



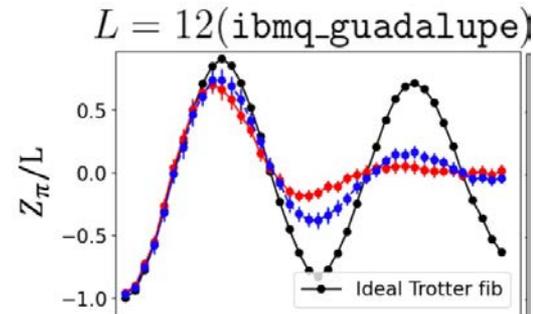
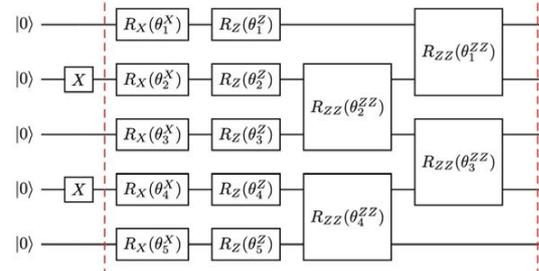
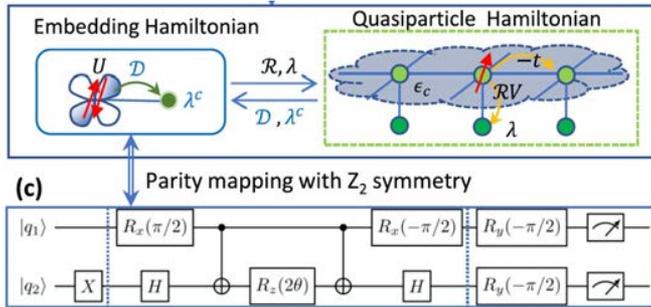
# Quantum Error Correction and Applications in Condensed Matter Physics

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# Outline and Take-Home Messages

- Quantum Computing Applications to Condensed Matter Physics
  - Condensed Matter & Material Science provides a rich & relevant set of problems
    - Difficulty level is often tunable
    - Many classical computational approaches are known to compare to
    - Open question which problems are best suited to demonstrate quantum advantage
  - Hybrid quantum-classical simulations leverage both classical & quantum computing power
    - One example is the variational quantum eigensolver (VQE) (see tutorial yesterday)
  - Simulations of nonequilibrium dynamics are classically hard due to entanglement growth
    - Opportunity for quantum computing



# Outline and Take-Home Messages

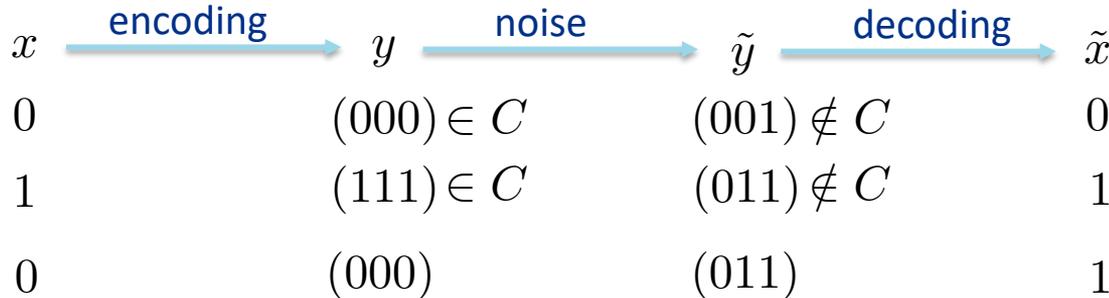
- Quantum Computing Applications to Condensed Matter Physics
  - Condensed Matter & Material Science provides a rich & relevant set of problems
    - Difficulty level is often tunable
    - Many classical computational approaches are known to compare to
    - Open question which problems are best suited to demonstrate quantum advantage
  - Hybrid quantum-classical simulations leverage both classical & quantum computing power
    - One example is the variational quantum eigensolver (VQE) (see tutorial yesterday)
  - Simulations of nonequilibrium dynamics are classically hard due to entanglement growth
    - Opportunity for quantum computing
- Quantum Error Correction (QEC)
  - Primary goal of the field that is required to unlock the full potential of quantum computing
  - Main idea: Protect quantum memory from noise and perform fault-tolerant operations
  - Many flavors and QEC codes exist (e.g. QEC Zoo<sup>1</sup>): Here focus on the basic principles.

[1] [www.quantumerrorcorrectionzoo.org](http://www.quantumerrorcorrectionzoo.org)

# Quantum Error Correction: Basics

# Motivation and repetition codes

- Errors in a quantum computation are unavoidable due to
  - Contact with environment  $\triangleright$  leads to decoherence
  - Unitary gate set is continuous  $\triangleright$  gate errors can be arbitrarily small  $U = U_{\text{ideal}}[1 + \mathcal{O}(\epsilon)]$
- Quantum Error Correction (QEC) protects quantum information by adding redundant information
  - Same idea as in Classical Error Correction



Code distance

$$d = \min_{x, y \in C} D_H(x, y)$$

Errors of weight up to  $\frac{d-1}{2}$  can be corrected

1 Single bit flips can be corrected

1 Two bit flips result in logical error

Failure probability:  $3p^2(1 - p) + p^2 < p \Rightarrow p < 1/2$

# Challenges for QEC

- Phase errors occur in addition to bit flip errors

$$\begin{array}{l}
 |0\rangle \rightarrow |0\rangle \\
 |1\rangle \rightarrow -|1\rangle
 \end{array}
 \quad \longrightarrow \quad
 |+\rangle = \frac{1}{\sqrt{2}}[|0\rangle + |1\rangle] \rightarrow \frac{1}{\sqrt{2}}[|0\rangle - |1\rangle] = |-\rangle$$

Phase flips act as bit flips of X eigenstates!

- Errors can be arbitrarily small and are continuous
- Measurement necessarily causes disturbance
  - Projective measurement projects onto eigenspace of measurement operator
- No cloning theorem (cannot copy quantum information)

## 3-qubit bit flip code

$$|0\rangle \rightarrow |\bar{0}\rangle = |000\rangle$$

$$|1\rangle \rightarrow |\bar{1}\rangle = |111\rangle$$

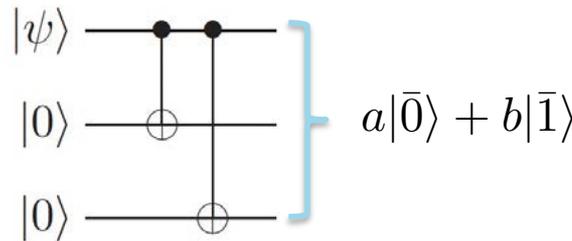
$$|\psi\rangle = a|0\rangle + b|1\rangle$$

Logical operators

$$X_L = X_1 X_2 X_3$$

$$Z_L = Z_1 Z_2 Z_3$$

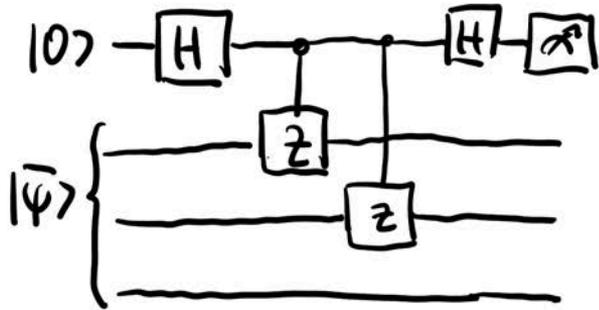
Encoding circuit:



Protected against  $\{X_1, X_2, X_3\}$  errors.

# Bit flip code: error detection via syndrome measurement

- Measure Pauli strings  $(Z_1 Z_2, Z_1 Z_3)$  yields error syndrome  $(\pm 1, \pm 1)$



$Z_1 Z_2$	$Z_2 Z_3$	Error type	Action
+1	+1	no error	no action
+1	-1	bit 3 flipped	flip bit 3
-1	+1	bit 1 flipped	flip bit 1
-1	-1	bit 2 flipped	flip bit 2

by majority vote

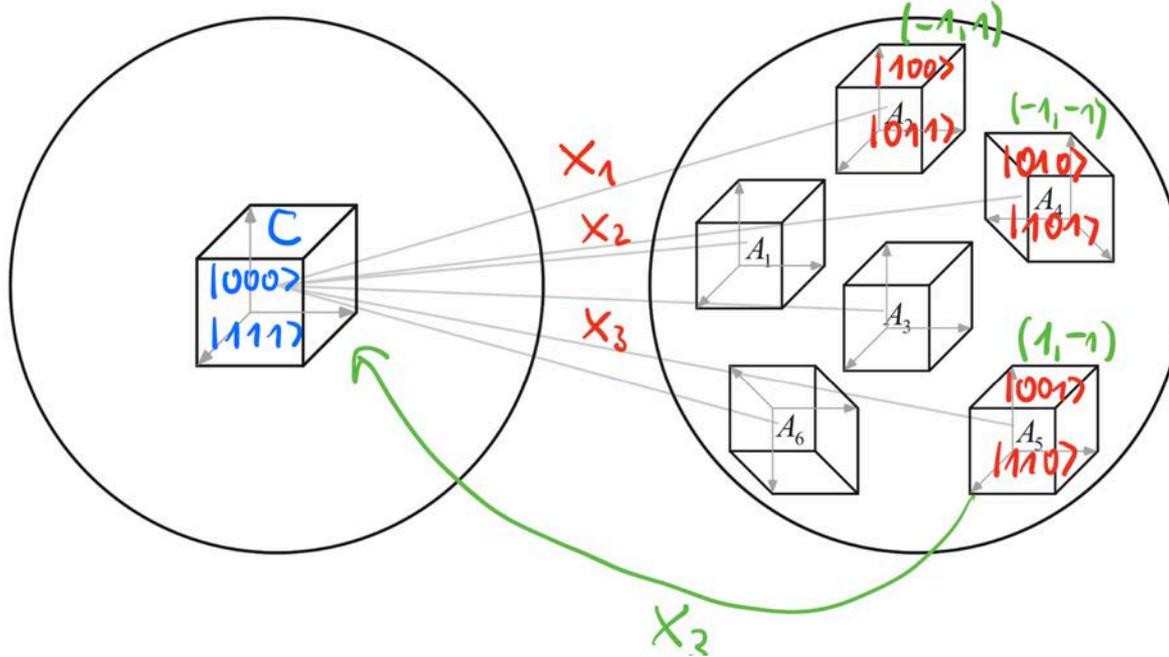
$$|0\rangle|\bar{\psi}\rangle \rightarrow \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)|\bar{\psi}\rangle \rightarrow \frac{1}{\sqrt{2}}(|0\rangle|\bar{\psi}\rangle + Z_1 Z_2 |1\rangle|\bar{\psi}\rangle)$$

$$\rightarrow \frac{1}{2} \left( (|0\rangle + |1\rangle)|\bar{\psi}\rangle + Z_1 Z_2 (|0\rangle - |1\rangle)|\bar{\psi}\rangle \right) = \frac{1}{2} (1 + Z_1 Z_2) |0\rangle|\bar{\psi}\rangle + \frac{1}{2} (1 - Z_1 Z_2) |1\rangle|\bar{\psi}\rangle$$

Measurement of ancilla collapses logical qubit to  $\frac{I \pm Z_1 Z_2}{2}$  orthogonal eigenspaces

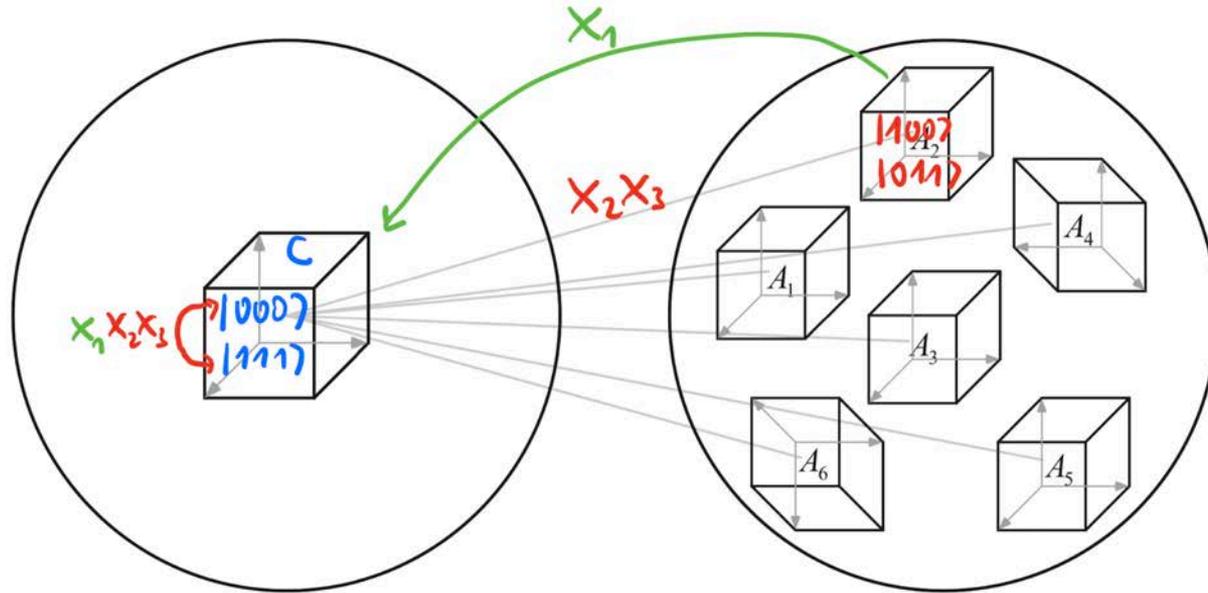
Digitization of error: bit flip either occurs (with small probability) or not.

