THE UNIVERSITY OF MELBOURNE

Noise-robust ground state energy estimates from deep quantum circuits

Harish Vallury

Lloyd Hollenberg
Charles Hill

AIP 2022

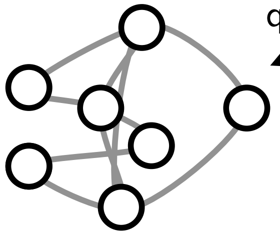
Overview

- Variational quantum computing and noise
- Ground state energy estimate from Hamiltonian moments
- The quantum computed moments (QCM) approach
- Application of QCM to Heisenberg model
- QCM noise robustness analysis
- Conclusion

IBM Quantum Network Hub
at the University of Melbourne

Hybrid quantum variational approach

Problem



e.g. molecule*, quantum magnet

Hamiltonian

$$H = \sum_i w_i \hat{P}_i$$

$$\hat{P}_i \in \{I, X, Y, Z\}^{\otimes N}$$

Solution

Ground state $|\psi_0\rangle$

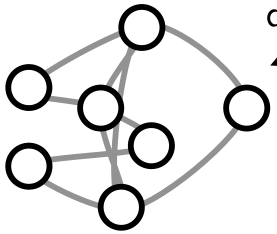
Ground energy E_0

*VQE method:
Peruzzo *et al.*, Nature communications **5**, 4213 (2014).
Kandala *et al.*, Nature **549**, 242–246 (2017).

Hybrid quantum variational approach

Problem

e.g. molecule*, quantum magnet



Hamiltonian

$$H = \sum_i w_i \hat{P}_i$$

$$\hat{P}_i \in \{I, X, Y, Z\}^{\otimes N}$$

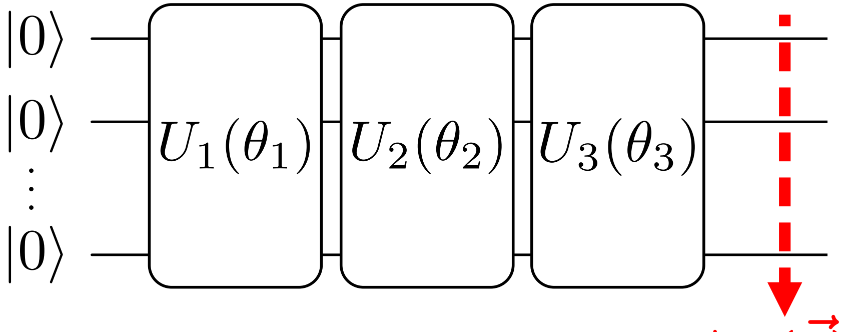
Solution

Ground state $|\psi_0\rangle$

Ground energy E_0

Role of quantum computer:

- Prepare trial state $|\psi(\vec{\theta})\rangle$



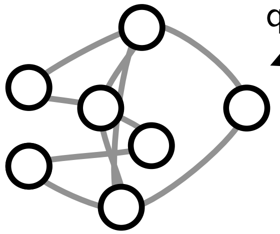
trial state $|\psi(\vec{\theta})\rangle$

*VQE method:
Peruzzo *et al.*, Nature communications **5**, 4213 (2014).
Kandala *et al.*, Nature **549**, 242–246 (2017).

Hybrid quantum variational approach

Problem

e.g. molecule*, quantum magnet



Hamiltonian

$$H = \sum_i w_i \hat{P}_i$$

$$\hat{P}_i \in \{I, X, Y, Z\}^{\otimes N}$$

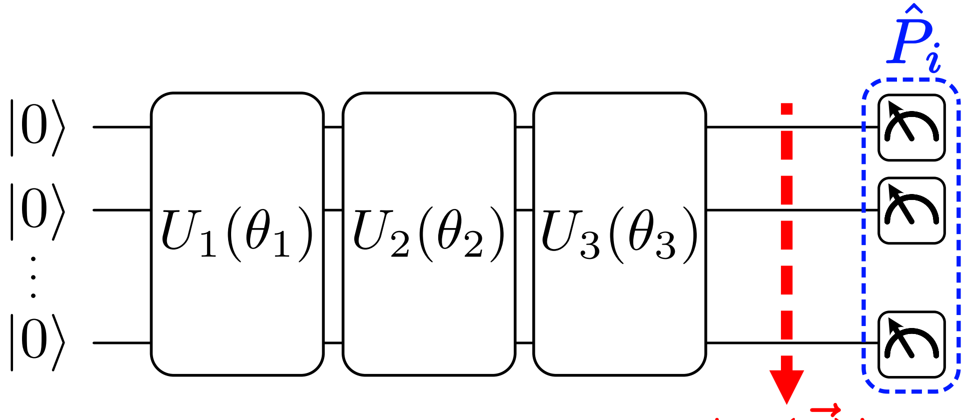
Solution

Ground state $|\psi_0\rangle$

Ground energy E_0

Role of quantum computer:

- Prepare trial state $|\psi(\vec{\theta})\rangle$
- Measure energy expectation value $\langle H \rangle_{\vec{\theta}}$ (cost function)

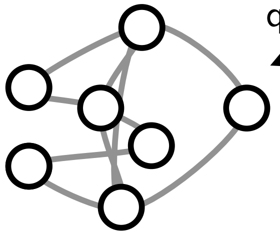


trial state $|\psi(\vec{\theta})\rangle$

*VQE method:
Peruzzo *et al.*, Nature communications **5**, 4213 (2014).
Kandala *et al.*, Nature **549**, 242–246 (2017).

Hybrid quantum variational approach

Problem e.g. molecule*, quantum magnet



Hamiltonian

$$H = \sum_i w_i \hat{P}_i$$

$$\hat{P}_i \in \{I, X, Y, Z\}^{\otimes N}$$

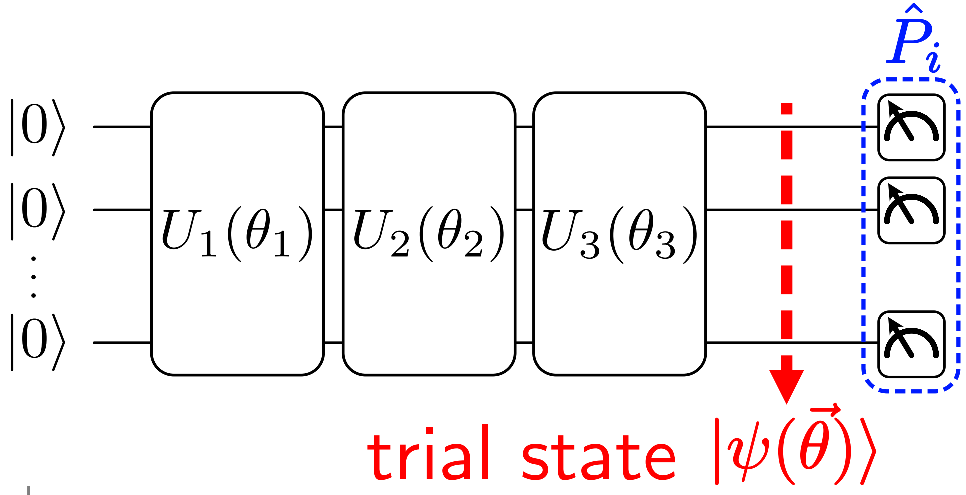
Solution

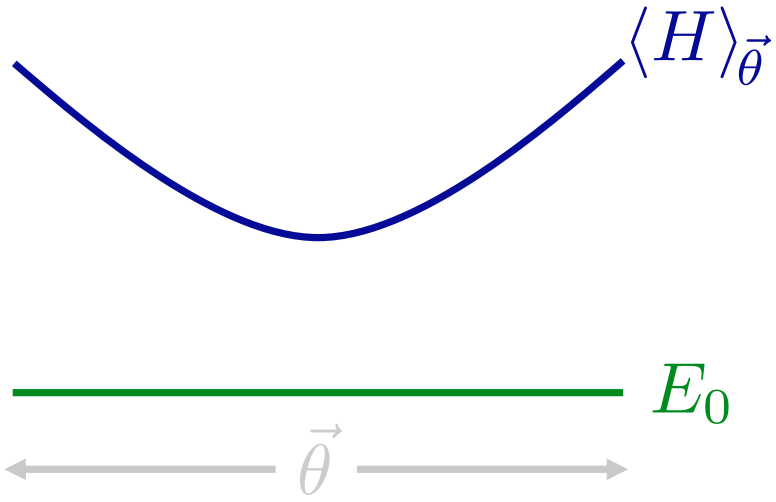
Ground state $|\psi_0\rangle$

Ground energy E_0

Role of quantum computer:

- Prepare trial state $|\psi(\vec{\theta})\rangle$
- Measure energy expectation value $\langle H \rangle_{\vec{\theta}}$ (cost function)



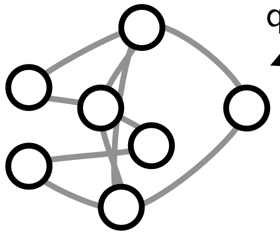


*VQE method:
Peruzzo *et al.*, Nature communications **5**, 4213 (2014).
Kandala *et al.*, Nature **549**, 242–246 (2017).

Hybrid quantum variational approach

Problem

e.g. molecule*, quantum magnet



Hamiltonian

$$H = \sum_i w_i \hat{P}_i$$

$$\hat{P}_i \in \{I, X, Y, Z\}^{\otimes N}$$

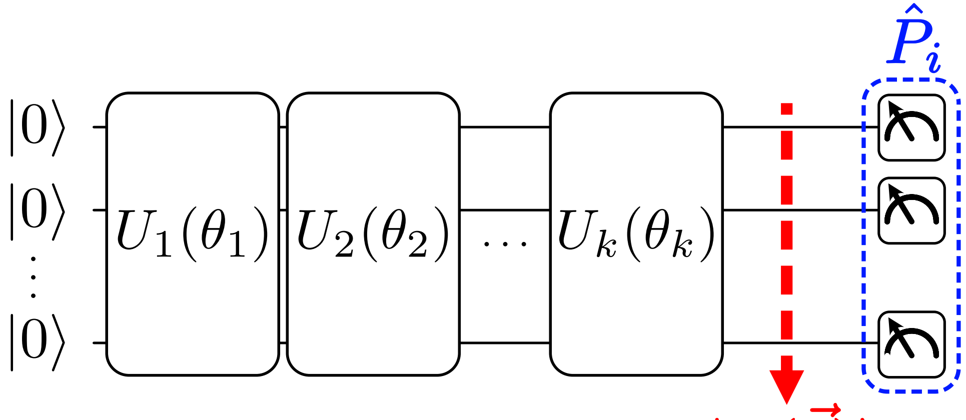
Solution

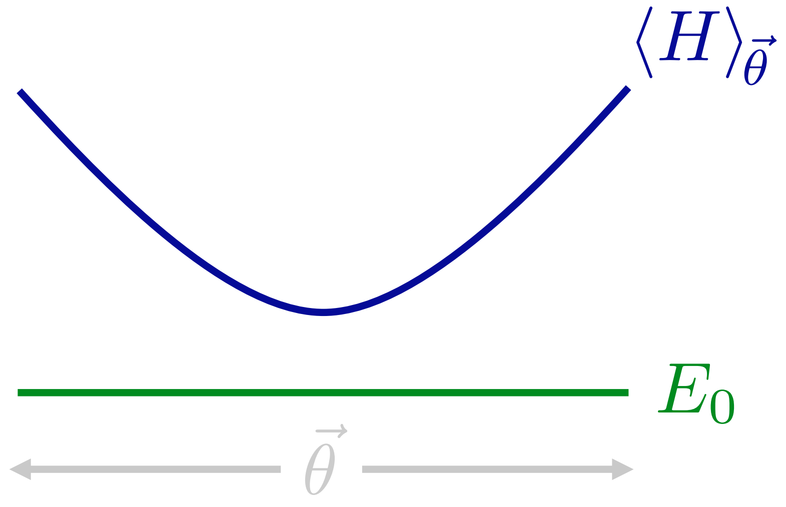
Ground state $|\psi_0\rangle$

Ground energy E_0

Role of quantum computer:

- Prepare trial state $|\psi(\vec{\theta})\rangle$
- Measure energy expectation value $\langle H \rangle_{\vec{\theta}}$ (cost function)



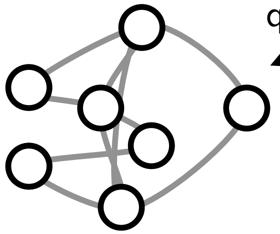


*VQE method:
Peruzzo *et al.*, Nature communications **5**, 4213 (2014).
Kandala *et al.*, Nature **549**, 242–246 (2017).

Hybrid quantum variational approach

Problem

e.g. molecule*, quantum magnet



Hamiltonian

$$H = \sum_i w_i \hat{P}_i$$

$$\hat{P}_i \in \{I, X, Y, Z\}^{\otimes N}$$

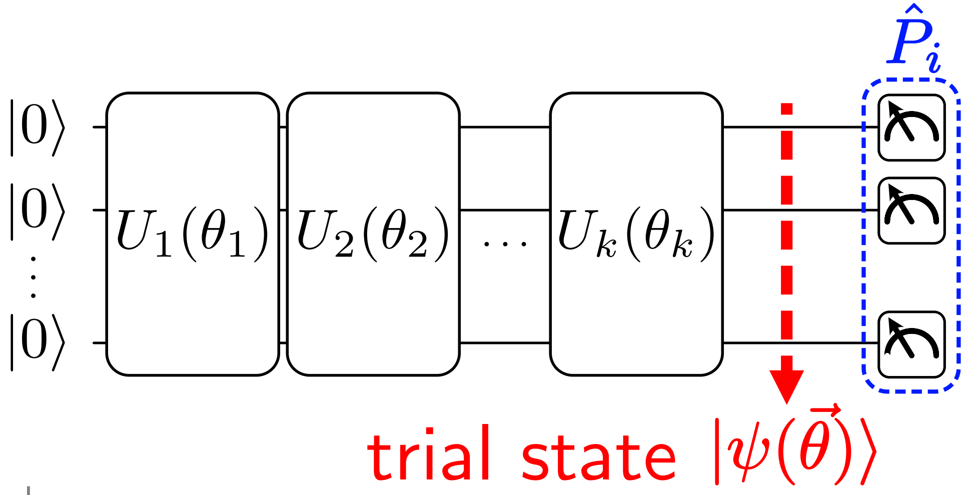
Solution

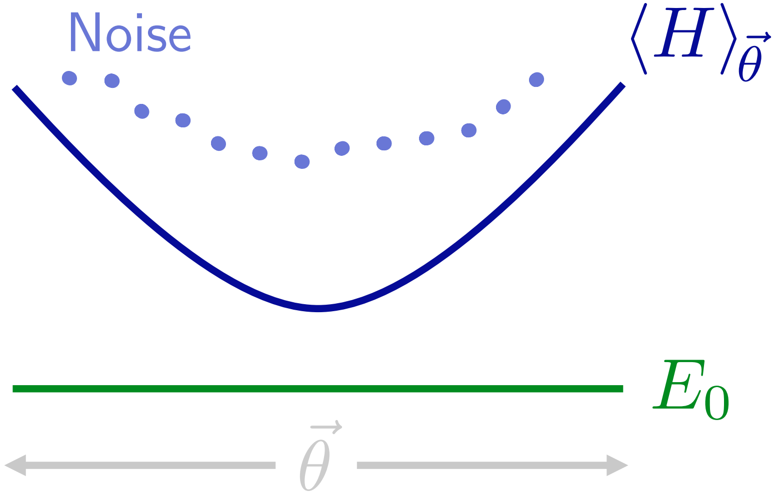
Ground state $|\psi_0\rangle$

Ground energy E_0

Role of quantum computer:

- Prepare trial state $|\psi(\vec{\theta})\rangle$
- Measure energy expectation value $\langle H \rangle_{\vec{\theta}}$ (cost function)



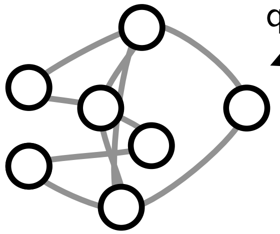


*VQE method:
Peruzzo *et al.*, Nature communications **5**, 4213 (2014).
Kandala *et al.*, Nature **549**, 242–246 (2017).

Hybrid quantum variational approach

Problem

e.g. molecule*, quantum magnet



Hamiltonian

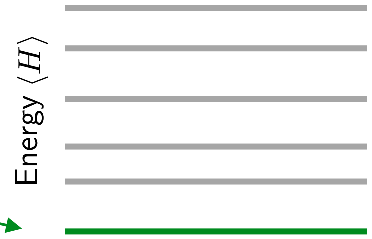
$$H = \sum_i w_i \hat{P}_i$$

$$\hat{P}_i \in \{I, X, Y, Z\}^{\otimes N}$$

Solution

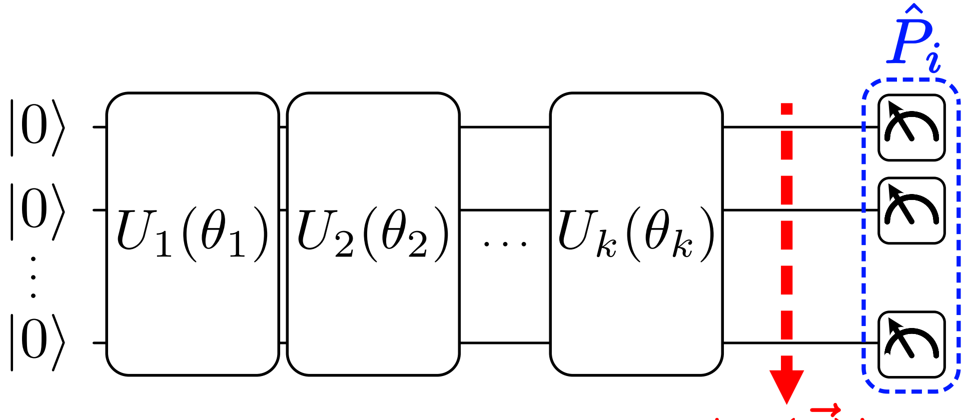
Ground state $|\psi_0\rangle$

Ground energy E_0

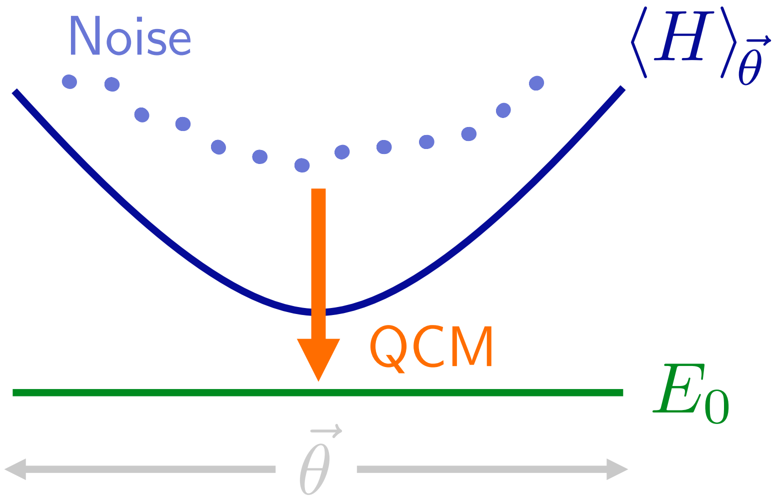


Role of quantum computer:

- Prepare trial state $|\psi(\vec{\theta})\rangle$
- Measure energy expectation value $\langle H \rangle_{\vec{\theta}}$ (cost function)



trial state $|\psi(\vec{\theta})\rangle$



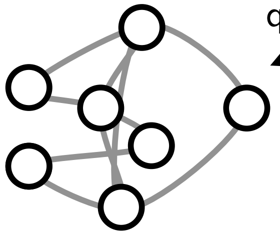
*VQE method:

Peruzzo *et al.*, Nature communications **5**, 4213 (2014).
Kandala *et al.*, Nature **549**, 242–246 (2017).

