Cloud Quantum Computing of an Atomic Nucleus

CCWang, Journal Club @2316
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References

PhysRevLett120(2018)210501 E. F. Dumitrescu, *et al.*

PhysRevX6(2016)031007 P. J. J. O'Malley, *et al*.

https://hiq.huaweicloud.com/portal/programming/hiq-composer

Abstract

We report a quantum simulation of the deuteron binding energy on quantum processors accessed via cloud servers. We use a Hamiltonian from pionless effective field theory at leading order. We design a low-depth version of the unitary coupled-cluster ansatz, use the variational quantum eigensolver algorithm, and compute the binding energy to within a few percent. Our work is the first step towards scalable nuclear structure computations on a quantum processor via the cloud, and it sheds light on how to map scientific computing applications onto nascent quantum devices.

Key words

Quantum computing

Pionless EFT

Unitary coupled-cluster (UCC)

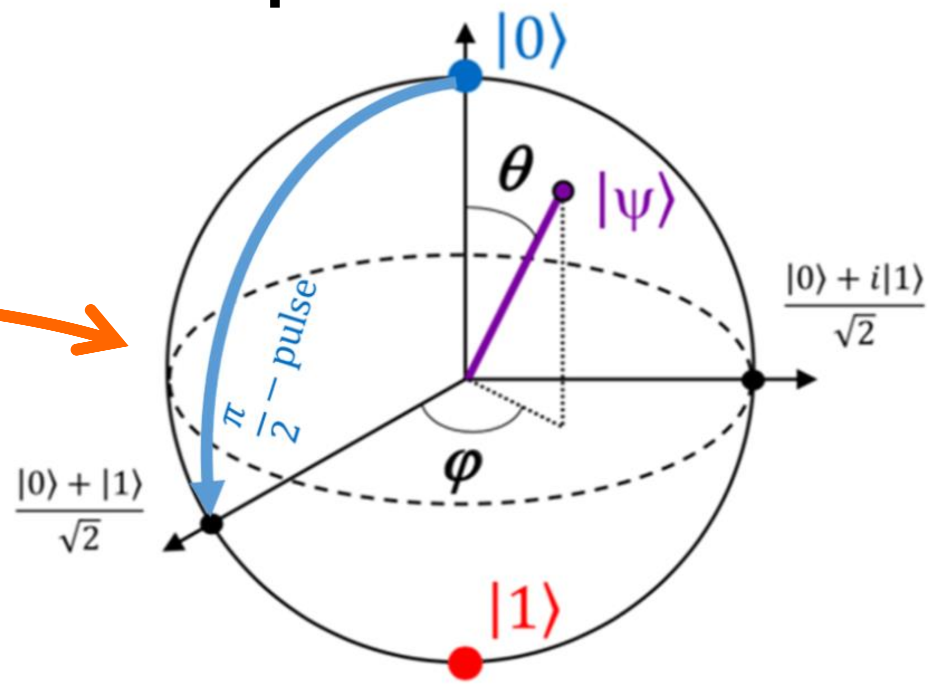
Variational quantum eigensolver (VQE) algorithm

A Qubit

$$|0\rangle := \begin{pmatrix} 1 \\ 0 \end{pmatrix}; \quad |1\rangle := \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$|\psi\rangle := \alpha\,|0\rangle + \beta\,|1\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

Bloch sphere



Quantum Gate & Circuit

Hadamard门（H门）

$$H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

π/8门（T门）

$$T = \begin{bmatrix} e^{-\frac{\pi}{8}i} & 0 \\ 0 & e^{\frac{\pi}{8}i} \end{bmatrix}$$

相位门（S门）

$$S = \begin{bmatrix} 1 & 0 \\ 0 & e^{\frac{\pi}{2}i} \end{bmatrix}$$

Pauli-X门（X门）

$$X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

Pauli-Y门（Y门）

$$Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

Pauli-Z门（Z门）

$$Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

Quantum Gate & Circuit, Cont'd

Rx门

$$Rx(\theta) = \begin{bmatrix} \cos(\frac{\theta}{2}) & -i\sin(\frac{\theta}{2}) \\ -i\sin(\frac{\theta}{2}) & \cos(\frac{\theta}{2}) \end{bmatrix}$$

