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Subject: **Parametrization of a three-qubit pure state**

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Consider a three-qubit pure state  $|\Psi\rangle$ . First do a Schmidt decomposition between qubit  $A$  and qubits  $B$  and  $C$ ,

$$|\Psi\rangle = \cos\theta|e_1\rangle \otimes |\psi_1\rangle + \sin\theta|e_2\rangle \otimes |\psi_2\rangle, \quad (1)$$

where  $0 \leq \theta \leq \pi/2$ . Now Schmidt decompose  $|\psi_1\rangle$ , and write  $|\psi_2\rangle$  in the resulting Schmidt basis,

$$\begin{aligned} |\Psi\rangle = & \cos\theta|e_1\rangle \otimes \left( \underbrace{\cos\chi|f_1\rangle \otimes |g_1\rangle + \sin\chi|f_2\rangle \otimes |g_2\rangle}_{=|\psi_1\rangle} \right) \\ & + \sin\theta|e_2\rangle \otimes \left( \underbrace{ae^{i\theta}|f_1\rangle \otimes |g_1\rangle + be^{i\phi}|f_2\rangle \otimes |g_2\rangle + ce^{i\alpha}|f_1\rangle \otimes |g_2\rangle + de^{i\beta}|f_2\rangle \otimes |g_1\rangle}_{=|\psi_2\rangle} \right), \end{aligned} \quad (2)$$

where  $0 \leq \chi \leq \pi/2$ ,  $a, b, c$ , and  $d$  are real and nonnegative, and the phases are arbitrary. Re-phase  $|e_2\rangle = |e'_2\rangle e^{-i\theta}$ , giving

$$\begin{aligned} |\Psi\rangle = & \cos\theta|e_1\rangle \otimes \left( \cos\chi|f_1\rangle \otimes |g_1\rangle + \sin\chi|f_2\rangle \otimes |g_2\rangle \right) \\ & + \sin\theta|e'_2\rangle \otimes \left( a|f_1\rangle \otimes |g_1\rangle + be^{i\phi'}|f_2\rangle \otimes |g_2\rangle + ce^{i\alpha'}|f_1\rangle \otimes |g_2\rangle + de^{i\beta'}|f_2\rangle \otimes |g_1\rangle \right), \end{aligned} \quad (3)$$

where  $\phi' = \phi - \theta$ ,  $\alpha' = \alpha - \theta$ , and  $\beta' = \beta - \theta$ . The orthogonality of  $|\psi_1\rangle$  and  $|\psi_2\rangle$  gives

$$0 = a \cos\chi + be^{i\phi'} \sin\chi \implies e^{i\phi'} = -1 \quad \text{and} \quad 0 = a \cos\chi - b \sin\chi, \quad (4)$$

and normalization of  $|\psi_2\rangle$  gives

$$1 = a^2 + b^2 + c^2 + d^2. \quad (5)$$

Re-phase

$$|f_1\rangle = |f'_1\rangle e^{-i\alpha'/2}, \quad |f_2\rangle = |f'_2\rangle e^{-i\beta'/2}, \quad |g_1\rangle = |g'_1\rangle e^{i\alpha'/2}, \quad |g_2\rangle = |g'_2\rangle e^{i\beta'/2}, \quad (6)$$

giving

$$\begin{aligned} |\Psi\rangle = & \cos\theta|e_1\rangle \otimes \left( \cos\chi|f'_1\rangle \otimes |g'_1\rangle + \sin\chi|f'_2\rangle \otimes |g'_2\rangle \right) \\ & + \sin\theta|e'_2\rangle \otimes \left( a|f'_1\rangle \otimes |g'_1\rangle - b|f'_2\rangle \otimes |g'_2\rangle + ce^{i\delta}|f'_1\rangle \otimes |g'_2\rangle + de^{i\delta}|f'_2\rangle \otimes |g'_1\rangle \right), \end{aligned} \quad (7)$$

where  $\delta = (\alpha' + \beta')/2$  is the one remaining phase. It is a relative phase that can take on the values  $0 \leq \delta \leq 2\pi$ .

We can now use local unitaries to transform to a standard basis for each qubit. Our conclusion is that any three-qubit pure state is equivalent under local unitaries to a state of the form

$$\begin{aligned} & \cos \theta |0\rangle \otimes \left( \cos \chi |0\rangle \otimes |0\rangle + \sin \chi |1\rangle \otimes |1\rangle \right) \\ & + \sin \theta |1\rangle \otimes \left( a |0\rangle \otimes |0\rangle - b |1\rangle \otimes |1\rangle + c e^{i\delta} |0\rangle \otimes |1\rangle + d e^{i\delta} |1\rangle \otimes |0\rangle \right), \end{aligned} \quad (8)$$

where the parameters are constrained by two relations,

$$a \cos \chi = b \sin \chi \quad \text{and} \quad c^2 + d^2 = 1 - a^2 - b^2. \quad (9)$$

Defining  $a^2 + b^2 = \cos^2 \xi$ , with  $0 \leq \xi \leq \pi/2$ , we have

$$a = \sin \chi \cos \xi, \quad b = \cos \chi \cos \xi, \quad c^2 + d^2 = 1 - \cos^2 \xi = \sin^2 \xi. \quad (10)$$