Hybrid quantum variational approach

Problem

e.g. molecule*, quantum magnet



Hamiltonian

$$H = \sum_i w_i \hat{P}_i$$

$$\hat{P}_i \in \{I, X, Y, Z\}^{\otimes N}$$

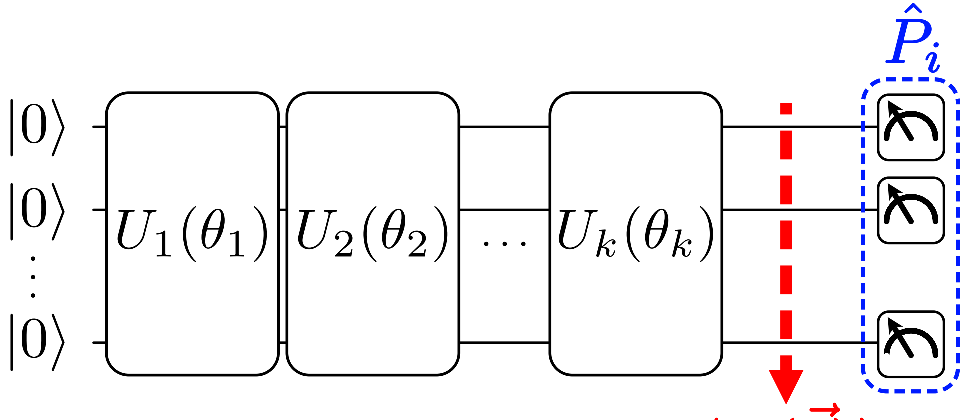
Solution

Ground state $|\psi_0\rangle$

Ground energy E_0

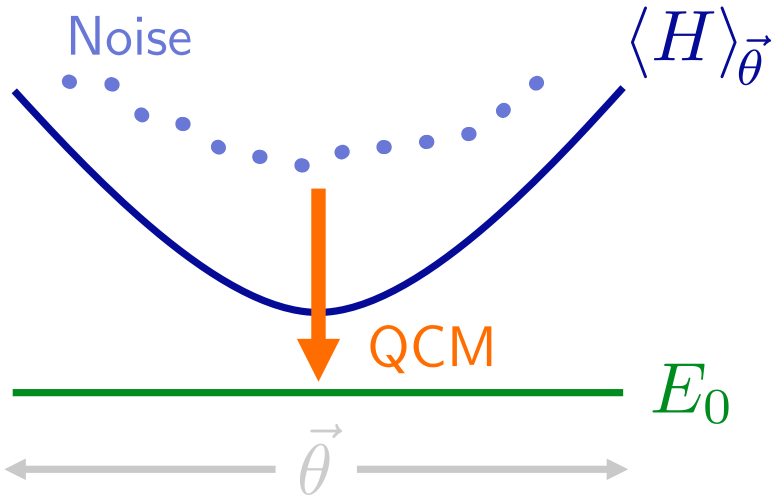
Role of quantum computer:

- Prepare trial state $|\psi(\vec{\theta})\rangle$
- Measure energy expectation value $\langle H \rangle_{\vec{\theta}}$ (cost function)



Hamiltonian moments

$$\{\langle H \rangle, \langle H^2 \rangle, \langle H^3 \rangle, \langle H^4 \rangle \dots\}$$



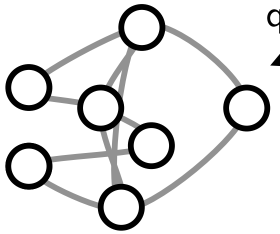
*VQE method:

Peruzzo *et al.*, Nature communications **5**, 4213 (2014).

Kandala *et al.*, Nature **549**, 242–246 (2017).

Hybrid quantum variational approach

Problem — e.g. molecule*, quantum magnet



Hamiltonian

$$H = \sum_i w_i \hat{P}_i$$

$$\hat{P}_i \in \{I, X, Y, Z\}^{\otimes N}$$

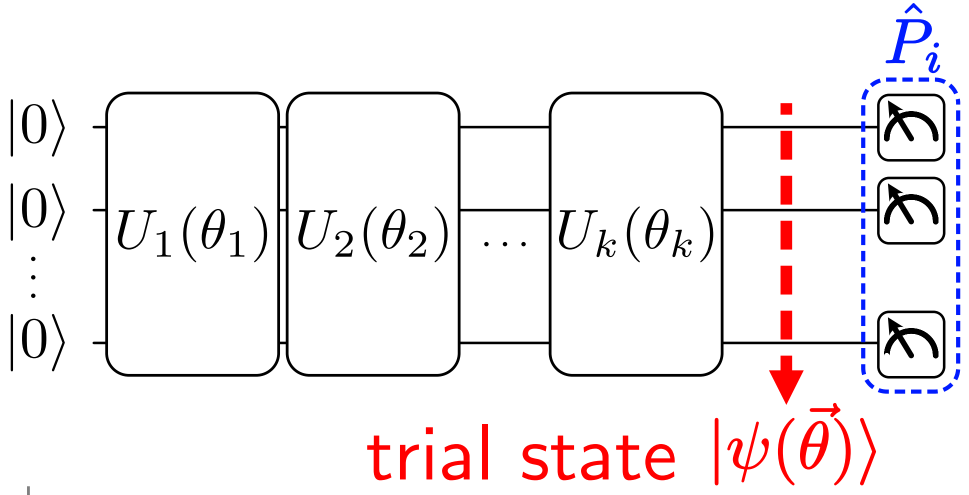
Solution

Ground state $|\psi_0\rangle$

Ground energy E_0

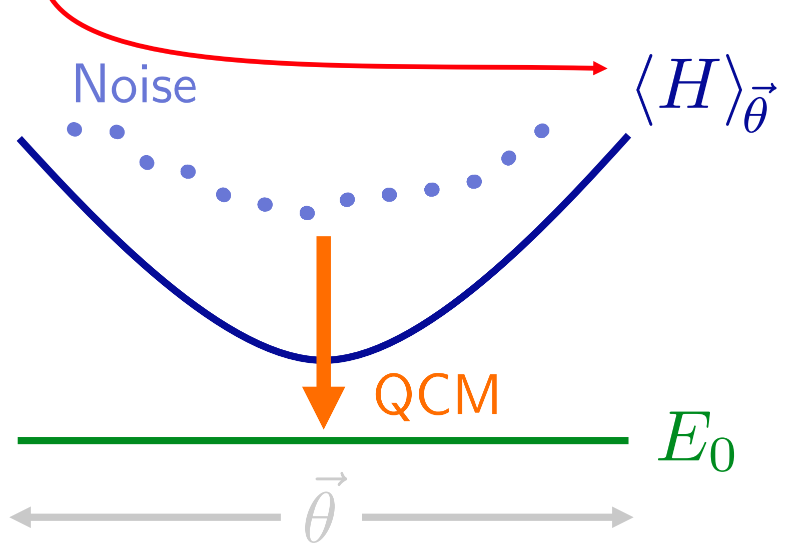
Role of quantum computer:

- Prepare trial state $|\psi(\vec{\theta})\rangle$
- Measure energy expectation value $\langle H \rangle_{\vec{\theta}}$ (cost function)



Hamiltonian moments

$$\{\langle H \rangle, \langle H^2 \rangle, \langle H^3 \rangle, \langle H^4 \rangle \dots\}$$



*VQE method:
Peruzzo *et al.*, Nature communications **5**, 4213 (2014).
Kandala *et al.*, Nature **549**, 242–246 (2017).

Ground state energy estimate from Hamiltonian moments

- Rather than fully diagonalizing a matrix, Lanczos algorithm takes it to tri-diagonal form, from here can numerically compute lowest eigenvalues more easily than from original matrix

$$\begin{bmatrix} \\ H \\ 2^n \times 2^n \\ \text{Hermitian matrix} \\ \end{bmatrix} \longrightarrow \begin{bmatrix} \alpha_1 & \beta_2 & & & & \\ \beta_2 & \alpha_2 & \beta_3 & & 0 & \\ & \beta_3 & \alpha_3 & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ & & & \ddots & & \beta_{N-1} & \\ & 0 & & \beta_{N-1} & \alpha_{N-1} & \beta_N \\ & & & & \beta_N & \alpha_N \end{bmatrix}$$

IBM Quantum Network Hub
at the University of Melbourne

Ground state energy estimate from Hamiltonian moments

- Rather than fully diagonalizing a matrix, Lanczos algorithm takes it to tri-diagonal form, from here can numerically compute lowest eigenvalues more easily than from original matrix

$$\begin{bmatrix} \\ H \\ 2^n \times 2^n \\ \text{Hermitian matrix} \\ \\ \end{bmatrix} \longrightarrow \begin{bmatrix} \alpha_1 & \beta_2 & & & & 0 \\ \beta_2 & \alpha_2 & \beta_3 & & & \\ & \beta_3 & \alpha_3 & \ddots & & \\ & & \ddots & \ddots & \beta_{N-1} & \\ & & & \beta_{N-1} & \alpha_{N-1} & \beta_N \\ 0 & & & & \beta_N & \alpha_N \end{bmatrix}$$

- Cluster expansion of Lanczos matrix elements:

$$\alpha_i = c_1 + \frac{(i-1)}{V}\frac{c_3}{c_2} + \ldots \qquad \beta_i^2 = \frac{i}{V}c_2 + \frac{1}{2}\frac{i(i-1)}{V^2}\left(\frac{c_2 c_4 - c_3^2}{2c_2^2}\right) + \ldots$$

LCL Hollenberg, *Phys Rev. D* **47**, 1640 (1993).

cumulants are calculated directly from moments: $c_n = \langle H^n \rangle - \sum_{k=0}^{n-2} \binom{n-1}{k} c_{k+1} \langle H^{n-k-1} \rangle$

Ground state energy estimate from Hamiltonian moments

- Generalisation beyond extensive systems:

$$\alpha(z) = c_1 + z\left[\frac{c_3}{c_2}\right] + z^2\left[\frac{3c_3^3 - 4c_2c_3c_4 + c_2^2c_5}{4c_2^4}\right] + \dots \qquad \beta(z)^2 = zc_2 + z^2\left[\frac{c_2c_4 - c_3^2}{2c_2^2}\right] + \dots$$

LCL Hollenberg and NS Witte, *Phys Rev. D* **50**, 3382 (1994).

cumulants are calculated directly from moments: $c_n = \langle H^n \rangle - \sum_{k=0}^{n-2} \binom{n-1}{k} c_{k+1} \langle H^{n-k-1} \rangle$

Ground state energy estimate from Hamiltonian moments

- Generalisation beyond extensive systems:

$$\alpha(z) = c_1 + z\left[\frac{c_3}{c_2}\right] + z^2\left[\frac{3c_3^3 - 4c_2c_3c_4 + c_2^2c_5}{4c_2^4}\right] + \dots \qquad \beta(z)^2 = zc_2 + z^2\left[\frac{c_2c_4 - c_3^2}{2c_2^2}\right] + \dots$$

LCL Hollenberg and NS Witte, *Phys Rev. D* **50**, 3382 (1994).

cumulants are calculated directly from moments: $c_n = \langle H^n \rangle - \sum_{k=0}^{n-2} \binom{n-1}{k} c_{k+1} \langle H^{n-k-1} \rangle$

- Ground state energy known explicitly via infimum theorem: $E_0 = \inf_{z>0} \left[\alpha(z) - 2\beta(z)\right]$

LCL Hollenberg and NS Witte, *Phys. Rev. B* **54**, 16309 (1996)

Ground state energy estimate from Hamiltonian moments

- Generalisation beyond extensive systems:

$$\alpha(z) = c_1 + z\left[\frac{c_3}{c_2}\right] + z^2\left[\frac{3c_3^3 - 4c_2c_3c_4 + c_2^2c_5}{4c_2^4}\right] + \dots \qquad \beta(z)^2 = zc_2 + z^2\left[\frac{c_2c_4 - c_3^2}{2c_2^2}\right] + \dots$$

LCL Hollenberg and NS Witte, *Phys Rev. D* **50**, 3382 (1994).

cumulants are calculated directly from moments: $c_n = \langle H^n\rangle - \sum_{k=0}^{n-2}\binom{n-1}{k} c_{k+1}\langle H^{n-k-1}\rangle$

- Ground state energy known explicitly via infimum theorem: $E_0 = \inf_{z>0}\left[\alpha(z) - 2\beta(z)\right]$

LCL Hollenberg and NS Witte, *Phys. Rev. B* **54**, 16309 (1996)

- Truncate moments to order $n_{\max} = 4$ to obtain the following estimate of ground state energy in terms of moments (cumulants) alone:

$$E_0^{\mathrm{L}(4)} = c_1 - \frac{c_2^2}{c_3^2 - c_2c_4}\left[\sqrt{3c_3^2 - 2c_2c_4} - c_3\right]$$

LCL Hollenberg and NS Witte, *Phys. Rev. D* **50**, 3382 (1994).

Ground state energy estimate from Hamiltonian moments

- Generalisation beyond extensive systems:

$$\alpha(z) = c_1 + z\left[\frac{c_3}{c_2}\right] + z^2\left[\frac{3c_3^3 - 4c_2c_3c_4 + c_2^2c_5}{4c_2^4}\right] + \dots \qquad \beta(z)^2 = zc_2 + z^2\left[\frac{c_2c_4 - c_3^2}{2c_2^2}\right] + \dots$$

LCL Hollenberg and NS Witte, *Phys Rev. D* 50, 3382 (1994).

cumulants are calculated directly from moments: $c_n = \langle H^n \rangle - \sum_{k=0}^{n-2} \binom{n-1}{k} c_{k+1} \langle H^{n-k-1} \rangle$

c_n's come from moments w.r.t. some trial state

- Ground state energy known explicitly via infimum theorem: $E_0 = \inf_{z>0} [\alpha(z) - 2\beta(z)]$

LCL Hollenberg and NS Witte, *Phys. Rev. B* 54, 16309 (1996)

- Truncate moments to order $n_{\max} = 4$ to obtain the following estimate of ground state energy in terms of moments (cumulants) alone:

$$E_0^{\mathrm{L}(4)} = c_1 - \frac{c_2^2}{c_3^2 - c_2c_4}\left[\sqrt{3c_3^2 - 2c_2c_4} - c_3\right]$$

LCL Hollenberg and NS Witte, *Phys. Rev. D* 50, 3382 (1994).

IBM Quantum Network Hub at the University of Melbourne

Ground state energy estimate from Hamiltonian moments

- Generalisation beyond extensive systems:

$$\alpha(z) = c_1 + z\left[\frac{c_3}{c_2}\right] + z^2\left[\frac{3c_3^3 - 4c_2c_3c_4 + c_2^2c_5}{4c_2^4}\right] + \dots \qquad \beta(z)^2 = zc_2 + z^2\left[\frac{c_2c_4 - c_3^2}{2c_2^2}\right] + \dots$$

LCL Hollenberg and NS Witte, *Phys Rev. D* 50, 3382 (1994).

cumulants are calculated directly from moments: $c_n = \langle H^n\rangle - \sum_{k=0}^{n-2}\binom{n-1}{k} c_{k+1}\langle H^{n-k-1}\rangle$

c_n's come from moments w.r.t. some trial state

- Ground state energy known explicitly via infimum theorem: $E_0 = \inf_{z>0}\left[\alpha(z) - 2\beta(z)\right]$

LCL Hollenberg and NS Witte, *Phys. Rev. B* 54, 16309 (1996).

$c_1 = \langle H \rangle$

- Truncate moments to order $n_{\max} = 4$ to obtain the following estimate of ground state energy in terms of moments (cumulants) alone:

$$E_0^{\mathrm{L}(4)} = c_1 - \frac{c_2^2}{c_3^2 - c_2c_4}\left[\sqrt{3c_3^2 - 2c_2c_4} - c_3\right]$$

LCL Hollenberg and NS Witte, *Phys. Rev. D* 50, 3382 (1994).

IBM Quantum Network Hub
at the University of Melbourne

Ground state energy estimate from Hamiltonian moments

- Generalisation beyond extensive systems:

$$\alpha(z) = c_1 + z\left[\frac{c_3}{c_2}\right] + z^2\left[\frac{3c_3^3 - 4c_2c_3c_4 + c_2^2c_5}{4c_2^4}\right] + \dots \qquad \beta(z)^2 = zc_2 + z^2\left[\frac{c_2c_4 - c_3^2}{2c_2^2}\right] + \dots$$

LCL Hollenberg and NS Witte, *Phys Rev. D* 50, 3382 (1994).

cumulants are calculated directly from moments:

$$c_n = \langle H^n \rangle - \sum_{k=0}^{n-2} \binom{n-1}{k} c_{k+1} \langle H^{n-k-1} \rangle$$

c_n's come from moments w.r.t. some trial state

- Ground state energy known explicitly via infimum theorem:

$$E_0 = \inf_{z>0} [\alpha(z) - 2\beta(z)]$$

LCL Hollenberg and NS Witte, *Phys. Rev. B* 54, 16309 (1996).

- Truncate moments to order $n_{\max}$ … of ground state energy in terms of moments (cumulants) alone.

$c_1 = \langle H \rangle$

Correction based on Hamiltonian moments, less sensitive to choice of trial state

$$E_0^{\mathrm{L}(4)} = c_1 - \frac{c_2^2}{c_3^2 - c_2c_4}\left[\sqrt{3c_3^2 - 2c_2c_4} - c_3\right]$$

LCL Hollenberg and NS Witte, *Phys. Rev. D* 50, 3382 (1994).

Heisenberg model and operator reduction

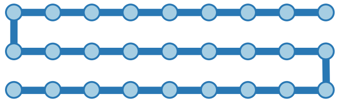
Heisenberg model Hamiltonian:

$$H = \frac{1}{q} \sum_{\langle ij \rangle} \left(J_{ij}^{(x)} X_i X_j + J_{ij}^{(y)} Y_i Y_j + J_{ij}^{(z)} Z_i Z_j \right)$$

Heisenberg model and operator reduction

Heisenberg model Hamiltonian:

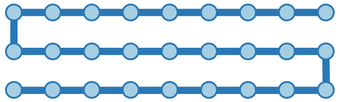
$$H = \frac{1}{q} \sum_{\langle ij \rangle} \left(J_{ij}^{(x)} X_i X_j + J_{ij}^{(y)} Y_i Y_j + J_{ij}^{(z)} Z_i Z_j \right)$$

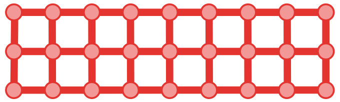


Heisenberg model and operator reduction

Heisenberg model Hamiltonian:

$$H = \frac{1}{q} \sum_{\langle ij \rangle} \left(J_{ij}^{(x)} X_i X_j + J_{ij}^{(y)} Y_i Y_j + J_{ij}^{(z)} Z_i Z_j \right)$$

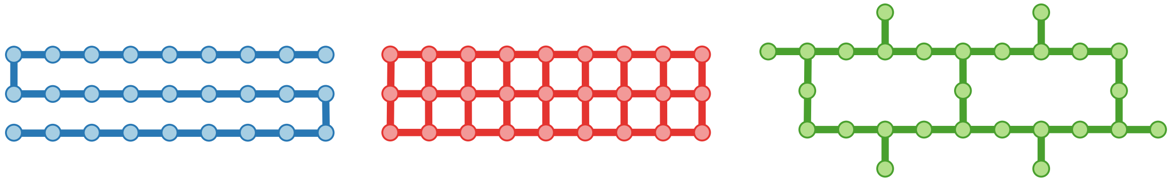




Heisenberg model and operator reduction

Heisenberg model Hamiltonian:

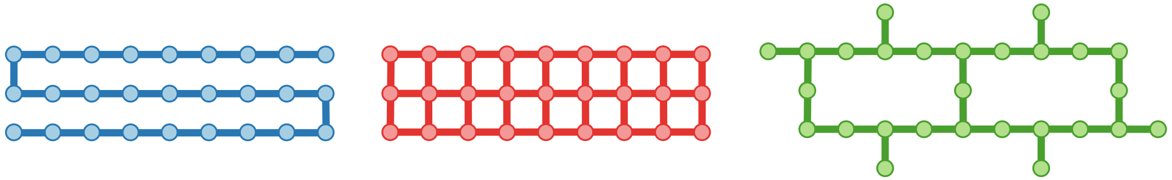
$$H = \frac{1}{q} \sum_{\langle ij \rangle} \left(J_{ij}^{(x)} X_i X_j + J_{ij}^{(y)} Y_i Y_j + J_{ij}^{(z)} Z_i Z_j \right)$$



Heisenberg model and operator reduction

Heisenberg model Hamiltonian:

$$H = \frac{1}{q} \sum_{\langle ij \rangle} \left(J_{ij}^{(x)} X_i X_j + J_{ij}^{(y)} Y_i Y_j + J_{ij}^{(z)} Z_i Z_j \right)$$

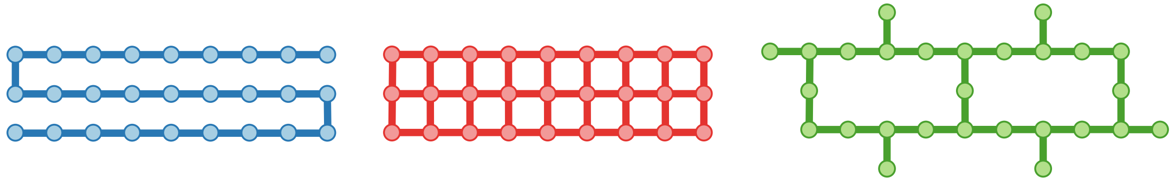


Need to multiply together terms in H to obtain H^2, H^3, H^4

Heisenberg model and operator reduction

Heisenberg model Hamiltonian:

$$H = \frac{1}{q} \sum_{\langle ij \rangle} \left(J_{ij}^{(x)} X_i X_j + J_{ij}^{(y)} Y_i Y_j + J_{ij}^{(z)} Z_i Z_j \right)$$



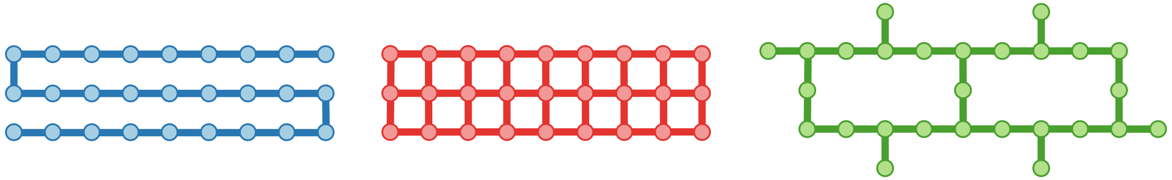
Need to multiply together terms in H to obtain H^2, H^3, H^4

H has m terms $\Longrightarrow H^4$ has $\sim m^4$ terms (Pauli strings)...

