Comment on "Universal quantum circuit for two-qubit transformations with three controlled-NOT gates" and "Recognizing small-circuit structure in two-qubit operators"

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Recent papers in Physical Review A have considered small quantum circuit decompositions in terms of a minimal number of controlled-NOT (CNOT) gates. Specifically, we point out errors in the papers by Vidal and Dawson [Phys. Rev. A **69**, 010301(R) (2004)] and by Shende *et al.* [Phys. Rev. A **70**, 012310 (2004)].

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Recently there has been interest in characterizing two-quantum-bit (qubit) operations in terms of certain invariants, and by other methods [1–6]. By such techniques one may discriminate whether a two-qubit operator is locally equivalent to zero, one, two, or three controlled-NOT (CNOT) gates. The equivalence for CNOT complexity is up to single-qubit rotations. This is very useful both in terms of the feasibility of achieving a single, double, or triple (SWAP) CNOT gate, and for constructing minimal two-qubit operator decompositions.

In a recent paper [3] building upon the magic basis results of Ref. [7], a decomposition for a two-qubit matrix exponential is given. We point out that Theorem 1 as stated in Ref. [3] is incorrect. All five operators u_2, v_2, u_3, v_3, and w in Eqs. (7)–(9) in that paper need to be modified. Correspondingly, certain intermediate results are also slightly but importantly modified. For instance, both the m and n dependencies of the phase ϕ_{mn} in Eq. (17) are modified. The corrected form of Eqs. (7)–(9) of Ref. [3], as kindly supplied to us by the authors, is given in Sec. 3.4 of the thesis [8,9]. One may also note that Ref. [3] also differs from the arXiv version [10] with respect to the matrix u_2.

The corrected single-qubit operators are given by

$$u_2 = He^{ih_x\sigma_x}, \quad v_2 = e^{ih_z\sigma_z}, \tag{1}$$

$$u_3 = HS, \quad v_3 = e^{-ih_y\sigma_z}, \tag{2}$$

$$w = e^{i\pi\sigma_x/4} = \frac{1}{\sqrt{2}}(I + i\sigma_x), \tag{3}$$

where H is the Hadamard gate, $S=\text{diag}(1,i)$, and σ_j are the Pauli matrices. Then it is readily verified that

$$\exp(iH_{xyz}) = (w \otimes w^{-1})U_{\text{CNOT}}(u_3 \otimes v_3) \times U_{\text{CNOT}}(u_2 \otimes v_2)U_{\text{CNOT}}, \tag{4}$$

where

$$H_{xyz} \equiv h_x\sigma_x \otimes \sigma_x + h_y\sigma_y \otimes \sigma_y + h_z\sigma_z \otimes \sigma_z. \tag{5}$$

As an example instance of change in the intermediate results incurred by Eqs. (1)–(3), we have now

$$\phi_{mn} = (-1)^{m+1}h_x + (-1)^{n+1}h_z, \tag{6}$$

replacing Eq. (17) in Ref. [3]. Equation (6) follows from

$$u_2|^x m\rangle = e^{(-1)^m ih_x}|m\rangle = e^{-(-1)^{m+1}ih_x}|m\rangle, \tag{7a}$$

and

$$v_2|n\rangle = e^{(-1)^n ih_z}|n\rangle = e^{-(-1)^{n+1}ih_z}|n\rangle, \tag{7b}$$

where $|^x0\rangle = H|0\rangle$ and $|^x1\rangle = H|1\rangle$. In stating Eqs. (6), (7a), and (7b) we have employed the convention of Ref. [3], wherein phases are written in the form $\exp(-i\phi_{mn})$.

As a complement to a special case of Ref. [3], we consider the CNOT complexity of the unitary evolution generated by the Hamiltonian

$$H_x = h_x\sigma_x \otimes \sigma_x, \tag{8}$$

wherein we may restrict consideration to values $0 \le h_x \le \pi/4$. We verify the single CNOT complexity induced by Eq. (8) at particular times, as well as provide the corresponding gate decomposition.

