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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,

$$|\Psi\rangle = \cos\theta|e_1\rangle \otimes |\psi_1\rangle + \sin\theta|e_2\rangle \otimes |\psi_2\rangle \ , \tag{1}$$

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

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

where $0 \le \chi \le \pi/2$, 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

$$\begin{aligned}|\Psi\rangle = {}& \cos\theta|e_1\rangle \otimes \Big(\cos\chi|f_1\rangle \otimes |g_1\rangle + \sin\chi|f_2\rangle \otimes |g_2\rangle\Big) \\ & + \sin\theta|e_2'\rangle \otimes \Big(a|f_1\rangle \otimes |g_1\rangle + be^{i\phi'}|f_2\rangle \otimes |g_2\rangle + ce^{i\alpha'}|f_1\rangle \otimes |g_2\rangle + de^{i\beta'}|f_2\rangle \otimes |g_1\rangle\Big) \ ,\end{aligned} \tag{3}$$

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

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

and normalization of $|\psi_2\rangle$ gives

$$1 = a^2 + b^2 + c^2 + d^2 \ . \tag{5}$$

Re-phase

$$|f_1\rangle = |f_1'\rangle e^{-i\alpha'/2} \ , \qquad |f_2\rangle = |f_2'\rangle e^{-i\beta'/2} \ , \qquad |g_1\rangle = |g_1'\rangle e^{i\alpha'/2} \ , \qquad |g_2\rangle = |g_2'\rangle e^{i\beta'/2} \ , \tag{6}$$

giving

$$\begin{aligned}|\Psi\rangle = {}& \cos\theta|e_1\rangle \otimes \Big(\cos\chi|f_1'\rangle \otimes |g_1'\rangle + \sin\chi|f_2'\rangle \otimes |g_2'\rangle\Big) \\ & + \sin\theta|e_2'\rangle \otimes \Big(a|f_1'\rangle \otimes |g_1'\rangle - b|f_2'\rangle \otimes |g_2'\rangle + ce^{i\delta}|f_1'\rangle \otimes |g_2'\rangle + de^{i\delta}|f_2'\rangle \otimes |g_1'\rangle\Big) \ ,\end{aligned} \tag{7}$$

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

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

$$\begin{aligned}&\cos\theta|0\rangle \otimes \Big(\cos\chi|0\rangle\otimes|0\rangle + \sin\chi|1\rangle\otimes|1\rangle\Big)\\ &+\sin\theta|1\rangle\otimes\Big(a|0\rangle\otimes|0\rangle - b|1\rangle\otimes|1\rangle + ce^{i\delta}|0\rangle\otimes|1\rangle + de^{i\delta}|1\rangle\otimes|0\rangle\Big)\ ,\end{aligned} \tag{8}$$

where the parameters are constrained by two relations,

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

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

$$a = \sin\chi\cos\xi\ , \qquad b=\cos\chi\cos\xi\ , \qquad c^2+d^2 = 1-\cos^2\xi = \sin^2\xi\ . \tag{10}$$

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

$$c = \sin\xi\cos\eta \qquad \text{and} \qquad d = \sin\xi\sin\eta\ , \tag{11}$$

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

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

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

$$0\le\theta,\chi,\xi,\eta\le\pi/2\ , \qquad 0\le\delta\le2\pi\ . \tag{13}$$

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

$$\cos^2\theta|0\rangle\langle 0|\otimes|\phi_0\rangle\langle\phi_0|+\sin^2\theta|1\rangle\langle 1|\otimes|\phi_1\rangle\langle\phi_1|+\cos\theta\sin\theta\big(|0\rangle\langle 1|\otimes|\phi_0\rangle\langle\phi_1|+|1\rangle\langle 0|\otimes|\phi_1\rangle\langle\phi_0|\big)\;. \tag{14}$$

The marginal density operator of qubit A is

$$\rho_A=\cos^2\theta|0\rangle\langle 0|+\sin^2\theta|1\rangle\langle 1|\;, \tag{15}$$

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

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

The marginal density operator of qubit B is

$$\begin{aligned}
\rho_B &= \mathrm{tr}_C(\rho_{BC})\\
&= \cos^2\theta\,\mathrm{tr}_C\big(|\phi_0\rangle\langle\phi_0|\big)+\sin^2\theta\,\mathrm{tr}_C\big(|\phi_1\rangle\langle\phi_1|\big)\\
&= \cos^2\theta\Big(\cos^2\chi|0\rangle\langle 0|+\sin^2\chi|1\rangle\langle 1|\Big)\\
&\quad+\sin^2\theta\Big(\big(\cos^2\xi\sin^2\chi+\sin^2\xi\cos^2\eta\big)|0\rangle\langle 0|+\big(\cos^2\xi\cos^2\chi+\sin^2\xi\sin^2\eta\big)|1\rangle\langle 1|\\
&\qquad\qquad+\cos\xi\sin\xi\big((e^{-i\delta}\sin\chi\sin\eta-e^{i\delta}\cos\chi\cos\eta)|0\rangle\langle 1|\\
&\qquad\qquad\qquad+(e^{i\delta}\sin\chi\sin\eta-e^{-i\delta}\cos\chi\cos\eta)|1\rangle\langle 0|\big)\Big)\\
&= \Big(\cos^2\theta\cos^2\chi+\sin^2\theta\big(\cos^2\xi\sin^2\chi+\sin^2\xi\cos^2\eta\big)\Big)|0\rangle\langle 0|\\
&\quad+\Big(\cos^2\theta\sin^2\chi+\sin^2\theta\big(\cos^2\xi\cos^2\chi+\sin^2\xi\sin^2\eta\big)\Big)|1\rangle\langle 1|\\
&\quad+\sin^2\theta\cos\xi\sin\xi\Big(\big(e^{-i\delta}\sin\chi\sin\eta-e^{i\delta}\cos\chi\cos\eta\big)|0\rangle\langle 1|\\
&\qquad\qquad+\big(e^{i\delta}\sin\chi\sin\eta-e^{-i\delta}\cos\chi\cos\eta\big)|1\rangle\langle 0|\Big)\;.
\end{aligned} \tag{17}$$

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