Heisenberg model and operator reduction

Heisenberg model Hamiltonian:

$$H = \frac{1}{q} \sum_{\langle ij \rangle} \left(J_{ij}^{(x)} X_i X_j + J_{ij}^{(y)} Y_i Y_j + J_{ij}^{(z)} Z_i Z_j \right)$$



Need to multiply together terms in H to obtain H^2, H^3, H^4

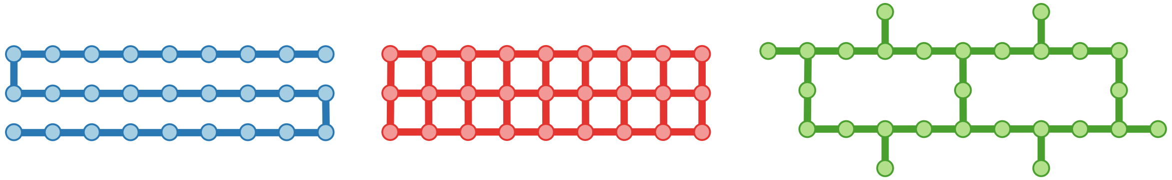
H has m terms $\Longrightarrow H^4$ has $\sim m^4$ terms (Pauli strings)...

- Most Pauli strings can be grouped into simultaneously measurable tensor product basis (TPB) sets

Heisenberg model and operator reduction

Heisenberg model Hamiltonian:

$$H = \frac{1}{q}\sum_{\langle ij\rangle}\left(J_{ij}^{(x)}X_iX_j + J_{ij}^{(y)}Y_iY_j + J_{ij}^{(z)}Z_iZ_j\right)$$



Need to multiply together terms in H to obtain H^2, H^3, H^4

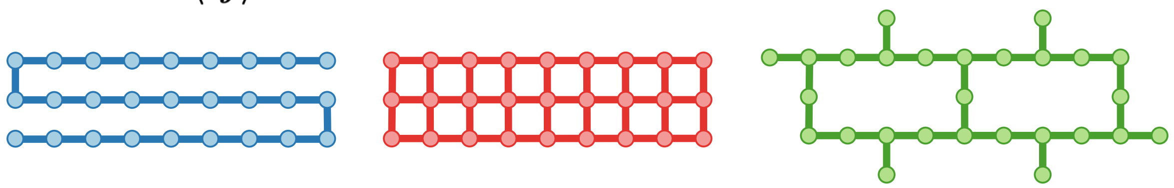
H has m terms $\implies H^4$ has $\sim m^4$ terms (Pauli strings)...

- Most Pauli strings can be grouped into simultaneously measurable tensor product basis (TPB) sets
- Number of required TPB sets: $\sim \log(m)$

Heisenberg model and operator reduction

Heisenberg model Hamiltonian:

$$H = \frac{1}{q} \sum_{\langle ij \rangle} \left(J_{ij}^{(x)} X_i X_j + J_{ij}^{(y)} Y_i Y_j + J_{ij}^{(z)} Z_i Z_j \right)$$

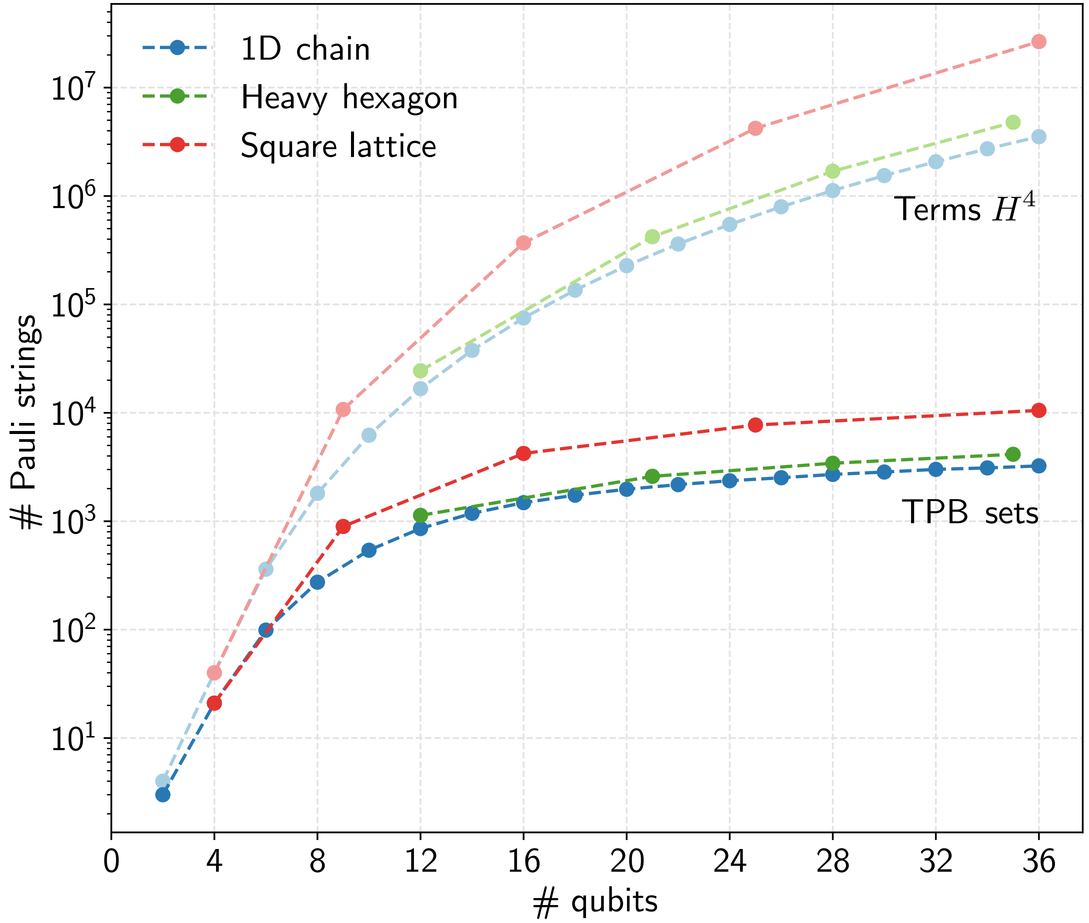


Need to multiply together terms in H to obtain H^2, H^3, H^4

H has m terms $\Longrightarrow H^4$ has $\sim m^4$ terms (Pauli strings)...

- Most Pauli strings can be grouped into simultaneously measurable tensor product basis (TPB) sets
- Number of required TPB sets: $\sim \log(m)$
- Have developed our own TPB grouping heuristic, as most alternatives in the literature are impractical at large scale

Problem graph	Terms in H^4	TPB sets
49 qubit (7 × 7) square	116712850	9296
65 qubit heavy hexagon	73331107	4249



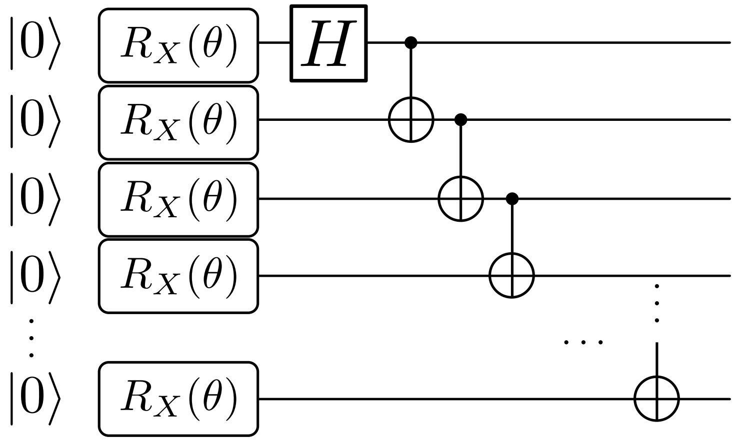
H Vallury, M Jones, C Hill, L Hollenberg, *Quantum* **4**, 373 (2020).

QCM on Heisenberg model: low fidelity trial state

$$H = \frac{1}{q}\sum_{\langle ij\rangle}\left(J_{ij}^{(x)}X_iX_j + J_{ij}^{(y)}Y_iY_j + J_{ij}^{(z)}Z_iZ_j\right)$$

A simple ansatz...

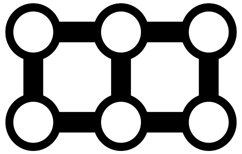
small parameter space,
poor ground state overlap



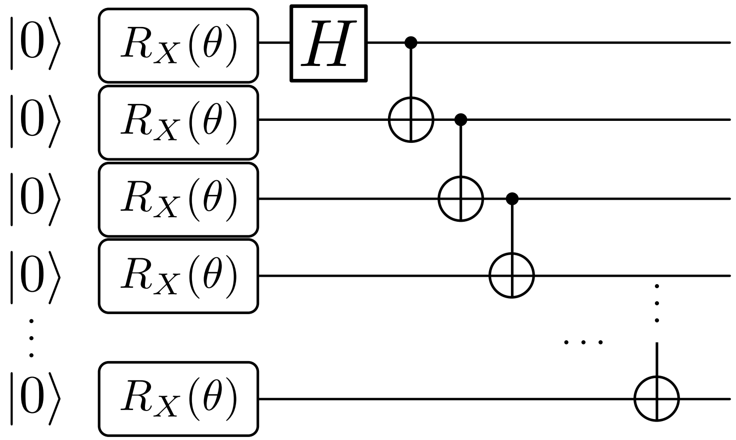
$$|\psi(\theta=\pi)\rangle = \frac{1}{\sqrt{2}}\left(|0101\ldots\rangle - |1010\ldots\rangle\right)$$

QCM on Heisenberg model: low fidelity trial state

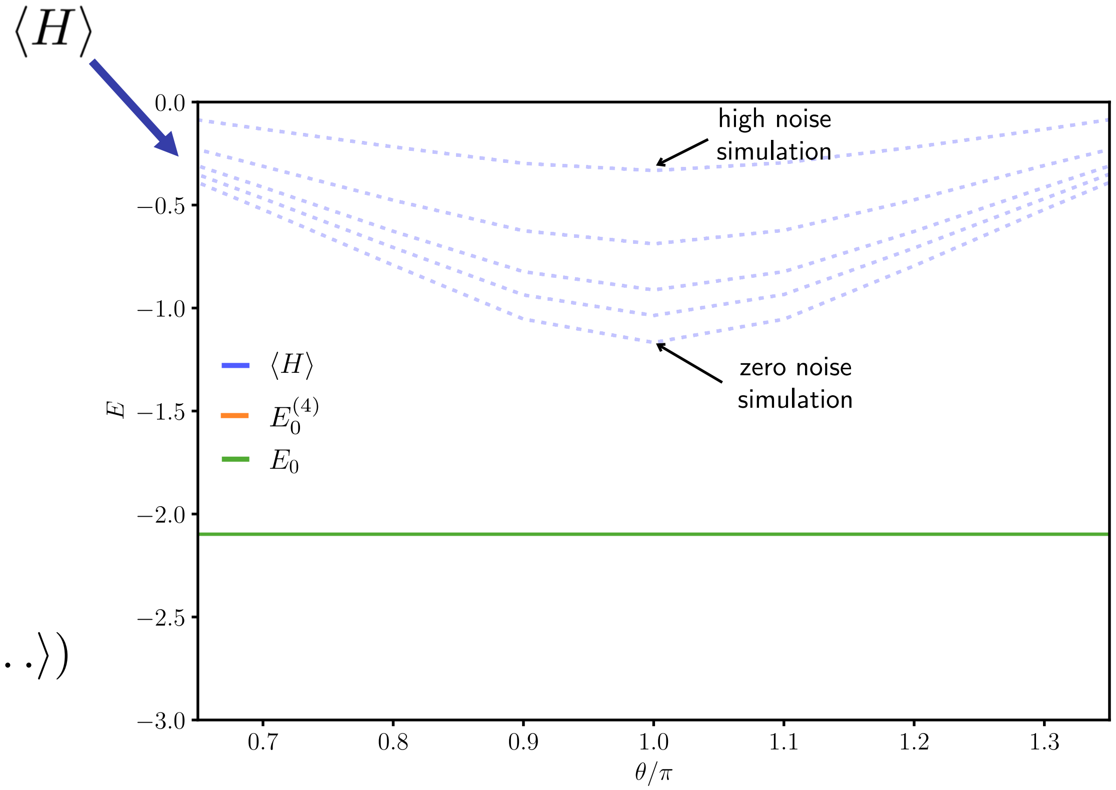
$$H = \frac{1}{q}\sum_{\langle ij\rangle}\left(J_{ij}^{(x)}X_iX_j + J_{ij}^{(y)}Y_iY_j + J_{ij}^{(z)}Z_iZ_j\right)$$



A simple ansatz...
small parameter space,
poor ground state overlap

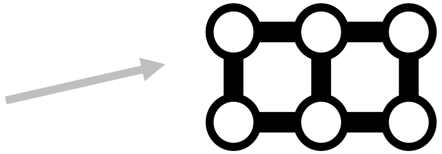


$$|\psi(\theta=\pi)\rangle = \frac{1}{\sqrt{2}}\left(|0101\ldots\rangle - |1010\ldots\rangle\right)$$

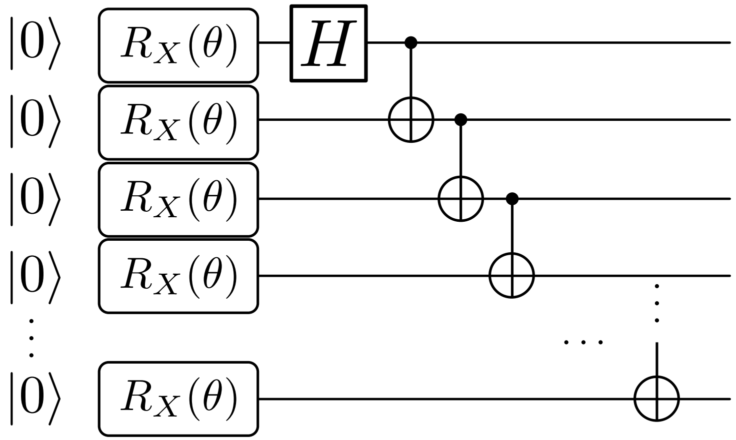


QCM on Heisenberg model: low fidelity trial state

$$H = \frac{1}{q}\sum_{\langle ij\rangle}\left(J_{ij}^{(x)}X_iX_j + J_{ij}^{(y)}Y_iY_j + J_{ij}^{(z)}Z_iZ_j\right)$$

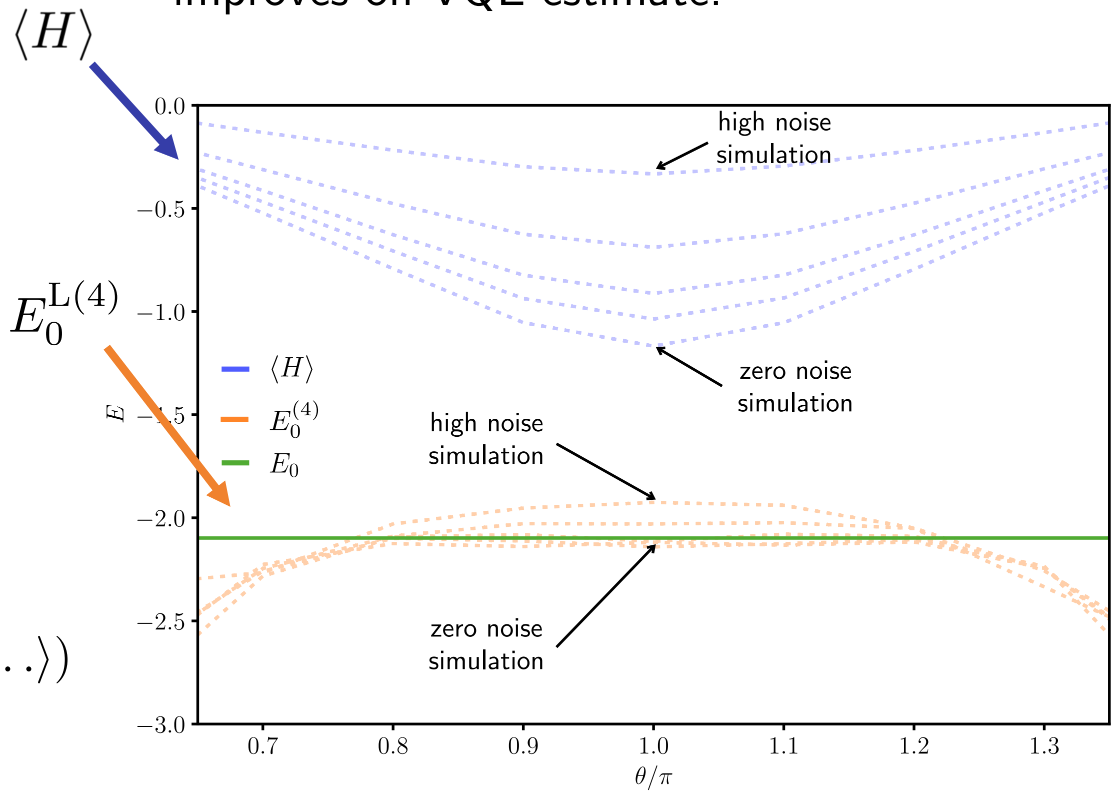


A simple ansatz...
small parameter space,
poor ground state overlap



$$|\psi(\theta=\pi)\rangle = \frac{1}{\sqrt{2}}\left(|0101\ldots\rangle - |1010\ldots\rangle\right)$$

Moments estimate
improves on VQE estimate:

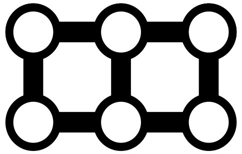


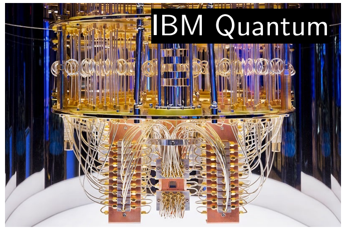
H Vallury, M Jones, C Hill, L Hollenberg, *Quantum* **4**, 373 (2020).

IBM Quantum Network Hub
at the University of Melbourne

QCM on Heisenberg model: low fidelity trial state

$$H = \frac{1}{q}\sum_{\langle ij\rangle}\left(J^{(x)}_{ij}X_iX_j + J^{(y)}_{ij}Y_iY_j + J^{(z)}_{ij}Z_iZ_j\right)$$



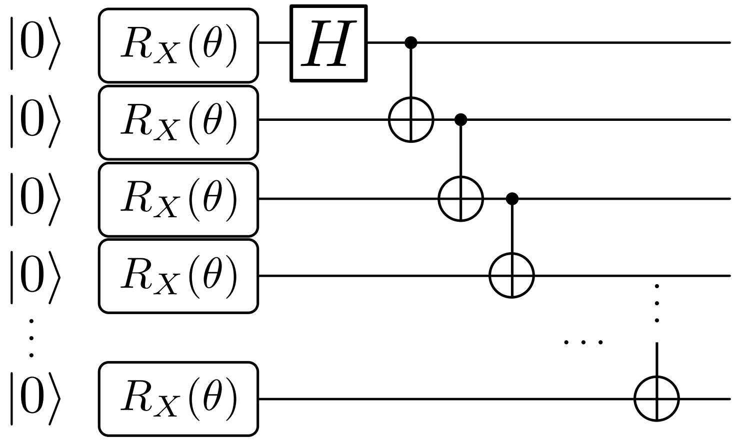


ibmq_montreal

Moments estimate improves on VQE estimate:

A simple ansatz...

