A unified quantum NOT gate

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Abstract
We study the universal quantum NOT machine (approximate) when the quantum state lies between two latitudes on the Bloch sphere and present an analytical formula for the optimized 1-to-M quantum NOT gate. Our result generalizes previous results concerning a quantum NOT gate for a quantum state distributed uniformly on the whole Bloch sphere as well as for the phase-covariant quantum state. We have also shown that such a 1-to-M optimized NOT gate can be implemented using a sequential generation scheme via matrix product states.

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1. Introduction

Recent developments in quantum information have resulted in an increasing number of applications, for instance quantum teleportation, quantum dense coding, quantum cryptography, quantum logic gates, quantum algorithms, etc [1–5]. Many tasks in quantum information processing (QIP) possess different properties from their classical counterparts. One such case is the quantum NOT gate. Classically, we can use the NOT gate to invert (complement) a bit, by changing the value of a bit from 0 to 1, and vice versa. Complementing a qubit, however, is another matter. The complement of a state |ψ⟩ is the state |ψ⟩⊥ that is orthogonal to it. In the quantum case, as shown in [6, 7], it is impossible to build a device that transforms an unknown quantum state into the state orthogonal to it. That is to say, we cannot design a perfect universal-NOT (U-NOT) gate. This is another difference between classical and quantum information processing, which is closely related to the no-cloning theorem [8]. However, such no-go theorems do not forbid imperfect quantum cloning [9–28]. Also, approximate quantum NOT gates do exist [6, 7] and it is interesting to know...
how well we can orthogonalize an unknown quantum state. Gisin and Popescu [6] present the so-called universal quantum spin-flip (UQSF) machine in their analysis of encoding of quantum information into pairs of spins. One important application of spin flips is the two-qubit concurrence entanglement measure [29]. In another paper, Bužek et al. [7] introduced a U-NOT gate that makes approximate NOT operation to an unknown quantum state $|\psi\rangle$ on the Bloch sphere and generates an output that is as close as possible to $|\psi^\perp\rangle$, which is orthogonal to $|\psi\rangle$. The spin-flip operator in [6] is in fact equivalent to the one-input qubit realization of the U-NOT gate [7].

In many real applications of the quantum information system, we often have partial information about a two-level quantum state, i.e. the state is distributed on a specific area on the Bloch sphere. Such partial information as in a phase-covariant 1-to-1 NOT gate allows us to orthogonalize such states by transforming $|0\rangle$ to $|1\rangle$ and $|1\rangle$ to $-|0\rangle$. Thus, any phase-covariant states can be orthogonalized perfectly. In this work, we study the problem of a 1-to-$M$ quantum NOT gate where the input state is uniformly distributed between two latitudes of the Bloch sphere rather than the whole Bloch sphere. By considering the case in which the two latitudes are brought to the poles, we obtain the U-NOT gate with the optimal fidelity $F = 2/3$ [7]. However, if the two latitudes collapse into a geodesic circle of the Bloch sphere, we obtain the phase-covariant NOT gate. As previously stated, the phase-covariant 1-to-1 NOT gate can be constructed perfectly. So we can achieve the 1-to-$M$ optimal phase-covariant NOT gate by combining the 1-to-1 perfect NOT gate and the 1-to-$M$ optimal phase-covariant quantum cloning machine (PQCM). Then the fidelity of the 1-to-$M$ optimal phase-covariant NOT gate and the fidelity of PQCM must be the same. A blow-by-blow description of this result will be presented in the following section.