# Orthogonal error subspaces



- Ancilla measurement **discretizes error** by projecting states onto orthogonal and undeformed error subspaces
- **Recovery operation** associated with each syndrome outcome  $(\pm 1, \pm 1)$

# Two and three bit flip errors are not correctable



- Two-bit flip errors are erroneously corrected → **logical error**
- Three-bit flip errors correspond to logical operations and cannot be detected

# Challenges for QEC: almost all addressed in bit flip code

- Phase errors occur in addition to bit flip errors **✗** (still need to be addressed)

$$\begin{array}{l} |0\rangle \rightarrow |0\rangle \\ |1\rangle \rightarrow -|1\rangle \end{array} \quad \longrightarrow \quad |+\rangle = \frac{1}{\sqrt{2}}[|0\rangle + |1\rangle] \rightarrow \frac{1}{\sqrt{2}}[|0\rangle - |1\rangle] = |-\rangle$$

Phase flips act as bit flips of X eigenstates!

- Errors can be arbitrarily small and are continuous
  - Ancilla measurement discretizes errors (either they occur or not) **✓**
- Measurement necessarily causes disturbance
  - Projective measurement projects onto eigenspace of measurement operator
  - Measurement of syndrome operators does not affect information encoded in code subspace C **✓**
  - Projection is actually a good thing **✓**
- No cloning theorem (cannot copy quantum information)
  - We never copied the state  $|\psi\rangle = a|0\rangle + b|1\rangle$  **✓**

# Phase flip code

- Phase errors occur in addition to bit flip errors ✓

$$\begin{aligned} |0\rangle &\rightarrow |0\rangle \\ |1\rangle &\rightarrow -|1\rangle \end{aligned} \quad \longrightarrow \quad |+\rangle = \frac{1}{\sqrt{2}}[|0\rangle + |1\rangle] \rightarrow \frac{1}{\sqrt{2}}[|0\rangle - |1\rangle] = |-\rangle$$

Phase flips act as bit flips of X eigenstates!

## 3-qubit phase flip code

$$|0\rangle \rightarrow |\bar{0}\rangle = |+++ \rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)^{\otimes 3}$$

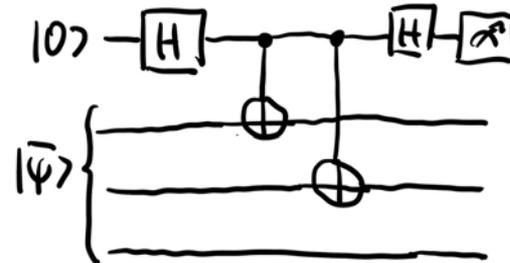
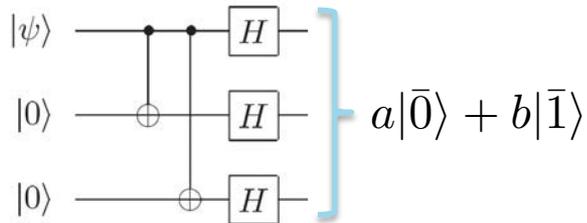
$$|1\rangle \rightarrow |\bar{1}\rangle = |--\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)^{\otimes 3}$$

Protected against  $\{Z_1, Z_2, Z_3\}$  errors.

Syndrome measurements

$$(X_1 X_2, X_1 X_3) = (\pm 1, \pm 1)$$

Encoding circuit:



Circuit to measure  $X_1 X_2$

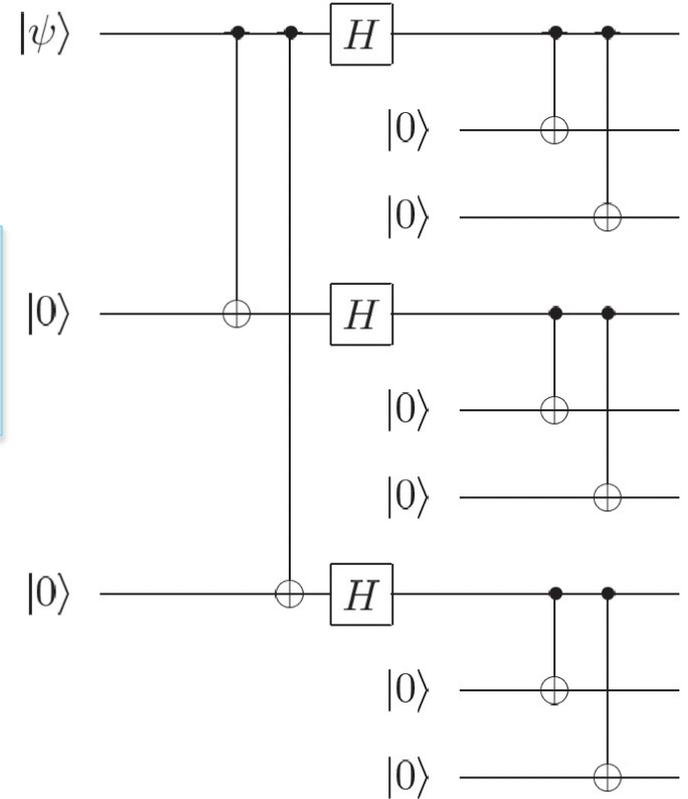
# Combine bit and phase flip code: Shor's 9-qubit code

- Shor's 9-qubit code protects against all single bit and phase flip errors and their combination
- Codewords

$$|0\rangle \rightarrow |\bar{0}\rangle = \frac{1}{2^{3/2}}(|000\rangle + |111\rangle)(|000\rangle + |111\rangle)(|000\rangle + |111\rangle)$$

$$|1\rangle \rightarrow |\bar{1}\rangle = \frac{1}{2^{3/2}}(|000\rangle - |111\rangle)(|000\rangle - |111\rangle)(|000\rangle - |111\rangle)$$

- Detect bit flips by syndrome measurements of  $(Z_1Z_2, Z_1Z_3, Z_4Z_5, Z_4Z_6, Z_7Z_8, Z_7Z_9)$
- Detect phase flips by syndrome measurements  $(X_1X_2X_3X_4X_5X_6, X_4X_5X_6X_7X_8X_9)$
- Information encoded nonlocally



# Code distance and uncorrectable errors

- Two bit flips in a single cluster of three qubits cannot be corrected (instead we incorrectly apply  $X_3$ )

$$\begin{aligned} X_3 X_1 X_2 |\bar{0}\rangle &= |\bar{0}\rangle \\ X_3 X_1 X_2 |\bar{1}\rangle &= -|\bar{1}\rangle \end{aligned} \quad \Rightarrow \quad Z_L(a|\bar{0}\rangle + b|\bar{1}\rangle) = a|\bar{0}\rangle - b|\bar{1}\rangle \quad \text{results in a logical phase flip}$$

- Two phase flips in different clusters cannot be corrected

$$\begin{aligned} Z_7 Z_1 Z_4 |\bar{0}\rangle &= |\bar{1}\rangle \\ Z_7 Z_1 Z_4 |\bar{1}\rangle &= |\bar{0}\rangle \end{aligned} \quad \Rightarrow \quad X_L(a|\bar{0}\rangle + b|\bar{1}\rangle) = a|\bar{1}\rangle + b|\bar{0}\rangle \quad \text{results in a logical bit flip}$$

- Only weight  $t=1$  Pauli errors can be corrected  $\Rightarrow$  **Code distance**  $d = 2t + 1 = 3$

Are there two qubit errors that can be corrected?

- Shor's code is a  $[[n, k, d]] = [[9, 1, 3]]$  code.

# Error probability

- Unencoded qubit: failure with probability  $p$
- Shor's logical qubit
  - Logical phase error requires two bits on the same cluster to flip

- Upper bounded by

$$p_{L,\text{phase}} \leq 3 \binom{3}{2} \left(\frac{2}{3}p\right)^2 = 4p^2$$

- Logical bit flip error requires two bits on different clusters to undergo phase error

- Upper bounded by

$$p_{L,\text{bit}} \leq \binom{3}{2} 3^2 \left(\frac{2}{3}p\right)^2 = 12p^2$$

- Encoding is advantageous for

$$p_{L,\text{tot}} = 16p^2 \leq p^2 \Rightarrow p < 1/16$$

- Encoded qubit has smaller failure rate for small enough physical failure rate

# Conditions for Quantum Error Correction

- Define set of correctable errors  $\mathcal{E} \subseteq \mathcal{P}_n = \{I, X, Y, Z\}^{\otimes n}$ 
  - Typical example: all Pauli errors of weight  $\leq t$
- Starting from any state  $|\bar{i}\rangle \in C$ , wish to undo any action composed of errors in  $\mathcal{E}$

Error map (Stinespring dilation representation):

$$|\bar{i}\rangle|0\rangle_E \rightarrow \sum_{\mu} M_{\mu}|\bar{i}\rangle|\mu\rangle_E$$

Error entangles system with environment!

orthonormal states

Kraus operators  $M_{\mu} = \sum_a c_{\mu a} P_a$

- Can reverse errors if there exists a **recovery superoperator** defined via  $\{R_{\nu}\}$  such that

$$\sum_{\nu, \mu} R_{\nu} M_{\mu} |\bar{i}\rangle |\mu\rangle_E |\nu\rangle_A = |\bar{i}\rangle |\text{stuff}\rangle_{EA}$$

- Entanglement has been shifted to occur between environment & ancillas
- State  $|\text{stuff}\rangle_{EA}$  must not depend on  $i$
- $R_{\nu} M_{\mu}$  acts as identity on codespace  $C$

$$R_{\nu} M_{\mu} |\bar{i}\rangle = \lambda_{\nu\mu} |\bar{i}\rangle$$

# Conditions for Quantum Error Correction

- Using completeness condition  $\sum_{\nu} R_{\nu}^{\dagger} R_{\nu} = I$ , we find

$$M_{\delta}^{\dagger} M_{\mu} |\bar{i}\rangle = M_{\delta}^{\dagger} \left( \sum_{\nu} R_{\nu}^{\dagger} R_{\nu} \right) M_{\mu} |\bar{i}\rangle = \sum_{\nu} \lambda_{\nu\delta}^* \lambda_{\nu\mu} |\bar{i}\rangle$$

↑ Also acts as identity on codespace C

$$R_{\nu} M_{\mu} |\bar{i}\rangle = \lambda_{\nu\mu} |\bar{i}\rangle$$

- Necessary and sufficient condition on codespace C for allowing errors in  $\mathcal{E}$  to be corrected is

$$\langle \bar{j} | M_{\delta}^{\dagger} M_{\mu} | \bar{i} \rangle = C_{\delta\mu} \delta_{ij}$$

Arbitrary Hermitian matrix that is independent of i,j

Since  $M_{\mu} = \sum_a c_{\mu a} P_a$

this implies

$$\langle \bar{j} | P_b P_a | \bar{i} \rangle = C_{ba} \delta_{ij} \text{ for } P_a, P_b \in \mathcal{E}$$

# Alternative derivation of QEC condition

- Consider the code block is in any state  $|\bar{\psi}\rangle$  and then an error acts:

$$|\bar{\psi}\rangle|0\rangle_E \rightarrow \sum_{\mu} M_{\mu}|\bar{\psi}\rangle|\mu\rangle_E$$

- The reduced density matrix of the environment must not carry any information about the state  $|\bar{\psi}\rangle$

$$\rho_E = \sum_{\mu, \nu} |\mu\rangle_E \langle \bar{\psi} | M_{\nu}^{\dagger} M_{\mu} | \bar{\psi} \rangle \langle \nu |_E$$

Must be independent of  $|\bar{\psi}\rangle = \sum_i c_i |\bar{i}\rangle$

$$\rho_E = \sum_{i, j} \sum_{\mu, \nu} c_i^* c_j |\mu\rangle_E \langle \bar{i} | M_{\nu}^{\dagger} M_{\mu} | \bar{j} \rangle \langle \nu |_E$$

Independence from  $c_i$  implies that  $\langle \bar{i} | M_{\nu}^{\dagger} M_{\mu} | \bar{j} \rangle = C_{\nu\mu} \delta_{ij}$ . Used that  $\sum_i |c_i|^2 = 1$ .

# Example: Shor's code and one weight Pauli errors

$$|0\rangle \rightarrow |\bar{0}\rangle = \frac{1}{2^{3/2}}(|000\rangle + |111\rangle)(|000\rangle + |111\rangle)(|000\rangle + |111\rangle)$$

$$|1\rangle \rightarrow |\bar{1}\rangle = \frac{1}{2^{3/2}}(|000\rangle - |111\rangle)(|000\rangle - |111\rangle)(|000\rangle - |111\rangle)$$

$$\langle \bar{j} | P_b P_a | \bar{i} \rangle = C_{ba} \delta_{ij} \text{ for } P_a, P_b \in \mathcal{E}$$

$$\langle \bar{0} | X_a X_b | \bar{0} \rangle = \delta_{ab}$$

$$\langle \bar{1} | X_a X_b | \bar{0} \rangle = 0$$

$$\langle \bar{1} | X_a X_b | \bar{1} \rangle = \delta_{ab}$$

$$\langle \bar{0} | Z_a Z_b | \bar{0} \rangle = \delta_{ab}$$

$$\langle \bar{1} | Z_a Z_b | \bar{0} \rangle = 0$$

$$\langle \bar{1} | Z_a Z_b | \bar{1} \rangle = \delta_{ab}$$

- Same holds for  $Y_a$  operators
- But, if one of the Paulis is  $X_2 X_3$

$$\langle \bar{0} | X_1 X_2 X_3 | \bar{0} \rangle = 1$$

$$\langle \bar{1} | X_1 X_2 X_3 | \bar{0} \rangle = 0$$

$$\langle \bar{1} | X_1 X_2 X_3 | \bar{1} \rangle = -1$$

No longer independent of  $i, j$ . Thus,  $X_2 X_3$  cannot be corrected.

