where $\gamma^* = \gamma_0$ or $\pi/2 - \gamma_0$ with γ_0 determined by $\cos \gamma_0 = 1/\sqrt{3}$, $\gamma_0 \in [0, \pi/2]$.

To establish equation (6), noting equation (5), it suffices to show that

$$M_{\max}(T_2 R_{\gamma^*}) = 1 + \sqrt{3}.$$

By direct calculations, we have

$$\begin{aligned} M(T_2 R_\gamma|\pm) &= 1 + \sin \gamma + \sqrt{2} \cos \gamma \\ &= 1 + \sqrt{3} \sin(\gamma + \gamma_0), \end{aligned}$$

$$M(T_2 R_\gamma|\pm i) = 1 + \sqrt{2},$$

$$\begin{aligned} M(T_2 R_\gamma|0) &= M(T_2 R_\gamma|1) = 1 + \sqrt{2} \sin \gamma + \cos \gamma \\ &= 1 + \sqrt{3} \cos(\gamma - \gamma_0), \end{aligned}$$

from which it can be readily checked that

$$\max_{\gamma} M_{\max}(T_2 R_\gamma) = M_{\max}(T_2 R_{\gamma^*}) = 1 + \sqrt{3}.$$

Of course, in view of the Clifford invariance of the quantifier of magic $M(\rho)$, the gate $VT_2 R_{\gamma^*} W$ also achieves the above maximal value for any Clifford unitaries $V, W \in \mathcal{C}_2$.

3.2. Qutrit T -gate

For a qutrit system ($d=3$) with computational basis $\{|0\rangle, |1\rangle, |2\rangle\}$, there are $3(3+1) = 12$ pure stabilizer states, which are

listed in table 2 together with the corresponding stabilizer generators. It is remarkable that these 12 stabilizer states can be partitioned into 4 mutually unbiased bases of \mathbb{C}^3 as

$$B_\mu = \{|\phi_{i+3\mu}\rangle : i = 1, 2, 3\}, \quad \mu = 0, 1, 2, 3.$$

The qutrit T -gate T_3 is defined as [23, 27]

$$T_3 = |0\rangle\langle 0| + e^{-2\pi i/9}|1\rangle\langle 1| + e^{2\pi i/9}|2\rangle\langle 2|$$

$$= \begin{pmatrix} 1 & 0 & 0 \\ 0 & e^{-2\pi i/9} & 0 \\ 0 & 0 & e^{2\pi i/9} \end{pmatrix}, \quad (7)$$

which is a diagonal unitary operator. This gate generates a group $\{T_3^k : k = 0, 1, \dots, 8\}$ consisting of elements of the forms Z^j (which are Pauli operators), $T_3 Z^j$ and $H^2 T_3 H^2 Z^j$ (which are Clifford equivalent to T_3). Here

$$H = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 1 & 1 \\ 1 & \omega & \omega^2 \\ 1 & \omega^2 & \omega \end{pmatrix}, \quad Z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \omega & 0 \\ 0 & 0 & \omega^2 \end{pmatrix}, \quad (8)$$

are the qutrit Hadamard gate H and the Z operator in a qutrit system (in the matrix form relative to the computational basis) and $\omega = e^{2\pi i/3}$ henceforth. Indeed, by noting that

$$T_3^2 = H^2 T_3 H^2 Z^2, \quad T_3 H^2 T_3 = H^2,$$

we readily derive that

$$T_3^3 = Z^2, \quad T_3^4 = T_3 Z^2, \quad T_3^5 = H^2 T_3 H^2 Z,$$

$$T_3^6 = Z, \quad T_3^7 = T_3 Z, \quad T_3^8 = H^2 T_3 H^2.$$

Consider the family of qutrit diagonal gates

$$U_{\theta_1, \theta_2} = |0\rangle\langle 0| + e^{i\theta_1}|1\rangle\langle 1| + e^{i\theta_2}|2\rangle\langle 2|$$

$$= \begin{pmatrix} 1 & 0 & 0 \\ 0 & e^{i\theta_1} & 0 \\ 0 & 0 & e^{i\theta_2} \end{pmatrix}, \quad (9)$$

where $\theta_1, \theta_2 \in [-\pi, \pi)$. Without loss of generality, we may assume that $\theta_1 \leq \theta_2$. We have the following optimal characterization of T_3 , the qutrit version of the T -gate.