Taking qubit $|\psi\rangle = \cos \frac{\theta}{2} |0\rangle + \sin \frac{\theta}{2} e^{i\phi} |1\rangle$ with $\phi \in [0, 2\pi]$ and $\theta_1 \leq \theta \leq \theta_2$ as an input, the outputs of our 1-to-$M$ NOT gate will always be some multipartite entangled states. As a result, the controllable generation of these entangled states becomes very important. But in general, it is extremely difficult to generate experimentally multipartite entangled states through a single global unitary operation. For this purpose, the sequential generation of the entangled states appears to be a promising avenue [30], where at each step one qubit is allowed to interact with an ancilla; a lot of effort has been made in recent years [30–36]. The essence of this sequential scheme is the successive interaction of each qubit initialized in the standard state with an ancilla of a suitable dimension to generate the desired multiqubit state. It is pointed out that photonic multiqubit states can be generated by letting a source emit photonic qubits in a sequential manner [31]. The general sequential generation of entangled multiqubit states in the realm of cavity QED was systematically studied in [30, 32]. It is also shown that the class of sequentially generated states is identical to the matrix-product state (MPS), which is very useful in the study of spin chains of condensed matter physics [33]. Moreover, it is indicated that the 1-to-$M$ sequential quantum cloning is available [34]. Dang and Fan [36] extend the sequential quantum cloning to the general $N$-to-$M$ case, and the $d$-level quantum states’ sequential cloning is also presented.

To this end, we consider the following state:

$$|\psi\rangle = \cos \frac{\theta}{2} |0\rangle + \sin \frac{\theta}{2} e^{i\phi} |1\rangle,$$

where $\phi \in [0, 2\pi]$ and $\theta_1 \leq \theta \leq \theta_2$ with constants $\theta_1, \theta_2$. The states we considered here are distributed uniformly between two latitudes on the Bloch sphere. When $\theta_1 = 0$ and $\theta_2 = \pi$, we get the situation of the U-NOT gate. In this way, the result of the U-NOT gate is recovered as special cases of our NOT gate. When $\theta_1 = \pi/2$ and $\theta_2 = \pi/2$, we obtain the NOT gate for phase-covariant states.
This paper is arranged as follows. We formulate our problem and present analytical results to our situation in the following section. In section 3, we analyze the 1-to-$M$ NOT gate within a sequential generation scheme and express the sequential NOT gate in an explicit form. We end the paper with some concluding remarks.

2. Quantum NOT gate for qubits between two latitudes on the Bloch sphere

The state we wish to orthogonalize can be written as

$$|\psi\rangle = \cos \frac{\theta}{2} |0\rangle + \sin \frac{\theta}{2} e^{i\phi} |1\rangle,$$  \hspace{1cm} (2)

where $\phi \in [0, 2\pi]$ and $\theta_1 \leq \theta \leq \theta_2$, i.e. the states we considered here are distributed uniformly within a region enclosed by two latitudes on the Bloch sphere. We assume the following unitary transformation for our NOT gate:

$$U: |0\rangle|X\rangle \rightarrow \sum_{k=0}^{M} (|M-k\rangle|0\rangle \otimes |A_k\rangle)$$
$$|1\rangle|X\rangle \rightarrow \sum_{k=0}^{M} |k\rangle (M-k) |1\rangle \otimes |A_{M+k+1}\rangle, \hspace{1cm} (3)$$

where $|(M-k)0, k1\rangle$ denotes symmetric and normalized states with $M-k$ qubits in $|0\rangle$ and $k$ qubits in $|1\rangle$. This ensures a symmetric NOT gate and that all the first $M$ qubits at the output of the NOT gate are the same. $|A_{l}\rangle (l=0, 1, \ldots, 2M+1)$ are unnormalized states. Let $a_{k,l} = \langle A_{l}|A_{k}\rangle$ and denote $a_k = \langle A_k|A_k\rangle$ for short where $a_{k,l}$ are the parameters that we want to determine.

After applying the unitary operation $U$, we can get the following state with the input qubit $|\psi\rangle$ described by equation (2):

$$|\psi_{\text{out}}\rangle = \cos \frac{\theta}{2} \sum_{k=0}^{M} (|M-k\rangle|0\rangle \otimes |A_k\rangle + \sin \frac{\theta}{2} e^{i\phi} \sum_{k=0}^{M} |k\rangle (M-k) |1\rangle \otimes |A_{M+k+1}\rangle. \hspace{1cm} (4)$$

