Symbolic Pauli Propagation for Gradient Enabled Pre-Training of Quantum Circuits

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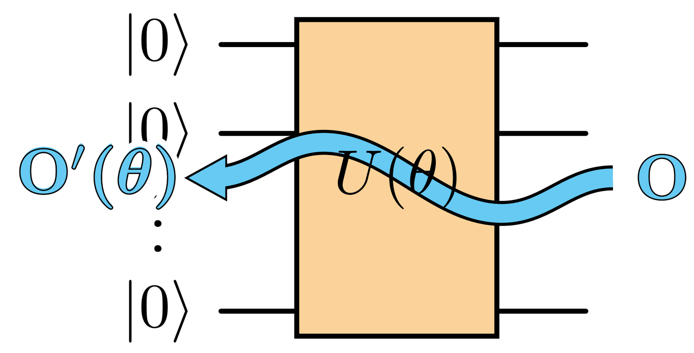
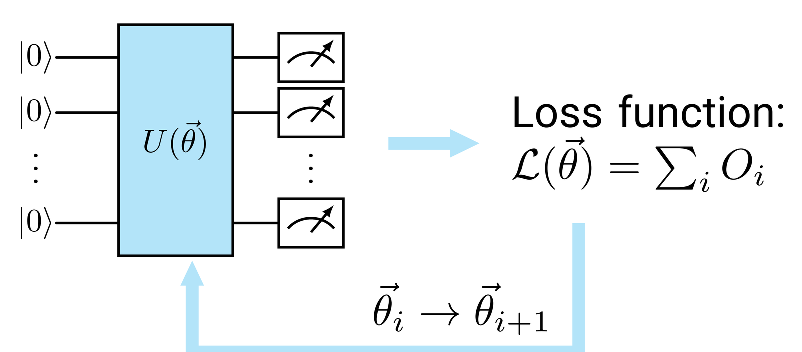


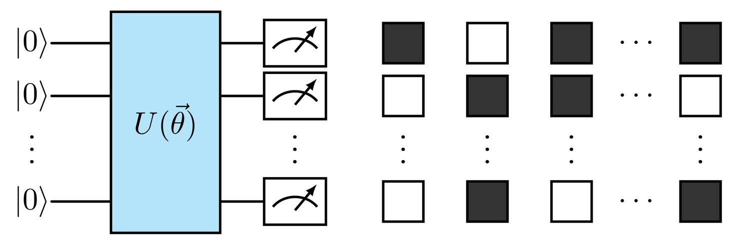
Use case

Obtain the **explicit** expectation value function of a circuit's observable in terms of its parameters. Useful when the loss is defined via expectation values but the output is a single measurement.

Training:



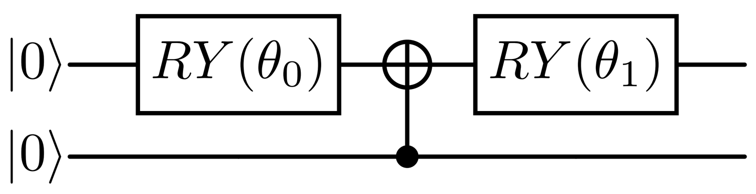
Output:



Propagation

Propagation of observables in the *Heisenberg picture*:

Circuit example:



Propagation rules:

$RY(\theta)$: $X \to \cos\theta X + \sin\theta Z$, $Z \to \cos\theta Z - \sin\theta X$

CNOT: $Z \otimes I \to Z \otimes Z$, $X \otimes I \to X \otimes I$

Propagation of Z ⊗ I:

1 Action of $RY(\theta_1) \otimes I$

$$Z \otimes I \to \cos(\theta_1) Z \otimes I - \sin(\theta_1) X \otimes I$$

2 Action of $\mathrm{CNOT}(1,0)$

$$\cos(\theta_1) Z \otimes I - \sin(\theta_1) X \otimes I \to \cos(\theta_1) Z \otimes Z - \sin(\theta_1) X \otimes I$$