# Shor's code as stabilizer code

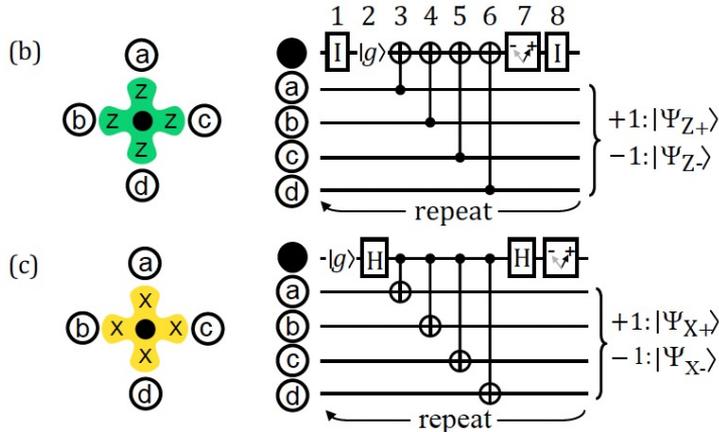
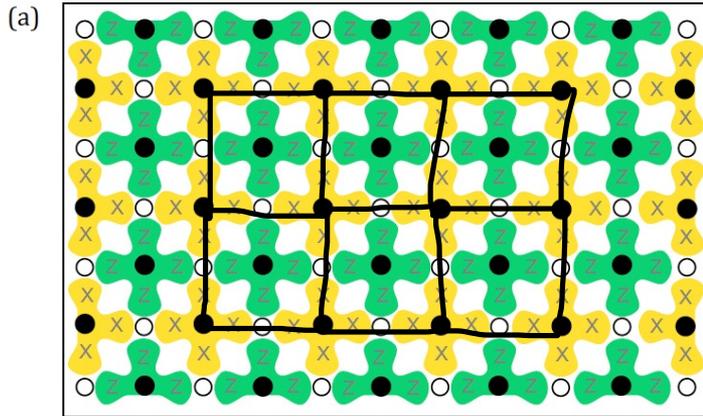
- Pauli group  $\mathcal{P}_n = \{\pm 1, \pm i\} \times \{I, X, Y, Z\}^{\otimes n}$
- Stabilizer code subspace is defined by a (stabilizer) subgroup  $\mathcal{S} \subset \mathcal{P}_n$  as the vector subspace that is fixed by all the elements in  $\mathcal{S} \subset \mathcal{P}_n$

$$\mathcal{C} = \{|\psi\rangle \in \mathcal{H} \mid S|\psi\rangle = |\psi\rangle \forall S \in \mathcal{S}\}$$

Joint +1 eigenspace of set of commuting Pauli strings

- Stabilizer group must not contain (-I) and it is Abelian
- Sufficient to define the codespace via the generators of the stabilizer group only
- For 3-qubit bit flip code:  $\mathcal{S} = \langle Z_1 Z_2, Z_1 Z_3 \rangle$
- For Shor's 9-qubit code:  
 $\{Z_1 Z_2, Z_2 Z_3, Z_4 Z_5, Z_5 Z_6, Z_7 Z_8, Z_8 Z_9, X_1 X_2 X_3 X_4 X_5 X_6, X_4 X_5 X_6 X_7 X_8 X_9\}$ .
- Set of logical Pauli gates = set of Pauli operators that commute with all stabilizers = centralizer of  $\mathcal{S} \subset \mathcal{P}_n$   
Alternatively:  $\bar{Z} = X_1 X_2 X_3$   $\bar{X} = Z_1 Z_4 Z_7$ 
  - Example:  $\bar{Z} = X_1 X_2 X_3 X_4 X_5 X_6 X_7 X_8 X_9$  and  $\bar{X} = Z_1 Z_2 Z_3 Z_4 Z_5 Z_6 Z_7 Z_8 Z_9$

# Surface code



- Planar version of Kitaev's toric code

$$H = - \sum_v A_v - \sum_p B_p$$

$$A_v = \prod_{i \in v} X_i, \quad B_p = \prod_{i \in p} Z_i$$

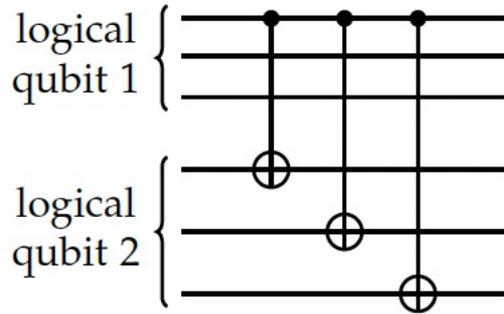
- Data qubits (open circles) on bonds of square lattice
- Local Z and X stabilizers
  - Z checks are product of four Z's around plaquette
  - X checks are product of four X's along star
- GS space is stabilizer space

Kitaev (1997); Dennis et al. (2002); Fowler et al. (2012);  
Cleland, Sci. Post Lecture Notes (2022)

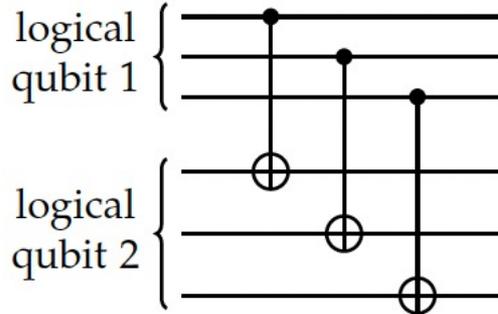


# Fault-tolerant quantum computations

- Compute directly on encoded logical qubits (no decoding necessary)
- Must prevent propagation and accumulation of errors
- Example: logical CNOT for 3-qubit bit flip code



Implementation A



Implementation B

Further reading:

- Nielsen, Chuang, Ch. 10.6
- Cleland, Sci. Post Lecture notes on fault-tolerant gate implementation in surface code

Assume that the only sources of errors are individual controlled-not gates which produce bit-flip errors in their outputs. Which of the two implementations is fault-tolerant?

# Summary of Quantum Error Correction part

- Quantum Error Correction protects quantum memory from a chosen set of correctable errors
  - Typically chosen as Pauli errors below some weight
- Quantum information is encoded nonlocally (locality assumption of the errors)
- Failure probability reduced for sufficient small failure rate of physical qubits
- Different codes exist  $[[n, k, d]]$ , specified by  $n$  = number of physical qubits per block,  $k$  = number of logical qubits per block,  $d$  = distance determines the maximal weight of errors that can be corrected:  $d = 2t + 1$
- Examples discussed: bit-flip, phase-flip, Shor code, surface code
- Outlook:
  - Classical codes, CSS codes, stabilizer codes, Qudit codes,
  - Bosonic codes for continuous variable systems
  - Fault-tolerant implementation of universal gate set

Check out:

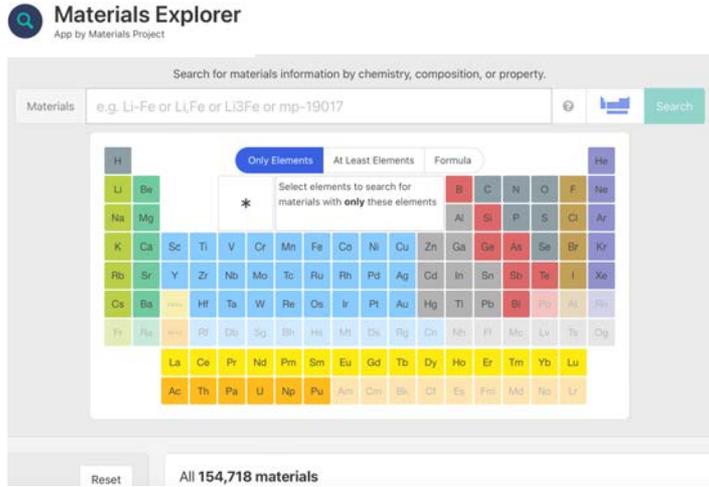
- [arthurpesah.me/blog](https://arthurpesah.me/blog)
- J. Roffe, arXiv:1907.11157
- Nielsen, Chuang, Ch. 10
- Preskill, Lecture Notes, Ch.6
- Rieffel, Polak “Introduction to QC” book

# Quantum Computing Applications in Condensed Matter Physics

Focus on near-term applications in pre-fault-tolerant era

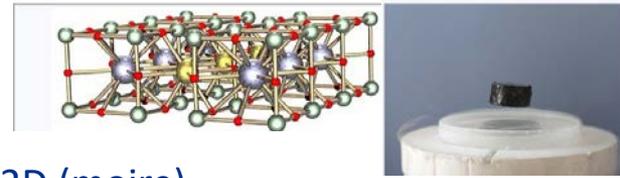
# Condensed Matter Physics & Materials Science

- Fueled by the many possibilities to combine atoms into (periodic) structures



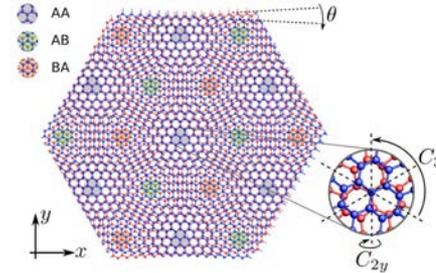
Unconventional superconductors

Yttrium barium copper oxide

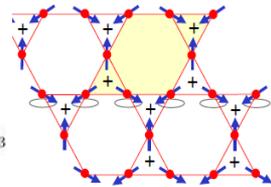


+ emergence due to electronic correlations

2D (moire) materials



Exotic magnets



- Goal: Understand & predict quantum materials' properties
  - Equilibrium behavior: phase diagrams, response functions at  $T=0$  and  $T>0$
  - Nonequilibrium behavior: driven systems, quenches, metastable states, kinetic pathways

# Common theoretical approach: separation of scales

- Workflow of building realistic effective models for solids
  - Start with atomistic description (theory of everything)

$$H' = T_e + V_{ee} + T_i + V_{ii} + V_{ei} + H_{so} + H_{hyper} + H_{rel} + H_{ext}$$

$$T_e + V_{ee} = - \sum_j \frac{\hbar^2}{2m_e} \nabla_j^2 + \frac{1}{2} \sum_{j \neq k} \frac{e^2}{|r_j - r_k|}$$

$$T_i + V_{ii} = - \sum_J \frac{\hbar^2}{2M_J} \nabla_J^2 + \frac{1}{2} \sum_{J \neq K} \frac{Z_J Z_K e^2}{|R_J - R_K|}$$

$$V_{ei} = - \sum_{j,J} \frac{Z_J e^2}{|r_j - R_J|},$$

- so: spin-orbit coupling
- hyper: hyperfine coupling
- rel: relativistic corrections
- ext: external fields

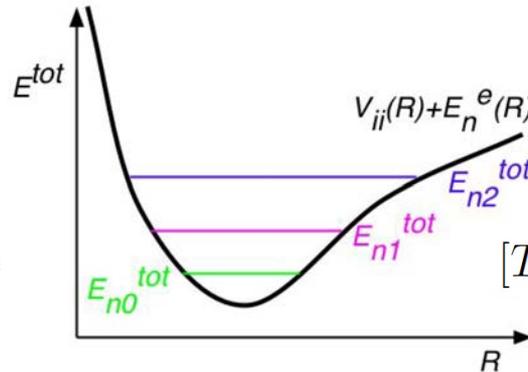
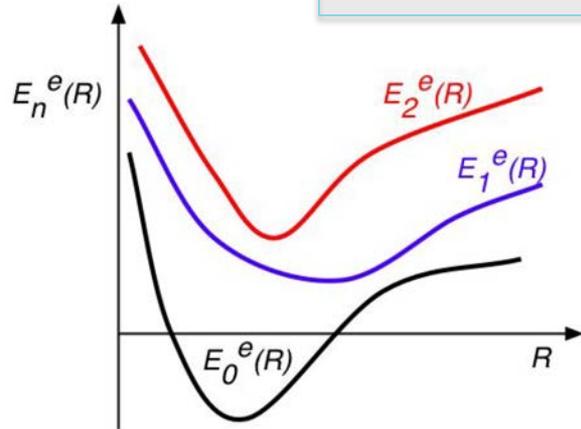
Neglect of simplicity on following slides, but can be quite important, e.g. in topological materials

# Common theoretical approach: separation of scales

- Workflow of building realistic effective models for solids
  - Start with atomistic description (theory of everything)  $\supset$  Born-Oppenheimer approximation
    - $\supset$  treat Coulomb interactions approximately, e.g. within Density Functional Theory (DFT)

$$[T_e + V_{ee} + T_i + V_{ii} + V_{ei}] \Phi(\mathbf{r}, \mathbf{R}) = E^{tot} \cdot \Phi(\mathbf{r}, \mathbf{R})$$

$$\Phi(\mathbf{r}, \mathbf{R}) \cong \Psi_n(\mathbf{r}; \mathbf{R}) \chi_{np}(\mathbf{R})$$



Oppenheimer, c. 1944

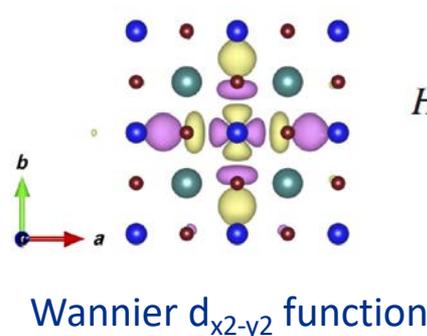
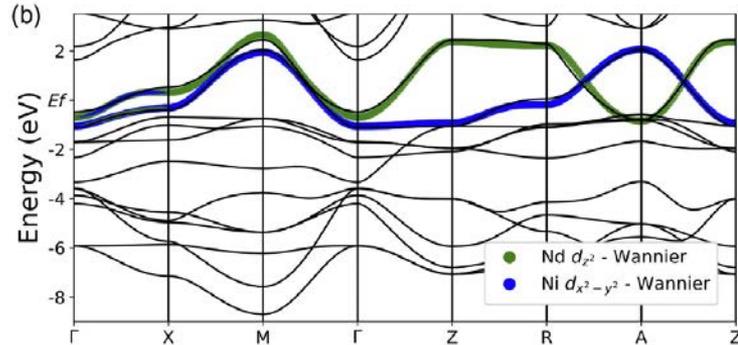
$$[T_i + V_{ii} + E_n^e(\mathbf{R})] \chi_{np}(\mathbf{R}) = E_{np}^{tot} \cdot \chi_{np}(\mathbf{R})$$

$$[T_e + V_{ee} + V_{ei}] \Psi_n(\mathbf{r}; \mathbf{R}) = E_n^e(\mathbf{R}) \cdot \Psi_n(\mathbf{r}; \mathbf{R})$$

# Downfolding to most important electronic orbitals

- Workflow of building realistic effective models for solids
  - Start with atomistic description (theory of everything)  $\supset$  Born-Oppenheimer approximation
    - $\supset$  treat Coulomb interactions approximately, e.g. within Density Functional Theory (DFT)
  - Downfold to low-energy states near Fermi surface (e.g. derive electronic Wannier wavefunctions) and build an effective (Hubbard-like) model
  - Effective model treats Coulomb interactions more accurately

Example for illustration: NdNiO<sub>2</sub>, taken from Been et al, PRX (2021).