Ry门

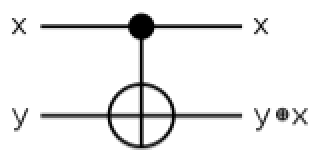
$$Ry(\theta) = \begin{bmatrix} \cos(\frac{\theta}{2}) & -\sin(\frac{\theta}{2}) \\ \sin(\frac{\theta}{2}) & \cos(\frac{\theta}{2}) \end{bmatrix}$$

Rz门

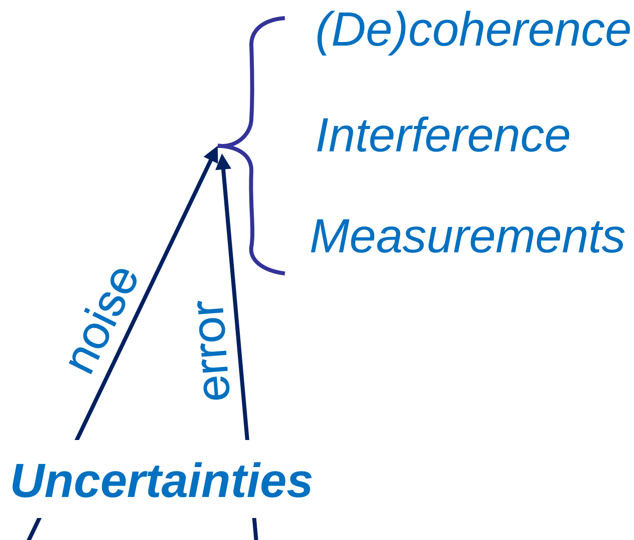
$$Rz(\theta) = \begin{bmatrix} e^{-\frac{i\theta}{2}} & 0 \\ 0 & e^{\frac{i\theta}{2}} \end{bmatrix}$$

受控非门（CNOT门）

$$CONT = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

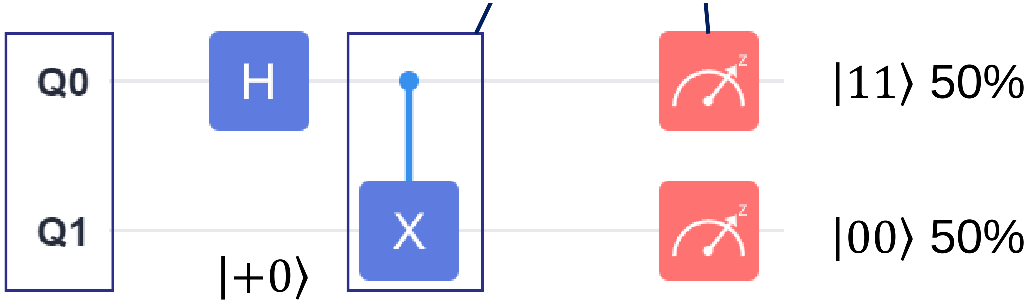


input		output	
x	y	x	y+x
$\|0\rangle$	$\|0\rangle$	$\|0\rangle$	$\|0\rangle$
$\|0\rangle$	$\|1\rangle$	$\|0\rangle$	$\|1\rangle$
$\|1\rangle$	$\|0\rangle$	$\|1\rangle$	$\|1\rangle$
$\|1\rangle$	$\|1\rangle$	$\|1\rangle$	$\|0\rangle$



Circuit Sample: Bell State

$|00\rangle = |0\rangle_{Q0} \otimes |0\rangle_{Q1}$



Pionless EFT in momentum-space

PhysRevC**98**(2018)054301

$$V_{NN}^{(0)}(\vec{p}', \vec{p}) = C_S + C_T \vec{\sigma}_1 \cdot \vec{\sigma}_2,$$

$$V_{NN}^{(2)}(\vec{p}', \vec{p}) = \mathrm{C}_1 q^2 + \mathrm{C}_2 k^2 + (C_3 q^2 + C_4 k^2)\vec{\sigma}_1 \cdot \vec{\sigma}_2 - iC_5 \frac{\vec{\sigma}_1 + \vec{\sigma}_2}{2} \cdot (\vec{q} \times \vec{k}) + C_6(\vec{\sigma}_1 \cdot \vec{q})(\vec{\sigma}_2 \cdot \vec{q}) + C_7(\vec{\sigma}_1 \cdot \vec{k})(\vec{\sigma}_2 \cdot \vec{k}).$$

