

Quantum chemistry on near-term devices

Anton Nykänen, Walter Talarico, Roberto Di Remigio Eikås | QAS2023, Göteborg | 27.10.2023



algorithmiq

Bringing quantum to life

Our mission is to revolutionise life sciences by
exploiting the potential of quantum computing
to solve currently inaccessible problems

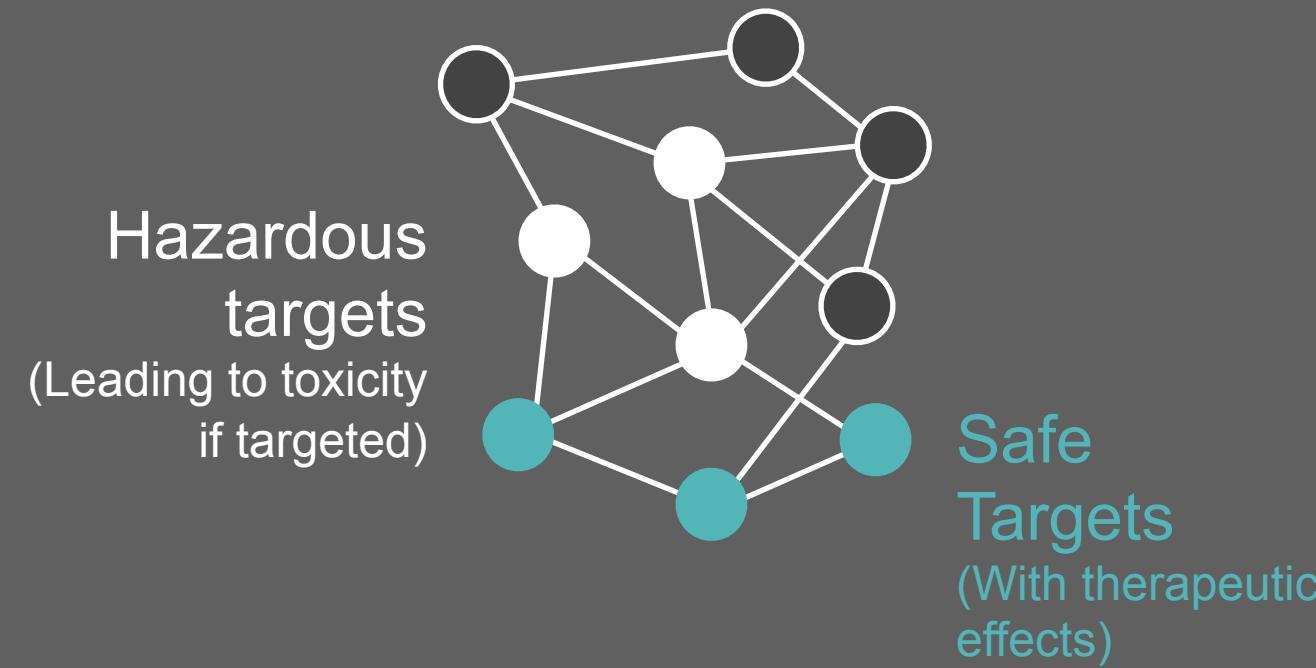
Quantum Network Medicine

Algorithmiq's multiscale approach to tackle the complexity of the cell biology

1

Classical & Quantum - inspired (proprietary)

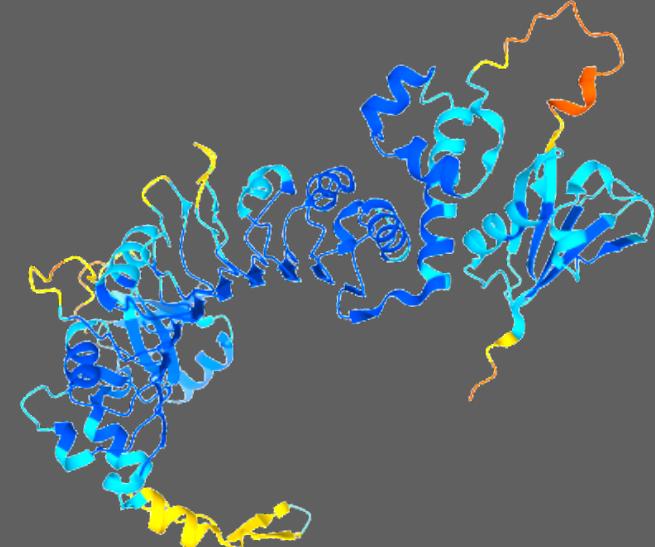
Data-driven identification of the relevant network biology



2

Classical

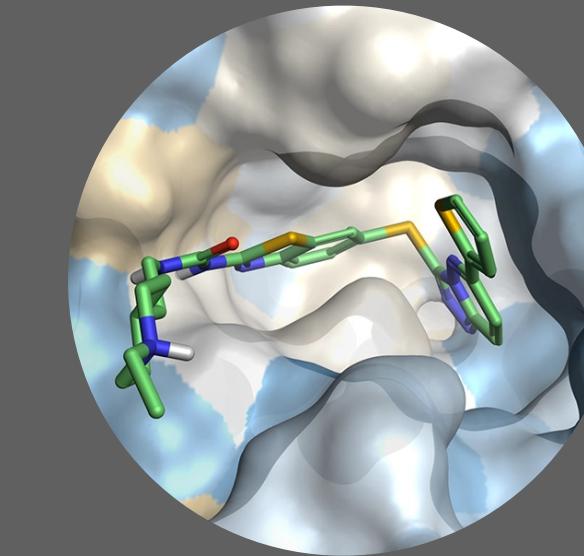
Modelling protein structures
machine learning and crystallographic data



3

Quantum (proprietary)