By taking partial trace, we obtain the reduced density matrix $\rho_m$ for the $m$th output qubit, and all the reduced density matrix are the same for $m=1, 2, \ldots, M$:

$$\rho_m = \text{tr}_{-m}(|\psi_{\text{out}}\rangle\langle \psi_{\text{out}}|)$$

$$= \cos^2 \frac{\theta}{2} \sum_{k=0}^{M} \frac{M-k}{M} a_k |0\rangle \langle 0| + B_0 |0\rangle \langle 1| + B_1 |1\rangle \langle 0| + \sum_{k=0}^{M-1} \frac{k+1}{M} a_{k+1} |1\rangle \langle 1|$$
$$+ e^{-i\phi} \sin \frac{\theta}{2} \cos \frac{\theta}{2} \left[ B_2 |0\rangle \langle 0| + B_3 |1\rangle \langle 0| + B_4 |1\rangle \langle 1| \right]$$
$$+ \sum_{k=0}^{M-1} \frac{\sqrt{(k+1)(M-k)}}{M} a_{M-k-1,M+k+1} |0\rangle \langle 1|$$
$$+ e^{i\phi} \sin \frac{\theta}{2} \cos \frac{\theta}{2} \left[ B_5 |0\rangle \langle 0| + B_6 |0\rangle \langle 1| + B_7 |1\rangle \langle 1| \right]$$
$$+ \sum_{k=0}^{M-1} \frac{\sqrt{(k+1)(M-k)}}{M} a_{M+k+1,M-k-1} |1\rangle \langle 0|.$$
\[ F = \langle \psi^\perp | \rho_m | \psi^\perp \rangle \]
\[ = \sin^2 \theta \cos^2 \theta \frac{1}{2} \sum_{k=0}^{M-1} \frac{M-k}{M} (a_k + a_{M+k+1}) + 2 \sum_{k=0}^{M-1} \frac{\sqrt{(M-k)(K+1)}}{M} \sqrt{|a_{M+k+1}a_{M-k-1}|^2} \]
\[ + \sin^2 \theta \cos^2 \theta \frac{1}{2} \sum_{k=0}^{M-1} \frac{m-1}{M} \frac{M-k}{M} (a_M + a_{M+k+2}) + 2 \sum_{k=0}^{M-1} \frac{\sqrt{(M-k)(K+1)}}{M} \sqrt{|a_{M+k+1}a_{M-k-1}|^2} \]
\[ + \sin^4 \theta \frac{1}{2} \sum_{k=0}^{M-1} \left( \frac{M-k}{M} \right) a_{M+k+2} + \cos^4 \theta \sum_{k=0}^{M-1} \left( \frac{M-k}{M} \right) a_{M+k+2} \]
\[ + e^{i\phi} C_1 + e^{-i\phi} C_1^* + e^{2i\phi} C_2 + e^{-2i\phi} C_2^*, \tag{6} \]
where \( C_1^* \) is the complex conjugation of \( C_1 \) and the same for \( C_2^* \). Since the input state \( |\psi\rangle \) given by equation (2) is arbitrary, the parameters \( \phi \in [0, 2\pi] \) and \( \theta \in [\theta_1, \theta_2] \) are unknown and are distributed uniformly on a belt of the Bloch sphere. We need to average the fidelity over all possible cases. The last four terms in equation (6) disappear as a consequence of the averaging over all possible angles \( \phi \). Moreover, we obtain the same optimal NOT gate by assuming that \( C_1 \) and \( C_2 \) are equal to zero. On the other hand, by using the definitions of \( a_{k,l} \), we can easily get that \( a_{k,l} = a_{k,l}^* \) and \( |a_{k,l}|^2 \leq a_k a_l \). Equality is obtained if and only if \( a_{k,l} = a_{k,l}^* \) are real numbers. Using equation (6), the fidelity becomes
\[ F = \sin^2 \theta \cos^2 \theta \frac{1}{2} \sum_{k=0}^{M-1} \frac{M-k}{M} (a_k + a_{M+k+1}) + 2 \sum_{k=0}^{M-1} \frac{\sqrt{(M-k)(K+1)}}{M} \sqrt{|a_{M+k+1}a_{M-k-1}|^2} \]
\[ + \sin^4 \theta \frac{1}{2} \sum_{k=0}^{M-1} \left( \frac{M-k}{M} \right) a_{M+k+2} + \cos^4 \theta \sum_{k=0}^{M-1} \left( \frac{M-k}{M} \right) a_{M+k+2} \tag{7} \]

