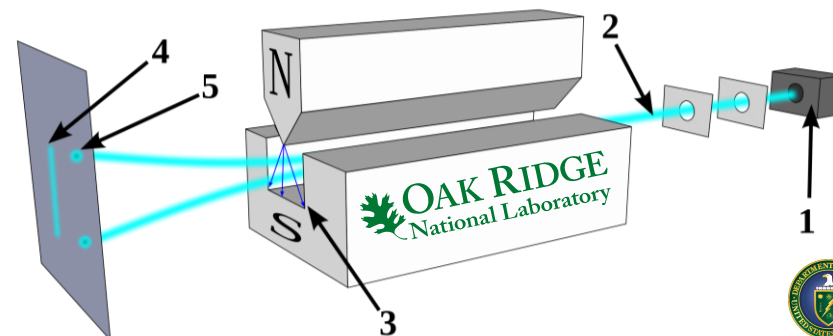


Arithmetic Quantum Algorithms

Eugene Dumitrescu

QIS Summer School, Wednesday July 17th



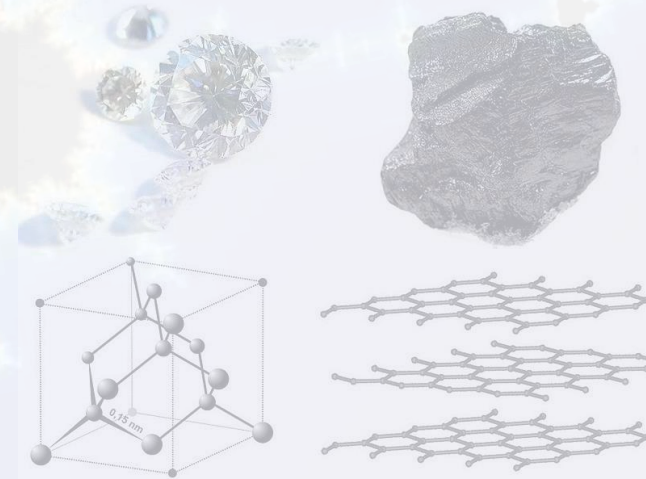
U.S. DEPARTMENT OF
ENERGY

Office of
Science



Outline

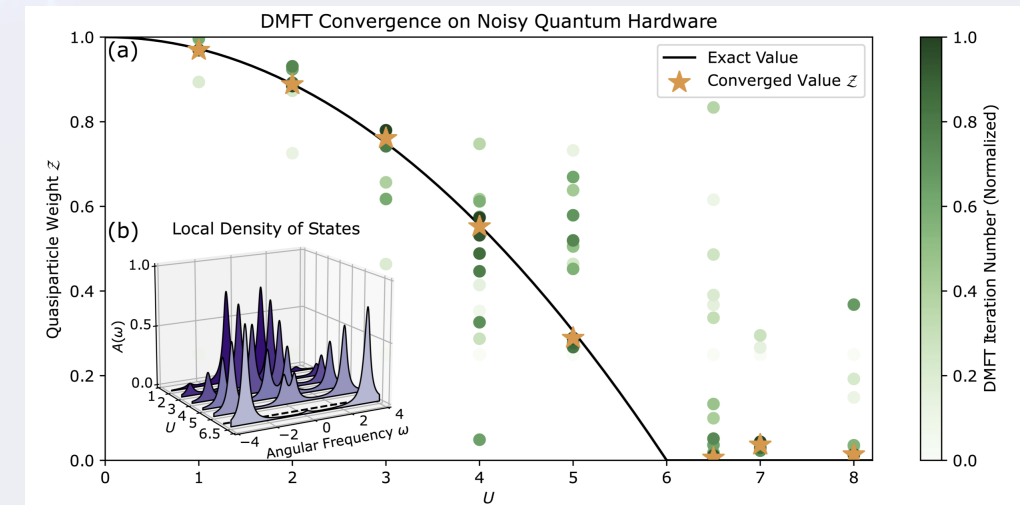
1. Introduction to Computation & Algorithms
 1. Quantum Facts of Life
 2. Motivation
 3. Ingredients of a Quantum Computation
2. Quantum Arithmetic – A guide for crafting algorithms
 1. Classical Arithmetic
 2. Classification of Quantum Algorithms
 3. Multiplicative Factorizations, Approximation Error
 4. Block Encoding Integral Transformations
 1. Projection operator $\hat{F} = e^{-\frac{1}{2}t^2\hat{H}^2}$
 2. Resolvent operator $\hat{R} = \frac{1}{\omega - \hat{H}}$
3. Multiplicative Optimal Control via Algebraic Factorization
 1. Anderson localization in TFX model
 1. Algorithm: 10.1103/PhysRevLett.129.070501
 2. Code: github.com/kemperlab/cartan-quantum-synthesizer
 2. Quantum dynamical mean field theory
 1. Experiment: 10.1103/PhysRevResearch.5.023198
 2. A working definition for NISQ?
4. Unification of multiplicative and additive forms
 1. Inversion symmetric Trotter formula
 2. Applications to measurement



3

17

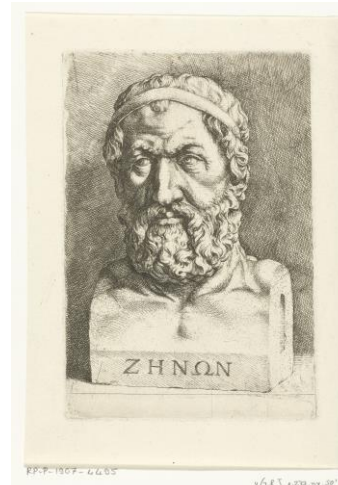
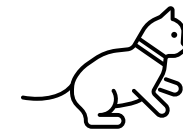
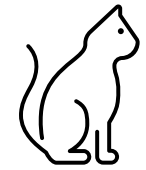
19





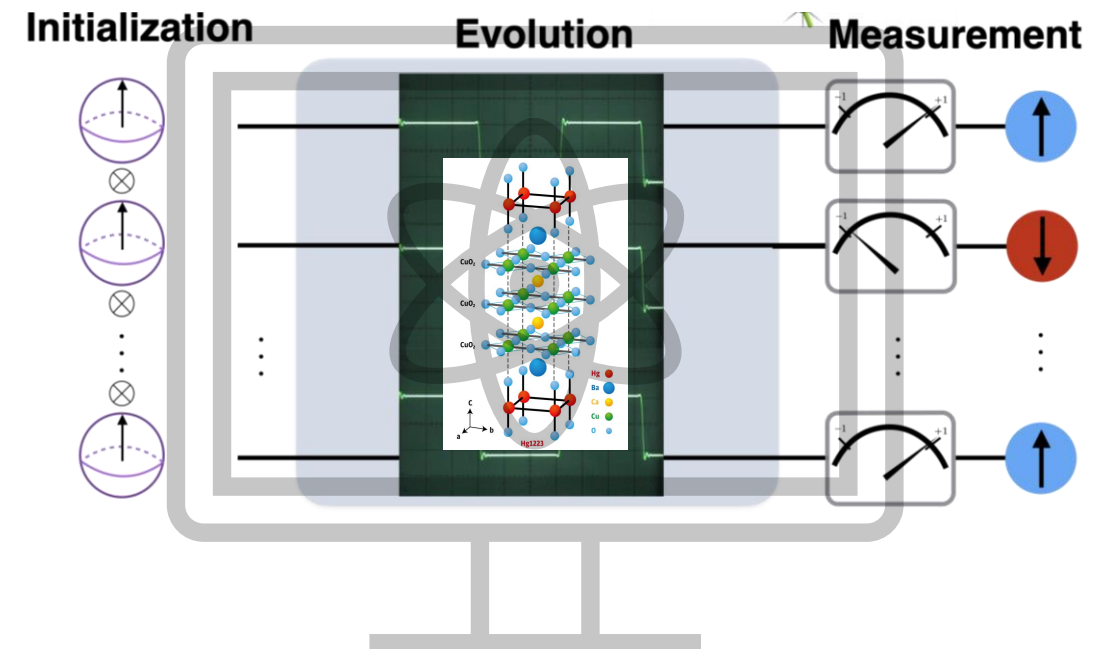
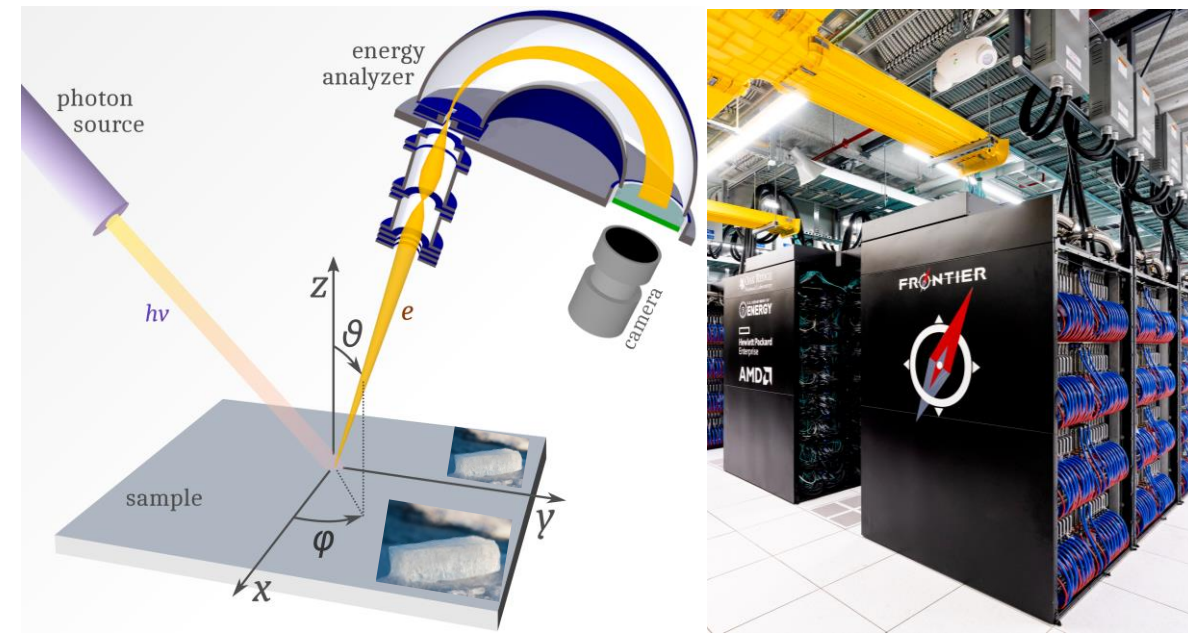
Paradoxical Cat States

- $|\text{Quantum Computing}\rangle =$
 - perfectly $|\text{isolated from}\rangle + |\text{controllable via}\rangle$ the outside environment
 - $\frac{1}{\sqrt{2}} [|\text{physics}\rangle + |\text{computer science}\rangle] \sim \frac{1}{\sqrt{2}} [|\text{analog}\rangle + |\text{digital}\rangle]$
 - $\frac{1}{\sqrt{3}} [|\text{qubit}\rangle + |\text{error correction}\rangle + |\text{algorithm}\rangle]$
 - $\frac{1}{\sqrt{2}} [|\text{NISQ}\rangle + |\text{BQP}\rangle] = \frac{1}{\sqrt{2}} [|\varepsilon_{\text{physical}} = 0.2\rangle + |\varepsilon_{\text{algorithmic}} = 2 \times 10^{-10}\rangle]$
 - $\frac{1}{\sqrt{2}} [|\text{physical error}\rangle + |\text{algorithmic error}\rangle]$
 - $\frac{1}{\sqrt{2}} [|\text{uses heat producing fridges}\rangle + |\text{reversible (zero heat loss)}\rangle]$
 - $\frac{1}{\sqrt{2}} [|\text{experimental demonstrations quantifying physical error}\rangle + |\text{experimentally impossible (today) exponentially fast matrix algorithms}\rangle]$
- Measurement-based Zeno-Effect \leftrightarrow Quantum Error Correction



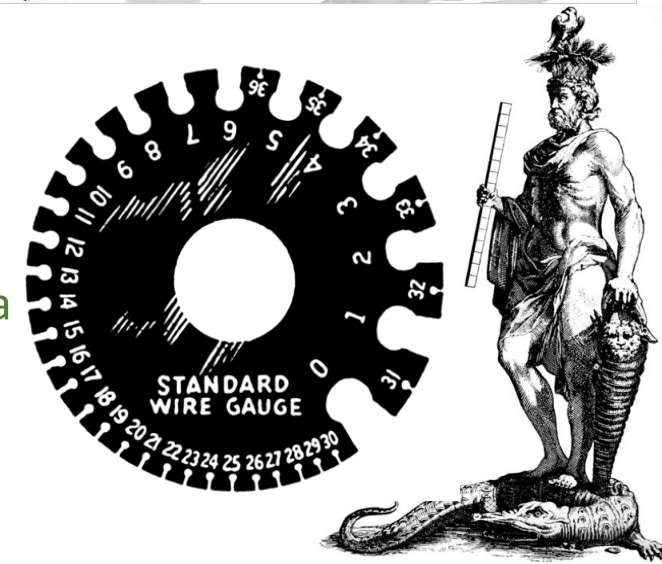
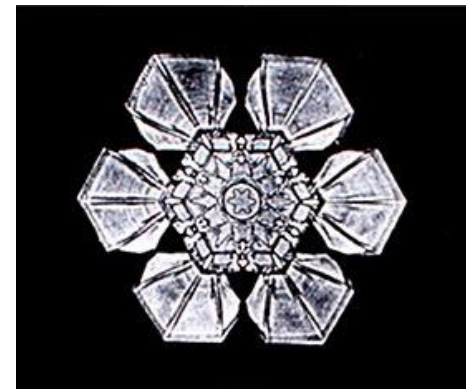
Simulation Scenarios:

- **Physical Experiment:**
 - Chemistry, lithography, etc. Make perfect sample. Cool to low T .
 - Probe system from external environment.
 - e.g. electro/thermal transport, ARPES, beams of all sorts
- **Classical Computation:**
 - Memory management in right panel
- **Quantum Computation:**
 - Model *target* system/Explicit problem encoding
 - Discretize quantized fields on a lattice e.g. in 2nd quantization:
 - Electrons $\{c_p, c_q^\dagger\} = \delta_{pq}$; $\{c_p^\dagger, c_q^\dagger\} = \{c_p, c_q\} = 0$
 - $\sim N$ qubits for N fermion modes
 - Phonons, photons $[a_p, a_q^\dagger] = \delta_{pq}$; $[a_p^\dagger, a_q^\dagger] = [a_p, a_q] = 0$
 - Truncation with $N \times \log(\Lambda)$ qubits
 - Use boson modes, linear scaling in N
 - Initialize
 - Begin with a simple & suitable input state.
 - Evolve *simulator* system
 - Real $U(t) \sim e^{i\hat{H}t}$ (or imaginary $V(\tau) = e^{-H\tau}$) time evolution
 - Measure Response Functions $\langle \hat{O} \rangle$



Ingredients of a Quantum Computation

- Initialize system (cool until relaxed into a lowest quantum mode)
- Generate entanglement (quantum correlations)
 - Volume law entanglement appears in
 - i) critical states
 - ii) nuclear matter [2303.04799](#)
 - iii) Shor's algorithm PhysRevA.96.062322 E.F.D.
- Interfere coherences constructively and destructively
 - Quantum gates offer a systematic way to do this:
 - E.g. Hadamard test on next slide
 - E.g. bosonic $\hat{D}(\alpha) = e^{\alpha a^\dagger - \alpha^* a}$
 - Definition:
 - Quantum Algorithm -- a sequence of quantum gates applied to perform a computational task
- Measurements: \mathbb{R} data



The Only Quantum Circuit You'll Ever Need

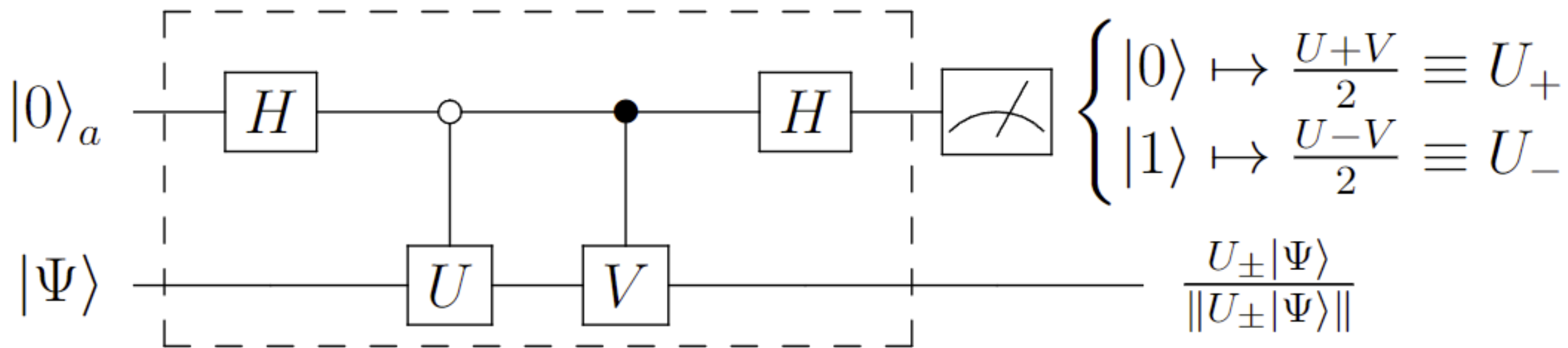


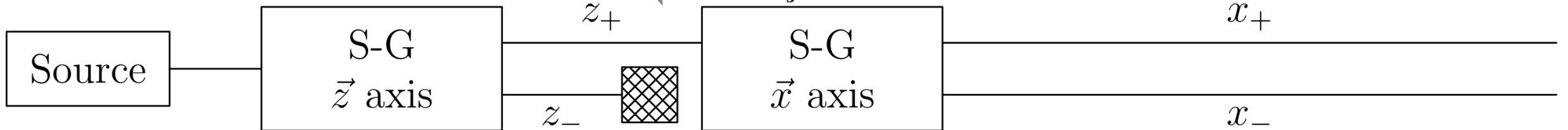
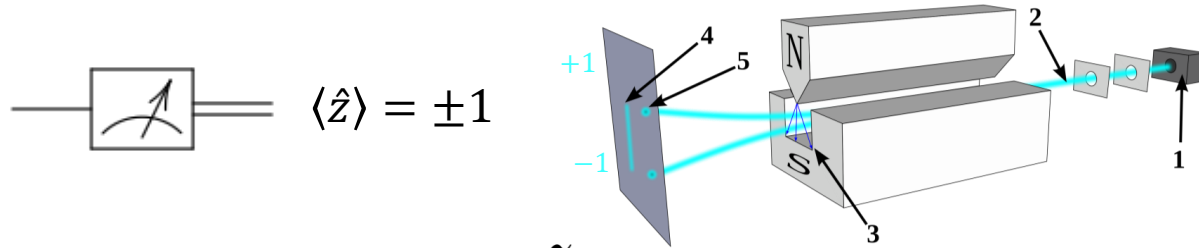
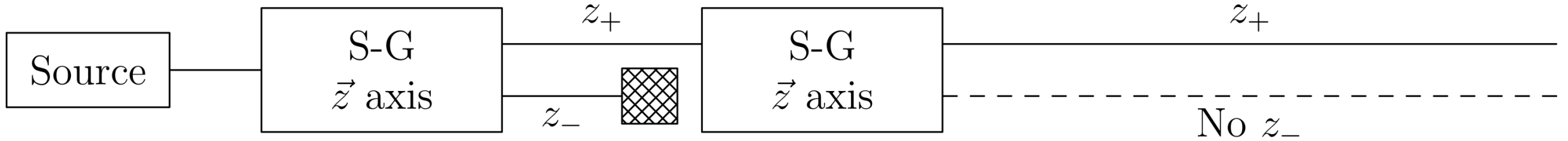
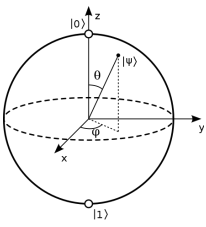
FIG. 1. Selecting $U = V^\dagger = e^{-itH}$ we define a random spectral walk (Sec. III A). Using $U = e^{tA}e^{tB}$ and $V = e^{tB}e^{tA}$, the quantum circuit acts by the BCH-like series that is symmetric with respect to the inversion $A \leftrightarrow B$. This is used to factorize time-evolution (Sec. III B). Setting different times ($t \rightarrow \theta_1, \theta_2$) enables a symmetric variational ansatz (Sec. III C). Last, setting $U = X_l$ and $V = iY_l$ for an array of qubits $\{q_l\}_{l=1}^N$ and concatenating the gadget N -times performs the measurement of Mermin polynomial M_N with a linear depth circuit (Sec. III D). The symmetry of the operator applied to $|\Psi\rangle$ is contingent on a measurement observing the ancillary qubit in the ($|1\rangle$) $|0\rangle$ state. Note that U_{\pm} are not unitary and that the principle system's final state $U_{\pm}|\Psi\rangle$ is normalized upon measurement of the ancilla qubit, due to the measurement postulate.

*Trotter (product) decompositions are recovered when $U=V$.