***Ab-initio* molecular simulations**
Quantum computer simulation



a u r o r a
Network Medicine

a u r o r a
Chemistry

Quantum computing is evolving very quickly

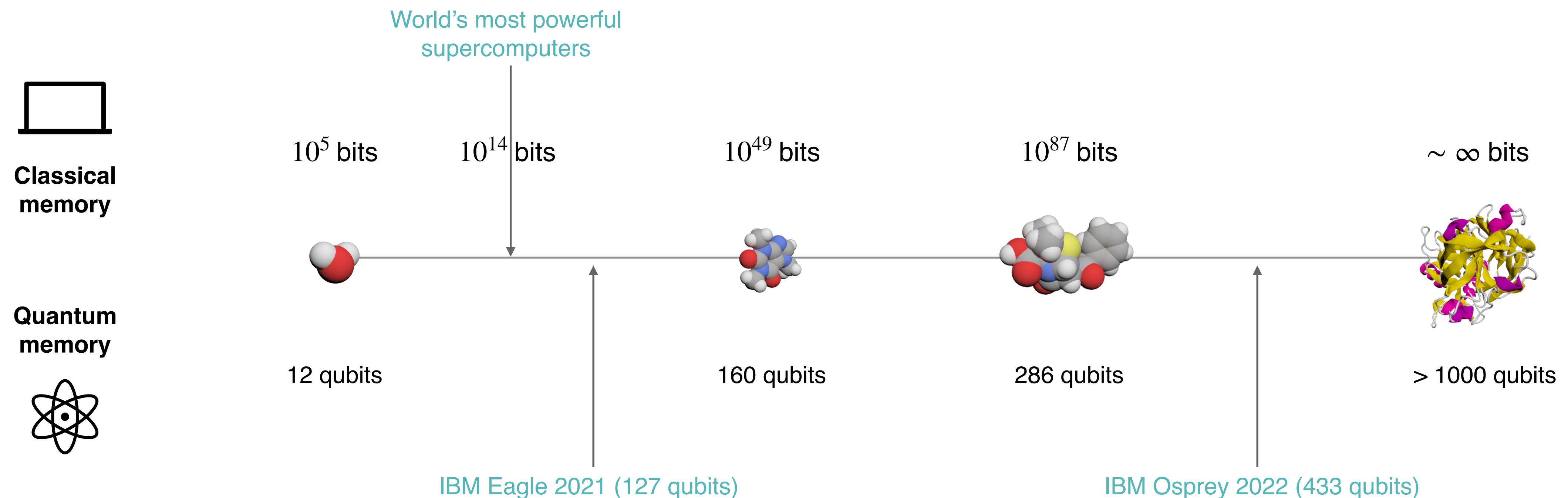


Billions are being invested

Hardware is improving fast

Drug discovery is emerging
as a promising area of application

Despite advances in high performance computing it is challenging to model complex molecules on classical computers

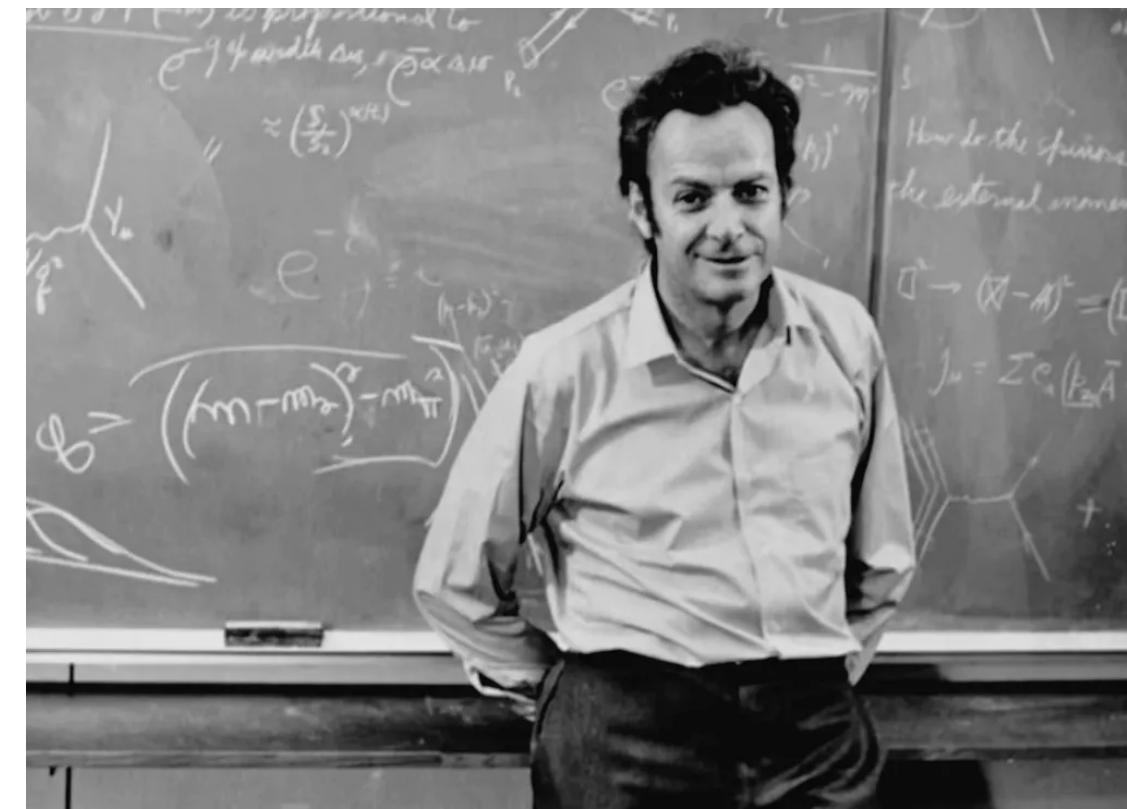


The origins of quantum computing

Simulating quantum physics



Yuri Manin
1980



Richard Feynman
1982

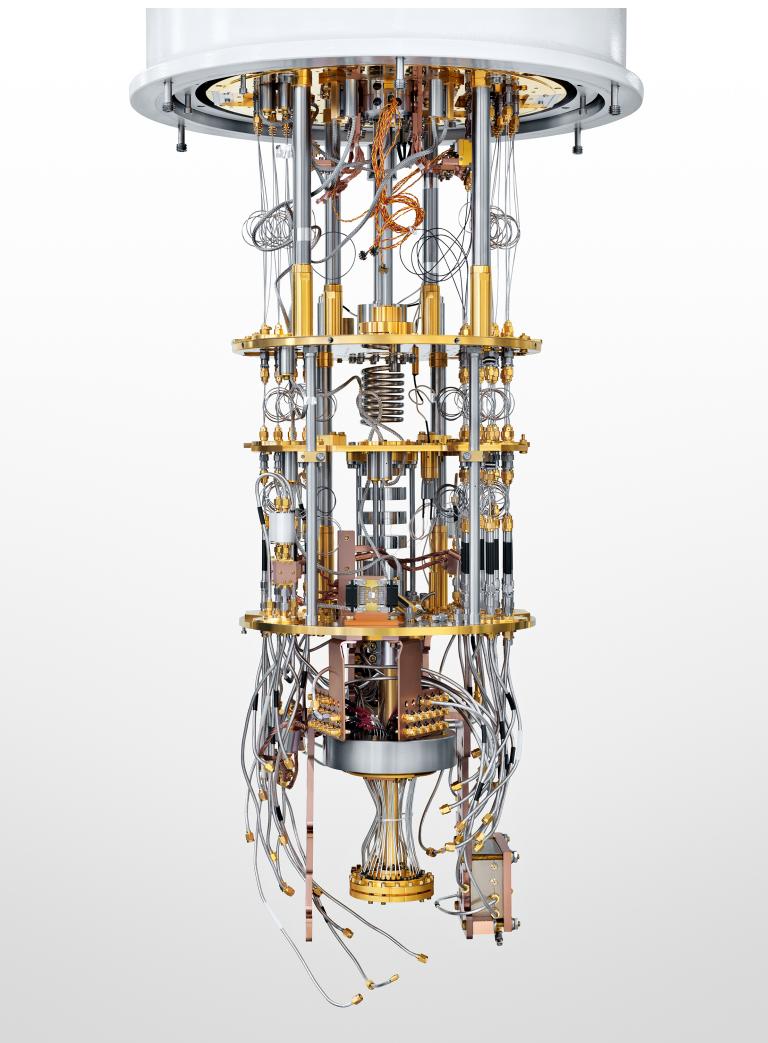
Simulating some quantum mechanical effects
on a classical computer is unfeasible



Use a quantum one!