Averaging the fidelity over all possible angles \( \theta \) [10], and observing that \( \sum_{k=0}^{M} a_k = \sum_{k=0}^{M} a_{M+k+1} = 1 \), we have
\[ \bar{F} = \int_{\theta_1}^{\theta_2} F \sin \theta \, d\theta \int_{\theta_1}^{\theta_2} \sin \theta \, d\theta \]
\[ = \frac{1}{2} + \frac{1}{6} K + P \sum_{k=0}^{M-1} \frac{(M-k)(K+1)}{M} \sqrt{|a_{M+k+1}a_{M-k-1}|^2} \]
\[ - Q \sum_{k=0}^{M-1} \frac{M-k}{M} a_k - R \sum_{k=0}^{M-1} \frac{M-k}{M} a_{M+k+1} \tag{8} \]
where \( K = \cos^2 \theta_1 + \cos \theta_1 \cos \theta_2 + \cos^2 \theta_2, P = \frac{3-K}{6}, Q = \frac{K}{\theta_1} + \frac{1}{2} (\cos \theta_1 + \cos \theta_2), R = \frac{K}{\theta_2} - \frac{1}{2} (\cos \theta_1 + \cos \theta_2) \) and \( K, P, Q, R \) are constants with given \( \theta_1 \) and \( \theta_2 \). In order to get the optimal quantum NOT gate, we should maximize \( \bar{F} \) with respect to \( a_k(k = 0, 1, \ldots, M - 1, M + 1, M + 2, \ldots, 2M) \).

We now seek a solution of \( a_k \) with maximum \( \bar{F} \). It is interesting to note that if the state lies somewhere on the whole Bloch sphere, \( \theta_1 = 0 \) and \( \theta_2 = \pi \), and we have \( K = 1, P = \frac{1}{3} \).
and $Q = R = \frac{1}{2}$. The optimal fidelity is $F = \frac{1}{2}$ with $a_{M+1} = a_{M-k-1}(k = 0, 1, \ldots, M-1)$, recovering the well-known result for the 1-to-M U-NOT gate in [7]. In this case, the fidelity is constant and the optimal universal NOT gate can be realized via a ‘measurement + repreparation’ scheme [7]. In the general situation, with states uniformly distributed in a belt on the Bloch sphere, the fidelity is dependent on the number of output qubits $M$ as shown below in this paper. So we cannot realize via a ‘measurement + repreparation’ scheme for the general case.

For the case in which the state is phase covariant, $\theta_1 = \theta_2 = \frac{\pi}{2}$, and we have $K = 0$, $P = \frac{1}{2}$ and $Q = R = 0$. The optimal fidelity is $F = \frac{1}{2} + \sqrt{\frac{M+1}{2M}}$ for even $M$ and $F = \frac{1}{2} + \frac{M+1}{2M}$ for odd $M$. This fidelity is just equal to the fidelity of the optimal 1-to-1 phase- covariant quantum cloning machine [15, 25, 37]. As mentioned above, the 1-to-1 phase-covariant NOT gate can be constructed perfectly. So we can achieve the 1-to-$M$ optimal phase- covariant NOT gate by combining the 1-to-1 perfect NOT gate with the 1-to-$M$ optimal phase-covariant cloning machine. The fidelities of the 1-to-$M$ optimal phase-covariant NOT gate and QCM must be the same as analyzed before.

In the general situation, we need to optimize the fidelity in equation (8) under the restrictions $0 \leq a_k \leq 1(k = 0, 1, \ldots, M-1, M + 1, \ldots, 2M)$, $\sum_{k=0}^{M-1} a_k \leq 1$ and $\sum_{k=0}^{M+1} a_{M+k+1} \leq 1$. By considering the smoothness of $\tilde{F}$, the maximum value should be achieved at the extremal points or on the boundary. We analyze the optimization problem with restrictions and get an optimal NOT gate for the following situations.