In this case the ancilla is not required as it will always be measured in the 0 state and may be removed.

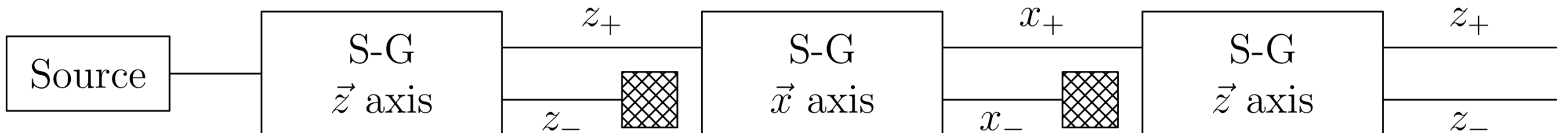
1st Q. Algorithm: Stern Gerlach Apparatus

or local-, SU(2), basis rotations and measurement



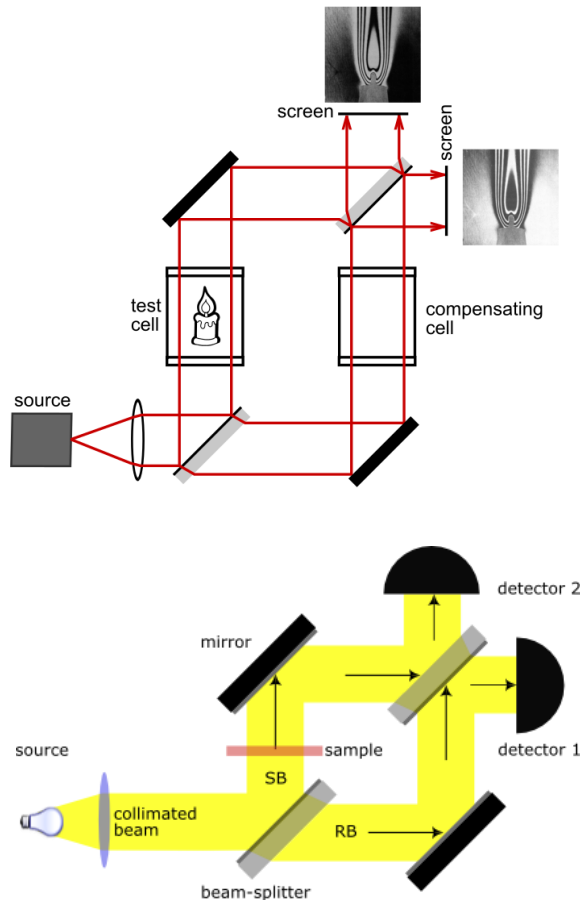
Pauli/XYZ-basis transformations \subset S-G gate

Non-commuting observables! $[\sigma^x, \sigma^z] \neq 0$



2nd Quantum Algorithm: Interferometry

Mach Zehnder



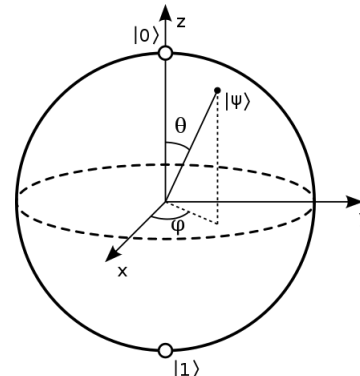
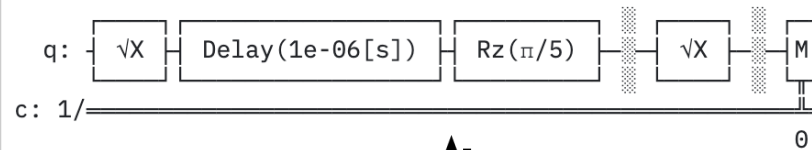
Ramsey

```
import numpy as np
import qiskit
from qiskit_experiments.library import T2Ramsey
```

```
qubit = 0
# set the desired delays
delays = list(np.arange(1e-6, 50e-6, 2e-6))
```

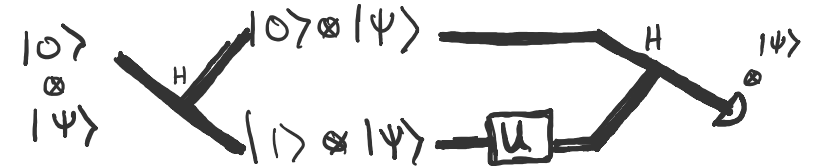
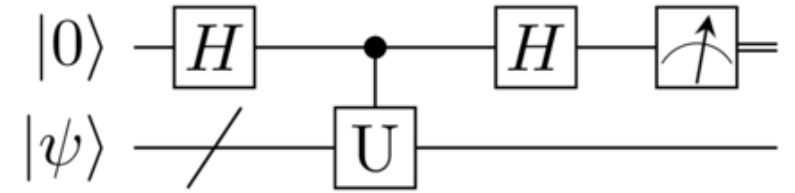
```
# Create a T2Ramsey experiment. Print the first circuit as a circuit
exp1 = T2Ramsey((qubit,), delays, osc_freq=1e5)

print(exp1.circuits()[0])
```

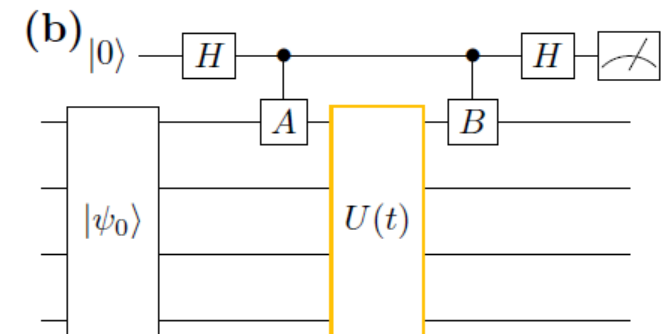


$$\frac{1}{\sqrt{2}}(|0\rangle - i|1\rangle) \otimes |\psi\rangle$$

$$\frac{1}{2} \langle \psi | (U^\dagger + U) | \psi \rangle = \text{Re} \langle \psi | U | \psi \rangle$$



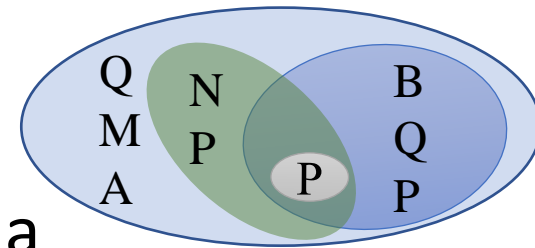
Generalized “Hadamard” Test



3rd, & Ultimate, Quantum Algorithm: Linear Algebra over exponentially large spaces



- A quantum system/computer performs matrix (linear) algebra with exponentially reduced memory resources:
 - n qubits used to **represent** exponentially large, $\mathcal{O}(\exp(n))$, matrix algebra. Exponential reduction in **memory** requirements.
 - To be efficient, a **polynomial**, $\mathcal{O}(\text{poly}(n))$, number of gate operations suffices to prepare the quantum algorithm's output.
 - This is BQP which is $\sim P$ as $\text{QMA} \sim \text{NP}$
- Main takeaway/perspective is that quantum algorithms is a venue where we can (theoretically) perform, and compute with, linear algebra in exponentially large vector spaces with only $\mathcal{O}(\text{poly}(n))$ resources.



INTEGER ARITHMETIC INTUITION

- Fundamental Theorem of Arithmetic:
 - Every positive integer $n > 1$ can be represented uniquely as $n = p_1^{n_1} p_2^{n_2} \cdots p_k^{n_k} = \prod_{i=1}^k p_i^{n_i}$
 - Can use *decompose*, and *represent*, integers as a **product** factorization.
 - Multiplicative Extensions:
 - Alternatively, complex numbers, multiplicative roots of unity.
 - E.g., with the modulo operation (e.g. $\text{mod}_5(12) = 2$) we have multiplicative groups $\mathbb{Z}_n = \mathbb{Z} / n\mathbb{Z}$. Elements represented as multiplication by generators of group cosets.
 - Represent group elements in terms of smaller set of *generating* elements.
- Numbers can also be **added**.
 - For example, every positive number can be (non-uniquely) represented as $n = \sum_{i=1}^n 1$. But this is way less efficient, especially if n is a large prime number (equipped with a succinct, and low entropy, product factorization representation)!
 - We can add (and subtract) integers to get the group \mathbb{Z}_n
- We can add **and** multiply numbers together.
 - Ex 1: $5001 \times 3001 = 5001 \times (3000 + 1) = 5000 \times 3000 + 3^2 \times 7 \times 127 = 15,008,001$
 - But then again $5001 = 3 \times 1667$ and 3001 is prime; so $15008001 = 3 \times 1667 \times 3001$ is simpler ☺
 - Ex 2: Integers: + operation, w/ inverse, and \times operation, w/o divisive inverse, == mathematical ring
- Matrices are the objects built from numbers and representing quantum operators.
 - You learned how to add, multiply, and decompose matrices in the past.
- Unitary operations/matrices (or unitaries) will be constructed by similar techniques!
 - Appropriate unitarity constraints apply.
 - $U^\dagger U = U U^\dagger = \mathbb{I}$

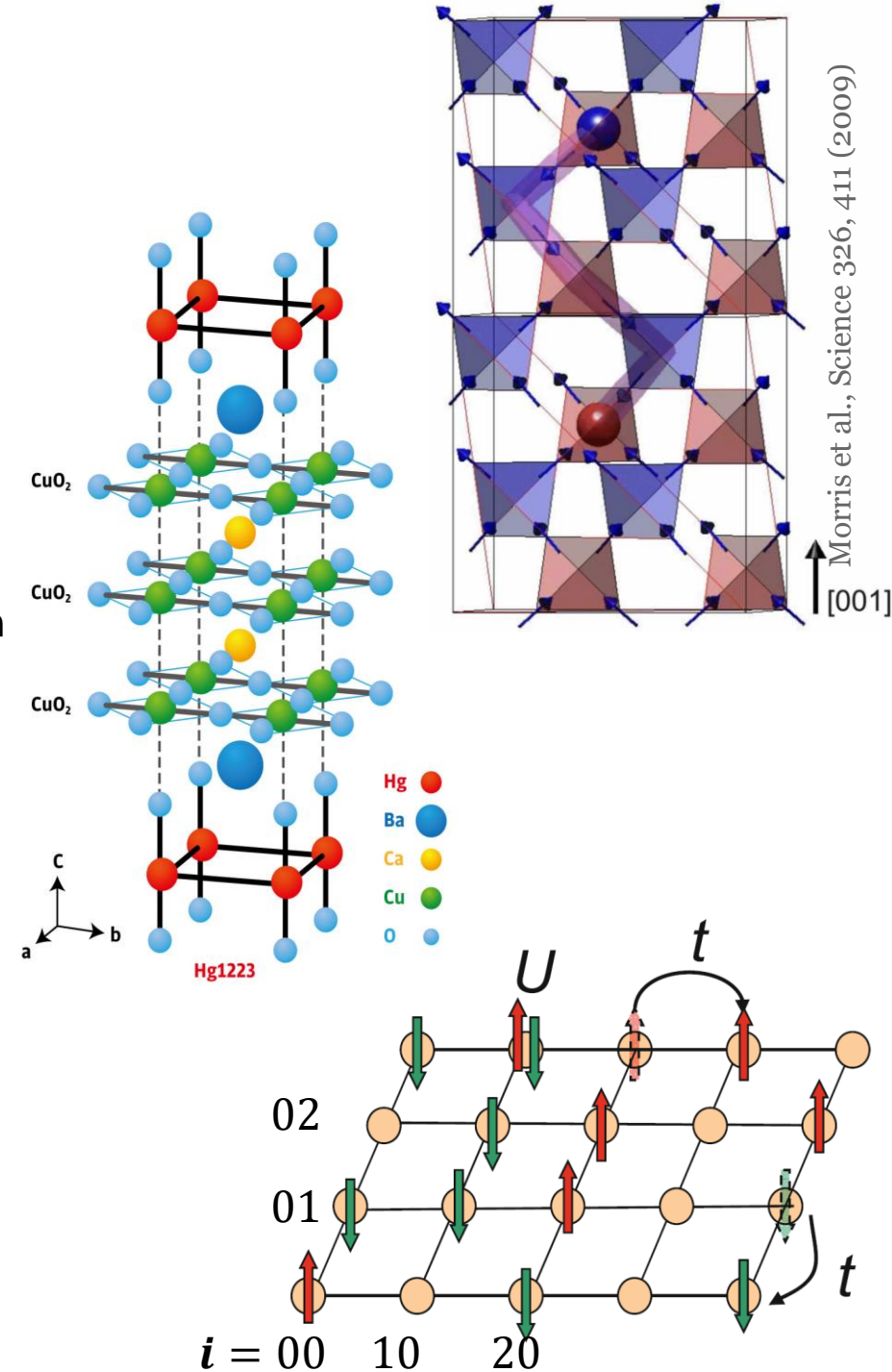
A PHYSICAL MOTIVATION

- $\approx 10^{23}$ particles condense into a discrete, symmetry-broken, crystalline configuration. Want to also study impurities, defects, etc therein.
- Negatively charged valence electrons electromagnetically interact with positively charged atomic lattice. Ab-initio Hamiltonian $\hat{H} = \hat{T} + \hat{V} + \hat{V}_{\text{ext}}$:

$$\hat{H} = -\sum_i \frac{\hbar^2 \nabla_i^2}{2m_e} + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{|\hat{r}_i - \hat{r}_j|} - \sum_{i,j} \frac{Z_j e^2}{|\hat{r}_i - \hat{R}_j|}$$

- Lattice model Hamiltonian: e.g., Hubbard model

$$\hat{H} = -t \sum_{\langle i,j \rangle, \sigma} (\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \hat{c}_{j\sigma}^\dagger \hat{c}_{i\sigma}) + U \sum_i \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\uparrow} \hat{c}_{i\downarrow}^\dagger \hat{c}_{i\downarrow} - \mu \sum_{i,\sigma} \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma}$$



(real) Time-Evolution

- Many quantum algorithms aim to simulate the time evolution of a quantum system. And this is a paradigmatic and complexity theoretically important task.
 - But even if you doing another algorithm TE is either i) an algorithmic subroutine and/or ii) being used to realize each of the algorithm's individual gates.
 - Hence, semi-tautologically, time evolution is the only quantum algorithm.

Schrodinger equation is first order differential equation:

$$i\hbar\partial_t|\Psi(t)\rangle = H(t)|\Psi(t)\rangle$$

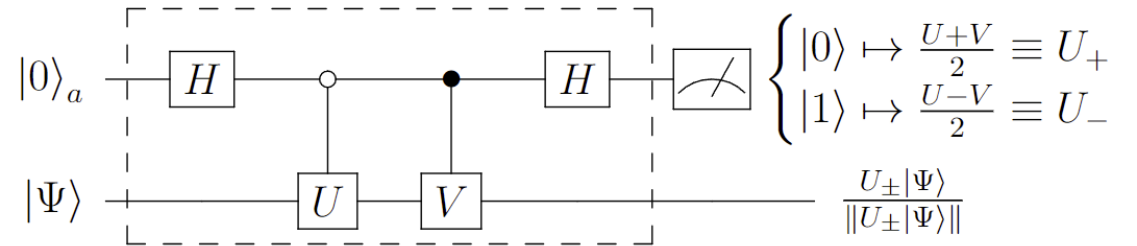
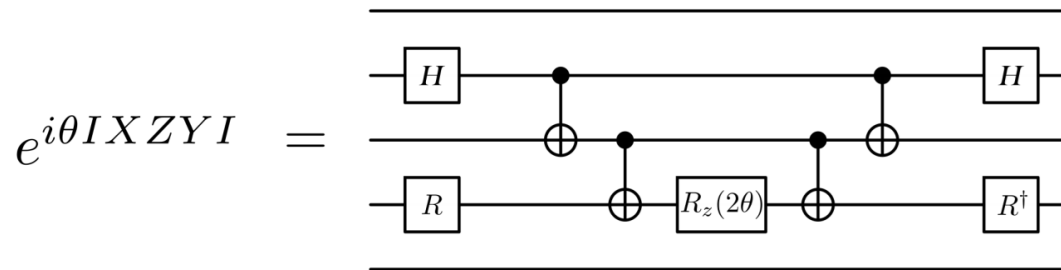
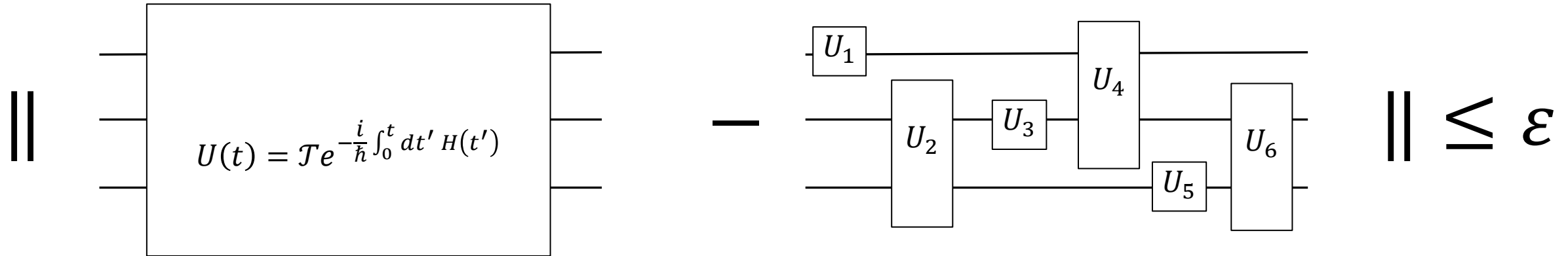
Formal solution is given by time ordered integral:

$$U(t) = \mathcal{T}e^{-\frac{i}{\hbar}\int_0^t dt' H(t')}$$

This acts as :

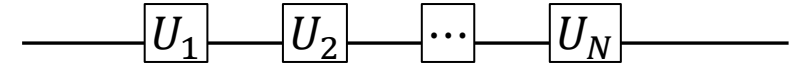
$$U(t)|\Psi(0)\rangle = |\Psi(t)\rangle$$

Unitary Synthesis: Does it factorize?



Then we can implement, e.g., $e^{i\theta XYIZ} \cdot e^{i\theta IXYZYI}$

Error Analysis



$$\varepsilon_{tot} = \varepsilon_{alg} + \varepsilon_{phys}$$

- You have ε error per gate. The gate fidelity is $F_U = 1 - \varepsilon$
- After applying N gates, the resulting fidelity is $F_{tot} = F^{\odot N} = (1 - \varepsilon)^N$.
- Can re-express in distinct limits:
 - If $|\varepsilon| \ll 1$, using binomial expansion, we have $(1 - \varepsilon)^N \approx 1 - N\varepsilon$.
 - So, if your error is very low, and you don't apply too many gates, error scales linearly with ε .
 - “Error correction” reduces $|\varepsilon_{phys}|$ to exponentially small rates. In that case, algorithmic trotter product error rates are well defined, dominant, and scaling as above.
 - I won't go into error correction (see earlier presentations and topological tutorials)
 - If $|\varepsilon| \ll 1$ but $|N\varepsilon| \gg 1$, then $(1 - \varepsilon)^N \approx e^{-\varepsilon N}$.
 - If error is too large, or low but applied too much, fidelity exponentially *decays* with εN
 - In a pre-error-corrected world, typical experimental error sources $|\varepsilon_{phys}| \sim 0.05$.
 - So, goal is $|\varepsilon| \ll 1$ and $|N\varepsilon| \ll 1$
- In most theoretical algorithms one assumes physical error $\varepsilon_{phys} \rightarrow 0^*$.
 - *Assuming some error correction mechanism.
- One then optimizes gates applied to minimize the algorithmic error $\varepsilon_{alg} \rightarrow 0$.