Using a quantum computer

As a quantum physics simulator

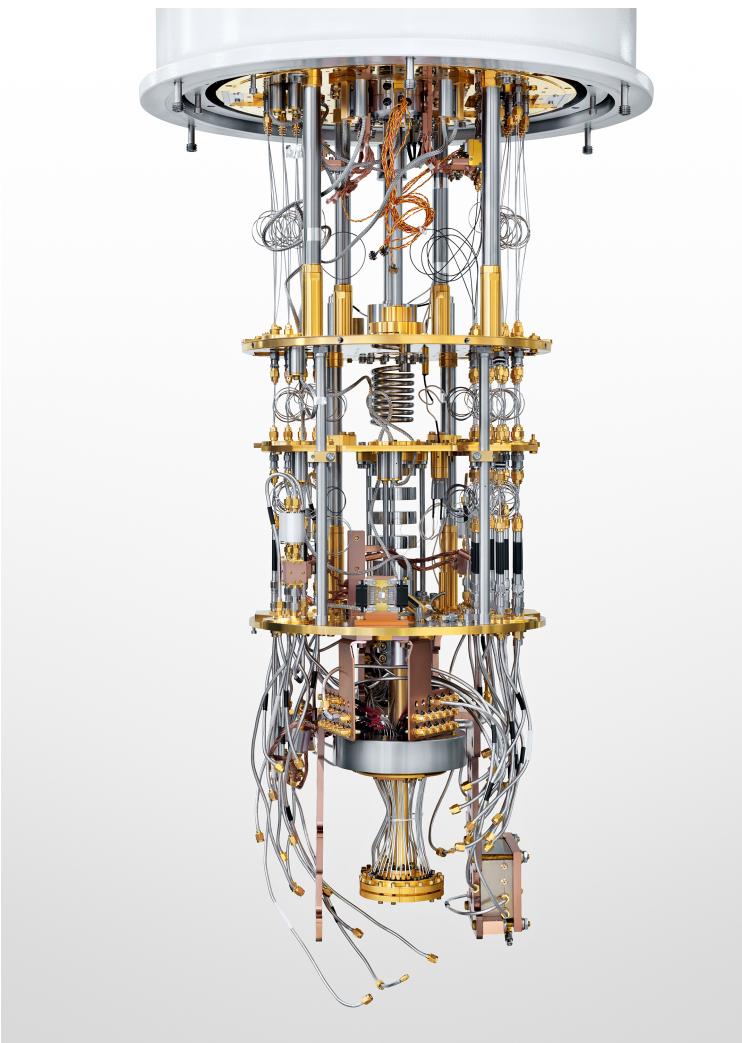


Arbitrary state of its quantum bits (qubits)

$$\rightarrow |\Psi\rangle = \sum_{\vec{f}} \alpha_{\vec{f}} |f_1 f_2 \dots f_M\rangle$$

Using a quantum computer

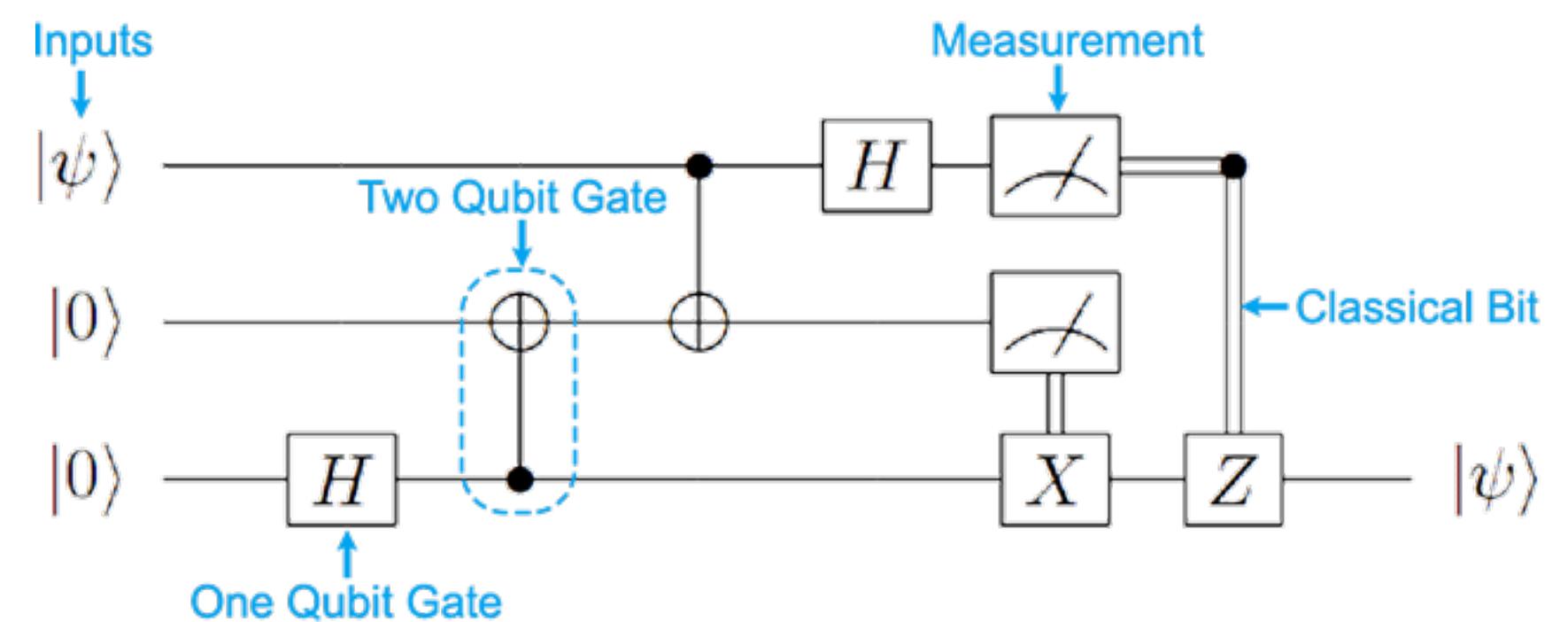
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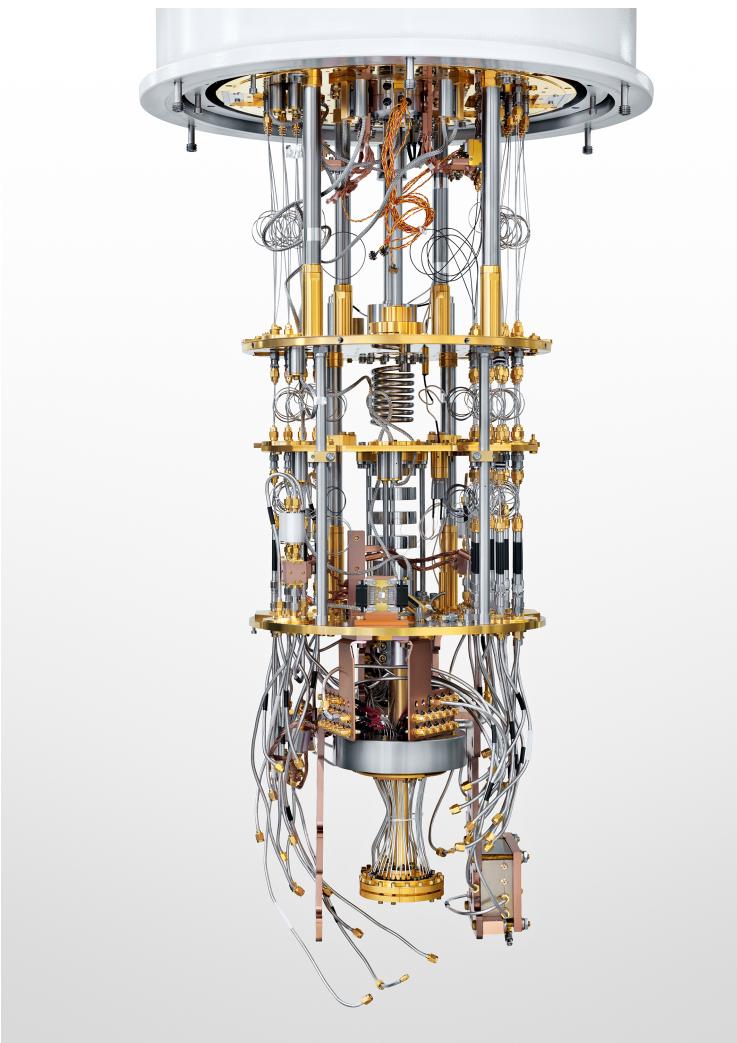
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A universal quantum computer can solve problems beyond quantum simulation (e.g. factorisation)



