

Institute for  
**Robust Quantum  
Simulation**

Lattice 2024, University of Liverpool

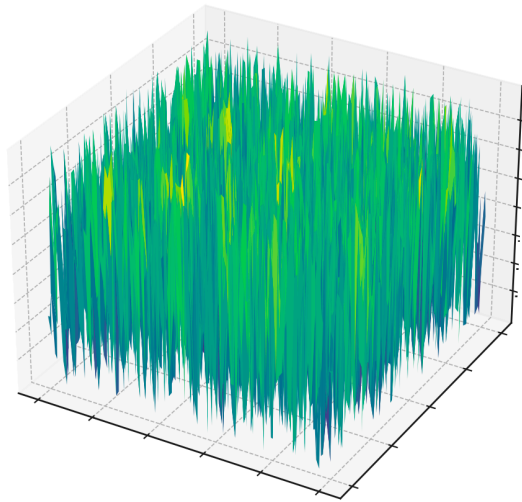
# Euclidean Monte Carlo informed ground state preparation for quantum simulation

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University of Maryland, College Park

*(Manuscript in preparation)*

**Lattice QCD gives us static correlation functions.**

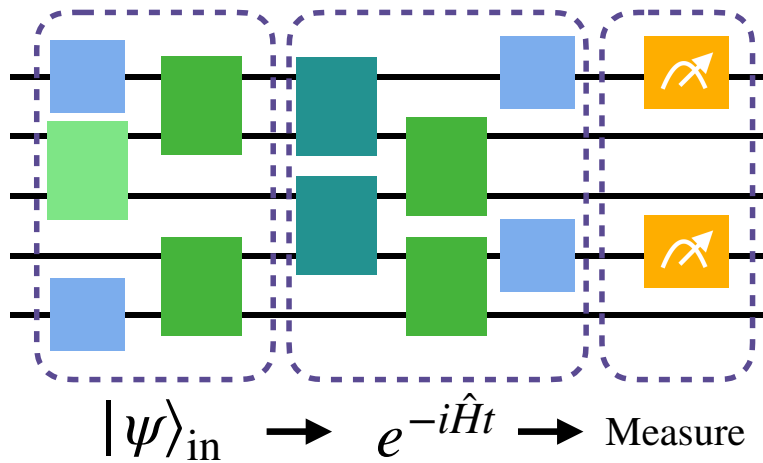


$$\langle O \rangle = \frac{1}{Z} \int \mathcal{D}\phi e^{-S[\phi]} O$$

# Hamiltonian methods can compute dynamical correlation functions.

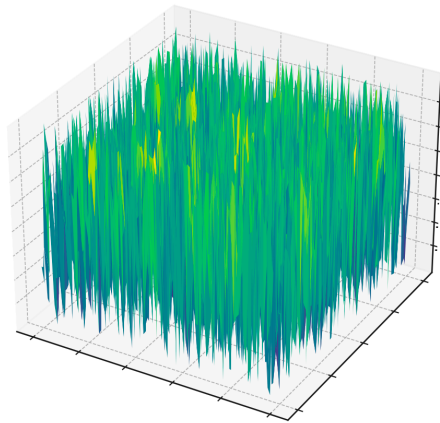
$$|\psi\rangle_{\text{in}} \rightarrow e^{-i\hat{H}t} \rightarrow \text{Measure} \quad \langle O(t) \rangle = \langle \psi | e^{i\hat{H}t} \hat{O} e^{-i\hat{H}t} | \psi \rangle$$

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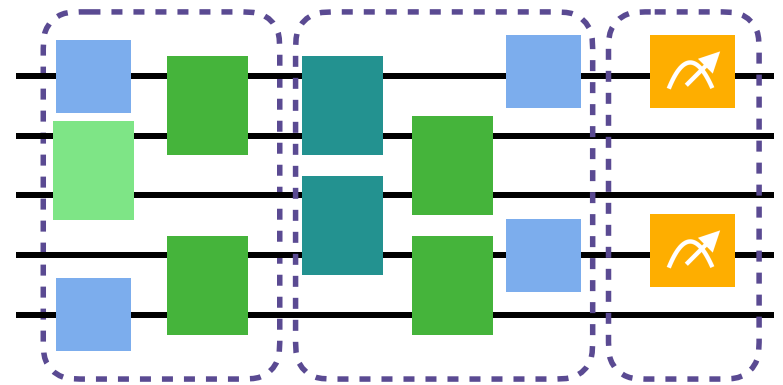
# Can we bridge lattice QCD and quantum simulation?



$$\langle O \rangle = \frac{1}{Z} \int \mathcal{D}\phi e^{-S[\phi]} O$$



Static correlators  
inform state  
preparation.

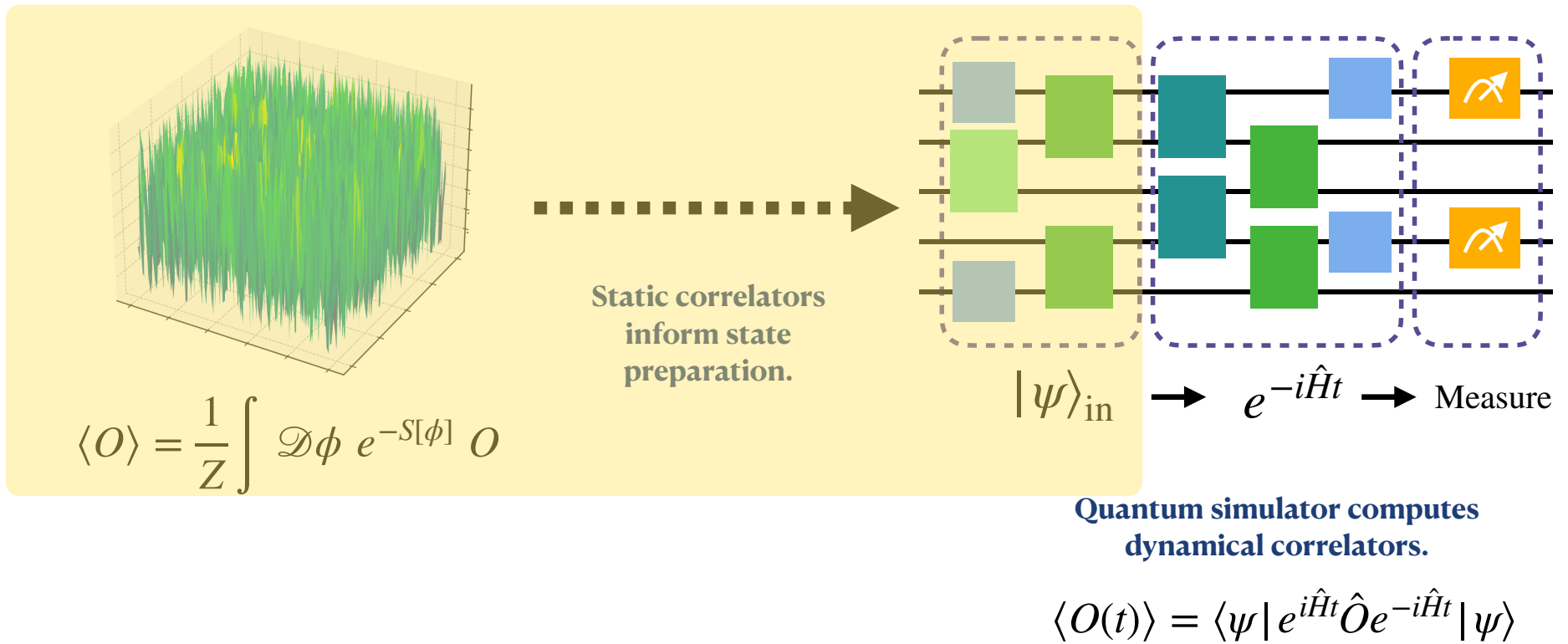


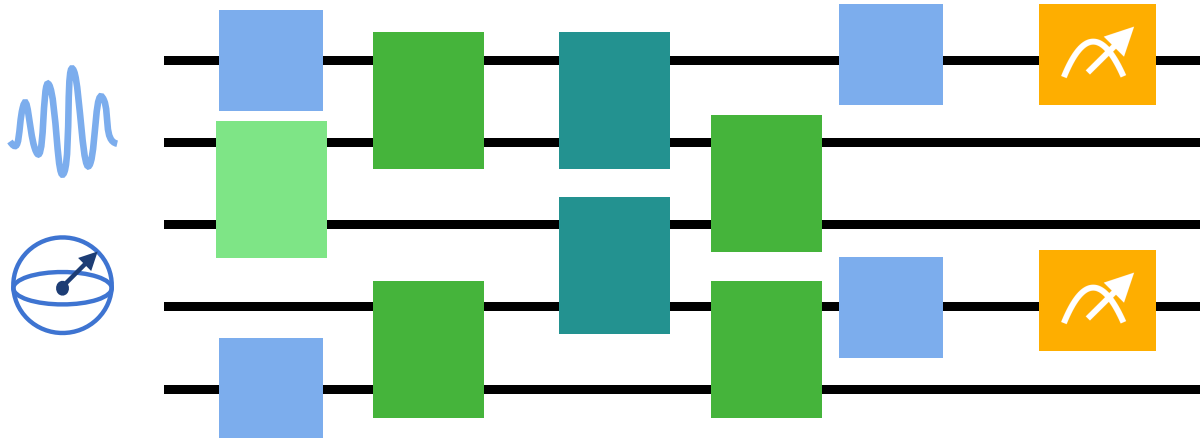
$$|\psi\rangle_{\text{in}} \rightarrow e^{-i\hat{H}t} \rightarrow \text{Measure}$$

Quantum simulator computes  
dynamical correlators.

