

Erratum: Faster Quantum Chemistry Simulations on a Quantum Computer with Improved Tensor Factorization and Active Volume Compilation [PRX Quantum 6, 030337 (2025)]

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The quantum circuits in the original Figs. 1 and 12 lacked the final controlled SWAP gate that is indicated between waypoints (C) and (D) in Fig. 1 in this document. The gate is necessary to maintain the self-inverse property of the block encoding and does not affect the resource counts in the tables noticeably. The gate swaps the qubits y and z in the $|0\rangle$ subspace of c and results in a new state:

$$\begin{aligned}
 (D): & \frac{1}{\sqrt{8}} \sum_{\nu=0}^{M-1} \sum_{\mu=0}^{\nu-1} \sqrt{|\hat{\zeta}_{\mu\nu}|} \sum_{\sigma\tau} (|\mu\rangle_{b_0} |\nu\rangle_{b_1} |0\rangle_i \tilde{Z}_{\nu,\tau} \tilde{Z}_{\mu,\sigma} + |\nu\rangle_{b_0} |\mu\rangle_{b_1} |1\rangle_i \tilde{Z}_{\mu,\tau} \tilde{Z}_{\nu,\sigma}) |0\rangle_c Z_m |\text{sign}(\hat{\zeta}_{\mu\nu})\rangle_m |0\rangle_x |\tau\rangle_y |\sigma\rangle_z \\
 & + \frac{1}{\sqrt{2}} \sum_{\nu=0}^{M-1} \sqrt{|\hat{\zeta}_{\nu\nu}|} |\nu\rangle_{b_0} |\nu\rangle_{b_1} |+\rangle_i |0\rangle_c Z_m |\text{sign}(\hat{\zeta}_{\nu\nu})\rangle_m |1\rangle_x (|1\rangle_y |0\rangle_z \tilde{Z}_{\nu,\downarrow} \tilde{Z}_{\nu,\uparrow} + |0\rangle_y |1\rangle_z \tilde{Z}_{\nu,\uparrow} \tilde{Z}_{\nu,\downarrow}) \\
 & + \frac{1}{\sqrt{2}} \sum_{\mu=0}^{N/2-1} \sqrt{|\hat{\zeta}_{\mu M}|} |\mu\rangle_{b_0} |M\rangle_{b_1} |+\rangle_i |1\rangle_c Z_m |\text{sign}(\hat{\zeta}_{\mu M})\rangle_m |0\rangle_x (|0\rangle_y \tilde{T}_{\mu,\uparrow} + |1\rangle_y \tilde{T}_{\mu,\downarrow}) |+\rangle_z.
 \end{aligned} \quad (1)$$

In the last stage, we undo the swap of the second stage, flip qubit i and uncompute i , x , y and z . Using $H|x\rangle = 2^{-1/2} \sum_y (-1)^{xy} |y\rangle$ for bits $x, y \in \{0, 1\}$, the state at waypoint (E) is

$$\begin{aligned}
 (E): & \frac{1}{8} \sum_{i,y,z} \sum_{\nu=0}^{M-1} \sum_{\mu=0}^{\nu-1} \sqrt{|\hat{\zeta}_{\mu\nu}|} |\mu\rangle_{b_0} |\nu\rangle_{b_1} |i\rangle_i \sum_{\sigma\tau} ((-1)^i \tilde{Z}_{\nu,\tau} \tilde{Z}_{\mu,\sigma} + \tilde{Z}_{\mu,\tau} \tilde{Z}_{\nu,\sigma}) |0\rangle_c Z_m |\text{sign}(\hat{\zeta}_{\mu\nu})\rangle_m |0\rangle_x (-1)^{y\tau+z\sigma} |y\rangle_y |z\rangle_z \\
 & + \frac{1}{2} \sum_y \sum_{\nu=0}^{M-1} \sqrt{|\hat{\zeta}_{\nu\nu}|} |\nu\rangle_{b_0} |\nu\rangle_{b_1} |0\rangle_i |0\rangle_c Z_m |\text{sign}(\hat{\zeta}_{\nu\nu})\rangle_m ((-1)^y \tilde{Z}_{\nu,\downarrow} \tilde{Z}_{\nu,\uparrow} + \tilde{Z}_{\nu,\uparrow} \tilde{Z}_{\nu,\downarrow}) |0\rangle_x |y\rangle_y |0\rangle_z \\
 & + \frac{1}{2} \sum_y \sum_{\mu=0}^{N/2-1} \sqrt{|\hat{\zeta}_{\mu M}|} |\mu\rangle_{b_0} |M\rangle_{b_1} |0\rangle_i |1\rangle_c Z_m |\text{sign}(\hat{\zeta}_{\mu M})\rangle_m (\tilde{T}_{\mu,\uparrow} + (-1)^y \tilde{T}_{\mu,\downarrow}) |0\rangle_x |y\rangle_y |0\rangle_z.
 \end{aligned} \quad (2)$$