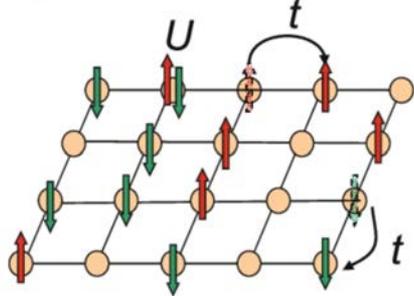
Multiorbital Hubbard model

$$H = \sum_{k,\sigma} (\epsilon_k^R n_{k,\sigma}^R + \epsilon_k^{\text{Ni}} n_{k,\sigma}^{\text{Ni}}) + U \sum_i n_{i,\uparrow}^{\text{Ni}} n_{i,\downarrow}^{\text{Ni}} + \sum_{k,i,\sigma} (V_{k,i} c_{k,\sigma}^\dagger d_{i,\sigma} + \text{H.c.}),$$

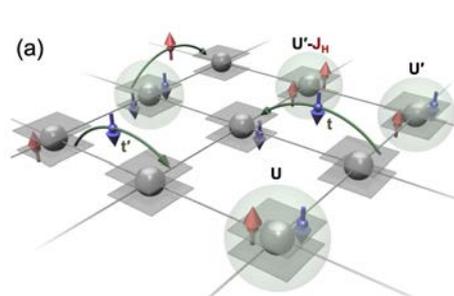
# Effective multiorbital Hubbard-Hund models & spin models

- Workflow of building realistic effective models for solids
  - Start with atomistic description (theory of everything)  $\supset$  Born-Oppenheimer approximation  $\supset$  treat Coulomb interactions approximately, e.g. within Density Functional Theory (DFT)
  - Downfold to low-energy states near Fermi surface (e.g. derive electronic Wannier wavefunctions) and build an effective (Hubbard-like) model
  - Effective model treats Coulomb interactions more accurately
  - Apply further approximations to the model, e.g. derive spin model in strong interaction limit
  - Compute phase diagram and response functions of effective model

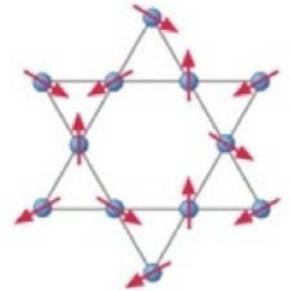
Single-band Hubbard model



Multiorbital Hubbard model



Strong coupling  
→  
obtain spin models



$$H = \sum_{i,j} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j + \dots$$

# Numerical approaches to effective models

- Solve a small instance of the effective model
  - Exact Diagonalization, Quantum Monte Carlo, Matrix Product States, Tensor Networks, QC
  - Extrapolate to larger systems

Example: Exact diagonalization of spin-1/2 models. Limited to  $N < 40$ .

$$|0\rangle = |\downarrow, \downarrow, \downarrow, \dots, \downarrow\rangle \quad (= 0 \dots 000)$$

$$|1\rangle = |\uparrow, \downarrow, \downarrow, \dots, \downarrow\rangle \quad (= 0 \dots 001)$$

$$|2\rangle = |\downarrow, \uparrow, \downarrow, \dots, \downarrow\rangle \quad (= 0 \dots 010)$$

$$|3\rangle = |\uparrow, \uparrow, \downarrow, \dots, \downarrow\rangle \quad (= 0 \dots 011)$$

$$H_{ij} = \langle i | H | j \rangle$$

$$i, j = 0, \dots, 2^N - 1$$

## The Lanczos method

If we need only the ground state and a small number of excitations

- can use “Krylov space” methods, which work for much larger matrices
- basis states with  $10^7$  states or more can be easily handled (30-40 spins)

## The Krylov space and “projecting out” the ground state

Start with an arbitrary state  $|\Psi\rangle$

- it has an expansion in eigenstates of  $H$ ; act with a high power  $\Lambda$  of  $H$

$$H^\Lambda |\Psi\rangle = \sum_n c_n E_n^\Lambda |n\rangle = E_0^\Lambda \left( c_0 |0\rangle + c_1 \left( \frac{E_1}{E_0} \right)^\Lambda |1\rangle + \dots \right)$$

For large  $\Lambda$ , if the state with largest  $|E_n|$  dominates the sum

- one may have to subtract a constant,  $H-C$ , to ensure ground state
- even better to use linear combination of states generated for different  $\Lambda$

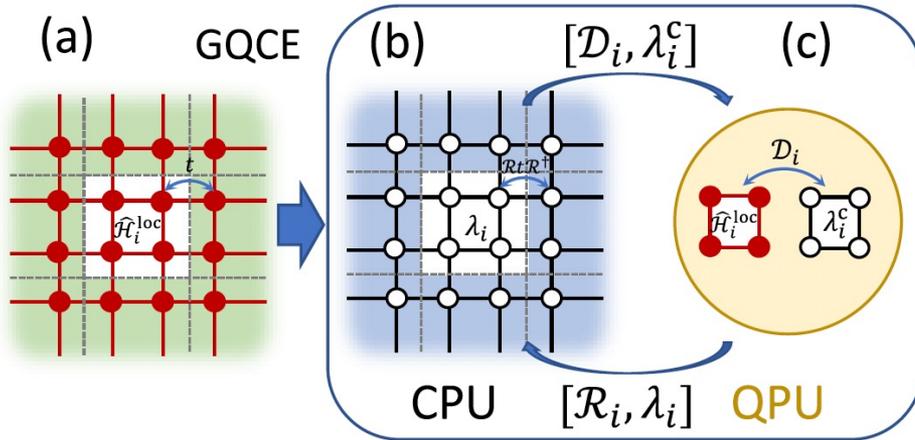
$$|\psi_a\rangle = \sum_{m=0}^{\Lambda} \psi_a(m) H^m |\Psi\rangle, \quad a = 0, \dots, \Lambda$$

- diagonalize  $H$  in this basis

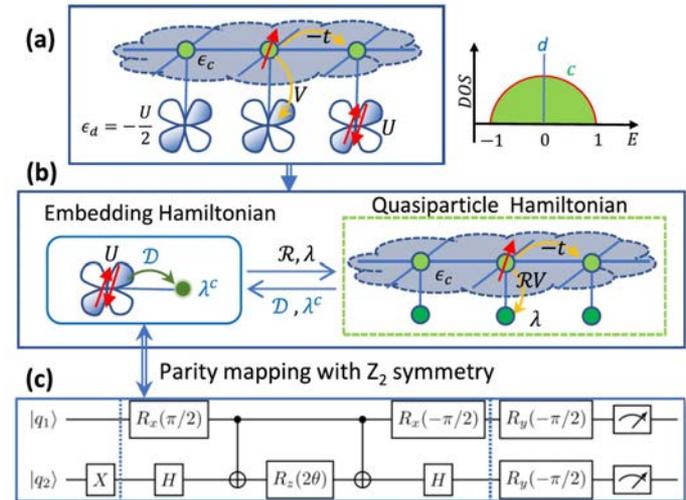
From Sandvik, Lecture Notes (2009)

# Numerical approaches to effective models

- Embedding Methods
  - Map lattice problem onto impurity model (= small part of the system) coupled to a reservoir (= the rest of the system)
  - Solve self-consistently using ED, QMC, etc to treat the interacting impurity model
  - Becomes exact as the size of the impurity cluster increases



From Yao, ..., PPO, PRR (2021).



# Opportunities for Quantum Computing

- QC avoids memory bottleneck of classical methods
  - Exponential growth of Hilbert space with system size limits classical methods such as ED
  - Instead: quantum computer can handle exponentially many wavefunction amplitudes (“Nature is not classical”, Feynman)

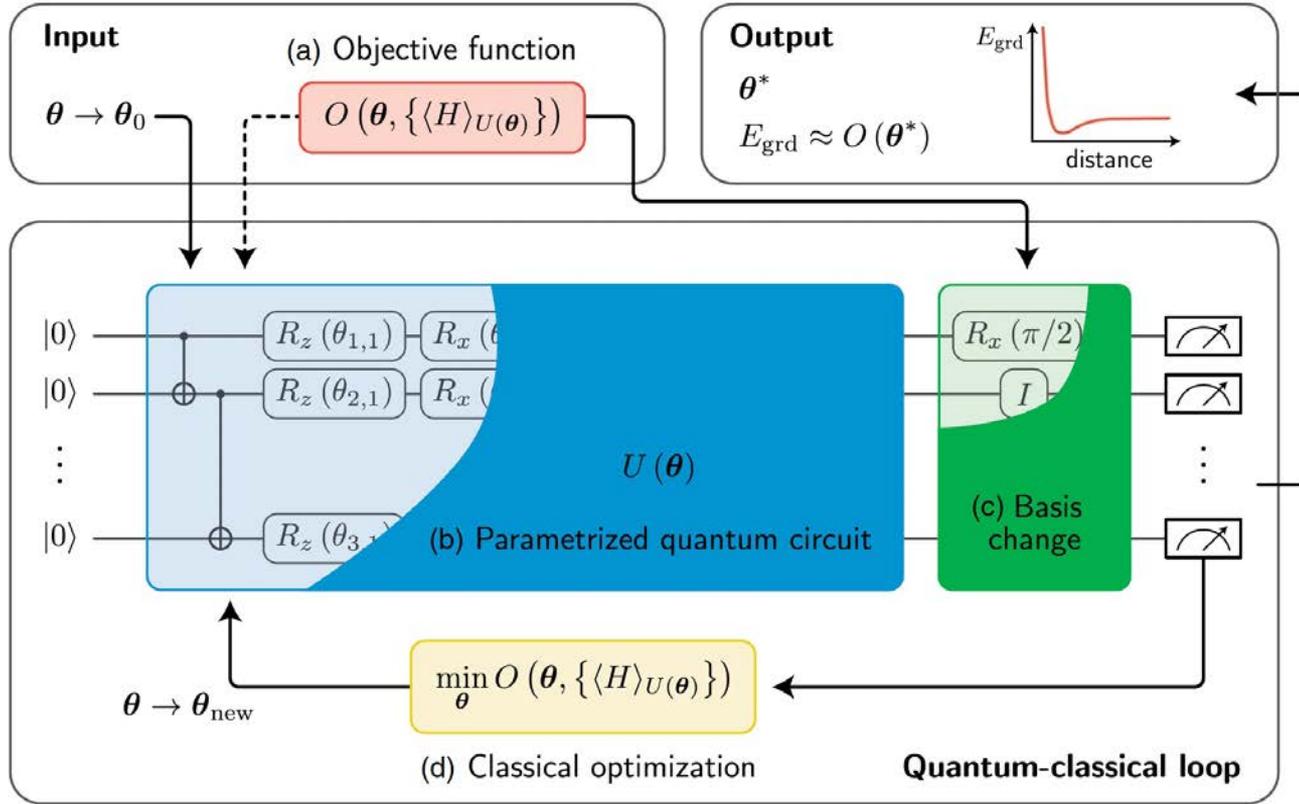
# Opportunities for Quantum Computing

- **QC avoids memory bottleneck of classical methods**
  - Exponential growth of Hilbert space with system size limits classical methods such as ED
  - Instead: quantum computer can handle exponentially many wavefunction amplitudes (“Nature is not classical”, Feynman)
- **QC can deal with highly entangled states**
  - Matrix Product States and Tensor Networks are efficient ways to compress a wavefunction
  - The memory requirement is set by the bond dimension that grows as  $e^S$ , where  $S$  is the entanglement entropy after tracing out part of the system
  - Essentially exact if the wavefunction carries a limited amount of entanglement: constant or logarithmically growing  $S$  with system size
  - Breaks down if  $S$  grows with system size (volume law)
  - Ground states are often area law entangled (1D gapped states)
  - Excited states generically carry volume law entanglement
    - Relevant at  $T>0$  & in nonequilibrium

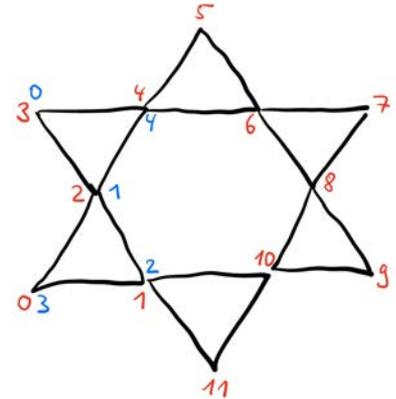
## Algorithms for Ground State Preparation

- Variational quantum eigensolver (VQE)
- Other notable directions (not covered here)
  - Quantum imaginary time evolution
    - Motta *et al.*, Nature Physics (2020); Ardle *et al.*, (2019)
    - Gomes *et al.*, Adv. Qu. Tech. (2021)
  - Subspace expansion techniques
    - McClean *et al.*, (2017)
    - Bharti *et al.*, Review of Modern Physics (2022).