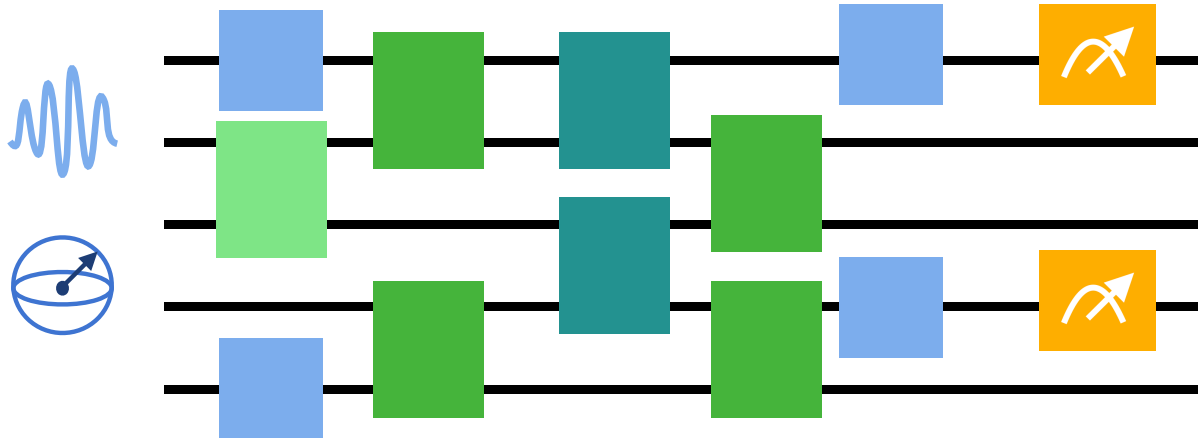
$$\langle O(t) \rangle = \langle \psi | e^{i\hat{H}t} \hat{O} e^{-i\hat{H}t} | \psi \rangle$$

# Can we bridge lattice QCD and quantum simulation?



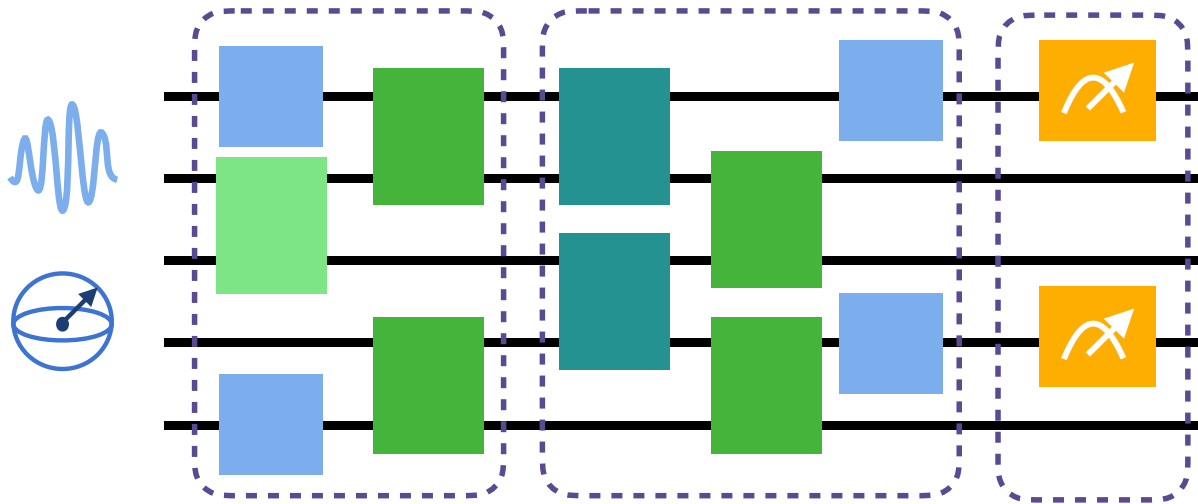


$$|\psi\rangle_{\text{in}} \rightarrow e^{-i\hat{H}t} \rightarrow \text{Measure}$$

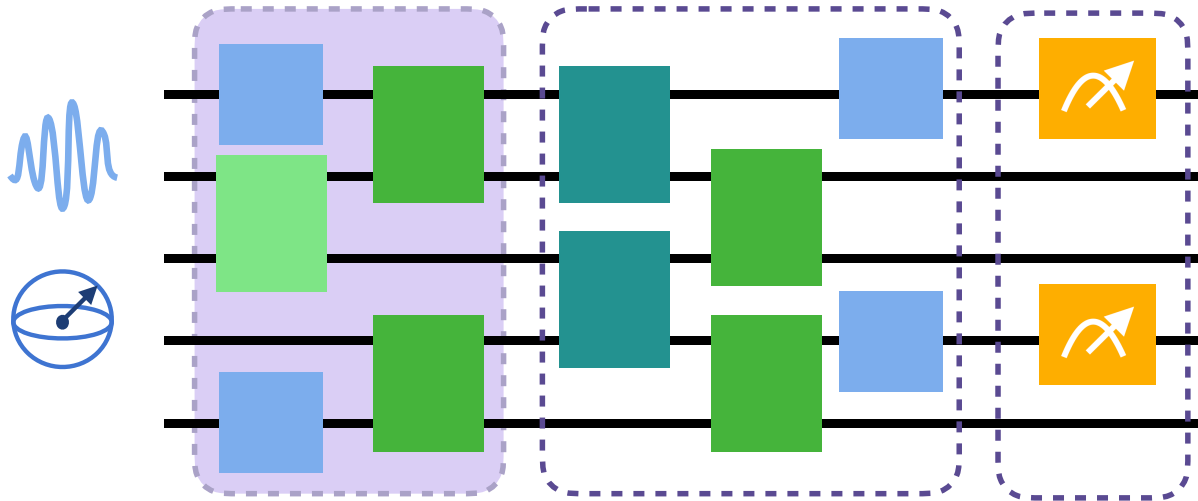




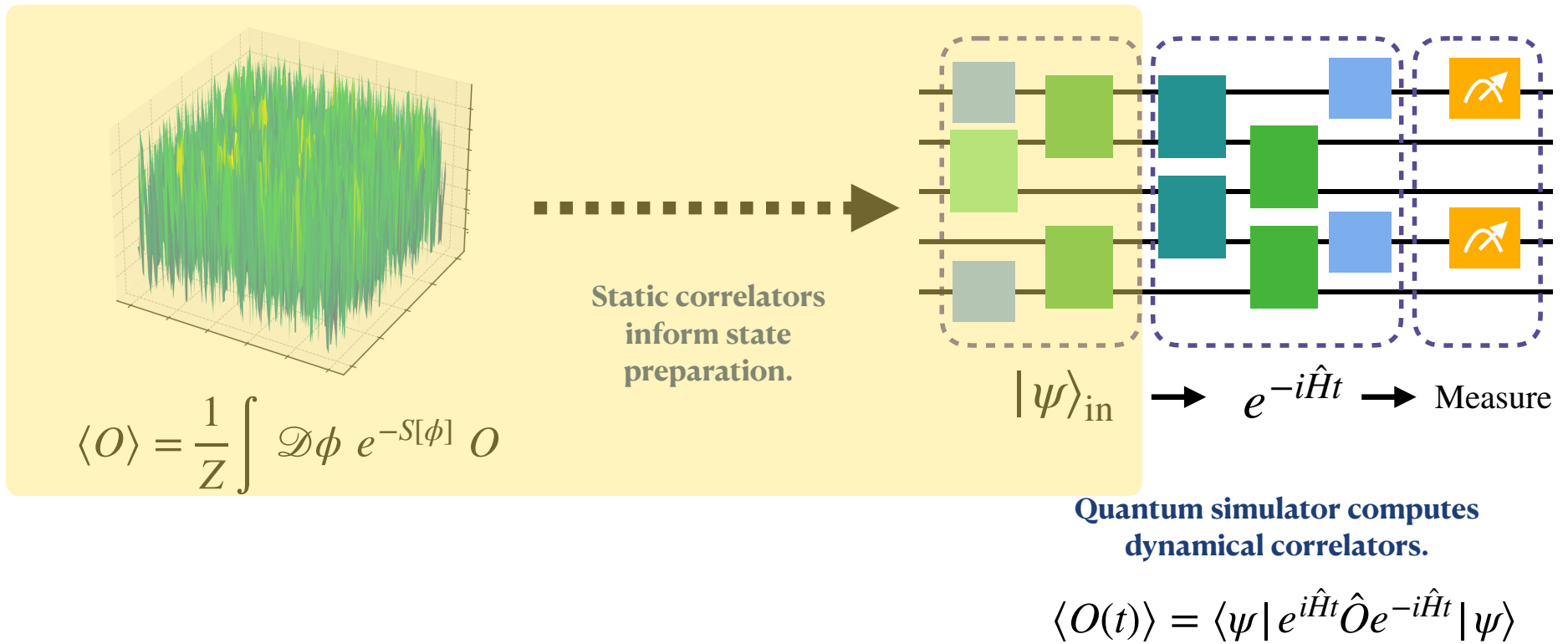
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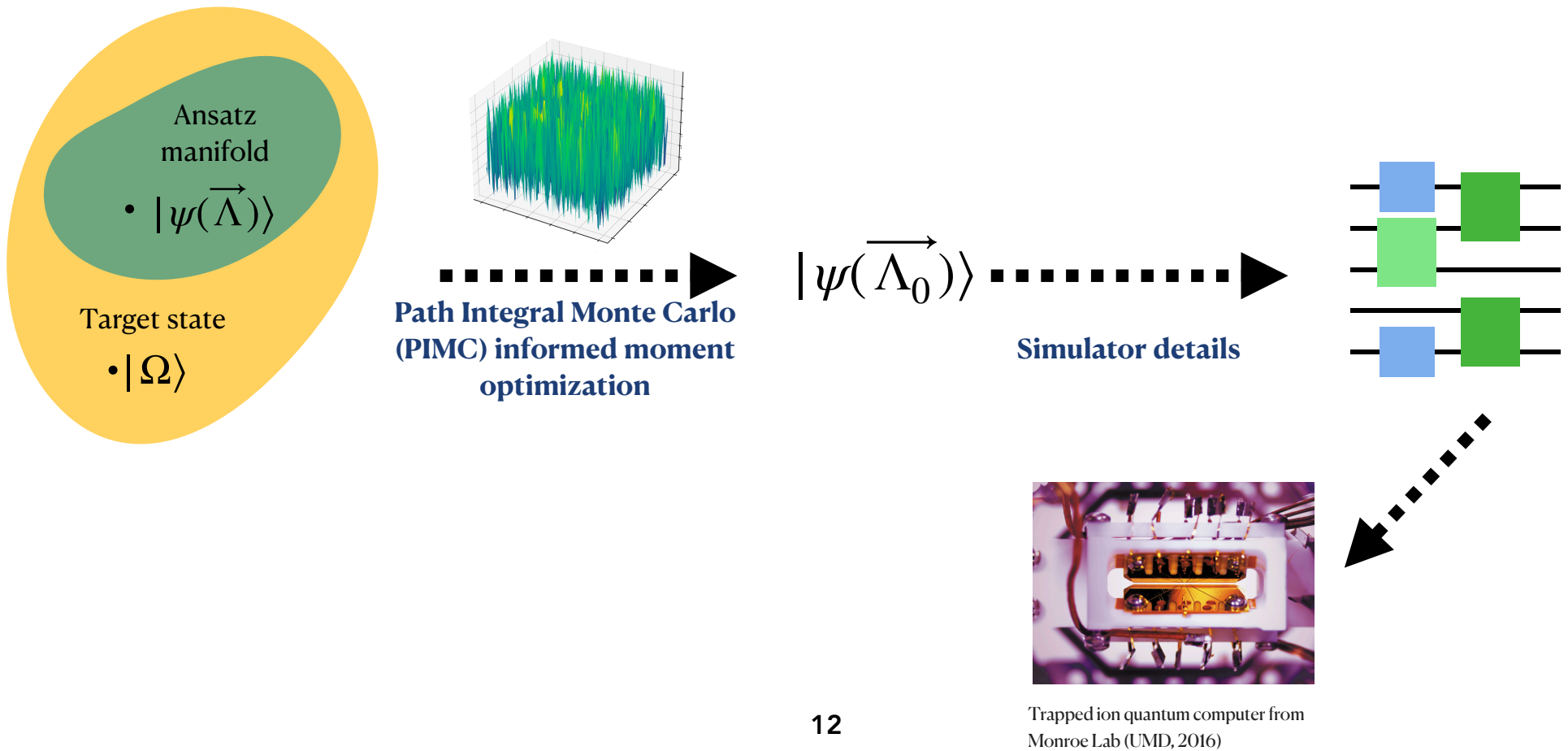
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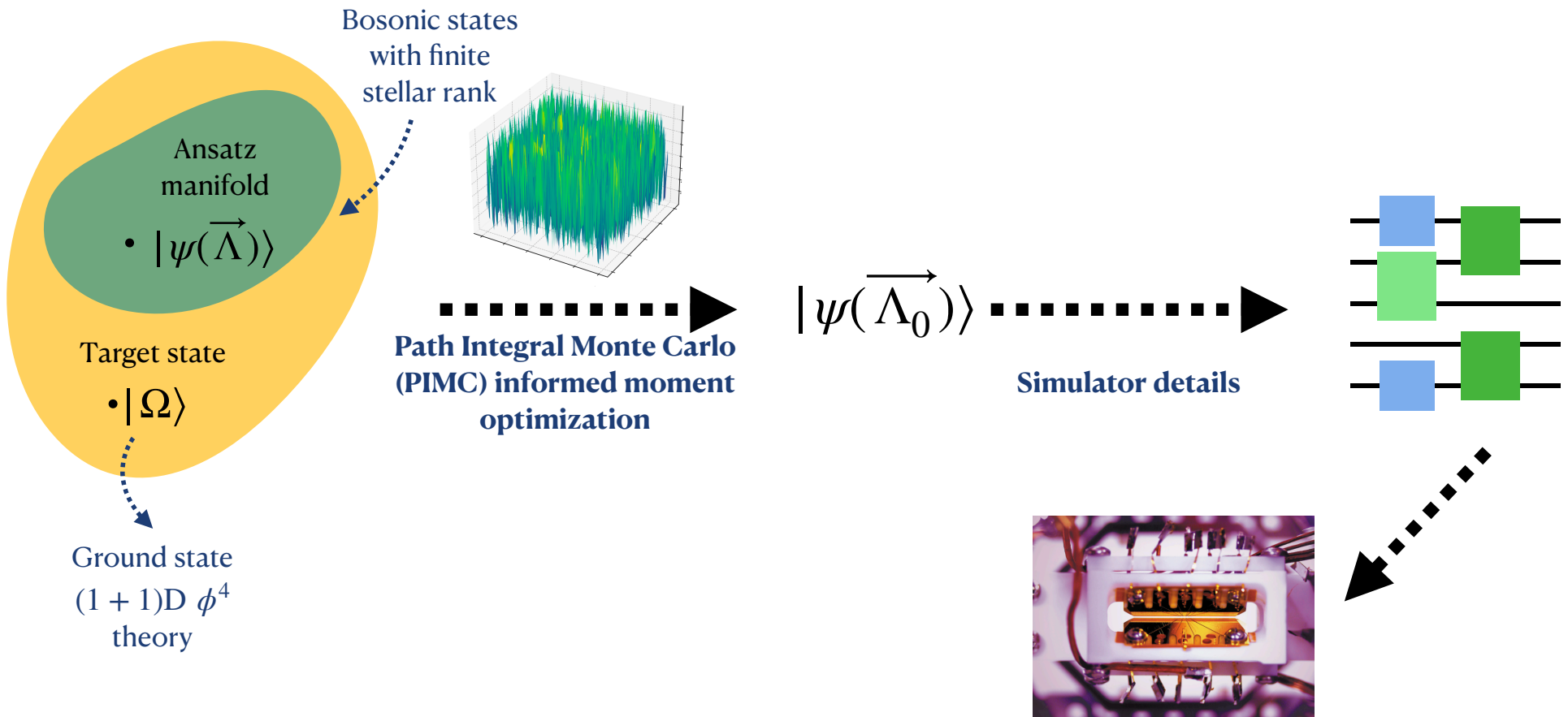
# Can we bridge lattice QCD and quantum simulation?