Arithmetic Classification of Quantum Simulation

2) Dynamics:

Hamiltonians vary greatly in their complexity. In turn, this complexity is inherited by the *time dynamics*:

- *Efficient quantum Hamiltonian simulation*: Given which an input state $|\psi(0)\rangle$, prepare $|\psi(t)\rangle = U_I(H,t) |\psi(0)\rangle$ to approximate $U_A(H,t) |\psi(0)\rangle$ with polynomial scaling resources (in system size and time) and a precision ϵ such that $\|U_I(H,t) - U_A(H,t)\| \leq \epsilon$

Product Encodings \times

- (Lie-)Trotter(-Suzuki) – approximate U as *product* of simpler unitaries $\text{poly}(N, t, \frac{1}{\epsilon})$

- Random walk on graph — sparse interactions


Block Encodings \oplus

- LCU — Factorize into a *sum* of terms $\|h\|t \log \frac{1}{\epsilon}$
- QSP — An efficient way to process information with a single ancilla $t + \log \frac{1}{\epsilon}$
- Oracles — Often *literally* defined in terms of matrix elements too obfuscated to say
- Fast Forwarding — use of underlying symmetry $\text{poly}(N) + \text{const}(t)$

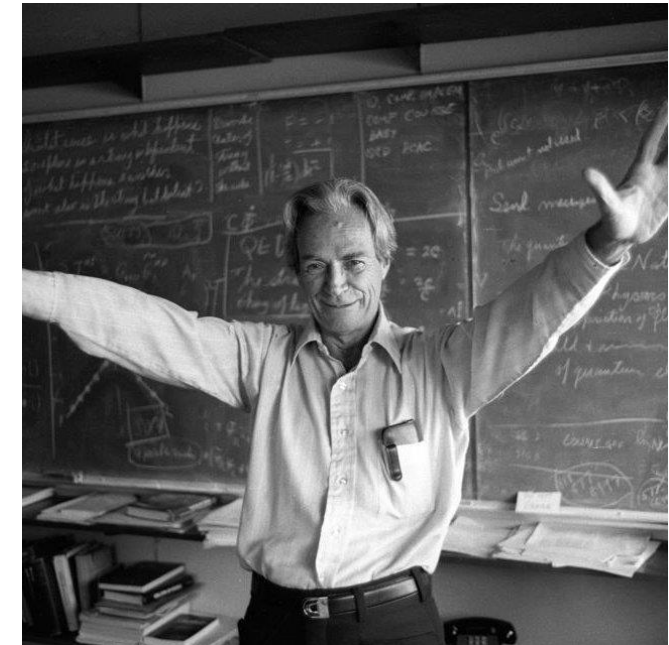
1) State Preparation

Constructively interfering into ground-, or more difficult excited- and thermal-, states is likewise generically (QMA) hard. Given $|\psi(0)\rangle$ prepare $|\psi_{Ideal}\rangle \approx |\psi_\theta\rangle = U(\theta) |\psi(0)\rangle$ such that $\| |\psi_{Target}\rangle - |\psi_\theta\rangle \| \leq \epsilon$. Often ψ is defined as being a (lowest) eigenstate corresponding to a parent Hamiltonian H .

$$H = \sum c_j \hat{h}_j$$

Exp \downarrow  \uparrow log

$$U(H, t) = \mathcal{T}e^{\frac{-it}{\hbar}H}$$



Trotter (Product) Error Analysis Continued

The Baker-Campbell-Hausdorff formula, or its related forms, imply

$$e^{t(X+Y)} = e^{tX} e^{tY} \times e^{-\frac{t^2}{2!}[X,Y]} \times e^{-\frac{t^3}{3!}\{[X,[X,Y]]+[Y,[Y,X]]\}} \times \dots = \prod_n e^{\frac{t^n}{n!}\hat{C}_n}$$

Then, $e^{t(X+Y)} = e^{tX} e^{tY} \times (\text{multiplicative error})$

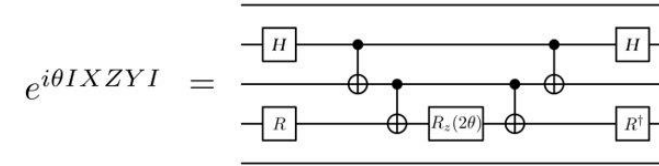
Alternatively, $e^{t(X+Y)} = e^{tX} e^{tY} + (\text{additive error})$

Where “m.e.” and “a.e.” are functions of nested commutators $([X, Y])$ of X and Y

Trotter Error for *Product* Decompositions

Existence: $U(t) = e^{-it\mathcal{H}} = \prod_{\bar{\sigma}^i \in \mathfrak{su}(2^n)} e^{i\kappa_i \bar{\sigma}^i}$ More systematic/intuitive approach?

$H = c_j \hat{p}^j$ For each individual term:



Lie-Trotter: $e^{t(A+B)} = \lim_{n \rightarrow \infty} (e^{\delta t A} e^{\delta t B})^n$ with $\delta t = \frac{t}{n}$ implies $\rightarrow e^{tA} e^{tB} = e^{t(A+B)} + O(t^2 f(A, B)) + \dots$
 * convergent series when $tA, tB < 1$

Hale. F. Trotter, *Proc. Am. Math. Phys.* 10, 545 (1959).

Suzuki 1970-90s:

m^{th} -order formulas

$$\varepsilon_{\text{Add}} \propto \mathcal{O}(t^{m+1})$$

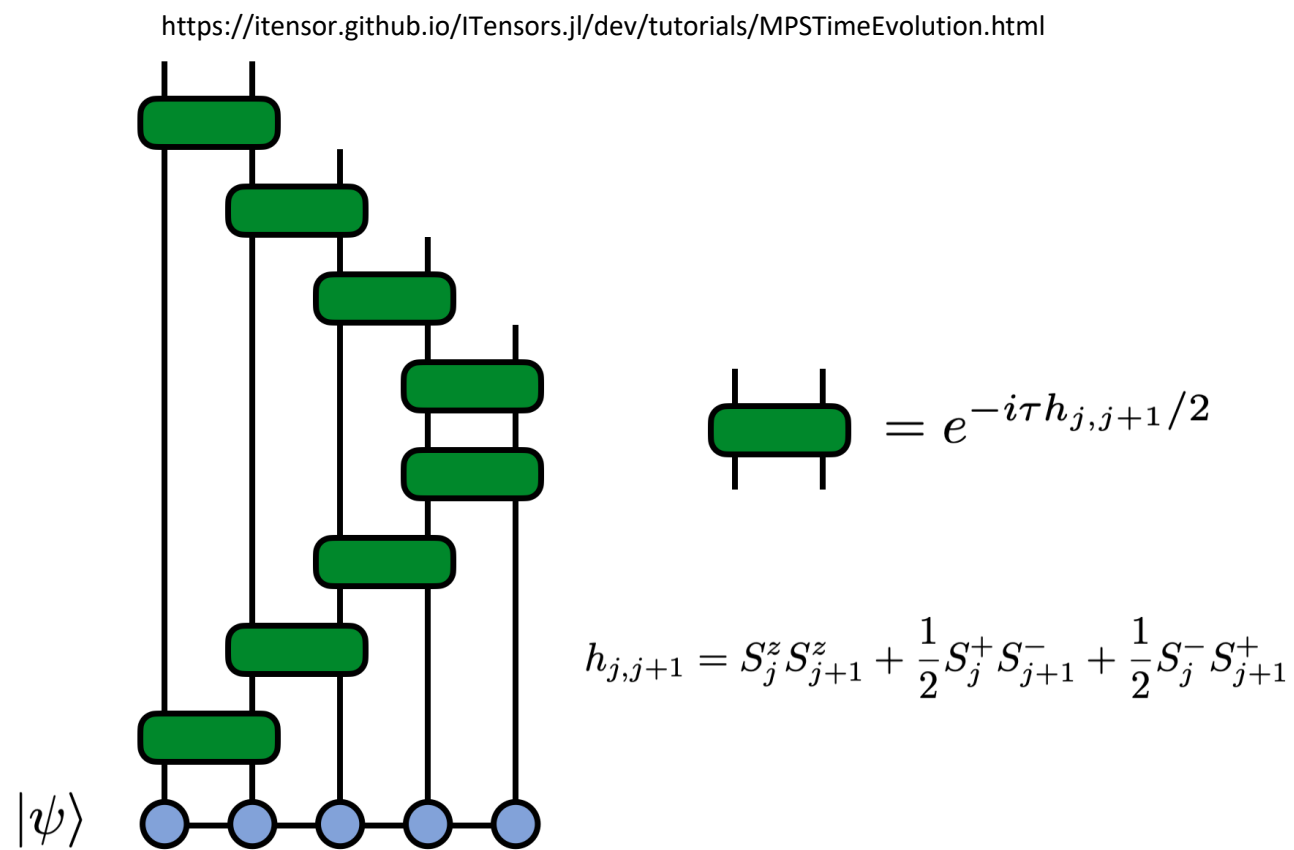
$$\exp[x(A+B)] = \left[f_m\left(\frac{A}{n}, \frac{B}{n}\right) \right]^n + O\left(\frac{x^{m+1}}{n^m}\right) \quad (1.3)$$

for the approximant $f_m(A, B)$ in (1.2). Thus we find that the convergence of our new scheme is extremely rapid for $x/n \ll 1$. This choice of decomposition is practically important in quantum Monte Carlo simulations.⁴⁻⁷

Childs, Su, et. al., Theory of Trotter Error *with Commutator Scaling*, PRX 2021

More related techniques emerging recently.

Trotter Decomposition Zoo



Tranter A, Love PJ, Mintert F, Wiebe N, Coveney PV. *Ordering of Trotterization: Impact on Errors in Quantum Simulation of Electronic Structure*. Entropy (Basel). 2019 doi: 10.3390/e21121218

Grimsley HR, Claudino D, Economou SE, Barnes E, Mayhall NJ. *Is the Trotterized UCCSD Ansatz Chemically Well-Defined?* J Chem Theory Comput. 2020 doi: 10.1021/acs.jctc.9b01083

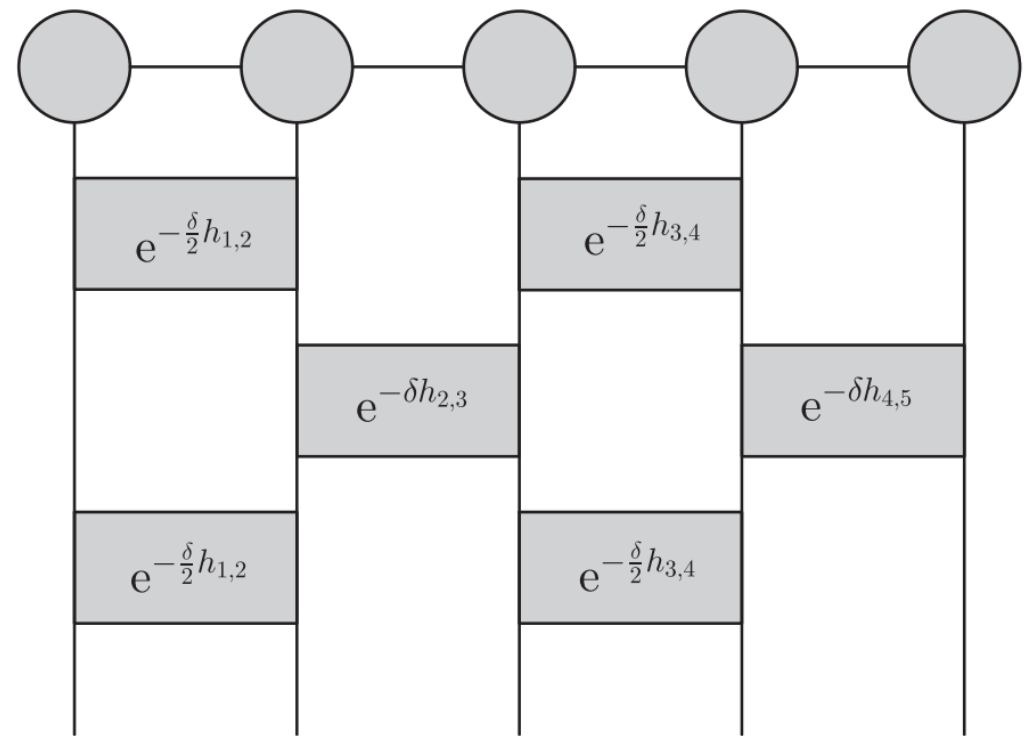
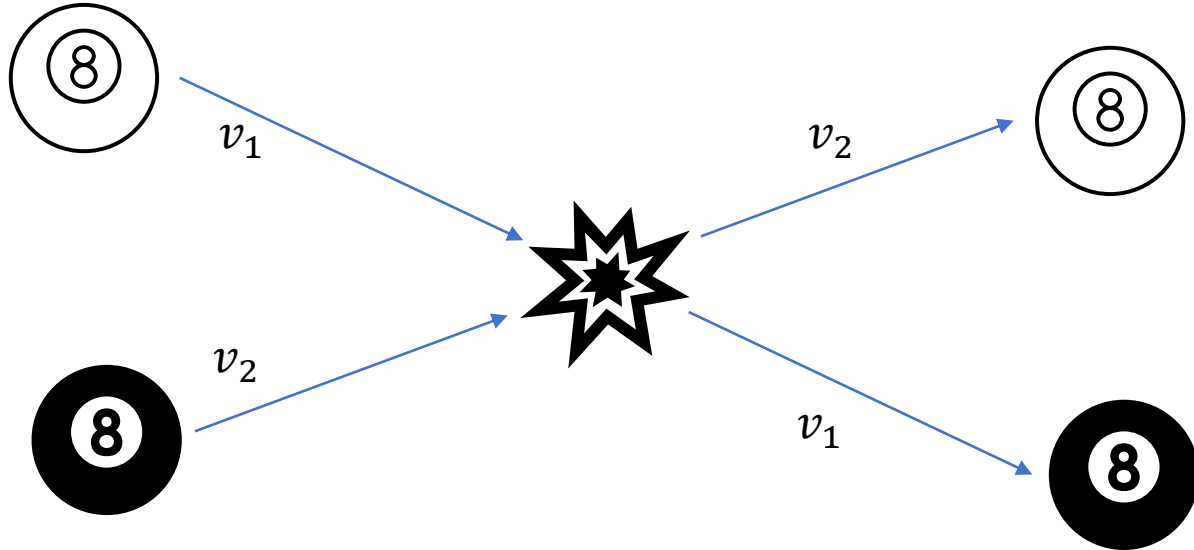


FIG. 1. Diagrammatic representation of the TEBD algorithm for a quantum lattice system of five sites with nearest-neighbor interactions. The full Hamiltonian is split into two parts, $H = H_{\text{odd}} + H_{\text{even}}$ with $H_{\text{odd}} = h_{1,2} + h_{3,4}$ and $H_{\text{even}} = h_{2,3} + h_{4,5}$. The odd and even numbered two-site local evolution operators are alternatively applied to the wave function represented by a matrix product state (MPS) [74].

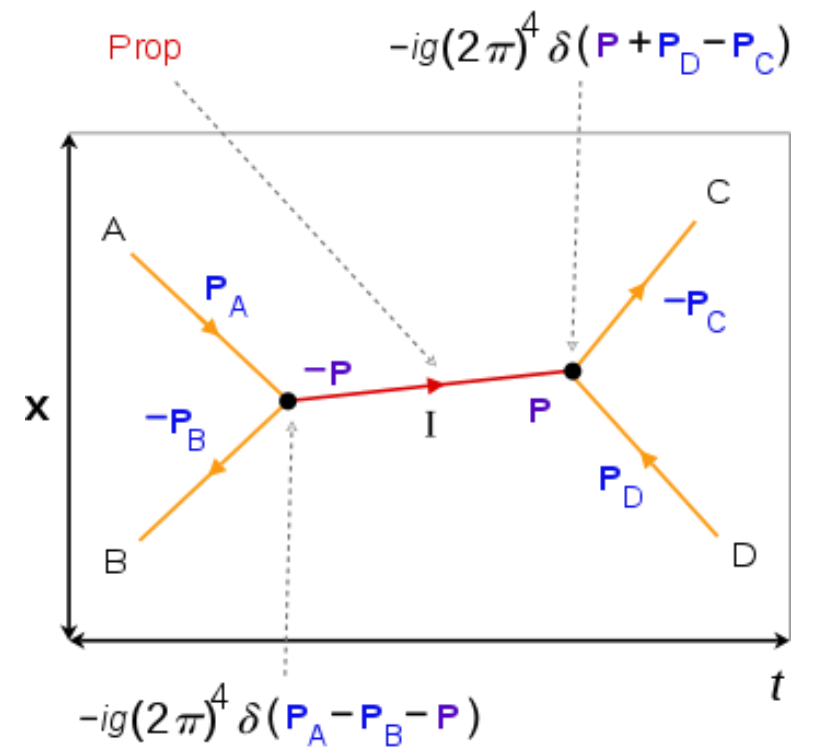


Up Next: Scattering

The inelastic scattering event on highway I-40 causing traffic today



Classical elastic scattering event with energy and momenta conserved

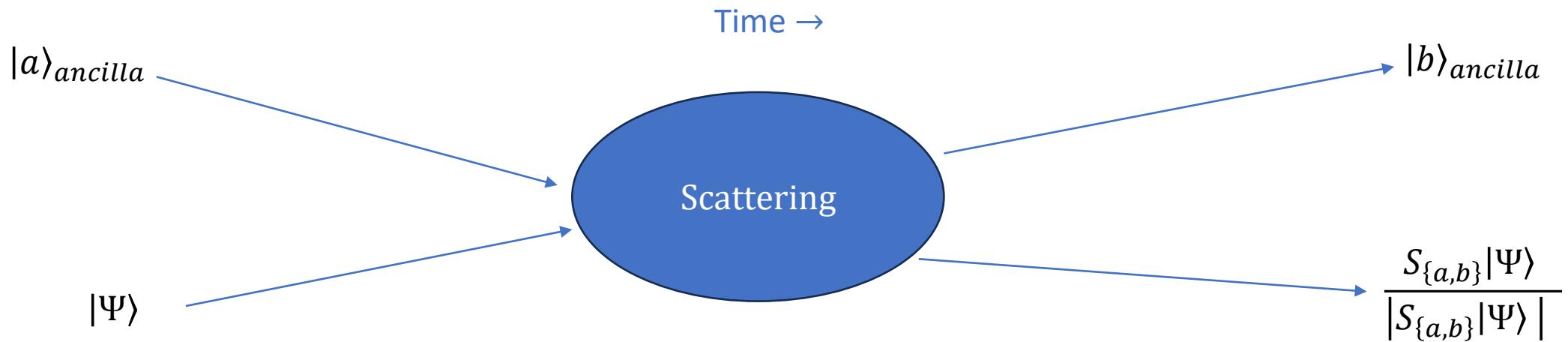
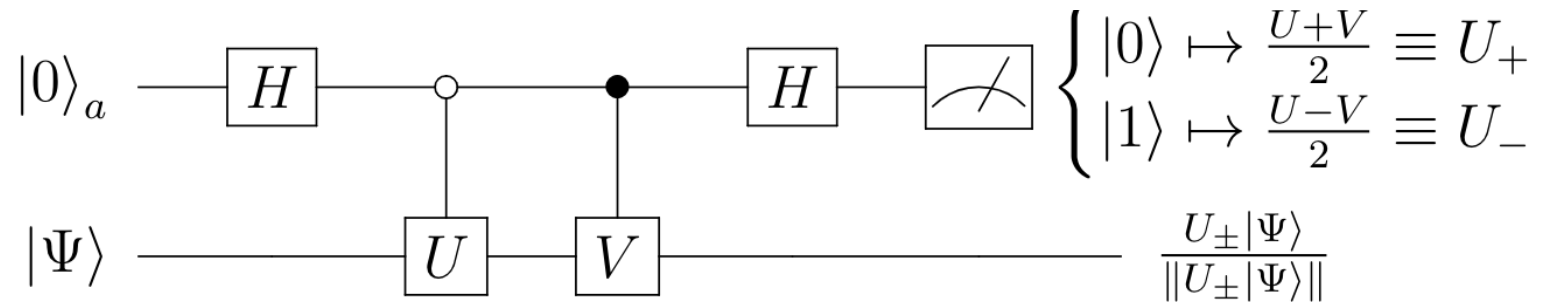


Feynman diagram depicting a quantum scattering process

4th quantum algorithm: Ancilla/Reservoir/Environment-Scattering

← time

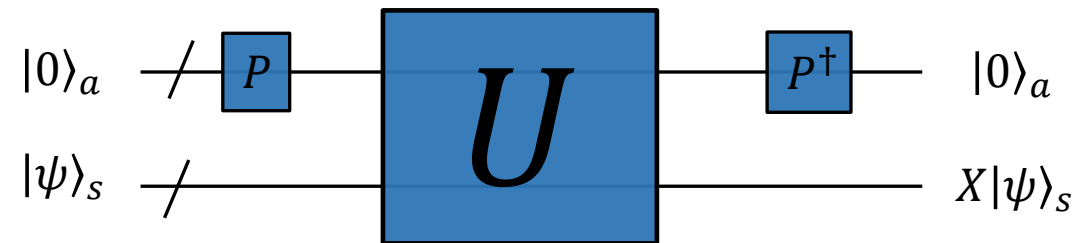
$$\begin{aligned}
 & \left\{ \begin{array}{l} \langle 0|_a H_a \\ \langle 1|_a H_a \end{array} \right\} \otimes \mathbb{1} \cdot \left(|0\rangle\langle 0|_a \otimes U + |1\rangle\langle 1|_a \otimes V \right) \left(|0\rangle\langle 0|_a \otimes \mathbb{1} + |1\rangle\langle 1|_a \otimes V \right) \cdot (H_a |0\rangle_a) \otimes \mathbb{1} \\
 &= \frac{\langle 0|_a \pm \langle 1|_a}{\sqrt{2}} \otimes \mathbb{1} \cdot \left(|0\rangle\langle 0|_a \otimes U + |1\rangle\langle 1|_a \otimes V \right) \cdot \frac{|0\rangle_a + |1\rangle_a}{\sqrt{2}} \otimes \mathbb{1} \\
 &= \frac{\langle 0|0\rangle_a U \pm \langle 1|1\rangle_a V}{2} = \frac{U \pm V}{2} \equiv U_{\pm}.
 \end{aligned}$$



(Additive matrix-element) Block Encodings

- An operator X is *block encoded* in a *standard form* (Low, Chuang 2019) if \exists a unitary-oracle U such that
- $(\langle p|_a \otimes \mathbb{1}_s) U(|p\rangle_a \otimes \mathbb{1}_s) = X$
- U acts on $\mathcal{H}_a \otimes \mathcal{H}_s$ where $a(s)$ refers to the ancilla (system) and we can prepare $|p\rangle_a = P|0\rangle_a$

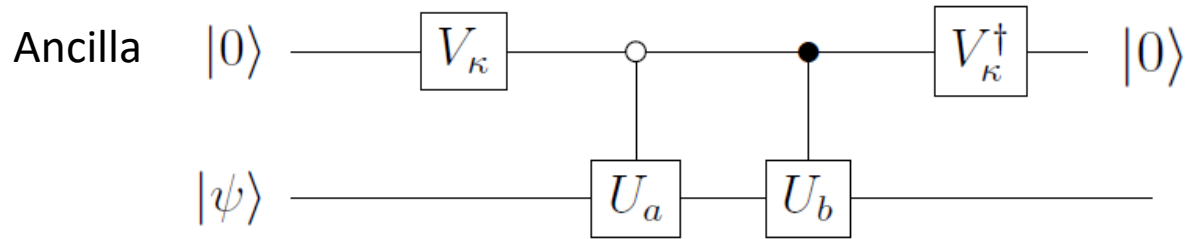
$$U = \begin{pmatrix} X & \cdot \\ \cdot & \cdot \end{pmatrix}$$



- LCU (next slide)
- Quantum walk, sparse Hamiltonian (Childs)
- Quantum signal processor (Low, Chuang 2019)
 - These algorithms provide an exponential improvement in precision $\frac{1}{\varepsilon} \rightarrow \frac{1}{\log(\varepsilon)}$.
 - From convergence of Taylor series $e^{iHt} = \sum_{k=0}^{k=\Lambda} \frac{(iHt)^k}{k!} + \varepsilon$

Linear combination of unitaries (LCU)*

Example: sum of two unitaries



Quantum circuit applying an operator $U = \kappa U_a + U_b$ given a measurement outcome of zero.

