

Digital quantum simulation and Time Evolution

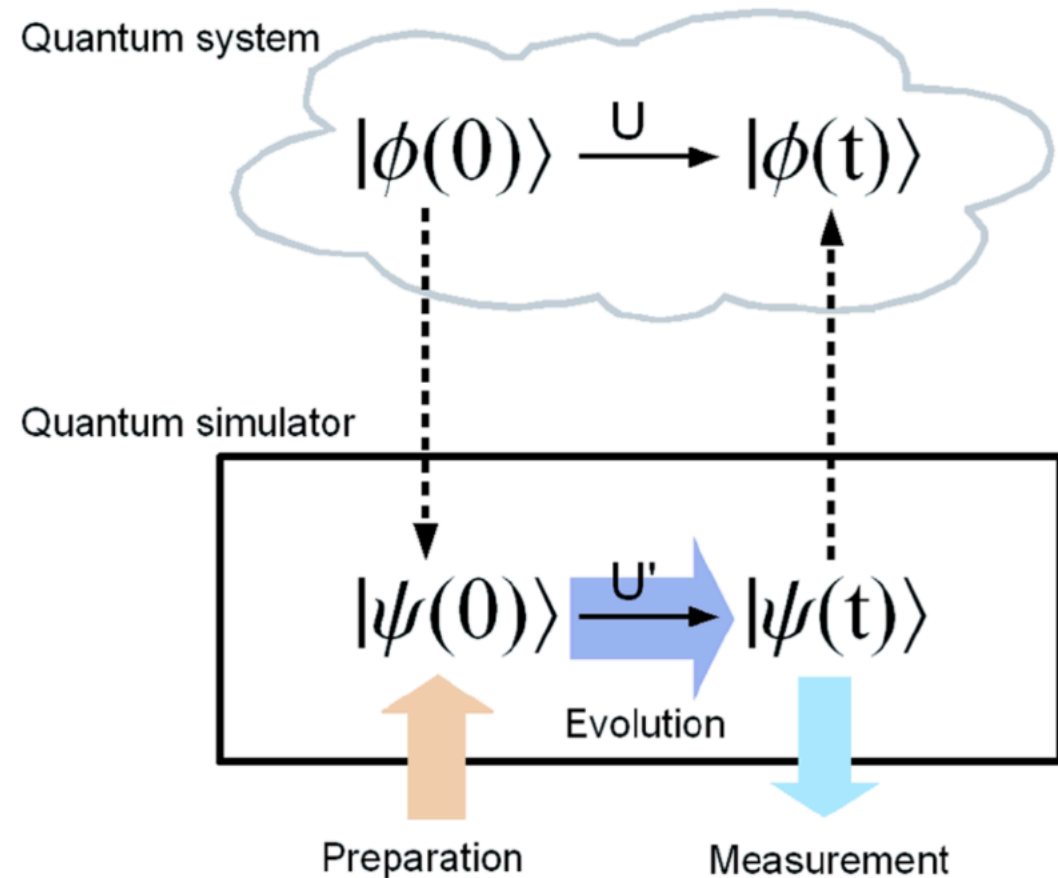
2 December 2020

Michele Grossi – *Quantum Ambassador, Qiskit Advocate*
Luca Crippa – *IT Architect, Qiskit Advocate*



Digital quantum simulation

Time Evolution



- **Analog quantum simulation:** quantum system that emulates a target system
- **Digital quantum simulation:** quantum computation of Time Evolution through a circuit model

Digital quantum simulators

After encoding $|\psi(0)\rangle$ on the computational basis, $|\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle$ is directly computed through a sequence of single and two qubits gates

Digital quantum simulation

Suzuki-Trotter decomposition

- Most Hamiltonians of physical interest can be mapped into a sum of L local terms: $\hat{\mathcal{H}} = \sum_k^L \hat{\mathcal{H}}_k$
- Then, map the original Hamiltonian into the QC algebra (i.e. SU2):