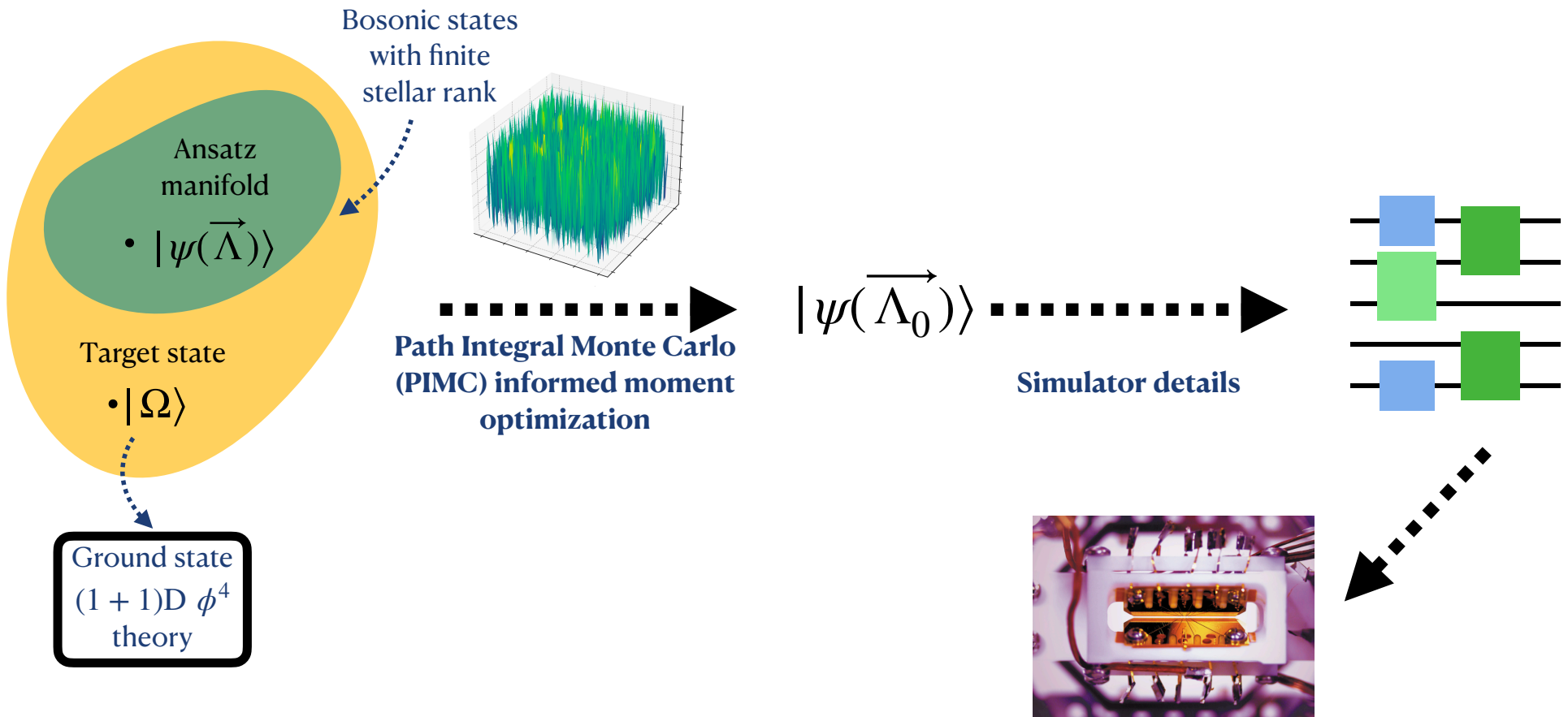
# Classically determined quantum circuit for ground states



# Classically determined quantum circuit for ground states

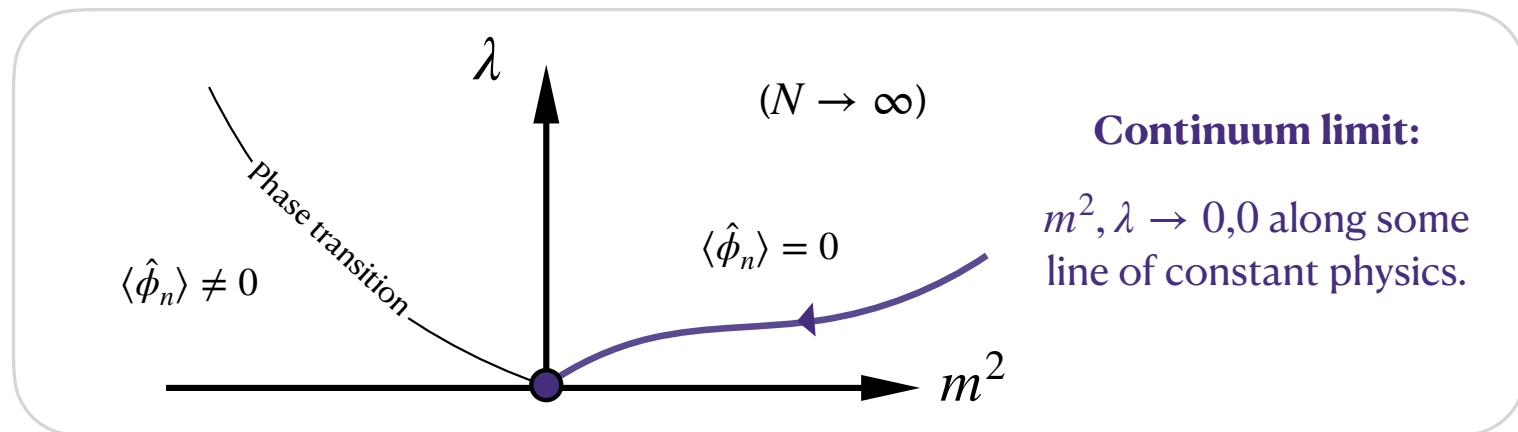


# Classically determined quantum circuit for ground states

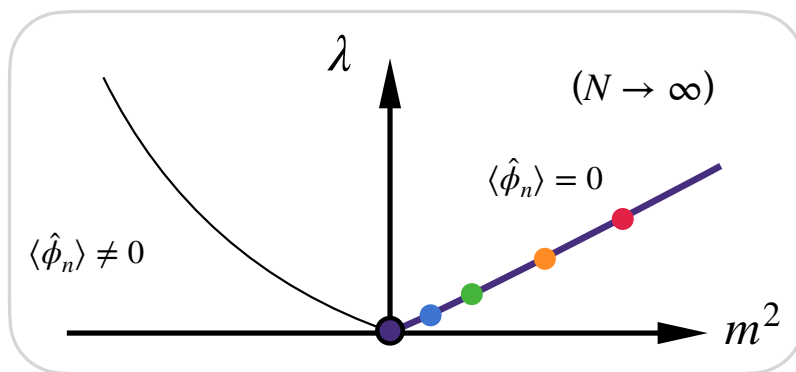


# Ground state of (1 + 1)D $\phi^4$ theory

$$\hat{H} = \sum_{n=0}^{N-1} \left( \frac{\hat{\pi}_n^2}{2} + \frac{(\hat{\phi}_{n+1} - \hat{\phi}_n)^2}{2} + \frac{1}{2}m^2\hat{\phi}_n^2 + \frac{\lambda}{4}\hat{\phi}_n^4 \right)$$