$$V_{NN}^{\mathrm{LO}}({}^1S_0) = \tilde{C}_{{}^1S_0} = C_S - 3C_T,$$

$$V_{NN}^{\mathrm{LO}}({}^3S_1) = \tilde{C}_{{}^3S_1} = C_S + C_T,$$

$$V_{NN}^{\mathrm{NLO}}({}^1S_0) = C_{{}^1S_0}(p^2 + p'^2),$$

$$V_{NN}^{\mathrm{NLO}}({}^3S_1) = C_{{}^3S_1}(p^2 + p'^2).$$

Low-energy observables: $k \cot \delta_0(k) = -\frac{1}{a_0} + \frac{1}{2} r_0 k^2 + \cdots$ and deuteron

Coupled-cluster method

PhysRevC**82**(2010)034330

$$\overline{H} = e^{-T} H e^{T}$$

$H \rightarrow \{\phi_0\}$ reference state

$$T_k = \frac{1}{(k!)^2} \sum_{i_1,\ldots,i_k;a_1,\ldots,a_k} t_{i_1\ldots i_k}^{a_1\ldots a_k} a_{a_1}^{\dagger} \cdots a_{a_k}^{\dagger} a_{i_k} \cdots a_{i_1}$$

singles-and-doubles excitations (CCSD) $T \approx T_1 + T_2$.

t_i^a $\quad 0 = \langle \phi_i^a | \overline{H} | \phi_0 \rangle,$

t_{ij}^{ab} $\quad 0 = \langle \phi_{ij}^{ab} | \overline{H} | \phi_0 \rangle.$

→ $E = \langle \phi_0 | \overline{H} | \phi_0 \rangle.$

Quantum process for Molecular H_2 Solutions

PhysRevX6(2016)031007

$$H = \sum_{pq} h_{pq} a_p^\dagger a_q + \frac{1}{2} \sum_{\text{pqrs}} h_{\text{pqrs}} a_p^\dagger a_q^\dagger a_r a_s,$$

with

$$h_{pq} = \int d\sigma \phi_p^*(\sigma) \left(\frac{\nabla_r^2}{2} - \sum_i \frac{Z_i}{|R_i - r|} \right) \phi_q(\sigma)$$

$$h_{\text{pqrs}} = \int d\sigma_1 d\sigma_2 \frac{\phi_p^*(\sigma_1)\phi_q^*(\sigma_2)\phi_s(\sigma_1)\phi_r(\sigma_2)}{|r_1 - r_2|}$$

Effective 2-qubit Hamiltonian

$$H = g_0 \mathbb{1} + g_1 Z_0 + g_2 Z_1 + g_3 Z_0 Z_1 + g_4 X_0 X_1 + g_5 Y_0 Y_1$$