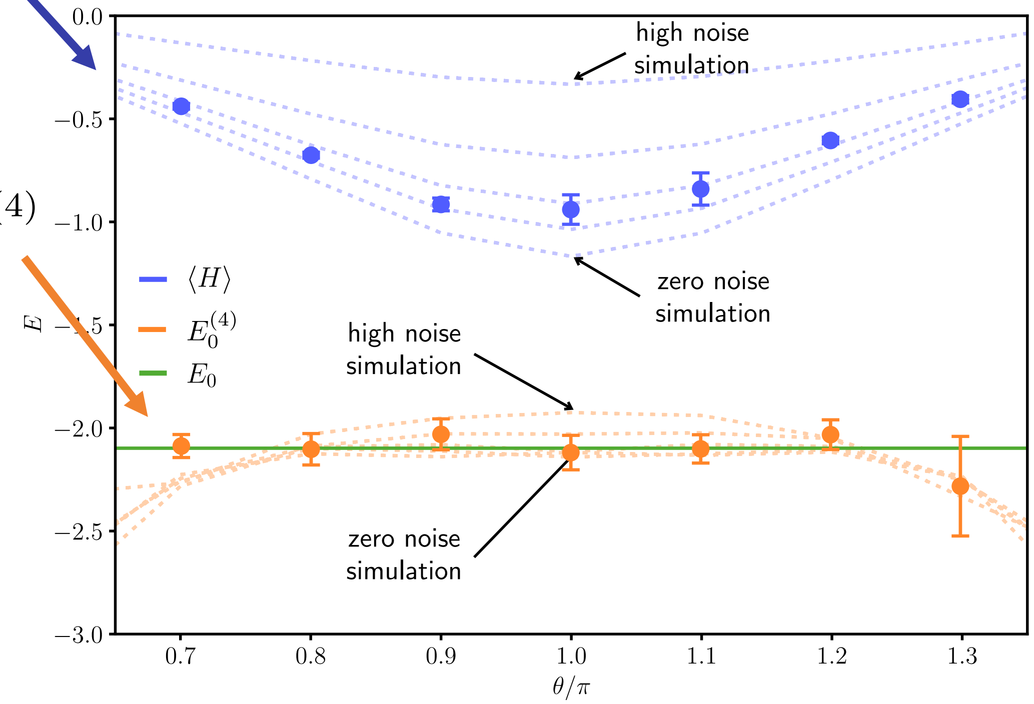
small parameter space,
poor ground state overlap



$$|\psi(\theta = \pi)\rangle = \frac{1}{\sqrt{2}}\left(|0101\ldots\rangle - |1010\ldots\rangle\right)$$

$\langle H \rangle$

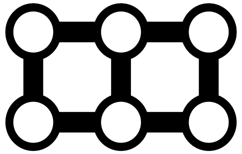
$E_0^{\mathrm{L}(4)}$



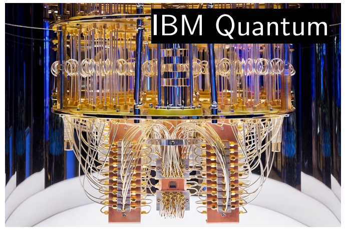
H Vallury, M Jones, C Hill, L Hollenberg, *Quantum* **4**, 373 (2020).

QCM on Heisenberg model: low fidelity trial state

$$H = \frac{1}{q}\sum_{\langle ij \rangle}\left(J_{ij}^{(x)}X_iX_j + J_{ij}^{(y)}Y_iY_j + J_{ij}^{(z)}Z_iZ_j\right)$$



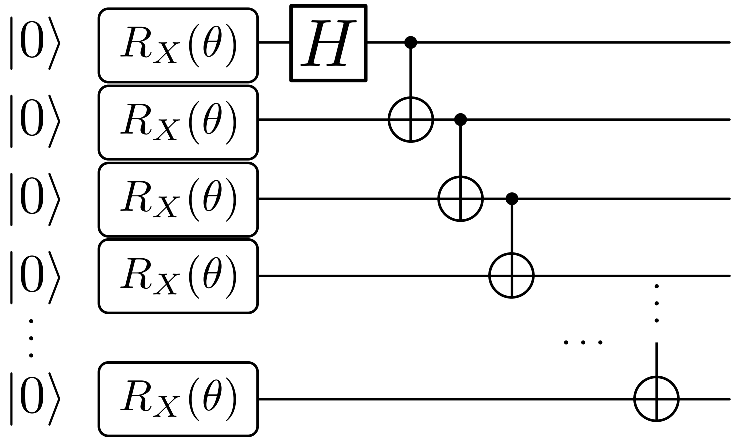
Moments estimate improves on VQE estimate:



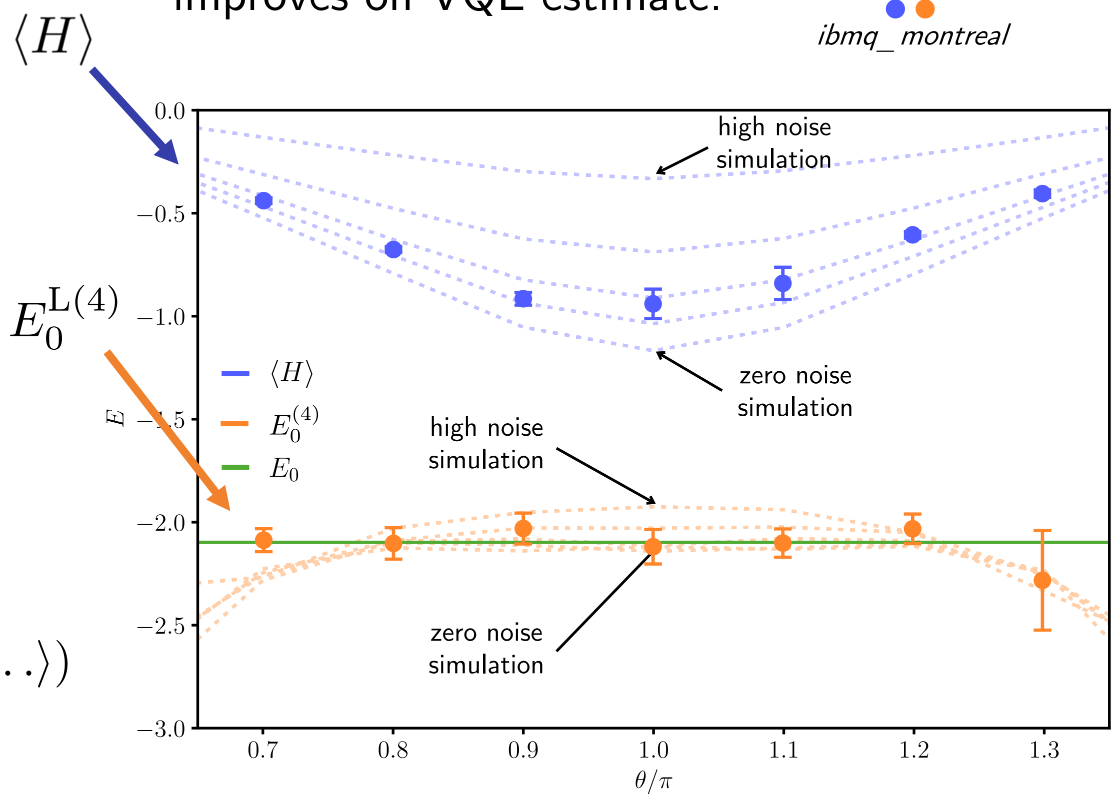
ibmq_montreal

Behaviour persists for larger instances:

A simple ansatz...
small parameter space,
poor ground state overlap



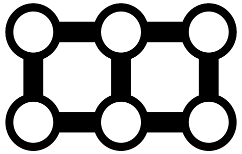
$$|\psi(\theta=\pi)\rangle = \frac{1}{\sqrt{2}}\left(|0101\ldots\rangle - |1010\ldots\rangle\right)$$

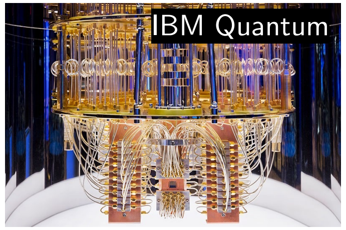


H Vallury, M Jones, C Hill, L Hollenberg, *Quantum* **4**, 373 (2020).

QCM on Heisenberg model: low fidelity trial state

$$H = \frac{1}{q}\sum_{\langle ij\rangle}\left(J_{ij}^{(x)}X_iX_j + J_{ij}^{(y)}Y_iY_j + J_{ij}^{(z)}Z_iZ_j\right)$$

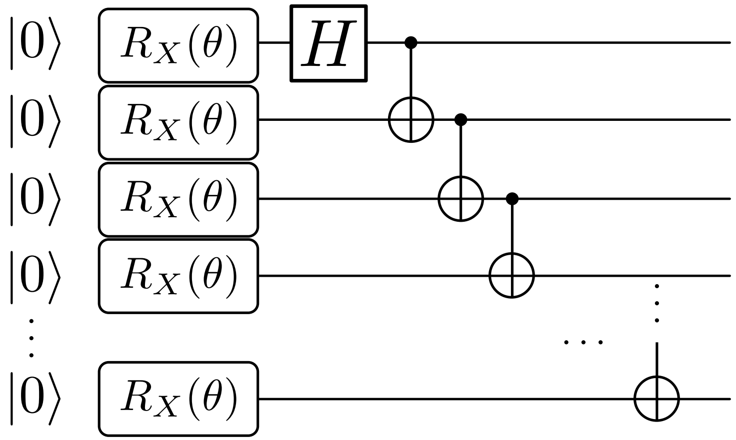




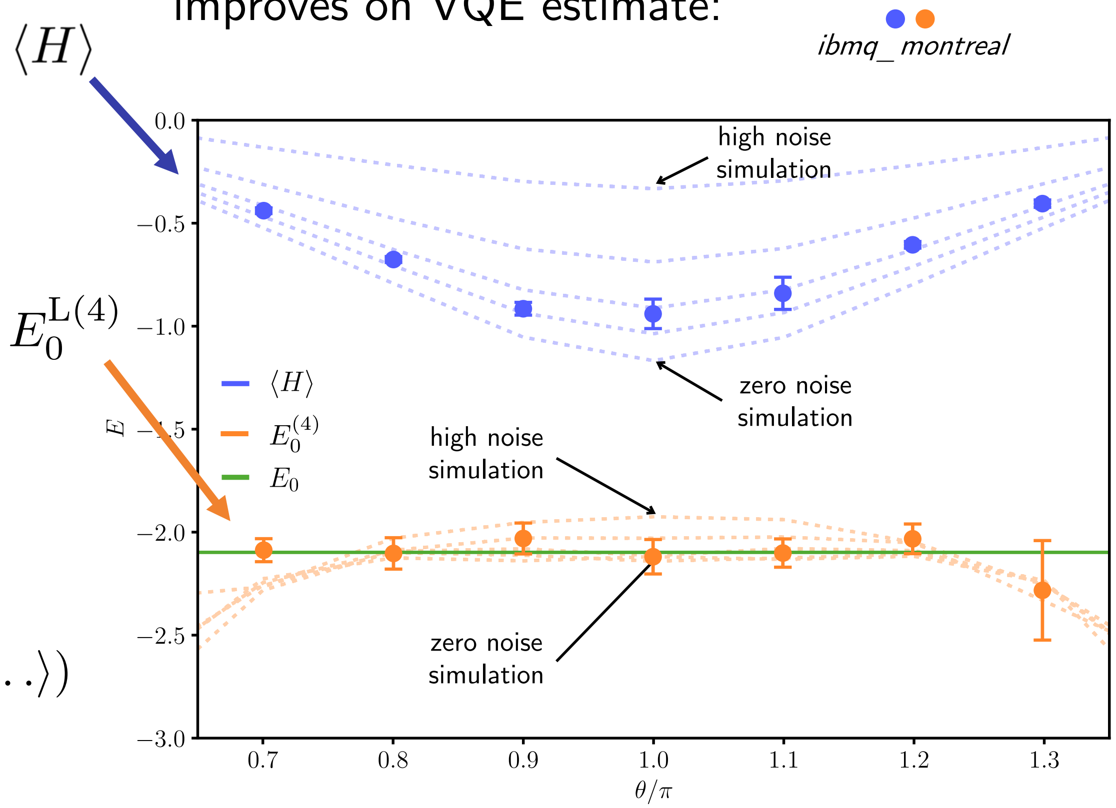
Moments estimate improves on VQE estimate:

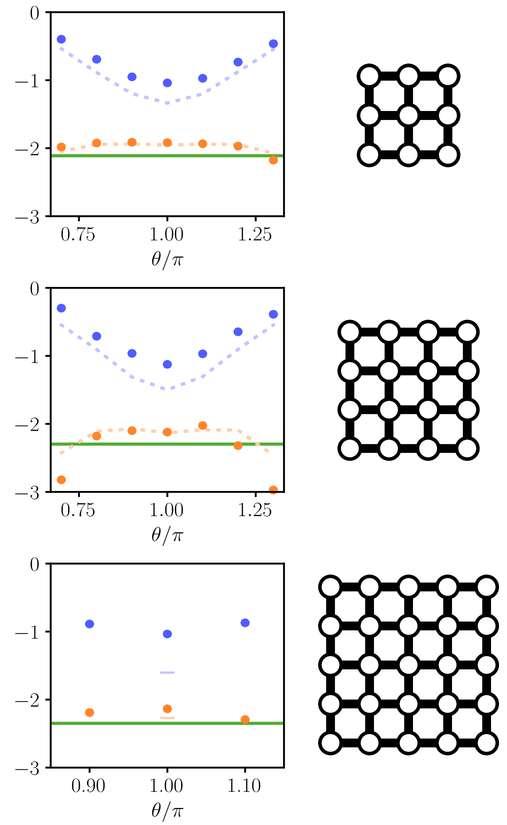
Behaviour persists for larger instances:

A simple ansatz...
small parameter space,
poor ground state overlap



$$|\psi(\theta=\pi)\rangle = \frac{1}{\sqrt{2}}\left(|0101\ldots\rangle - |1010\ldots\rangle\right)$$





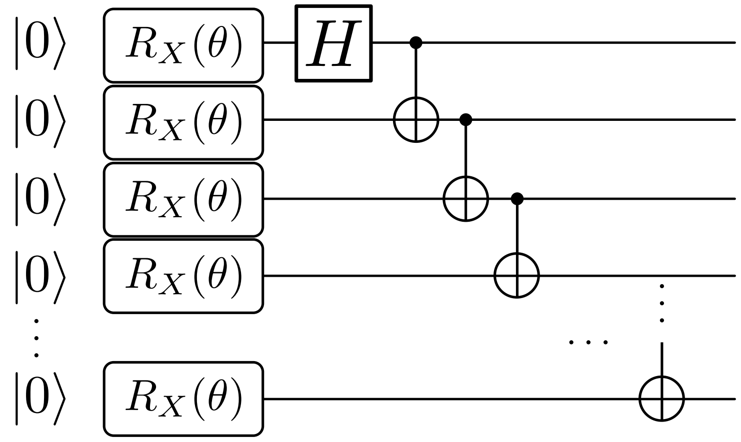
H Vallury, M Jones, C Hill, L Hollenberg, *Quantum* **4**, 373 (2020).

IBM Quantum Network Hub at the University of Melbourne

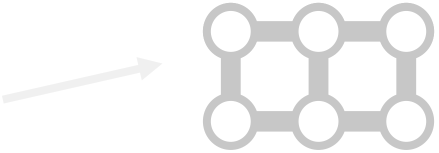
QCM on Heisenberg model: low fidelity trial state

$$H = \frac{1}{q}\sum_{\langle ij\rangle}\left(J_{ij}^{(x)}X_iX_j + J_{ij}^{(y)}Y_iY_j + J_{ij}^{(z)}Z_iZ_j\right)$$

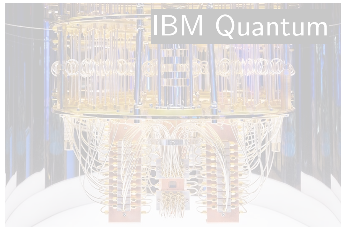
A simple ansatz...
small parameter space,
poor ground state overlap

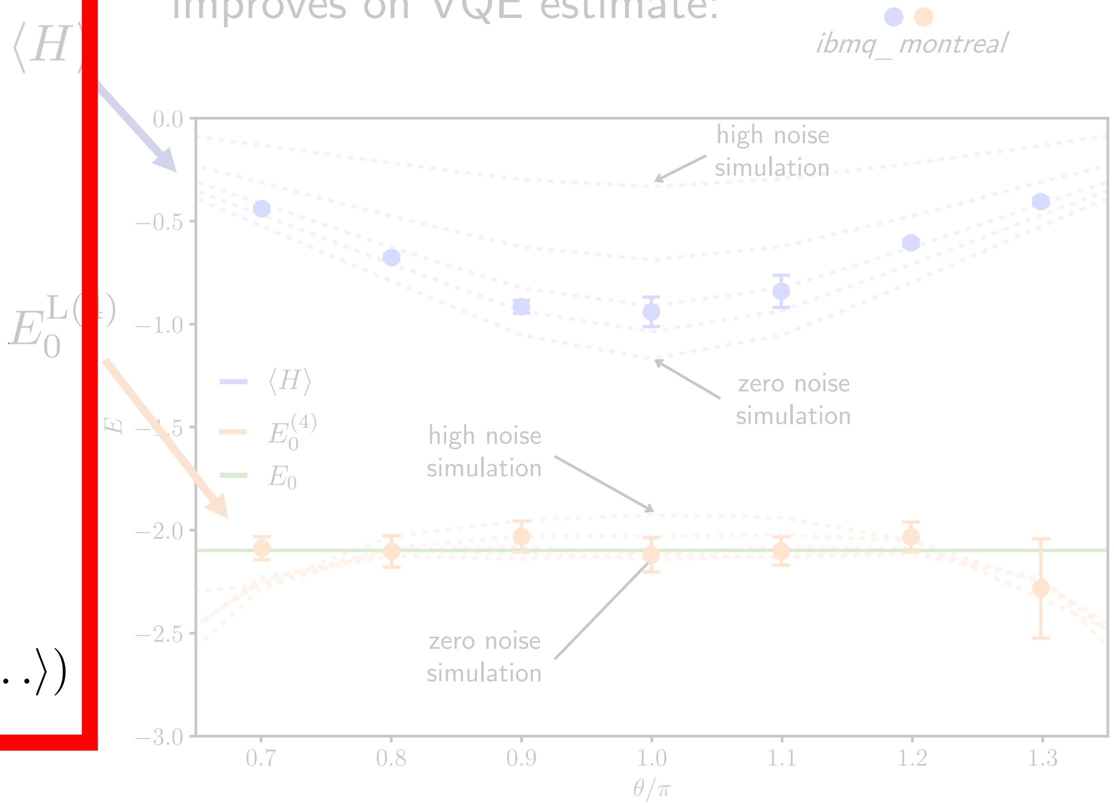


$$|\psi(\theta=\pi)\rangle = \frac{1}{\sqrt{2}}\left(|0101\ldots\rangle - |1010\ldots\rangle\right)$$

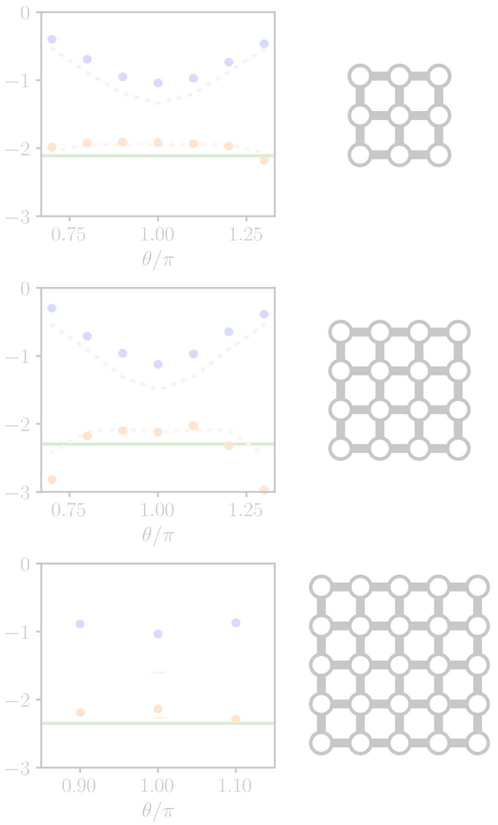


Moments estimate improves on VQE estimate:





Behaviour persists for larger instances:

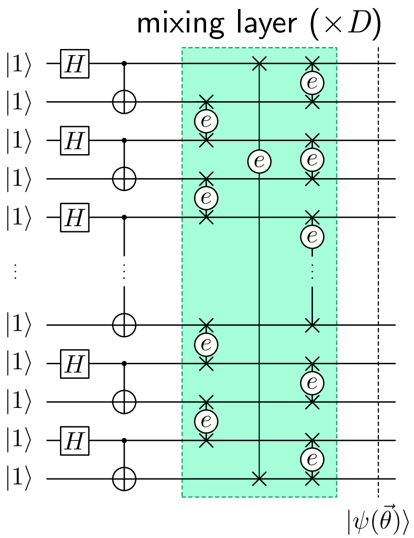


H Vallury, M Jones, C Hill, L Hollenberg, *Quantum* **4**, 373 (2020).