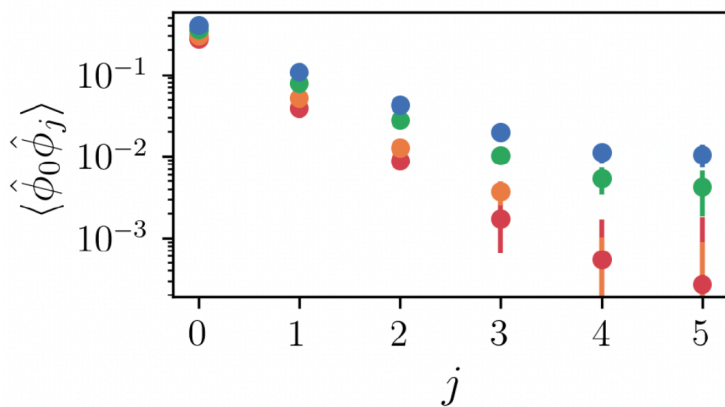


# Ground state of (1 + 1)D $\phi^4$ theory: Monte Carlo results

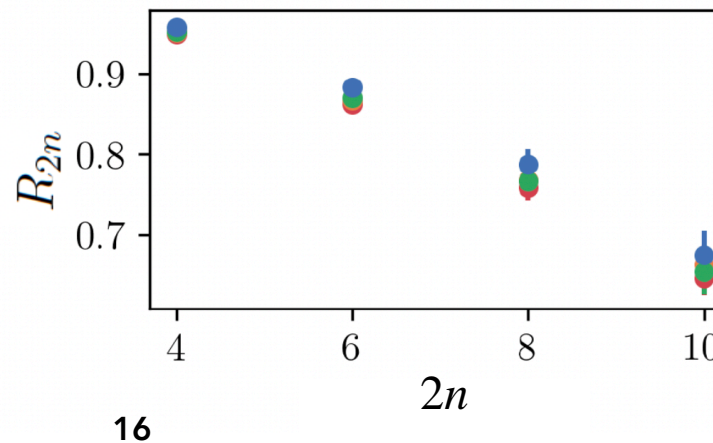


$(m^2, \lambda)$			
<span style="color: red;">●</span>	(0.6, 1.5)	<span style="color: green;">●</span>	(0.2, 0.5)
<span style="color: orange;">●</span>	(0.4, 1.0)	<span style="color: blue;">●</span>	(0.1, 0.25)

## Correlations



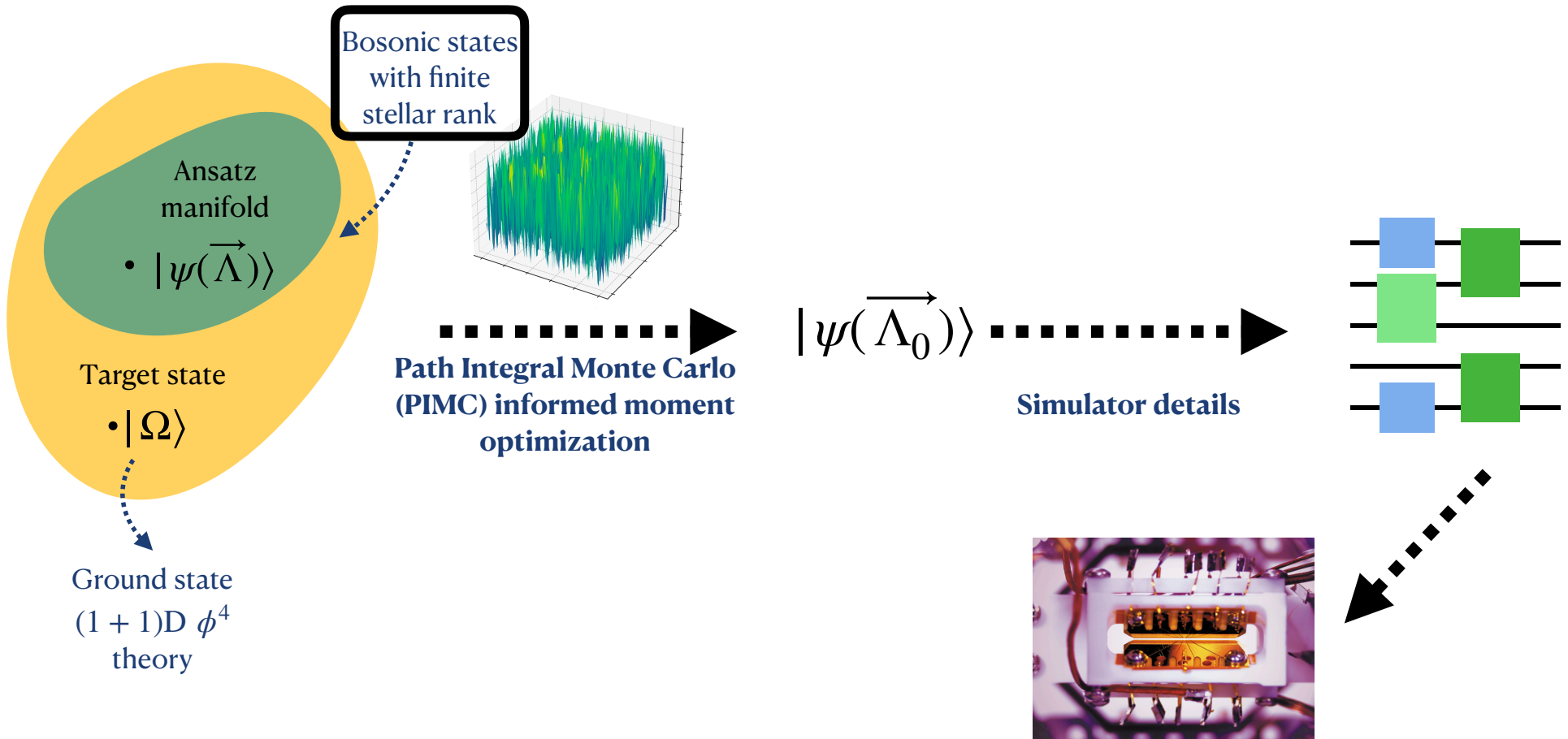
## Non-Gaussianity



$$R_{2n} \equiv \frac{\langle \hat{\phi}^{2n} \rangle}{(n-1)!! \langle \hat{\phi}^2 \rangle^n}$$