- if $[H_l, H_{l'}] = 0$ then $U = \prod_l \exp\{-i H_l t\}$ is exact

- otherwise, it is needed to apply the Suzuki-Trotter decomposition

$$\hat{U}(t) = e^{-i\hat{\mathcal{H}}t} \approx (e^{-i\hat{\mathcal{H}}_1\tau} \dots e^{-i\hat{\mathcal{H}}_L\tau})^n \quad \tau = t/n$$

- Program the Time Evolution through simple and two-qubit gates on the real hardware

Steps to Time Evolve your models

Time Evolution through Suzuki-Trotter decomposition

Original Hubbard model fermionic Hamiltonian

$$\mathcal{H} = -t \sum_{\langle i,j \rangle} (\hat{b}_i^\dagger \hat{b}_j + \hat{b}_j^\dagger \hat{b}_i) + V \sum_i (\hat{n}_{i\uparrow} \hat{n}_{i\downarrow})$$



Jordan-Wigner
Transform

OR

Built-in Aqua
functions

Spin Hamiltonian

$$\mathcal{H}_{spin}$$



Unitary evolution with Suzuki-Trotter decomposition

Original Ising transverse field model spin Hamiltonian

$$\mathcal{H}_t = b(S_1^x + S_2^x) + j(S_1^z S_2^z)$$



Unitary evolution with Suzuki-Trotter decomposition

Choose your own problem to Time Evolve!

- 2 to n sites Hubbard model
- 2 to n sites Ising model (transverse magnetic field)
- 2 to n sites Heisenberg model
- ...

Heisenberg model, n=2

Time Evolution through Suzuki-Trotter decomposition

Original Heisenberg model Hamiltonian

$$\mathcal{H} = J'(s_{x1}s_{x2} + s_{y1}s_{y2} + s_{z1}s_{z2}) + Bg(s_{z1} + s_{z2})$$

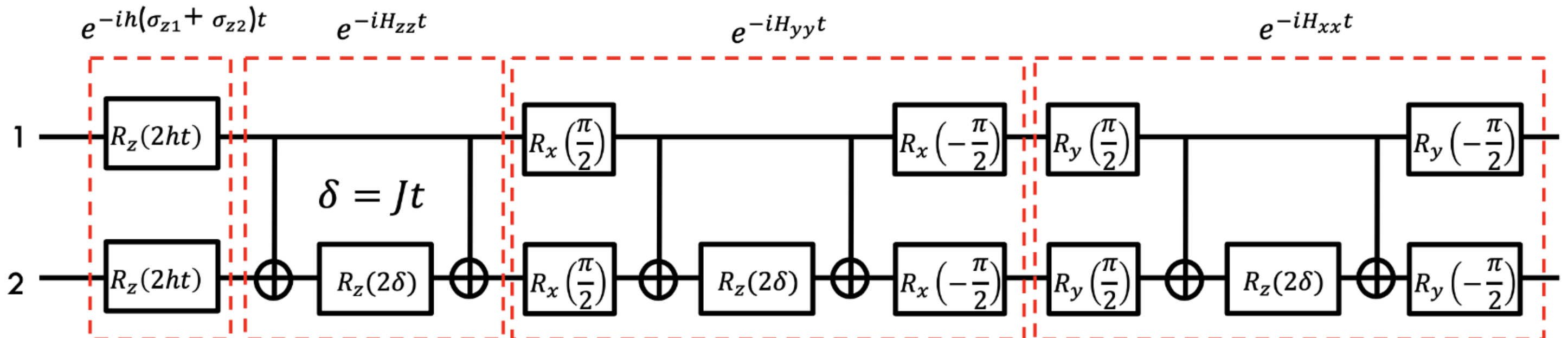
Mapped Hamiltonian

$$H_2 = J(\sigma_{x1}\sigma_{x2} + \sigma_{y1}\sigma_{y2} + \sigma_{z1}\sigma_{z2}) + h(\sigma_{z1} + \sigma_{z2})$$

Unitary evolution

$$e^{-iH_2t} = e^{-iH_{xx}t} e^{-iH_{yy}t} e^{-iH_{zz}t} e^{-ih(\sigma_{z1} + \sigma_{z2})t}$$

