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Abstract. We study quantum cloning machines (QCM) that act on an unknown N-level quantum state and make M copies. We give a formula for the maximum of the fidelity of cloning and exhibit the unitary transformations that realize this optimal fidelity. We also extend the results to treat the case of M copies from N' (M > N') identical N-level quantum systems.

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A major difference between cloning of classical and quantum information is that whereas the copies of the classical information can be made perfect the copies of the quantum information are always imperfect, by the very principles of quantum theory. More precisely the classical information about the input state is available through measurement and can be cloned by making a measurement on the input state and using the result of the measurement to make an arbitrary number M of identical copies. In contrast, from the very superposition principle of quantum mechanics, an unknown quantum state can not be perfectly copied (see e.g., [1,2]). Consider an N-level quantum state. Let $|i\rangle$, i = 1, ..., N, be the basis vectors spanning the Hilbert space of quantum states. A quantum state is a complex linear combination of the bases vectors. For an arbitrary (unknown) input state $|\Phi\rangle$ and another given initial state $|\Phi\rangle_0$ of the blank copy, the no-cloning theorem (see e.g. [1]) says that there is no unitary transformation U of two quantum states $|\Phi\rangle$ and $|\Phi\rangle_0$, such that $U|\Phi\rangle|\Phi\rangle_0 = |\Phi\rangle|\Phi\rangle$ (where $|\Phi\rangle|\Phi\rangle_0$ denotes the tensor product of $|\Phi\rangle$ and $|\Phi\rangle_0$). Hence in cloning quantum states one has to drop the requirement that the copies be perfect. The concept of quantum cloning machines (QCM) which act on an unknown quantum state and make one, or more, imperfect copies of it has been introduced [3]. To make the copies as good as possible the transformations used by the quantum cloning machines should be optimal, in the sense that they maximize the average fidelity between the input and the output states.

The transformation that produces two copies of one qubit state $(N = 2, i.e. a \text{ spin } \frac{1}{2} \text{ state})$, with a fidelity independent of the state of the input qubit, was first given in [3]. This transformation was shown to be optimal [4–6]. In [4] the transformations that produce M copies from N' (M > N') identical states of qubits are also studied. Its optimality is generally proved in [6]. To clone entangled states of two or more qubits, a transformation that produces two copies (M = 2) from one N-level quantum state was given in [7]. In [8] Werner studied optimal cloning of pure states for turning a finite number of N-level quantum systems in the same unknown state σ into M systems of the state σ .

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In this article we study QCM that transform one N-level quantum state into M identical copies by using the representation of the algebra SU(N), a different approach from the one used in [8]. We first compute the maximum of the fidelity for these QCM. Then we present the unitary transformation that realizes this fidelity. More general QCM that produce M copies from N' identical N-level quantum systems $(M > N' \ge 1)$ are also studied, by giving explicitly the unitary transformations and the related fidelity. The optimal cloning of entangled states of many qubits to M copies are discussed. Our results recover the ones obtained in [4,7,8] by taking different values of N and M.

For an N-level quantum state with basis $|j\rangle$, j = 1, ..., N, an input state is of the form

$$|\Psi\rangle = \sum_{j=1}^{N} \xi_j |j\rangle, \qquad (1)$$

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where $(\xi_1, ..., \xi_N)$ is a point in the complex sphere $S_{\mathbf{C}}^{N-1}$ with

$$\xi_1 = e^{i\varphi_1} \sin \theta_{N-1} \dots \sin \theta_2 \sin \theta_1$$

$$\xi_2 = e^{i\varphi_2} \sin \theta_{N-1} \dots \sin \theta_2 \cos \theta_1$$

$$\dots$$

$$\xi_{N-1} = e^{i\varphi_{N-1}} \sin \theta_{N-1} \cos \theta_{N-2}$$

$$\xi_N = e^{i\varphi_N} \cos \theta_{N-1}$$

where $i = \sqrt{-1}, 0 \le \varphi_j < 2\pi, 0 \le \theta_j < \frac{\pi}{2}, j = 1, ..., N.$