# Variational Quantum Eigensolver



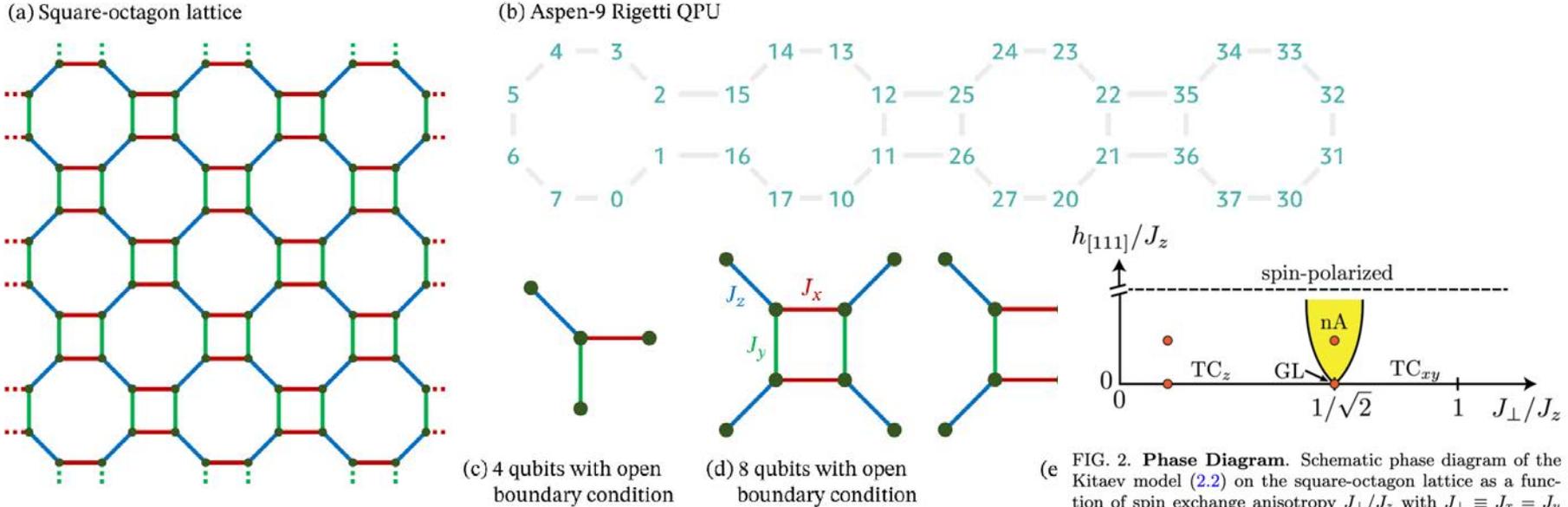
Example from tutorial yesterday (Kagome\_gs.ipynb):



Early work: Peruzzo et al., (2013)

From Bharti et al., RMP (2022)

# VQE for Kitaev square-octagon lattice model in magnetic field



Kitaev model on square-octagon lattice matches Rigetti's QPU geometry. No SWAP gates needed as connectivities match.

From:  
Li et al. (SQMS), PRR (2023).

# Parametrized quantum circuit (HVA ansatz)

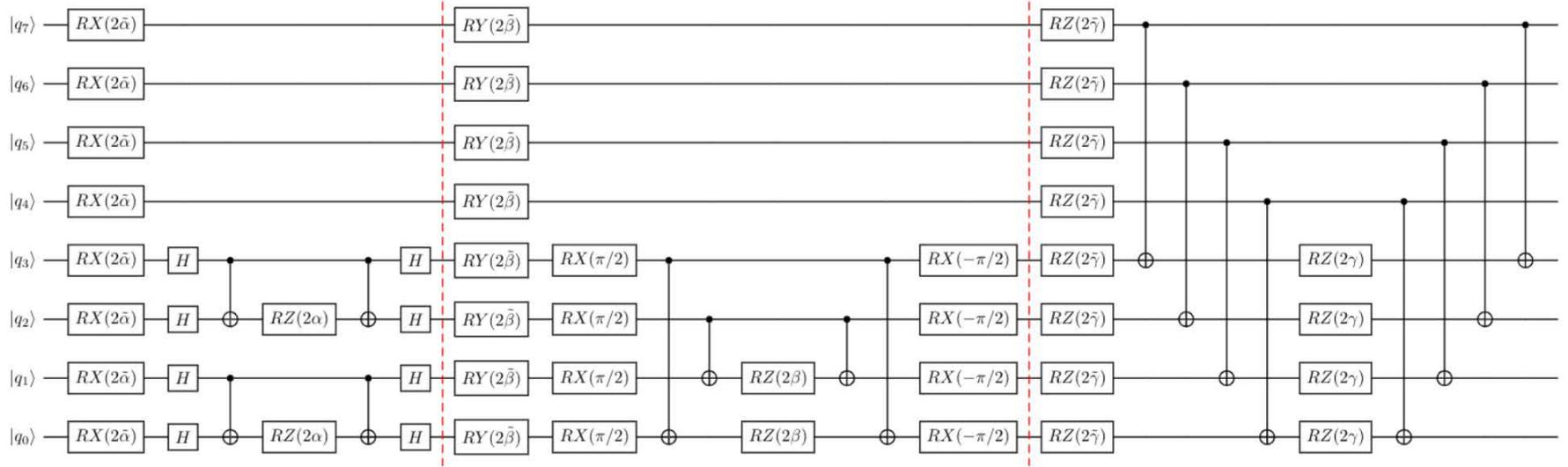
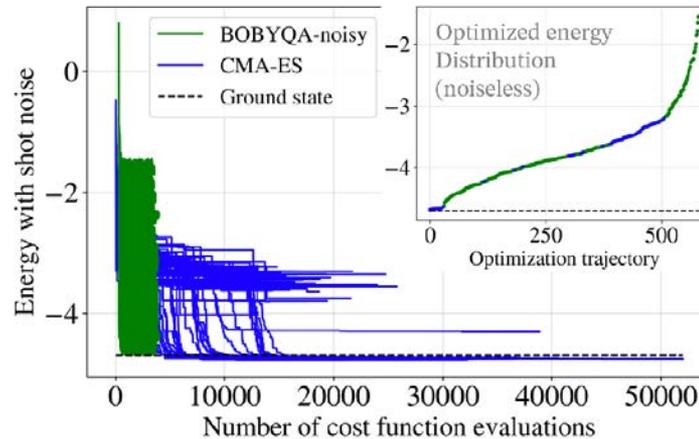
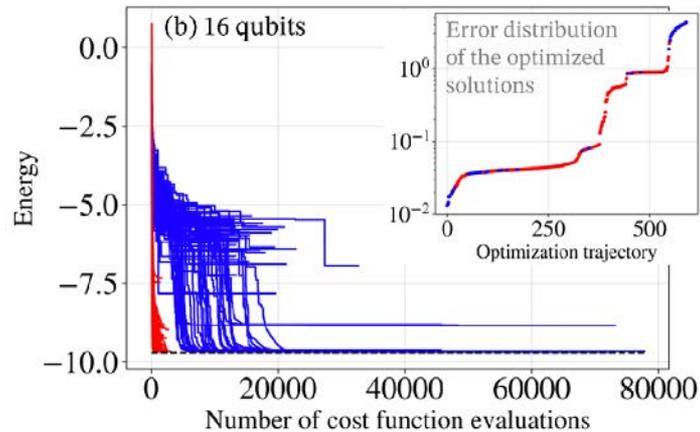


FIG. 3. **HVA with one layer on eight qubits.** The Hamiltonian Variational Ansatz (HVA) with one layer on eight qubits, split into commuting blocks. The first block corresponds to the operation  $e^{-i\bar{\alpha} \sum_q X_q} e^{-i\bar{\alpha} \sum_{(i,j) \in X\text{-links}} X_i X_j}$ , the second to  $e^{-i\bar{\beta} \sum_q Y_q} e^{-i\bar{\beta} \sum_{(i,j) \in Y\text{-links}} Y_i Y_j}$ , and the third to  $e^{-i\bar{\gamma} \sum_q Z_q} e^{-i\bar{\gamma} \sum_{(i,j) \in Z\text{-links}} Z_i Z_j}$ . For the circuit shown here, we used  $X\text{-links} = \{(q_0, q_1), (q_2, q_3)\}$ ,  $Y\text{-links} = \{(q_0, q_3), (q_1, q_2)\}$ , and  $Z\text{-links} = \{(q_0, q_4), (q_1, q_5), (q_2, q_6), (q_3, q_7)\}$ .

# Statevector and QASM simulations



Noiseless: 16 qubits  
 Noisy: 8 qubits  
 (8000 shots)

From:  
 Li et al. (SQMS),  
 PRR (2023).

## Conclusions

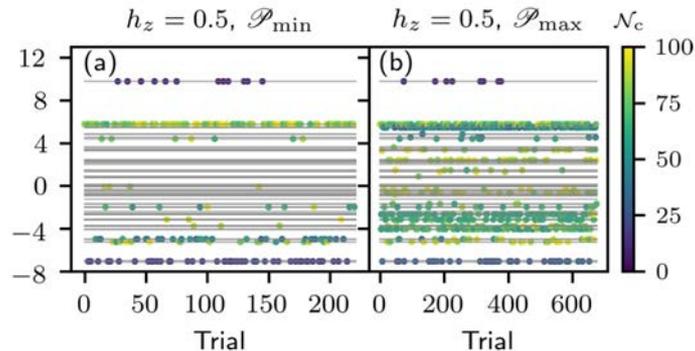
- Shot noise makes optimization more challenging
- Start from preoptimized solutions for larger systems
- Subspace expansion techniques avoid classical optimization loop (still require many measurements)

Optimizer	Error (noiseless)	Measured deviation	Cost function evaluations
BFGS, 501 initial values	0.45069	0.42052	mean: 747, max: 1994
BOBYQA, 501 initial values	0.27485	0.21843	mean: 471, max: 610
BOBYQA-noisy, 501 initial values	0.07989	-0.00453	mean: 3532, max: 4004
CMA-ES	0.02416	-0.06462	37570
CMA-ES, 80 initial values	0.01610	-0.07125	mean: 21042, max: 52000
Dual annealing	0.04534	-0.01631	60101
SPSA	0.00612	0.00879	100000 (cutoff)

# Variational quantum eigensolver for excited states

- Variational quantum eigensolver to prepare highly excited states (VQE-X)
- Minimize energy variance (instead of energy):

$$C(|\psi(\theta)\rangle) = \langle \psi(\theta) | H^2 | \psi(\theta) \rangle - \langle \psi(\theta) | H | \psi(\theta) \rangle^2$$



- Adaptive ansatz construction instead of fixed ansatz
- Nontrivial pool dependence

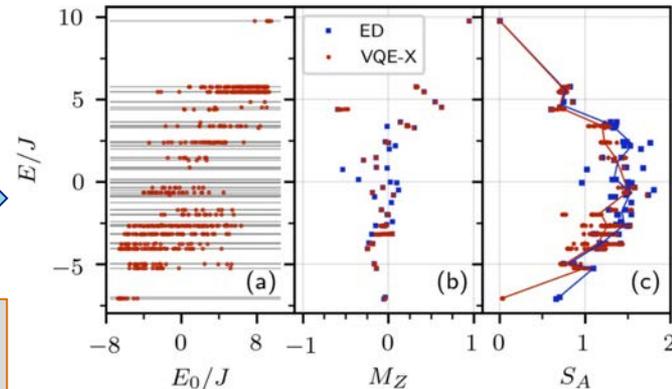


Can investigate properties of volume law highly excited states

Full coverage of energy spectrum for operator pool with long-range Pauli strings

$$\mathcal{P}_{\max} = \{Y_i\}_{i=1}^N \cup \{Y_i Z_j\}_{i,j=1}^N \cup \{Y_i X_j\}_{i,j=1}^N$$

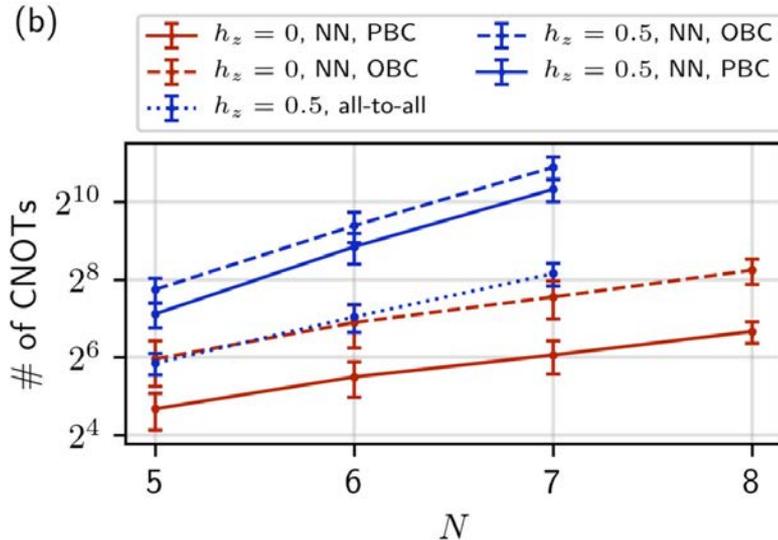
Zhang, Gomes, Yao, PPO, Iadecola, PRB **104**, 075159 (2021).



# Variational quantum eigensolver for excited states

- Variational quantum eigensolver to prepare highly excited states (VQE-X)
- Minimize energy variance (instead of energy):

$$\mathcal{C}(|\psi(\boldsymbol{\theta})\rangle) = \langle \psi(\boldsymbol{\theta}) | H^2 | \psi(\boldsymbol{\theta}) \rangle - \langle \psi(\boldsymbol{\theta}) | H | \psi(\boldsymbol{\theta}) \rangle^2$$



- Exponential scaling of # CNOTs with system size
- Relax convergence condition to represent microcanonical averages instead, see Pollock, PPO, Iadecola, arXiv:2301.04129 (2023).

Zhang, Gomes, Yao, PPO, Iadecola, PRB **104**, 075159 (2021).