Proposition 2. *In the qutrit gate set $\{U_{\theta_1, \theta_2} : -\pi \leq \theta_1 \leq \theta_2 < \pi\}$ defined by equation (9), the qutrit T -gate $T_3 = U_{-2\pi/9, 2\pi/9}$ has the maximal magic-resource-generating power in the sense that*

$$\max_{\theta_1, \theta_2} M_{\max}(U_{\theta_1, \theta_2}) = M_{\max}(T_3) = 1 + 2\sqrt{3}, \quad (10)$$

$$\max_{\theta_1, \theta_2} M_{\text{ave}}(U_{\theta_1, \theta_2}) = M_{\text{ave}}(T_3) = \frac{3}{2}(1 + \sqrt{3}), \quad (11)$$

where the max is over $\theta_1, \theta_2 \in [-\pi, \pi)$. Moreover, all solutions of (θ_1, θ_2) in the domain $\pi \leq \theta_1 \leq \theta_2 < \pi$ for U_{θ_1, θ_2} achieving the maximal values of magic-resource-generating power are listed in table 3. Any gate VT_3W also achieves the above maximal value for any Clifford unitaries $V, W \in \mathcal{C}_3$.

The detailed proof is deferred to the appendix.

For numerical illustration, we depict the graph of $M_{\max}(U_{\theta_1, \theta_2})$ in figure 1, which clearly exhibits the same feature for the maximal value as in proposition 2.

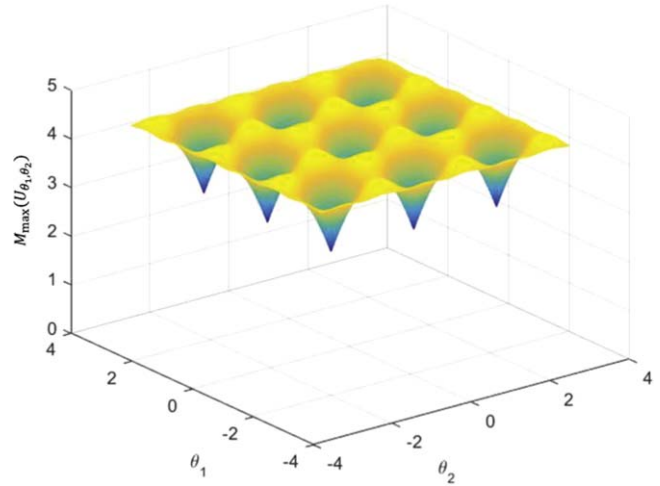


Figure 1. The graph of $M_{\max}(U_{\theta_1, \theta_2})$ on the domain $\theta_1, \theta_2 \in [-\pi, \pi)$. We see that there are 18 pairs of (θ_1, θ_2) achieving the same maximal value $1 + 2\sqrt{3} \approx 4.4641$. In the region $-\pi \leq \theta_1 \leq \theta_2 < \pi$, there are 9 pairs of (θ_1, θ_2) , as listed in table 3, which achieve the maximal value. We also observe that $M_{\max}(U_{\theta_1, \theta_2}) \geq 3$.

Table 3. Gates $U_{\theta_1, \theta_2} = |0\rangle\langle 0| + e^{i\theta_1}|1\rangle\langle 1| + e^{i\theta_2}|2\rangle\langle 2|$ with the maximal magic-resource-generating power, which include the qutrit T -gate $T_3 = U_{-2\pi/9, 2\pi/9}$. All gates U_{θ_1, θ_2} with (θ_1, θ_2) in the following table are optimal for generating magic resource among the diagonal set of unitary gates, and yield the same value $1 + 2\sqrt{3}$ of maximal magic-resource-generating power. Actually, all these gates are Clifford equivalent to T_3 .

θ_1	$-\frac{2\pi}{9}$	$-\frac{4\pi}{9}$	$-\frac{8\pi}{9}$	$-\frac{8\pi}{9}$	$-\frac{8\pi}{9}$	$-\frac{4\pi}{9}$	$-\frac{2\pi}{9}$	$\frac{2\pi}{9}$	$\frac{4\pi}{9}$
θ_2	$\frac{2\pi}{9}$	$\frac{4\pi}{9}$	$\frac{8\pi}{9}$	$-\frac{4\pi}{9}$	$\frac{2\pi}{9}$	$-\frac{2\pi}{9}$	$\frac{8\pi}{9}$	$\frac{4\pi}{9}$	$\frac{8\pi}{9}$

Let (noting here $\omega = e^{2\pi i/3}$)

$$S = |0\rangle\langle 0| + |1\rangle\langle 1| + \omega|2\rangle\langle 2| = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \omega \end{pmatrix} \quad (12)$$

be the qutrit phase gate, which is a Clifford unitary since $SXS^\dagger = XZ$ and $SZS^\dagger = Z$. The following result shows that up to Clifford equivalence, the gate T_3 is essentially the only gate among the diagonal unitary gates for optimally generating the magic resource: All the gates listed in table 3 are Clifford equivalent to the gate T_3 , i.e. are of the forms VT_3W for some Clifford unitaries $V, W \in \mathcal{C}_3$. More explicitly