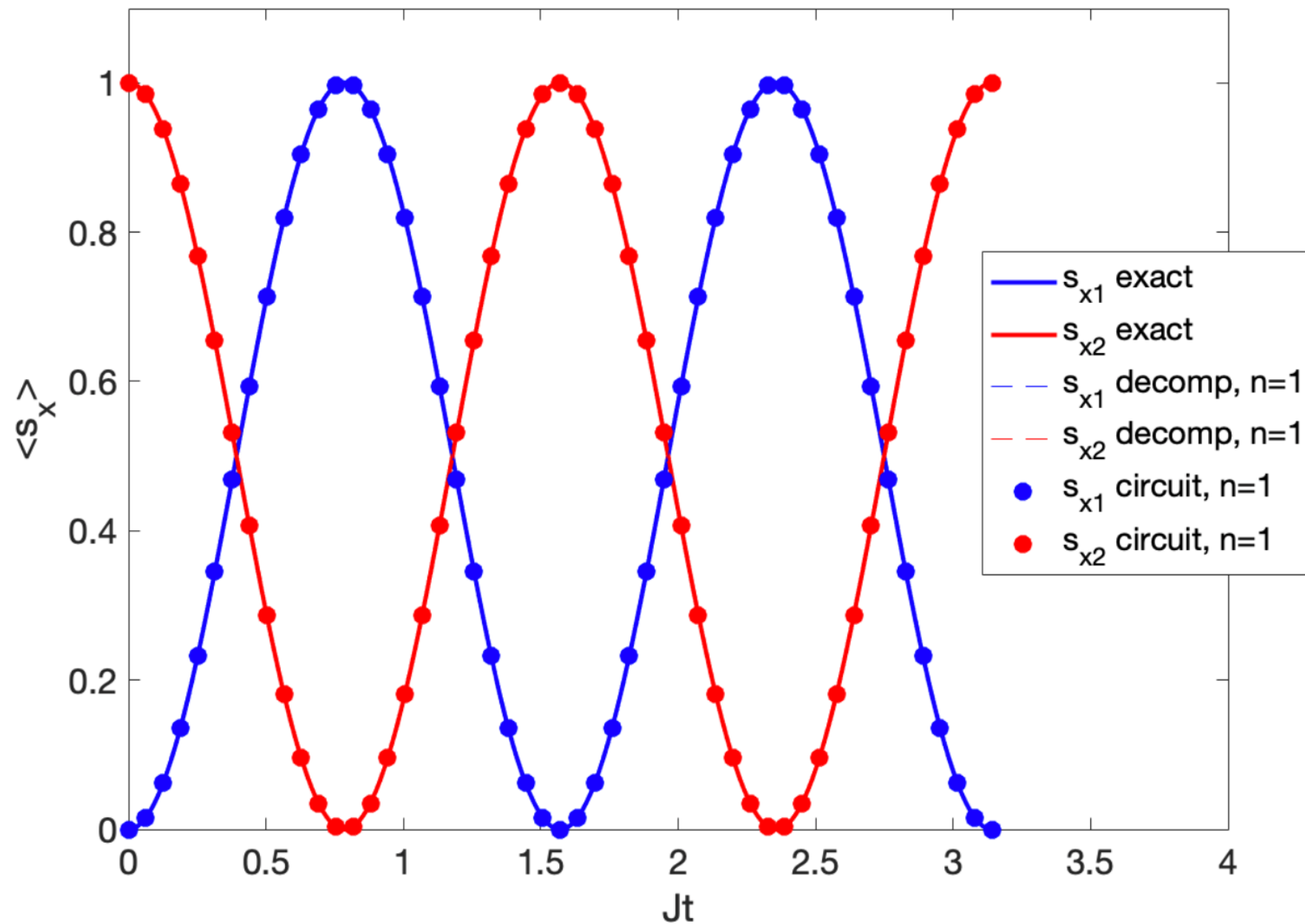
Circuit model for the unitary evolution



Heisenberg model, n=2

Time Evolution through Suzuki-Trotter decomposition

$h=0$



Mapped Hamiltonian

$$H_2 = J(\sigma_{x1}\sigma_{x2} + \sigma_{y1}\sigma_{y2} + \sigma_{z1}\sigma_{z2}) + h(\sigma_{z1} + \sigma_{z2})$$