Special cases

$$V_\kappa := \begin{pmatrix} \sqrt{\frac{\kappa}{\kappa+1}} & \frac{-1}{\sqrt{\kappa+1}} \\ \frac{1}{\sqrt{\kappa+1}} & \sqrt{\frac{\kappa}{\kappa+1}} \end{pmatrix}$$

$$\begin{aligned} c_q^\dagger &\sim X_q + i Y_q \\ c_q &\sim X_q - i Y_q \end{aligned}$$

[*] A. M. Childs and N. Wiebe, Quantum Infor. Comput. **12**, 901 (2012).

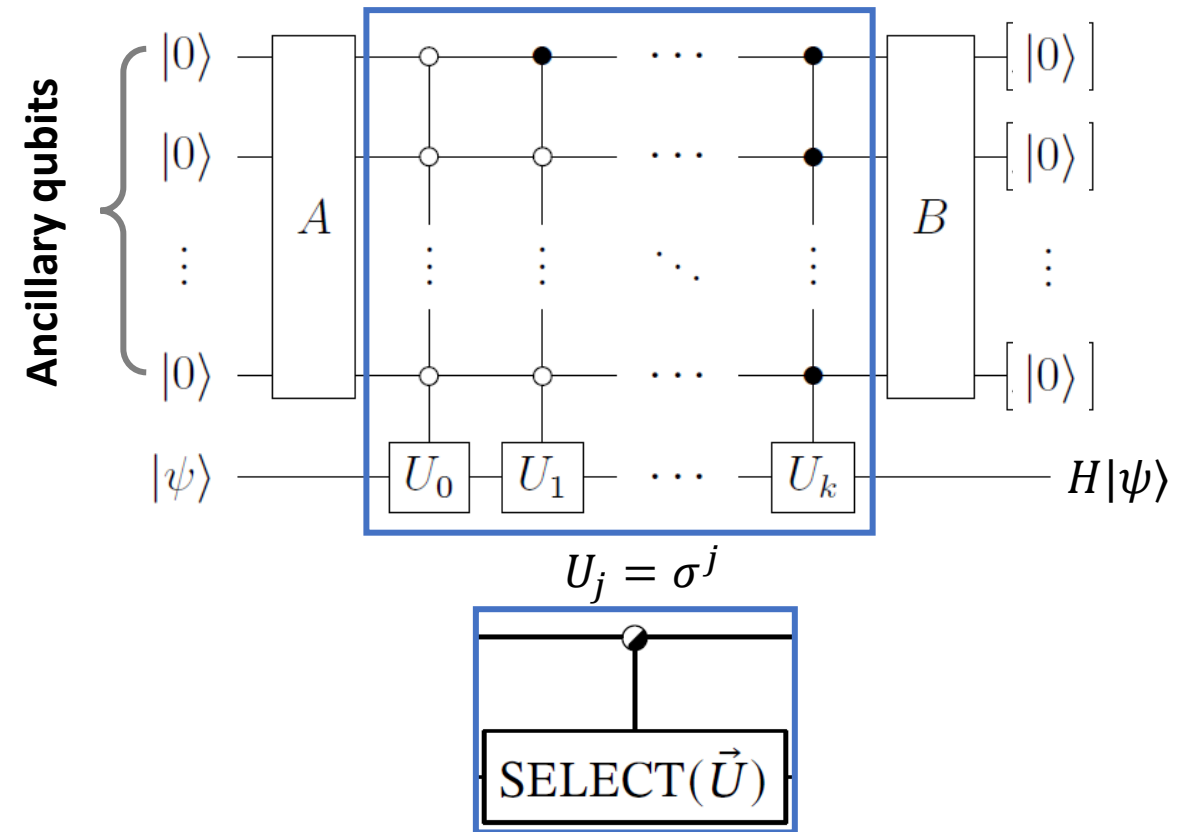
$$\mathcal{H} = \sum_j h_j \sigma^j$$

$$A = \sum_{j=1,\dots,d} \sqrt{\frac{h_j}{\|h\|}} |j\rangle\langle 0|$$

$$\text{SEL} = \sum_{j=1,\dots,d} |j\rangle\langle j| \otimes \sigma^j \quad U_{B.E.} = \begin{pmatrix} \mathcal{H} & \cdot \\ \cdot & \cdot \end{pmatrix}$$

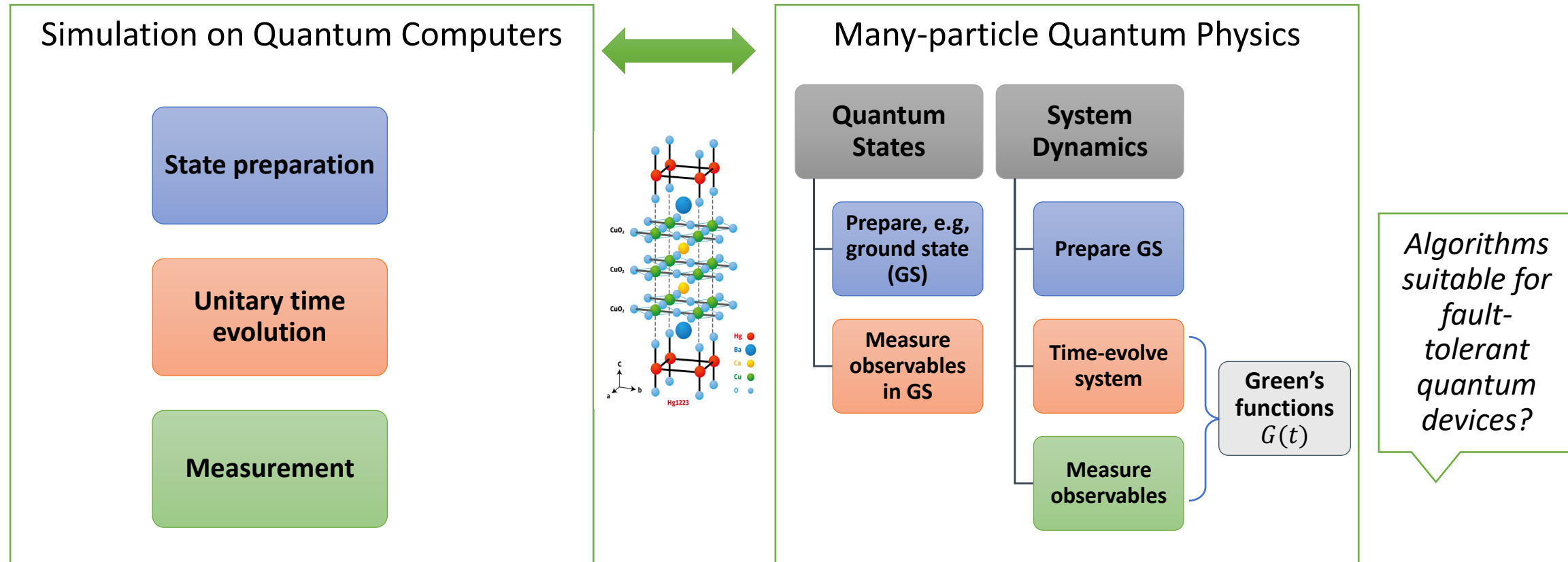
LCU: sum of many unitaries

$$B = A^{-1}$$



$$\langle 0 \cdots 0 | U_{B.E.} (| 0 \cdots 0 \rangle_A \otimes |\psi\rangle) = H|\psi\rangle$$

General workflow for simulating quantum many-particle systems



How To Evaluate My Correlation Function?

LCU expansion

- Measuring single-particle correlation function $\langle c_q^\dagger c_{q+1} \rangle$
- Modulo the fermionic \mathbb{Z}_2 phases, the field operators are $c_q^\dagger \sim X_q + i Y_q$; $c_q \sim X_q - i Y_q$
 - 2 term LCU
- $\langle c_q^\dagger c_{q+1} \rangle \propto \langle X_q X_{q+1} + Y_q Y_{q+1} + i (Y_q X_{q+1} - X_q Y_{q+1}) \rangle$
 - 4 term LCU

Quantum Sum

Linear expansion

- $\langle c_q^\dagger c_{q+1} \rangle \sim \langle X_q X_{q+1} \rangle + \langle Y_q Y_{q+1} \rangle + +i (\langle Y_q X_{q+1} \rangle - \langle X_q Y_{q+1} \rangle)$
- Measure each term individually and sum together *classically*

Classical Sum

Projection, $\hat{F} = e^{-\frac{1}{2}t^2\hat{H}^2}$, and Resolvent, $\hat{R} = \frac{1}{\omega - \hat{H}}$, operators

1. Prepare ground state (**GS**) by $\hat{F}|\psi_{\text{trial}}\rangle \approx |\psi_{\text{GS}}\rangle$

$$= |E_0\rangle\langle E_0| + \sum_{n \neq 0} e^{-\frac{1}{2}(E_n - E_0)^2 \tau^2} |E_n\rangle\langle E_n|$$

- Requires: GS energy estimate to shift the spectrum as $\hat{H} - E_0$
- \hat{F} nonunitary: implement via LCU of the Fourier transform (for Gaussian, also called Hubbard-Stratonovich transform)

2. Dynamics:

$$G_{ij}(\omega) = \int_0^\infty dt G_{ij}(t) e^{i(\omega + i\Gamma)t} = \langle \psi_{\text{GS}} | \hat{c}_i (\omega + i\Gamma - \hat{H})^{-1} \hat{c}_j^\dagger | \psi_{\text{GS}} \rangle$$

- Direct computation of frequency-domain Green's function (G)
- $\hat{R} = (\omega + i\Gamma - \hat{H})^{-1}$ nonunitary: implement via LCU of the Fourier-Laplace transform

LCU unified quantum framework with time-evolution oracle

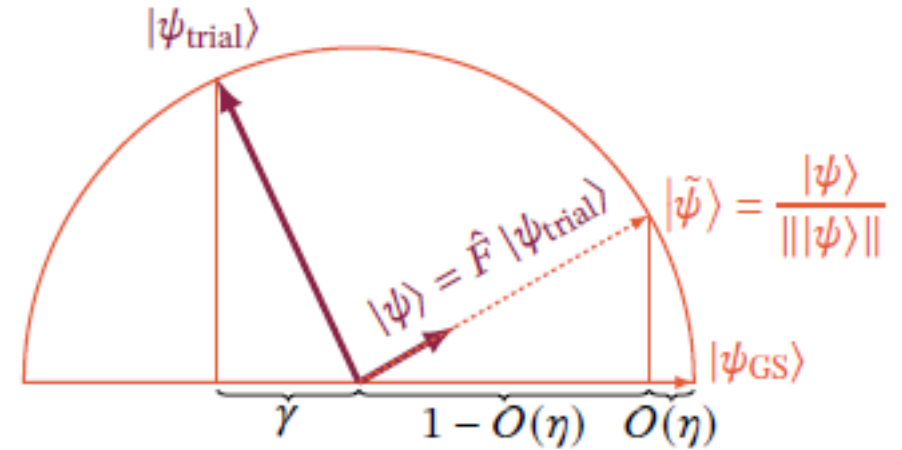
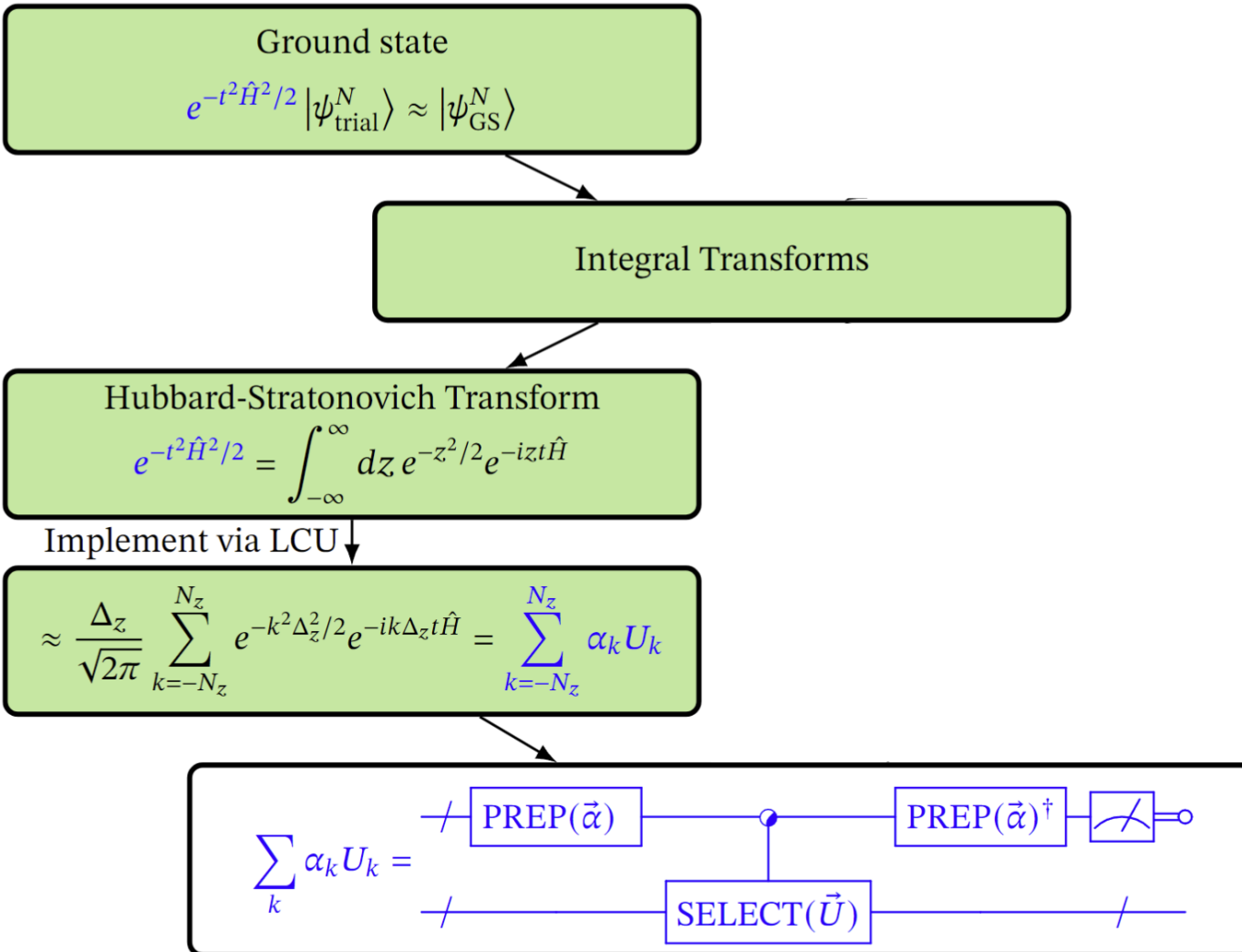
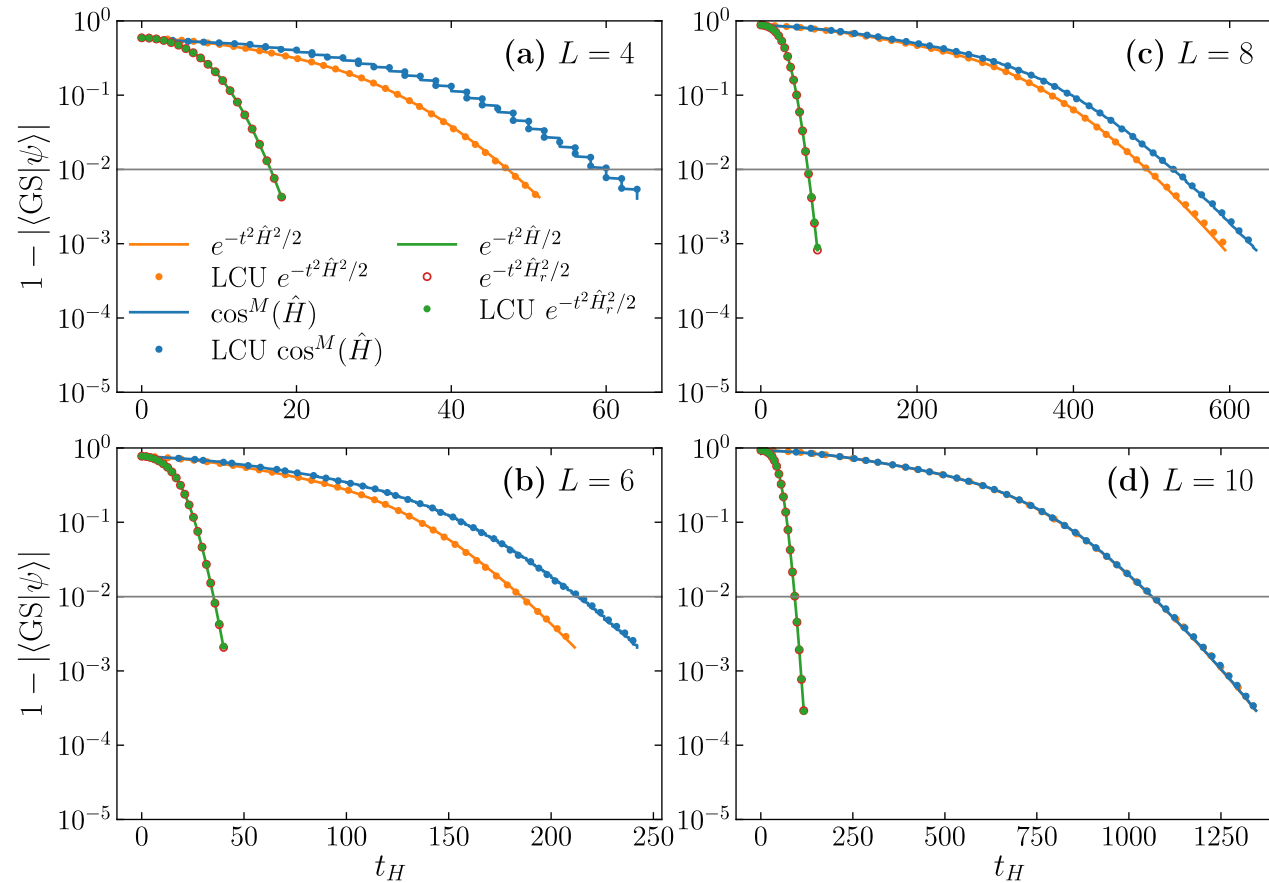


Fig. 1: Illustration of the projective ground state preparation algorithm. $\hat{F} = e^{-t^2 \hat{H}^2 / 2}$ and the error on the fidelity of the prepared ground $1 - |\langle \psi_{\text{GS}} | \tilde{\psi} \rangle| = O(\eta)$.