QCM on Heisenberg model: noise robustness

$$H = \frac{1}{q}\sum_{\langle ij\rangle}\left(J_{ij}^{(x)} X_i X_j + J_{ij}^{(y)} Y_i Y_j + J_{ij}^{(z)} Z_i Z_j\right)$$

A better ansatz



Lots of parameters, good overlap with Heisenberg ground state

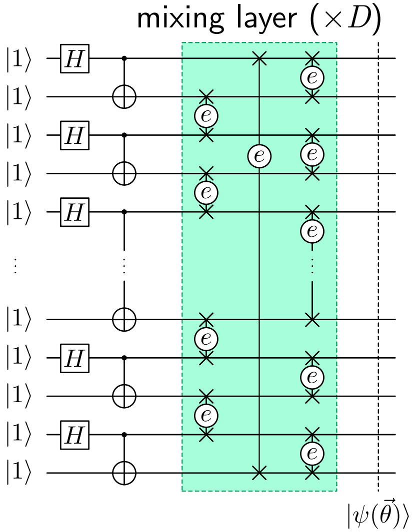
$$|\psi(\vec{\theta})\rangle = \sum_{\mathcal{C}[\psi(\vec{\theta})]} w(\mathcal{C}[\psi(\vec{\theta})]) \bigotimes_{[i,j]\in\mathcal{C}[\psi(\vec{\theta})]} |s_{ij}\rangle$$

RVB ansatz: K. Seki *et al.*, Phys Rev A (2020).

QCM on Heisenberg model: noise robustness

$$H = \frac{1}{q}\sum_{\langle ij\rangle}\left(J_{ij}^{(x)}X_iX_j + J_{ij}^{(y)}Y_iY_j + J_{ij}^{(z)}Z_iZ_j\right)$$

A better ansatz…?



Lots of parameters, good overlap with Heisenberg ground state

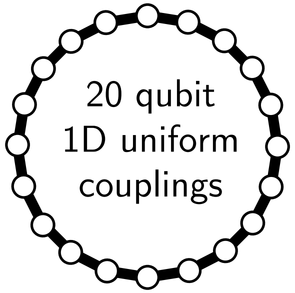
BUT many more gates required, introducing noise

$$|\psi(\vec{\theta})\rangle = \sum_{\mathcal{C}[\psi(\vec{\theta})]} w(\mathcal{C}[\psi(\vec{\theta})]) \bigotimes_{[i,j]\in\mathcal{C}[\psi(\vec{\theta})]} |s_{ij}\rangle$$

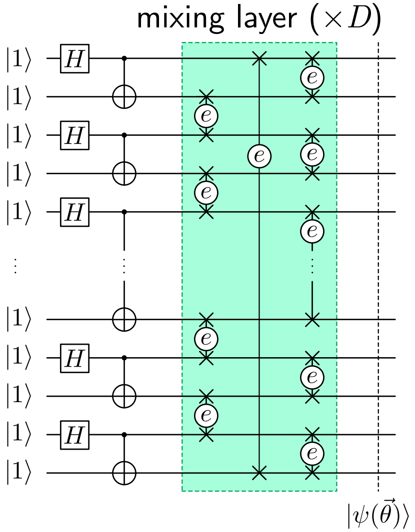
RVB ansatz: K. Seki *et al.*, Phys Rev A (2020).

QCM on Heisenberg model: noise robustness

$$H = \frac{1}{q} \sum_{\langle ij \rangle} \left(J_{ij}^{(x)} X_i X_j + J_{ij}^{(y)} Y_i Y_j + J_{ij}^{(z)} Z_i Z_j \right)$$



A better ansatz…?

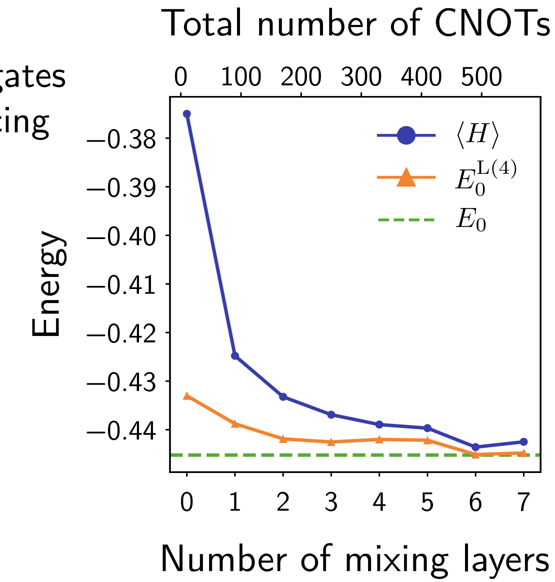


Lots of parameters, good overlap with Heisenberg ground state

BUT many more gates required, introducing noise

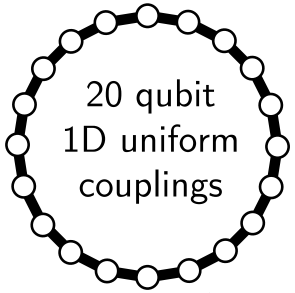
$$|\psi(\vec{\theta})\rangle = \sum_{\mathcal{C}[\psi(\vec{\theta})]} w(\mathcal{C}[\psi(\vec{\theta})]) \bigotimes_{[i,j]\in\mathcal{C}[\psi(\vec{\theta})]} |s_{ij}\rangle$$

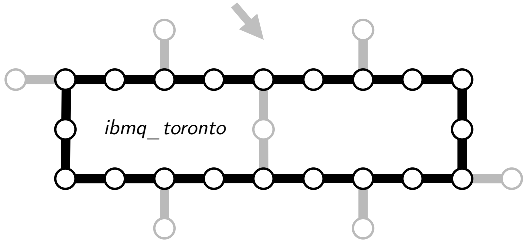
RVB ansatz: K. Seki *et al.*, Phys Rev A (2020).



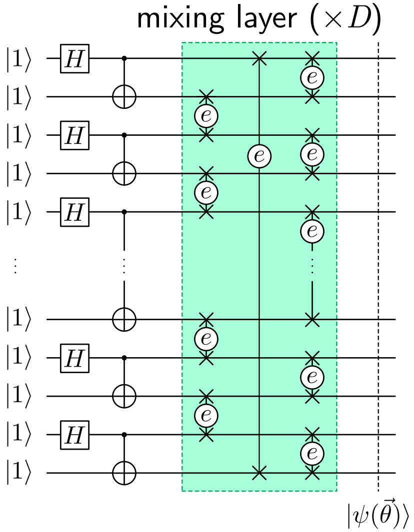
QCM on Heisenberg model: noise robustness

$$H = \frac{1}{q}\sum_{\langle ij\rangle}\left(J_{ij}^{(x)}X_iX_j + J_{ij}^{(y)}Y_iY_j + J_{ij}^{(z)}Z_iZ_j\right)$$





A better ansatz...?

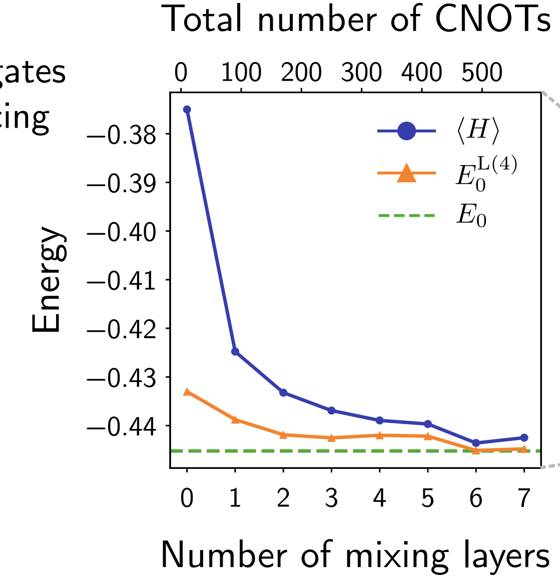


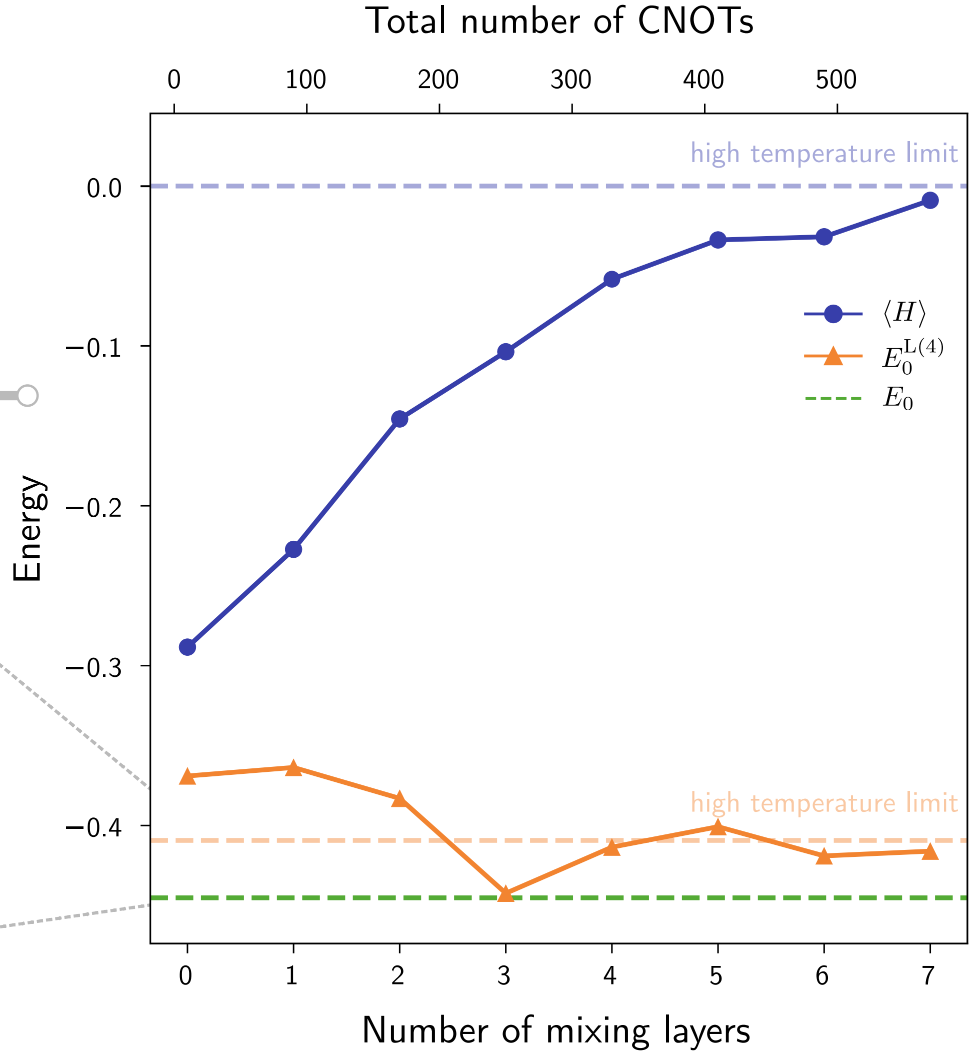
Lots of parameters, good overlap with Heisenberg ground state

BUT many more gates required, introducing noise

$$|\psi(\vec{\theta})\rangle = \sum_{\mathcal{C}[\psi(\vec{\theta})]} w(\mathcal{C}[\psi(\vec{\theta})]) \bigotimes_{[i,j]\in\mathcal{C}[\psi(\vec{\theta})]} |s_{ij}\rangle$$

RVB ansatz: K. Seki *et al.*, Phys Rev A (2020).



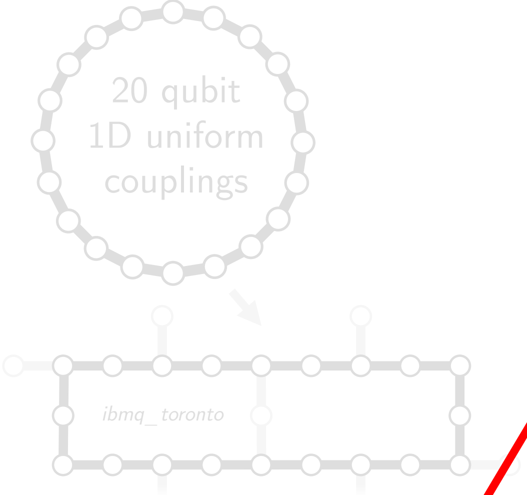


H Vallury, M Jones, G White, F Creevey, C Hill, L Hollenberg, arXiv preprint arXiv:2211.08780 (2022).

IBM Quantum Network Hub
at the University of Melbourne

QCM on Heisenberg model: noise robustness

$$H = \frac{1}{q}\sum_{\langle ij\rangle}\left(J^{(x)}_{ij}X_iX_j + J^{(y)}_{ij}Y_iY_j + J^{(z)}_{ij}Z_iZ_j\right)$$



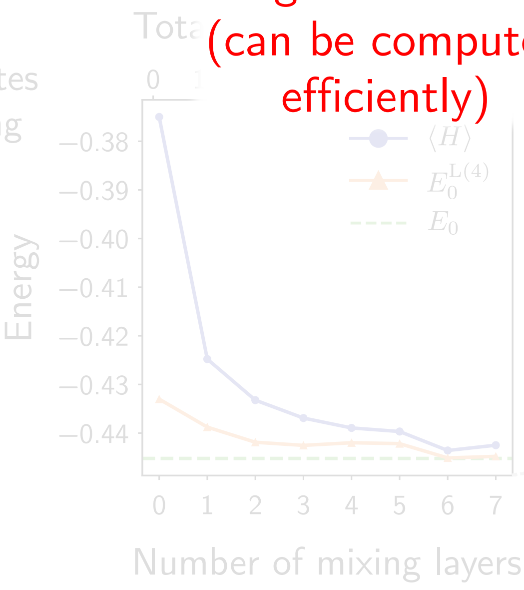
A better ansatz…?

Lots of parameters, good overlap with Heisenberg ground state

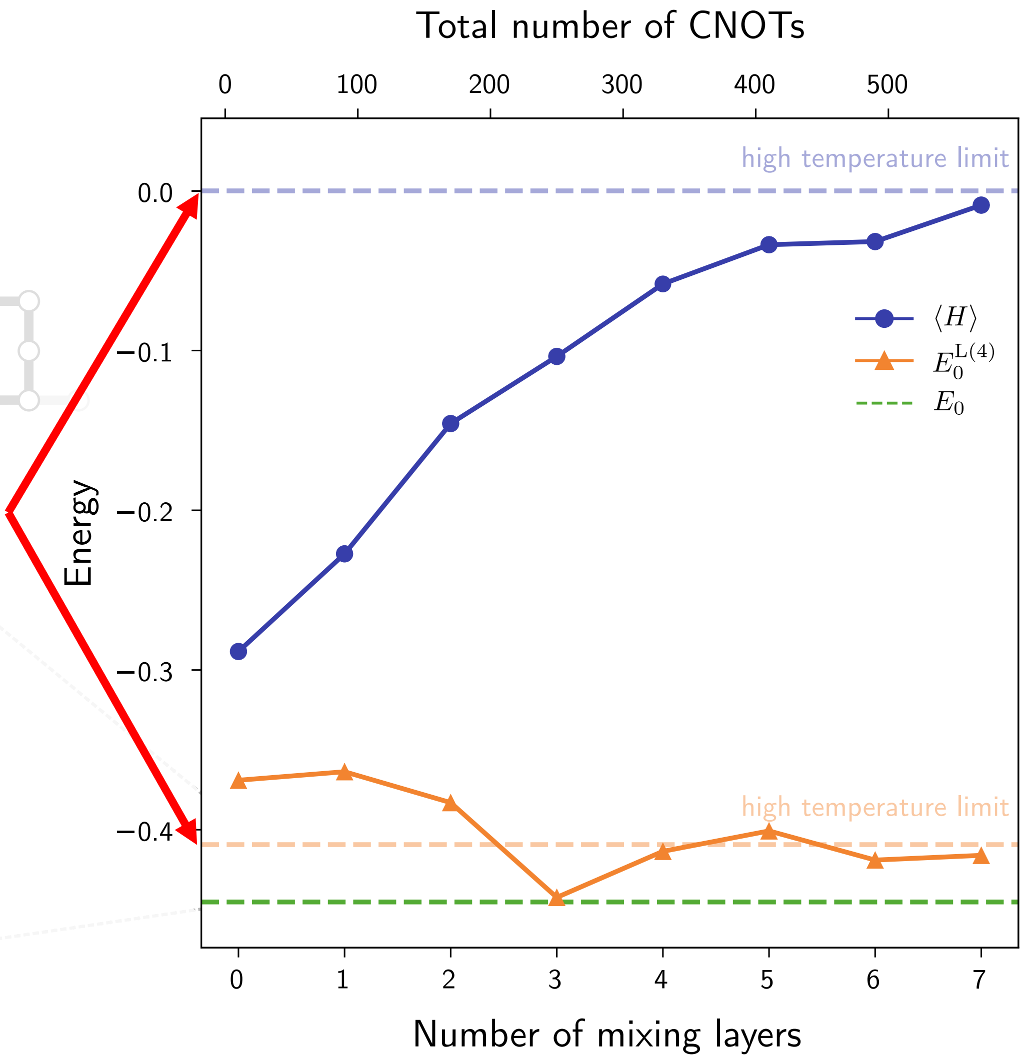
BUT many more gates required, introducing noise

$$|\psi(\vec{\theta})\rangle = \sum_{\mathcal{C}[\psi(\vec{\theta})]} w(\mathcal{C}[\psi(\vec{\theta})]) \bigotimes_{[i,j]\in\mathcal{C}[\psi(\vec{\theta})]} |s_{ij}\rangle$$

RVB ansatz: K. Seki *et al.*, Phys Rev A (2020).



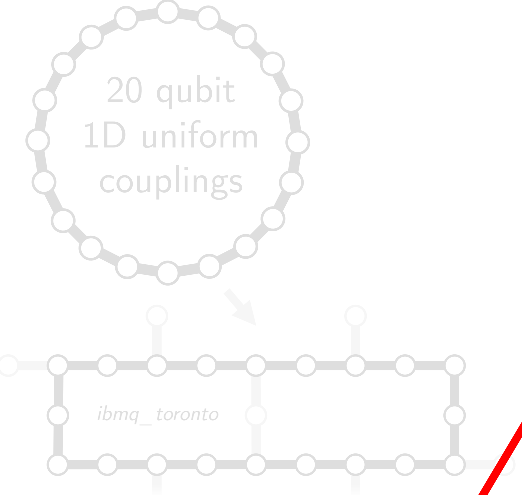
High-noise limit (can be computed efficiently)



H Vallury, M Jones, G White, F Creevey, C Hill, L Hollenberg, arXiv preprint arXiv:2211.08780 (2022).

QCM on Heisenberg model: noise robustness

$$H = \frac{1}{q}\sum_{\langle ij\rangle}\left(J_{ij}^{(x)}X_iX_j + J_{ij}^{(y)}Y_iY_j + J_{ij}^{(z)}Z_iZ_j\right)$$



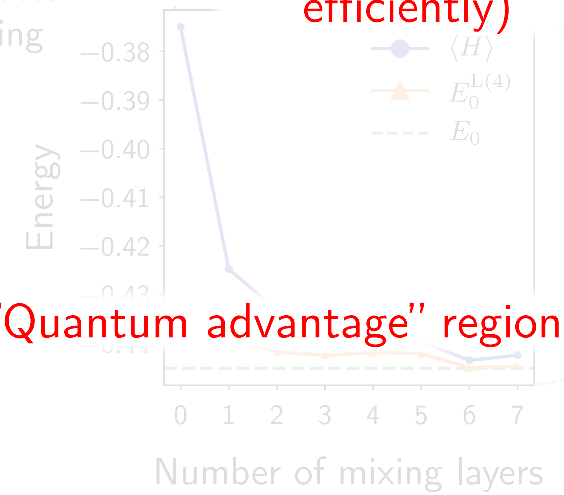
A better ansatz…?

