Dual quantum time evolution

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Can we reduce the cost of variational time evolution?
arXiv:2303.12830

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in collaboration with

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Outline

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- Recap on Quantum Time Evolution
- Variational approach and its bottlenecks
- Dual formulation
- Resource benchmark

Quantum Time Evolution

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Note
- $\hbar \equiv 1$
- H is static

Real time evolution

How does the system evolve in time?

$$\frac{\partial}{\partial t}|\psi(t)\rangle = -iH|\psi(t)\rangle$$

Observable $\langle O \rangle$

Thermalization
$\lim_{t\to\infty} |\psi(t)\rangle$

Phase transitions

Quantum Time Evolution

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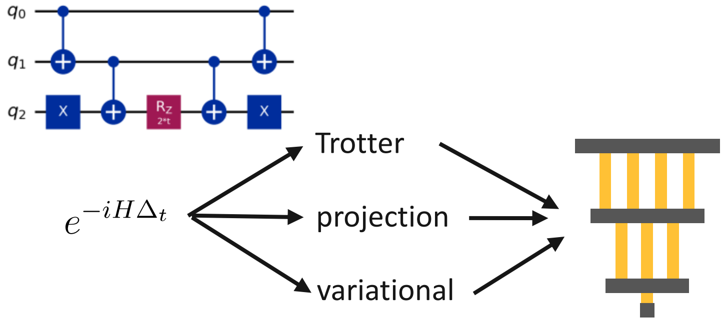

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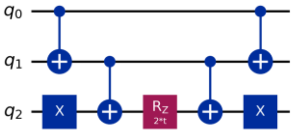
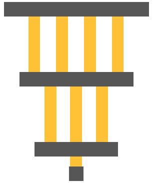


$e^{-iH\Delta_t}$ → Trotter / projection / variational →

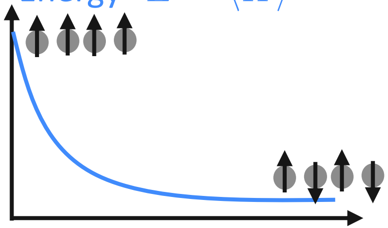


Imaginary time evolution

Evolve for *imaginary* time $\tau = it$

$$\frac{\partial}{\partial \tau}|\psi(\tau)\rangle = -(H - E)|\psi(\tau)\rangle$$

Energy $E = \langle H \rangle$



Ground states

$$|\psi(\tau)\rangle = c_0 e^{-E_0\tau}|\psi_0\rangle + \ldots$$

Gibbs states

$$\rho(\beta) = \frac{e^{-\beta H}}{Z(\beta)}$$

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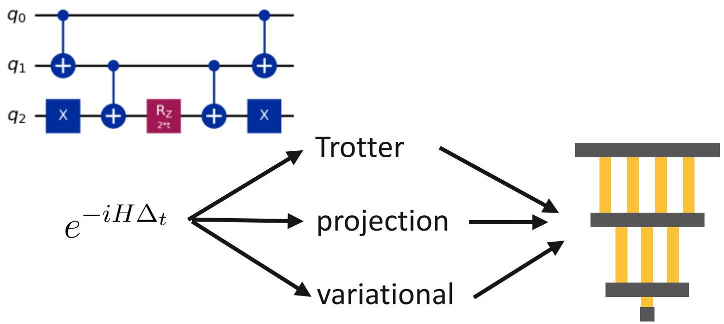

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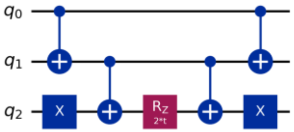