Results and complexity scaling

- Projection operator $\hat{F} = e^{-\frac{1}{2}t^2\hat{H}^2}$
 - $O\left(\frac{\alpha}{\gamma\Delta} \log \frac{1}{\gamma\eta}\right)$ queries to the time evolution oracle
 - $O\left(\log \frac{1}{\Delta} + \log \log \frac{1}{\gamma\eta}\right)$ ancilla qubits
 - α is L_1 norm of coefficients in LCU
 - Δ is a lower bound on the spectral gap Δ_s of the system
 - γ is a lower bound on the overlap of the trial state and true GS
 - η is the additive error in the state vector
- Resolvent operator $\hat{R} = (\omega + i\Gamma - \hat{H})^{-1}$
 - $O\left(\frac{1}{\Gamma^2} \log \frac{2}{\Gamma\epsilon}\right)$ queries to the time evolution oracle
 - $O\left(\log \frac{1}{\Gamma\epsilon} + \log \log \frac{2}{\Gamma\epsilon}\right)$ ancilla qubits
 - Γ is the artificial broadening
 - ϵ is the allowable error in constructing the resolvent

Isotropic, ferromagnetic Heisenberg model



L-site chain (OBC)

$$\hat{H} = \sum_{j=1}^L \hat{H}_{j,j+1}$$

where

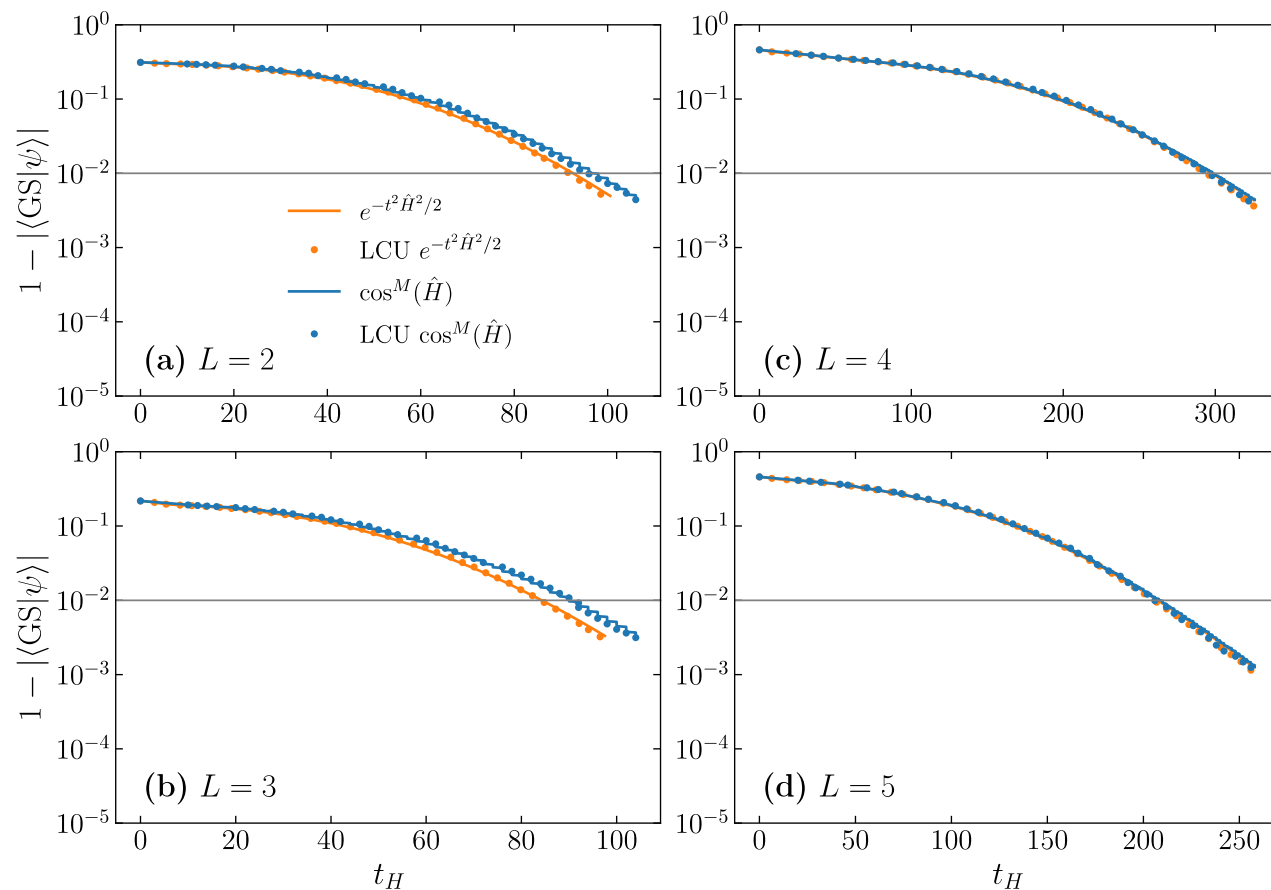
$$\hat{H}_{j,j+1} = -\frac{1}{4}(X_j X_{j+1} + Y_j Y_{j+1}) + \frac{1}{4}(1 - Z_j Z_{j+1})$$

Trial State: $|1 \dots 10 \dots 0\rangle$

A. N. Chowdhury and R. D. Somma, Quantum Information and Computation
17, 41 (2017)

Ge, Tura, and Cirac, J. Math. Phys. 60, 022202 (2019)

Hubbard Model



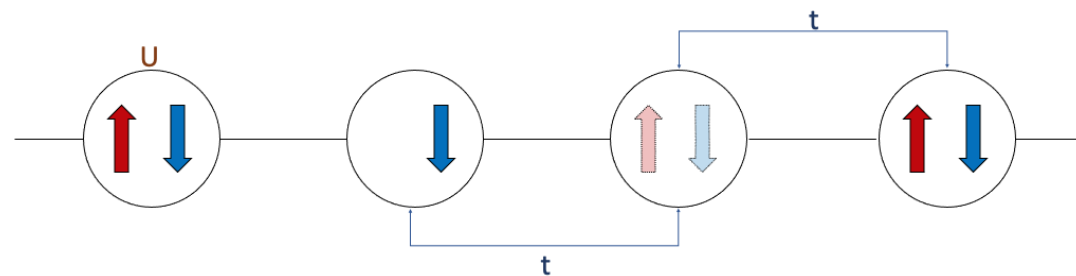
We want to implement

$$e^{-\frac{t^2}{2} \hat{H}^2} |\psi_{\text{trial}}\rangle \approx |\psi_{\text{GS}}\rangle$$

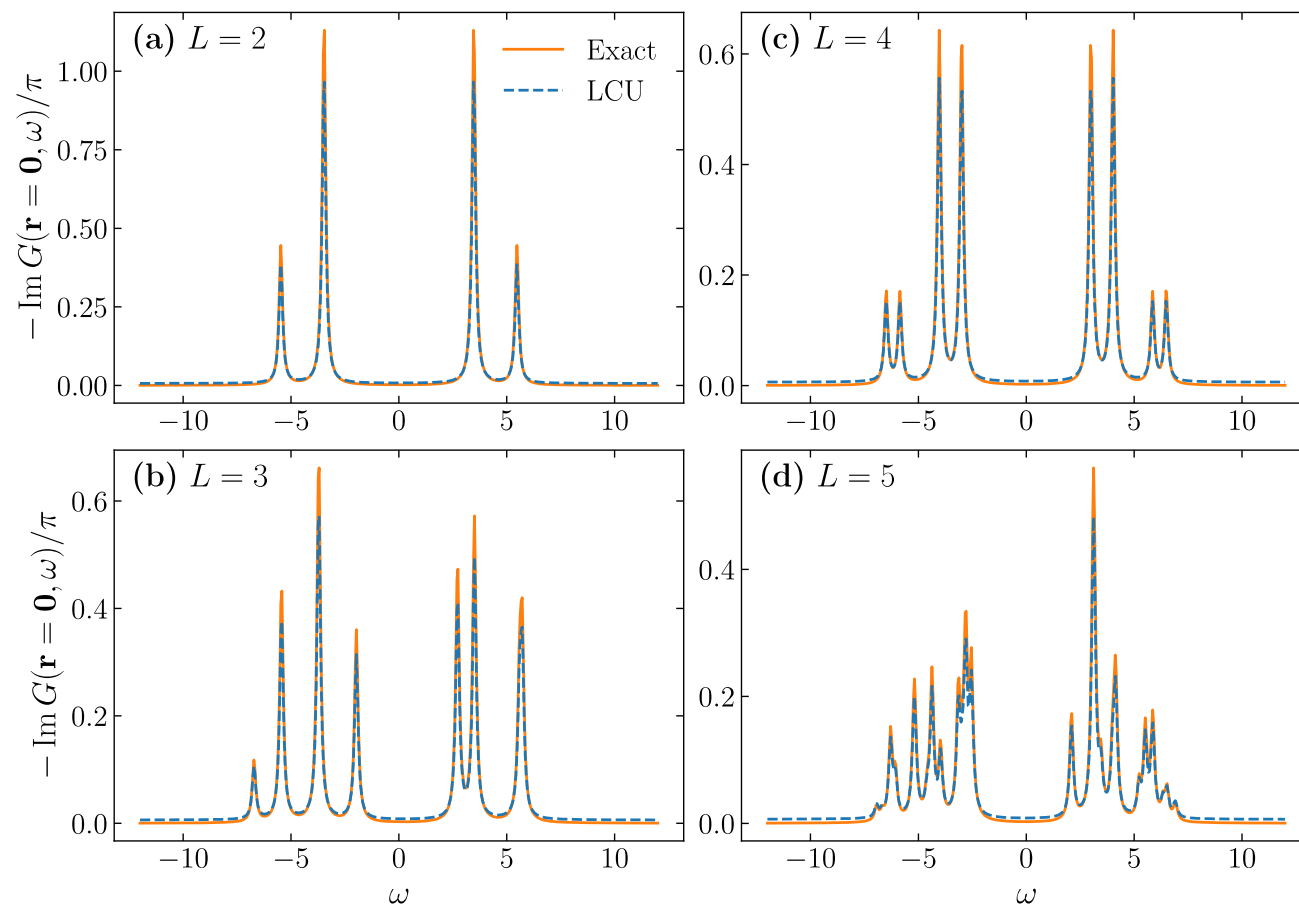
Trial State:

- $|\uparrow_0 \downarrow_1 \cdots \uparrow_{L-1} \downarrow_L\rangle, L \text{ even}$
- $|\uparrow_0 \downarrow_1 \cdots \uparrow_{L-1}\rangle, L \text{ odd}$

$$\hat{H}_{\text{Hubbard}} = -t \sum_{\langle ij \rangle, \sigma} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$



Hubbard Model Dynamics



$$G_{ij}^{(e)}(z) = \langle \psi_{\text{GS}} | \hat{c}_i \frac{1}{\omega + i\Gamma - \hat{H}} \hat{c}_j^\dagger | \psi_{\text{GS}} \rangle$$

$$(\omega + i\Gamma - \hat{H})^{-1} \rightarrow -i \int_0^\infty dt e^{i(\omega + i\Gamma - \hat{H})t}$$

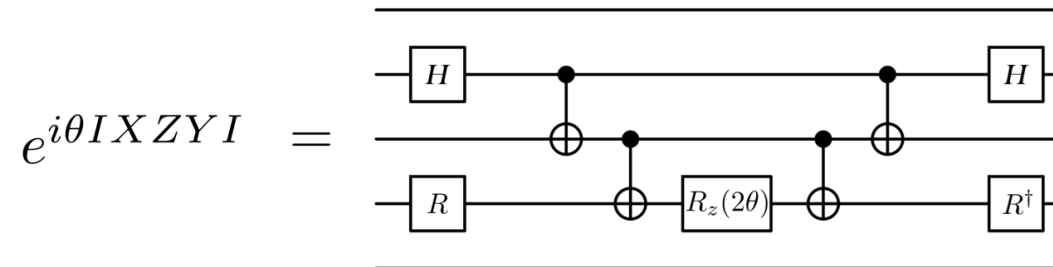
$$\approx -i \sum_{k=0}^{N_c} \Delta_t e^{i(\omega + i\Gamma - \hat{H})k\Delta_t}$$

ALGEBRAIC PRODUCT DECOMPOSITIONS

Simulation of a time independent Hamiltonian: $\mathcal{H} = \sum_j h_j \sigma^j$

Time evolution operator is: $U(t) = e^{-it\mathcal{H}} = \prod_{\bar{\sigma}^i \in \mathfrak{su}(2^n)} e^{i\kappa_i \bar{\sigma}^i}$

Single exponential circuit is given as:



Two main issues:

1) $4^n - 1$ many generators ☹️

2) How to determine angles? κ_i

Hamiltonian Algebra

- We don't have to work in full $\mathfrak{su}(2^n)$

$$\mathcal{H} = \sum_j h_j \sigma^j$$

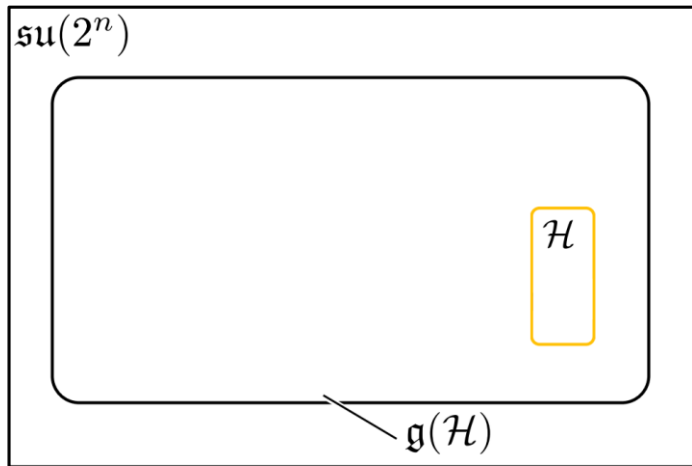
$$U(t) = e^{-it\mathcal{H}} = \prod_{\bar{\sigma}^i \in \mathfrak{su}(2^n)} e^{i\kappa_i \bar{\sigma}^i}$$

Hamiltonian Algebra

- We don't have to work in full $\mathfrak{su}(2^n)$
- Get the closure of the Pauli strings within the Hamiltonian under commutation i.e. the “Hamiltonian algebra” $\mathfrak{g}(\mathcal{H})$

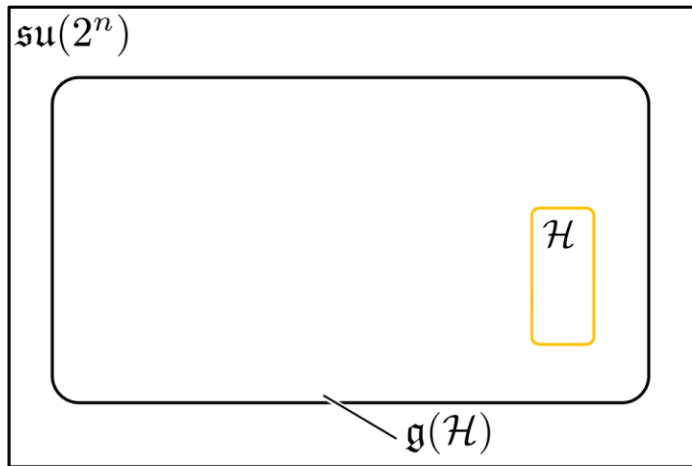
$$\mathcal{H} = \sum_j h_j \sigma^j$$

$$U(t) = e^{-it\mathcal{H}} = \prod_{\bar{\sigma}^i \in \mathfrak{su}(2^n)} e^{i\kappa_i \bar{\sigma}^i}$$



Hamiltonian Algebra

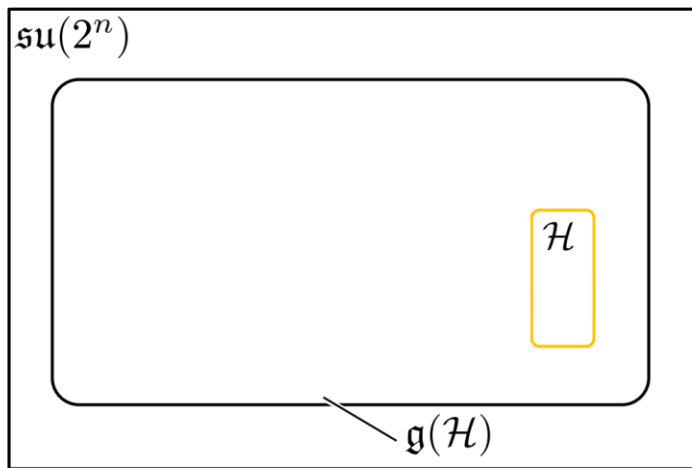
- We don't have to work in full $\mathfrak{su}(2^n)$
- Get the closure of the Pauli strings within the Hamiltonian under commutation i.e. the “Hamiltonian algebra” $\mathfrak{g}(\mathcal{H})$



$$\mathcal{H} = \sum_j h_j \sigma^j$$
$$U(t) = e^{-it\mathcal{H}} = \prod_{\substack{\bar{\sigma}^i \in \mathfrak{su}(2^n) \\ \bar{\sigma}^i \in \mathfrak{g}(\mathcal{H})}} e^{i\kappa_i \bar{\sigma}^i}$$

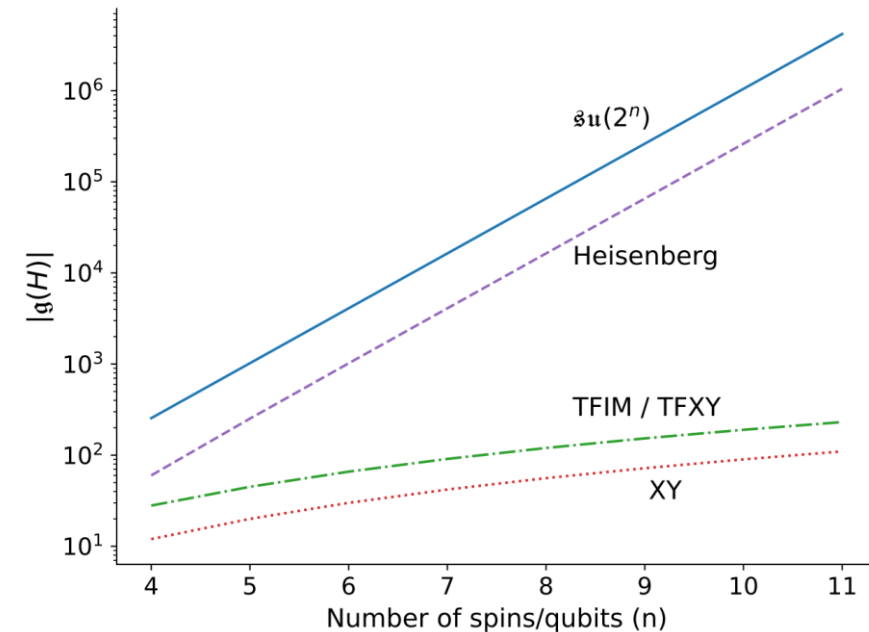
Hamiltonian Algebra

- We don't have to work in full $\mathfrak{su}(2^n)$
- Get the closure of the Pauli strings within the Hamiltonian under commutation i.e. the “Hamiltonian algebra” $\mathfrak{g}(\mathcal{H})$



$$\mathcal{H} = \sum_j h_j \sigma^j$$

$$U(t) = e^{-it\mathcal{H}} = \prod_{\substack{\bar{\sigma}^i \in \mathfrak{su}(2^n) \\ \bar{\sigma}^i \in \mathfrak{g}(\mathcal{H})}} e^{i\kappa_i \bar{\sigma}^i}$$



Cartan Decomposition and KHK Theorem

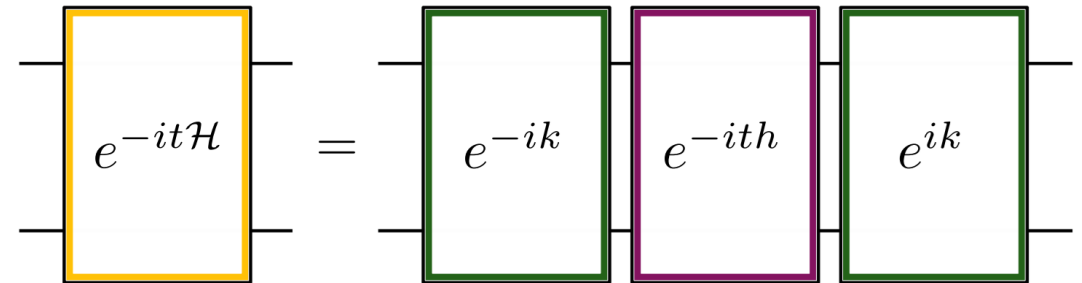
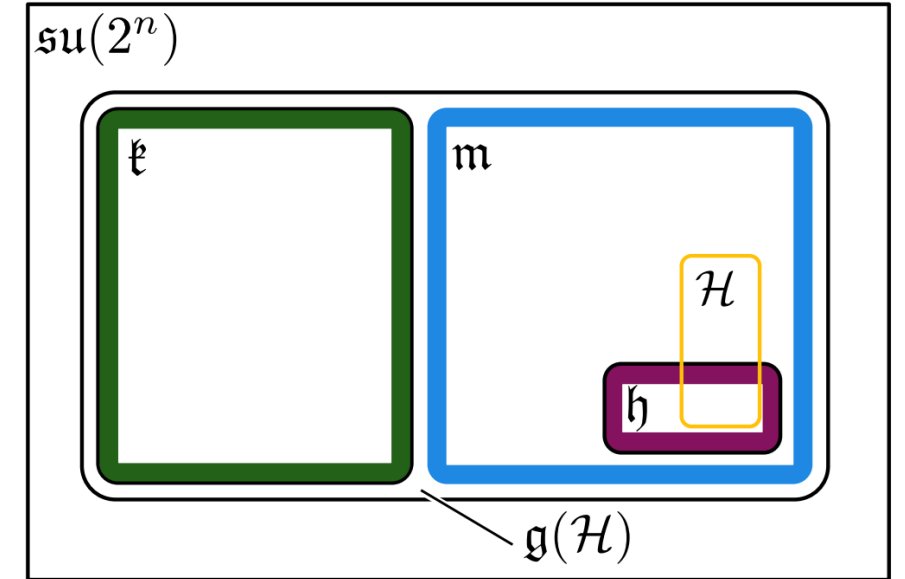
Definition 1 Consider a compact semi-simple Lie subgroup $G \subset SU(2^n)$, which has a corresponding Lie subalgebra \mathfrak{g} . A **Cartan decomposition** on \mathfrak{g} is defined as an orthogonal split $\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{m}$ satisfying

$$[\mathfrak{k}, \mathfrak{k}] \subset \mathfrak{k} \quad [\mathfrak{m}, \mathfrak{m}] \subset \mathfrak{k} \quad [\mathfrak{k}, \mathfrak{m}] = \mathfrak{m} \quad (4)$$

and is referred as $(\mathfrak{g}, \mathfrak{k})$. **Cartan subalgebra** of this decomposition is defined as one of the maximal Abelian subalgebras of \mathfrak{m} , and denoted as \mathfrak{h} .