Lots of parameters, good overlap with Heisenberg ground state

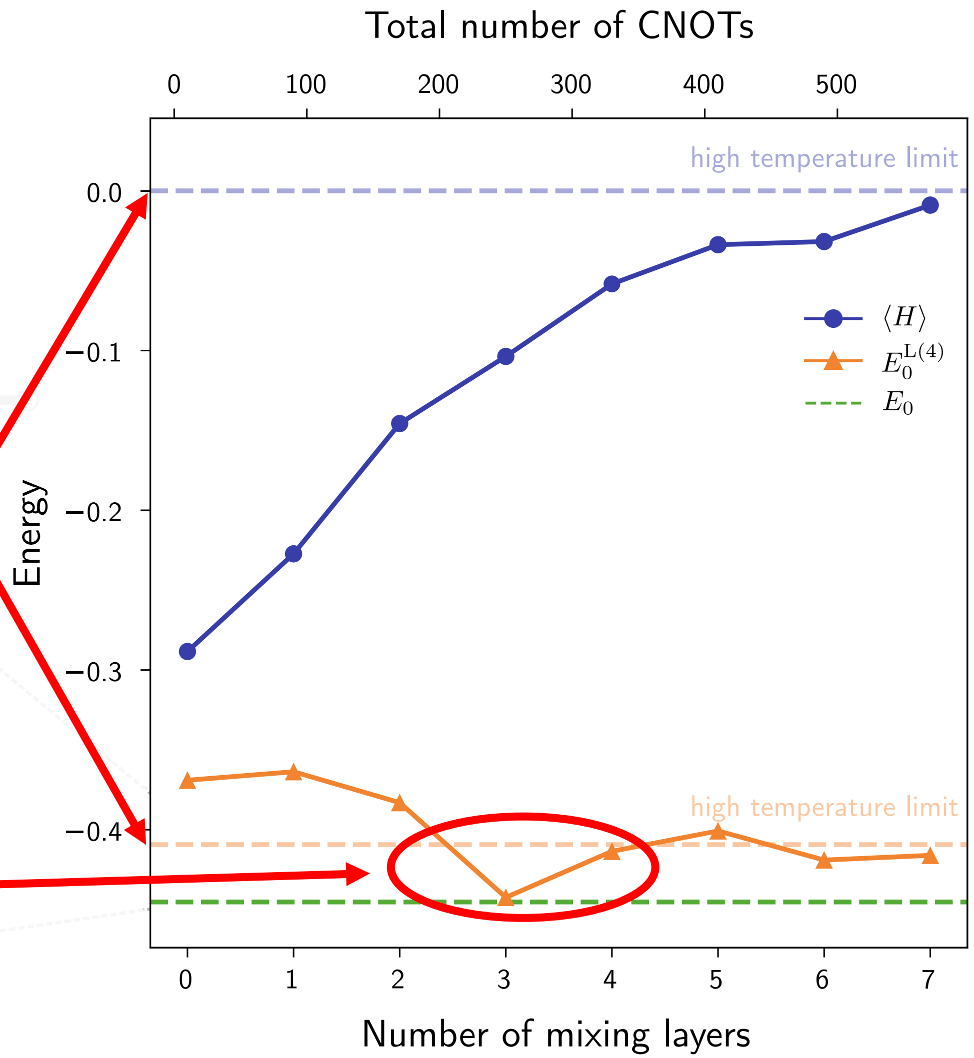
BUT many more gates required, introducing noise

$$|\psi(\vec{\theta})\rangle = \sum_{\mathcal{C}[\psi(\vec{\theta})]} w(\mathcal{C}[\psi(\vec{\theta})]) \bigotimes_{[i,j]\in\mathcal{C}[\psi(\vec{\theta})]} |s_{ij}\rangle$$

RVB ansatz: K. Seki *et al.*, Phys Rev A (2020).



High-noise limit (can be computed efficiently)

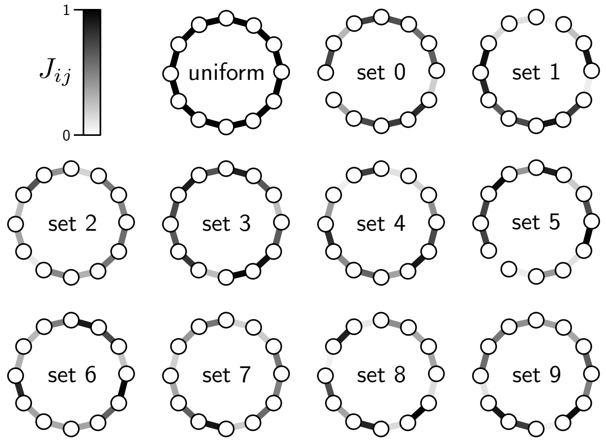


"Quantum advantage" region?

H Vallury, M Jones, G White, F Creevey, C Hill, L Hollenberg, arXiv preprint arXiv:2211.08780 (2022).

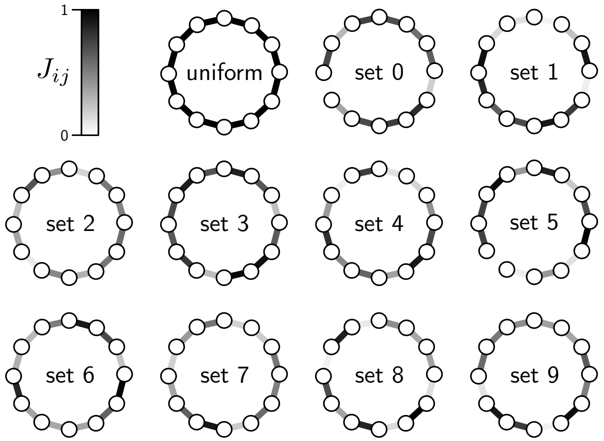
A noise-robust quantum heuristic

$$H = \sum_{\langle i\, j \rangle} J_{ij}(X_i X_j + Y_i Y_j + Z_i Z_j)$$

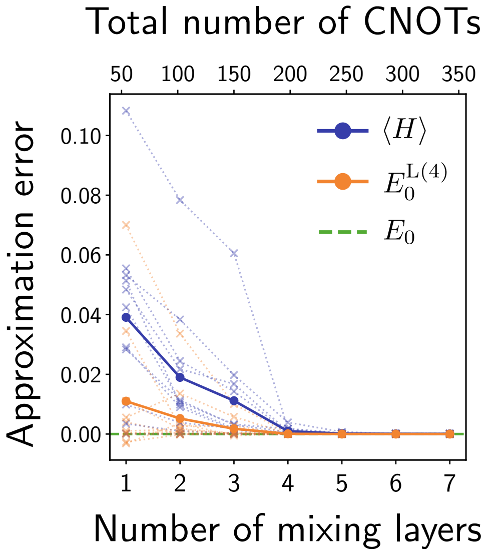


A noise-robust quantum heuristic

$$H = \sum_{\langle i\,j \rangle} J_{ij}(X_iX_j + Y_iY_j + Z_iZ_j)$$

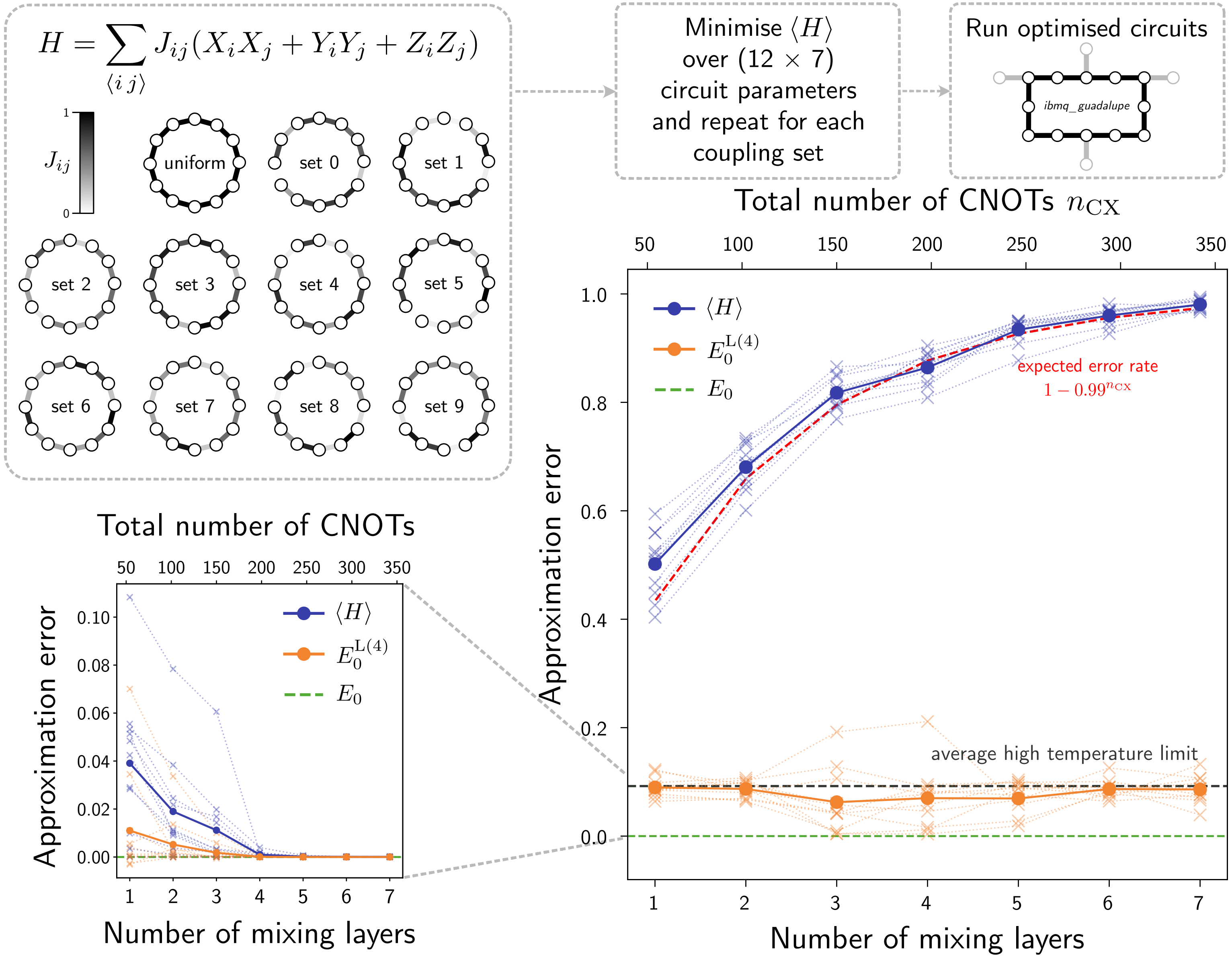


Minimise $\langle H \rangle$ over (12×7) circuit parameters and repeat for each coupling set



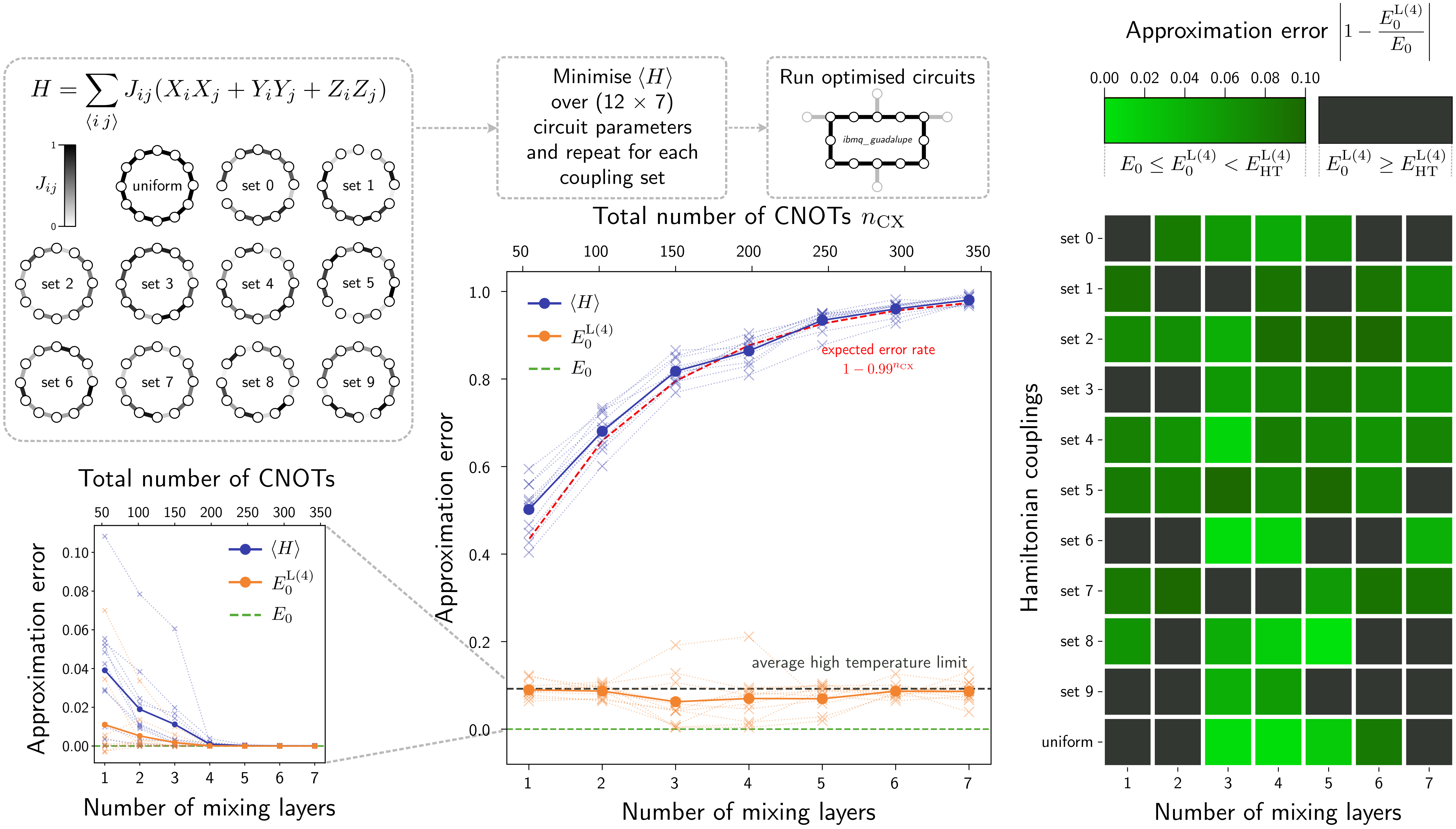
IBM Quantum Network Hub
at the University of Melbourne

A noise-robust quantum heuristic



IBM Quantum Network Hub at the University of Melbourne

A noise-robust quantum heuristic



Noisy toy model

- N-level system with fixed energy gap Δ under simple white noise with parameter $p \in [0,1]$:

$$E_j = E_0 + j\Delta, \quad j = 0, 1, \ldots, N.$$

$$\langle H^k \rangle \mapsto \langle H^k \rangle_{\text{noisy}} = (1-p)\langle H^k \rangle + \frac{p}{N}\text{tr}(H^k)$$

  - As it turns out, this error model isn't entirely unrealistic for certain randomised circuits
    Dalzell *et al.*, arXiv:2111.14907 (2021)

Noisy toy model

- N-level system with fixed energy gap Δ under simple white noise with parameter $p \in [0,1]$:

$$E_j = E_0 + j\Delta, \quad j = 0, 1, \ldots, N.$$

$$\langle H^k \rangle \mapsto \langle H^k \rangle_{\text{noisy}} = (1-p)\langle H^k \rangle + \frac{p}{N}\text{tr}(H^k)$$

  - As it turns out, this error model isn't entirely unrealistic for certain randomised circuits
    Dalzell *et al.*, arXiv:2111.14907 (2021)

- Evaluate moments with respect to exact ground state: $\langle H^k \rangle = E_0^k$

$$\implies \langle H^k \rangle_{\text{noisy}} \approx E_0^k (1 - p + \frac{p}{2} N k \frac{\Delta}{E_0})$$

Noisy toy model

$$c_n = \langle H^n \rangle - \sum_{k=0}^{n-2} \binom{n-1}{k} c_{k+1} \langle H^{n-k-1} \rangle$$

- N-level system with fixed energy gap Δ under simple white noise with parameter $p \in [0,1]$:

$$E_j = E_0 + j\Delta, \quad j = 0, 1, \ldots, N.$$

$$\langle H^k \rangle \mapsto \langle H^k \rangle_{\text{noisy}} = (1 - p)\langle H^k \rangle + \frac{p}{N} \mathrm{tr}(H^k)$$

  - As it turns out, this error model isn't entirely unrealistic for certain randomised circuits
    Dalzell *et al.*, arXiv:2111.14907 (2021)

- Evaluate moments with respect to exact ground state: $\langle H^k \rangle = E_0^k$

$$\implies \langle H^k \rangle_{\text{noisy}} \approx E_0^k (1 - p + \frac{p}{2} N k \frac{\Delta}{E_0})$$

$$E_0^{\mathrm{L}(4)} = c_1 - \frac{c_2^2}{c_3^2 - c_2 c_4}\left[\sqrt{3c_3^2 - 2c_2c_4} - c_3\right]$$

$$E_0^{\mathrm{CMX}(5)} = c_1 - \frac{c_2^2}{c_3} - \frac{1}{c_3}\frac{(c_2c_4 - c_3^2)^2}{c_3c_5 - c_4^2}$$

Seen recently in quantum computing context:
K. Seki and S. Yunoki, *PRX Quantum* **2**, 010333 (2021).

Noisy toy model

$$c_n = \langle H^n \rangle - \sum_{k=0}^{n-2} \binom{n-1}{k} c_{k+1} \langle H^{n-k-1} \rangle$$

- N-level system with fixed energy gap Δ under simple white noise with parameter $p \in [0,1]$:

$$E_j = E_0 + j\Delta, \quad j = 0, 1, \ldots, N.$$

$$\langle H^k \rangle \mapsto \langle H^k \rangle_{\text{noisy}} = (1-p)\langle H^k \rangle + \frac{p}{N}\text{tr}(H^k)$$

  - As it turns out, this error model isn't entirely unrealistic for certain randomised circuits
    Dalzell *et al.*, arXiv:2111.14907 (2021)

- Evaluate moments with respect to exact ground state: $\langle H^k \rangle = E_0^k$

$$\implies \langle H^k \rangle_{\text{noisy}} \approx E_0^k (1 - p + \frac{p}{2} N k \frac{\Delta}{E_0})$$

$$E_0^{\text{L}(4)} = c_1 - \frac{c_2^2}{c_3^2 - c_2 c_4}\left[\sqrt{3c_3^2 - 2c_2c_4} - c_3\right]$$

$$E_0^{\text{CMX}(5)} = c_1 - \frac{c_2^2}{c_3} - \frac{1}{c_3}\frac{(c_2c_4 - c_3^2)^2}{c_3c_5 - c_4^2}$$

Seen recently in quantum computing context:
K. Seki and S. Yunoki, *PRX Quantum* **2**, 010333 (2021).

- Resulting expressions for energy estimates:

$$\langle H \rangle \mapsto E_0 + p(|E_0| + \frac{1}{2}\Delta N)$$

$$E_0^{\text{CMX}(5)} \mapsto E_0 + \frac{p}{3}(|E_0| + \frac{1}{2}\Delta N) + \mathcal{O}\left[\frac{1}{N}\right]$$

$$E_0^{\text{L}(4)} \mapsto E_0 + \sqrt{\frac{2|E_0|^3}{\Delta N}} + \mathcal{O}\left[\frac{1}{N}\right]$$

Noisy toy model

$$c_n = \langle H^n \rangle - \sum_{k=0}^{n-2} \binom{n-1}{k} c_{k+1} \langle H^{n-k-1} \rangle$$

- N-level system with fixed energy gap Δ under simple white noise with parameter $p \in [0,1]$:

$$E_j = E_0 + j\Delta, \quad j = 0, 1, \ldots, N.$$

$$\langle H^k \rangle \mapsto \langle H^k \rangle_{\text{noisy}} = (1 - p)\langle H^k \rangle + \frac{p}{N}\text{tr}(H^k)$$

  - As it turns out, this error model isn't entirely unrealistic for certain randomised circuits
    Dalzell *et al.*, arXiv:2111.14907 (2021)

- Evaluate moments with respect to exact ground state: $\langle H^k \rangle = E_0^k$

$$\implies \langle H^k \rangle_{\text{noisy}} \approx E_0^k (1 - p + \frac{p}{2} N k \frac{\Delta}{E_0})$$

$$E_0^{\text{L}(4)} = c_1 - \frac{c_2^2}{c_3^2 - c_2 c_4}\left[\sqrt{3c_3^2 - 2c_2 c_4} - c_3\right]$$

$$E_0^{\text{CMX}(5)} = c_1 - \frac{c_2^2}{c_3} - \frac{1}{c_3}\frac{(c_2 c_4 - c_3^2)^2}{c_3 c_5 - c_4^2}$$

Seen recently in quantum computing context:
K. Seki and S. Yunoki, *PRX Quantum* **2**, 010333 (2021).