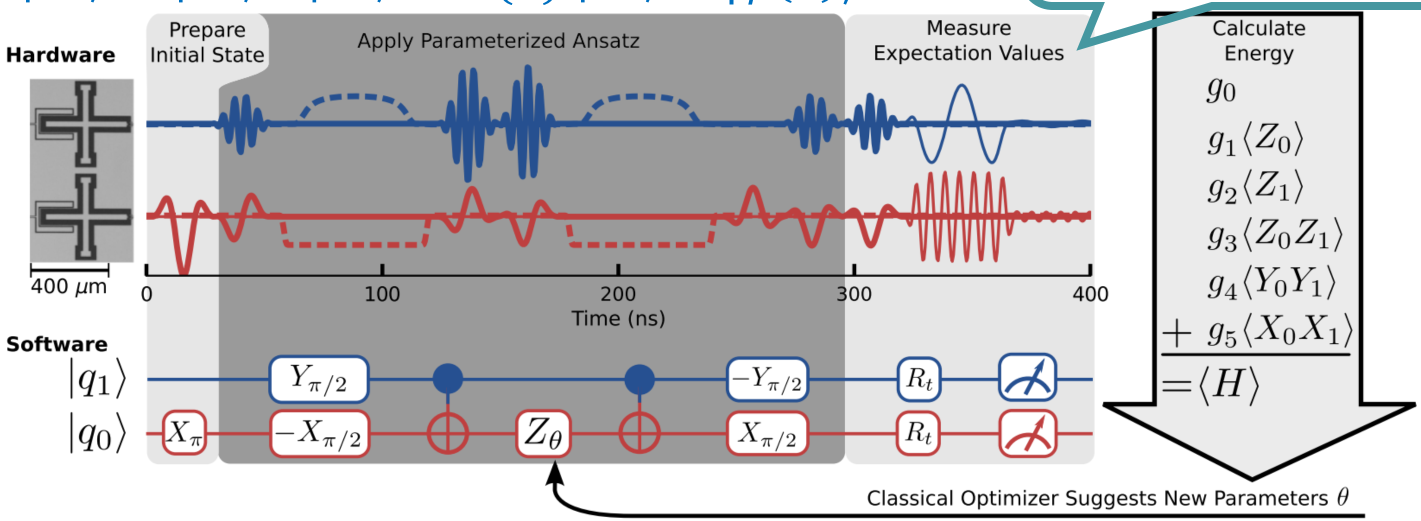
2-qubit state for electron

$$|\varphi(\vec{\theta})\rangle = U(\vec{\theta})|\varphi\rangle = e^{T(\vec{\theta}) - T(\vec{\theta})^\dagger}|\phi\rangle$$

Measurement & variation

$$\frac{\langle \varphi(\vec{\theta})|H|\varphi(\vec{\theta})\rangle}{\langle \varphi(\vec{\theta})|\varphi(\vec{\theta})\rangle} \geq E_0$$

$|00\rangle \rightarrow |01\rangle$ $\quad |01\rangle \rightarrow U(\theta)\,|01\rangle = |\varphi(\theta)\rangle$



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Construction of Hamiltonian

$$H_N = \sum_{n,n'=0}^{N-1} \langle n'|(T+V)|n\rangle a_{n'}^{\dagger} a_n$$

$$\langle n'|T|n\rangle = \frac{\hbar\omega}{2}\Big[(2n+3/2)\delta_n^{n'} - \sqrt{n(n+1/2)}\delta_n^{n'+1} - \sqrt{(n+1)(n+3/2)}\delta_n^{n'-1}\Big],$$

$$\langle n'|V|n\rangle = V_0\delta_n^0\delta_n^{n'}. \qquad V_0 = -5.68658111\ \mathrm{MeV}$$

Jordan-Wigner transformation

$$a_n^{\dagger} \rightarrow \frac{1}{2}\left[\prod_{j=0}^{n-1} -Z_j\right](X_n - iY_n)$$

$$a_n \rightarrow \frac{1}{2}\left[\prod_{j=0}^{n-1} -Z_j\right](X_n + iY_n)$$

⇒

$$H_1 = 0.218\,291(Z_0 - I)$$

$$H_2 = 5.906\,709 I + 0.218\,291 Z_0 - 6.125 Z_1 - 2.143\,304(X_0X_1 + Y_0Y_1),$$

$$H_3 = H_2 + 9.625(I - Z_2) - 3.913\,119(X_1X_2 + Y_1Y_2)$$

Construction of initial variational state

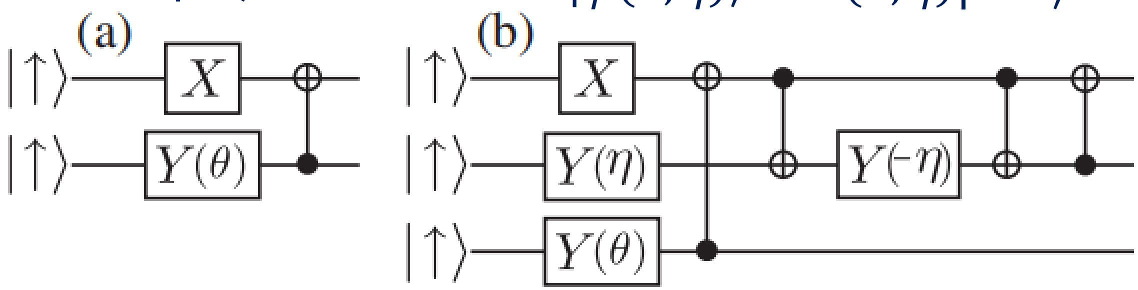
$$U(\theta) \equiv e^{\theta(a_0^\dagger a_1 - a_1^\dagger a_0)} = e^{i(\theta/2)(X_0 Y_1 - X_1 Y_0)},$$