# Classically determined quantum circuit for ground states



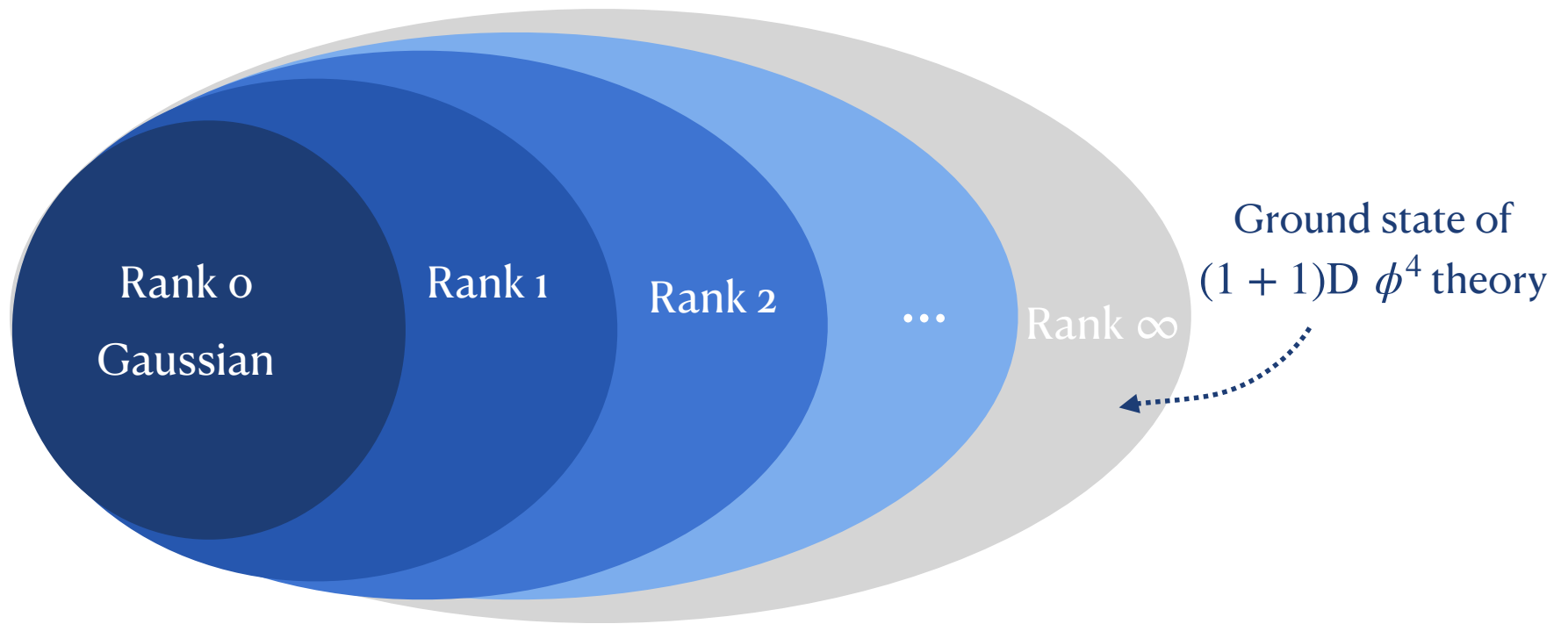
# Quantum states of $N$ bosons

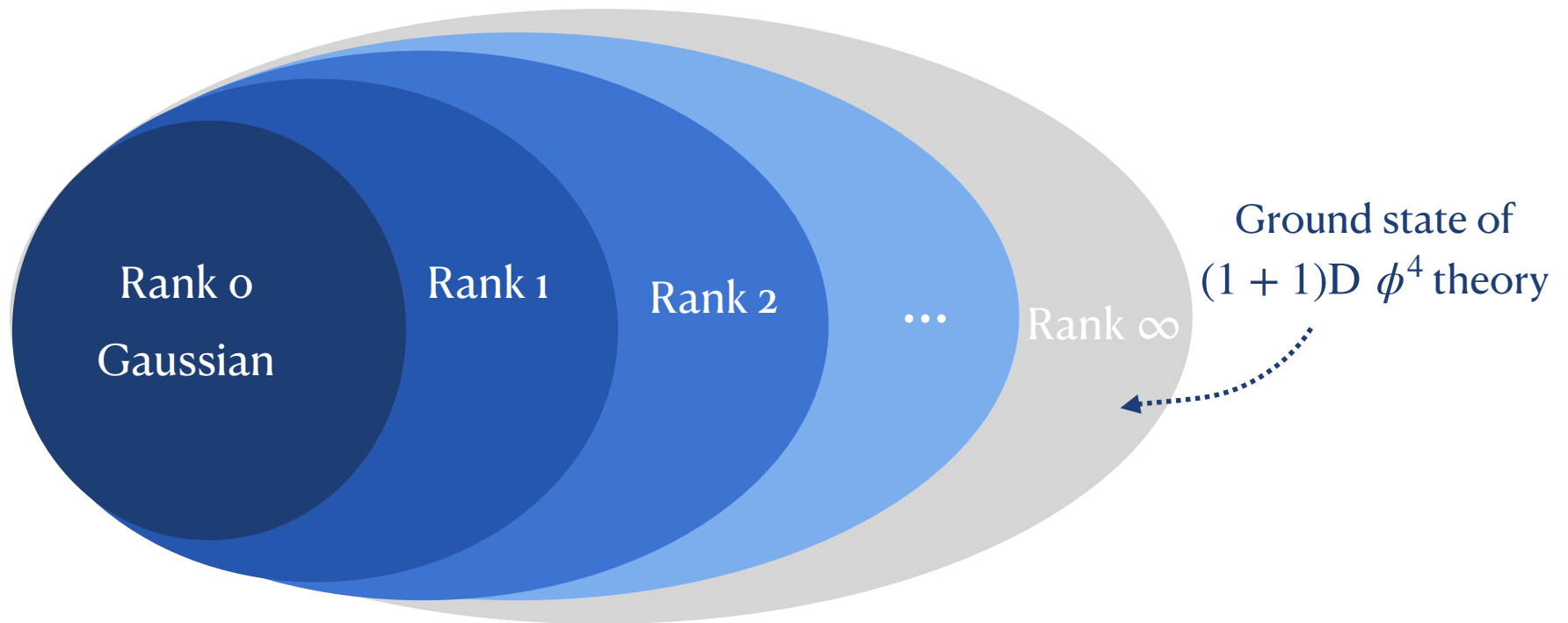
Most states of  $N$  bosons admit the decomposition

$$|\psi\rangle = \hat{U}_G \sum_{\substack{\vec{n} = n_1, \dots, n_N \\ n_1 + \dots + n_N \leq R}} c_{\vec{n}} \hat{a}_1^{\dagger n_1} \dots \hat{a}_N^{\dagger n_N} |\vec{0}\rangle$$

$n_1 + \dots + n_N \leq R$  .....  $R \in \mathbb{N} \cup \{0\}$  is the **stellar rank** of this state.

The bosonic states which do not admit the above decomposition are said to have an infinite rank.





**Finite rank states can get arbitrarily close to infinite-rank states (in trace distance).**

## Simpler choices of finite rank states

$$|\psi\rangle = \hat{U}_G \sum_{\substack{\vec{n} = n_1, \dots, n_N \\ n_1 + \dots + n_N \leq R}} c_{\vec{n}} \hat{a}_1^{\dagger n_1} \dots \hat{a}_N^{\dagger n_N} |\vec{0}\rangle$$

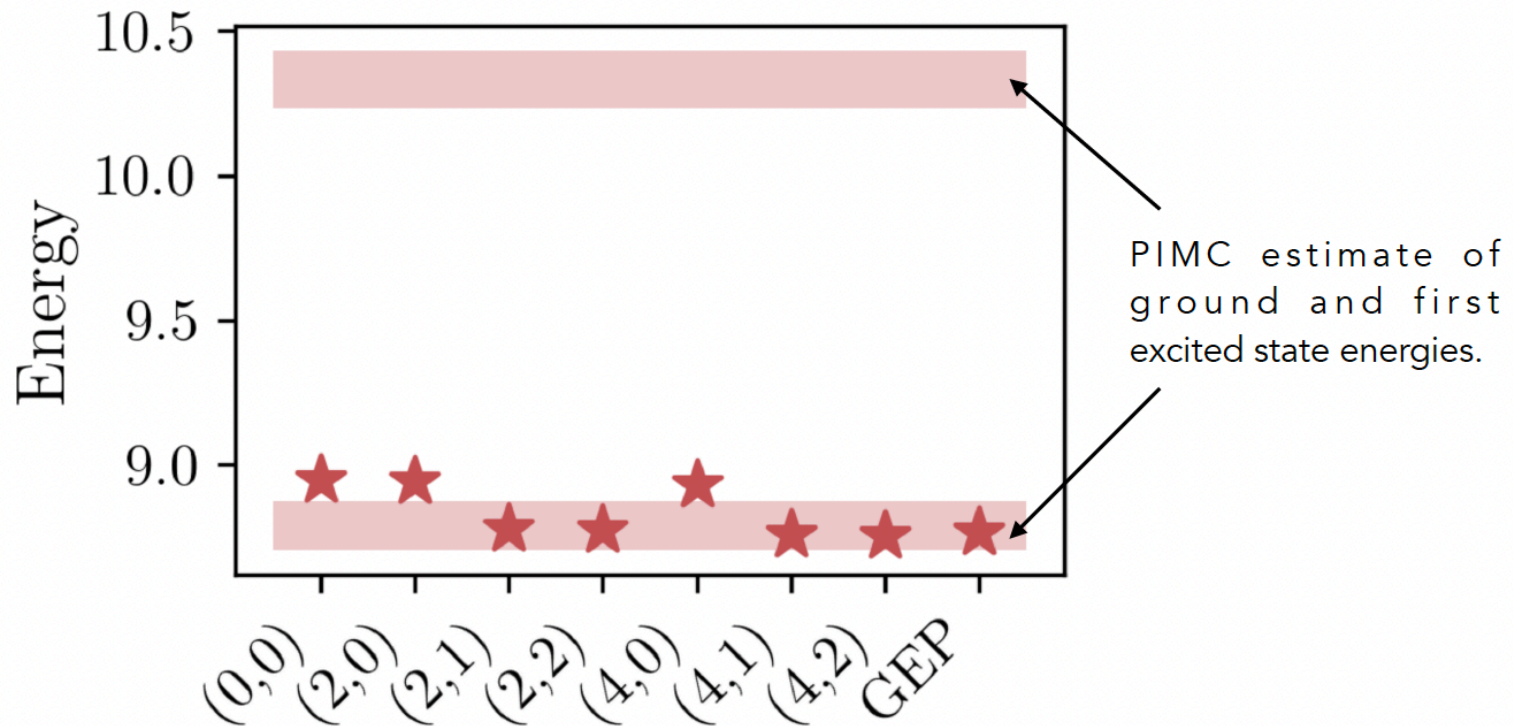


$$|\psi\rangle_{GEP} = \hat{U}_G |\vec{0}\rangle$$

$$|\psi\rangle_{(R,Q)} = \bigotimes_{i=0}^N \hat{S}_i(r) \sum_{\substack{\vec{n} = n_1, \dots, n_q \\ n_1 + \dots + n_q \leq R \\ q \leq Q}} d_{\vec{n}} \hat{a}_i^{\dagger n_0} \dots \hat{a}_{i+q}^{\dagger n_q} |\vec{0}\rangle$$

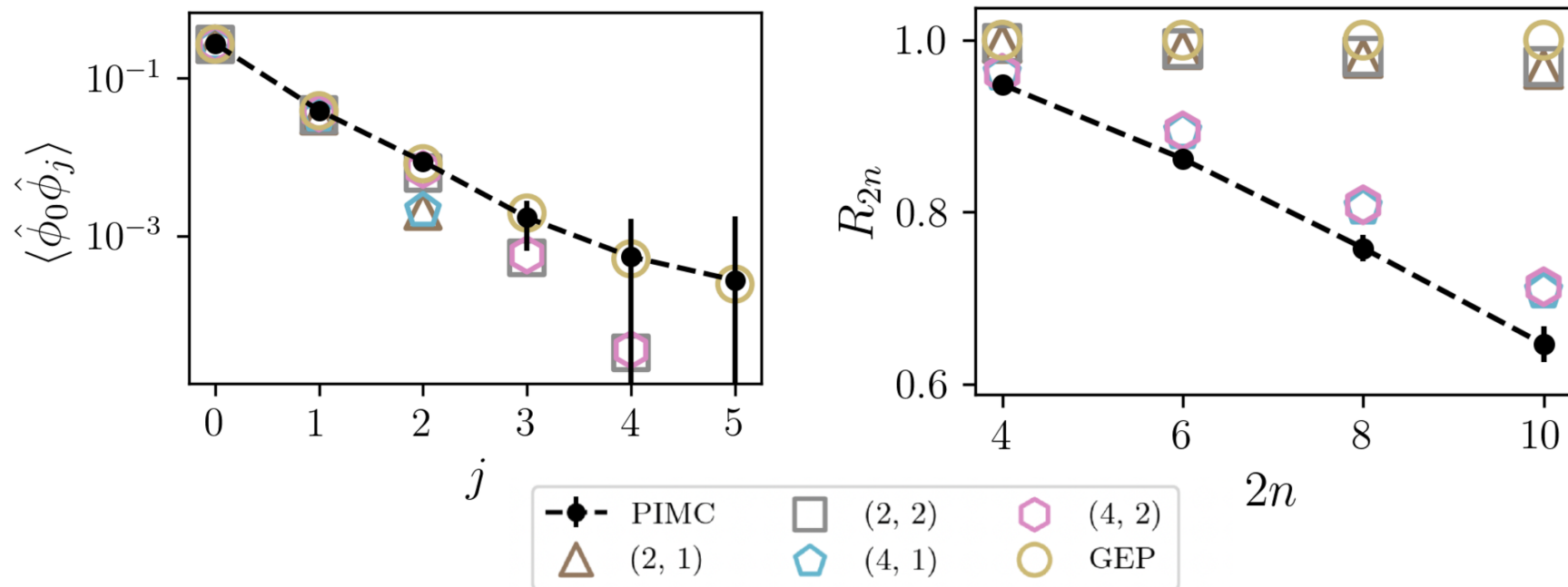
# Energy minimization results in comparable ansatz energies...