Using a quantum computer

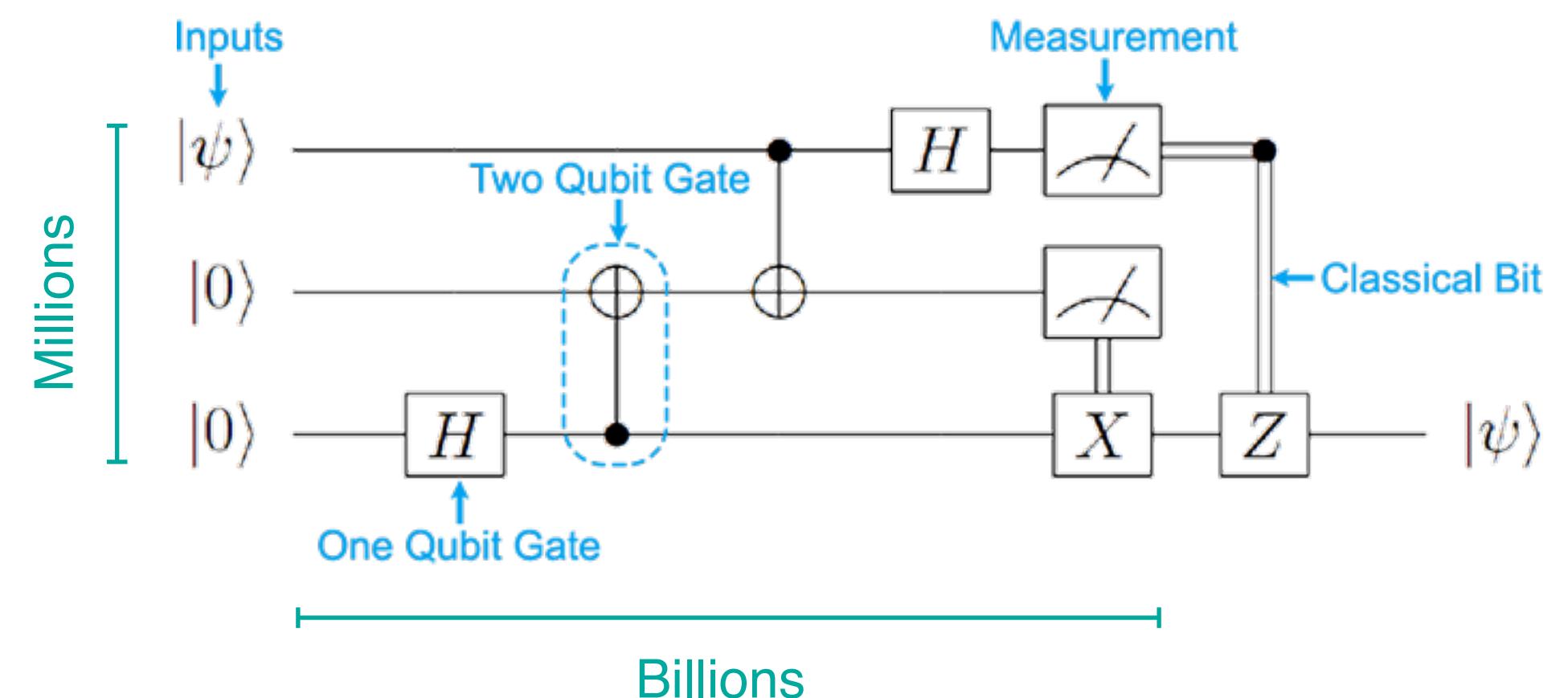
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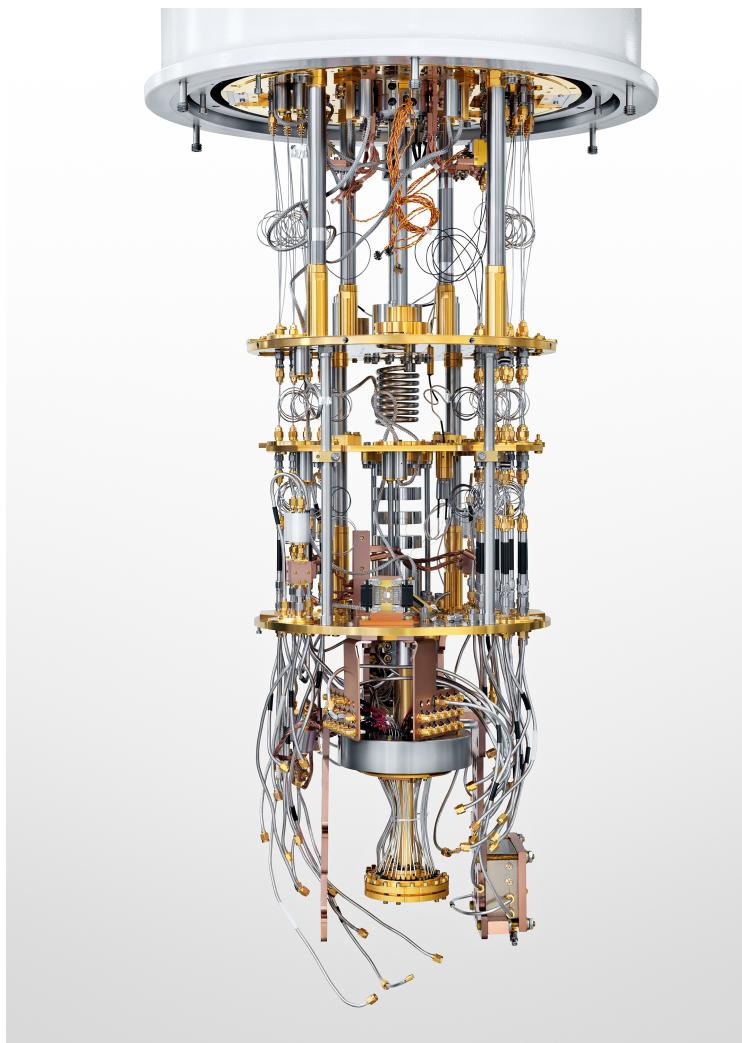
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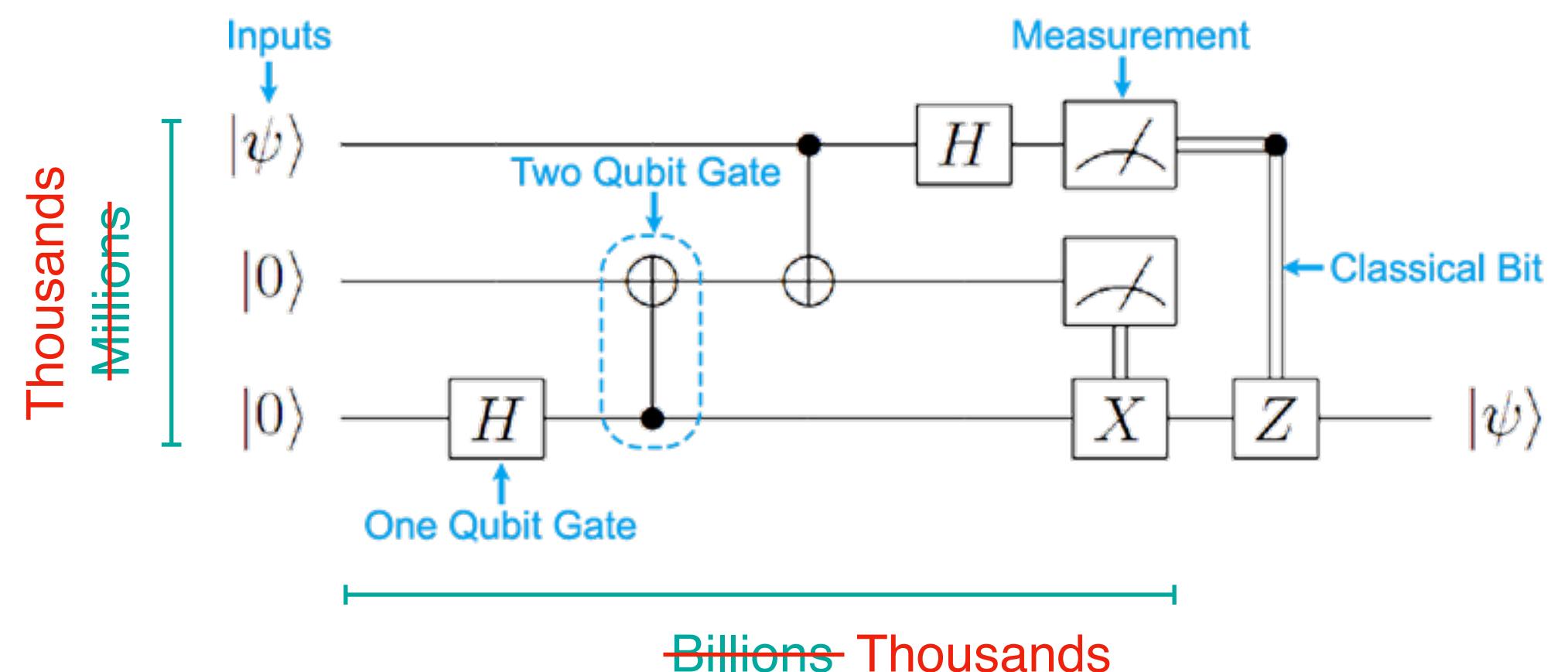