Theorem 1 Given a Cartan decomposition $\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{m}$, for any element $\mathcal{H} \in \mathfrak{m}$ there exist a $K \in e^{\mathfrak{k}}$ and $h \in \mathfrak{h}$ such that

$$\mathcal{H} = KhK^\dagger \quad (5)$$



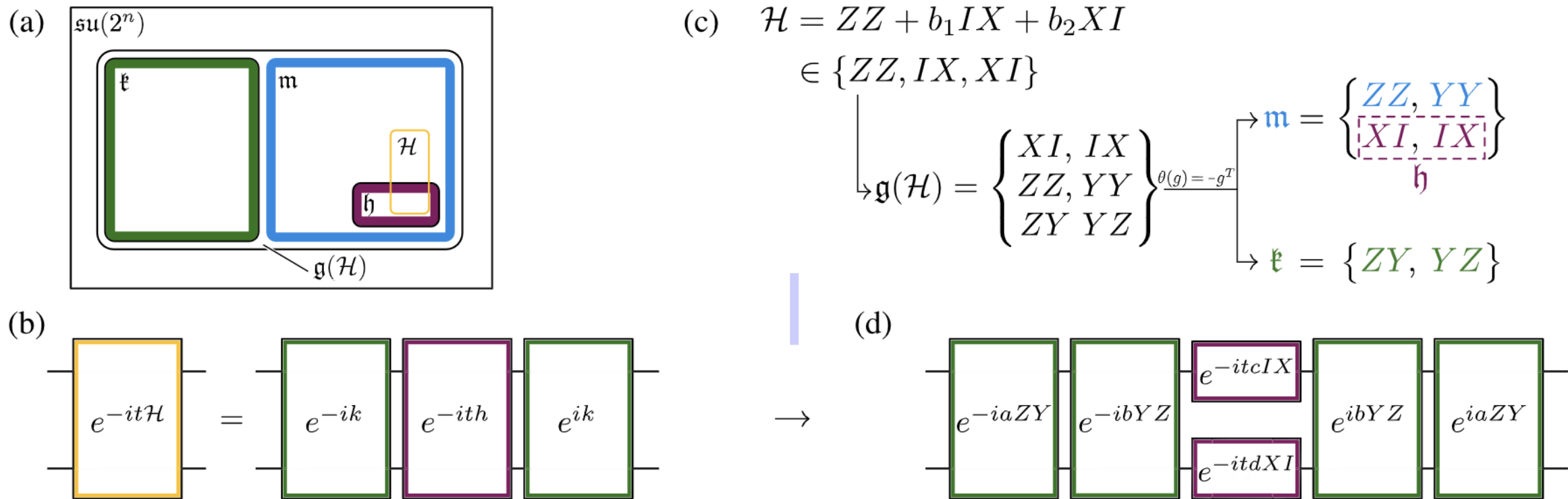


FIG. 2. (a) Schematic relationship of the Hamiltonian algebra $\mathfrak{g}(\mathcal{H})$ and its partitioning into a subalgebra \mathfrak{k} , its complement \mathfrak{m} , and the Cartan subalgebra \mathfrak{h} . (b) KHK decomposition (Theorem 1) applied to a time-evolution operator generated by an element of \mathfrak{m} . (c) Hamiltonian algebra $\mathfrak{g}(\mathcal{H})$ for the two-site TFIM and the Cartan decomposition generated by the involution $\theta(\mathfrak{g}) = -\mathfrak{g}^T$. Here we list the bases that span $\mathfrak{g}(\mathcal{H})$ and its Cartan decomposition. (d) Decomposed time evolution for the two-site TFIM.

Determining Parameters

Have $H \in \mathfrak{m}$, and consider the following function

$$f(K) = \langle K v K^\dagger H \rangle$$

where

$$K = e^{\theta_1 k_1} e^{\theta_2 k_2} \dots e^{\theta_{n_k} k_{n_k}}$$

$$v = h_1 + \pi h_2 + \pi^2 h_3 + \dots + \pi^{n_h-1} h_{n_h}$$

Then for any local minimum or maximum of the function f denoted by K_0 will satisfy

$$K_0^\dagger H K_0 \in \mathfrak{h}$$

Determining Parameters

Have $H \in \mathfrak{m}$, and consider the following function

$$f(K) = \langle KvK^\dagger, \mathcal{H} \rangle$$

where

$$K = e^{\theta_1 k_1} e^{\theta_2 k_2} \dots e^{\theta_{n_k} k_{n_k}}$$

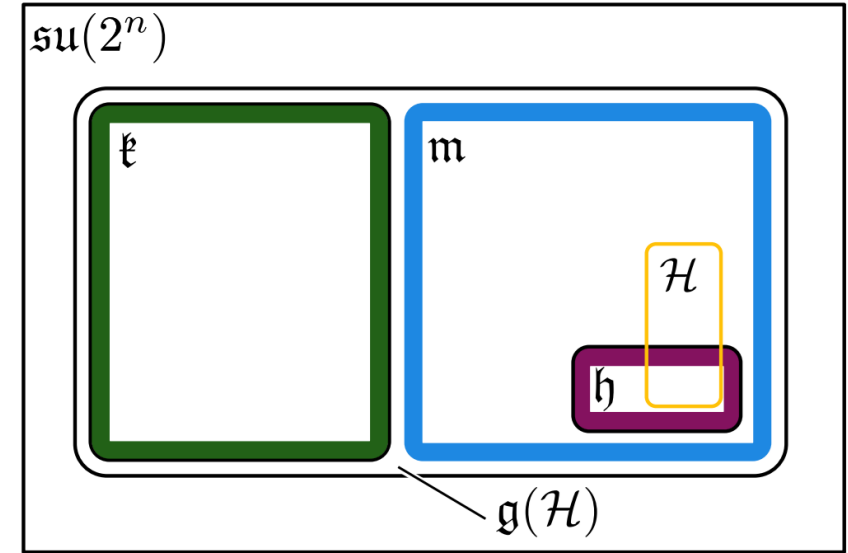
$$v = h_1 + \pi h_2 + \pi^2 h_3 + \dots + \pi^{n_h-1} h_{n_h}$$

Then for any local minimum or maximum of the function f denoted by K_0 will satisfy

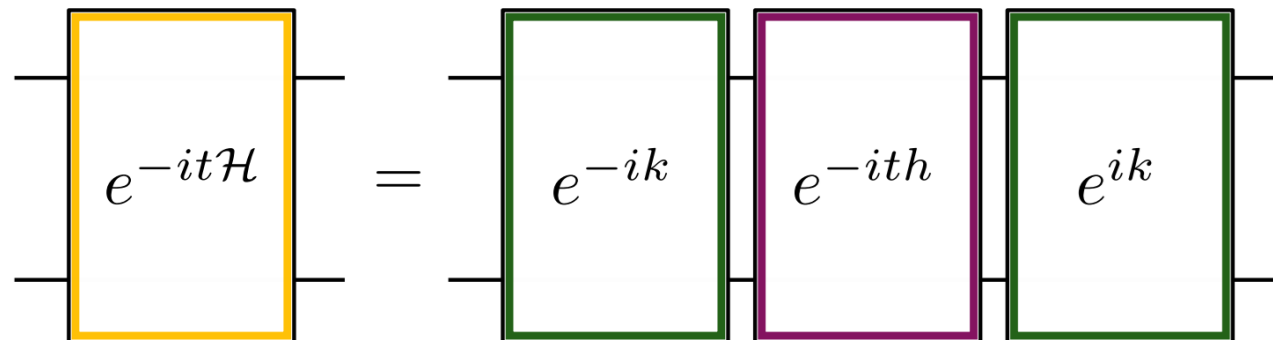
$$K_0^\dagger H K_0 \in \mathfrak{h}$$

Algorithm

- 1) Generate Hamiltonian algebra $\mathfrak{g}(\mathcal{H})$
- 2) Find a Cartan decomposition such that \mathcal{H} is in \mathfrak{m}
- 3) Fit parameters via minimizing $f(K)$
- 4) Build the circuit using K and h
- 5) Then simulate for any time you want!



$$f(K) = \langle K v K^\dagger, \mathcal{H} \rangle$$



Application: Anderson Localization

- We apply our method to the following Hamiltonian for $n = 10$, with random magnetic fields to the initial state $|\psi\rangle = |\downarrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\rangle$:

$$H = \sum_{j=1}^{n-1} (X_j X_{j+1} + Y_j Y_{j+1}) + \sum_{j=1}^n B_j Z_j$$

- In the presence of, e.g. a random magnetic field, the spin excitations are Anderson localized*. We measure

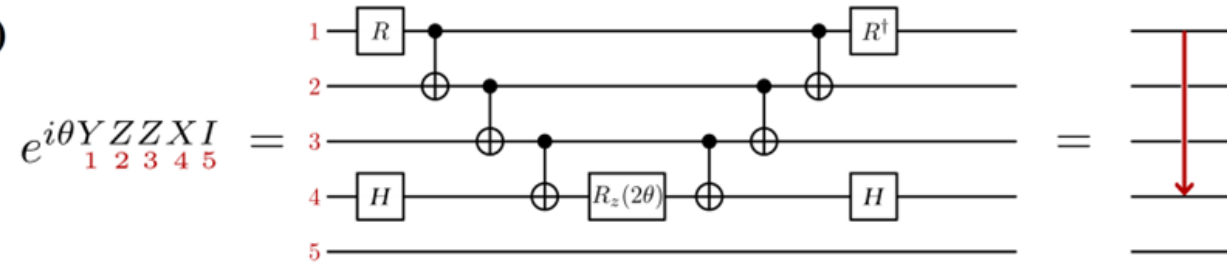
$$\langle n^2 \rangle = \sum_n |\psi(t, n)|^2 |n|^2$$

(*) Bucaj, Valmir. (2016). arXiv: Spectral Theory : 1608.01379

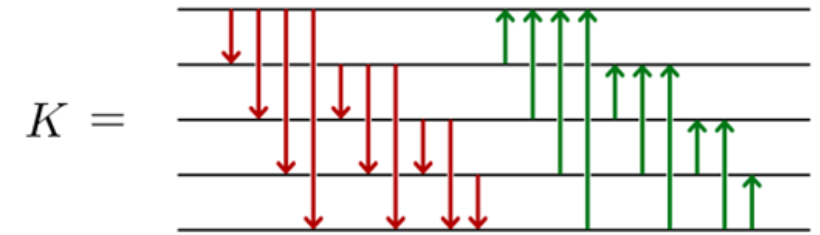
(**) Jović Savić, Dragana & Kivshar, Yuri & Denz, Cornelia & Belić, Milivoj. (2011). Phys. Rev. A. 83.10.1103/PhysRevA.83.033813.

Circuits

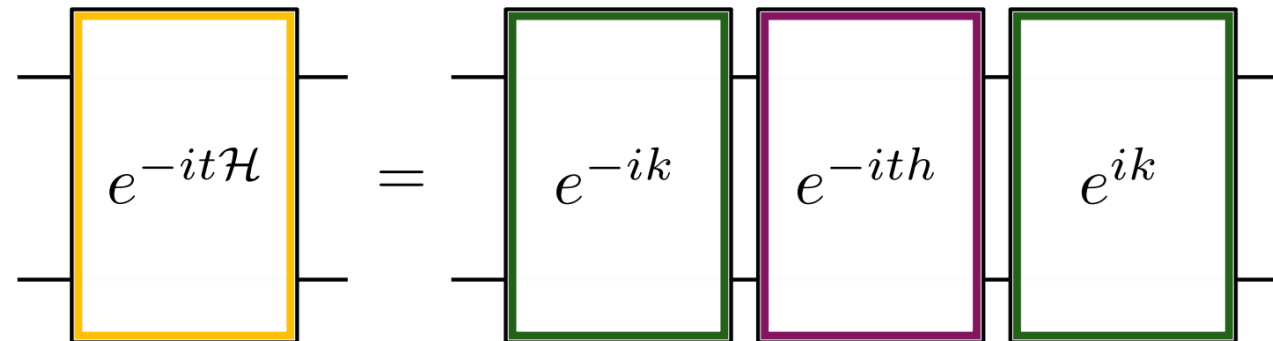
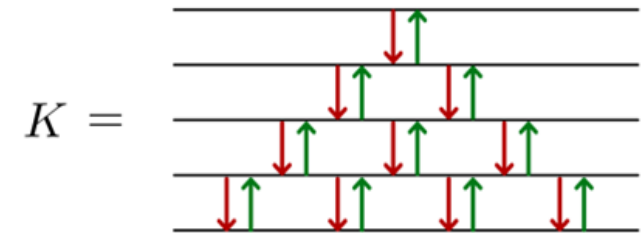
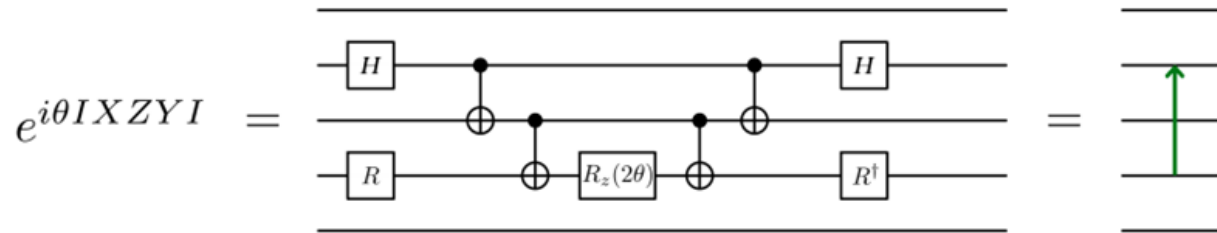
a)



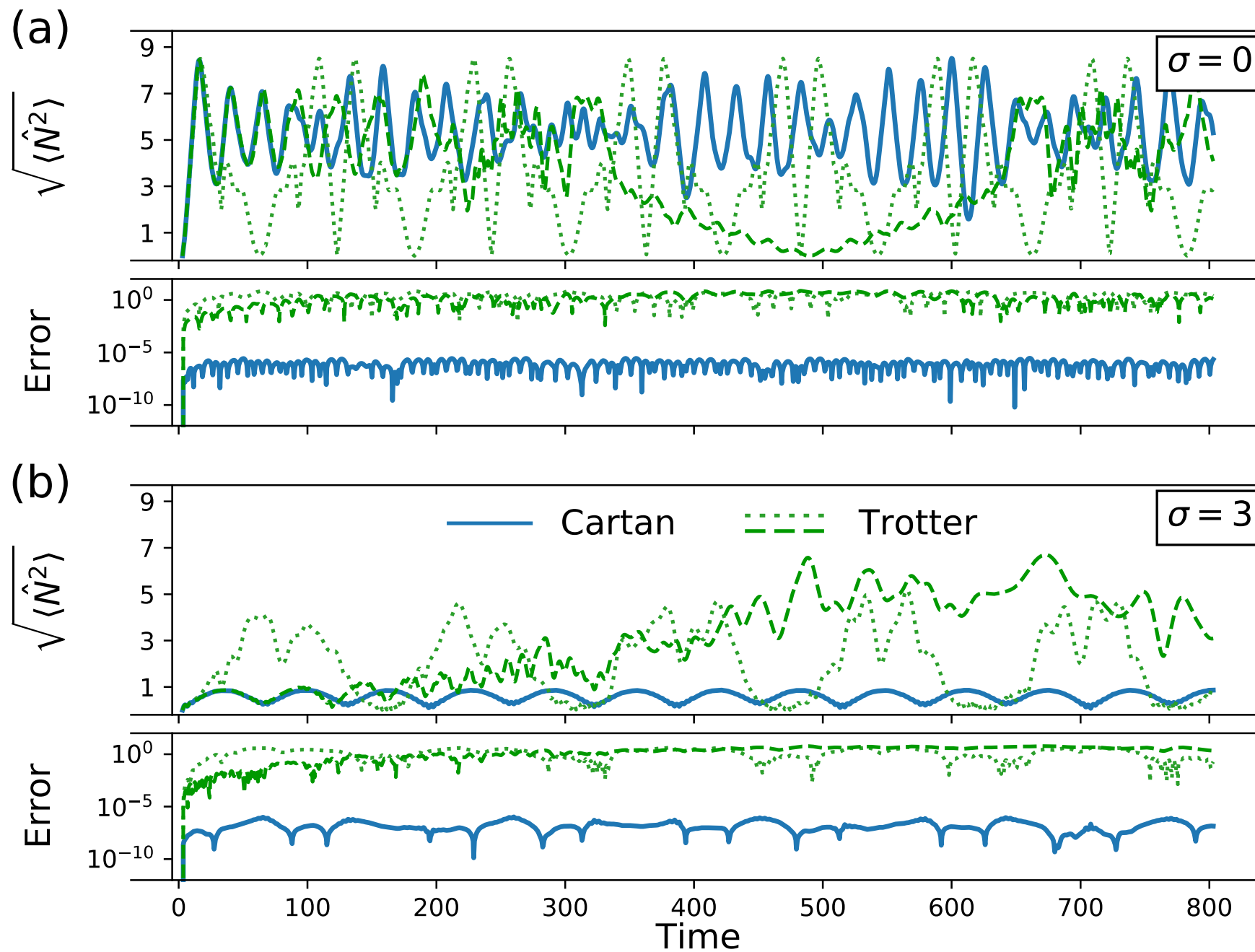
b)



c)

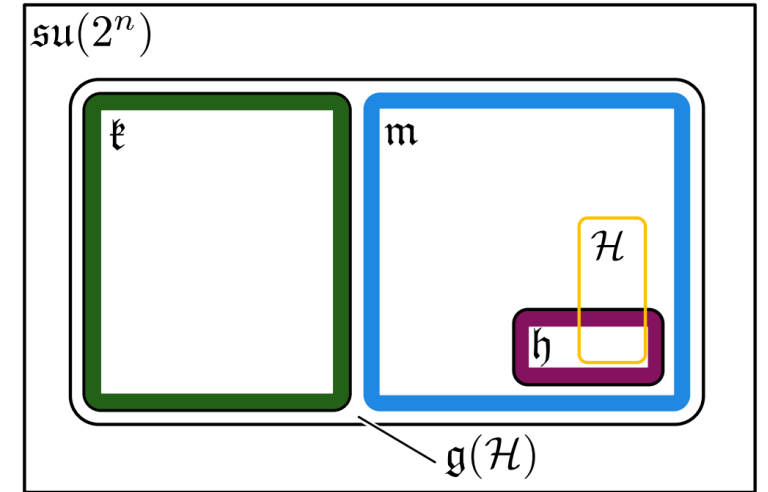


Results



Cartan Conclusions

- We provide a generic method to build circuits for time evolution of spin systems.
- $O(N^2, t^0 = 1)$ circuit for TFIM, TFX, XY
- Only local minimum needed for optimization
- Optimize only *once*



$$f(K) = \langle K v K^\dagger, \mathcal{H} \rangle$$

The diagram shows the decomposition of the time evolution operator $e^{-it\mathcal{H}}$ into three sequential gates: e^{-ik} , e^{-ith} , and e^{ik} .