1. When $|\theta_1 - \frac{\pi}{2}| \geq |\theta_2 - \frac{\pi}{2}|$ and $M$ is odd, we have $a_{\frac{M+1}{2}} = \min (\frac{P}{2\theta_2})^2, 1)$, $a_M = 1 - a_{\frac{M+1}{2}}, a_{\frac{M-1}{2}} = 1$, $a_{\frac{M+1}{2}} a_{\frac{M-1}{2}} = a_{\frac{M+1}{2}} a_{\frac{M-1}{2}} = -\sqrt{a_{\frac{M+1}{2}}} \sqrt{a_{\frac{M-1}{2}}} \sqrt{a_{\frac{M+1}{2}}} \sqrt{a_{\frac{M-1}{2}}} = 0$ otherwise. The fidelity is $F = \frac{1}{2} + K + \frac{M+1}{2M}(\frac{P}{2\theta_2} - R)$ for $a_{\frac{M+1}{2}} = \frac{P}{2\theta_2}$ and $F = \frac{1}{2} + K + \frac{M+1}{2M}(P - Q - R)$ for $a_{\frac{M+1}{2}} = 1$.

2. When $|\theta_1 - \frac{\pi}{2}| < |\theta_2 - \frac{\pi}{2}|$ and $M$ is odd, we have $a_{\frac{M+1}{2}} = 1, a_{\frac{M+1}{2}} = \min (\frac{P}{2\theta_2})^2, 1)$, $a_{\frac{M+1}{2}} = 1 - a_{\frac{M+1}{2}}, a_{\frac{M+1}{2}} = a_{\frac{M+1}{2}}, a_{\frac{M+1}{2}} = -a_{\frac{M+1}{2}} \sqrt{a_{\frac{M+1}{2}}} \sqrt{a_{\frac{M+1}{2}}} = 0$ otherwise. The fidelity is $F = \frac{1}{2} + K + \frac{M+1}{2M}(\frac{P}{2\theta_2} - Q)$ for $a_{\frac{M+1}{2}} = \frac{P}{2\theta_2}$ and $F = \frac{1}{2} + K + \frac{M+1}{2M}(P - Q - R)$ for $a_{\frac{M+1}{2}} = 1$.

3. When $|\theta_1 - \frac{\pi}{2}| \geq |\theta_2 - \frac{\pi}{2}|$ and $M$ is even, we have $a_{\frac{M}{2}} = \min (\frac{P}{2\theta_2})^2, 1)$, $a_M = 1 - a_{\frac{M}{2}}, a_{\frac{M}{2}} = 1, a_{\frac{M}{2}} a_{\frac{M}{2}} = a_{\frac{M}{2}} a_{\frac{M}{2}} = -a_{\frac{M}{2}} \sqrt{a_{\frac{M}{2}}} \sqrt{a_{\frac{M}{2}}} = 0$ otherwise. The fidelity is $F = \frac{1}{2} + K + \frac{M+1}{2M}(\frac{P}{2\theta_2} - R)$ for $a_{\frac{M}{2}} = \frac{P}{2\theta_2}$ and $F = \frac{1}{2} + K + \frac{P}{2\theta_2}M - R\frac{M+1}{2M} + \frac{1}{2}Q$ for $a_{\frac{M}{2}} = 1$.

4. When $|\theta_1 - \frac{\pi}{2}| < |\theta_2 - \frac{\pi}{2}|$ and $M$ is even, we have $a_{\frac{M}{2}} = 1, a_{\frac{M}{2}} = \min (\frac{P}{2\theta_2})^2, 1)$, $a_{M+1} = 1 - a_{\frac{M}{2}} a_{\frac{M}{2}} = a_{\frac{M}{2}} a_{\frac{M}{2}} = -a_{\frac{M}{2}} \sqrt{a_{\frac{M}{2}}} \sqrt{a_{\frac{M}{2}}} = 0$ otherwise. The fidelity is $F = \frac{1}{2} + K + \frac{M+1}{2M}(\frac{P}{2\theta_2} - Q)$ for $a_{\frac{M}{2}} = \frac{P}{2\theta_2}$ and $F = \frac{1}{2} + K + \frac{P}{2\theta_2}M - R\frac{M+1}{2M} + \frac{1}{2}Q$ for $a_{\frac{M}{2}} = 1$.