Theorem. The maximal value of the fidelity F for optimal cloning of an N-level quantum state to Mcopies is

$$F_{\max} = \frac{2M+N-1}{M(N+1)} \,. \tag{2}$$

Proof. Let $|R\rangle$ be the initial state of the QCM and the M-1 blank copies. The most general action of the QCM on $|\Psi\rangle$ defined by (1) is given by a unitary operator U such that

$$U|\Psi\rangle|R\rangle \equiv |\Psi_{\text{out}}\rangle = \sum_{i=1}^{N} \sum_{n_{1},...,n_{N}=0}^{M} \langle \xi_{i}|n_{1},...,n_{N}\rangle|R_{i,n_{1},...,n_{N}}\rangle$$
$$\equiv \sum_{i=1}^{N} \sum_{\mathbf{n}=0}^{M} \langle \xi_{i}|\mathbf{n}\rangle|R_{i,\mathbf{n}}\rangle,$$
(3)

where **n** denotes $n_1, ..., n_N$, $\sum_{i=1}^{M} i^{\prime}$ means to sum over the variables under the condition that the sum of all the variables should be equal to M, *i.e.* $\sum_{i=1}^{N} n_i = M$, $|\mathbf{n}\rangle = |n_1, ..., n_N\rangle$ is a completely symmetric (normalized) state with n_i quantum systems in the state $|i\rangle$ (we have postulated that the output of the QCM is completely symmetric, which does not affect the conclusions, see the discussions in [4] for the case N = 2), $|R_{i,\mathbf{n}}\rangle$ are unnormalized final states of the additional N-level quantum systems contributing to the copies of the original quantum system. By the unitarity of the evolution, the states $|R_{i,\mathbf{n}}\rangle$ satisfy the relations

$$\sum_{\mathbf{n}=0}^{M} \langle R_{j',\mathbf{n}} | R_{j,\mathbf{n}} \rangle = \delta_{j',j} \tag{4}$$

(with \langle , \rangle the scalar product in the Hilbert space).

As the output state is symmetric under permutations, the fidelity of the copies is obtained by calculating the overlap of the reduced density matrix of one copy, say the

first, with the input state $|\Psi\rangle$ and averaging over all input states:

$$F = \operatorname{Tr}\left[\sum_{i,i'=1}^{N} \langle \Psi_{\mathrm{out}} | \xi_{i'} | i' \rangle \langle i | \xi_i^* | \Psi_{\mathrm{out}} \rangle\right]$$

$$\equiv \sum_{j,j'=1}^{N} \sum_{\mathbf{n}'=\mathbf{0}}^{M'} \sum_{\mathbf{n}=0}^{M'} \langle R_{j',\mathbf{n}'} | R_{j,\mathbf{n}} \rangle A_{j',\mathbf{n}',j,\mathbf{n}},$$
(5)

where
$$A_{j',\mathbf{n}',j,\mathbf{n}} = \sum_{i,i'=1}^{N} \int \mathrm{d}\xi \, \xi_{j'}^* \xi_{i'} \xi_i^* \xi_j \operatorname{Tr}\left[\langle \mathbf{n}' | i' \rangle \langle i | \mathbf{n} \rangle\right]$$
 and

d ξ is the invariant measure on $S_{\mathbb{C}}^{N-1}$, *i.e.*, in above spherical coordinates $\varphi = (\varphi_1, ..., \varphi_N), \ \theta = (\theta_1, ..., \theta_{N-1})$:

$$d\xi \equiv d\xi(\varphi,\theta) = \frac{(N-1)!}{2\pi^N} \prod_{r=1}^N d\varphi_r \prod_{k=1}^{N-1} \sin^{2k-1} \theta_k \cos \theta_k d\theta_k.$$