- $U_{-2\pi/9, 2\pi/9} = T_3$,
- $U_{-4\pi/9, 4\pi/9} = H^2 T_3 H^2 Z^2$,
- $U_{-8\pi/9, 8\pi/9} = T_3 Z^2$,
- $U_{-8\pi/9, -4\pi/9} = T_3 Z^2 S$,
- $U_{-8\pi/9, 2\pi/9} = T_3 Z^2 S^2$,
- $U_{-4\pi/9, -2\pi/9} = H^2 T_3 H^2 Z^2 S^2$,
- $U_{-2\pi/9, 8\pi/9} = T_3 S$,
- $U_{2\pi/9, 4\pi/9} = H^2 T_3 H^2 S$,
- $U_{4\pi/9, 8\pi/9} = T_3 Z S^2$.

Here H is the qutrit Hadamard gate defined by equation (8), and S is the qutrit phase gate defined by equation (12). The proof is via direct verification.

Table 4. Comparison between magic-resource-generating power for diagonal and general (non-diagonal) unitary gates in qubit and qutrit systems. Here \mathcal{D}_d is the set of diagonal unitary operators, which is a subgroup of the set \mathcal{U}_d of all unitary operators.

d	$\max_{U \in \mathcal{D}_d} M_{\max}(U) = M_{\max}(T_d)$	$\max_{U \in \mathcal{U}_d} M_{\max}(U)$
2 (qubit)	$1 + \sqrt{2}$	$1 + \sqrt{3}$
3 (qutrit)	$1 + 2\sqrt{3}$	5

We emphasize that although in the gate set $\{U_{\theta_1, \theta_2}: \theta_1, \theta_2 \in [-\pi, \pi)\}$, the qutrit T -gate T_3 has the maximal magic-resource-generating power, there exist *non-diagonal* gates possessing higher magic-resource-generating power since, for a qutrit system ($d=3$)

$$\begin{aligned} \max_{\rho} M(\rho) &= 1 + (3-1)\sqrt{3+1} \\ &= 5 > M_{\max}(T_3) = 1 + 2\sqrt{3}. \end{aligned}$$

For example, any unitary operator $U_0 \in \mathcal{U}_3$ satisfying

$$U_0|0\rangle = \frac{1}{\sqrt{2}}(|1\rangle - |2\rangle)$$

has the maximal magic-resource-generating power

$$M_{\max}(U_0) = \max_{U \in \mathcal{U}_d} M_{\max}(U) = 5.$$

We summarize the results in table 4.

4. Summary

In the stabilizer formalism of fault-tolerant quantum computation, the Clifford + T gate set is usually adapted as the basic structure. Since by the Gottesman–Knill theorem, the Clifford circuits can be efficiently simulated by classical means, the quantum power comes from the T -gate and its interaction with Clifford circuits. The T -gate is widely employed to generate magic resource (magic states) from stabilizer states. Consequently, it is desirable to study the power of the T -gate for generating magic resource, and to ask whether it is optimal in some sense.

By employing a natural quantifier of magic (non-stabilizerness), we have shown that the qubit T -gate and qutrit T -gate are indeed optimal for generating magic resource among the class of diagonal unitaries, and furthermore, up to Clifford equivalence, they are essentially the only ones. This highlights a fundamental and optimal feature of the T -gate, and provides new support for the utilization of the T -gate.

For higher dimensional systems, the calculation is considerably more complicated, and we may expect similar results. However, this calls for further investigations. It is certainly worthwhile to classify and identify the optimal gates for generating magic resource in the general case for other quantifiers of magic, such as the relative entropy of magic and sum negativity.

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Appendix

Here we present the detailed proof of proposition 2 in section 3.