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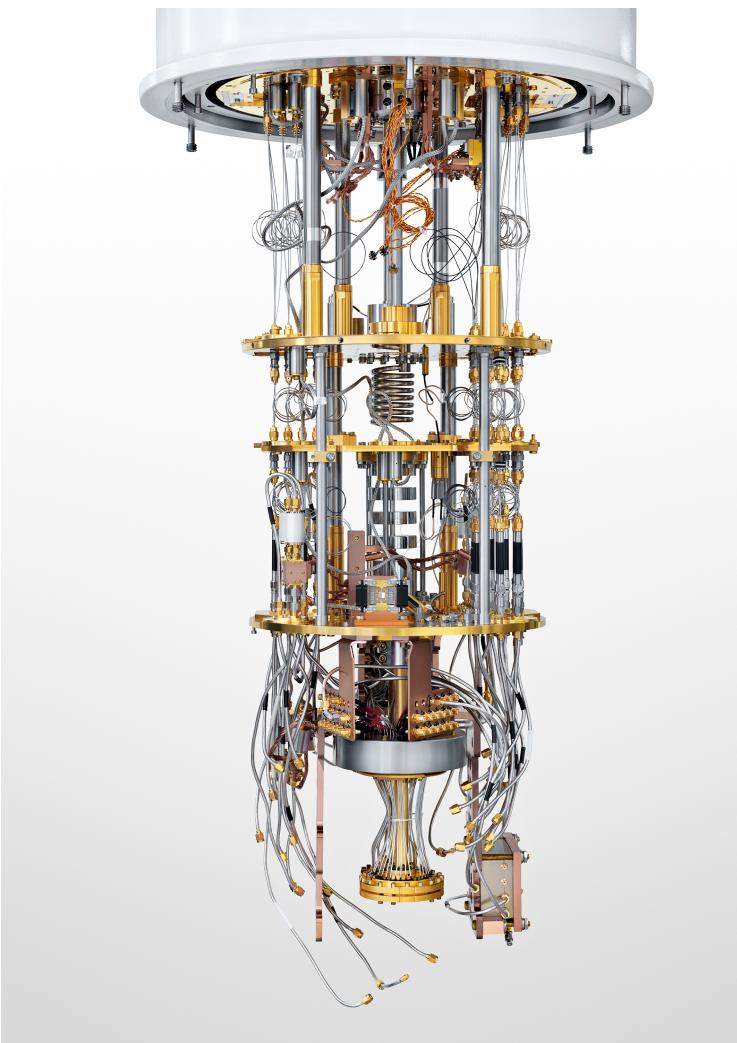
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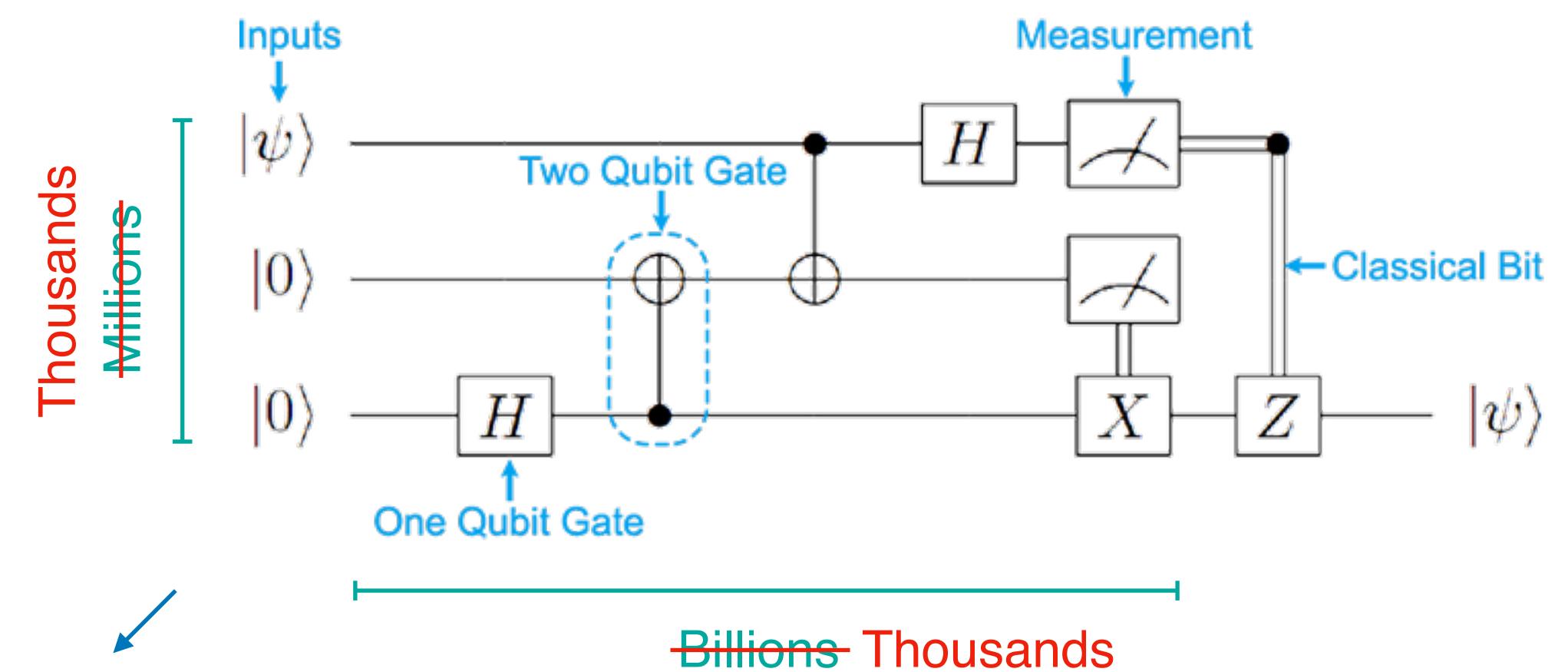
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We are in the era of the Noisy Intermediate-Scale Quantum computers:
soon useful for simulation!