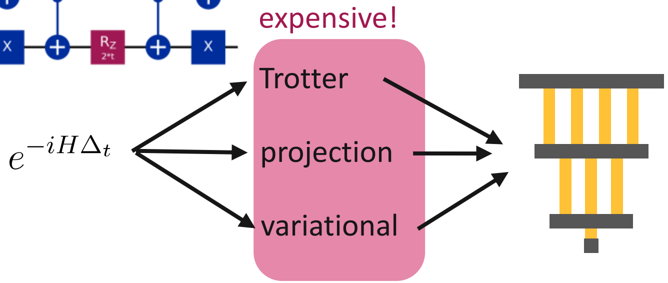

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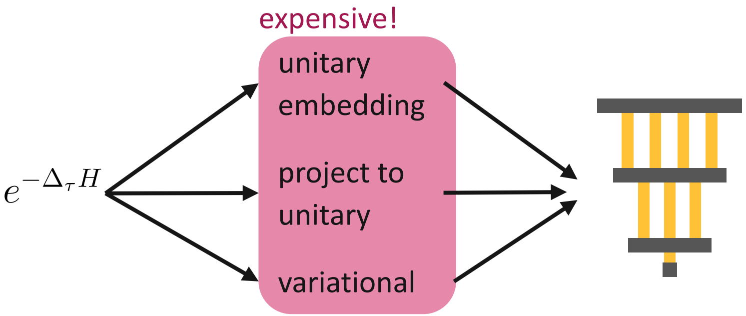

Slattery et al. PRR 4 023072 (2022)
Motta et al. Nature Physics 16 205-210 (2020)
McArdle et al. npj Quantum Information 5 75 (2019)

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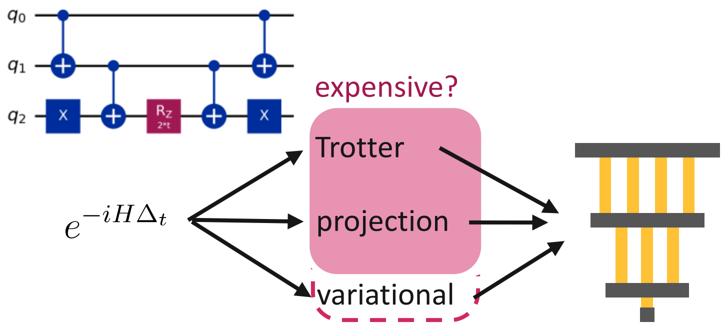

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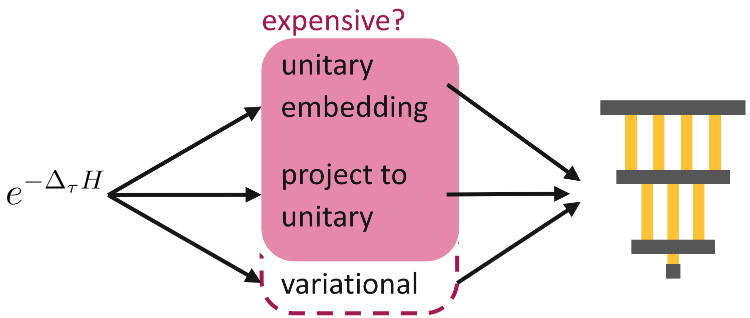

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Variational time evolution

Notation
$$\partial_i \equiv \frac{\partial}{\partial \theta_i}$$

Projection

Project the state-evolution onto parameter-evolution

$$|\psi(\tau)\rangle \approx |\phi(\theta(\tau))\rangle \qquad \theta(\tau) \in \mathbb{R}^d$$

with $|\phi(\theta)\rangle = U(\theta)|0\rangle$ acting in the device's capabilities.

