

# QUANTUM ALGORITHMS FOR SIMULATING PHYSICAL SYSTEMS

THE HEART OF SIMULATION OF PHYSICAL SYSTEMS IS SOLVING SCHRODINGER EQUATION OF MOTION

$$i \frac{\partial |\psi\rangle}{\partial t} = H |\psi\rangle$$

WHERE  $H$  IS THE HAMILTONIAN THAT DEFINES THE INTERACTION BETWEEN THE SYSTEM COMPONENTS IN POSITION REPRESENTATION, A 1D SYSTEM MAY BE SIMULATED BY SOLVING THE EQUATION

$$i \frac{\partial |\psi\rangle}{\partial t} = \left( \sum_l \frac{p_l^2}{2m_l} + V(x_1, x_2, \dots, x_n) \right) |\psi\rangle$$

SUPPOSED  $|\psi\rangle$  REPRESENTS AN  $n$ -PARTICLE SYSTEM STATE A SINGLE PARTICLE MAY BE SIMULATED BY SOLVING THE EQUATION

$$i \frac{\partial |\psi\rangle}{\partial t} = \left( \frac{p^2}{2m} + V(x) \right) |\psi\rangle$$

A CLASSICAL SIMULATION WOULD IMPLY A FINE DISCRETIZATION OF POSITION BASIS

$$|x\rangle \text{ FOR } x \in [0, L] \rightarrow |k\Delta x\rangle \text{ FOR } k=0, \dots, n-1$$

THIS DISCRETIZATION LEADS TO A REPRESENTATION OF THE SINGLE PARTICLE STATE

$$|\psi\rangle = \sum_{k=0}^{n-1} a_k |k\Delta x\rangle, \quad \Delta x = \frac{L}{n}$$

MOMENTUM OPERATOR APPROXIMATED USING  $P = \partial_x$ , COULD BE FINITE DIFFERENCE FORMULAS

THUS LEADING TO A DIFFERENTIAL EQUATION

$$i \frac{d\alpha_k}{dt} = H_{k\ell} \alpha_\ell$$

THIS SYSTEM OF EQUATIONS MAY BE SOLVED ITERATIVELY, YIELDING TIME EVOLUTION OF THE 1D 1-PARTICLE SYSTEM

$$|\psi(t)\rangle \approx \sum_{k=0}^{N-1} \alpha_k(t) |k\Delta x\rangle$$

PROVIDED THE PROPER INITIAL CONDITIONS  $\alpha_k(0)$  ARE GIVEN A QUANTUM ALGORITHM FOR SIMULATING THIS SYSTEM WOULD APPROXIMATE THE SYSTEM'S STATE ALSO AS

$$|\psi\rangle = \sum_{k=0}^{N-1} \alpha_k |k\Delta x\rangle$$

HOWEVER, DUE TO NATURE OF QUANTUM BITS, ENCODING THIS STATE WOULD REQUIRE  $\log N$  SPACE IF HAMILTONIAN IS TIME INDEPENDENT, THEN IT IS TRUE THAT

$$|\psi(t)\rangle = e^{-iHt} |\psi(0)\rangle$$

$$|\psi(t)\rangle = e^{-iP^2/2mt - iV(x)t} |\psi(0)\rangle$$

IN MOST CASES,  $V(x)$  IS EFFICIENTLY COMPUTABLE, AND THUS ITS EXPONENTIAL IS ALSO EFFICIENTLY COMPUTABLE ALSO, SINCE  $X$  AND  $P$  ARE CONJUGATE OPERATORS

$$P = QFT \times QFT^\dagger$$

$$e^{-iP^2/2mt} = QFT e^{-ix^2/2mt} QFT^\dagger$$

AS A RESULT, BOTH UNITARIES

$$e^{-iP^2/2mt}, e^{-iV(x)t}$$

ARE EFFICIENTLY COMPUTABLE HOWEVER, SINCE

$$\left[ \frac{P^2}{2m}, V(x) \right] \neq 0$$

IT IS SO THAT

$$e^{-iP^2/2mt - iV(x)t} \neq e^{-iP^2/2mt} e^{-iV(x)t}$$

AS WILL BE SHOWN LATER, THOUGH, IT IS POSSIBLE TO ESTIMATE THE UNITARY

$$U(t) = e^{-iP^2/2mt - iV(x)t}$$

BY A SEQUENCE OF APPLICATIONS OF OPERATORS

$$U_P(\Delta t) = e^{-iP^2 \Delta t / 2m}$$

$$U_x(\Delta t) = e^{-iV(x) \Delta t}$$

THIS SEQUENCE OF APPLICATIONS CAN BE IMPLEMENTED EFFICIENTLY FOR ALL  $t$  SUCH THAT  $t = k\Delta t$ ,  $k \in \mathbb{Z}^+$  AS A RESULT, STATE

$$|\psi(t)\rangle = U(t) |\psi(0)\rangle$$

WILL BE EFFICIENTLY COMPUTED USING A QUANTUM CIRCUIT !!! THE PROBLEM OF SOLVING A SYSTEM OF  $k$  COMPLEX ODE'S HAS BEEN SUBSTITUTED BY THE PROBLEM OF ESTIMATING A UNITARY

REGARDING AN  $n$ -PARTICLE SYSTEM, WHILE CLASSICAL ALGORITHMS HAVE SPACE COMPLEXITY THAT SCALES  $O(2^n)$ , QUANTUM ALGORITHMS HAVE SPACE COMPLEXITY  $O(n)$ . THIS IS A STRONG ARGUMENT IN FAVOR OF QUANTUM ALGORITHMS.

