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

$$i \frac{\partial |\psi\rangle}{\partial t} = \left(\sum_i \frac{p_i^2}{2m_i} + V(x_1, x_2, \ldots, x_N) \right) |\psi\rangle$$

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

$$|x\rangle \text{ FOR } x \in [0, L] \longrightarrow |k\Delta x\rangle \text{ FOR } k = 0, \ldots, N-1$$

THIS DISCRETIZATION LEADS TO A REPRESENTATION OF THE SINGLE PARTICLE STATE

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

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

THUS LEADING TO A DIFFERENTIAL EQUATION

$$i \frac{\partial a_k}{\partial t} = H_{kl} a_l$$

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

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

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

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

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

$$p = QFT \, x \, QFT^{+}$$

$$e^{-ip^2/2mt} = QFT \, e^{-ix^2/2mt} \, QFT^{+}$$

AS A RESULT, BOTH UNITARIES

$$e^{-ip^2/2mt} \quad , \quad e^{-iV(x)t}$$

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

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

MAY 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 ALGORITMS HAVE SPACE COMPLEXITY THAT SCALES $O(2^n)$, QUANTUM ALGORITMS 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

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

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 $\longrightarrow$ CONSIDER OPERATORS H_1, H_2 WITH $[H_1, H_2] \neq 0$ THEN

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

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

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

DEFINE $k = l + m$ THE DOUBLE SUM ABOVE AMOUNTS TO

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

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

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 ARE 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 Δt 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 $A_1, A_2, \ldots, A_m$ DEFINE

$$f(t) = \prod_{k=1}^{m} e^{tA_k} = e^{tA_1} e^{tA_2} \cdots e^{tA_m}$$

IF $|t| \ll 1$, THEN

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

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

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

BAKER-HAUSDORF FORMULA $\longrightarrow$ DEFINE THE PARAMETRISED FUNCTION

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

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

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

$$f(t) = 1 + t(A+B) + \frac{t^2}{2}\left(A + B^2 + AB + BA\right) + O(t^3)$$

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

AND THUS

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

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

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

DEM DEFINE $A_1 = A/2$, $A_2 = B$, $A_3 = A/2$
DEFINE $f(t)$ AS BEFORE

$$f(t) = 1 + t(A+B)$$
$$+ \frac{t^2}{2}\left[\frac{A^2}{2} + B^2 + AB + \frac{A^2}{2} + BA\right] + O(t^3)$$

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

FROM WHICH THE DESIRED FORMULA FOLLOWS

GENERAL FORMULA $\longrightarrow$ A GENERAL HAMILTONIAN

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

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

$$e^{tH} \approx e^{tH_1/2} e^{tH_2/2} \quad e^{tH_L/2} e^{tH_L/2} \quad e^{tH_2/2} e^{tH_1/2}$$

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

$$\sum_{k=1}^{M} A_m = \sum_{k=1}^{L} \frac{H_k^2}{2}$$

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

EXACT SOLUTION OF 1D ISING MODEL

$$H = \underbrace{\sum_{i=1}^{N} X_i X_{i+1}}_{\text{SPIN INTERACTIONS}} + \underbrace{Y_1 \bigotimes_{i=2}^{N-1} Z_i \, Y_N}_{\text{BOUNDARY TERMS}} + \underbrace{\lambda \sum_{i=1}^{N} Z_i}_{\text{TRANSVERSE FIELD}}$$

CONSIDER THE JORDAN-WIGNER TRANSFORMATION, GIVEN BY

$$c_i = \left(\bigotimes_{j=1}^{i-1} Z_j \right) \sigma_i$$

$$c_i^{+} = \left(\bigotimes_{j=1}^{i-1} Z_j \right) \sigma_i^{+}$$

WITH

$$\sigma_i = \frac{1}{2}(X + iY)$$

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

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

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

$$\{c_i, c_j^{+}\} = \begin{cases} 0 & i \neq j \\ \{\sigma_i, \sigma_i^{+}\} \quad \text{IF} & i = j \end{cases}$$