Parameter dynamics

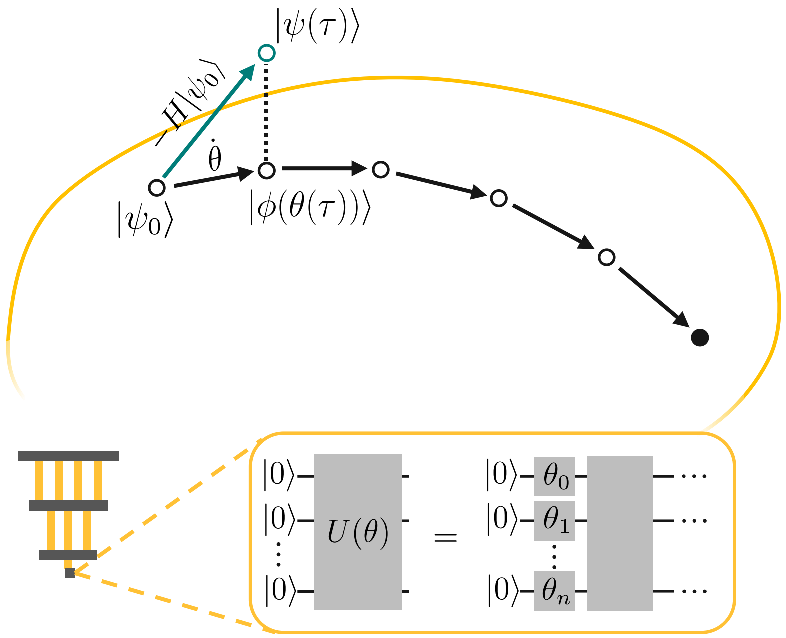
$$g(\theta)\dot{\theta} = b(\theta)$$

Quantum geometric tensor (QGT) O(d^2)

$$g_{ij}(\theta) = \mathrm{Re}\left\{\langle \partial_i \phi | \partial_j \phi \rangle - \langle \partial_i \phi | \phi \rangle \langle \phi | \partial_j \phi \rangle \right\}$$

Evolution gradient

$$b_i(\theta) = -\frac{\partial_i E(\theta)}{2}$$



Yuan et al. "Theory of variational quantum simulation" Quantum 3, 191 (2019)

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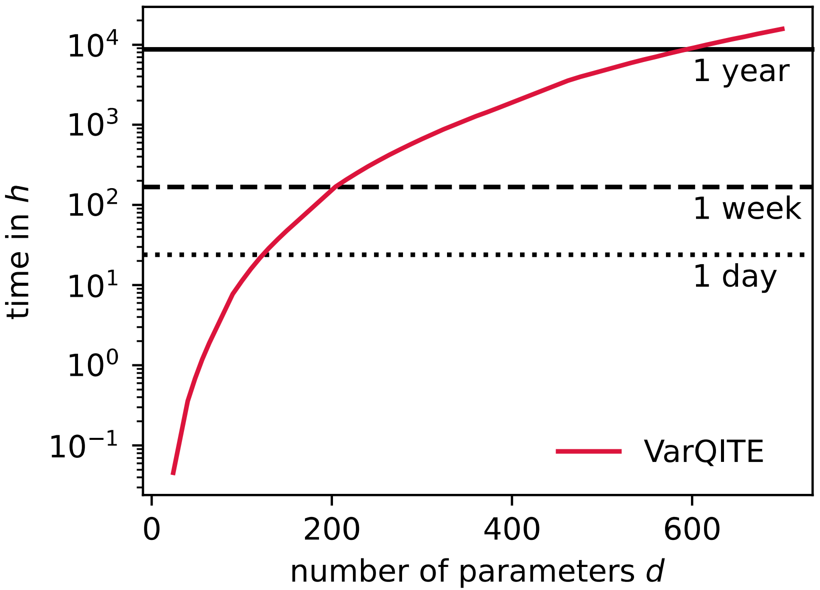
Benchmark