INTERESTING SYSTEMS



ALTHOUGH SEVERAL SIMPLE SYSTEMS MAY BE SIMULATED EFFICIENTLY, QUITE IMPORTANT

SYSTEMS ARE NOT IN THIS SET IN THE CONTEXT OF SOLID STATE PHYSICS, THE HUBBARD MODEL

$$H = \sum_{k=1}^n V_0 \underbrace{n_{k\uparrow} n_{k\downarrow}}_{\text{OCCUP # FERMIONIC OPERATORS}} + \sum_{\langle ij \rangle} t_0 \underbrace{c_{i\sigma}^* c_{j\sigma}}_{\text{LADDER FERMIONIC OPERATORS}}$$

AND ISING-LIKE MODELS

$$H = \sum_{\langle ij \rangle} J_{ij} \vec{\sigma}_i \cdot \vec{\sigma}_j + h \sum_i \vec{\sigma}_i$$

ARE NOT EFFICIENTLY SIMULATED USING CLASSICAL ALGORITHMS IN GENERAL, LATTICE MODELS ARE BELIEVED TO BE EFFICIENTLY SIMULATED BY QUANTUM ALGORITHMS. THIS HAS MOTIVATED PHYSICISTS TO APPLY QUANTUM ALGORITHMS TO QED AND QCD.

REALLY IMPORTANT FERMIONIC HAMILTONIANS DEFINED ON ARBITRARY GRAPHS ARE NOT PROVEN TO BE EFFICIENTLY SIMULATED BY QUANTUM ALGORITHMS.

REFS arXiv 1804.03023v4  
 arXiv 1801.03922v4  
 arXiv 1807.07112v3

# SYSTEMS WITH LOCAL INTERACTIONS

CONSIDER A SYSTEM WHOSE HAMILTONIAN IS SUCH THAT

$$H = \sum_{k=1}^L H_k$$

WHERE  $H_k$  ACTS ON AT MOST  $C$  SUBSYSTEMS AND  $L$  IS SOME POLYNOMIAL ON THE NUMBER OF PARTICLES

IF  $[H_i, H_j] = 0$  FOR ALL  $i, j$ , THEN THESE OPERATORS HAVE A COMMON EIGENBASIS AND THUS IT IS TRIVIAL TO SEE THAT

$$e^{-iH\Delta t} = \prod_{k=1}^L e^{-iH_k \Delta t}$$

IN GENERAL, HOWEVER  $[H_i, H_j] \neq 0$  FOR SOME  $i, j$ . IN WORST CASE,  $[H_i, H_j] \neq 0$  FOR ALL  $i, j$ .

TROTTER FORMULAS → CONSIDER OPERATORS  $H_1, H_2$  WITH  $[H_1, H_2] \neq 0$  THEN

$$e^{iH_1 \Delta t} = \sum_{m=0}^{\infty} \frac{(i\Delta t)^m}{m!} H_1^m$$

$$e^{iH_2 \Delta t} = \sum_{l=0}^{\infty} \frac{(i\Delta t)^l}{l!} H_2^l$$

$$e^{iH_1 \Delta t} e^{iH_2 \Delta t} = \sum_{m=0}^{\infty} \sum_{l=0}^{\infty} \frac{(i\Delta t)^{l+m}}{l! m!} H_1^m H_2^l$$

DEFINE  $K = l + m$  THE DOUBLE SUM ABOVE SHOUTS TO

$$e^{i\Delta t H_1} e^{i\Delta t H_2} = \sum_{k=0}^{\infty} \frac{(i\Delta t)^k}{k!} \sum_{m=0}^k \frac{k!}{(k-m)! m!} H_1^m H_2^{k-m}$$

$$= \sum_{k=0}^{\infty} \frac{(i\Delta t)^k}{k!} \sum_{m=0}^k \binom{k}{m} H_1^m H_2^{k-m}$$

IT WOULD BE DESIRABLE TO WRITE

$$\sum_{m=0}^k \binom{k}{m} H_1^m H_2^{k-m} = (H_1 + H_2)^k$$

BUT THIS IS ONLY TRUE FOR COMMUTING OPERATORS WHAT IS THE ERROR OF ASSUMING THE EQUATION ABOVE? THE PROBLEM HERE THAT TO GO FROM  $(H_1 + H_2)^k$  TO THE LEFT HAND SIDE, PERMUTATIONS SHOULD BE MADE FOR NON COMMUTING OPERATORS, IT IS POSSIBLE TO PERFORM THOSE PERMUTATIONS AT COST OF ADDING TERMS THAT DEPEND ON THE COMMUTATOR

THEREFORE

$$\sum_{m=0}^k \binom{k}{m} H_1^m H_2^{k-m} = (H_1 + H_2)^k + f_k(H_1, H_2)$$

WHERE  $f_k(H_1, H_2)$  DEPENDS ON THE COMMUTATORS ASSOCIATED TO THE PERMUTATIONS DISCUSSED BEFORE SINCE  $f_1(H_1, H_2) = 0$

$$e^{i\Delta t H_1} e^{i\Delta t H_2} = e^{i\Delta t (H_1 + H_2)} + O(\Delta t^2)$$

IF  $\Delta t$  IS SMALL, THE PRODUCT OF EXPONENTIALS ESTIMATE THE EVOLUTION OPERATOR WITH AN ERROR  $O(\Delta t^2)$

THIS IS A PARTICULAR CASE OF THE SO CALLED TROTTER FORMULAS

CONSIDER OPERATORS  $\Delta_1, \Delta_2, \dots, \Delta_m$  DEFINE

$$f(t) = \prod_{k=1}^m e^{t\Delta_k} = e^{t\Delta_1} e^{t\Delta_2} \dots e^{t\Delta_m}$$

IF  $|t| \ll 1$ , THEN

$$f(t) \approx \prod_{k=1}^m \left( 1 + t\Delta_k + \frac{t^2}{2}\Delta_k^2 \right) + O(t^3)$$

$$f(t) \approx 1 + t \sum_k \Delta_k + \frac{t^2}{2} \left[ \sum_{k=1}^m \Delta_k^2 + 2 \sum_{j>k} \Delta_k \Delta_j \right] + O(t^3)$$