# Algorithms for Quantum Dynamics Simulations

# Applications of real-time dynamics

- Investigate nonequilibrium behavior
  - Chemical reactions
  - Scattering experiments
  - Phase transformations, synthesis, metastable states, kinetic pathways, quenches
  - Fundamental questions: thermalization of a closed quantum system (eigenstate thermalization hypothesis, many-body localization)
  - Scaling behavior in nonequilibrium: transport, nonequilibrium dynamics of order parameters and correlation functions (coarsening, aging)
- Adiabatic state preparation
  - Preparing ground states of Hamiltonians

$$H(t) = H_0(1 - t/T) + H_1 t/T, \quad 0 \leq t \leq T$$



Here, we focus on far-from-equilibrium behavior

# Quantum dynamics simulations

Initial state

$$|\Psi(0)\rangle = \sum_n c_n |n\rangle$$



Energy eigenstate of many-body  $H$

Dynamics

$$|\Psi(t)\rangle = \sum_n c_n e^{-iE_n t} |n\rangle$$

Dynamics of an observable  $O$

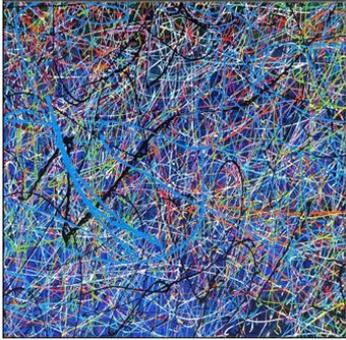
$$\langle O(t) \rangle = \sum_{n,m} c_n c_m^* e^{i(E_m - E_n)t} \langle m | O | n \rangle$$

$$|\Psi(t)\rangle = \sum_n c_n e^{-iE_n t} |n\rangle$$



- Classically hard due to rapid growth of entanglement in nonequilibrium for generic  $H$ 
  - Reason: contains highly excited states  $\triangleright$  Volume-law entanglement entropy.
  - Need many parameters to classically represent the quantum state
- Quantum simulators and computers can naturally time-evolve a quantum state

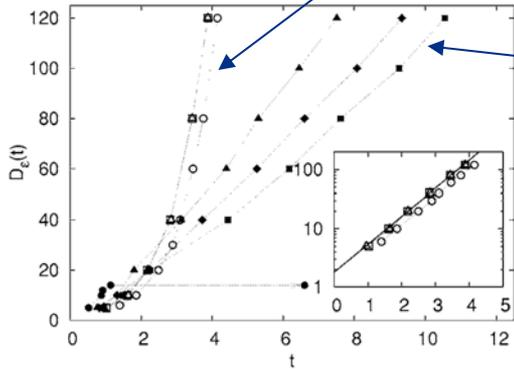
# Entanglement growth makes classical simulations hard



- Time-evolved state  $|\Psi(t)\rangle = \sum_n c_n e^{-iE_n t} |n\rangle$  is strongly entangled
- Contains highly excited states of  $H \succ$  Volume-law entanglement

Minimal **dimension** of matrix product operators (MPO) **grows exponentially in time** for nonintegrable models (mixed-field Ising model)

Bond dimension



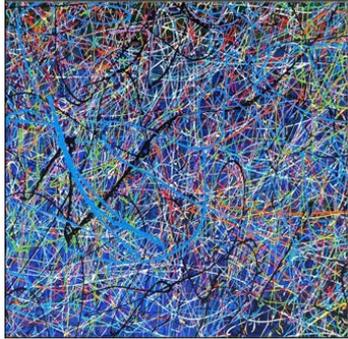
Growth is polynomially for **integrable** models (transverse-field Ising model)

$$H(h^x, h^z) = \sum_{j=0}^{n-2} \sigma_j^x \sigma_{j+1}^x + \sum_{j=0}^{n-1} (h^x \sigma_j^x + h^z \sigma_j^z)$$

FIG. 3.  $D_\epsilon(t)$  for local initial operators. We consider three cases  $O(0) = \sigma_{n/2}^{x,y,z}$  (empty circles, squares, and triangles), for nonintegrable evolution  $H_C$ , and four cases,  $O(0) = \sigma_{n/2}^{x,y}$  (full squares, diamonds),  $\sigma_{n/2-1}^z \sigma_{n/2}^y$  (full triangles) with infinite index, and  $O(0) = \sigma_{n/2-1}^z \sigma_{n/2}^x$  (full circles) with index 2, for integrable evolution  $H_R$ .

Prosen, Znidaric (2007)

# Entanglement growth makes classical simulations hard



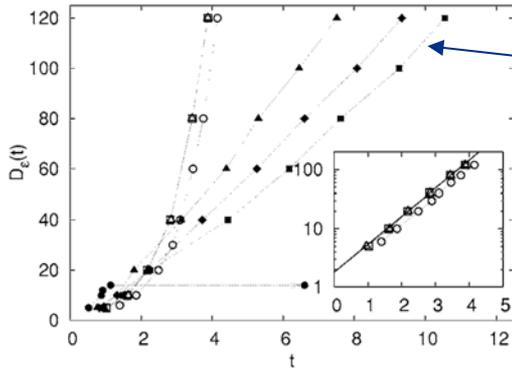
- Time-evolved state  $|\Psi(t)\rangle = \sum_n c_n e^{-iE_n t} |n\rangle$  is strongly entangled
- Contains highly excited states of  $H \rhd$  Volume-law entanglement

Minimal **dimension** of matrix product operators (MPO) **grows exponentially in time** for nonintegrable models (mixed-field Ising model)

Entanglement entropy  $S_A = -\text{Tr}[\rho_A \ln \rho_A]$

Reduced density matrix  $\rho_A = \text{Tr}_B \rho$

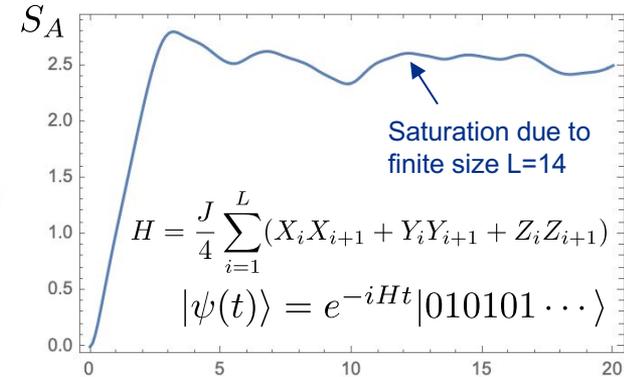
Bond dimension



Growth is polynomially for **integrable** models (transverse-field Ising model)

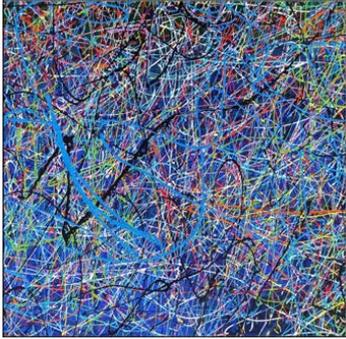
**Entanglement entropy grows ballistically  $\propto t$**  after global quench

## Quench dynamics in Heisenberg model



Prosen, Znidaric (2007)

# Dynamics simulations are opportunity for quantum advantage



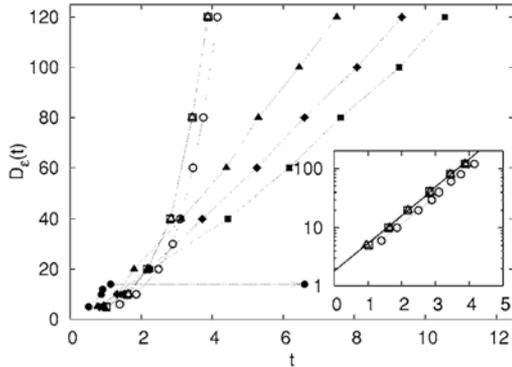
- Time-evolved state  $|\Psi(t)\rangle = \sum_n c_n e^{-iE_n t} |n\rangle$  is strongly entangled
- Contains highly excited states of  $H \gg$  Volume-law entanglement

**Entanglement = complexity of classical calculation**

Exponential growth of classical resources like the bond dimension in tensor networks. Exact diagonalization is limited by memory.

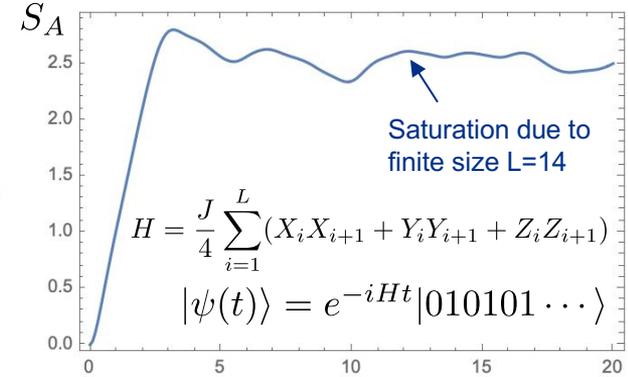
**Opportunity for quantum computing**

Bond dimension



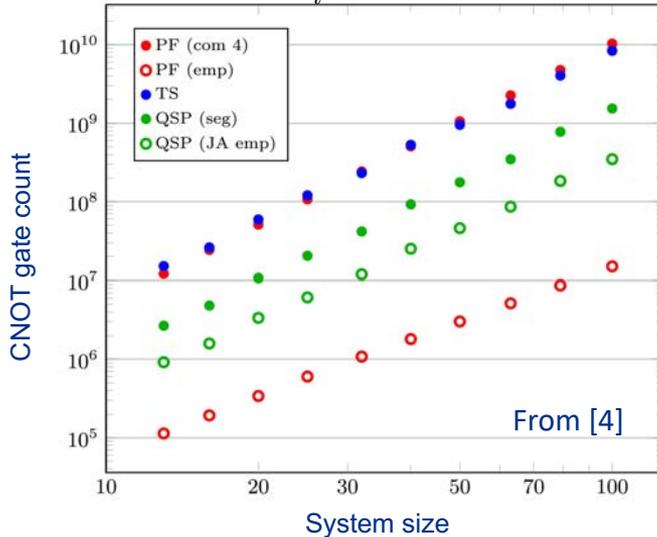
Prosen, Znidaric (2007)

Quench dynamics in Heisenberg model



# Overview of quantum algorithms for dynamics simulations

$$H = J \sum_i (Z_i Z_{i+1} + h_i Z_i)$$



- Lie-Suzuki-Trotter Product formulas (PF)
  - Simple yet limited to early times for current hardware noise
  - Trotter circuit depth scales as  $\mathcal{O}(t^{1+1/k})$  for fixed  $t_f$
- Algorithms with best asymptotic scaling have significant overhead
  - Linear combination of unitaries (TS) [1], quantum walk methods [2], quantum signal processing (QSP) [3]
- Hybrid quantum-classical variational methods [5,6]
  - Work with fixed gate depth  $\rightarrow$  ideally tailored for NISQ hardware
  - Trading gate depth for doing many QPU measurements

[1] Berry et al. (2015); [2] Childs (2004); [3] Low, Chuang (2017); [4] Childs et al., PNAS (2018); [5] Li, Benjamin, Endo, Yuan (2019); Y. Yao, PPO, T. Iadecola *et al.* (2021).

# Trotter Product Formula approach

- Trotter decomposition of time evolution operator
- Decompose Hamiltonian into sum of terms that include commuting operators
- Example: Mixed-field quantum Ising model

$$H = H_{ZZ} + H_Z + H_X = V \sum_{i=1}^{L-1} Z_i Z_{i+1} - 2V \sum_{i=2}^{L-1} Z_i - V(Z_1 + Z_L) + \Omega \sum_{i=1}^L X_i.$$

Time evolution operator in 1<sup>st</sup> order Trotter approximation

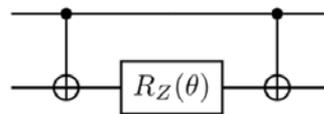
$$U(\Delta t) \approx e^{-iH_{ZZ}\Delta t} e^{-iH_Z\Delta t} e^{-iH_X\Delta t}$$

$$R_X(\theta_i^X) = e^{-i\theta_i^X X_i/2}$$

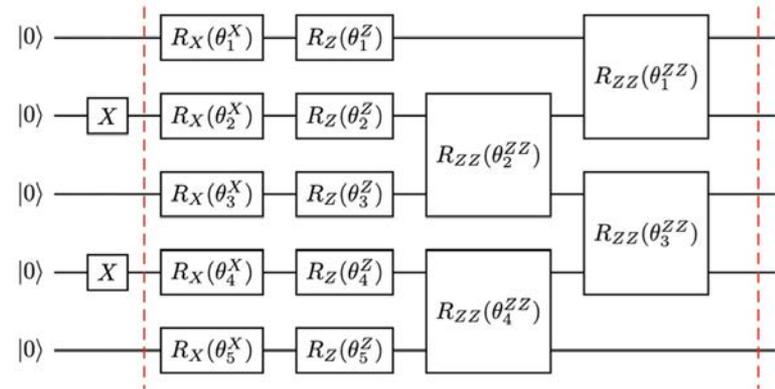
$$R_Z(\theta_i^Z) = e^{-i\theta_i^Z Z_i/2}$$

$$R_{ZZ}(\theta_i^{ZZ}) = e^{-i\theta_i^{ZZ} Z_i Z_{i+1}/2}$$

Standard decomposition of RZZ into CNOT and RZ



One step of Trotter circuit in L=5 system, starting in Neel state.