$$U(\eta,\theta) \equiv e^{\eta(a_0^\dagger a_1 - a_1^\dagger a_0) + \theta(a_0^\dagger a_2 - a_2^\dagger a_0)}$$

$$\approx e^{i(\eta/2)(X_0 Y_1 - X_1 Y_0)} e^{i(\theta/2)(X_0 Z_1 Y_2 - X_2 Z_1 Y_0)}$$

$|\varphi(\theta)\rangle = U(\theta)|00\rangle$

$|\varphi(\theta,\eta)\rangle = U(\theta,\eta)|000\rangle$



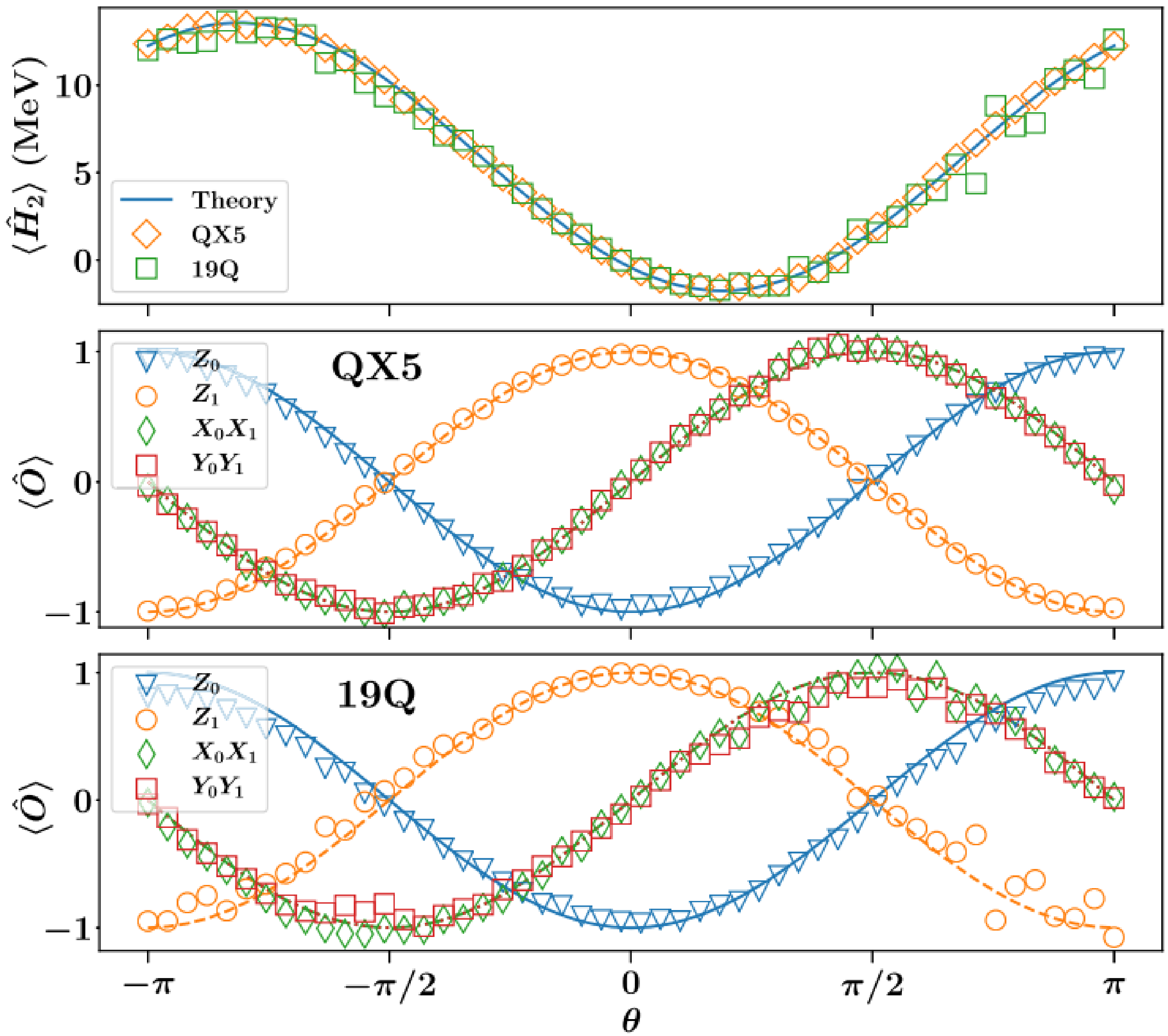
Matching finite model-space to infinite-basis: Luescher's formula