USING THE IDENTITY ABOVE, IT IS POSSIBLE TO DERIVE  $O(t^3)$  APPROXIMATIONS FOR THE EVOLUTION UNITARY

BAKER-HAUSDORF FORMULA  $\rightarrow$  DEFINE THE PRODUCT-TRISED FUNCTION

$$f(t) = e^{t\Delta} e^{tB} e^{-\frac{1}{2}[\Delta, B]t^2}$$

IF  $|t| \ll 1$ , THE ABOVE REASONING YIELDS

$$f(t) = 1 + t(\Delta+B) + \frac{t^2}{2} (\Delta^2 + B^2 - [\Delta, B] + 2\Delta B) + O(t^3)$$

$$f(t) = 1 + t(\Delta+B) + \frac{t^2}{2} (\Delta + B^2 + \Delta B + B\Delta) + O(t^3)$$

$$f(t) = 1 + t(\Delta+B) + \frac{t^2}{2} (\Delta+B)^2 + O(t^3)$$

AND THUS

$$e^{t\Delta} e^{tB} e^{-\frac{1}{2}[\Delta, B]} = e^{t(\Delta+B)} + O(t^3)$$

IMPORTANT THIS FORMULA IS PARTICULARLY USEFUL TO APPROXIMATE HAMILTONIANS THAT ARE COMPOSED OF OPERATORS THAT FORM A LIE ALGEBRA

A CLOSELY RELATED APPROXIMATION FORMULA IS NEXT DERIVED

$$e^{t(\Delta+B)} = e^{\frac{t}{2}\Delta} e^{tB} e^{\frac{t}{2}\Delta} + O(t^3)$$

**DEFINITION**  $\Delta_1 = \Delta/2$ ,  $\Delta_2 = B$ ,  $\Delta_3 = \Delta/2$   
**DEFINE**  $f(t)$  **AS BEFORE**

$$f(t) = 1 + t(\Delta+B)$$

$$+ \frac{t^2}{2} \left[ \frac{\Delta^2}{2} + B^2 + \Delta B + \frac{\Delta^2}{2} + B\Delta \right] + O(t^3)$$

$$f(t) = 1 + t(\Delta+B) + \frac{t^2}{2} (\Delta+B)^2 + O(t^3)$$

FROM WHICH THE DESIRED FORMULA FOLLOWS

**GENERAL FORMULA**  $\rightarrow$  **GENERAL HAMILTONIAN**

$$H = \sum_{k=1}^L H_k$$

CAN BE ESTIMATED WITH ERROR  $O(t^3)$  USING THE FORMULA

$$e^t H \approx e^{tH_1/2} e^{tH_2/2} e^{tH_L/2} e^{tH_L/2} e^{tH_2/2} e^{tH_1/2}$$

**DEM** USE THE REASONING DISCUSSED BEFORE AND THE IDENTITY

$$\left( \sum_{k=1}^L H_k \right)^2 = \sum_{k=1}^L H_k^2 + \sum_{j>k} (H_k H_j + H_j H_k)$$

THE MATCH TO FIRST ORDER IS TRIVIAL THE MATCH TO SECOND ORDER FOLLOWS FROM

$$\sum_{k=1}^m \Delta_m = \sum_{k=1}^L \frac{H_k^2}{2}$$

$$2 \sum_{j>k} \Delta_k \Delta_j = \sum_{k=1}^L \frac{H_k^2}{2} + \sum_{j>k} (H_k H_j + H_j H_k)$$

# EXACT SOLUTION OF 1D ISING MODEL

$$H = \underbrace{\sum_{l=1}^N X_l X_{l+1}}_{\text{SPIN INTERACTIONS}} + \underbrace{Y_1 \otimes_{l=2}^{N-1} Z_l Y_N}_{\text{BOUNDARY TERMS}} + \underbrace{h \sum_{l=1}^N Z_l}_{\text{TRANSVERSE FIELD}}$$

CONSIDER THE JORDAN-WIGNER TRANSFORMATION, GIVEN BY

$$C_l = \left( \bigotimes_{j=1}^{l-1} Z_j \right) \sigma_l^-$$

$$C_l^+ = \left( \bigotimes_{j=1}^{l-1} Z_j \right) \sigma_l^+$$

WITH

$$\sigma_l^\pm = \frac{1}{2}(X + iY)$$

THESE ARE FERMIONIC OPERATORS IN THE SENSE THAT IT SATISFIES ANTICOMMUTATION RELATIONS

$$\{C_l, C_j\} = \{\sigma_\ell, Z_\ell\} \left( \bigotimes_{k=\ell+1}^{h-1} Z_k \right) \sigma_h = 0$$

WITH  $h = \max(l, j)$ ,  $\ell = \min(l, j)$   $\neq j$  AND

$$\{C_l, C_j^+\} = \begin{cases} 0 & l \neq j \\ \{\sigma_l, \sigma_l^+\} & \text{IF } l=j \end{cases}$$

THIS OPERATORS GIVE RISE TO THE FERMIONIC DESCRIPTION OF THE PROBLEM IN THE SENSE

THAT EACH SITE MIGHT BE THOUGHT OF AS OCCUPIED BY A FERMION, AND THE ENERGY OF INTERACTION DEPENDS ON THE OCCUPATION NUMBER THERE EXISTS A VACUUM STATE

$$c_l^+ c_l | \underline{\underline{\underline{0}}} \rangle = 0 \quad \text{FOR } 1 \leq l \leq n$$

OPERATORS  $c_l^+ c_l$  ARE NUMBER OPERATORS FOR SITE  $l$ , AND HAVE EIGENVALUES 0 OR 1 SOME IMPORTANT PROPERTIES OF  $c_l^+ c_l$ ,  $c_l$  AND  $c_l^+$  ARE