Heisenberg model on superconducting hardware



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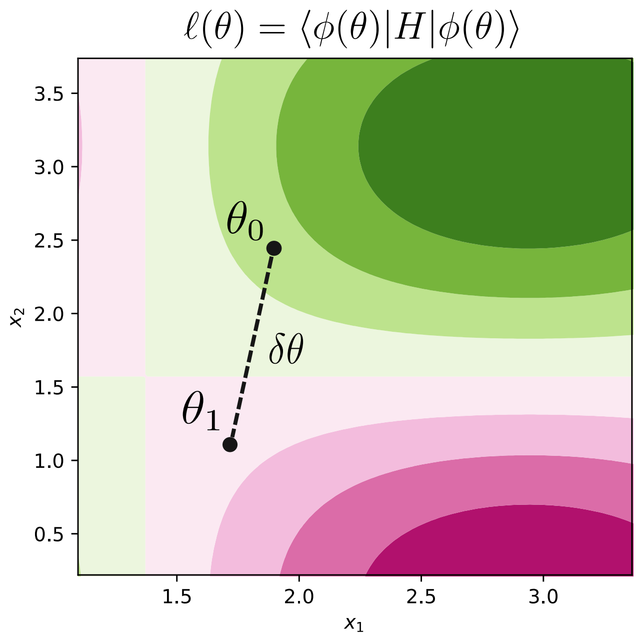
Understanding the QGT



What's the distance of the parameters?

Model-independent measure:

$$\|\theta_0 - \theta_1\|_2^2$$

Model-aware measure:

$$F(\theta_0, \theta_1) = |\langle \phi(\theta_0)|\phi(\theta_1)\rangle|^2$$

For small $\delta\theta$ we can expand the fidelity using the QGT

$$F(\theta_0, \theta_0 + \delta\theta) = 1 - \delta\theta^T g(\theta_0)\delta\theta + \mathcal{O}(\|\delta\theta\|_2^3)$$

➡ the QGT is a measure for model sensitivity

➡ leveraged e.g. in Quantum Natural Gradients

Stokes et al. 2019, "Quantum Natural Gradient"

Avoiding the QGT

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A dual formulation

$$g(\theta)\dot{\theta} = b(\theta)$$

$\dot{\theta} = \frac{\delta\theta}{\delta\tau}$, $\delta\tau > 0$ ↓

$$g(\theta)\frac{\delta\theta}{\delta\tau} = b(\theta)$$

as quadratic problem ↓

O(d^2)

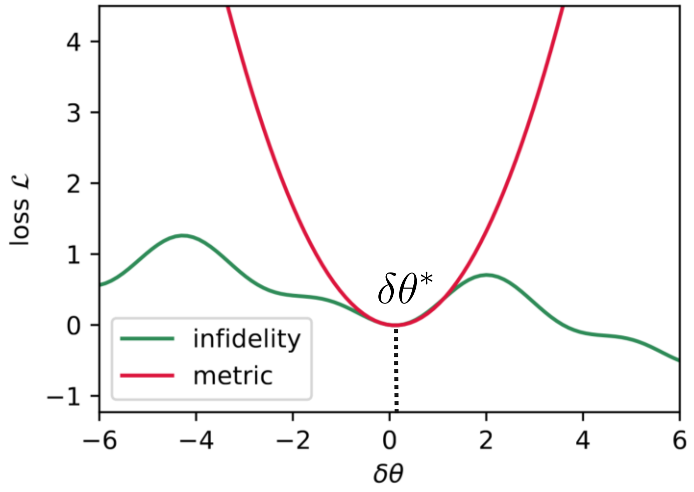
$$\delta\theta = \underset{\delta\theta}{\operatorname{argmin}} \frac{\delta\theta^T g(\theta)\delta\dot{\theta}}{2} - \delta\tau \cdot \delta\theta^T b(\theta)$$

previous slide ↓

O(1)

$$\delta\theta \approx \underset{\delta\theta}{\operatorname{argmin}} \underbrace{\frac{1 - F(\theta, \theta + \delta\theta)}{2} - \delta\tau \cdot \delta\theta^T b(\theta)}_{\mathcal{L}(\delta\theta)}$$