# NISQ Trotter simulations of mixed field Ising model

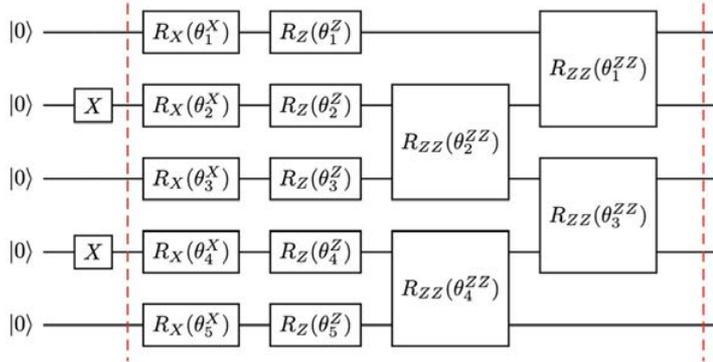
- Benchmark Trotter simulations of mixed-field Ising model on current NISQ hardware

$$H = H_{ZZ} + H_Z + H_X = V \sum_{i=1}^{L-1} Z_i Z_{i+1} - 2V \sum_{i=2}^{L-1} Z_i - V(Z_1 + Z_L) + \Omega \sum_{i=1}^L X_i.$$

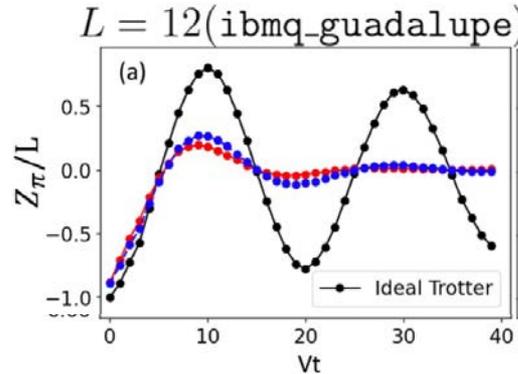
Displays many-body coherent dynamics for  $V \gg \Omega$

Bernien, Lukin (2017)

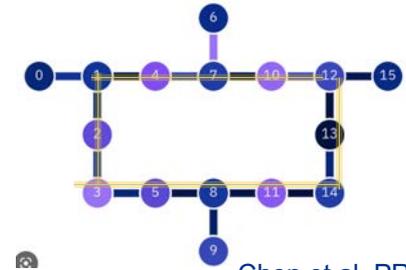
- Naïve Trotter simulation limited to short times due to finite device coherence time



One step of Trotter circuit in  $L=5$  system, starting from Neel state.



Trotter simulation on QPU  
ibmq\_guadalupe  
12 qubits, periodic boundary conditions



Chen et al, PRR (2022)

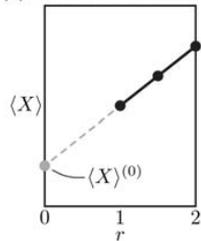
**Use pulse level control and error mitigation to extend simulation time**

# Pulse level control and quantum error mitigation (QEM)

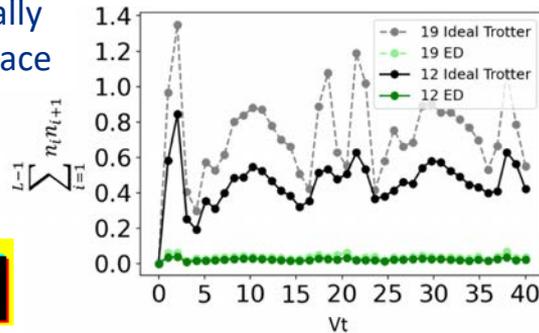
- Pulse level control allows to make optimal use of finite coherence time on device
  - Direct implementation of  $RZZ$  gate via cross-resonance pulse  $\triangleright$  cuts program in half
- Quantum error mitigation further extends final time of simulation
  - Readout error mitigation (tensor product assumption):  $C_{\text{ideal}} = M^{-1}C_{\text{noisy}}$ .  $M = \begin{bmatrix} 1 - \epsilon_1 & \eta_1 \\ & \eta_1 \end{bmatrix} \otimes \dots$
  - Zero-noise extrapolation (ZNE) after increasing noise via gate folding  $G \mapsto GG^\dagger G$ .
  - Pauli twirling: transforming noise to Pauli error channel  $\mathcal{N}_{\Lambda} \rho = \sum_h E_h \rho E_h^\dagger$   $E_h = \sum_{a=0}^3 \sum_{b=0}^3 \alpha_{h;a,b} \sigma_c^a \sigma_t^b$
  - Dynamical decoupling: apply  $X(\pi)$  and  $X(-\pi)$  during qubit idle time
  - Symmetry-based postselection: physically motivated

Postselection into physically relevant part of Hilbert space

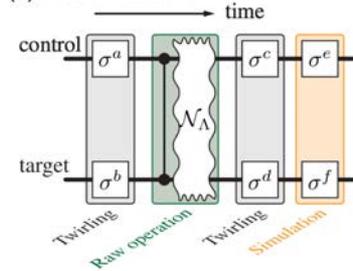
(a) Error reduction



ZNE using



(b) Error simulation

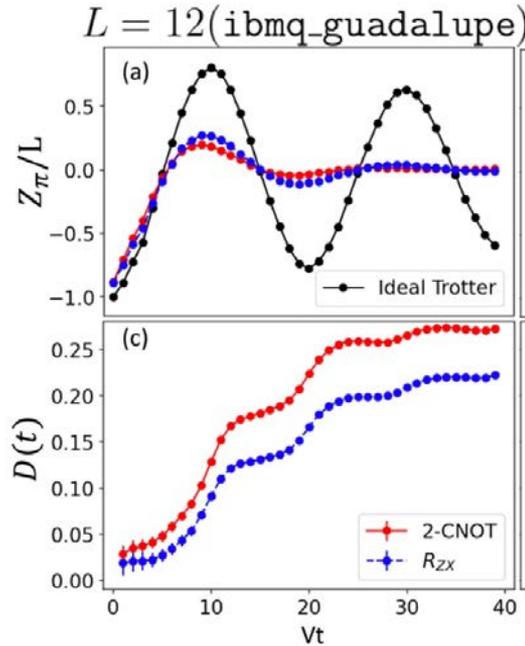


$$\tilde{\mathcal{N}}_{\Lambda} = F_{\Lambda}[1] + \sum_{(a,b) \neq (0,0)} \epsilon_{a,b} [\sigma_c^a \sigma_t^b],$$

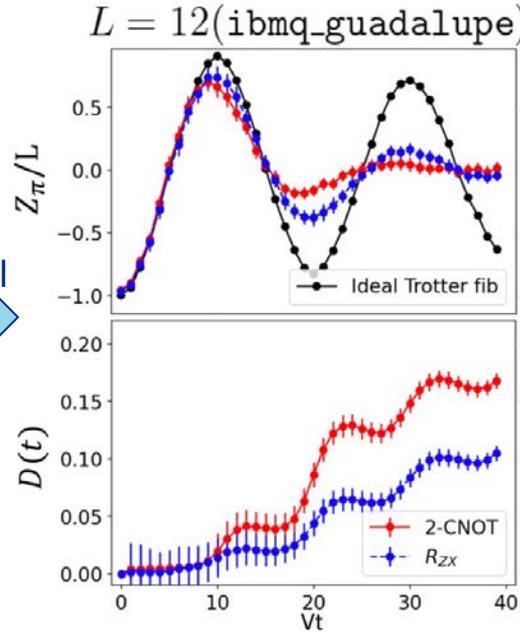
Pauli twirling converts noise to stochastic form  $\triangleright$  justification for ZNE

Wallmann, Emerson; Li, Benjamin (2017)

# Extending simulation time using pulse control and QEM

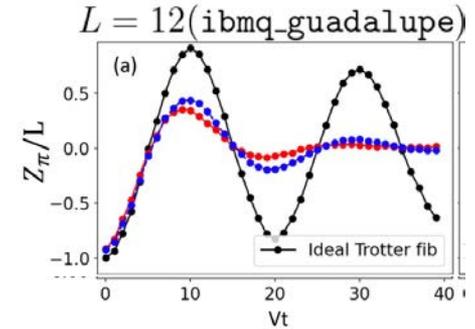


Pulse control  
  
 QEM



Chen *et al.*, PRR (2022)

Postselection only



See also the work by the IBM group

Article | Published: 06 February 2023

**Scalable error mitigation for noisy quantum circuits produces competitive expectation values**

Youngeok Kim, Christopher J. Wood, Theodore J. Yoder, Seth T. Merkel, Jay M. Gambetta, Kristan Temme & Abhinav Kandala

Nature Physics 19, 752–759 (2023) | Cite this article

**Pulse and zero-noise extrapolation (ZNE) are effective strategies to reduce errors.  
 But: ZNE is heuristic and cannot extend simulation time beyond coherence time of device.**

# Scaled up simulations: approaching quantum utility regime

- Recent Nature publication from the IBM group: transverse-field Ising model dynamics simulations on 127 qubits
- Uses Zero-Noise Extrapolation (ZNE) informed by sparse Pauli noise tomography

Article | [Open Access](#) | [Published: 14 June 2023](#)

## Evidence for the utility of quantum computing before fault tolerance

[Youngseok Kim](#) ✉, [Andrew Eddins](#) ✉, [Sajant Anand](#), [Ken Xuan Wei](#), [Ewout van den Berg](#), [Sami Rosenblatt](#), [Hasan Nayfeh](#), [Yantao Wu](#), [Michael Zaletel](#), [Kristan Temme](#) & [Abhinav Kandala](#) ✉

[Nature](#) **618**, 500–505 (2023) | [Cite this article](#)

**88k** Accesses | **6** Citations | **631** Altmetric | [Metrics](#)

Hamiltonian

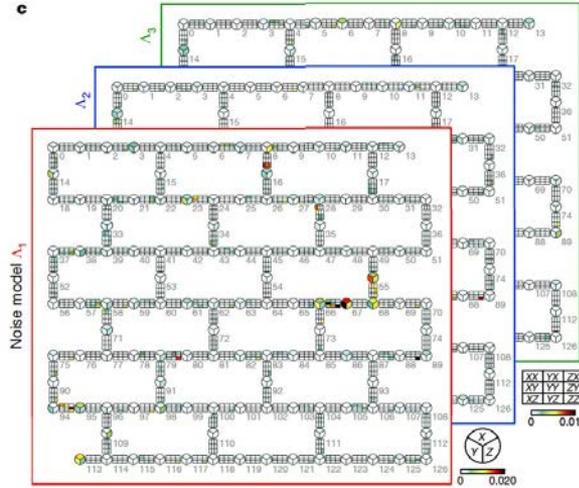
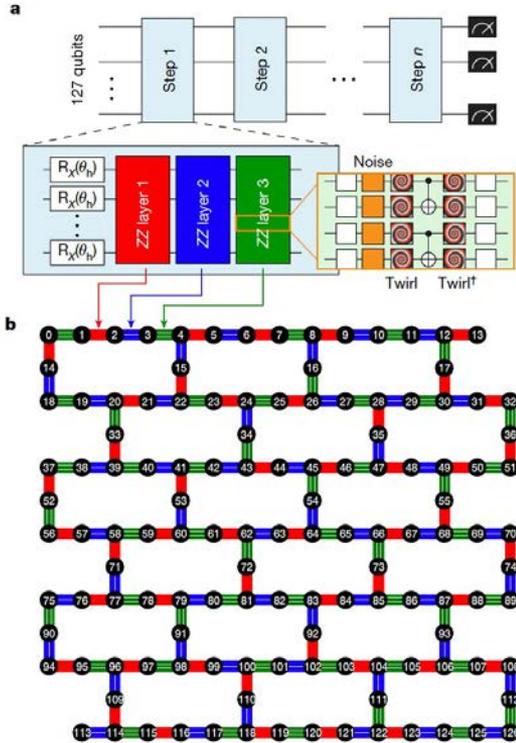
$$H = -J \sum_{\langle i,j \rangle} Z_i Z_j + h \sum_i X_i,$$

Initial state

$$|\psi(t=0)\rangle = |0\rangle^{\otimes 127}$$

- Stimulated several classical simulation works, e.g. Tindall et al., arXiv:2306.14887; Begusic, Chan, arXiv:2306.16372.
- Demonstration of fruitful interplay of quantum and classical simulations

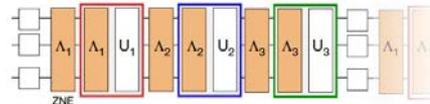
# Trotter dynamics of 127 qubit transverse-field Ising model



**d**

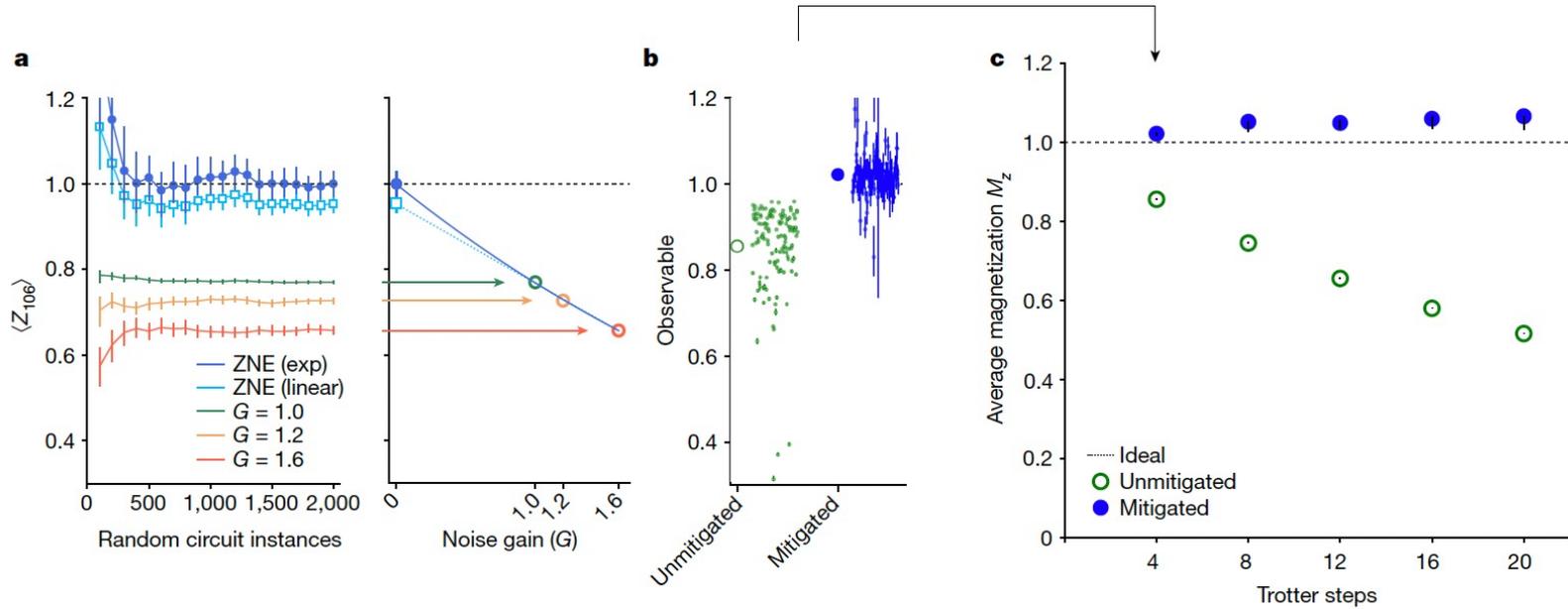
$$e^{-iH_{ZZ}\delta t} = \prod_{\langle i,j \rangle} e^{iJ\delta t Z_i Z_j} = \prod_{\langle i,j \rangle} R_{ZZ}(-2J\delta t)$$

$$e^{-iH_X\delta t} = \prod_i e^{-ih\delta t X_i} = \prod_i R_{X_i}(2h\delta t),$$