1  $(c_l^+ c_l)^2 = c_l^+ c_l$  THIS IS A CONSEQUENCE OF THE COMMUTATION RELATIONS

$$\begin{aligned} c_l^+ c_l c_l^+ c_l &= c_l^+ (1 - c_l^+ c_l) c_l \\ &= c_l^+ c_l - (c_l^2)^+ (c_l^2) \\ &= c_l^+ c_l \end{aligned}$$

FOR  $c_l^2 = 0$  THIS IMPLIES  $c_l^+ c_l$  HAS EIGENVALUES 0 OR 1, AND THUS IS A FERMIONIC OCCUPATION NUMBER OPERATOR

2  $c_l^+$  AND  $c_l$  ARE RAISING AND LOWERING OPERATORS SUPPOSE A STATE  $| \psi \rangle$  SUCH THAT  $c_l^+ c_l | \psi \rangle = 0$  GIVEN THAT

$$c_l^+ c_l c_l^+ = c_l^+ (1 - c_l^+ c_l) = c_l^+$$

IT IS SO THAT  $c_l^+ | \psi \rangle$  IS AN EIGENSTATE OF  $c_l^+ c_l$  WITH EIGENVALUE 1 BY THE SAME TOKEN, IT IS SO THAT IF  $c_l^+ c_l | \psi \rangle = | \psi \rangle$ , THEN  $c_l^+ | \psi \rangle = (c_l^2)^+ | \psi \rangle = 0$

IN A SIMILAR MANNER, IF  $c_l^+ c_l | \psi \rangle = | \psi \rangle$  THEN  $c_l | \psi \rangle$  IS EIGENSTATE OF  $c_l^+ c_l$  WITH EIGENVALUE 0 THIS IS SO BECAUSE

$$c_l^+ c_l c_l = c_l^+ c_l^2 = 0$$

OCCUPATION NUMBER IS EITHER 0 OR 1 FOR EACH LATTICE SITE

3  $C_L + C_L^\dagger$  ARE A SET OF COMMUTING OPS  
CONSIDER THE COMMUTATION RELATIONS

$$\begin{aligned} C_L + C_L^\dagger, C_J + C_J^\dagger &= -C_L + C_J + C_L C_J \\ &= C_J + C_L + C_L C_J \\ &= C_J + C_J^\dagger, C_L + C_L^\dagger \end{aligned}$$

THIS IMPLIES THERE SHOULD EXIST A COMMON ORTHONORMAL EIGENBASIS FOR OPERATORS  $C_L + C_L^\dagger$ . IN PARTICULAR, A VACUUM EIGENSTATE SHOULD EXIST CONSIDER

$$\prod_{l=1}^N (C_l +)^{\alpha_l} \quad \text{WITH } \alpha_l = 0, 1$$

SINCE IT IS SO THAT

$$\begin{aligned} &\left( \prod_{l=1}^N (C_l +)^{\alpha'_l} \right)^\dagger \prod_{l=1}^N (C_l +)^{\alpha_l} \\ &= C_N^{\alpha'_N} C_{N-1}^{\alpha'_{N-1}} \quad C_1^{\alpha'_1} C_1^{\alpha'_1} \quad C_{N-1}^{\alpha'_{N-1}} C^{\alpha_N} \\ &= \prod_{l=1}^N C_l^{\alpha'_l} C_l^{\alpha_l} \end{aligned}$$

STATES DEFINED BY

$$|\alpha\rangle = |\alpha_1, \alpha_{N-1}, \alpha_N\rangle = \prod_{l=1}^N (C_l +)^{\alpha_l} |0\rangle$$

SINCE

$$\sigma_i + \sigma_i^+ = X_i$$
$$i(\sigma_i^+ - \sigma_i) = Y_i$$

AND  $Y_i Z_i = -Z_i Y_i = i X_i$

$$X_i Z_i = -Z_i X_i = -i Y_i$$

IT IS SO THAT

$$X_i X_{i+1} = (\underline{c}_i^+ - \underline{c}_i)(\underline{c}_{i+1} + \underline{c}_{i+1}^+)$$
$$Y_i Y_{i+1} = (\underline{c}_i^+ + \underline{c}_i)(\underline{c}_{i+1} - \underline{c}_{i+1}^+)$$

CONSIDER AN INTERACTION HAMILTONIAN

$$H = -\frac{J_x}{2} \sum_{i=1}^N X_i X_{i+1} - \frac{J_y}{2} \sum_{i=1}^N Y_i Y_{i+1}$$

$$X_i X_{i+1} = c_i^+ c_{i+1} + c_i^+ c_{i+1}^+ - c_i c_{i+1} - c_i c_{i+1}^+$$
$$= c_i^+ c_{i+1} + c_i^+ c_{i+1}^+ + c_{i+1} c_i + c_{i+1}^+ c_i$$

$$Y_i Y_{i+1} = c_i^+ c_{i+1} - c_i^+ c_{i+1}^+ + c_i c_{i+1} - c_i c_{i+1}^+$$
$$= c_i^+ c_{i+1} + c_{i+1}^+ c_i - c_i^+ c_{i+1}^+ - c_{i+1} c_i$$

IF  $J_x = J_y$ , IT IS THE INTERACTION CORRESPONDS TO THE XY HEISENBERG MODEL

$$H = -\frac{J}{2} \sum_{i=1}^N (c_i^+ c_{i+1} + c_{i+1}^+ c_i)$$

LETS TRANSFORM TO MOMENTUM SPACE IN ORDER TO SIMPLIFY THE HAMILTONIAN

$$C_L = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} S_{\mathbf{k}} e^{i \mathbf{k} \cdot \mathbf{R}_L}$$