- Resulting expressions for energy estimates:

$$\langle H \rangle \mapsto E_0 + p(|E_0| + \frac{1}{2}\Delta N)$$

$$E_0^{\text{CMX}(5)} \mapsto E_0 + \frac{p}{3}(|E_0| + \frac{1}{2}\Delta N) + \mathcal{O}\left[\frac{1}{N}\right]$$

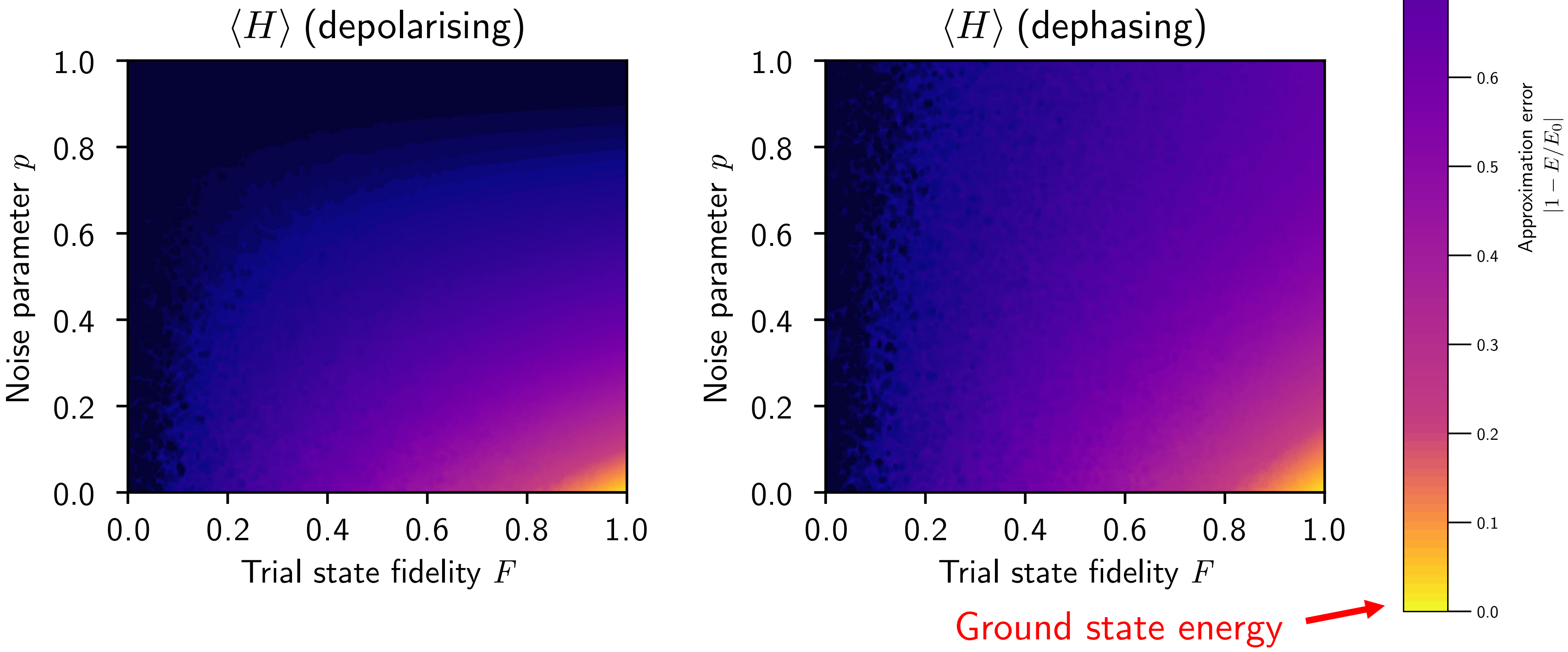
$$E_0^{\text{L}(4)} \mapsto E_0 + \sqrt{\frac{2|E_0|^3}{\Delta N}} + \mathcal{O}\left[\frac{1}{N}\right]$$

No p dependence!

More realistic error modelling

What does noisy quantum simulation reveal about the noise robustness of $E_0^{\mathrm{L}(4)}$?

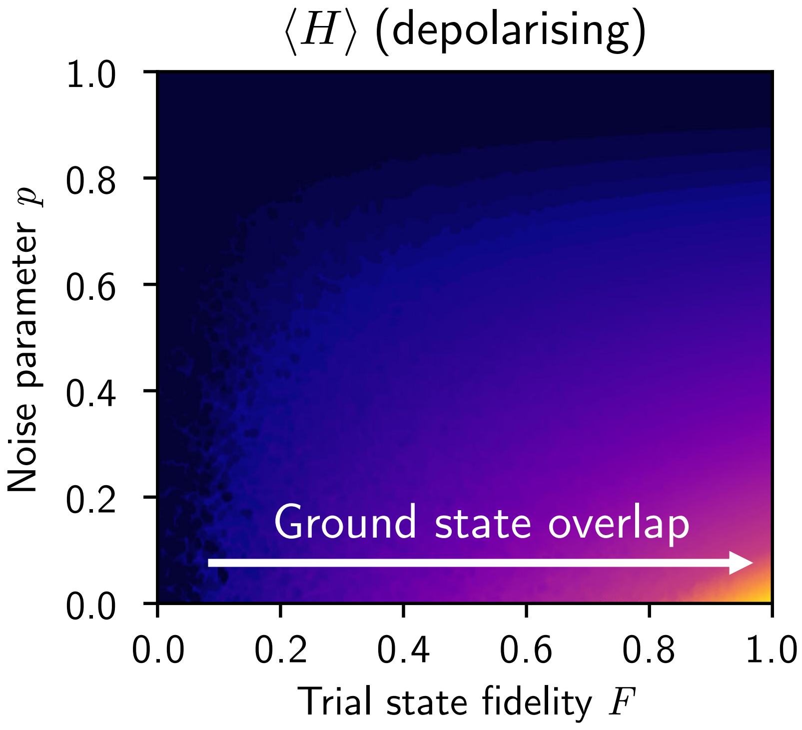
$$\boldsymbol{\rho} \mapsto (1 - \frac{3p}{4})\boldsymbol{\rho} + \frac{p}{4}(X\boldsymbol{\rho}X + Y\boldsymbol{\rho}Y + Z\boldsymbol{\rho}Z) \qquad \boldsymbol{\rho} \mapsto (1 - \frac{p}{2})\boldsymbol{\rho} + \frac{p}{2}Z\boldsymbol{\rho}Z$$

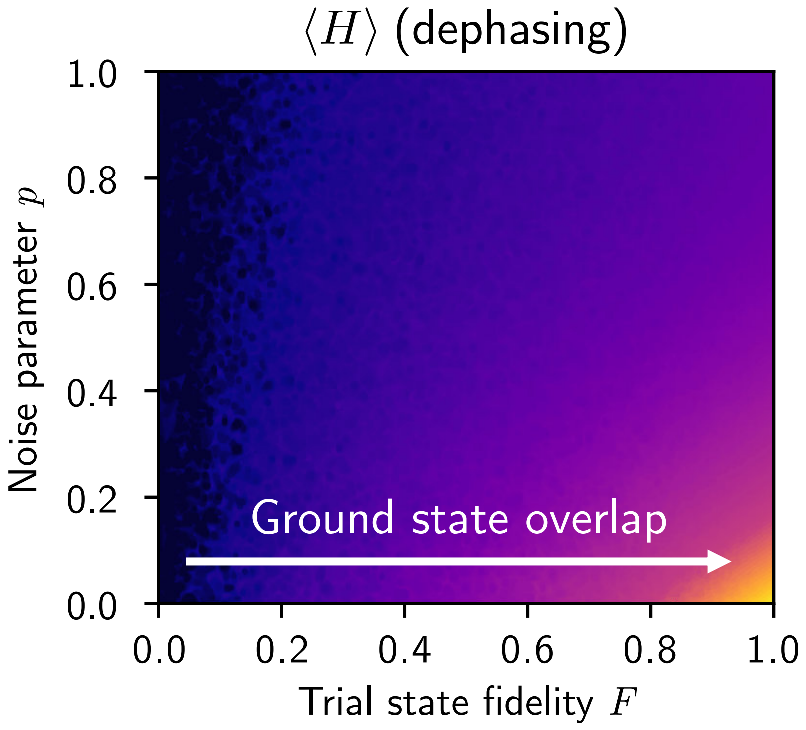


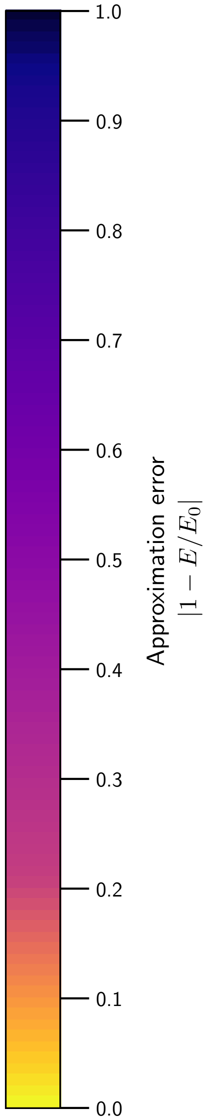
More realistic error modelling

What does noisy quantum simulation reveal about the noise robustness of $E_0^{\mathrm{L}(4)}$?

$$\boldsymbol{\rho} \mapsto (1 - \frac{3p}{4})\boldsymbol{\rho} + \frac{p}{4}(X\boldsymbol{\rho}X + Y\boldsymbol{\rho}Y + Z\boldsymbol{\rho}Z) \qquad \boldsymbol{\rho} \mapsto (1 - \frac{p}{2})\boldsymbol{\rho} + \frac{p}{2}Z\boldsymbol{\rho}Z$$



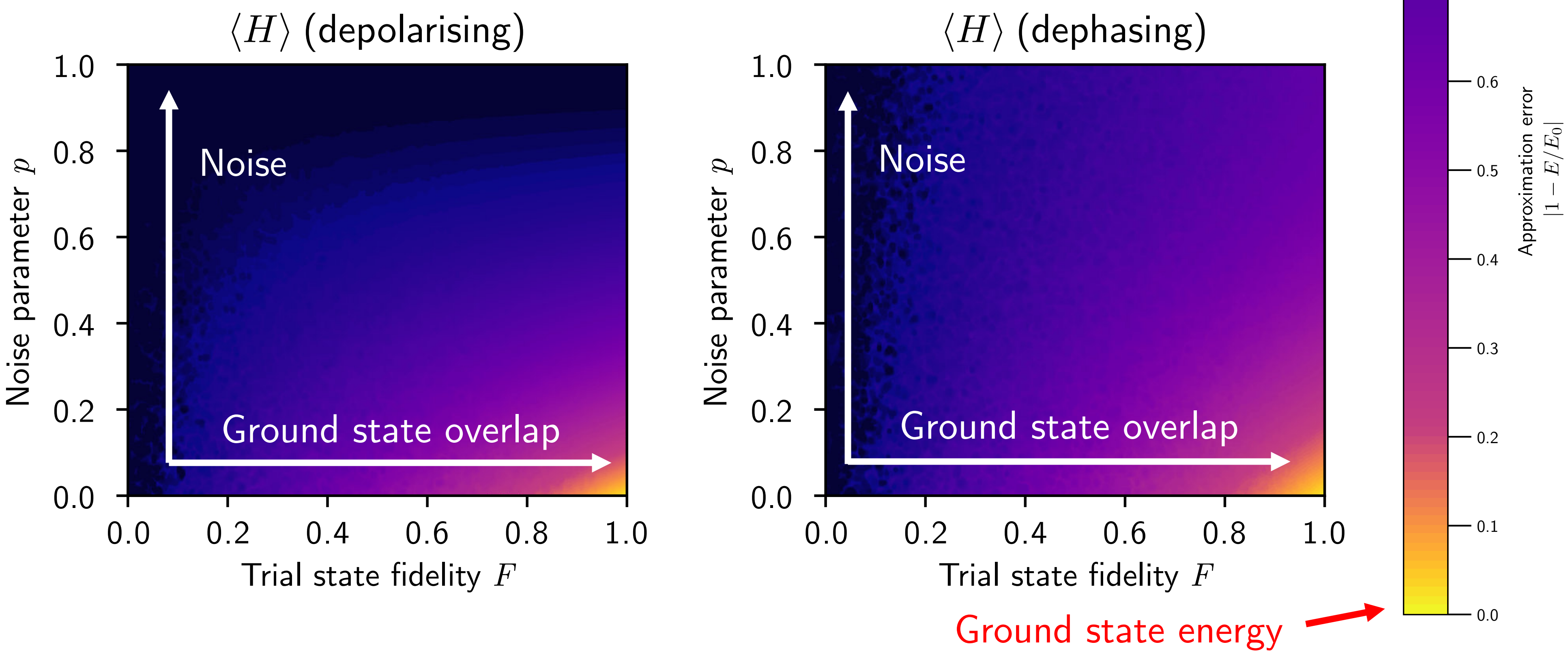




More realistic error modelling

What does noisy quantum simulation reveal about the noise robustness of $E_0^{\mathrm{L}(4)}$?

$$\boldsymbol{\rho} \mapsto (1 - \frac{3p}{4})\boldsymbol{\rho} + \frac{p}{4}(X\boldsymbol{\rho}X + Y\boldsymbol{\rho}Y + Z\boldsymbol{\rho}Z) \qquad \boldsymbol{\rho} \mapsto (1 - \frac{p}{2})\boldsymbol{\rho} + \frac{p}{2}Z\boldsymbol{\rho}Z$$

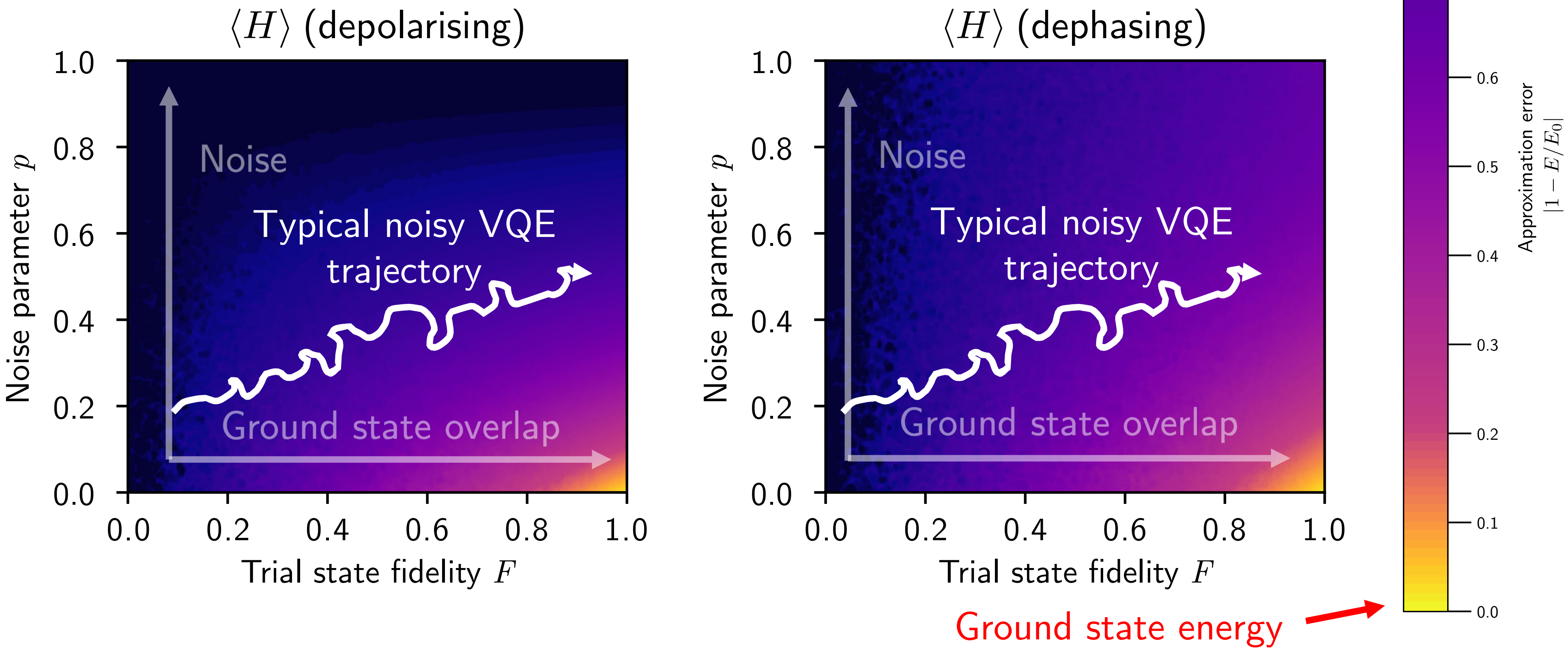


IBM Quantum Network Hub at the University of Melbourne

More realistic error modelling

What does noisy quantum simulation reveal about the noise robustness of $E_0^{\mathrm{L}(4)}$?

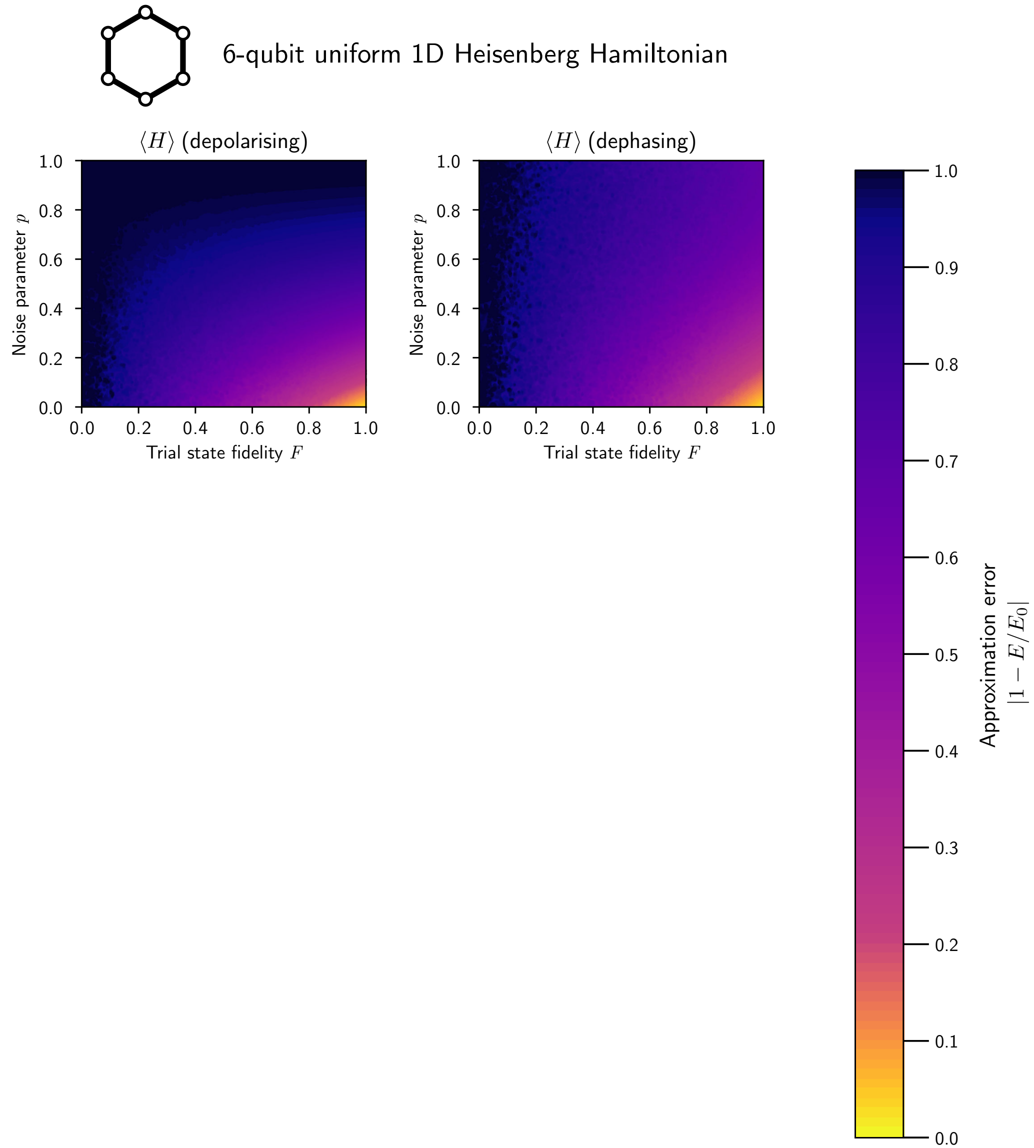
$$\boldsymbol{\rho} \mapsto (1 - \frac{3p}{4})\boldsymbol{\rho} + \frac{p}{4}(X\boldsymbol{\rho}X + Y\boldsymbol{\rho}Y + Z\boldsymbol{\rho}Z) \qquad \boldsymbol{\rho} \mapsto (1 - \frac{p}{2})\boldsymbol{\rho} + \frac{p}{2}Z\boldsymbol{\rho}Z$$