$$(m^2, \lambda) = (0.6, 1.5)$$

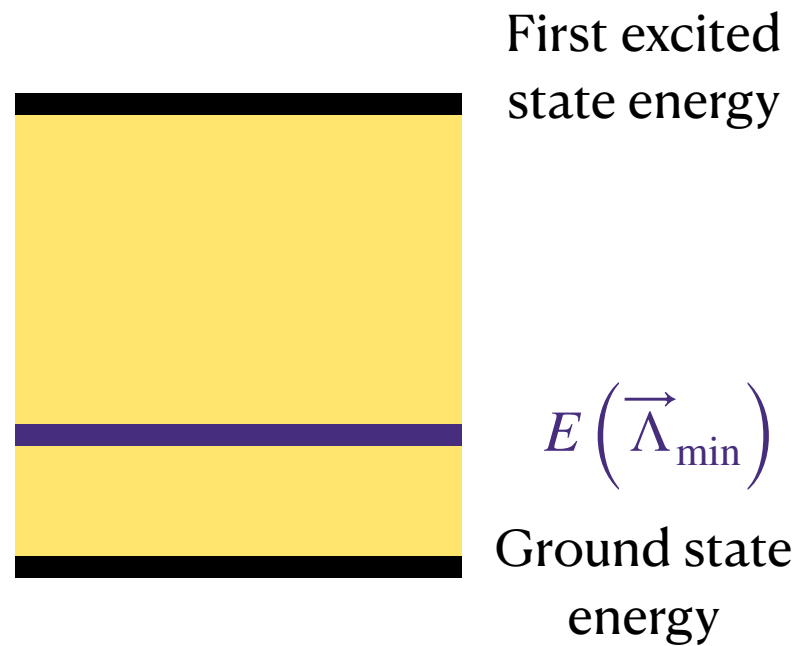
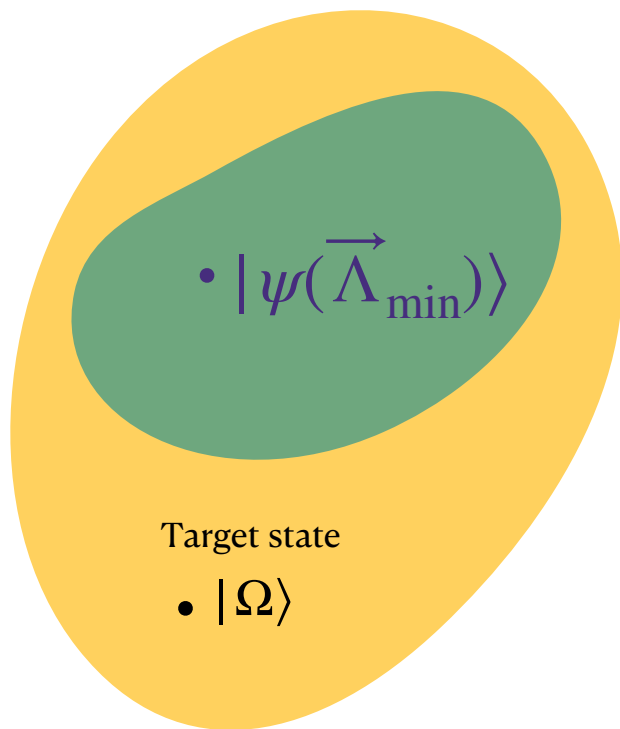


**...but exhibit distinct levels of non-local correlations and non-gaussianity.**

$$(m^2, \lambda) = (0.6, 1.5)$$

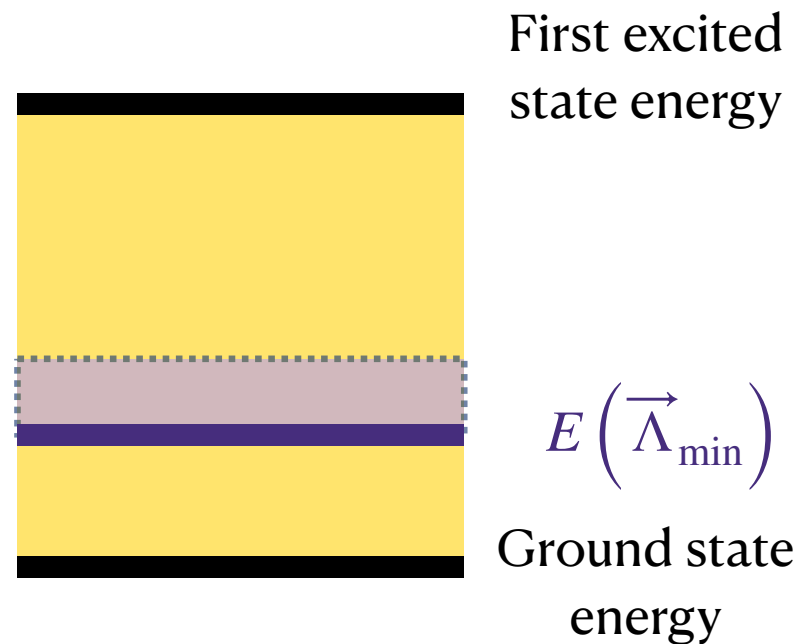
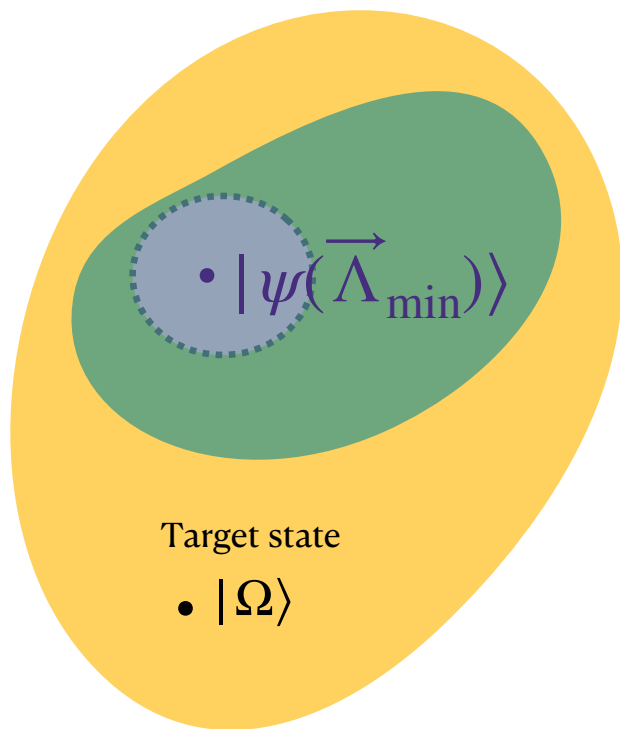


**It is desirable to go beyond the single-dimensional metric of energy.**

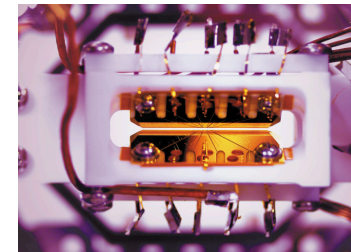
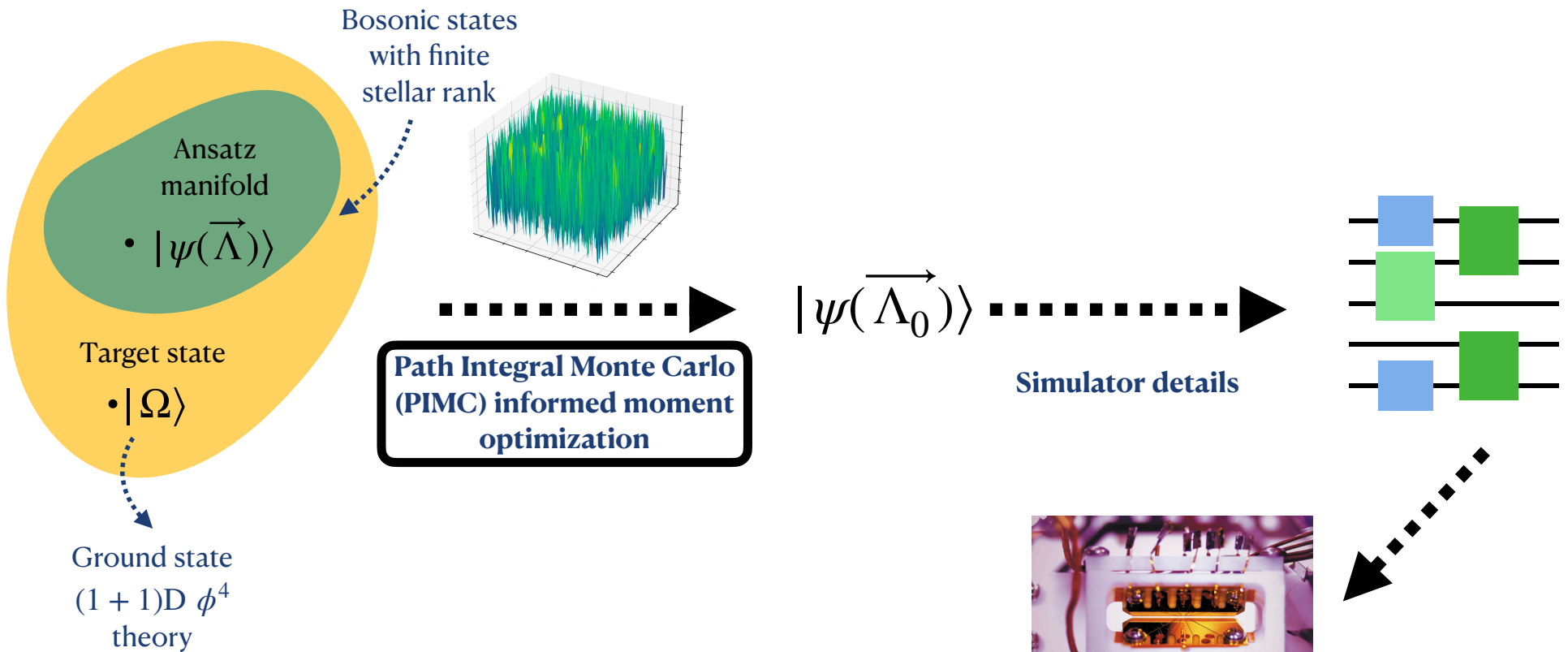




**It is desirable to go beyond the single-dimensional metric of energy.**



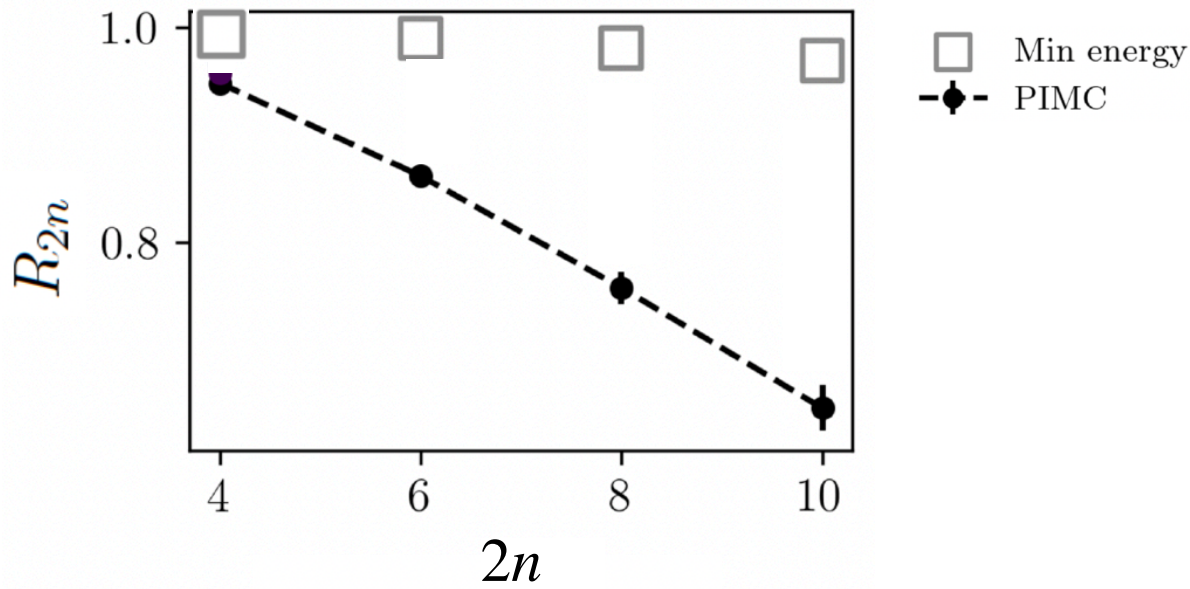
# Classically determined quantum circuit for ground states