The evolution operator $U(t) \equiv \exp(-iH_x t)$ ($\hbar=1$) is given by

$$U(t) = \cos(h_x t)I - i\sin(h_x t)\sigma_x \otimes \sigma_x. \tag{9}$$

Using the classification procedure of Ref. [11], we apply the operator, for matrices in SU(2), $\gamma(w) = w\sigma_y^{\otimes 2}w^T\sigma_y^{\otimes 2}$, wherein T denotes transposition. Since in this case H_x and U are symmetric, we have $\gamma[U(t)] = [U(t)\sigma_y \otimes \sigma_y]^2$ and find

$$\gamma[U(t)] = \cos 2h_x tI - i\sin 2h_x t\sigma_x \otimes \sigma_x. \tag{10}$$

Calculating the characteristic polynomial $\chi(g)(x) = \det(xI - g)$, we have

$$\chi\{\gamma[U(t)]\} = (x^2 - 2x\cos 2h_x t + 1)^2. \tag{11}$$

According to the classification of Ref. [1], the evolution of H_x is generally equivalent to a double CNOT gate. In addition, there are special times when χ assumes the form $\chi = (x^2+1)^2$. In this case, $t_n = \pi(n+1/2)/2h_x$ for nonnegative integers n, and the smallest such is $t_0 = \pi/4h_x$. At these times, the evolution is equivalent to a single CNOT gate.

At the particular time t_0, when $\gamma[U(t_0)] = -i\sigma_x \otimes \sigma_x$, we have

$$U(t_0) = \frac{1}{\sqrt{2}}(I - i\sigma_x \otimes \sigma_x) = e^{-i\pi\sigma_x \otimes \sigma_x/4}. \tag{12}$$

We introduce the single-qubit operators

$$w_x \equiv \frac{1}{\sqrt{2}}(I - i\sigma_x) = e^{-i\pi\sigma_x/4}, \quad w_y^{(\pm)} \equiv \frac{1}{\sqrt{2}}(I \pm i\sigma_y) = e^{\pm i\pi\sigma_y/4}. \tag{13}$$

We then determine the decomposition

$$U(t_0) = e^{-i\pi\sigma_x\otimes\sigma_x/4} = (w_y^{(-)}S \otimes w_x)U_{\text{CNOT}}(w_y^{(+)} \otimes I). \tag{14}$$

In this equation, we have given the explicit tensor product pre- and postfactors for the single CNOT equivalence. We may note that Eq. (14) does not simply correspond to either $u_2 \otimes v_2 = I$ or $u_3 \otimes v_3 = I$ in Eq. (4), in which case we could apply the fact $U_{\text{CNOT}}^2 = I$.

The CNOT complexity that we have illustrated may also be determined directly in terms of the operator γ [1]. In fact, from Eq. (9) $\text{tr}[U(t)]$ is real, implying the equivalence of $U(t)$ to two CNOT gates. As concerns $U(t_n)$, we have that $\gamma[U(t_n)]$ is not proportional to the identity matrix, while $\gamma^2[U(t_n)] = -I$, implying equivalence to a single CNOT gate.

Reference [1] considered two-qubit operators with respect to CNOT complexity and presented a series of algebraic results and some numerical examples. We nonexhaustively describe some corrections and clarifications that are in order for this paper.

In example 3 for the two-qubit Fourier transform, the 42 entry of the matrix $\mathcal{F}$ should read $-i$, thereby making this operator symmetric and unitary, as it must be. Most importantly, neither the written nor the corrected matrix has determinant 1. Therefore, one does not literally compute the characteristic polynomial $\chi[\gamma(\mathcal{F})]$ as stated, but must first divide $\mathcal{F}$ by the normalizing factor $[\det(\mathcal{F})]^{1/4}$.

The numerical example matrix decomposition given in Sec. V of Ref. [1] is incorrect. That is, with C_2^1 denoting a CNOT gate with control on the second qubit, $C_2^1 = (a_2 \otimes b_2)\exp(iH_{42}t_{\text{CNOT}})(c_2 \otimes d_2)$ does not hold for the given local gates a_2, b_2, c_2, and d_2, which may be readily confirmed by performing the matrix product in question. (Compare the paper [12], which contains the very same example.)

In the last paragraph of Sec. III of Ref. [1], "nonscalar" should be taken to mean "not proportional to the identity," and after $\text{tr}[\gamma(u)]$ "is real" should be inserted. Other examples of typographical errors in this paper include the (here revised) statements $\text{tr}[\gamma(C_1^2)] = \text{tr}[\gamma(C_2^1)] = 0$ on p. 2 and $-\sigma^y \otimes \sigma^y = EE^T$ in the fourth paragraph of the Appendix on p. 4.

In conclusion, (i) explicit quantum circuit decompositions are very useful, and indeed necessary in order to take quantum logic circuits to an engineering physics level and further (ii) although it may be difficult at times to arrive at the desired gate decomposition, a candidate decomposition may be swiftly verified.

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