Simulated error model results

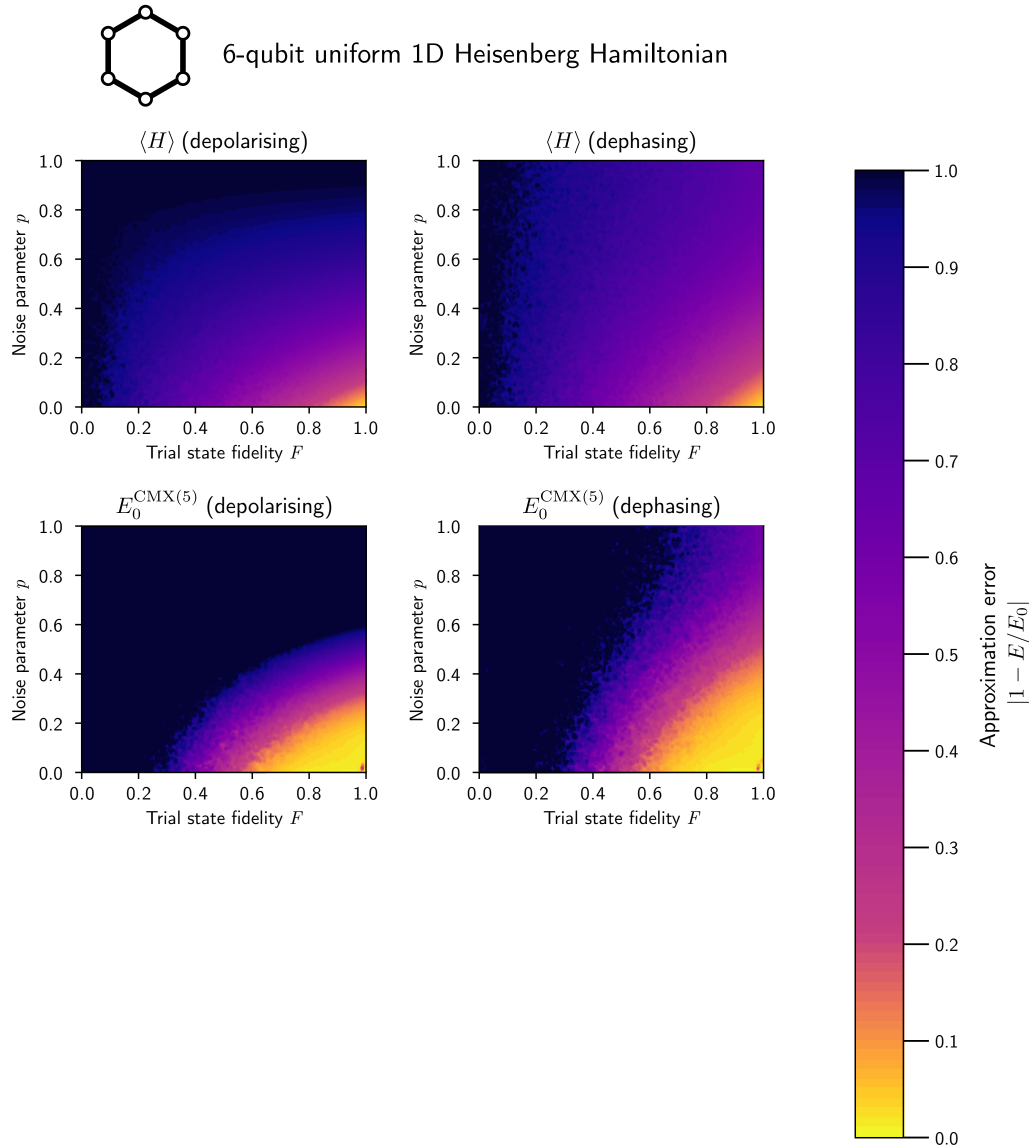
IBM Quantum Network Hub at the University of Melbourne

$\langle H \rangle$



$$\langle H \rangle = c_1$$

Simulated error model results



$\langle H \rangle$

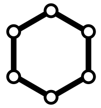
$E_0^{\mathrm{CMX}(5)}$

$$\langle H \rangle = c_1$$

$$E_0^{\mathrm{CMX}(5)} = c_1 - \frac{c_2^2}{c_3} - \frac{1}{c_3}\frac{(c_2 c_4 - c_3^2)^2}{c_3 c_5 - c_4^2}$$

IBM Quantum Network Hub
at the University of Melbourne

Simulated error model results

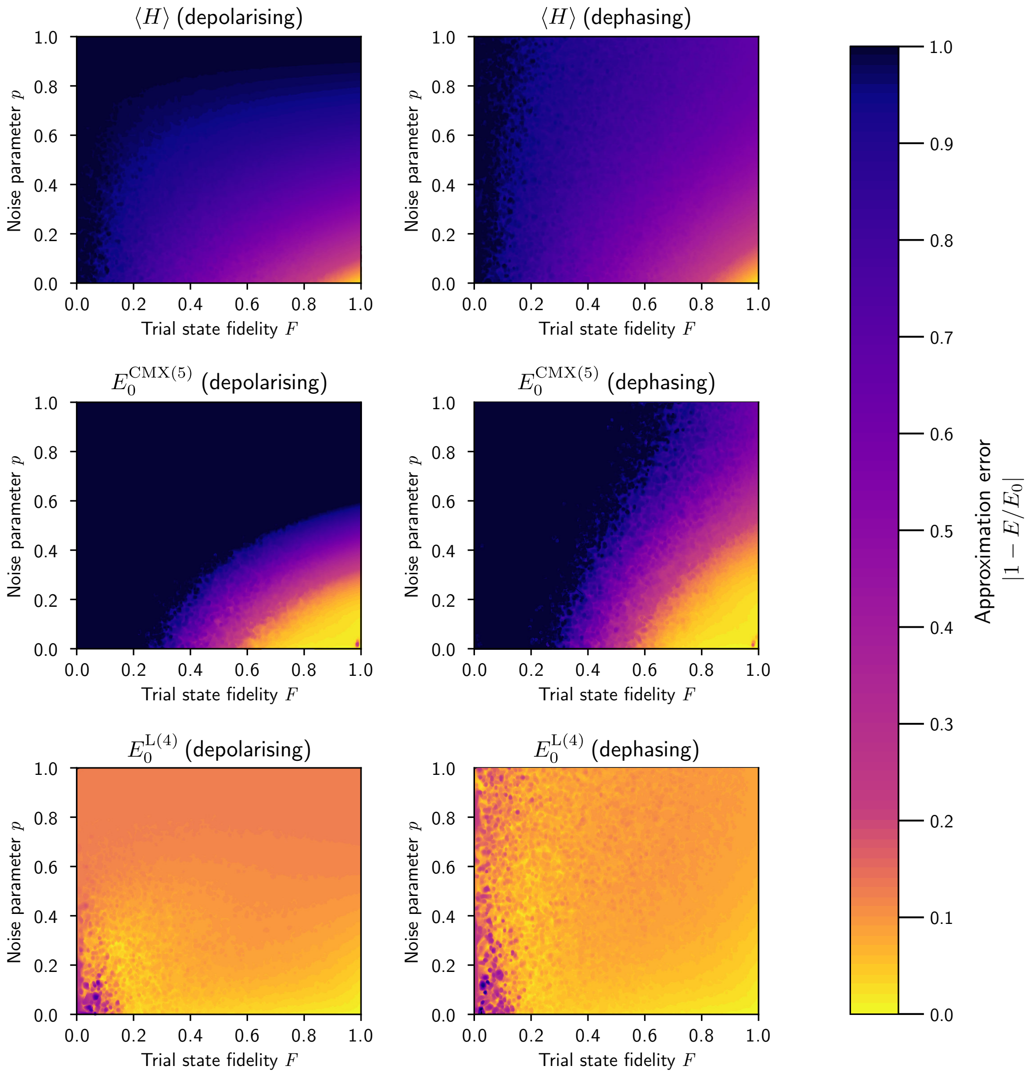


6-qubit uniform 1D Heisenberg Hamiltonian

$\langle H \rangle$

$E_0^{\mathrm{CMX}(5)}$

$E_0^{\mathrm{L}(4)}$

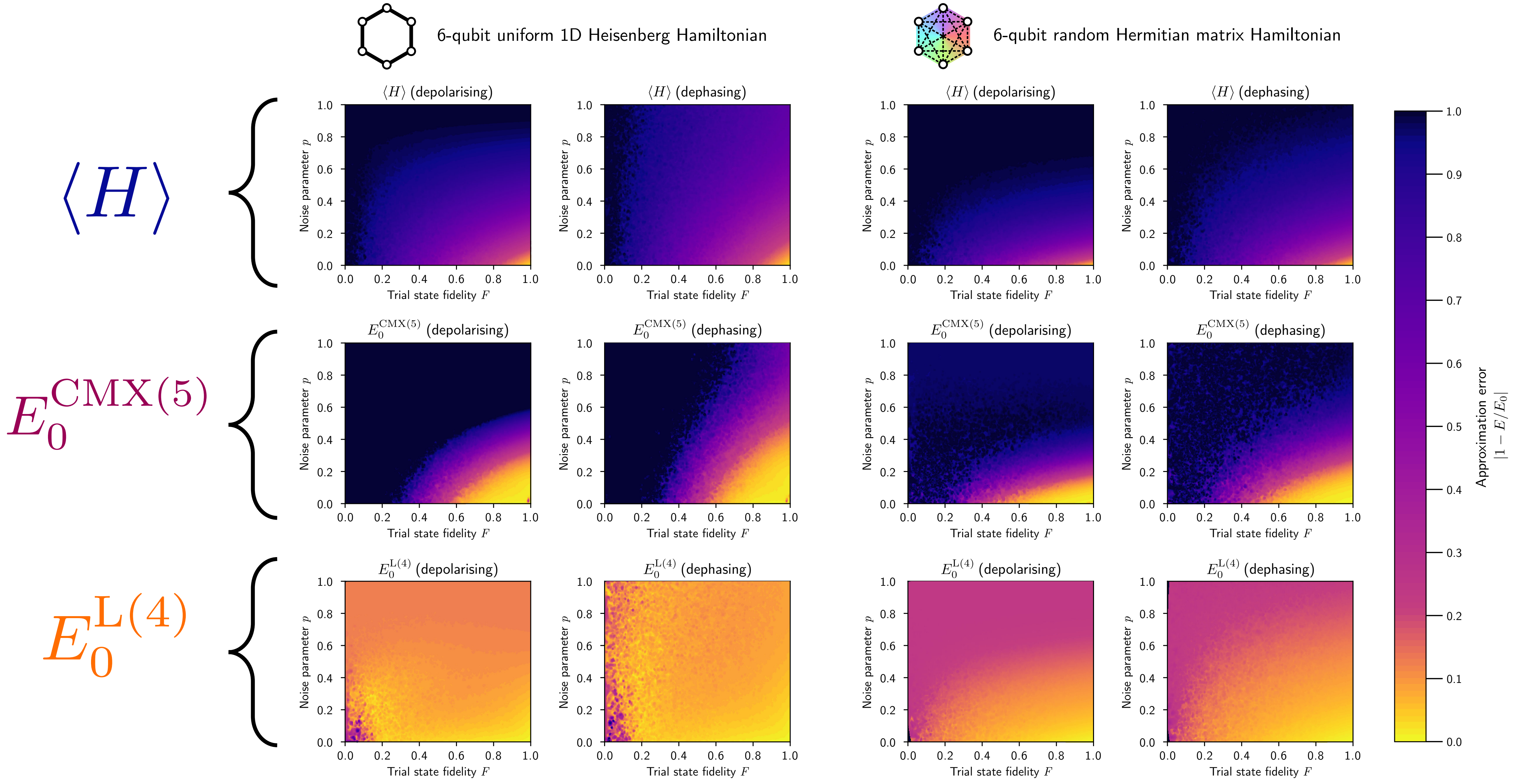


$$\langle H \rangle = c_1$$

$$E_0^{\mathrm{CMX}(5)} = c_1 - \frac{c_2^2}{c_3} - \frac{1}{c_3}\frac{(c_2 c_4 - c_3^2)^2}{c_3 c_5 - c_4^2}$$

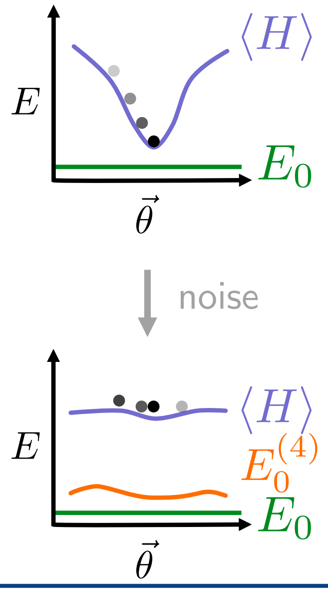
$$E_0^{\mathrm{L}(4)} = c_1 - \frac{c_2^2}{c_3^2 - c_2 c_4}\left[\sqrt{3c_3^2 - 2c_2 c_4} - c_3\right]$$

Simulated error model results



Summary

- Variational quantum algorithms have near-term utility, but right now still heavily impacted by noise
- Computing additional Hamiltonian moments improves on variational ground state energy estimate
- This method can handle suboptimal trial states and circumvent noise on present-day hardware



- QCM method: HJV, MAJ, CDH, LCLH, *Quantum* **4**, 373 (2020).
- Chemistry application: MAJ, HJV, CDH, LCLH, *Sci Rep* **12**, 8985 (2022).
- Noise robustness: HJV, MAJ, GALW, FMC, CDH, LCLH, arXiv:2211.08780 (2022).

- Demonstrated noise robustness for deep circuits on real quantum computer (~500 CNOTs)
- Error-filtering behaviour of QCM studied via analytical model and noisy simulation
- Hardware error rate improvement by 2 orders of magnitude required for VQE results to match

arXiv:2211.08780

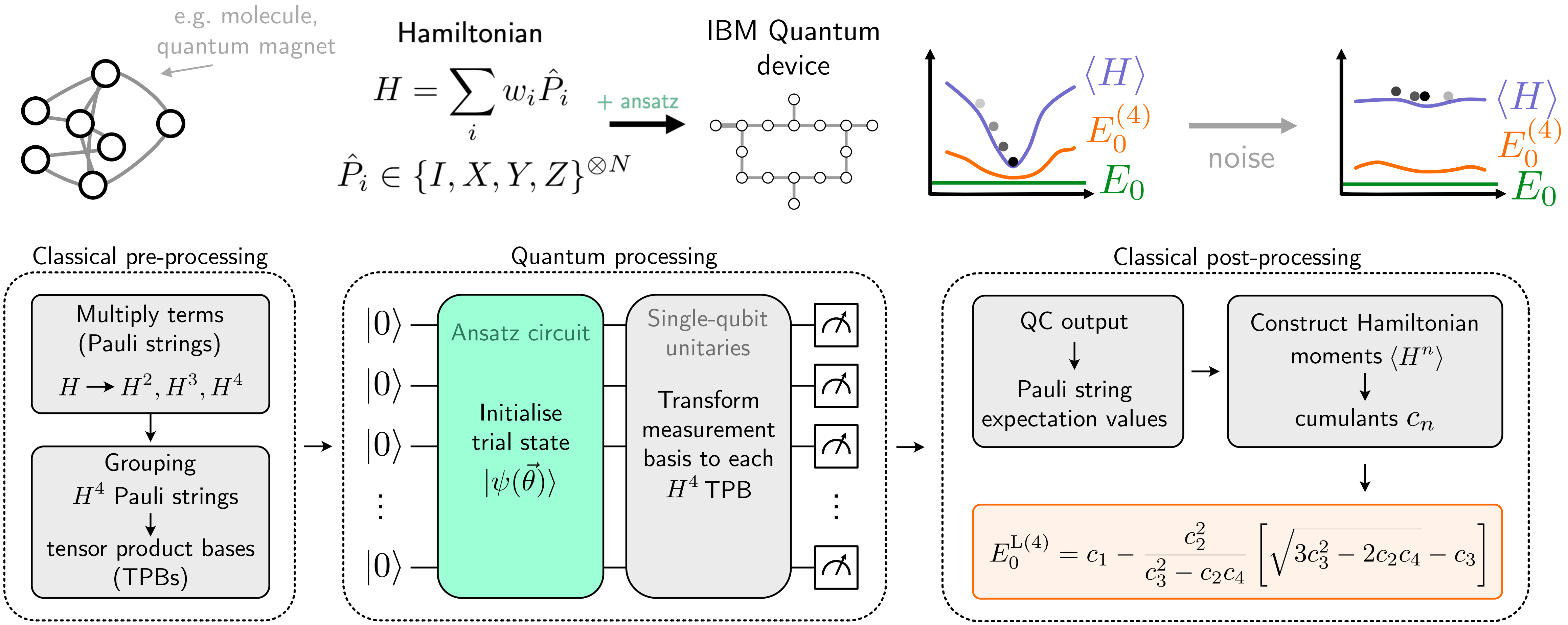
Future work:

- Larger instances of quantum many-body problems
- Classify computational complexity vs. classical methods (e.g. DMRG)
- Moments-based estimates for other ground state observables and excited states

Thank you

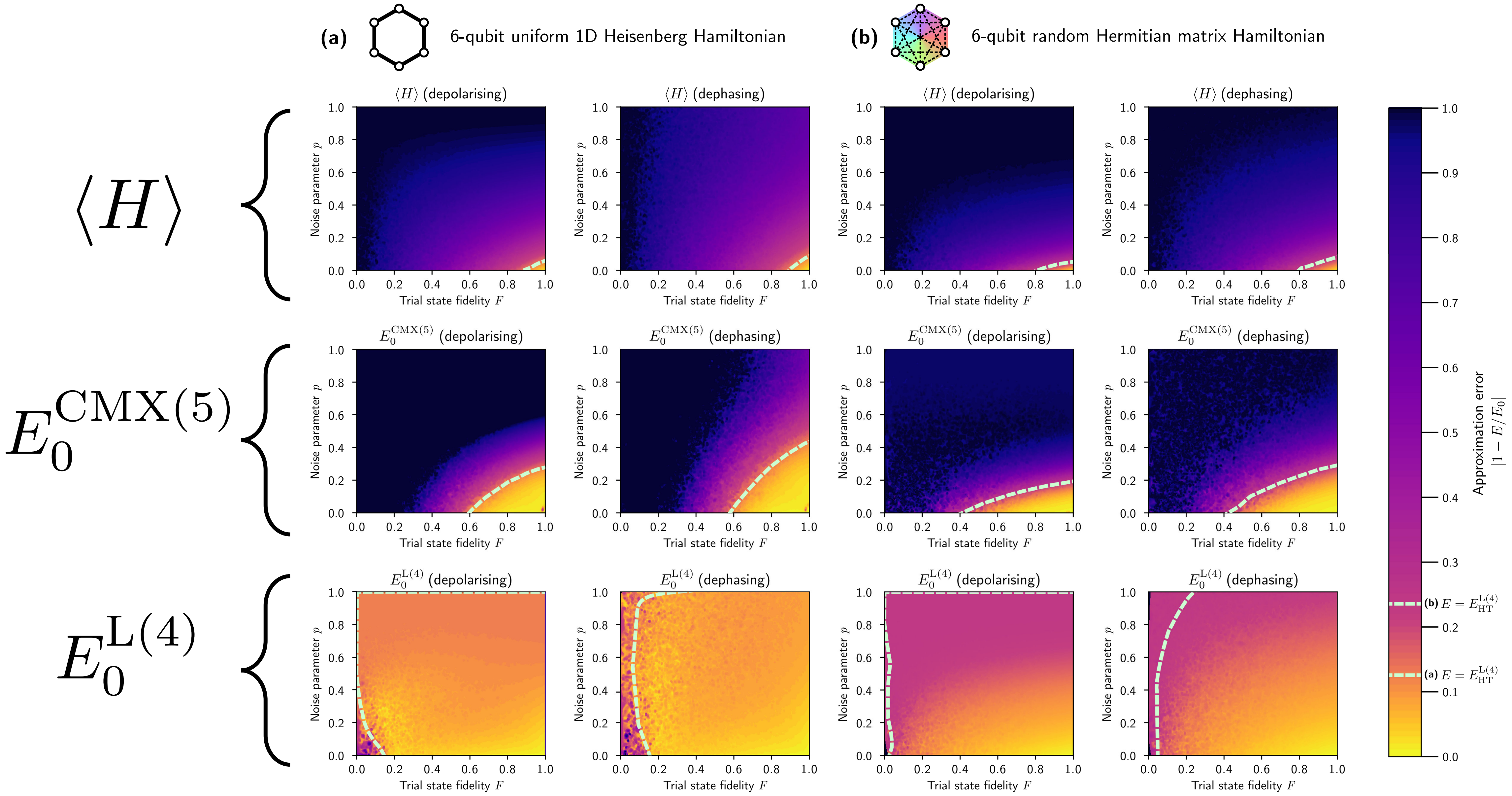
IBM Quantum Network Hub
at the University of Melbourne

The quantum computed moments (QCM) approach



H Vallury, M Jones, C Hill, L Hollenberg,
Quantum **4**, 373 (2020).

Simulated error model results



More noisy simulation

- Have implemented a circuit-based error model to match the results obtained from the real device
- Current QC hardware error rates need to reduce by two orders of magnitude for $\langle H \rangle$ to match accuracy of $E_0^{\mathrm{L}(4)}$