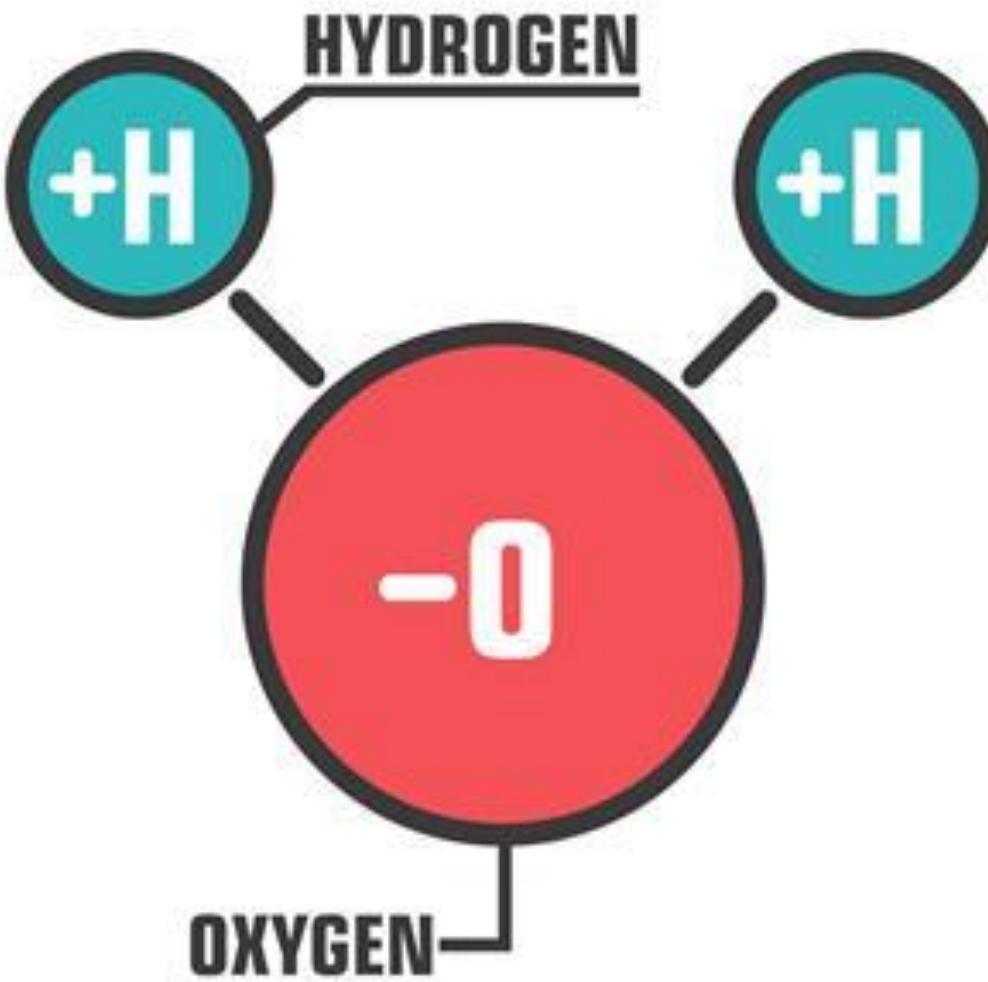
Variational Quantum Eigensolver

(General) problem statement

Molecular ground-state energy

- Composition of the molecule is given

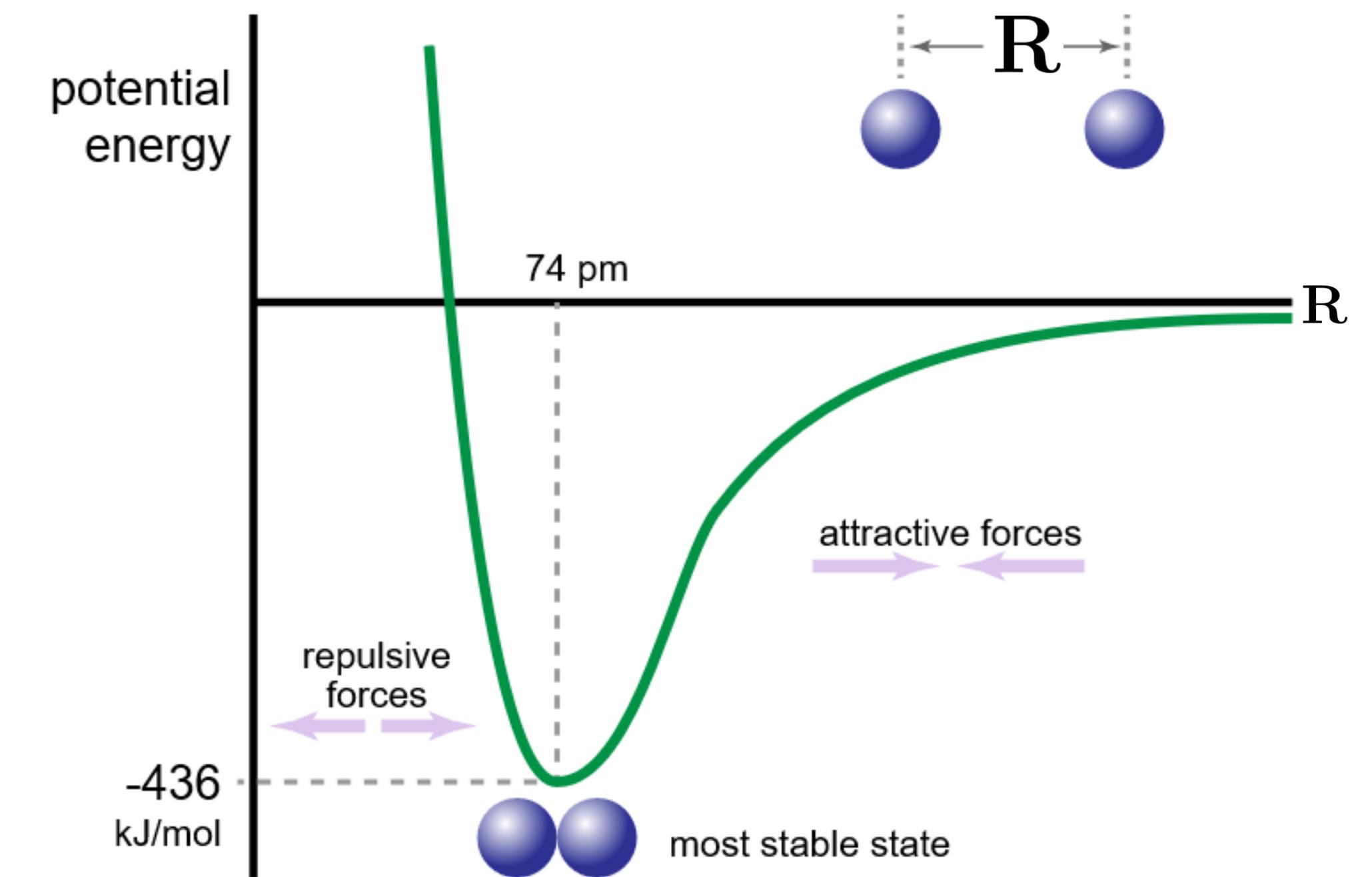