3 Action of $RY(\theta_0) \otimes I$

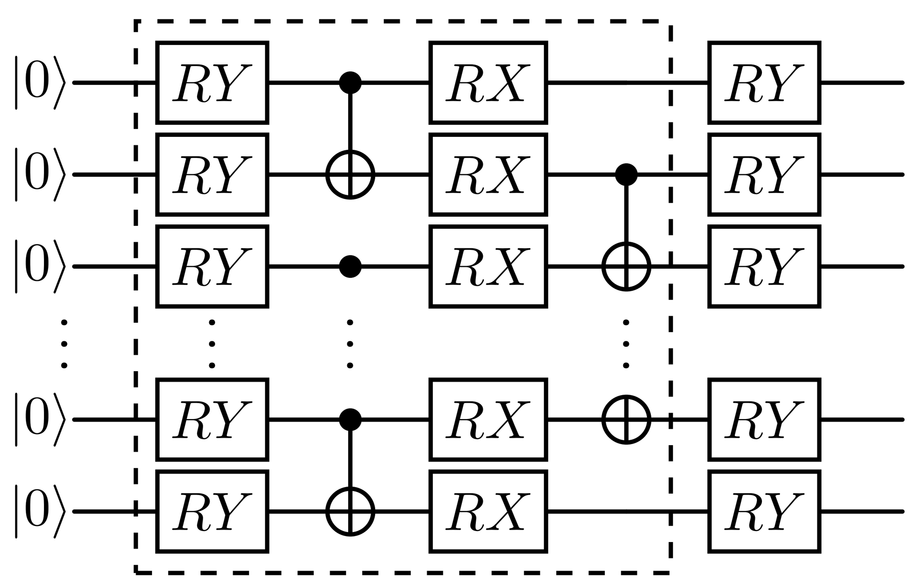
$$\cos(\theta_1) Z \otimes Z - \sin(\theta_1) X \otimes I \to$$
$$\to + \cos(\theta_0)\cos(\theta_1) Z \otimes Z - \sin(\theta_0)\cos(\theta_1) X \otimes Z +$$
$$- \cos(\theta_0)\sin(\theta_1) X \otimes I - \sin(\theta_0)\sin(\theta_1) Z \otimes I$$

4 **Trimming:** Computing the expectation value of the Pauli Obs.

$$\langle Z \otimes I \rangle(\vec{\theta}) = + \cos(\theta_0)\cos(\theta_1) - \sin(\theta_0)\sin(\theta_1)$$