Multiplying this state from the left-hand side with $\langle\Lambda_1| \cdot$ finally gives us

$$H' = \frac{1}{8} \sum_{\mu=0}^{M-1} \sum_{\nu \neq \mu} \hat{\zeta}_{\mu\nu} \sum_{\sigma\tau} \tilde{Z}_{\nu,\tau} \tilde{Z}_{\mu,\sigma} + \frac{1}{2} \sum_{\nu=0}^{M-1} \hat{\zeta}_{\nu\nu} \sum_{\sigma} \tilde{Z}_{\nu,\sigma} \tilde{Z}_{\nu,\bar{\sigma}} + \frac{1}{2} \sum_{k=0}^{N/2-1} \hat{\zeta}_{kM} \sum_{\sigma} \tilde{T}_{k,\sigma},$$

where $\bar{\sigma}$ is the flipped version of σ . This is the Hamiltonian we have encoded, while the Hamiltonian we were aiming to encode is

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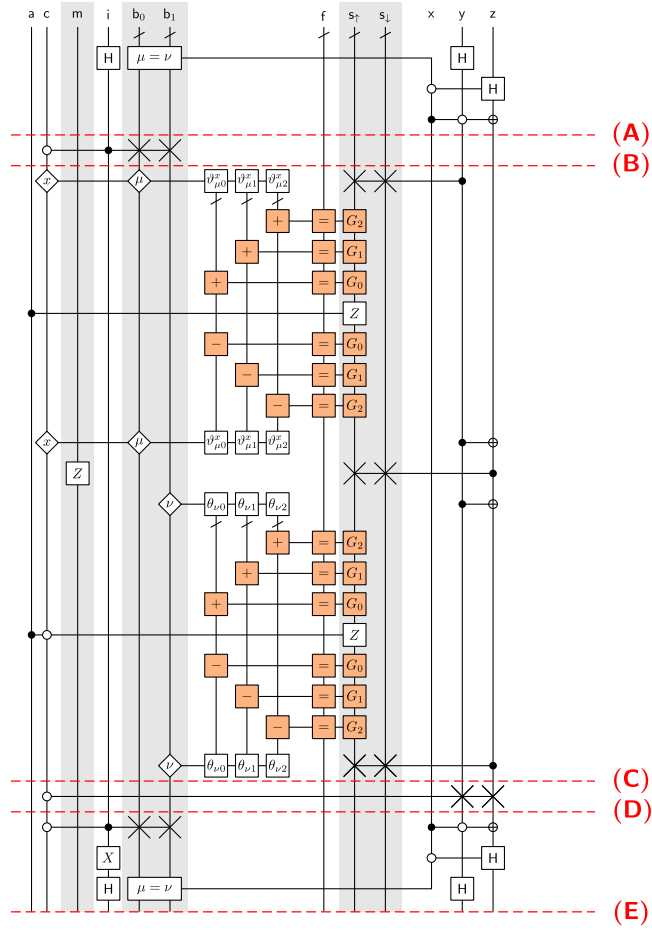


FIG. 1. Select to replace Figs. 1 and 12 divided into sections with the waypoints (A), (B), (C), (D) and (E).

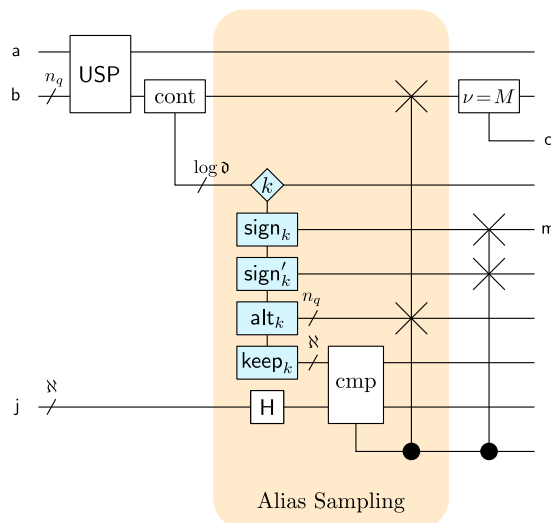


FIG. 2. The Prepare to replace Fig. 2.