$$E_N = -\frac{\hbar^2 k^2}{2m}\left(1 - 2\frac{\gamma^2}{k} e^{-2kL} - 4\frac{\gamma^4 L}{k} e^{-4kL}\right) + \frac{\hbar^2 k \gamma^2}{m}\left(1 - \frac{\gamma^2}{k} - \frac{\gamma^4}{4k^2} + 2 w_2 k \gamma^4\right) e^{-4kL}$$

⇒

$$E_\infty = -\hbar^2 k^2/(2m)$$

Results of $H_2 = 5.906\,709 I + 0.218\,291 Z_0 - 6.125 Z_1 - 2.143\,304 (X_0 X_1 + Y_0 Y_1)$

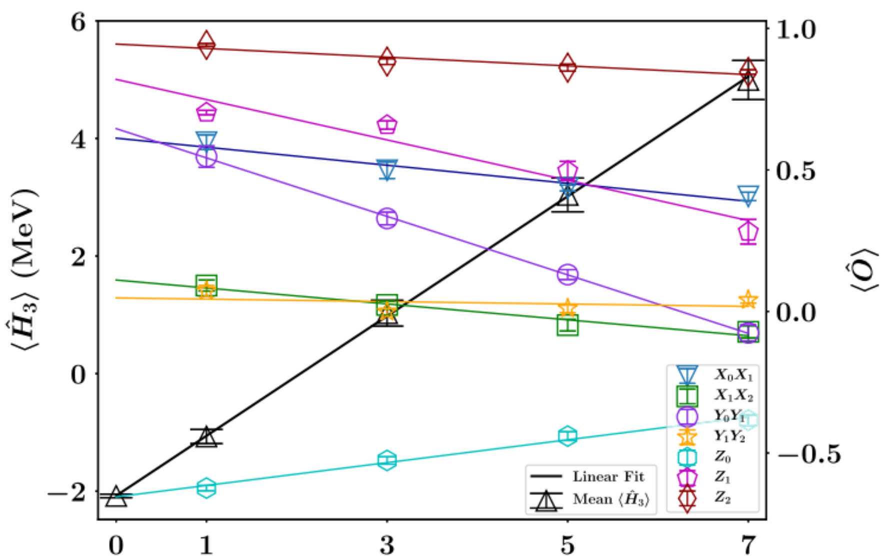


Results of H_3 , Noise estimator

Ansatz: $\mathcal{E}(\rho) = (1-\varepsilon)\rho + \varepsilon I/4$

$$\rho = |\varphi(\theta)\rangle\langle\varphi(\theta)|$$

$$\mathcal{E}_r(\rho) = (1 - r\varepsilon)C_X \rho C_X + r\varepsilon I/4 + O(\varepsilon^2)$$



E from exact diagonalization				
N	E_N	$O(e^{-2kL})$	$O(kLe^{-4kL})$	$O(e^{-4kL})$
2	−1.749	−2.39	−2.19	
3	−2.046	−2.33	−2.20	−2.21
E from quantum computing				
N	E_N	$O(e^{-2kL})$	$O(kLe^{-4kL})$	$O(e^{-4kL})$
2	−1.74(3)	−2.38(4)	−2.18(3)	
3	−2.08(3)	−2.35(2)	−2.21(3)	−2.28(3)

Thank you for your attentions!