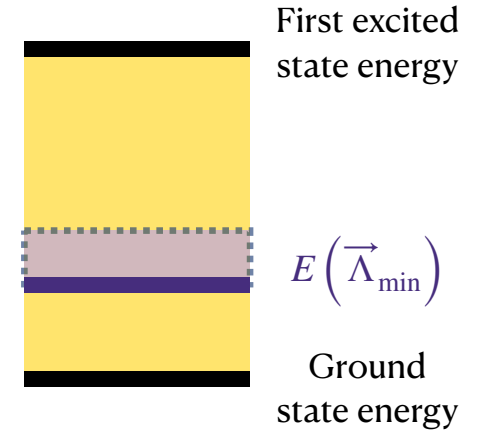
Trapped ion quantum computer from Monroe Lab (UMD, 2016)

# PIMC informed moment optimization

$(m^2, \lambda) = (0.6, 1.5), (R, Q) = (2, 2)$



$$R_{2n} \equiv \frac{\langle \hat{\phi}^{2n} \rangle}{(n-1)!! \langle \hat{\phi}^2 \rangle^n}$$

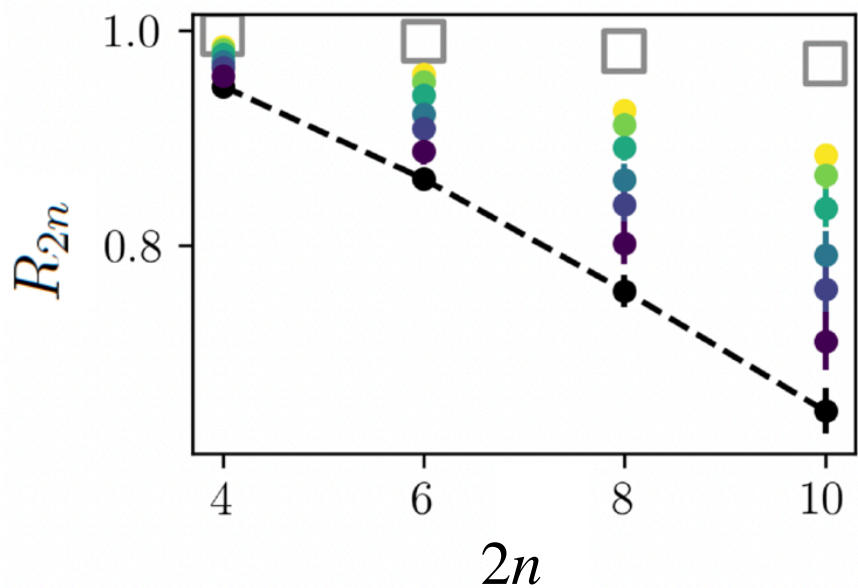


**Minimize:**

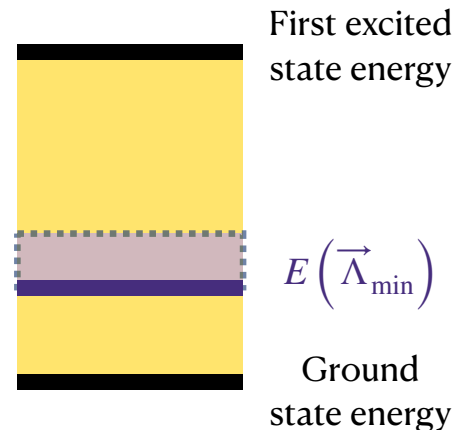
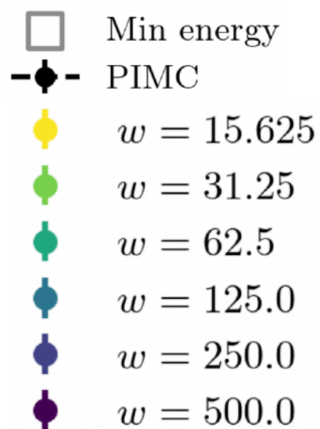
$$w \sum_{2n=6,8,10} \left( \langle \hat{H} \rangle_{\vec{\Lambda}} + \left( \langle \hat{\phi}^{2n} \rangle_{\vec{\Lambda}} - \langle \hat{\phi}^{2n} \rangle_{\text{PIMC}} \right)^2 \right)$$

# PIMC informed moment optimization

$(m^2, \lambda) = (0.6, 1.5), (R, Q) = (2, 2)$



$$R_{2n} \equiv \frac{\langle \hat{\phi}^{2n} \rangle}{(n-1)!! \langle \hat{\phi}^2 \rangle^n}$$

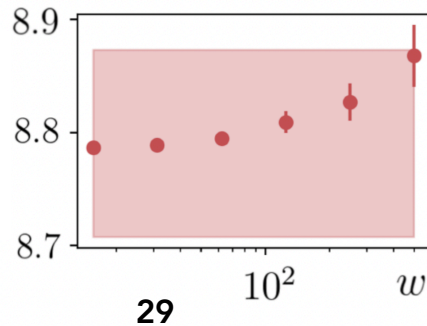
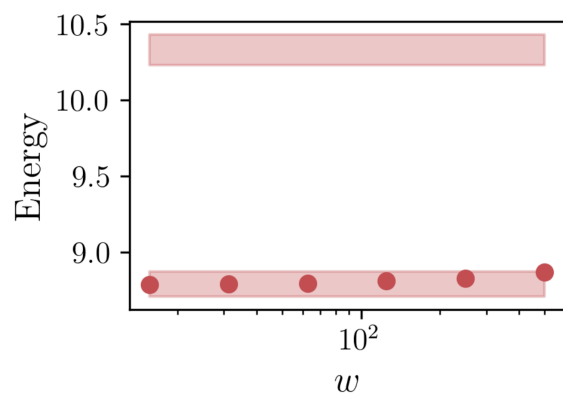
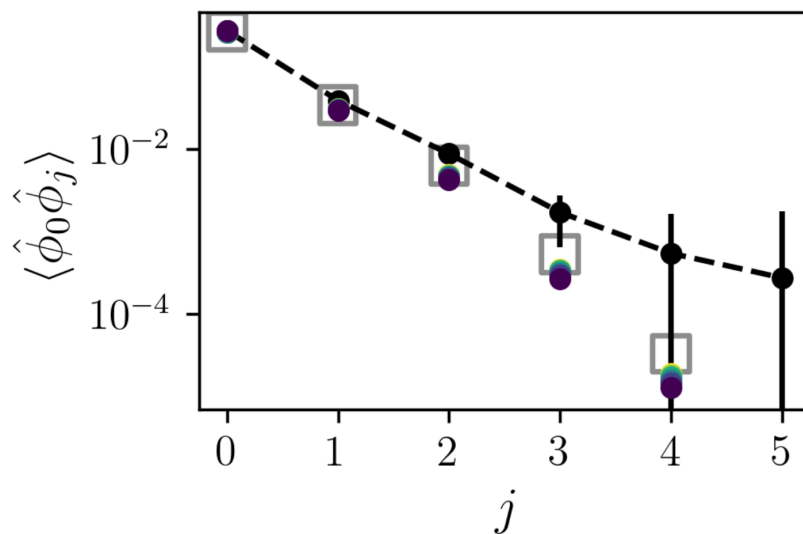
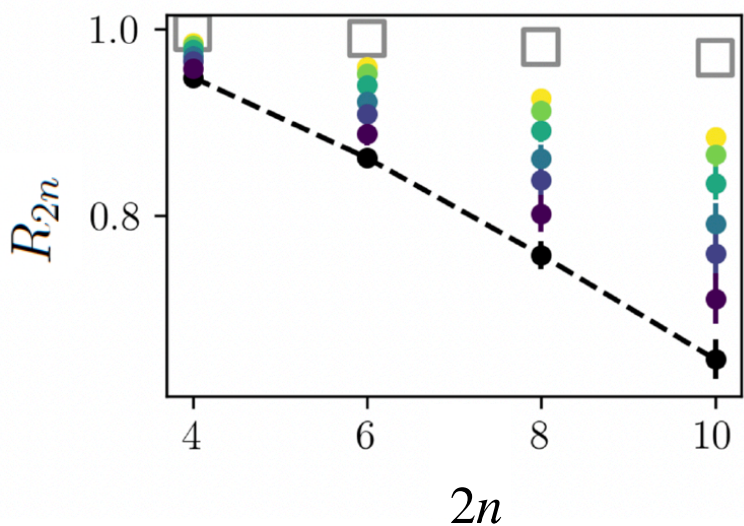


**Minimize:**

$$w \sum_{2n=6,8,10} \left( \langle \hat{H} \rangle_{\vec{\Lambda}} + \left( \langle \hat{\phi}^{2n} \rangle_{\vec{\Lambda}} - \langle \hat{\phi}^{2n} \rangle_{\text{PIMC}} \right)^2 \right)$$

# PIMC informed moment optimization

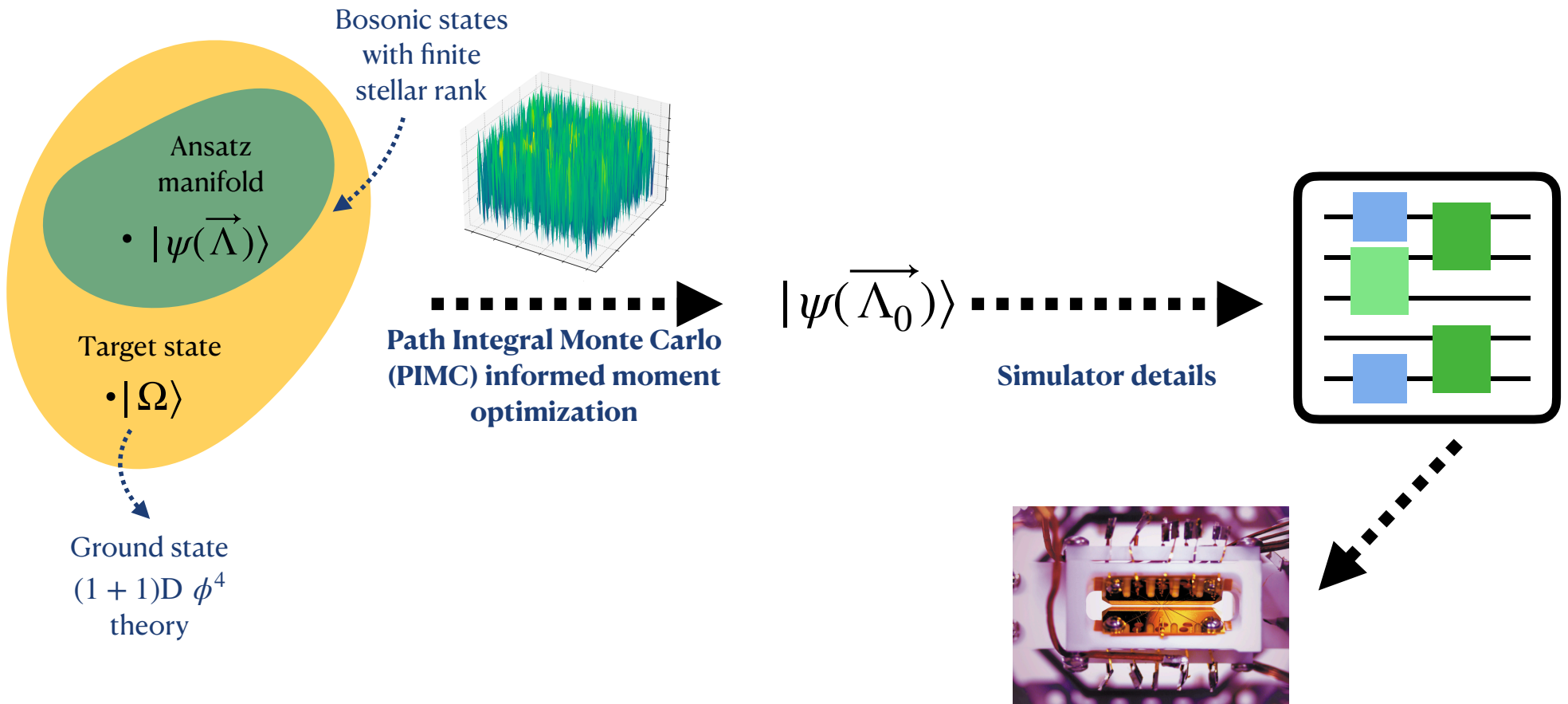
$(m^2, \lambda) = (0.6, 1.5)$ ,  $(R, Q) = (2, 2)$