To get the maximum of F as given by (5), we impose the constraint of the trace of equation (4), which gives the extrema of the fidelity that is greater or equal to the one using the constraint of equation (4). Using a corresponding Lagrange multiplier $\lambda \in \mathbb{R}$, we have to extremize

$$F_{\lambda} = \sum_{j,j'=1}^{N} \sum_{\mathbf{n}'=\mathbf{0}}^{M} \sum_{\mathbf{n}=\mathbf{0}}^{M'} \langle R_{j',\mathbf{n}'} | R_{j,\mathbf{n}} \rangle A_{j',\mathbf{n}',j,\mathbf{n}} -\lambda \left(\langle R_{j',\mathbf{n}'} | R_{j,\mathbf{n}} \rangle \delta_{j',j} \delta_{\mathbf{n}',\mathbf{n}} - N \right),$$

where $\delta_{\mathbf{n}',\mathbf{n}} = \prod_{k=1}^{N} \delta_{n'_k,n_k}$. Varying with respect to

Varying with respect to the components of $\langle R_{j',n'_1,...,n'_N} |$ one gets

$$\sum_{j=1}^{N} \sum_{\mathbf{n}=0}^{M'} \left(A_{j',\mathbf{n}',j,\mathbf{n}} - \lambda \delta_{\mathbf{n}',\mathbf{n}} \delta_{j',j} \right) |R_{j,\mathbf{n}}\rangle = 0.$$
(6)

Hence the possible value of λ are the eigenvalues of the matrix $A_{j',\mathbf{n}',j,\mathbf{n}}$, with corresponding eigenvectors $|R_{j,\mathbf{n}}\rangle$. Multiplying the above equation on the left by $\langle R_{j',\mathbf{n}'}|$ and summing over j', \mathbf{n}' we have

$$\sum_{j,j'=1}^{N} \sum_{\mathbf{n}'=\mathbf{0}}^{M'} \sum_{\mathbf{n}=0}^{M'} \langle R_{j',\mathbf{n}'} | R_{j,\mathbf{n}} \rangle A_{j',\mathbf{n}',j,\mathbf{n}} = \sum_{j,j'=1}^{N} \sum_{\mathbf{n}'=\mathbf{0}}^{M'} \sum_{\mathbf{n}=0}^{M'} \langle R_{j',\mathbf{n}'} | R_{j,\mathbf{n}} \rangle \lambda \delta_{\mathbf{n}',\mathbf{n}} \delta_{j',j} = N\lambda.$$
(7)

Comparing (5) and (7) we get $F_{\lambda} = N\lambda$. Therefore the maximum of F_{λ} is proportional to the largest eigenvalue of the matrix $A_{j',\mathbf{n}',j,\mathbf{n}}$.

$$B = \frac{1}{MN(N+1)} \begin{pmatrix} M+n_1 & \sqrt{(n_2+1)n_1} & \sqrt{(n_3+1)n_1} & \dots & \sqrt{(n_N+1)n_1} \\ \sqrt{n_1(n_2+1)} & M+n_2+1 & \sqrt{(n_3+1)(n_2+1)} & \dots & \sqrt{(n_N+1)(n_2+1)} \\ \sqrt{n_1(n_3+1)} & \sqrt{(n_2+1)(n_3+1)} & M+n_3+1 & \dots & \sqrt{(n_N+1)(n_3+1)} \\ \vdots & & \vdots \\ \sqrt{n_1(n_N+1)} & \sqrt{(n_2+1)(n_N+1)} & \sqrt{(n_3+1)(n_N+1)} & \dots & M+n_N+1 \end{pmatrix}$$