We first establish equation (10). For the qutrit stabilizer states listed in table 2, by direct calculations, we have

$$M(U_{\theta_1, \theta_2}|\phi_j\rangle) = 3, \quad j = 1, 2, 3 \quad (\text{A1})$$

and

$$M(U_{\theta_1, \theta_2}|\phi_j\rangle) = 1 + \frac{2}{3} \sum_{k=0}^2 \sqrt{3 + 2x_k}, \quad j = 4, \dots, 12 \quad (\text{A2})$$

with

$$\begin{aligned} x_k &= \cos\left(\alpha + \frac{2k\pi}{3}\right) + \cos\left(-\frac{\alpha}{2} + \frac{3\beta}{2} + \frac{2k\pi}{3}\right) \\ &\quad + \cos\left(-\frac{\alpha}{2} - \frac{3\beta}{2} + \frac{2k\pi}{3}\right), \quad k = 0, 1, 2, \end{aligned}$$

and

$$\alpha = \theta_1 + \theta_2 \in [-2\pi, 2\pi), \quad \beta = \theta_1 - \theta_2 \in (-2\pi, 0].$$

Noting that

$$\sum_{k=0}^2 \cos\left(x + \frac{2k\pi}{3}\right) = 0, \quad \forall x \in [0, 2\pi),$$

we obtain

$$\sum_{k=0}^2 x_k = 0. \quad (\text{A3})$$

We need to maximize the quantity

$$M_{\max}(U_{\theta_1, \theta_2}) = 1 + \frac{2}{3} \sum_{k=0}^2 \sqrt{3 + 2x_k}$$

over the region $-\pi \leq \theta_1 \leq \theta_2 < \pi$. By the Cauchy–Schwarz inequality, we have

$$\left(\sum_{k=0}^2 \sqrt{3 + 2x_k}\right)^2 \leq \left(\sum_{k=0}^2 (3 + 2x_k)\right) \left(\sum_{k=0}^2 1^2\right) = 27,$$

with the equality holding if and only if

$$x_0 = x_1 = x_2.$$

Combined with equation (A3), we have

$$x_0 = x_1 = x_2 = 0.$$

From $x_0 = 0$ we obtain

$$\cos \alpha + \cos\left(-\frac{\alpha}{2} + \frac{3\beta}{2}\right) + \cos\left(-\frac{\alpha}{2} - \frac{3\beta}{2}\right) = 0. \quad (\text{A4})$$

From $x_1 = 0$ we obtain

$$\begin{aligned} & \left(\cos \alpha + \cos \left(-\frac{\alpha}{2} + \frac{3\beta}{2} \right) \right. \\ & \quad \left. + \cos \left(-\frac{\alpha}{2} - \frac{3\beta}{2} \right) \right) \cos \frac{2\pi}{3} \\ & \quad + \left(\sin \alpha + \sin \left(-\frac{\alpha}{2} + \frac{3\beta}{2} \right) \right. \\ & \quad \left. + \sin \left(-\frac{\alpha}{2} - \frac{3\beta}{2} \right) \right) \sin \frac{2\pi}{3} = 0. \end{aligned}$$

Combined with equation (A4), we obtain

$$\sin \alpha + \sin \left(-\frac{\alpha}{2} + \frac{3\beta}{2} \right) + \sin \left(-\frac{\alpha}{2} - \frac{3\beta}{2} \right) = 0. \quad (\text{A5})$$

Now equations (A4) and (A5) can be equivalently rewritten as

$$2 \cos^2 \frac{\alpha}{2} - 1 + 2 \cos \frac{\alpha}{2} \cos \frac{3\beta}{2} = 0, \quad (\text{A6})$$

$$2 \sin \frac{\alpha}{2} \left(\cos \frac{\alpha}{2} - \cos \frac{3\beta}{2} \right) = 0, \quad (\text{A7})$$

respectively. The solutions of equations (A6) and (A7) can be directly obtained by considering the following exhaustive cases:

- (i) From equation (A7), we conclude that either $\sin \frac{\alpha}{2} = 0$ or $\cos \frac{\alpha}{2} - \cos \frac{3\beta}{2} = 0$. First consider the case $\sin \frac{\alpha}{2} = 0$, then $\alpha = -2\pi, 0$ (noting that $\alpha \in [-2\pi, 2\pi]$). We have two subcases
 - (a) $\alpha = -2\pi$, then $\theta_1 = \theta_2 = -\pi$ and $\beta = \theta_1 - \theta_2 = 0$. This subcase is excluded by equation (A6) since it cannot be satisfied.
 - (b) $\alpha = 0$, then $\cos \frac{\alpha}{2} = 1$, and by equation (A6), $\cos \frac{3\beta}{2} = -\frac{1}{2}$, which in turn implies that $\frac{3\beta}{2} = -\frac{2\pi}{3}, -\frac{4\pi}{3}, -\frac{8\pi}{3}$ (noting that $\beta \in (-2\pi, 0]$), that is,

$$\beta = -\frac{4\pi}{9}, -\frac{8\pi}{9}, -\frac{16\pi}{9}.$$

Consequently, in this subcase, we obtain three solutions of equations (A6) and (A7) as

$$\theta_1 = -\theta_2 = -\frac{2\pi}{9}, -\frac{4\pi}{9}, -\frac{8\pi}{9}.$$

In particular, the qutrit T -gate T_3 corresponds to U_{θ_1, θ_2} with

$$\theta_1 = -\theta_2 = -\frac{2\pi}{9}.$$

This establishes equation (10).