WATER (H_2O)



(General) problem statement

Molecular ground-state energy

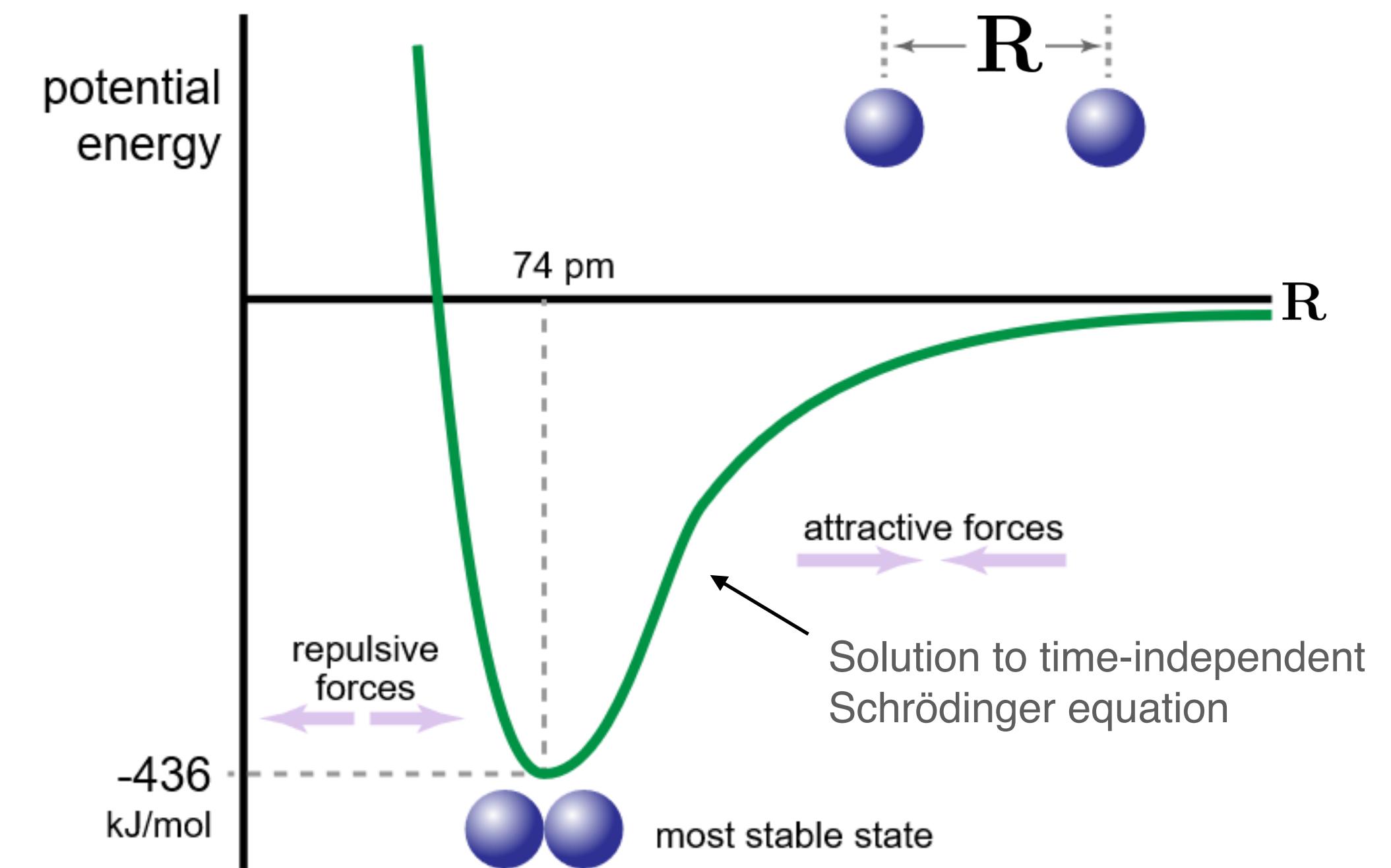
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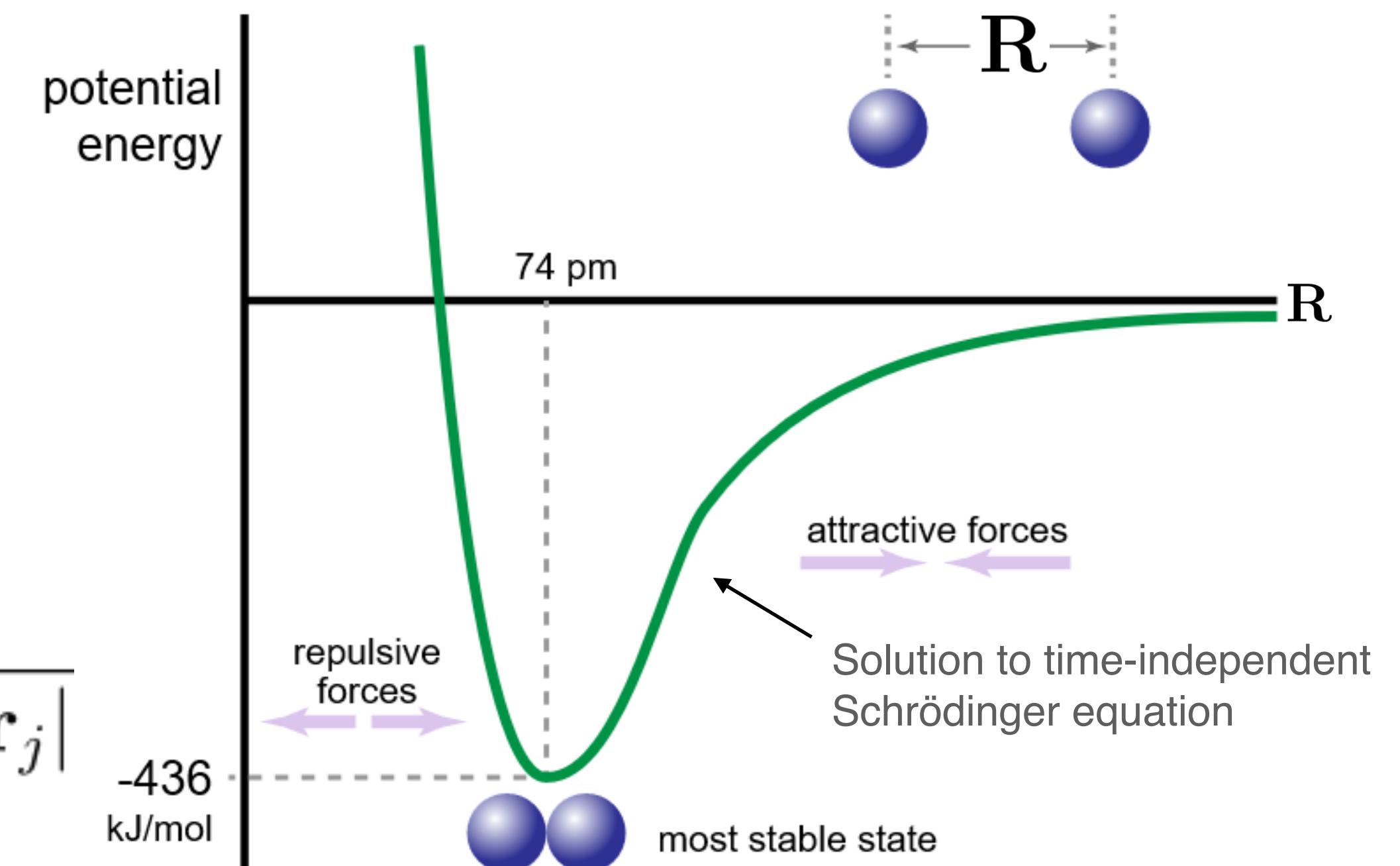