**Minimize:**

$$\langle \hat{H} \rangle_{\bar{\Lambda}} + w \sum_{2n=6,8,10} \left( \langle \hat{\phi}^{2n} \rangle_{\bar{\Lambda}} - \langle \hat{\phi}^{2n} \rangle_{\text{PIMC}} \right)^2$$

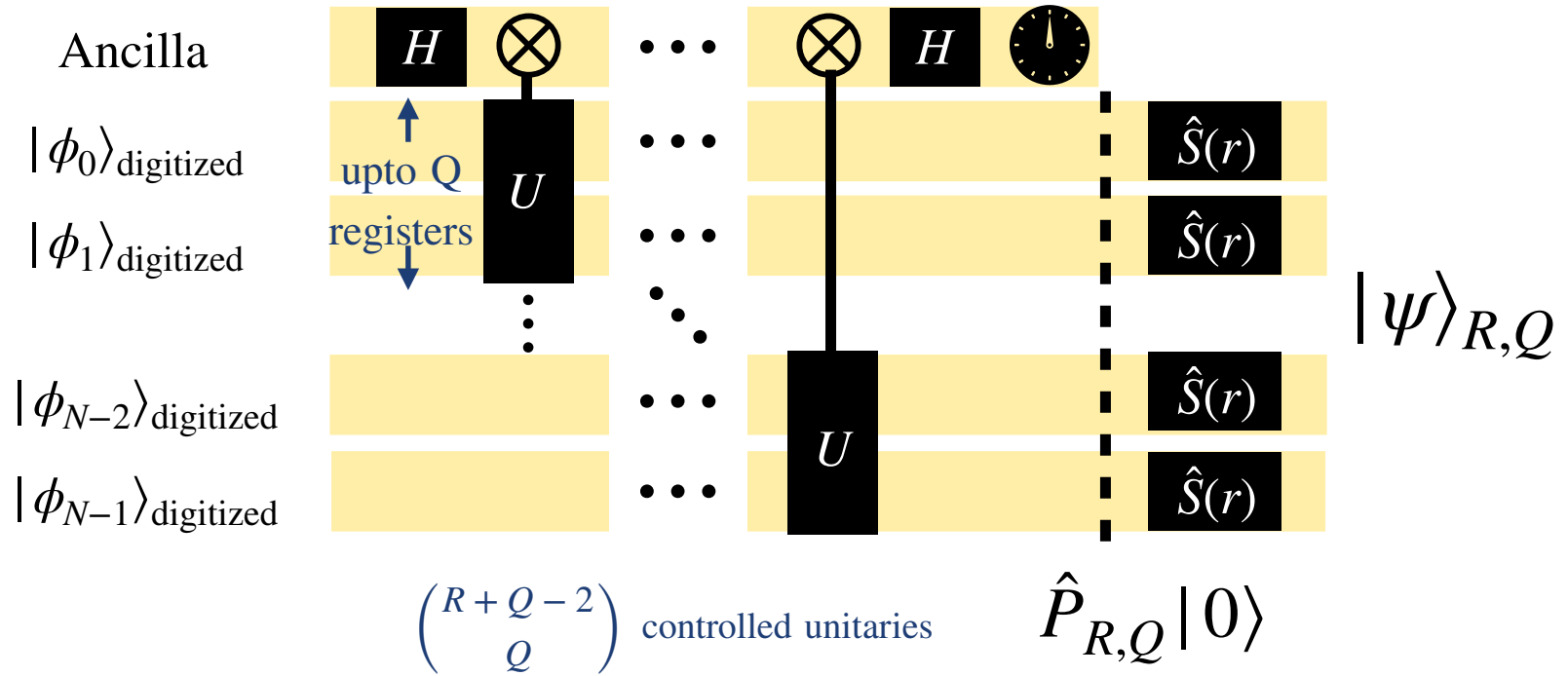
# Classically determined quantum circuit for ground states



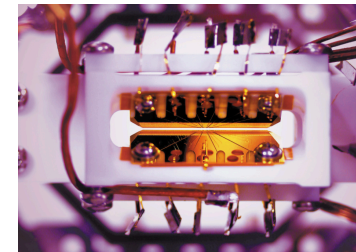
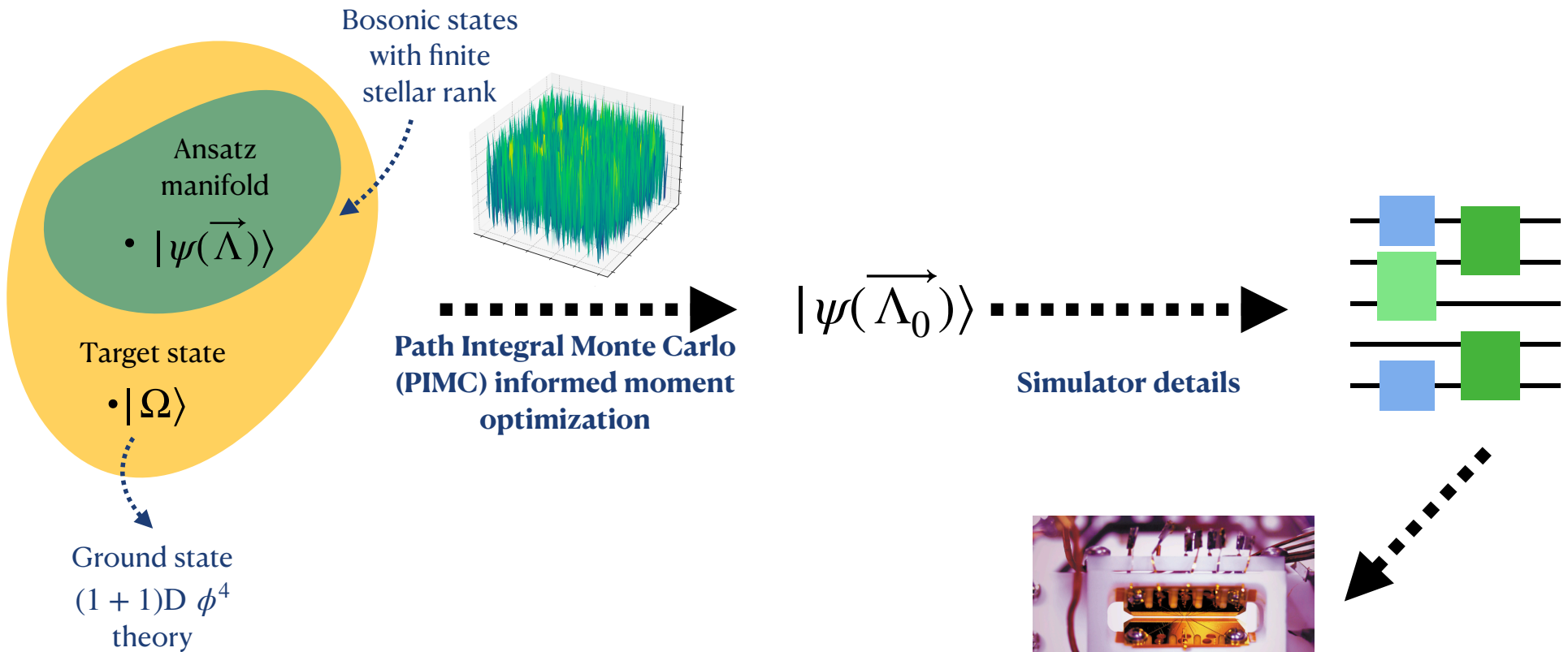
Trapped ion quantum computer from Monroe Lab (UMD, 2016)

# Circuit blueprint

$$|\psi\rangle_{(R,Q)} = \hat{U}_G \sum_{\substack{\vec{n} = n_1, \dots, n_q \\ n_1 + \dots + n_q \leq R \\ q \leq N/2}} d_{\vec{n}} \hat{a}_i^{\dagger n_0} \dots \hat{a}_{i+q}^{\dagger n_q} |0\rangle_R$$



# Classically determined quantum circuit for ground states



Trapped ion quantum computer from Monroe Lab (UMD, 2016)



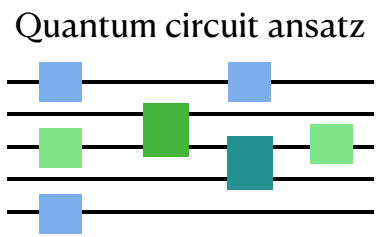
## Outlook

- Systematic study of the moment optimization landscape.
- Development of continuous variable state preparation strategies.
- Application of moment optimization to gauge theories.
- Utility of moment optimization in simulations of dynamics.
- Implementation on actual quantum hardware.

# **Supplementary slides**

## Variational Quantum Eigensolver

### Input



### Computation

Minimizing the energy of the state represented by the circuit using hybrid classical and quantum computing.

Optimized state misses certain ground state moments.

## Path-integral Monte Carlo assisted moment optimization

- Wavefunction ansatz:  $|\psi(\vec{\Lambda})\rangle$
- Spectral gap and ground state moments (determined by PIMC)

Optimize  $|\psi(\vec{\Lambda})\rangle$  to accurately represent a set of target ground state moments.

Determine circuit encoding of moment optimized ansatz.

GROUND STATE KNOWLEDGE NEEDED

## Direct circuit encoding

Ground state wavefunction.

Determining the quantum circuit which encodes this known wavefunction.

Wavefunction known only for a limited set of cases.

Minimal

Maximal