- Trotter circuit contains three layers
- Pauli twirling transforms the noise to Pauli noise
- Efficient noise tomography using a sparse Pauli noise model ansatz
- Can precisely tune the noise for ZNE since noise is well characterized (probabilistic noise amplification)

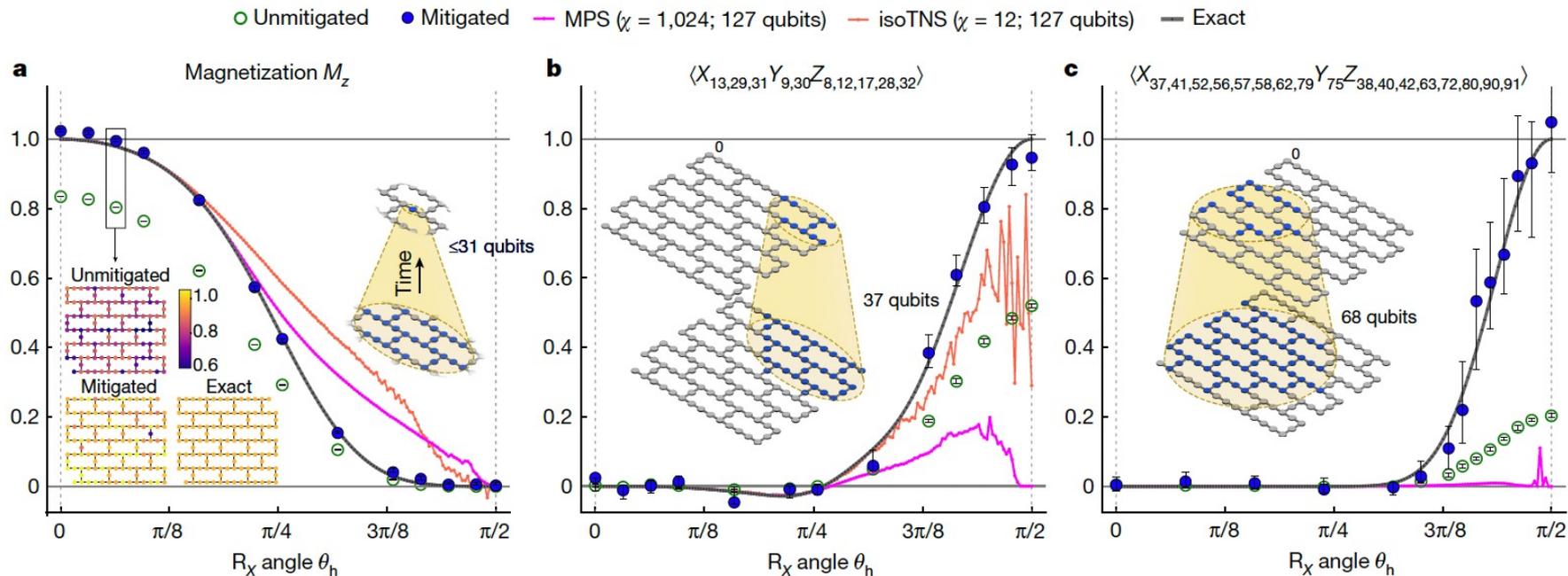
# Trotter dynamics of 127 qubit transverse-field Ising model



**Fig. 2 | Zero-noise extrapolation with probabilistic error amplification.** Mitigated expectation values from Trotter circuits at the Clifford condition  $\theta_h = 0$ . **a**, Convergence of unmitigated ( $G = 1$ ), noise-amplified ( $G > 1$ ) and noise-mitigated (ZNE) estimates of  $\langle Z_{106} \rangle$  after four Trotter steps. In all panels, error bars indicate 68% confidence intervals obtained by means of percentile bootstrap. Exponential extrapolation (exp, dark blue) tends to outperform

linear extrapolation (linear, light blue) when differences between the converged estimates of  $\langle Z_{106} \rangle_{G \neq 0}$  are well resolved. **b**, Magnetization (large markers) is computed as the mean of the individual estimates of  $\langle Z_q \rangle$  for all qubits (small markers). **c**, As circuit depth is increased, unmitigated estimates of  $M_z$  decay monotonically from the ideal value of 1. ZNE greatly improves the estimates even after 20 Trotter steps (see Supplementary Information II for ZNE details).

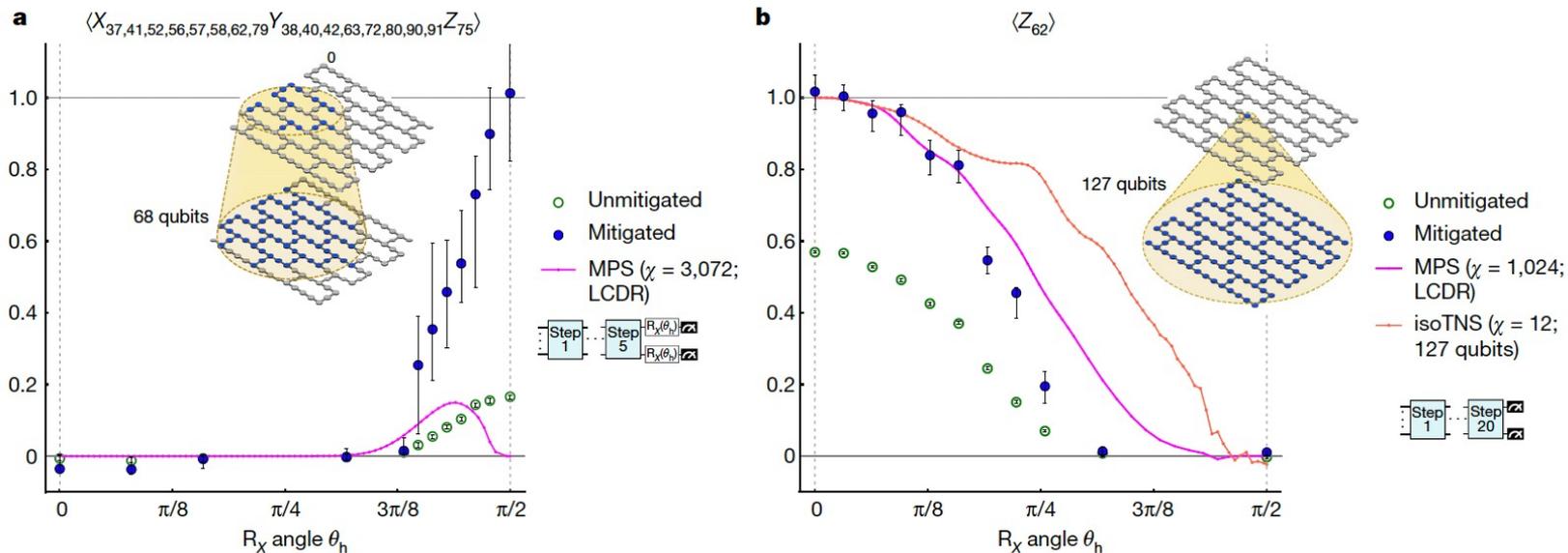
# Classically verifiable regime



**Fig. 3 | Classically verifiable expectation values from 127-qubit, depth-15 Clifford and non-Clifford circuits.** Expectation value estimates for  $\theta_h$  sweeps

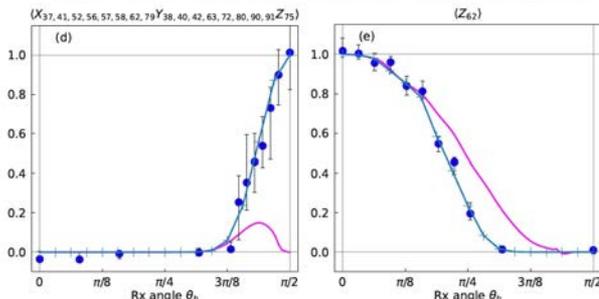
Upper insets in all panels illustrate causal light cones, indicating in blue the final qubits measured (top) and the nominal set of initial qubits that can

# Classically “challenging” regime



**Fig. 4 | Estimating expectation values beyond exact verification.** Plot

Even if this work is not yet beyond classical capabilities, it is clear that Trotter dynamics is a leading candidate for quantum advantage



Classical simulations using sparse Pauli dynamics method (Begusic, Chan, arXiv (2023)).

# Variational Quantum Dynamics

Variational form of quantum state

$$|\Psi[\boldsymbol{\theta}]\rangle = \prod_{\mu=0}^{N_{\boldsymbol{\theta}}-1} e^{-i\theta_{\mu}\hat{A}_{\mu}} |\Psi_0\rangle.$$

Variational parameters evolve in time

Von Neumann equation

$$\frac{d\rho}{dt} = \mathcal{L}(\rho) = -i[\mathcal{H}, \rho]$$

MacLachlan distance b/w exact  
and variational time evolution

$$L^2 \equiv \left\| \sum_{\mu} \frac{\partial \rho[\boldsymbol{\theta}]}{\partial \theta_{\mu}} \dot{\theta}_{\mu} - \mathcal{L}[\rho] \right\|^2$$

$$= \sum_{\mu\nu} M_{\mu\nu} \dot{\theta}_{\mu} \dot{\theta}_{\nu} - 2 \sum_{\mu} V_{\mu} \dot{\theta}_{\mu} + \text{Tr}[\mathcal{L}[\rho]^2].$$

[1] Li, Benjamin, Endo, Yuan (2019).

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Minimize  $L^2$

M measures state change under parameter change

$$M_{\mu\nu} \equiv \text{Tr} \left[ \frac{\partial \rho[\theta]}{\partial \theta_{\mu}} \frac{\partial \rho[\theta]}{\partial \theta_{\nu}} \right]$$

$$V_{\mu} \equiv \text{Tr} \left[ \frac{\partial \rho[\theta]}{\partial \theta_{\mu}} \mathcal{L}[\rho] \right]$$

V depends on Hamiltonian

EOM for variational parameters

$$\sum_{\nu} M_{\mu\nu} \dot{\theta}_{\nu} = V_{\mu}.$$

Matrix  $M_{\mu\nu}$  and vector  $V_{\mu}$  measured on QPU

Scaling to large system sizes challenging as  $N_{meas} \propto N_{\theta}^2$  and  $N_{\theta}$  can grow exponentially with system size for nonintegrable models

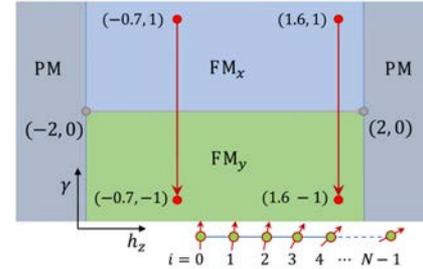
👉 Opportunity at early times and for integrable models

[1] Li, Benjamin, Endo, Yuan (2019).

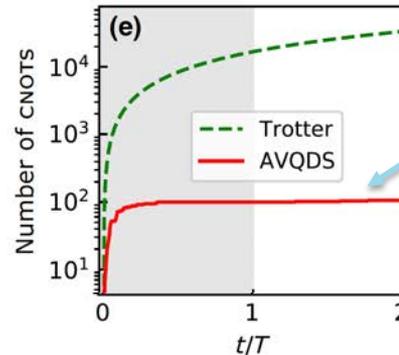
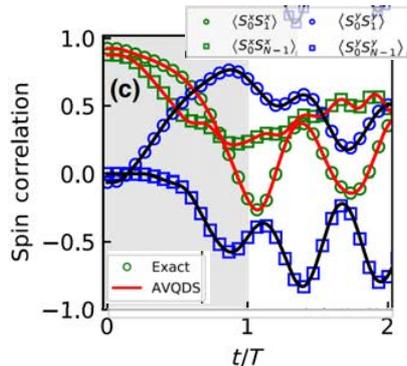
# Application: continuous quench in spin chain

- Linear quench of anisotropic XY chain in transverse magnetic field

$$\hat{\mathcal{H}} = -J \sum_{i=0}^{N-2} \left[ (1 + \gamma) \hat{X}_i \hat{X}_{i+1} + (1 - \gamma) \hat{Y}_i \hat{Y}_{i+1} \right] + h_z \sum_{i=0}^{N-1} \hat{Z}_i \quad \text{with} \quad \gamma(t) = 1 - \frac{2t}{T}$$



- Follows exact solution during and after quench, shown for  $N=8$
- Circuit depth saturates at 100 CNOTs  $\ll$  Trotter circuit depth  $[[10]]^4$  CNOTs
- Simulate system with gate depth independent of time  $t \gg$  can simulate to arbitrary times!



Y. Yao, .., PPO, PRX Quantum (2021)

# Summary of CMP applications part

- Condensed Matter Physics provides a rich set of problems that are relevant for domain specialists in physics, chemistry, material science
- Problems are often tunable and thus ideal for benchmarking and tuning into the quantum advantage regime
- Promising directions:
  - Simulation of nonequilibrium quantum dynamics
    - Trotter product formula approach is conceptually simple: combined with quantum error mitigation this is good candidate to reach beyond classical regime soon (maybe already)
    - Multi-product formulas (2207.11268, 2212.14144)
    - Variational methods can in principle extend simulation time further out, but suffer from measurement overhead and difficult classical optimization task
  - Subspace expansion methods avoid classical optimization and are closer in spirit to ED: not covered here, but promising approach both for ground state and dynamics simulations
  - Finite temperature simulations in  $d > 1$ : hard classically, so worth trying QC approaches

**Thanks for your attention!**