Exact Propagation

Studied circuit

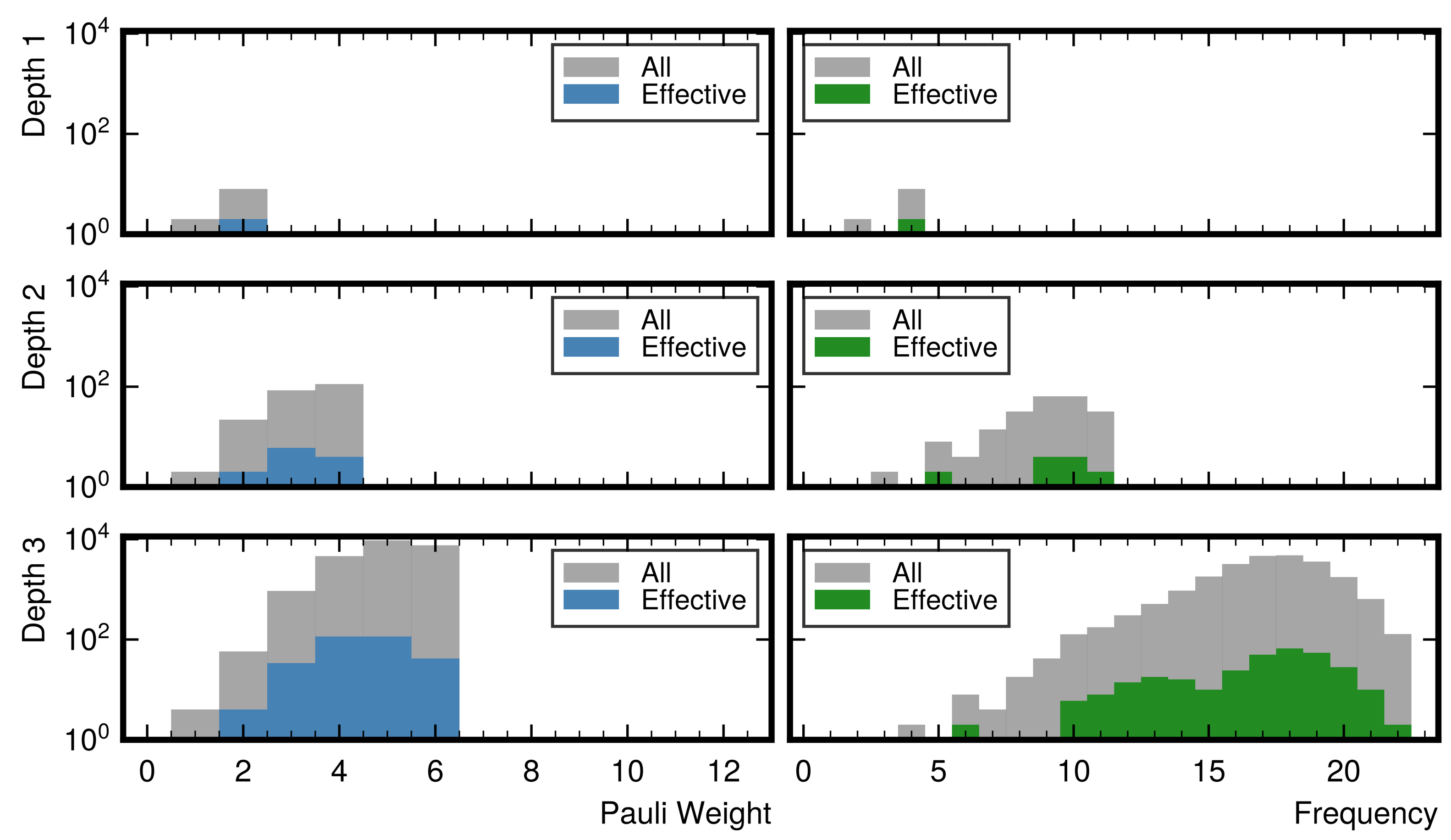


Quantities

- **Pauli weight**: number of non-identity Pauli-Op
- **Frequency**: number of trigonometric functions multiplied

Example:

$$\underbrace{\sin\theta_8 \sin\theta_1 \cos\theta_0}_{\text{Frequency (3)}} \; \underbrace{X_0 Z_1}_{\text{Weight (2)}}$$

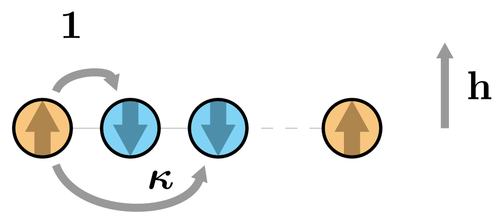


★ The number of terms grows rapidly → necessity of cutoffs: cut-off on Pauli weight w_{cut} and frequency ν_{cut}

Application: VQE

- **Goal of VQE: (ANNNI model)**

Find the ground state of the Hamiltonian:

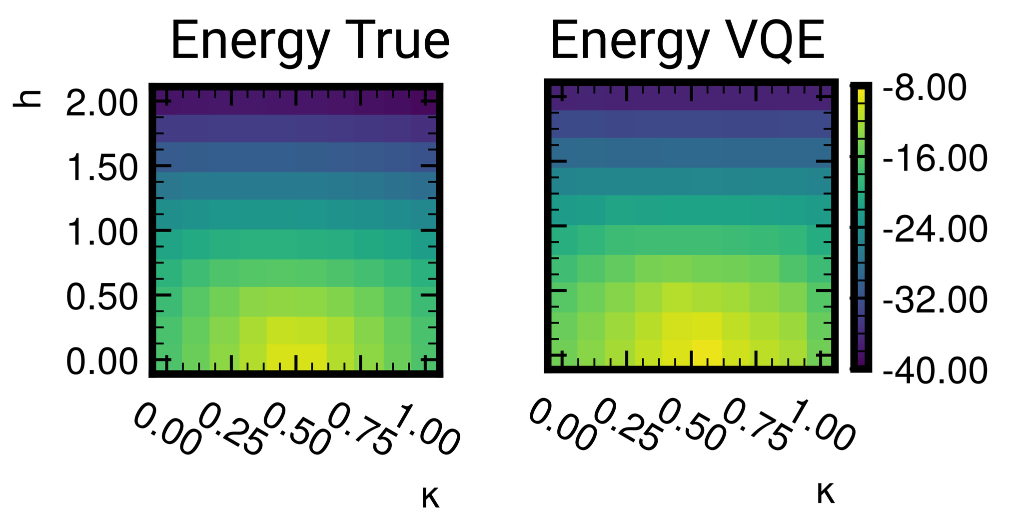


$$H(\kappa, h) = -J \sum_{i=1}^{N} \Big(X(i)X(i+1) - \kappa\, X(i)X(i+2) + h\, Z(i) \Big),$$

by minimizing the **expectation value of the observable**

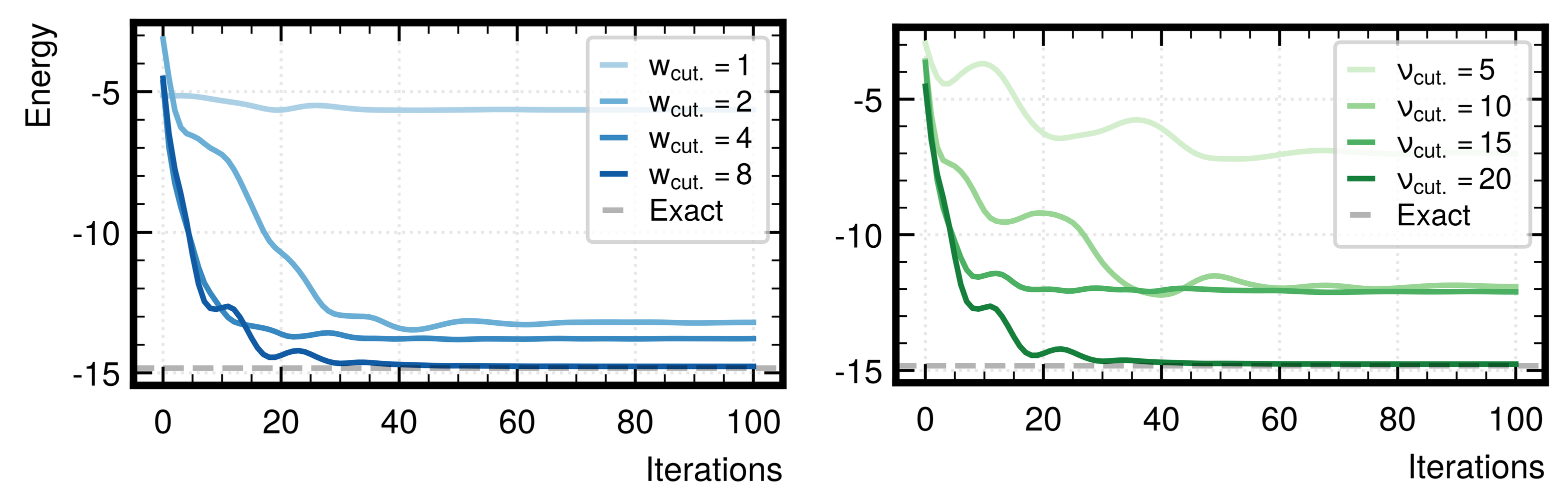
$$E(\boldsymbol{\theta}) = \langle \psi(\boldsymbol{\theta}) | H | \psi(\boldsymbol{\theta}) \rangle$$