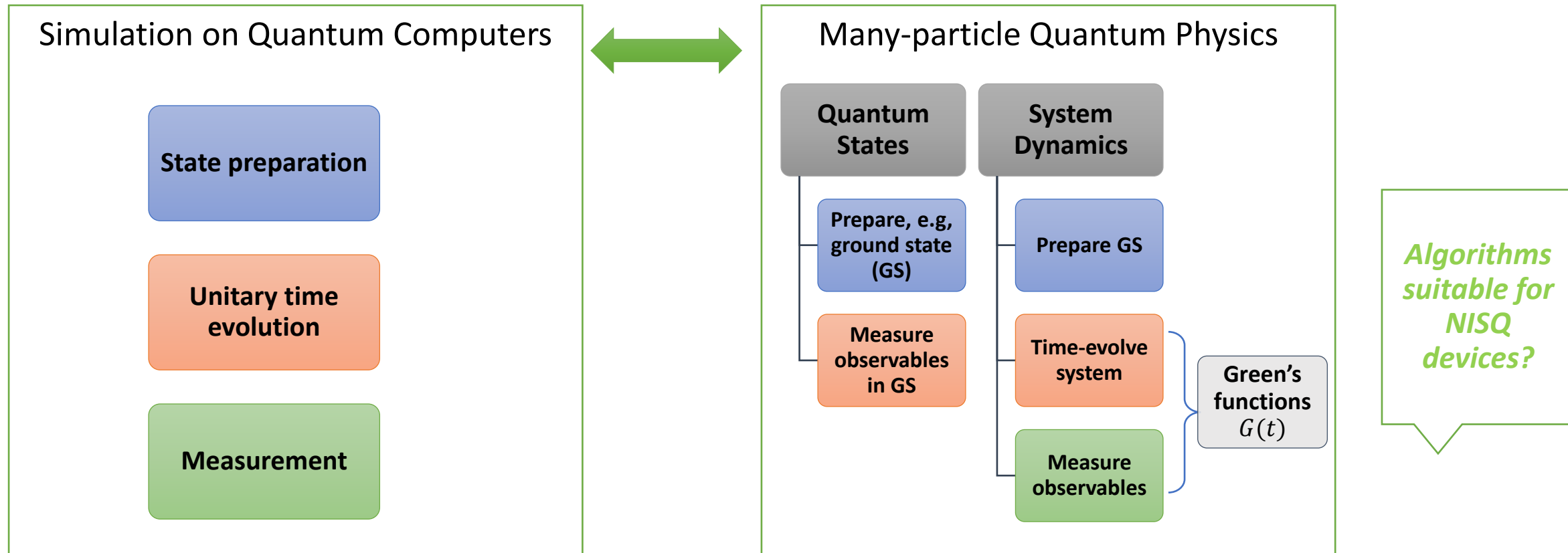
Fast Forwarding Application: DMFT

NISQ algorithms: simulate GF of dynamical mean-field theory (DMFT) for the Hubbard model on noisy intermediate-scale quantum (NISQ) devices

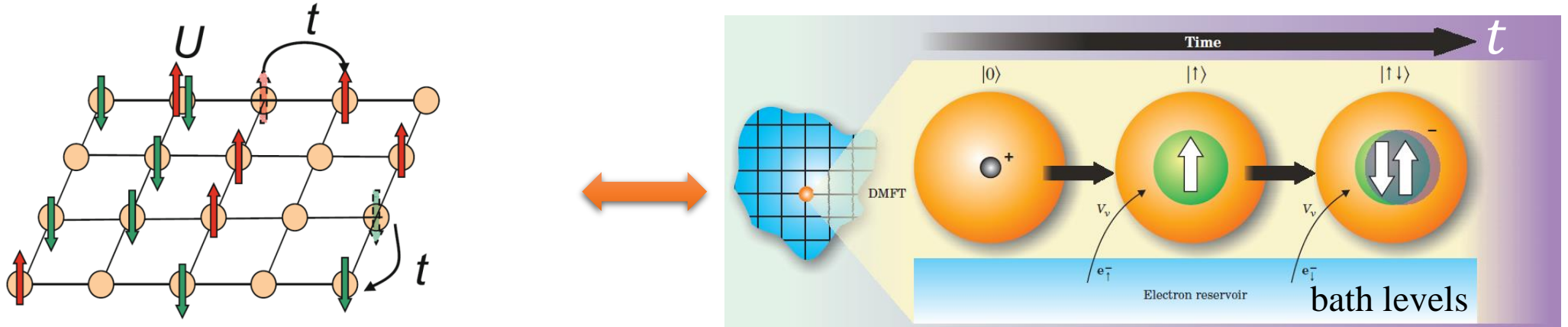
- Intro to DMFT (a map from Hubbard model to Anderson Impurity model via GF)
- Fast-forwarding circuit by Cartan decomposition of dynamical unitary group

Ref: arXiv:2112.05688

10.1103/PhysRevResearch.5.023198



3.2 DMFT: a map from Hubbard model to Anderson Impurity model



$$\hat{H}_{\text{Hub}} = -\tilde{t} \sum_{\langle i,j \rangle, \sigma} (\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \hat{c}_{j\sigma}^\dagger \hat{c}_{i\sigma}) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} - \mu \sum_{i,\sigma} \hat{n}_{i,\sigma} \longleftrightarrow \hat{H}_{\text{AIM}} = \sum_{i=1, \sigma}^{N_b} V_i (\hat{c}_{0,\sigma}^\dagger \hat{c}_{i,\sigma} + \hat{c}_{i,\sigma}^\dagger \hat{c}_{0,\sigma}) + U \hat{n}_{0,\uparrow} \hat{n}_{0,\downarrow} + \sum_{i=0, \sigma}^{N_b} (\epsilon_i - \mu) \hat{n}_{i,\sigma}$$

$$\Sigma(\omega) = \Sigma_{\text{imp}}(\omega) \xrightarrow{\text{Dyson's Eqn.}} G(\mathbf{k}, \omega), G_{\text{imp}}(\omega)$$

$$\sum_{\mathbf{k}} G(\mathbf{k}, \omega) = G_{\text{imp}}(\omega)$$

2-site (1 impurity + 1 bath) Anderson Impurity Model:

$$\hat{H}_{\text{AIM}} = \frac{V}{2} (X_0 X_1 + Y_0 Y_1 + X_2 X_3 + Y_2 Y_3) + \frac{U}{4} Z_0 Z_2$$

3.3 New specific workflow for simulation DMFT/AIM GF

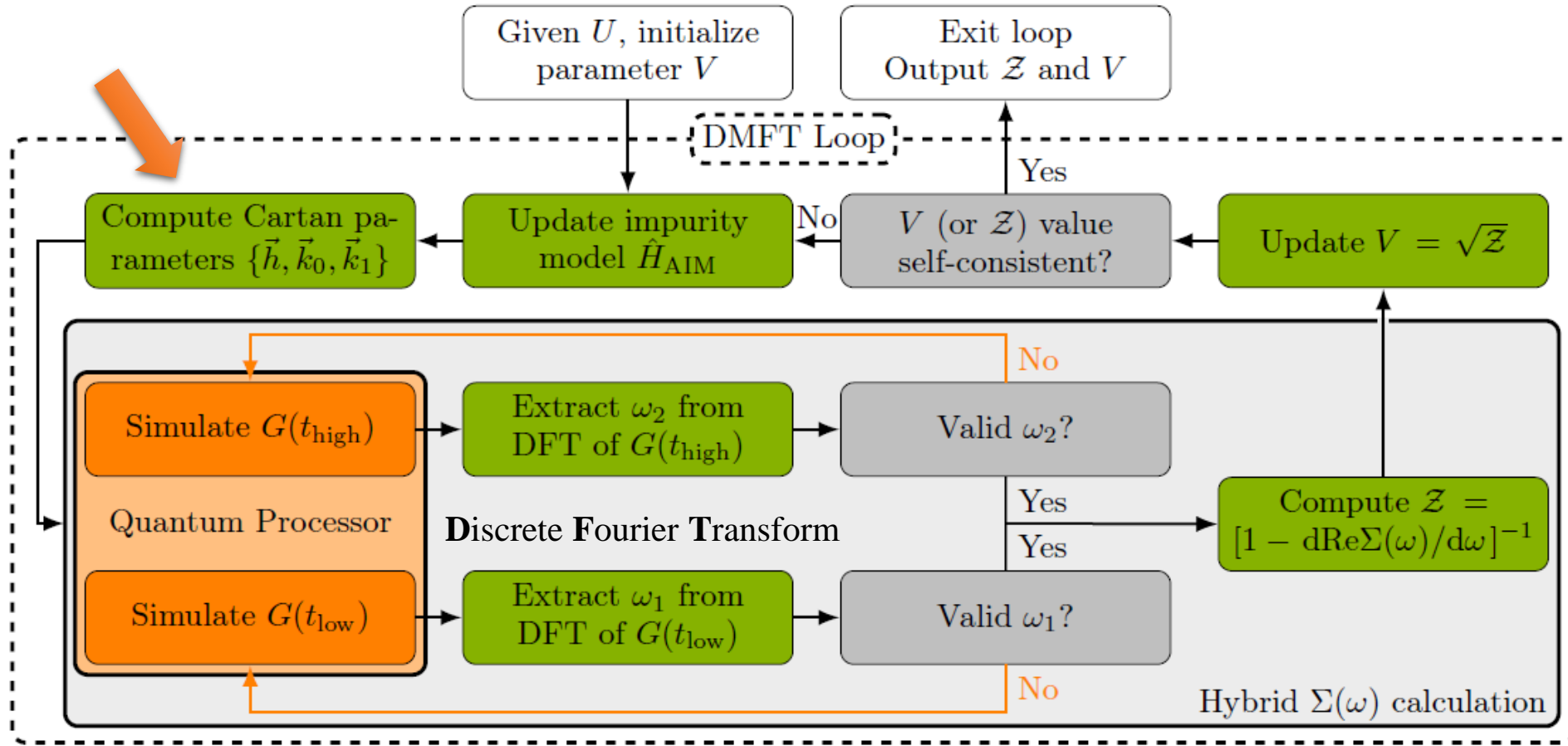


FIG. 1: Diagram of the DMFT loop specialized for the two-site calculation. Our calculations are initialized with $V = 0.5$. Each DMFT loop iteration also updates the time evolution Cartan parameters corresponding to the updated V . The hybrid computation of $\Sigma(\omega)$ evaluates the two frequencies ω_1 and ω_2 separately, in a procedure that is elaborated on in section IV(C).

3.4 Cartan decomposition of the Hamiltonian algebra

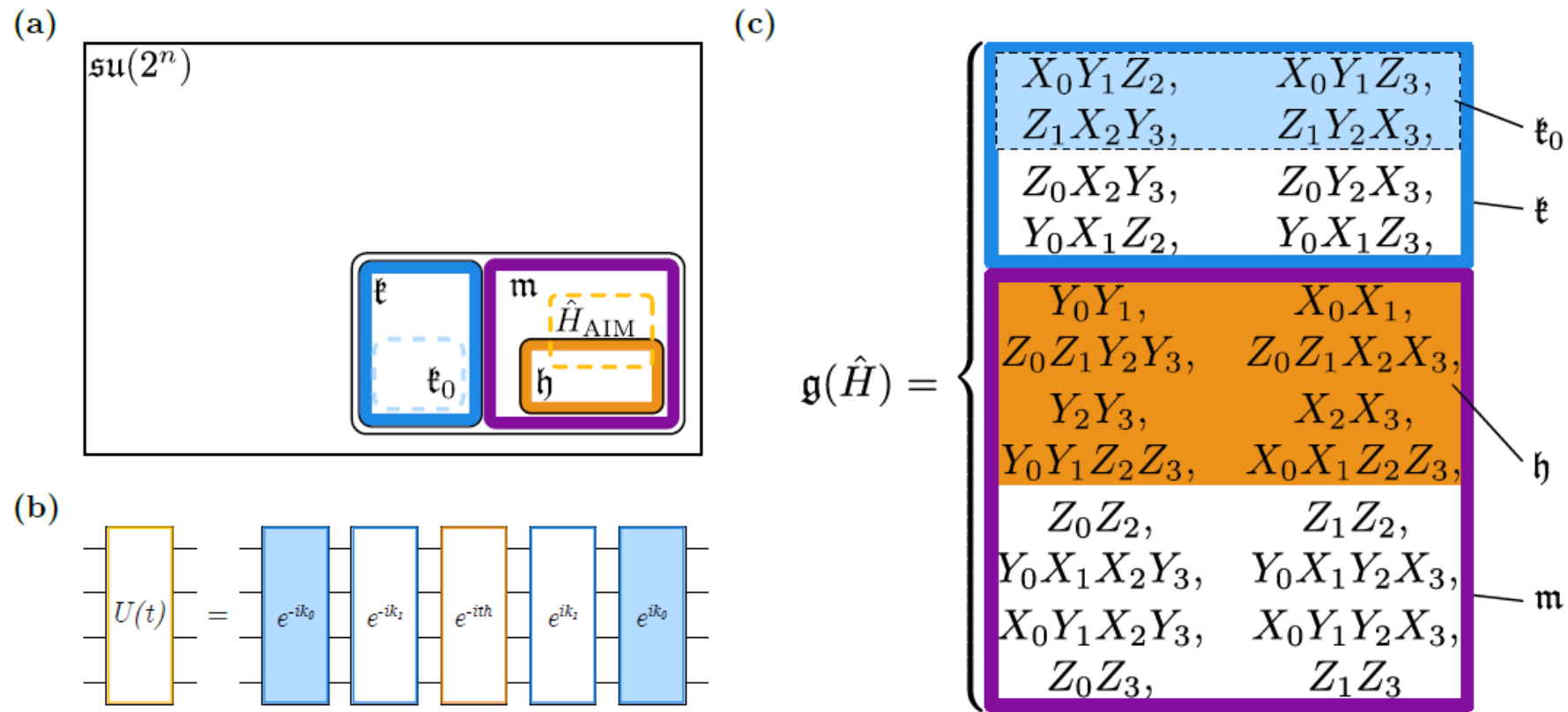


FIG. 2: (a) A generalized diagram of the Cartan decomposition of the Hamiltonian algebra with dimension = 24 within the special unitary algebra with dimension = 255. Here, \mathfrak{k}_0 is the set of basis elements which commute with X_0 , which is not a typical requirement of Cartan decomposition but results in a significant gate cost reduction in our application. (b) A block circuit diagram of the decomposed time evolution operator. (c) Cartan decomposition applied to the AIM Hamiltonian equation (A2), where the blue, shaded light blue, magenta, and shaded orange color regions correspond to the sets \mathfrak{k} , \mathfrak{k}_0 , \mathfrak{m} , and \mathfrak{h} .

3.5 Manually optimized circuits

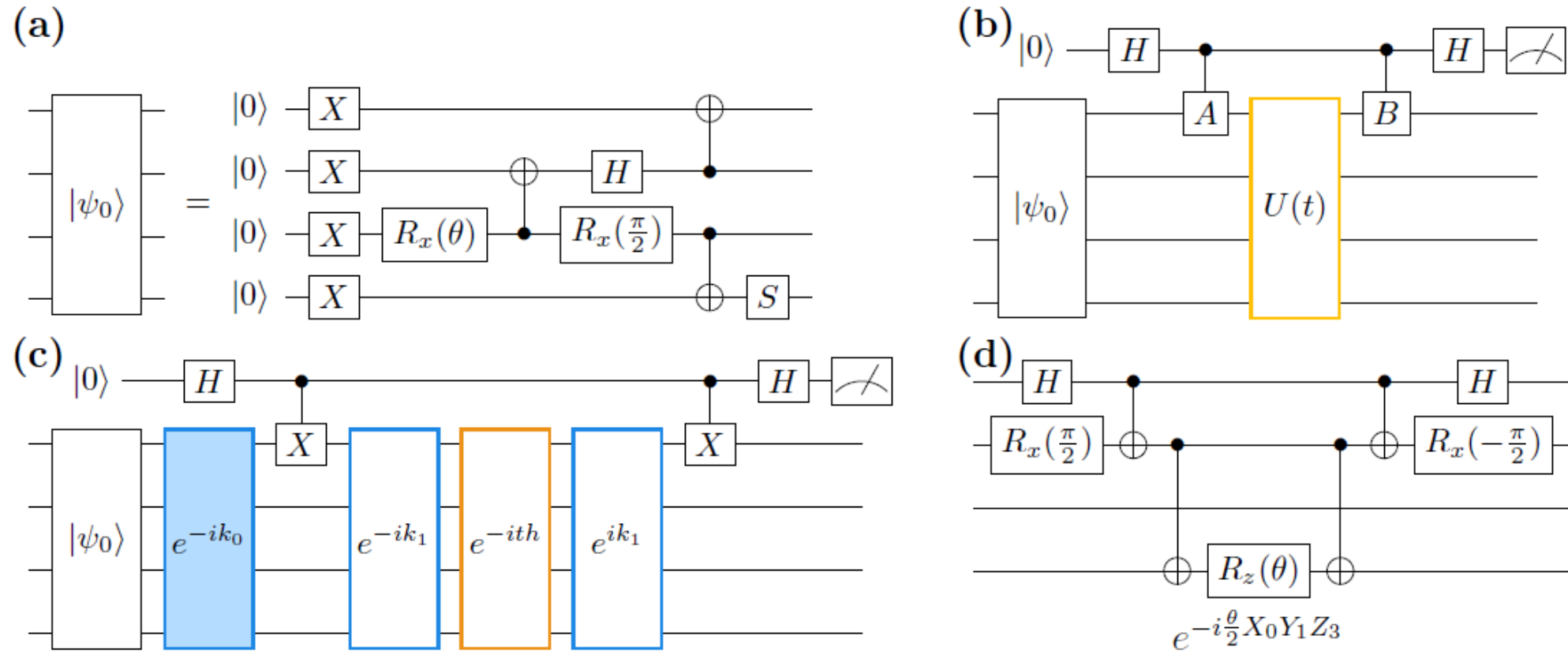


FIG. 3. (a) Ansatz circuit used to prepare the ground state. (b) General Hadamard interference type circuit used to implement a function circuit used in the final computation, except for the $e^{-i\frac{\theta}{2}X_0Y_1Z_3}$ gate. The property of k_0 allows for commuting through the CNOT gate so it need only be implemented once. (c) A general circuit showing the implementation of a Pauli gate exponential.