Illustrative example



A dual formulation: DualQTE

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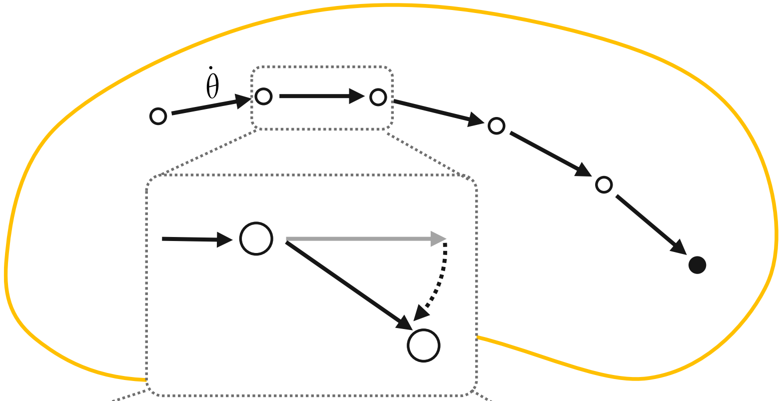


$\delta\theta^{(0)} =$ previous $\delta\theta^*$

until termination, do

$$\delta\theta^{(k+1)} = \delta\theta^{(k)} - \eta\nabla\mathcal{L}(\delta\theta^{(k)})$$

$$\theta(\tau + \delta\tau) = \theta(\tau) + \delta\theta^*$$

Gradients

Evaluate via parameter-shift rules or linear combination of unitaries

$$\nabla\mathcal{L}(\delta\theta) = -\frac{\nabla_{\delta\theta}F(\theta, \theta + \delta\theta)}{2} - \delta\tau \cdot b(\theta)$$

Trainability

+ Evolution gradient uses local expectations

− Fidelity gradient uses global projector

➡ can be initialized in Barren plateau-free setting

➡ supported by numerical benchmarks

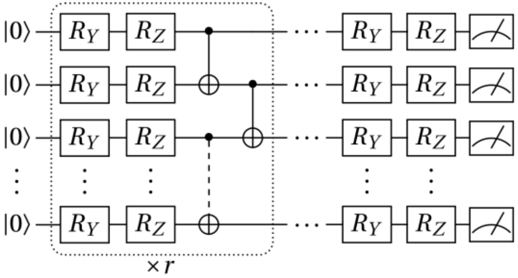
Grant et al. Quantum 3, 214 (2019)

Imaginary time evolution

Heisenberg model on a periodic chain

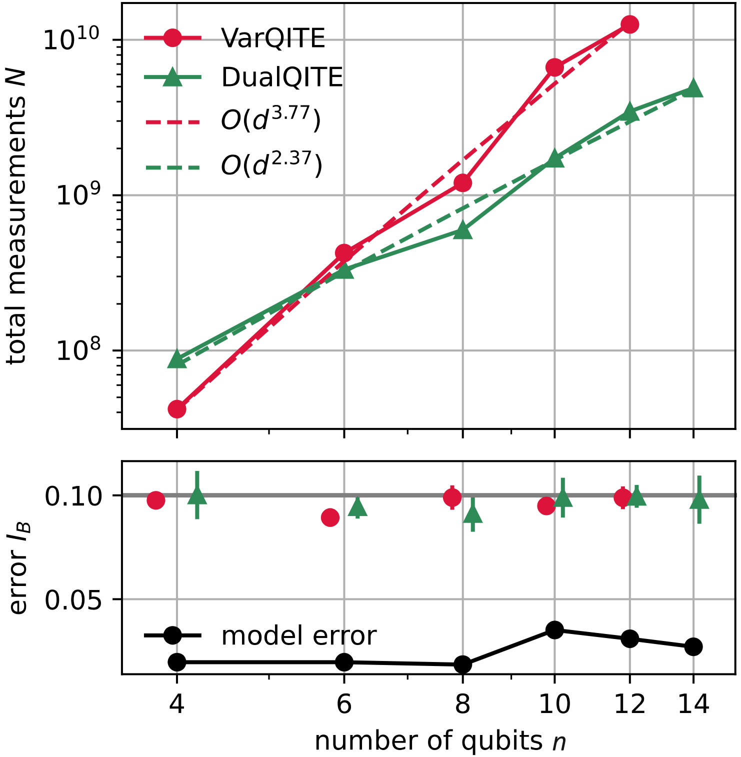
$$H = J \sum_{\langle ij \rangle} (X_i X_j + Y_i Y_j + Z_i Z_j) + h \sum_{i=1}^{n} Z_i$$