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 INTERACCTION DEPENDS ON THE OCCUPATION NUMBER THERE EXISTS A VACUUM STATE

$$c_i^+ c_i |\Omega\rangle = 0 \qquad \text{FOR} \quad 1 \leq i \leq N$$

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

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

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

$$= c_i^+ c_i - (c_i^2)^+ (c_i^2)$$

$$= c_i^+ c_i$$

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

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

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

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

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

$$c_i^+ c_i c_i = c_i^+ c_i^2 = 0$$

OCCUPATION NUMBER IS EITHER 0 OR 1 FOR EACH LATTICE SITE

3 $c_i^+ c_i$ ARE A SET OF COMMUTING OPS

CONSIDER THE COMMUTATION RELATIONS

$$
\begin{aligned}
c_i^+ c_i \, c_j^+ c_j &= - c_i^+ c_j^+ c_i c_j \\
&= c_j^+ c_i^+ c_i c_j \\
&= c_j^+ c_j \, c_i^+ c_i
\end{aligned}
$$

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

$$\prod_{i=1}^{N} (c_i^+)^{\alpha_i} \qquad \text{WITH} \quad \alpha_i = 0, 1$$

SINCE IT IS SO THAT

$$\left(\prod_{i=1}^{N} (c_i^+)^{\alpha'_i} \right)^+ \prod_{i=1}^{N} (c_i^+)^{\alpha_i}$$

$$= c_N^{\alpha'_N} c_{N-1}^{\alpha'_{N-1}} \quad c_1^{\alpha'_i} c_1^{+\alpha_i} \quad c_{N-1}^{+\alpha_N'} c^{+\alpha_N}$$

$$= \prod_{i=1}^{N} c_i^{\alpha'_i} c_i^{+\alpha_i}$$

STATES DEFINED BY

$$|\alpha\rangle = |\alpha_1 \quad \alpha_{N-1}, \alpha_N\rangle = \prod_{i=1}^{N} (c_i^+)^{\alpha_i} |\Omega\rangle$$

SINCE

$$\sigma_l + \sigma_l^+ = X_l$$
$$\imath(\sigma_l^+ - \sigma_l) = Y_l$$

AND
$$Y_l Z_l = -Z_l Y_l = \imath X_l$$
$$X_l Z_l = -Z_l X_l = -\imath Y_l$$

IT IS SO THAT

$$X_l X_{l+1} = (c_l^+ - c_l)(c_{l+1} + c_{l+1}^+)$$
$$Y_l Y_{l+1} = (c_l^+ + c_l)(c_{l+1} - c_{l+1}^+)$$

CONSIDER AN INTERACTION HAMILTONIAN

$$H = -\frac{J_x}{2}\sum_{l=1}^{N} X_l X_{l+1} - \frac{J_y}{2}\sum_{l=1}^{N} Y_l Y_{l+1}$$

$$X_l X_{l+1} = c_l^+ c_{l+1} + c_l^+ c_{l+1}^+ - c_l c_{l+1} - c_l c_{l+1}^+$$
$$= c_l^+ c_{l+1} + c_l^+ c_{l+1}^+ + c_{l+1} c_l + c_{l+1}^+ c_l$$

$$Y_l Y_{l+1} = c_l^+ c_{l+1} - c_l^+ c_{l+1}^+ + c_l c_{l+1} - c_l c_{l+1}^+$$
$$= c_l^+ c_{l+1} + c_{l+1}^+ c_l - c_l^+ c_{l+1}^+ - c_{l+1} c_l$$