- **Result of VQE:** (number of qubits: 18)



VQE energies classically obtained through the propagated Hamiltonian show a close match to the true energies.

- **Effect of the cut-off parameters:** $(\kappa, h) = (0.2, 0.4)$



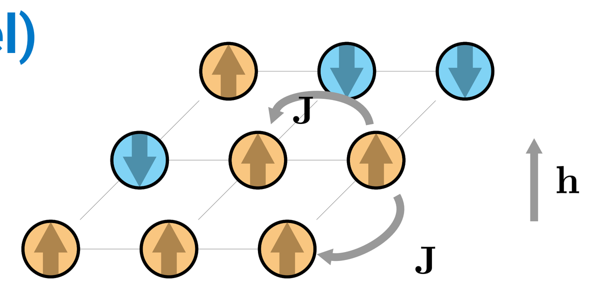
$\nu_{\text{cut}} = 20$, varying w_{cut} $w_{\text{cut}} = 8$, varying ν_{cut}

★ Relatively low ν_{cut} and w_{cut} suffice for good performance.

Application: Warm Start (VQE)

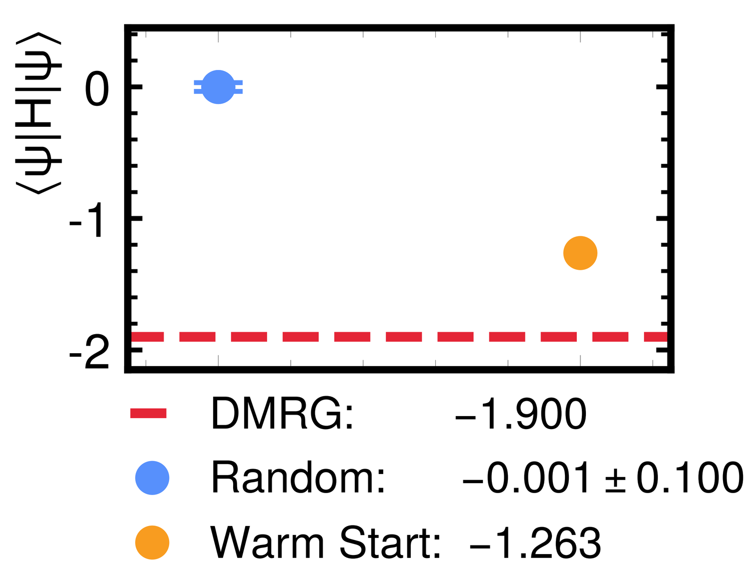
- **Hamiltonian: (2D Transverse Ising Model)**

$$H = -\frac{1}{N}\Big(J \sum_{\langle i,j \rangle} Z(i)Z(j) + h \sum_i X(i) \Big)$$



- **Result of VQE:** $(J = h = 1$, number of qubits: 64)

System size too large for classical simulation. Training (warm starting) through Pauli Propagation & deployment on Quantum (*ibm_fez*)



Info:

- Ansatz: 2D brickwork with alternating entanglers
- Number of parameters: 320
- Number of qubits: 64
- Deployed on *ibm_fez*
- Number of shots: 2048

★ For specific problems, Pauli Propagation proves **effective** at off-load initial costly computations from Quantum Computers

References

[1] S. Monaco et al.,: *Symbolic Pauli Propagation for Gradient-Enabled Pre-Training of Quantum Circuits*, ArXiv (2025)

ArXiv Github

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