The explicit NOT gate transformations have already been presented in equation (3) by letting $|A_1(\frac{\pi}{2})| = -\sqrt{a_{\frac{M}{2}}}, |A_{M+1}| = \sqrt{1 - a_{\frac{M}{2}}}, |A_{M+2}| = \frac{P}{2\theta_2}$ and $|A_2| = 0$ otherwise for cases 1 and 3, and by letting $|A_{\frac{M}{2}+1}| = |\uparrow\rangle, |A_{\frac{M}{2}+2}| = -\sqrt{a_{\frac{M}{2}+1}}, |A_{M+3}| = \sqrt{1 - a_{\frac{M}{2}+1}}$ and $|A_2| = 0$ otherwise for cases 2 and 4.

It is interesting to note that the output states of the NOT gate given by equation (3) are always entangled. As shown by Bužek et al [7], the optimal U-NOT gate can be realized via a ‘measurement + repreparation’ scheme. Moreover for each measurement result obtained,
that any multiqubit MPS can be sequentially generated \[30\]. The basic idea is to show that the final states therein, already comprehensively studied in \[30, 32–34, 36, 38–40\]. Moreover, it was proven that any multiqubit MPS can be sequentially generated. As shown in \[30, 34, 36\], the sequential generation of a multiqubit state is as follows. Let the prepared state can be taken to be a product one. In this case, it is an ‘easy’ operation, and requires no generation of entanglement nor unitary operations but just the measurement and preparation of product states. Unfortunately, there is no ‘measurement + repreparation’ scheme in the general situation, as the optimal fidelity is dependent on the number of output qubits \( M \). So the generation of entanglement is unavoidable. As a result, the controlled generation of these entangled states becomes very important. In the following section, we consider the generation of these entangled states and present the sequential quantum NOT gate.

3. The 1-to-\( M \) sequential quantum NOT gate

As shown in \[30, 34, 36\], the sequential generation of a multiqubit state is as follows. Let \( \mathcal{H}_A \cong C^D \) and \( \mathcal{H}_B \cong C^2 \) be the Hilbert spaces characterizing a \( D \)-dimensional ancillary system and a single qubit, respectively. At every step of the sequential generation of a multiqubit state, a unitary time evolution will be acting on the joint system \( \mathcal{H}_A \otimes \mathcal{H}_B \). Assuming that each qubit is initially in the state \( |0\rangle \), we disregard the qubit at the input and write the evolution in the form of an isometry \( V : \mathcal{H}_A \rightarrow \mathcal{H}_A \otimes \mathcal{H}_B \), where \( V = \sum_{i,a,\beta} V_{i,a,\beta} |\alpha, i\rangle \langle \beta| \), each \( V_i \) is a \( D \times D \) matrix and the isometry condition takes the form \( \sum_{i=0}^{n-1} V_i V_i^\dagger = 1 \). If we apply successively \( n \) operations of this form to an initial state \( |\psi_i\rangle \in \mathcal{H}_A \), we obtain the state \( |\Phi\rangle = V^{(n)} |\psi_1\rangle \cdots V^{(2)} |\psi_1\rangle |\psi_1\rangle \cdots |\psi_1\rangle \). The \( n \)-generated qubits are in general entangled. Assuming in the last step the ancilla decouples from the system, such that \( |\Phi\rangle = |\psi_F\rangle \otimes |\psi_e\rangle \), and we are left with the \( n \)-qubit state

\[
|\psi\rangle = \sum_{i_1,\ldots,i_n=0}^{1} \langle \psi_F| V^{(n)} |i_n\rangle \cdots V^{(1)} |i_1\rangle |i_1\rangle \cdots |i_1\rangle,
\]

where \( |\psi_F\rangle \) is the final state of the ancilla. The state (9) is a MPS (cf e.g. \[38\], and references therein), already comprehensively studied in \[30, 32–34, 36, 38–40\]. Moreover, it was proven that any multiqubit MPS can be sequentially generated \[30\].

The NOT gate given by equation (3) can approximately orthogonalize one input state to \( M \) copies. Next, we show that this general 1-to-\( M \) sequential quantum NOT gate can be generated through a sequential procedure. The basic idea is to show that the final states \( |\psi_{1,M}\rangle \) in equation (3) can be expressed in its MPS form. As presented in \[30\], any MPS can be sequentially generated. We shall follow the method as in \[34, 36, 39\].