IF $J_x = J_y$, I E THE INTERACTION CORRESPONDS TO AN XY HEISENBERG MODEL

$$H = -\frac{J}{2}\sum_{l=1}^{N}\left(c_l^+ c_{l+1} + c_{l+1}^+ c_l\right)$$

LETS TRANSFORM TO MOMENTUM SPACE IN ORDER TO SIMPLIFY THE HAMILTONIAN

$$c_l = \frac{1}{\sqrt{N}} \sum_k s_k e^{ikR_l}$$

WITH k IN THE 1ST BRILLOUIN ZONE

$$c_l^+ c_{l+1} = \frac{1}{N} \sum_{kk'} s_k^+ s_{k'} e^{-ik'} e^{i(k-k')R_l}$$

$$c_{l+1}^+ c_l = \frac{1}{N} \sum_{kk'} s_{k'}^+ s_k e^{ik} e^{i(k'-k)R_l}$$

FROM THE ABOVE EXPRESSIONS, AND USING

$$\sum_l e^{i(k-k')R_l} = N\delta_{k,k'}$$

THE INTERACTION HAMILTONIAN SIMPLIFIES TO

$$H = -J \sum_k \cos k \, s_k^+ s_k$$

$$\hat{\Delta} = \vec{S}_i \, \hat{S}_j = \sum_k \hat{\sigma}_k^{(i)} \otimes \hat{\sigma}_k^{(j)}$$

$$\hat{\Delta}^2 = \left(\sum_k \hat{\sigma}_k^{(i)} \otimes \hat{\sigma}_k^{(j)}\right)\left(\sum \hat{\sigma}_l^{(i)} \otimes \hat{\sigma}_l^{(j)}\right)$$

$$= \sum_{kl} \hat{\sigma}_k^{(i)} \hat{\sigma}_l^{(i)} \otimes \hat{\sigma}_k^{(j)} \hat{\sigma}_l^{(j)}$$

$$= \sum_{kl} (\delta_{kl} + i\epsilon_{klm} \hat{\sigma}_m^{(i)})(\delta_{kl} + i\epsilon_{kln} \hat{\sigma}_n^{(j)})$$

$$= \sum_{kl} \delta_{kl}\delta_{kl} + i \sum_{kl} \cancel{\delta_{kl}\epsilon_{klm}}\, \hat{\sigma}_m^{(i)} \quad 0$$

$$+ i \sum_{kl} \cancel{\delta_{kl}\epsilon_{kln}}\, \hat{\sigma}_n^{(j)} \quad 0$$

$$- \sum_{kl} \underbrace{\epsilon_{klm}\epsilon_{kln}} \hat{\sigma}_m^{(i)} \otimes \hat{\sigma}_n^{(j)}$$

$$= 3 - 2\vec{S}_i \, \vec{S}_j = 3 - 2\hat{\Delta}$$

$$e^{-i\theta\hat{\Delta}} = f(\theta) - ig(\theta)\hat{\Delta}$$

$$e^{-i\theta\hat{\Delta}}\Big|_{\theta=0} = f(0) - ig(0)\hat{\Delta}$$

$$\boxed{\begin{aligned} f(0) &= 1 \\ g(0) &= 0 \end{aligned}}$$

$$\frac{d e^{-i\theta\hat{\Delta}}}{d\theta} = -i\hat{\Delta} e^{-i\theta\hat{\Delta}} = f'(\theta) - ig'(\theta)\hat{\Delta}$$

$$e^{-\iota\theta\hat{\Delta}} = f(\theta) - \iota g(\theta)\hat{\Delta}$$
$$-\iota\hat{\Delta}e^{-\iota\theta\hat{\Delta}} = f'(\theta) - \iota g'(\theta)\hat{\Delta}$$
$$-\hat{\Delta}^2 e^{\iota\theta\hat{\Delta}} = f''(\theta) - \iota g''(\theta)\hat{\Delta}$$
$$-(3-2\Delta)e^{\iota\theta\hat{\Delta}} = f''(\theta) - \iota g''(\theta)\hat{\Delta}$$