By a straightforward calculation we have

some $\lambda' \in \mathbb{R}$, we have

$$\begin{split} \langle n'_1, \dots, n'_N | k \rangle \langle l | n_1, \dots, n_N \rangle &= \\ \begin{cases} \frac{1}{M} \sqrt{n_l (n_k + 1)} \delta n'_1, n_1 \dots \delta n'_l, n_l - 1 \dots \delta n'_k, n_k + 1 \dots \delta n'_N, n_N \\ & k \neq l \end{cases} \\ \\ \frac{n_l}{M} \delta_{\mathbf{n}', \mathbf{n}} \qquad k = l \end{split}$$

and

$$\int d\xi \xi_{j'}^* \xi_{i'} \xi_i^* \xi_j = \begin{cases} \frac{2}{N(N+1)} & i' = j' = i = j \\\\ \frac{1}{N(N+1)} & i' = i \neq j' = j \text{ or } i' = j' \neq i = j \\\\ 0 & \text{otherwise.} \end{cases}$$

Therefore

$$A_{j',n'_1,...,n'_N,j,n_1,...,n_N} = \sum_{i,i'=1}^N \int d\xi \xi_{j'}^* \xi_{i'} \xi_i^* \xi_j \left[\frac{n_l}{M} \delta_{i',i} + \frac{1}{M} \sqrt{n_l(n_k+1)} |_{i \neq i'} \right]$$
$$= \frac{1}{MN(N+1)} \left((m+n_j) \delta_{jj'} + \sqrt{n_j(n_{j'}+1)} |_{j \neq j'} \right)$$

For any given $n_1, ..., n_N$, if we arrange the matrix indices $(j, n_1, n_2, n_3, ..., n_N)$ as $(1, n_1, n_2, n_3, ..., n_N)$, $(2, n_1, n_2 + 1, n_3, ..., n_N)$, $(3, n_1, n_2, n_3 + 1, ..., n_N)$, ..., $(N, n_1, n_2, ..., n_N + 1)$, then A is a block diagonal matrix. The block matrix B is given by

see equation above

where $n_1 = M - \sum_{i=2}^{N} n_i$. Setting $\lambda = \frac{\lambda'}{MN(N+1)}$ for

$$|B - \lambda| = \frac{n_1}{MN(N+1)} \prod_{i=2}^{N} (n_i + 1)$$

$$\times \begin{vmatrix} 1 + \frac{M - \lambda'}{n_1} & 1 & 1 & \dots & 1 \\ 1 & 1 + \frac{M - \lambda'}{n_2 + 1} & 1 & \dots & 1 \\ 1 & 1 & 1 + \frac{M - \lambda'}{n_3 + 1} & \dots & 1 \\ \vdots & & & \vdots \\ 1 & 1 & 1 & \dots & 1 + \frac{M - \lambda'}{n_N + 1} \end{vmatrix}$$

$$=\frac{(M-\lambda')^{N-1}(\lambda'-2M-N+1)}{MN(N+1)}$$

Therefore the largest eigenvalue of the matrix A is $\lambda_{\max} = \frac{\lambda'_{\max}}{MN(N+1)} = \frac{2M+N-1}{MN(N+1)}$. The maximum of the fidelity is then obtained as

$$F_{\max} = F_{\lambda_{\max}} = N\lambda_{\max} = \frac{2M + N - 1}{M(N+1)}$$

From formula (2) we see that when N = 2 the fidelity is reduced to the one in [4]. For M = 2, formula (2) gives the fidelity obtained from the transformations in [7] where optimality had been tested numerically. For large N, the optimal fidelity is almost independent of the number of quantum levels of the qubit being copied, in fact we have $\lim_{N\to\infty} F_{\max} = \frac{1}{M}$. We also see that the fidelity of the copies decreases with N, tending to $\frac{1}{M}$ as N goes to infinity.