Take one output entangled state in case 1 for example. We have

\[
|\psi_{1,M}\rangle = -\sqrt{\gamma} \left( \frac{M + 1}{2} |0\rangle - \frac{M - 1}{2} |1\rangle \right) + \sqrt{1 - \gamma} |M1\rangle |1\rangle,
\]

where \( \gamma = a_{\alpha,\beta} \). By Schmidt decomposition, we first express the quantum state \( |\psi_{1,M}\rangle \) as a bipartite pure state in \( \mathcal{H}_{A_1} \otimes \mathcal{H}_{B_1} \) with two particle sets \( A_1 = \{1\} \) and \( B_1 = \{2, 3, \ldots, M + 1\} \) respectively:

\[
|\psi_{1,M}^0\rangle = \lambda_1^{[1]} |0\rangle |\psi_1^{[2,\ldots,M+1]}\rangle + \lambda_2^{[1]} |1\rangle |\psi_2^{[2,\ldots,M+1]}\rangle
\]

\[
= \sum_{a_1,j_1} \Gamma_{a_1}^{[1]} |\psi_{a_1,j_1}^{[1]}\rangle |\psi_{a_1,j_1}^{[2,\ldots,M+1]}\rangle,
\]

where \( \lambda_1^{[1]} \) are eigenvalues of the first qubit-reduced density operator and we find \( \lambda_1^{[1]} = \sqrt{\frac{M+1}{2M}} \) and \( \lambda_2^{[1]} = \sqrt{1 - \gamma} \frac{M+1}{2M} \). Matching indices in equation (11), we have \( \Gamma_{a_1}^{[1]} = \delta_{a_1,1} \) and \( \Gamma_{a_1}^{[2]} = \delta_{a_1,2} \). To correspond with the MPS form in equation (9), we define

\[
V_{a_1}^{[1]} = \Gamma_{a_1}^{[1]} \lambda_1^{[1]}.
\]
Comparing equation (16) with the following relation:

\[
\psi_n = \lambda_n \psi_{n+1}, \quad \text{where } \lambda_n = \sqrt{\frac{\lambda_{n+1}}{\lambda_n}}, \quad n = 1, 2, \ldots, M - 1.
\]

By successive Schmidt decomposition, the quantum state \( |\Psi_1^0 \rangle \) in equation (10) can be considered as a bipartite pure state in \( \mathcal{H}_A \otimes \mathcal{H}_B \) with particle sets \( A_n = \{1, 2, \ldots, n\} \) and \( B_n = \{n + 1, n + 2, \ldots, M + 1\} \), where \( 1 < n \leq M \). We have

\[
|\Psi_1^0 \rangle = \sum_{l=0}^{n} \lambda_{nl}^{|n\rangle |n-l\rangle 0} |\psi_{l+1}^{n+1} \rangle |\psi_{l}^{n+1} \rangle |\psi_{l+1}^{n+1} \rangle, \quad (13)
\]

where \( \lambda_{nl} \) are eigenvalues of the first \( n \) qubits-reduced density operator of \( |\Psi_1^0 \rangle \). We can obtain

\[
\begin{align*}
\lambda_{nl} & = \sqrt{\frac{\lambda_{n-1}^l}{\lambda_n^l}}, & 1 < n \leq M - 1, \quad l = 0, 1, \ldots, n - 1; \\
\lambda_{nl} & = \sqrt{\frac{\lambda_{n+1}^l}{\lambda_n^l}}, & M - \frac{1}{2} < n \leq M, \quad l = n - M + 1, \ldots, M - 1; \\
\lambda_{nl} & = 0, & \text{otherwise}
\end{align*}
\]