Ansatz with $r = \lceil \log_2(n) \rceil$ and initial state $|+\rangle^{\otimes n}$



Accuracy measure is the integrated Bures distance

$$I_B(T) = \frac{1}{T} \qquad \overset{!}{\leq} 0.1$$



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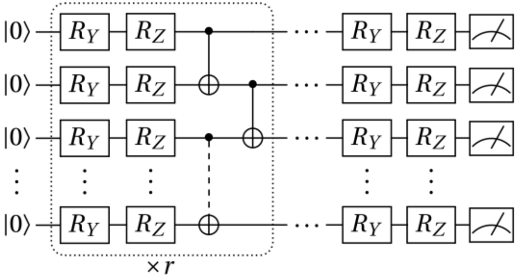

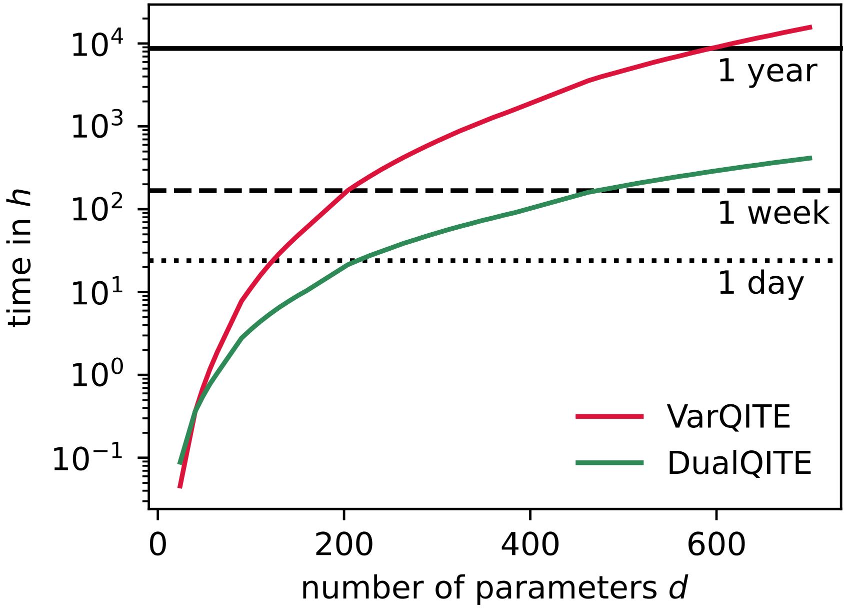

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Take-home message

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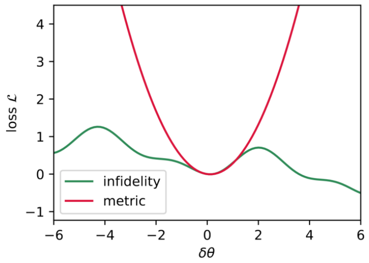
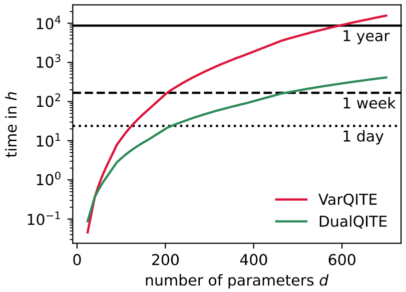
Duality

QGT and fidelity are closely connected: choose the suitable representation for your problem!



Improved scaling

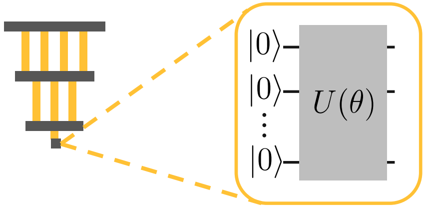
DualQTE promises a reduction in scaling



Open questions

Efficient fidelity measurements

Ansatz selection



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