In the following we give a unitary transformation that realizes the optimal fidelity given above. For any given $|i\rangle$, $i \in 1, ..., N$, the optimal cloning $|i\rangle$ to M copies is given by the following transformation:

$$U_{1,M}|i\rangle\otimes R=\sum_{\mathbf{n}_i=0}^{M}{}^{\prime\prime}\;\alpha_{\mathbf{n}_i}|\mathbf{n}\rangle\otimes R_{\mathbf{n}_i}$$

where \mathbf{n}_i denotes $n_1, ..., n_{i-1}, n_{i+1}, ..., n_N$, $\sum^{M''}$ means to sum over the variables under the condition that $m_i \equiv n_1 + ... + n_{i-1} + n_{i+1} + ... + n_N \leq M$, n_i in \mathbf{n} is given by $M - m_i$, $R_{\mathbf{n}_i}$ are orthogonal normalized internal states of QCM, and

$$\alpha_{\mathbf{n}_{i}} = \sqrt{M - m_{i}} \sqrt{\frac{N!(M-1)!}{(M+N-1)!}}$$

The fidelity given by the above copy machine is

$$F = \sum_{\mathbf{n}_{i}=0}^{M} \frac{M - m_{i}}{M} \alpha_{\mathbf{n}_{i}}^{2}$$

= $\frac{N!(M-1)!}{M(M+N-1)!} \sum_{n_{1}=0}^{M} \dots \sum_{n_{i-1}=0}^{M-n_{i-1}} \sum_{n_{i+1}=0}^{M-n_{i-1}}$
 $\dots \sum_{n_{N}=0}^{M-m_{i}} (M - m_{i})^{2}$
= $\frac{2M + N - 1}{M(N+1)} = F_{\text{max}}.$

Therefore F_{max} is truly the maximum of the fidelity that can be realized by optimal cloning. An optimal copy of an input state (1) can be obtained by the following unitary transformation,

$$U_{1,M}|\Psi\rangle\otimes R = \sum_{i=1}^{N}\sum_{\mathbf{n}_{i}=0}^{M}{}^{\prime\prime}\xi_{i}\,\alpha_{\mathbf{n}_{i}}|\mathbf{n}\rangle\otimes R_{\mathbf{n}_{i}}.$$
 (8)

We have discussed optimal cloning of an N-level quantum state to M copies. Formula (8) can be also applied for making M copies from a quantum register with N' qubits such that $2^{N'} = N$. In the following we consider a quantum cloning machine that takes N' identical N-level quantum systems into M identical copies (M > N'). Let $|N'i\rangle$, i = 1, ..., N, denote the input state consisting of N' quantum states all in the state $|i\rangle$. The quantum cloning machine is described by

$$U_{N',M}|N'i\rangle \otimes R = \sum_{\mathbf{n}_i=0}^{M-N'} \beta_{\mathbf{n}_i}|\mathbf{n}\rangle \otimes R_{\mathbf{n}_i}, \qquad (9)$$

$$\beta_{\mathbf{n}_i} = \sqrt{\frac{(M-m_i)!}{(M-N'-m_i)!}} \sqrt{\frac{(N'+N-1)!(M-N')!}{N'!(M+N-1)!}},$$

here $\sum_{i=1}^{M-N'} m_{i}$ means to sum over the variables under the condition that $m_i \leq M - N'$ so that the number m_i of errors in the copies is smaller or equal to the number M - N' of additional N-level qubits. The fidelity of each output qubit is

$$F_{N'M} = \sum_{\mathbf{n}_i=0}^{M''} \frac{M - m_i}{M} \beta_{\mathbf{n}_i}^2 = \frac{M + N'(M + N - 1)}{M(N + N')} \cdot$$
(10)

The unitary transformation (9) is a generalization of (8). Its optimality can be proved for small integer values of N'. We believe that the method used in proving the optimality for the case N = 2 can be used for a general proof of the optimality of the transformation (9). In fact, the dimension of the state space for N' N-level systems is $N^{N'}$. If we view the N' N-level systems as one of the states belonging to an $N^{N'}$ -level system, then (9) is just a special case of (8). However, with \tilde{F}_{\max} defined as F_{\max} with N replaced by $N^{N'}$, $\tilde{F}_{\max} = \frac{2M + N^{N'} - 1}{M(N^{N'} + 1)} \leq F_{N'M}$, which implies that the more one learns about the quantum input state, the better one can make a copy of it. The explicitly given unitary transformations (8) and (9) can help in constructing quantum computational networks for the kinds of cloning machine we described.

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