For clarity, we list the above optimal solutions in table A1.

- (ii) Now consider the case $\cos \frac{\alpha}{2} - \cos \frac{3\beta}{2} = 0$, then combined with equation (A6), we have $\cos \frac{3\beta}{2} = \pm \frac{1}{2}$. We have two subcases:

Table A1. Optimal solutions for the case (i).

θ_1	$-\frac{2\pi}{9}$	$-\frac{4\pi}{9}$	$-\frac{8\pi}{9}$
θ_2	$\frac{2\pi}{9}$	$\frac{4\pi}{9}$	$\frac{8\pi}{9}$

Table A2. Optimal solutions for the subcase (ii)(a).

θ_1	$-\frac{8\pi}{9}$	$\frac{4\pi}{9}$
θ_2	$-\frac{4\pi}{9}$	$\frac{8\pi}{9}$

Table A3. Optimal solutions for the subcase (ii)(b).

θ_1	$-\frac{8\pi}{9}$	$-\frac{4\pi}{9}$	$-\frac{2\pi}{9}$	$\frac{2\pi}{9}$
θ_2	$\frac{2\pi}{9}$	$-\frac{2\pi}{9}$	$\frac{8\pi}{9}$	$\frac{4\pi}{9}$

- (a) $\cos \frac{3\beta}{2} = -\frac{1}{2}$. In this subcase, $\cos \frac{\alpha}{2} = -\frac{1}{2}$. Consequently, $\frac{3\beta}{2} = -\pi \pm \frac{\pi}{3}, -3\pi \pm \frac{\pi}{3}$ (noting that $\beta \in (-2\pi, 0]$), i.e. $\beta = -\frac{4\pi}{9}, -\frac{8\pi}{9}, -\frac{16\pi}{9}$, and $\alpha = \pm \frac{4\pi}{3}$ (noting that $\alpha \in [-2\pi, 2\pi]$). In this subcase, we obtain the optimal solutions as listed in table A2 (noting that we require $\theta_1, \theta_2 \in [-\pi, \pi), \theta_1 \leq \theta_2$).
- (b) $\cos \frac{3\beta}{2} = \frac{1}{2}$. In this subcase, $\cos \frac{\alpha}{2} = \frac{1}{2}$. Consequently, $\frac{3\beta}{2} = -\frac{\pi}{3}, -2\pi - \frac{\pi}{3}, -2\pi + \frac{\pi}{3}$ (noting that $\beta \in (-2\pi, 0]$), i.e. $\beta = -\frac{2\pi}{9}, -\frac{10\pi}{9}, -\frac{14\pi}{9}$, and $\alpha = \pm \frac{\pi}{3}$ (noting that $\alpha \in [-2\pi, 2\pi]$). In this subcase, we obtain the optimal solutions as listed in table A3 (noting that we require $\theta_1, \theta_2 \in [-\pi, \pi), \theta_1 \leq \theta_2$).

We list all solutions (θ_1, θ_2) of equations (A6) and (A7) achieving the maximal magic-resource-generating power in table 3 in section 3. The maximal value is

$$\max_{\theta_1, \theta_2} M_{\max}(U_{\theta_1, \theta_2}) = 1 + \frac{2}{3}\sqrt{27} = 1 + 2\sqrt{3}.$$

From the above derivation, any gate U_{θ_1, θ_2} with (θ_1, θ_2) in table 3, as well as any of its Clifford equivalent, also has the maximal magic-resource-generating power, with the maximal value

$$\max_{\theta_1, \theta_2} M_{\max}(U_{\theta_1, \theta_2}) = M_{\max}(T_3) = 1 + 2\sqrt{3}.$$

Finally, equation (11) follows readily from equation (10) since from equations (A1) and (A2), we have

$$\begin{aligned} M_{\text{ave}}(U_{\theta_1, \theta_2}) &= \frac{1}{12} \left(3 \times 3 + 9 \left(1 + \frac{2}{3} \sum_{k=0}^2 \sqrt{3 + 2x_k} \right) \right) \\ &= \frac{3}{4} (1 + M_{\max}(U_{\theta_1, \theta_2})), \end{aligned}$$

which implies that the solutions of (θ_1, θ_2) for achieving the maximal value of $M_{\text{ave}}(U_{\theta_1, \theta_2})$ are the same as those for $M_{\max}(U_{\theta_1, \theta_2})$.

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