We are left with five parameters necessary to specify an arbitrary three-qubit pure state up to local unitaries. We can make these parameters explicit by defining

$$c = \sin \xi \cos \eta \quad \text{and} \quad d = \sin \xi \sin \eta, \quad (11)$$

where  $0 \leq \theta \leq \pi/2$ . This puts the arbitrary state (8) in the final form

$$\begin{aligned} & \cos \theta |0\rangle \otimes \underbrace{\left( \cos \chi |0\rangle \otimes |0\rangle + \sin \chi |1\rangle \otimes |1\rangle \right)}_{= |\phi_0\rangle} \\ & + \sin \theta |1\rangle \otimes \underbrace{\left( \cos \xi (\sin \chi |0\rangle \otimes |0\rangle - \cos \chi |1\rangle \otimes |1\rangle) + e^{i\delta} \sin \xi (\cos \eta |0\rangle \otimes |1\rangle + \sin \eta |1\rangle \otimes |0\rangle) \right)}_{= |\phi_1\rangle} \\ & = \cos \theta \cos \chi |0\rangle \otimes |0\rangle \otimes |0\rangle + \cos \theta \sin \chi |0\rangle \otimes |1\rangle \otimes |1\rangle \\ & \quad + \sin \theta \sin \chi \cos \xi |1\rangle \otimes |0\rangle \otimes |0\rangle - \sin \theta \cos \chi \cos \xi |1\rangle \otimes |1\rangle \otimes |1\rangle \\ & \quad + e^{i\delta} \sin \theta \sin \xi \cos \eta |1\rangle \otimes |0\rangle \otimes |1\rangle + e^{i\delta} \sin \theta \sin \xi \sin \eta |1\rangle \otimes |1\rangle \otimes |0\rangle. \end{aligned} \quad (12)$$

Here the  $BC$  states  $|\phi_0\rangle$  and  $|\phi_1\rangle$  are orthogonal (from the first Schmidt decomposition of  $A$  vs.  $BC$ ), and the ranges of the parameters are

$$0 \leq \theta, \chi, \xi, \eta \leq \pi/2, \quad 0 \leq \delta \leq 2\pi. \quad (13)$$

The Schmidt-like decomposition (12) puts qubit  $A$  on a special footing, different from qubits  $B$  and  $C$ . It treats qubits  $B$  and  $C$  symmetrically; swapping qubits  $B$  and  $C$  is the same as the exchange  $\cos \eta \leftrightarrow \sin \eta$ . The decomposition (12) is not a three-qubit Schmidt decomposition, because of the presence of four terms in  $|\phi_1\rangle$ , instead of just the first two terms or the second two terms. It becomes a three-qubit Schmidt decomposition when  $\xi = 0$  or  $\pi/2$ .

Writing the state (12) as a density operator, we have

$$\cos^2 \theta |0\rangle\langle 0| \otimes |\phi_0\rangle\langle \phi_0| + \sin^2 \theta |1\rangle\langle 1| \otimes |\phi_1\rangle\langle \phi_1| + \cos \theta \sin \theta (|0\rangle\langle 1| \otimes |\phi_0\rangle\langle \phi_1| + |1\rangle\langle 0| \otimes |\phi_1\rangle\langle \phi_0|) . \quad (14)$$

The marginal density operator of qubit  $A$  is

$$\rho_A = \cos^2 \theta |0\rangle\langle 0| + \sin^2 \theta |1\rangle\langle 1| , \quad (15)$$

as it must be from the original Schmidt decomposition. The marginal density operator of qubits  $B$  and  $C$  is

$$\rho_{BC} = \cos^2 \theta |\phi_0\rangle\langle \phi_0| + \sin^2 \theta |\phi_1\rangle\langle \phi_1| . \quad (16)$$

The marginal density operator of qubit  $B$  is

$$\begin{aligned} \rho_B &= \text{tr}_C(\rho_{BC}) \\ &= \cos^2 \theta \text{tr}_C(|\phi_0\rangle\langle \phi_0|) + \sin^2 \theta \text{tr}_C(|\phi_1\rangle\langle \phi_1|) \\ &= \cos^2 \theta \left( \cos^2 \chi |0\rangle\langle 0| + \sin^2 \chi |1\rangle\langle 1| \right) \\ &\quad + \sin^2 \theta \left( (\cos^2 \xi \sin^2 \chi + \sin^2 \xi \cos^2 \eta) |0\rangle\langle 0| + (\cos^2 \xi \cos^2 \chi + \sin^2 \xi \sin^2 \eta) |1\rangle\langle 1| \right. \\ &\quad \quad \left. + \cos \xi \sin \xi \left( (e^{-i\delta} \sin \chi \sin \eta - e^{i\delta} \cos \chi \cos \eta) |0\rangle\langle 1| \right. \right. \\ &\quad \quad \quad \left. \left. + (e^{i\delta} \sin \chi \sin \eta - e^{-i\delta} \cos \chi \cos \eta) |1\rangle\langle 0| \right) \right) \\ &= \left( \cos^2 \theta \cos^2 \chi + \sin^2 \theta (\cos^2 \xi \sin^2 \chi + \sin^2 \xi \cos^2 \eta) \right) |0\rangle\langle 0| \\ &\quad + \left( \cos^2 \theta \sin^2 \chi + \sin^2 \theta (\cos^2 \xi \cos^2 \chi + \sin^2 \xi \sin^2 \eta) \right) |1\rangle\langle 1| \\ &\quad + \sin^2 \theta \cos \xi \sin \xi \left( (e^{-i\delta} \sin \chi \sin \eta - e^{i\delta} \cos \chi \cos \eta) |0\rangle\langle 1| \right. \\ &\quad \quad \left. + (e^{i\delta} \sin \chi \sin \eta - e^{-i\delta} \cos \chi \cos \eta) |1\rangle\langle 0| \right) . \end{aligned} \quad (17)$$

As indicated above, the marginal density operator of qubit  $C$  is obtained from  $\rho_B$  by the exchange  $\cos \eta \leftrightarrow \sin \eta$ . Notice that these forms for  $\rho_B$  and  $\rho_C$  are diagonal when  $\xi = 0$  or  $\pi/2$ , i.e., when Eq. (12) is a three-qubit Schmidt decomposition.