$$-(3-2\Delta)(f(\theta) - \iota g(\theta)\hat{\Delta}) = f''(\theta) - \iota g''(\theta)\hat{\Delta}$$

$$3f(\theta) - 3\iota g(\theta)\hat{\Delta} - 2f(\theta)\Delta + 2\iota g(\theta)\hat{\Delta}^2 = -f''(\theta) + \iota g''(\theta)\hat{\Delta}$$

$$\hat{\Delta}^2 \rightarrow 3-2\hat{\Delta}$$

$$3f(\theta) + 6\iota g(\theta) - 3\iota g(\theta)\hat{\Delta} - 2f(\theta)\hat{\Delta} - 4\iota g(\theta)\hat{\Delta} = -f''(\theta) + \iota g''(\theta)\hat{\Delta}$$

$$f''(\theta) = -3f(\theta) - 6\iota g(\theta)$$
$$\iota g''(\theta) = -2f(\theta) - 7\iota g(\theta)$$

$$\begin{bmatrix} f''(\theta) \\ g''(\theta) \end{bmatrix} = \begin{bmatrix} -3 & -6\iota \\ -2\iota & 7 \end{bmatrix} \begin{bmatrix} f(\theta) \\ g(\theta) \end{bmatrix}$$

$$f(0) = 1, \quad g(0) = 0$$
$$f'(0) = 0, \quad g'(0) = 1$$

CONSIDER OPERATOR

$$\hat{H}_{ij} = \vec{\sigma}^{(i)} \, \bar{\bar{J}} \, \vec{\sigma}^{(j)} = \sum_{kl} J_{kl} \sigma_k^{(i)} \sigma_l^{(j)}$$

SUPPOSE $J_{kl} = J_l \delta_{kl}$ SO THAT

$$\hat{H}_{ij} = \sum_l J_l \hat{\sigma}_l^{(i)} \hat{\sigma}_l^{(j)}$$

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

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

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

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

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

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

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

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

1 CHANGE FROM COMPUTATIONAL BASIS TO BELL BASIS SUCH THAT

$$|00\rangle \longrightarrow |\phi^+\rangle$$
$$|01\rangle \longrightarrow |\phi^-\rangle$$
$$|10\rangle \longrightarrow |\Psi^+\rangle$$
$$|11\rangle \longrightarrow |\Psi^-\rangle$$