WITH  $\mathbf{k}$  IN THE 1ST BRILLOUIN ZONE

$$C_L^+ C_{L+1} = \frac{1}{N} \sum_{\mathbf{k}\mathbf{k}'} S_{\mathbf{k}}^+ S_{\mathbf{k}'} e^{-i \mathbf{k}' \cdot \mathbf{R}_L} e^{i (\mathbf{k}-\mathbf{k}') \cdot \mathbf{R}_L}$$

$$C_{L+1}^+ C_L = \frac{1}{N} \sum_{\mathbf{k}\mathbf{k}'} S_{\mathbf{k}'}^+ S_{\mathbf{k}} e^{i \mathbf{k}' \cdot \mathbf{R}_L} e^{i (\mathbf{k}'-\mathbf{k}) \cdot \mathbf{R}_L}$$

FROM THE ABOVE EXPRESSIONS, AND USING

$$\sum_L e^{i (\mathbf{k}-\mathbf{k}') \cdot \mathbf{R}_L} = N \delta_{\mathbf{k}, \mathbf{k}'}$$

THE INTERACTION HAMILTONIAN SIMPLIFIES TO

$$H = -J \sum_{\mathbf{k}} \cos \mathbf{k} S_{\mathbf{k}}^+ S_{\mathbf{k}}$$

CONSIDER OPERATOR

$$\hat{H}_{11} = \vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(1)} = \sum_{ke} J_{ke} \sigma_k^{(1)} \sigma_e^{(1)}$$

SUPPOSE  $J_{ke} = J_e \delta_{ke}$  SO THAT

$$\hat{H}_{11} = \sum_e J_e \hat{\sigma}_e^{(1)} \hat{\sigma}_e^{(1)}$$

CONSIDER THE BELL BASIS, IN COMPUTATIONAL BASIS

$$|\phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$

$$|\phi^-\rangle = \frac{1}{\sqrt{2}}(|00\rangle - |11\rangle)$$

$$|\Psi^+\rangle = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)$$

$$|\Psi^-\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$$

CONSIDER THE FOLLOWING IDENTITIES

$$|\phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) = \frac{1}{\sqrt{2}}(|++\rangle + |-+\rangle)$$

$$|\phi^-\rangle = \frac{1}{\sqrt{2}}(|00\rangle - |11\rangle) = \frac{1}{\sqrt{2}}(|+-\rangle - |+-\rangle)$$

$$|\Psi^+\rangle = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle) = \frac{1}{\sqrt{2}}(|++\rangle - |--\rangle)$$

$$|\Psi^-\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle) = \frac{1}{\sqrt{2}}(|-+\rangle - |+-\rangle)$$

$$\hat{\sigma}_x |0\rangle = |1\rangle$$

$$\hat{\sigma}_x |1\rangle = |0\rangle$$

$$\hat{\sigma}_y |0\rangle = i|1\rangle$$

$$\hat{\sigma}_y |1\rangle = -i|0\rangle$$

FROM WHICH IT IS CLEAR THAT

$$\hat{\sigma}_x^{(i)} \hat{\sigma}_x^{(j)} |\Psi^\pm\rangle = \pm |\Psi^\pm\rangle$$

$$\hat{\sigma}_y^{(i)} \hat{\sigma}_y^{(j)} |\Psi^\pm\rangle = \pm |\Psi^\pm\rangle$$

$$\hat{\sigma}_z^{(i)} \hat{\sigma}_z^{(j)} |\Psi^\pm\rangle = - |\Psi^\pm\rangle$$

$$\hat{\sigma}_x^{(i)} \hat{\sigma}_x^{(j)} |\phi^\pm\rangle = \pm |\phi^\pm\rangle$$

$$\hat{\sigma}_y^{(i)} \hat{\sigma}_y^{(j)} |\phi^\pm\rangle = \mp |\phi^\pm\rangle$$

$$\hat{\sigma}_z^{(i)} \hat{\sigma}_z^{(j)} |\phi^\pm\rangle = |\phi^\pm\rangle$$

AND THUS THE BELL BASIS IS THE EIGENBASIS OF THE 2QBIT HAMILTONIAN, WITH

$$\hat{H}_{ij} |\Psi^\pm\rangle = [-J_z \pm (J_x + J_y)] |\Psi^\pm\rangle$$

$$\hat{H}_{ij} |\phi^\pm\rangle = [J_z \pm (J_x - J_y)] |\phi^\pm\rangle$$

WITH THIS IN MIND, I BELIEVE IT IS POSSIBLE TO BUILD A QUANTUM CIRCUIT THAT PERFORMS EXACT TIME EVOLUTION UNDER THIS HAMILTONIAN

I CHANGE FROM COMPUTATIONAL BASIS TO BELL BASIS SUCH THAT

$$\begin{aligned} |00\rangle &\rightarrow |\phi^+\rangle \\ |01\rangle &\rightarrow |\phi^-\rangle \\ |10\rangle &\rightarrow |\Psi^+\rangle \\ |11\rangle &\rightarrow |\Psi^-\rangle \end{aligned}$$