and

\[
\begin{align*}
|\psi_{l+1}^{n+1} \rangle & = -\left| \frac{M+1}{2} - n + l \right\rangle 0 \left( \frac{M-1}{2} - l \right\rangle 1, & 1 < n \leq M - 1, \quad l = 0, 1, \ldots, n - 1; \\
|\psi_{l+1}^{n+1} \rangle & = -\sqrt{\frac{\lambda_{n+1}^l}{\lambda_n^l}} \left| \frac{M+1}{2} \right\rangle 0 \left( \frac{M-1}{2} - n \right\rangle 1 + \sqrt{\frac{\lambda_{n+1}^l}{\lambda_n^l}} \left( M - n \right\rangle 1, & 1 < n \leq M - 1; \\
|\psi_{l+1}^{n+1} \rangle & = -\left| \frac{M+1}{2} - n + l \right\rangle 0 \left( \frac{M-1}{2} - l \right\rangle 0, & M - \frac{1}{2} < n \leq M, \quad l = n - M + 1, \ldots, M - 1; \\
|\psi_{l+1}^{n+1} \rangle & = \left( M - n \right\rangle 1, & M - \frac{1}{2} \leq n \leq M; \\
|\psi_{l+1}^{n+1} \rangle & = 0, & \text{otherwise.}
\end{align*}
\]

According to the results in equations (14) and (15), we get the following recursion formula:

\[
|\psi_{l+1}^{n+1} \rangle = \sqrt{\frac{(n-1)}{l+1}} \left[ \lambda_{nl}^{|n\rangle |n-l\rangle 0} |\psi_{l+1}^{n+1} \rangle |\psi_{l}^{n+1} \rangle |\psi_{l+1}^{n+1} \rangle \right] + \lambda_{nl}^{|n\rangle |n-l\rangle 1} |\psi_{l+1}^{n+1} \rangle |\psi_{l}^{n+1} \rangle |\psi_{l+1}^{n+1} \rangle. \quad (16)
\]

Comparing equation (16) with the following relation:

\[
|\psi_{l+1}^{n+1} \rangle = \sum_{a_{nl}} \Gamma_{l+1}^{n+1} |\psi_{a_{nl}}^{n+1} \rangle |\psi_{l}^{n+1} \rangle |\psi_{l+1}^{n+1} \rangle,
\]

we have

\[
\Gamma_{l+1}^{n+1} |\psi_{l+1}^{n+1} \rangle = \delta_{l+1} |\psi_{l+1}^{n+1} \rangle \sqrt{\frac{(n-1)}{l+1}} \lambda_{nl}^{|n\rangle |n-l\rangle 0} |\psi_{l}^{n+1} \rangle |\psi_{l+1}^{n+1} \rangle. \quad (17)
\]
\[
\Gamma_{\{l+1\}a_0}^{[n]} = \delta_{[l+2]a_0} \sqrt{\binom{n-1}{l+1}} \frac{\lambda_{\{l+1\}}^{[n-1]} \sqrt{\binom{n}{l}}}{\lambda_{\{l+1\}}^{[n]}}.
\]  

In order to get the MPS form in equation (9), we define that
\[
V_{\{l+1\}a_0}^{[n]} = \Gamma_{\{l+1\}a_0}^{[n]} \lambda_{\{l+1\}}^{[n]} (1 < n \leq M).
\]

After performing \(M\) sequential Schmidt decompositions, the states on the rhs in equation (13) can be written as
\[
\ket{\psi^{[M+1]}_{k+1}} = \ket{0} \quad \text{and} \quad \ket{\psi^{[M+1]}_{k+1}} = \ket{1}.
\]

Checking the above-defined \(V\), we find that the isometry condition \(\sum_{\{l+1\}} V_{\{l+1\}a_0}^{[n]} V_{\{l+1\}a_0}^{[n]} = 1\) is satisfied.

Until now, we have found that the output state of the general quantum NOT gate can be expressed as a MPS as in form (9). So the sequential quantum NOT gate is obtainable.

4. Concluding remark

In summary, by applying quantum orthogonalizing transformations for the state uniformly distributed between two latitudes on the Bloch sphere, we present a general 1-to-\(M\) quantum NOT gate. The usual U-NOT gate is a special case and we find out that the optimal fidelity of the U-NOT gate is consistent with that studied in [7]. For another special case, we point out the relation between the phase-covariant 1-to-\(M\) NOT gate and the phase-covariant QCM. In the general situation, there is no ‘measurement + repreparation’ scheme as the U-NOT gate can be realized via it. Consequently, the generation of entanglement is unavoidable and the controlled generation of entangled states becomes very important. To this end, we analyze the NOT gate within a sequential generation scheme and show that the sequential quantum NOT gate is feasible.

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