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

3 USE AN ANCILLA QBIT TO ADD A PHASE ASSOCIATED TO J_x & J_y AS FOLLOWS

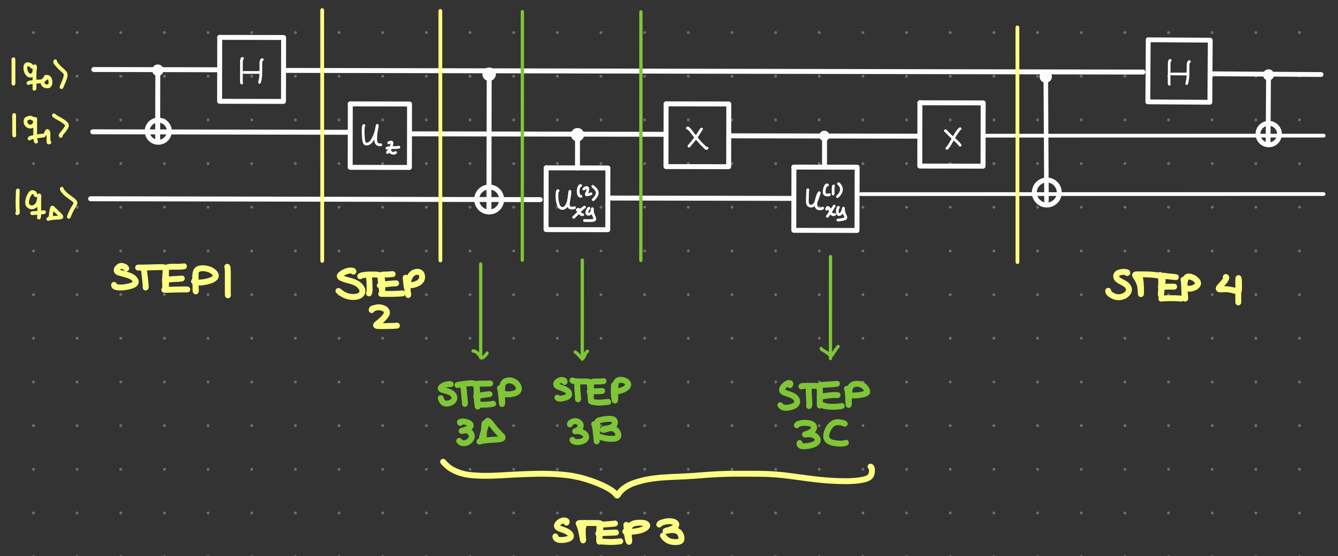
A APPLY A CNOT TO DETERMINE THE SIGN OF THE PHASE, WITH 1ST QBIT AS CONTROL

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

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

4 UNDO WORK ON ANCILLA, AND RETURN TO COMPUTATIONAL BASIS

NOTE 1 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 A STATE

<u>EXAMPLE 1</u> $|\psi_i\rangle = \frac{1}{\sqrt{2}}|\phi^+\rangle + \frac{1}{\sqrt{2}}|\phi^-\rangle = |00\rangle$

IF THIS STATE IS SIMULATED ON ARBITRARY t

$$U(t)|\psi_i\rangle = \frac{1}{\sqrt{2}}\left(U(t)|\phi^+\rangle + U(t)|\phi^-\rangle\right)$$

$$= \frac{1}{\sqrt{2}} e^{J_z t}\left(e^{(J_x-J_y)t}|\phi^+\rangle + e^{-(J_x-J_y)t}|\phi^-\rangle\right)$$

$$= \frac{1}{\sqrt{2}} e^{[J_z+J_x-J_y]t}\left(|\phi^+\rangle + e^{-2(J_x-J_y)t}|\phi^-\rangle\right)$$

THIS CIRCUIT IMPLEMENTS TIME EVOLUTION UNDER HAMILTONIAN

$$\hat{H}_{ij} = \vec{S}_i \bar{J} \vec{S}_j$$

HOWEVER, IF THE GOAL IS TO SIMULATE EVOLUTION OF A HEISENBERG CHAIN, THE FULL HAMILTONIAN IS:

$$\hat{H} = \sum_{i=0}^{N-1} H_{i,\, i+1 \bmod N} = \sum_{i=0}^{N} \hat{K}_i$$

SINCE INTERACTION IS NEAREST NEIGHBOUR, IT IS SO THAT $\hat{K}_i$ AND $\hat{K}_{i+n}$ WITH $n \geq 2$ ARE COMMUTING OPERATORS

ALSO, NOTICE THAT

$$\hat{K}_i \hat{K}_{i+1} = \left(\sum_{l} J_l \hat{\sigma}_l^{(i)} \hat{\sigma}_l^{(i+1)} \right) \left(\sum_{m} J_m \hat{\sigma}_m^{(i+1)} \hat{\sigma}_m^{(i+2)} \right)$$

$$\left[\hat{K}_i , \hat{K}_{i+1} \right] = \sum_{lm} J_l J_m \hat{\sigma}_l^{(i)} \left[\hat{\sigma}_l^{(i+1)}, \hat{\sigma}_m^{(i+1)} \right] \hat{\sigma}_m^{(i+2)}$$

$$= i \sum_{lmn} J_l J_m \hat{\sigma}_l^{(i)} \epsilon_{nlm} \hat{\sigma}_n^{(i+1)} \hat{\sigma}_m^{(i+2)}$$