2 ADD A PHASE ASSOCIATED TO  $J_z$  BY APPLYING AN  $R_z(-2J_z t)$  TO THE 2ND QBIT

3 USE AN SWAP QBIT TO ADD A PHASE ASSOCIATED TO  $J_x \& J_y$  AS FOLLOWS

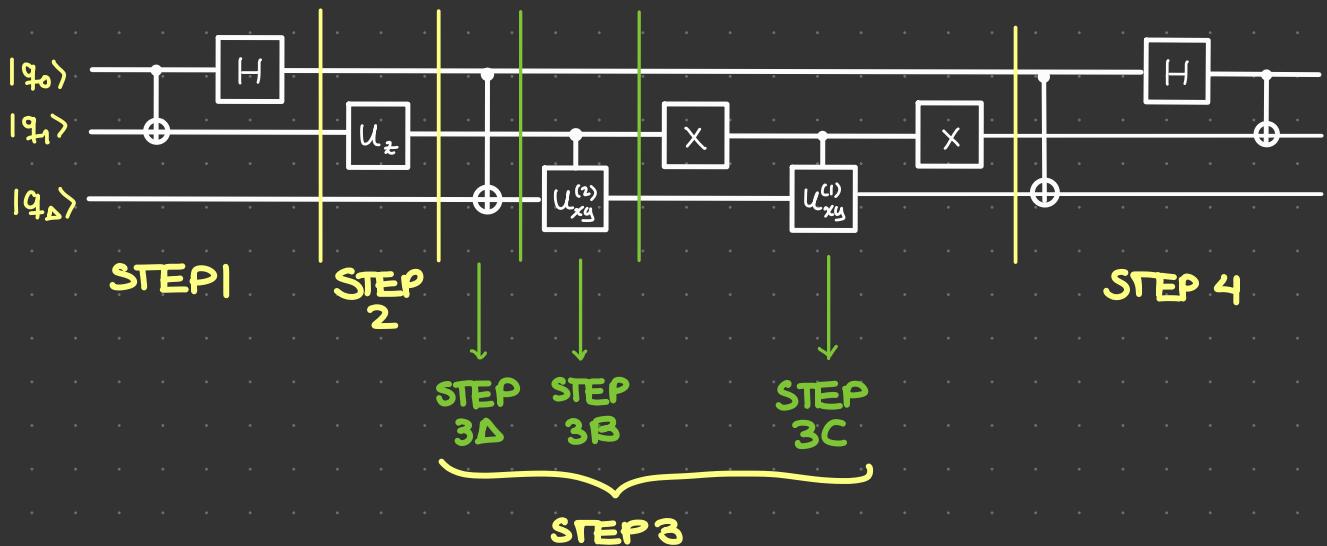
△ APPLY A CNOT TO DETERMINE THE SIGN OF THE PHASE, WITH 1ST QBIT AS CONTROL

B APPLY  $C[R_z(-2(J_x+J_y)t)]$  TO 2ND QBIT

C APPLY  $C[R_z(-2(J_x-J_y)t)]$  TO 2ND QBIT WITH INVERTED CONDITIONING

4 UNDO WORK ON ANCILLA, AND RETURN TO COMPUTATIONAL BASIS

NOTE I DEFINE  $U_{xy}^{(2)} = R_z(-2(J_x+J_y)t)$ ,  
 $U_{xy}^{(1)} = R_z(-2(J_x-J_y)t)$ ,  $U_z = R_z(-2J_z t)$



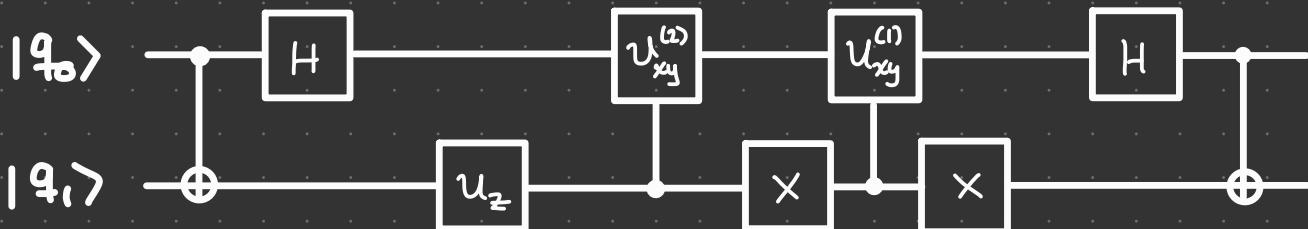
I PROBE THIS CIRCUIT USING QISKit CONSIDER STATE

EXAMPLE 1  $|\Psi_1\rangle = \frac{1}{\sqrt{2}}|\phi^+\rangle + \frac{1}{\sqrt{2}}|\phi^-\rangle = |00\rangle$

IF THIS STATE IS SIMULATED ON DEBINARY t

$$\begin{aligned}
 U(t)|\Psi_1\rangle &= \frac{1}{\sqrt{2}}(U(t)|\phi^+\rangle + U(t)|\phi^-\rangle) \\
 &= \frac{1}{\sqrt{2}}e^{J_z t}(e^{(J_x-J_y)t}|\phi^+\rangle + e^{-(J_x-J_y)t}|\phi^-\rangle) \\
 &= \frac{1}{\sqrt{2}}e^{[J_z+J_x-J_y]t}(|\phi^+\rangle + e^{-2(J_x-J_y)t}|\phi^-\rangle)
 \end{aligned}$$

I REALISE I CAN IMPLEMENT THIS CIRCUIT WITHOUT ANCILLA BITS THIS BECAUSE I ONLY APPLY ROTATIONS THAT ARE DIAGONAL ON COMPUTATIONAL BASIS



AS A RECAP, THE FIRST STAGE TRANSFORMS TO EIGENBASIS, THE SECOND PUSHES GLOBAL PHASES DEPENDING ON THE BELL BASIS MOP, AND THE LAST STAGE RETURNS TO COMPUTATIONAL BASIS

THIS MEANS THAT I CAN SIMULATE AN ANISOTROPIC SPIN CHAIN WITHOUT THE NEED OF ANCILLA BITS

THE SCHEME WOULD RELY ON A FIRST ST ITERATION CONSIDER A CHAIN WITH HAMILTONIAN

$$\hat{H} = \sum_{l=0}^{N-2} \sum_{k=1}^3 (J_k \sigma_k^{(l)} \otimes \sigma_k^{(l+1)} + h_k \sigma_k^{(l)})$$

REPRESENTATION OF THE STATE OF A SYSTEM WITH THIS HAMILTONIAN WOULD NEED N QUBITS TROTTERIZATION WOULD BE DEVELOPED BY PROMOVING THE HAMILTONIAN AS

$$\hat{H} = \sum_{l=0}^{N-2} \hat{H}_{l,l+1} + h_1 \underbrace{\sum_{l=0}^{N-1} \sigma_x^{(l)}}_{\hat{H}_1} + h_2 \underbrace{\sum_{l=0}^{N-1} \sigma_y^{(l)}}_{\hat{H}_2} + h_3 \underbrace{\sum_{l=1}^{N-1} \sigma_z^{(l)}}_{\hat{H}_3}$$