Initial state

$$(|00\rangle + |01\rangle) / \sqrt{2}$$

Results

$$\langle \sigma_{x1} \rangle (t); \langle \sigma_{x2} \rangle (t)$$

TO DO: change h

Native and decomposed gates implemented on IBM Q

Native gates

$$U_1(\lambda) = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\lambda} \end{pmatrix}$$

$$U_3(\vartheta, \lambda, \varphi) = \begin{pmatrix} \cos \frac{\vartheta}{2} & -e^{i\lambda} \sin \frac{\vartheta}{2} \\ e^{i\varphi} \sin \frac{\vartheta}{2} & e^{i(\lambda+\varphi)} \cos \frac{\vartheta}{2} \end{pmatrix}$$

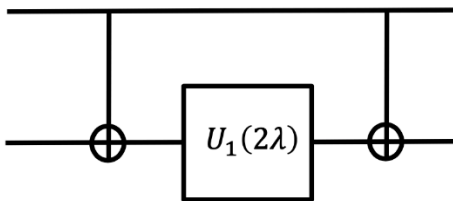
$$U_2(\varphi, \lambda) = \begin{pmatrix} \frac{1}{\sqrt{2}} & -e^{i\lambda} \frac{1}{\sqrt{2}} \\ e^{i\varphi} \frac{1}{\sqrt{2}} & e^{i(\lambda+\varphi)} \frac{1}{\sqrt{2}} \end{pmatrix}$$

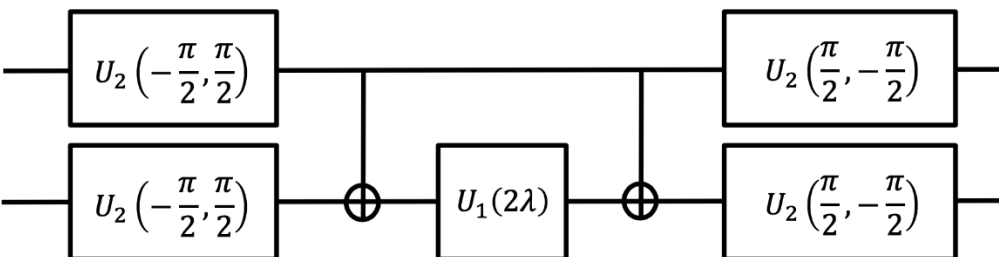
**Single
qubit
rotations**

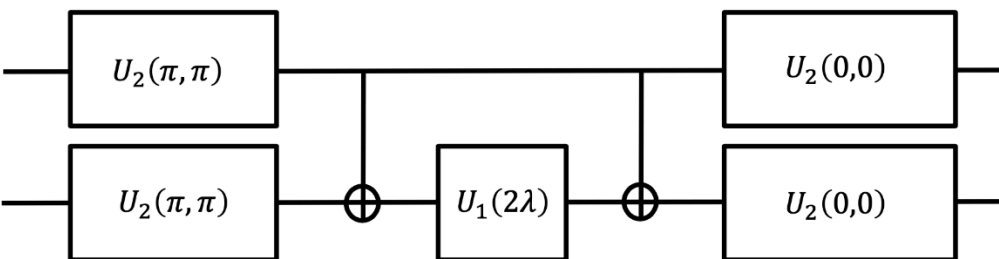
$$CX = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

**CNOT: two-qubit
entangling gate**

Decomposed gates

$$e^{-i\lambda\sigma_1^z\sigma_2^z} = \text{CNOT} \circ U_1(2\lambda) \circ \text{CNOT}$$


$$e^{-i\lambda\sigma_1^y\sigma_2^y} = U_2(-\frac{\pi}{2}, \frac{\pi}{2}) \circ \text{CNOT} \circ U_1(2\lambda) \circ \text{CNOT} \circ U_2(\frac{\pi}{2}, -\frac{\pi}{2})$$


$$e^{-i\lambda\sigma_1^x\sigma_2^x} = U_2(\pi, \pi) \circ \text{CNOT} \circ U_1(2\lambda) \circ \text{CNOT} \circ U_2(0, 0)$$


IBM