3.6 Noisy results (IBM device)

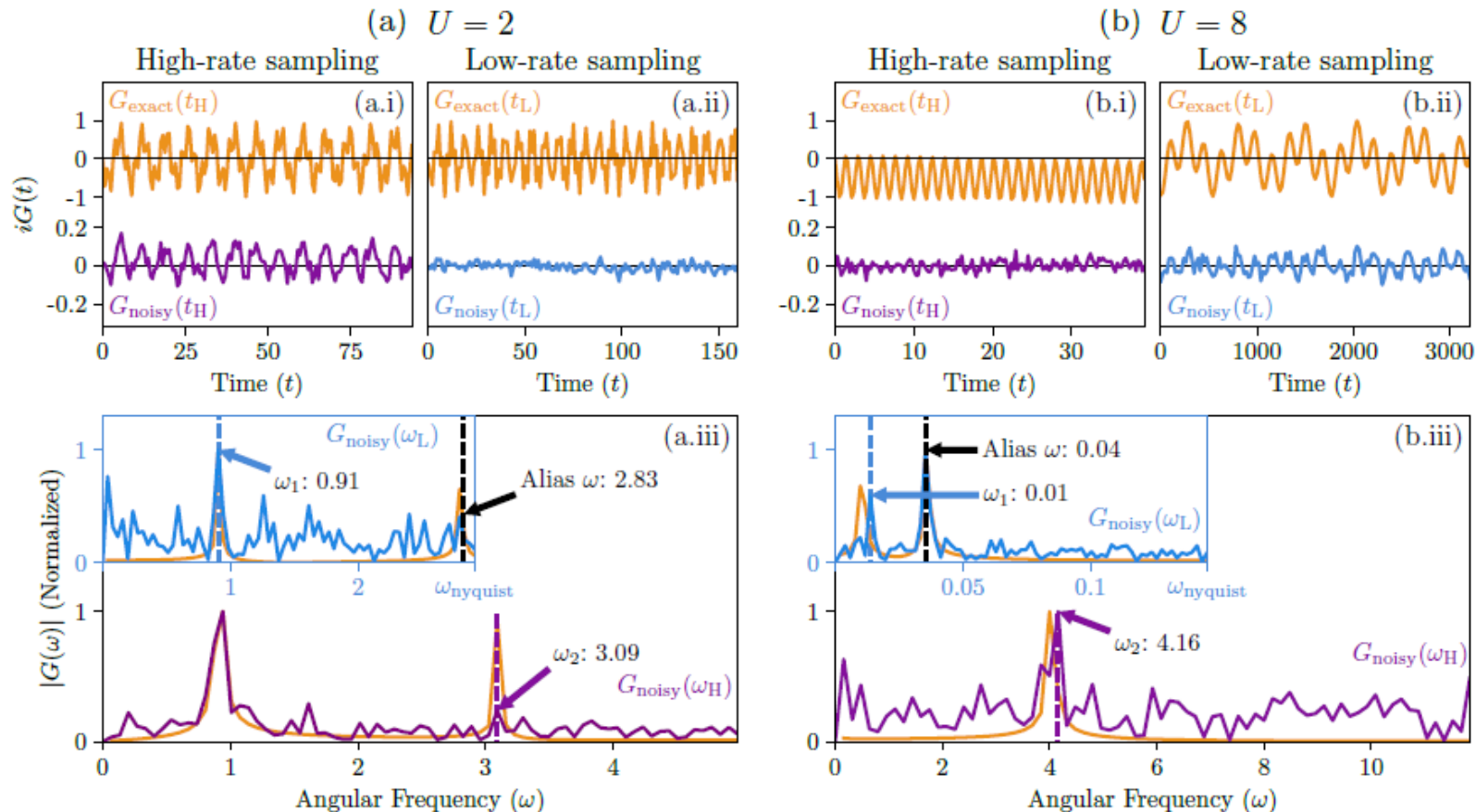
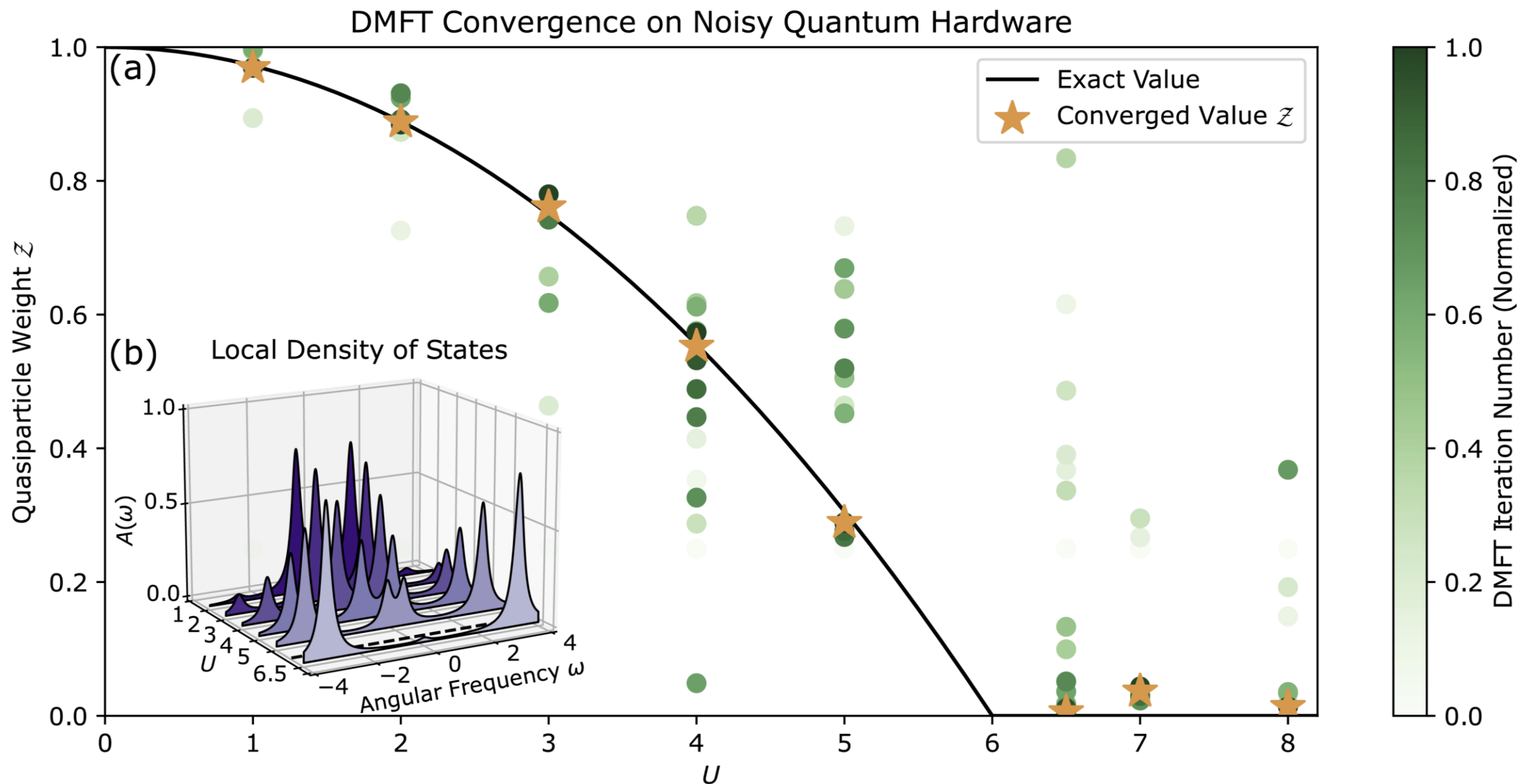


FIG. 4: Green's function sampled on the quantum computer *ibmq_manila* at self-consistency. Initial conditions: (a) $U = 2$ and $V_{\text{initial}} = 0.964$ and (b) $U = 8$ and $V_{\text{initial}} = 0.119$. (i/ii) The normalized Green's function with a phase correction (top, shifted vertically) and the actual, noisy results (bottom) with high (t_H) and low (t_L) sampling rates to evaluate the high frequency signal ω_2 and the low frequency signal ω_1 , respectively. (iii) The discrete Fourier transform showing the ideal frequencies (solid, orange) and the evaluated peaks (dashed) for both frequencies. Spurious peaks at $\omega = 0$ have been removed. (a) Returns a value of $V_{\text{new}} = 0.944$ and (b) returns a value of $V_{\text{new}} = 0.116$, both within the tolerance of 0.02.

3.7 Correct physical results



The first computation of metal-insulator phase diagram using noisy digital quantum hardware.

Quantum Arithmetic with Symmetry

- Intuition:

- Euler identity $e^A = \cos(A) + i\sin(A)$ is a decomposition into even (cos) and odd (sin) functions (or symmetric and anti-symmetric forms)

- $\cos(-x) = \cos(x)$; $\sin(-x) = -\sin(x)$

- ± 1 eigenvalues of spatial inversion operation $x \leftrightarrow -x$

- $\cos(Ht) = \frac{e^{-iHt} + e^{iHt}}{2}$

- $\sin(Ht) = \frac{e^{iHt} - e^{-iHt}}{2i}$

- A basis for engineering (spectral) quantum filter functions

- Application 1: $A \leftrightarrow B$ Inversion Symmetrized Trotter formula

- Application 2: Derivation of Ancilla as a measurement pointer state

Linear Combination of Trotter Unitaries: Sum and Product

- $H = A + B$

- $U(t) = e^{-\frac{it}{2}(A+B)}$

- $U_{AB}(t) = e^{-\frac{itA}{2}} e^{-\frac{itB}{2}}$

- $U - U_{AB} = \mathcal{O}(t^2 [A, B])$

- $U_{BA}(t) = e^{-\frac{itB}{2}} e^{-\frac{itA}{2}}$

- $U - U_{BA} = \mathcal{O}(t^2 [A, B])$

- $U_+ = \frac{U_{AB} + U_{BA}}{2}$

- $U - U_+ = \mathcal{O}(t^3 ([A, [A, B]] + B \leftrightarrow A))$

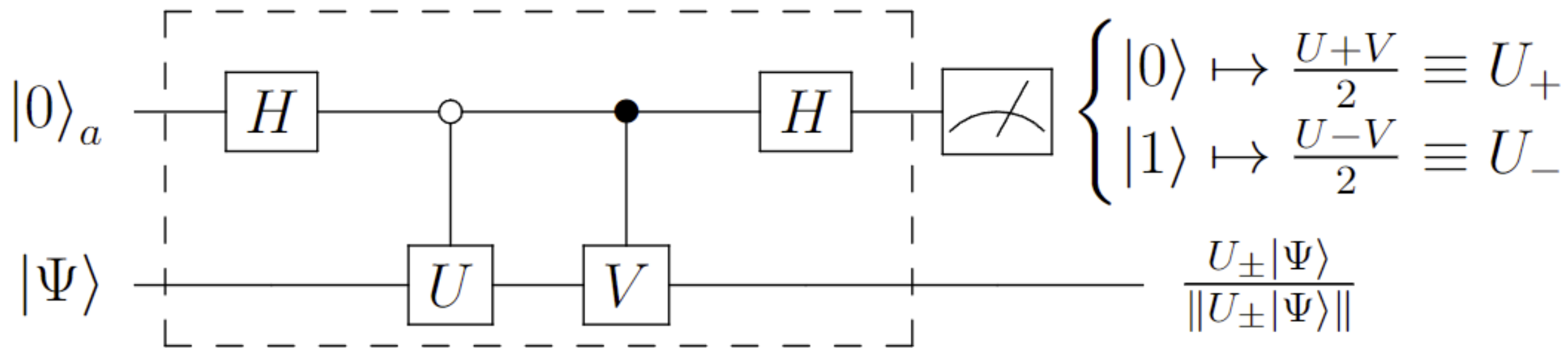
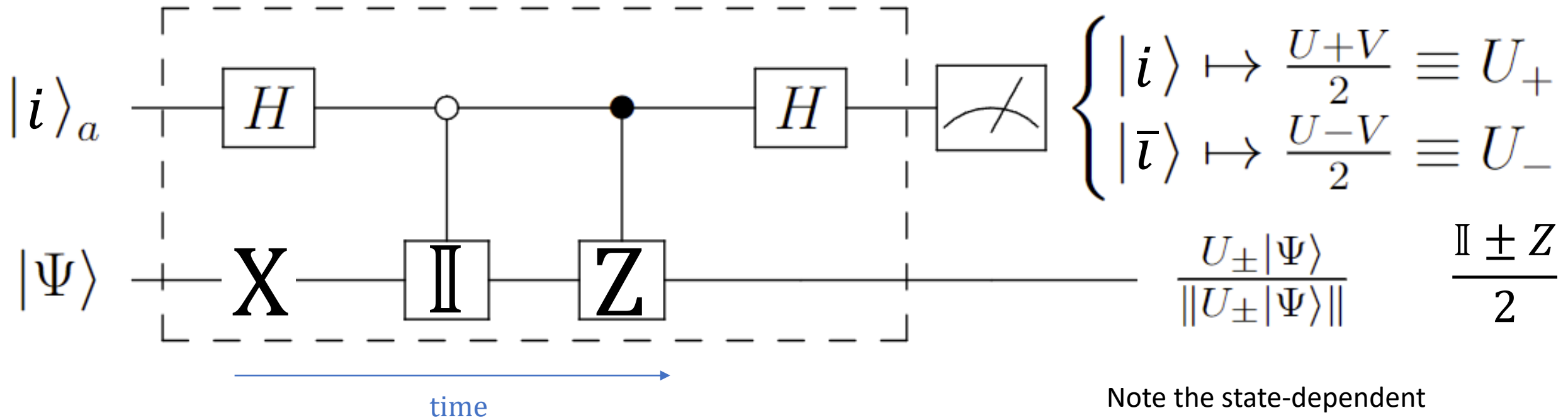


FIG. 1. Selecting $U = V^\dagger = e^{-itH}$ we define a random spectral walk (Sec. III A). Using $U = e^{tA}e^{tB}$ and $V = e^{tB}e^{tA}$, the quantum circuit acts by the BCH-like series that is symmetric with respect to the inversion $A \leftrightarrow B$. This is used to factorize time-evolution (Sec. III B). Setting different times ($t \rightarrow \theta_1, \theta_2$) enables a symmetric variational ansatz (Sec. III C). Last, setting $U = X_l$ and $V = iY_l$ for an array of qubits $\{q_l\}_{l=1}^N$ and concatenating the gadget N -times performs the measurement of Mermin polynomial M_N with a linear depth circuit (Sec. III D). The symmetry of the operator applied to $|\Psi\rangle$ is contingent on a measurement observing the ancillary qubit in the ($|1\rangle$) $|0\rangle$ state. Note that U_\pm are not unitary and that the principle system's final state $U_\pm |\Psi\rangle$ is normalized upon measurement of the ancilla qubit, due to the measurement postulate.

*Trotter (product) decompositions are recovered when $U=V$. The ancilla is not required, decouples and will *always* be measured in the 0 state. It may thus be removed.

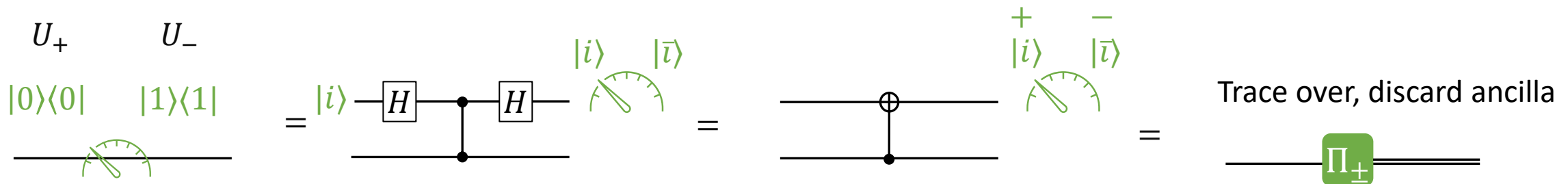
The Only Quantum Circuit You'll Ever Need

$$\overleftarrow{X \cdot (\mathbb{I} \mp Z)} = X \pm iY = (\mathbb{I} \pm Z) \cdot X$$



Note the state-dependent
weighting factors

$$\|U_i|\Psi\rangle\|$$



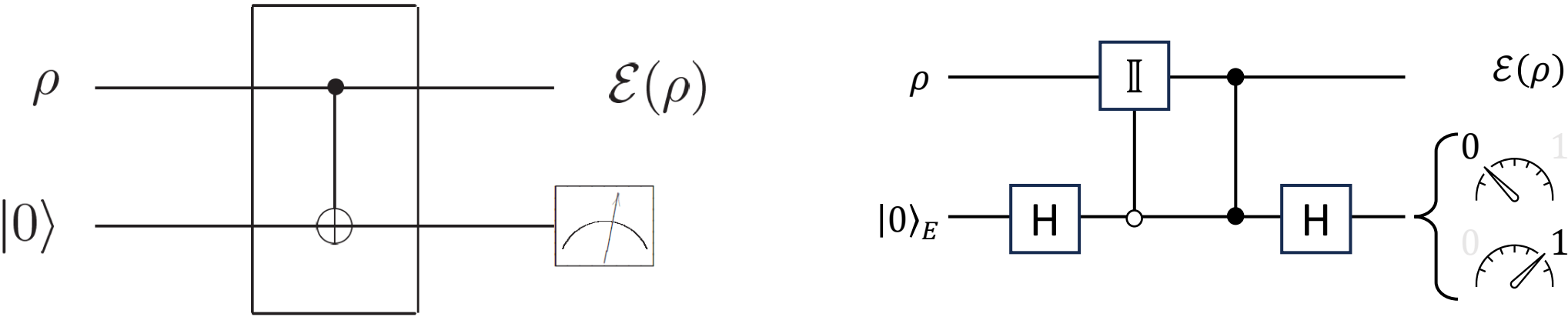


Figure 8.5. Controlled-NOT gate as an elementary model of single qubit measurement.

$$U = |0_P 0_E\rangle\langle 0_P 0_E| + |0_P 1_E\rangle\langle 0_P 1_E| + |1_P 1_E\rangle\langle 1_P 0_E| + |1_P 0_E\rangle\langle 1_P 1_E|. \tag{8.24}$$

Thus

$$E_0 = \langle 0_E | U | 0_E \rangle = |0_P\rangle\langle 0_P| \tag{8.25}$$

$$E_1 = \langle 1_E | U | 0_E \rangle = |1_P\rangle\langle 1_P|, \tag{8.26}$$

and therefore

$$\mathcal{E}(\rho) = E_0 \rho E_0 + E_1 \rho E_1, \tag{8.27}$$

$$\mathcal{E}(\rho) = \sum_{\sigma=\pm} \left(\frac{\mathbb{I}}{2} \sigma \frac{Z}{2} \right) \rho \left(\frac{\mathbb{I}}{2} \sigma \frac{Z}{2} \right)$$

0 1 1 + Z 1 - Z

0 1 2 2 = |0><0| = |1><1|

Summary

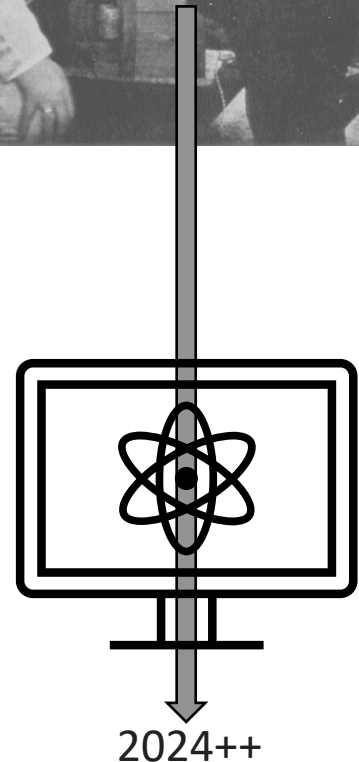
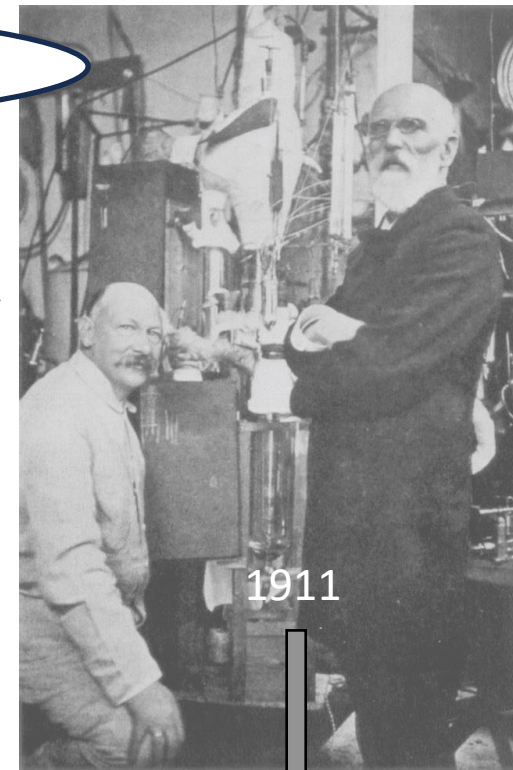
- Algorithmic perspective and classification of dynamic simulations.
- Unification of state-preparation and dynamics algorithms with ancilla-mediated quantum integral transformations (2112.05731):
 - Projection – Hubbard-Stratonovic
 - Propagation – Fourier-Laplace
- Algebra-based product encoding algorithm is used to recover a metal-insulator phase-transition (PhysRevLett.129.070501 , PhysRevResearch.5.023198).
- Considered all ancilla outcomes and the quantum channels they construct on the principal system (2403.05470).
 - Generalization of time-evolution operator decomposition in terms of addition *composed with* multiplication.
 - Defining projective measurements gives operational definition for ancilla measurement pointer states

"I gave the world quantum advantage 113 years ago....
And all I got was a lousy phenomenological theory of superconductivity"

Quantum Supremacy Outlook

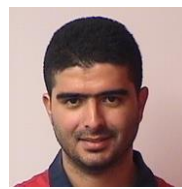
* a biased perspective

- Landau theory of symmetry breaking and phase transitions
 - (BCS) Superconductivity, Josephson junction, high- T_c , high- P_{ressure}
 - Transistor, STM, MFM, ..., Transmon 🏆
Phonons, polaritons, polarons, solitons, vortices, magnons, anyons,...
 - Onsager
Thermo-electrics, spin-tronics, valley-tronics, quantum information
 - QHE (topology, $R = \frac{h}{e^2 \nu}$) – K.V.K., Laughlin, Haldane 🍩
 - Graphene and Moire
WKB, BTK, BKT, ..., LTS, LCU, QSP, ETC
- Looking Forward:
It's a *long & challenging* road to *universal* quantum computing.
Luckily, \exists many big discoveries along the way.

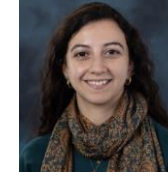




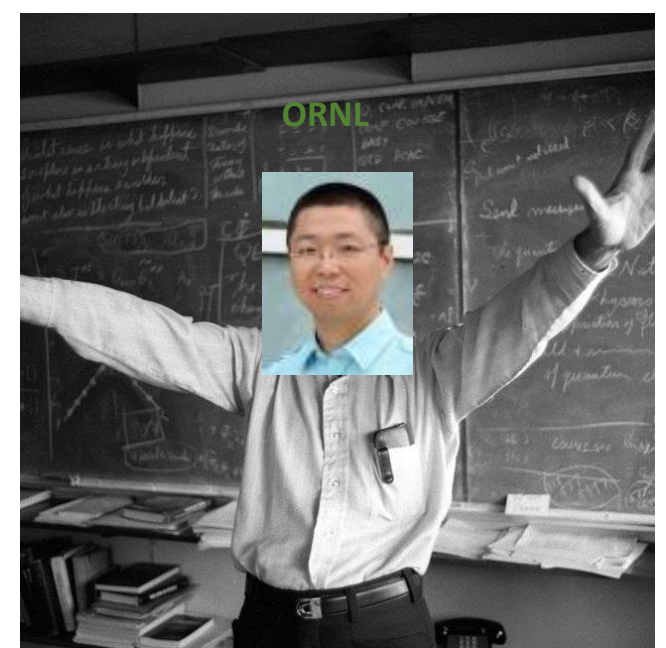
NSCU



Georgetown



ORNL



U.S. DEPARTMENT OF
ENERGY

Office of
Science

arXiv:2112.05731 – Integral Transformations

$U(2\text{years})| \text{PhysRevLett.129.070501} \rangle = | \text{PhysRevResearch.5.023198} \rangle$

arXiv:2403.05470 – Symmetric Forms