WITH

$$\hat{H}_{l,l} = \sum_{k=1}^3 J_k \sigma_k^{(l)} \otimes \sigma_k^{(l)}$$

I WOULD USE THE FIRST SUZUKI-TROTTER ITERATION AS MY SIMULATION STEP, AND IT WOULD BE IMPLEMENTED AS

$$\prod_{l=0}^{\lfloor N/2 \rfloor} e^{-i\hat{H}_{2l,2l+1}\frac{\Delta t}{2}} \prod_{l=0}^{\lfloor N/2 \rfloor} e^{-i\hat{H}_{2l+1,2l+2}\frac{\Delta t}{2}} e^{-i\hat{H}_1\frac{\Delta t}{2}} e^{-i\hat{H}_2\frac{\Delta t}{2}} \\ e^{-i\hat{H}_3\Delta t} e^{-i\hat{H}_1\frac{\Delta t}{2}} e^{-i\hat{H}_2\frac{\Delta t}{2}} \prod_{l=0}^{\lfloor N/2 \rfloor} e^{-i\hat{H}_{2l,2l+1}\frac{\Delta t}{2}}$$

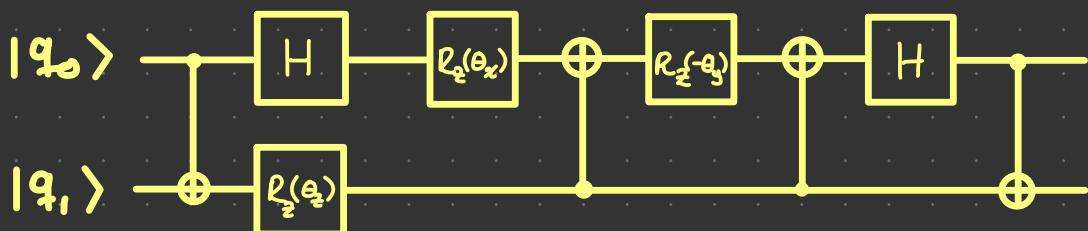
IF I COUPLE THIS TIME EVOLUTION WITH QPE, I CAN DIAGONALIZE THE CHAIN HAMILTONIAN

I WOULD LIKE TO REDUCE THE AMOUNT OF GATES REQUIRED BY MY SUBROUTINE FOR COMPUTING

$$e^{-i\hat{H}_y\frac{\Delta t}{2}}$$

AND SEE HOW WOULD I OPTIMIZE THE QPE ALGORITHM

I COULD SEE THAT  $J_x$ -PHASE CORRELATES TO  $|q_0\rangle$ , SO THAT CONTROLLED OPERATION IS UNNECESSARY ALSO,  $J_y$ -PHASE ANTI-CORRELATES / CORRELATES WITH  $|q_0\rangle$ , CONDITIONED ON  $|q_1\rangle$  AS A RESULT, I PROPOSE THE FOLLOWING ALGORITHM FOR COMPUTING THE Z PARTICLE SPIN UNITARY



WHERE  $\theta_i = J_i \Delta t / 2$  THE MINUS IN THE THIRD Z ROTATION IS PUT THERE TO REFLECT THE SIGN CHANGE OF  $J_y$  IN THE ENERGY, FROM  $| \Psi \rangle$  TO  $| \Phi \rangle$  STATES

I BELIEVE THIS IS THE BEST I CAN DO WITH MY CURRENT KNOWLEDGE OF QUANTUM COMPUTING I EMPLOY ONLY 5 SINGLE-QUBIT ROTATIONS AND 4 CNOT GATES

NOTE. THIS CIRCUIT RELIES ON LINEARITY OF QUANTUM GATES

I NOTICED THAT I CAN PACK AN X-ROTATION FOR  $| \Psi_i \rangle$  THIS LED ME TO A MORE EFFICIENT TROTTERIZATION THAT COULD REDUCE FURTHER CIRCUIT DEPTH SINCE

$$\text{CNOT } R_{x,2}(\theta) = R_{x,2}(\theta) \text{ CNOT}$$

IT IS POSSIBLE TO SET THE SUZUKI-TROTTER ITERATION SUCH THAT  $H_y$  AND  $H_z$  CAN BE SIMULATED SOMEWHAT IN PARALLEL TO THIS SINCE I PACK THE X FIELD-SPIN INTERACTION THIS CAN BE DONE BECAUSE

$$e^{-iH_z t} = \bigotimes_{l=0}^{N-1} R_{x,l}(\theta)$$

AND I CAN SEE A "POCKET" FOR PARALLELIZATION AT THE BASIS CHANGE STEPS I DEFINE NOTATION

$$\prod_{l=0}^{N-1} \chi_l^+ = \prod_{i=0}^{\lfloor N/2 \rfloor} \chi_{z_l}$$

$$\prod_{l=0}^{N-1} \chi_l^- = \prod_{i=0}^{\lfloor N/2 \rfloor} \chi_{z_{l+1}}$$

$$\text{AND } H_j^+ = \sum_{l=0}^{N-1} h_j \sigma_j^{(l)}, H_j^- = \sum_{l=0}^{N-1} h_j \sigma_j^{(l)}$$