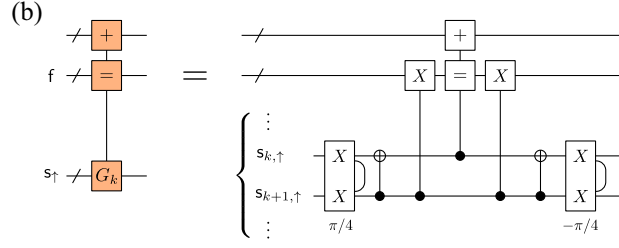


FIG. 3. (b) A programmable Givens rotation subcircuit that replaces Fig. 3(b). Here, the lower register, $\mathbf{s}_\uparrow$ fans out into singular qubits $\mathbf{s}_{0,\uparrow}, \mathbf{s}_{1,\uparrow}, \dots, \mathbf{s}_{N/2-1,\uparrow}$ of which this circuit uses exactly two subsequent qubits, determined by the index k of G_k . The circuit implements the product of rotations $\exp(-i\pi\theta X_{\mathbf{s}_{k+1,\uparrow}} Y_{\mathbf{s}_{k,\uparrow}})$ and $\exp(i\pi\theta Y_{\mathbf{s}_{k+1,\uparrow}} X_{\mathbf{s}_{k,\uparrow}})$ for fixed-point values $\theta < 1$ in the $|\theta\rangle$ subspace of the temporary register on top. This is done under catalytic use of a phase-gradient state in register $\mathbf{f}$. The circuit on the right-hand-side features $\pm\pi/4$ rotations of Pauli strings $X_{\mathbf{s}_{k+1,\uparrow}} X_{\mathbf{s}_{k,\uparrow}}$, controlled flips of all qubits in $\mathbf{f}$ denoted by the gates “X,” and a controlled Givens adder, which adds the binary number stored in the register under the “+” gate into the register under the “=” gate. For the Givens rotation uncomputations, this adder is replaced with an in-place subtractor, symbolized by “-.”

$$\tilde{H} = \frac{1}{8} \sum_{\mu=0}^{M-1} \sum_{\nu \neq \mu} \tilde{\zeta}_{\mu\nu} \sum_{\sigma\tau} \tilde{Z}_{\nu,\tau} \tilde{Z}_{\mu,\sigma} + \frac{1}{8} \sum_{\nu=0}^{M-1} \tilde{\zeta}_{\nu\nu} \sum_{\sigma} \tilde{Z}_{\nu,\sigma} \tilde{Z}_{\nu,\bar{\sigma}} - \frac{1}{2} \sum_{k=0}^{N/2-1} \tilde{t}_k \sum_{\sigma} \tilde{T}_{k,\sigma}, \quad (3)$$

where constant terms were eliminated with respect to Eq. (22).

This change removes the need for register $\mathbf{x}$ in Fig. 1 to be persistent and allows for the use of a left and right elbow at the beginning and the end of the Select circuit. This change is also reflected in the new Fig. 2 where the register $\mathbf{c}$ is initialized conditional on the outcome of the $\nu = M$ comparator through a left elbow.

The new version of Eq. (30) reads

$$G_k(\theta) = \exp(-i\pi\theta X_{k+1} Y_k) \exp(i\pi\theta Y_{k+1} X_k), \quad (4)$$

and reflects the correct sign for the Givens rotations and the correct qubits to act on (k and $k + 1$). This change is reflected in Fig. 3(b) where the registers $\mathbf{s}_{k-1,\uparrow}, \mathbf{s}_{k,\uparrow}$ are replaced with $\mathbf{s}_{k,\uparrow}, \mathbf{s}_{k+1,\uparrow}$ and the signs of the rotations over $\frac{\pi}{4}$ are flipped. This correction influences the numerical outcome of the circuits but not the resource estimates.