THE SCHEME I PROPOSE IS

$$\begin{aligned}
 & \prod_{l=0}^{N-1} e^{-iH_{l+1} \frac{\Delta t}{2}} e^{-i\hat{H}_l - \frac{\Delta t}{2}} \prod_{l=0}^{N-1} + e^{-iH_{l+1} \frac{\Delta t}{2}} \\
 & e^{-i\hat{H}_1 + \frac{\Delta t}{2}} e^{-i\hat{H}_2 \frac{\Delta t}{2}} e^{-i\hat{H}_3 \Delta t} e^{-i\hat{H}_2 \frac{\Delta t}{2}} \\
 & e^{-i\hat{H}_1 + \frac{\Delta t}{2}} \prod_{l=0}^{N-1} + e^{-iH_{l+1} \frac{\Delta t}{2}} e^{-i\hat{H}_1 - \frac{\Delta t}{2}}
 \end{aligned}$$

THE OPTIMIZATION STEEMS FROM THE FACT THAT

$$\begin{aligned}
 & \prod_{l=0}^{N-1} \pm e^{-iH_{l+1} \frac{\Delta t}{2}} e^{-i\hat{H}_l \pm \frac{\Delta t}{2}} \\
 & e^{-i\hat{H}_l \pm \frac{\Delta t}{2}} \prod_{l=0}^{N-1} \pm e^{-iH_{l+1} \frac{\Delta t}{2}}
 \end{aligned}$$

CAN BE COMPUTED AS A BLOCK, DUE TO CNOT COMMUTATION PROPERTIES ALSO, EACH OF THE BLOCKS CAN BE COMPUTED IN PARALLEL, SO THAT THE EFFECTIVE CIRCUIT DEPTH OF THIS STAGES IS CONSTANT

FIRST SUZUKI TROTTER ITERATION, THEREFORE, HAS A CIRCUIT DEPTH OF  $16 + 3 + 16 = 35$  AND IS ULTIMATELY CONSTANT

ULTIMATELY, I CLAIM THAT THIS CIRCUIT HAS A GATE COUNT THAT SCALES LINEARLY WITH THE SIZE OF THE SYSTEM

NOTE I NEED TO EVALUATE THE ERROR  
THAT A SINGLE TIME STEP IMPLIES THIS IS  
PREDOMINANT FOR EVOLVING THE ACTUAL COM-  
PLEXITY OF MY ALGORITHM

FOR THE MOMENT I WILL CONSIDER EVOLU-  
TION UNDER HAMILTONIAN

$$\hat{H}_0 = h_1 \hat{\sigma}_1^{(u)} + h_2 \hat{\sigma}_2^{(u)} + h_3 \hat{\sigma}_3^{(u)}$$

THIS IS A PARTICLE IN AN EXTERNAL FIELD  
FOR SIMPLICITY, I WILL CONSIDER

$$\hat{H}_0 = h \hat{n}(\theta, \phi) \vec{\sigma}^{(u)}$$

WITH THE DEFINITION

$$\hat{n} = \sin\theta \cos\phi \hat{x} + \sin\theta \sin\phi \hat{y} + \cos\theta \hat{z}$$

TO PERFORM EXACT SIMULATION UNDER THIS  
HAMILTONIAN, I NEED A SPIN ROTATION UNITARY  
TO THIS END, I SHOULD DIAGONALIZE THE  
OPERATOR

$$\hat{n}(\theta, \phi) \vec{\sigma}^{(u)}$$

WE NOTICE THAT THIS OPERATOR COMMU-  
TES WITH  $R_{\hat{n}}(\alpha)$  FOR ANY  $\alpha \in \mathbb{R}$ . THIS  
IMPLIES THAT BOTH OPERATORS ARE SIMUL-  
TANEOUSLY DIAGONALIZABLE. WE NOTE THAT  
THE EIGENSTATES OF ANY  $R_{\hat{n}}(\alpha)$  ARE  
THE STATES WHOSE BLOCH VECTORS ARE PAR-  
ALLEL OR ANTI-PARALLEL TO  $\hat{n}$ .

THOSE ARE

$$|\uparrow\rangle = \cos \frac{\theta}{2} |0\rangle + e^{i\phi} \sin \frac{\theta}{2} |1\rangle$$

$$|\downarrow\rangle = \sin \frac{\theta}{2} |0\rangle - e^{i\phi} \cos \frac{\theta}{2} |1\rangle$$

Therefore, the unitary that changes from computational basis to the eigenbasis is of the form

$$\begin{bmatrix} \cos \frac{\theta}{2} & \sin \frac{\theta}{2} \\ e^{i\phi} \sin \frac{\theta}{2} & -e^{i\phi} \cos \frac{\theta}{2} \end{bmatrix}$$

The operator that changes from eigenbasis to computational basis is

$$\begin{bmatrix} \cos \frac{\theta}{2} & e^{-i\phi} \sin \frac{\theta}{2} \\ \sin \frac{\theta}{2} & -e^{-i\phi} \cos \frac{\theta}{2} \end{bmatrix}$$

Once in the eigenbasis, an  $R_z(\hbar t)$  rotation performs time evolution. I would like to express the unitary in  $XZX$  decomposition. This would allow me to perform exact evolution under

$$\hat{H} = \hat{H}_1 + \hat{H}_2 + \hat{H}_3$$

Now, the operator is

$$\begin{bmatrix} \cos \frac{\theta}{2} & e^{-i\phi} \sin \frac{\theta}{2} \\ \sin \frac{\theta}{2} & -e^{-i\phi} \cos \frac{\theta}{2} \end{bmatrix} \begin{bmatrix} e^{-i\hbar t} & 0 \\ 0 & e^{i\hbar t} \end{bmatrix} \begin{bmatrix} \cos \frac{\theta}{2} & \sin \frac{\theta}{2} \\ e^{i\phi} \sin \frac{\theta}{2} & -e^{i\phi} \cos \frac{\theta}{2} \end{bmatrix}$$

The problem of finding the angles for the  $XZX$  decomposition seem excessively complicated. A detailed account of the error reduction that exact simulation of this part would yield is needed to establish if the decomposition is worth the effort.

For now, I remain studying the scheme with separated  $x, y, z$  field interaction.