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$$\hat{H}_e = -\frac{1}{2} \sum_i \nabla_i^2 - \sum_i \sum_{\alpha} \frac{Z_{\alpha}}{|\mathbf{R}_{\alpha} - \mathbf{r}_i|} + \frac{1}{2} \sum_{i \neq j} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}$$
$$\hat{H}_e |\Psi\rangle = E |\Psi\rangle$$



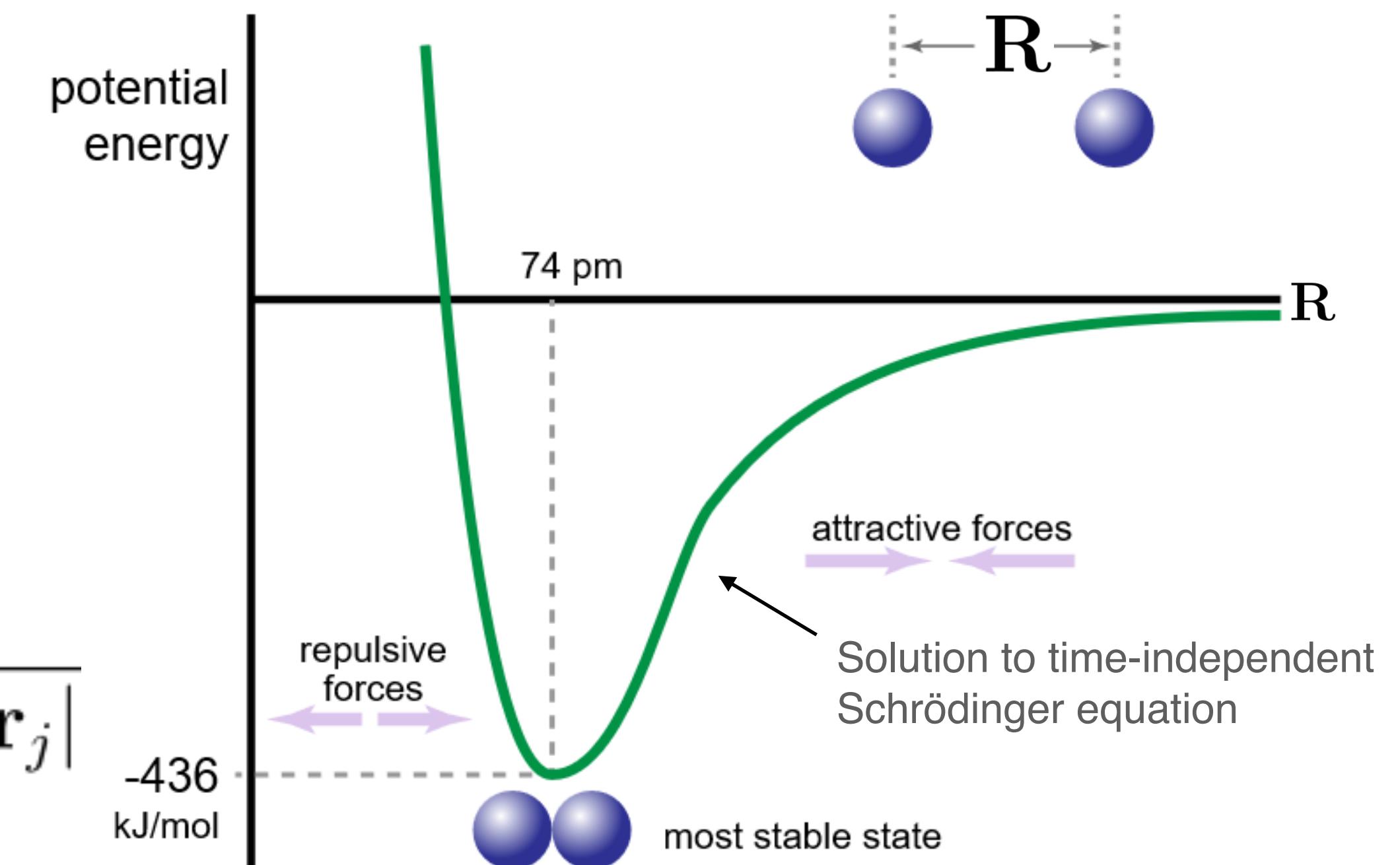
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High-dimensional vector
in Hilbert space



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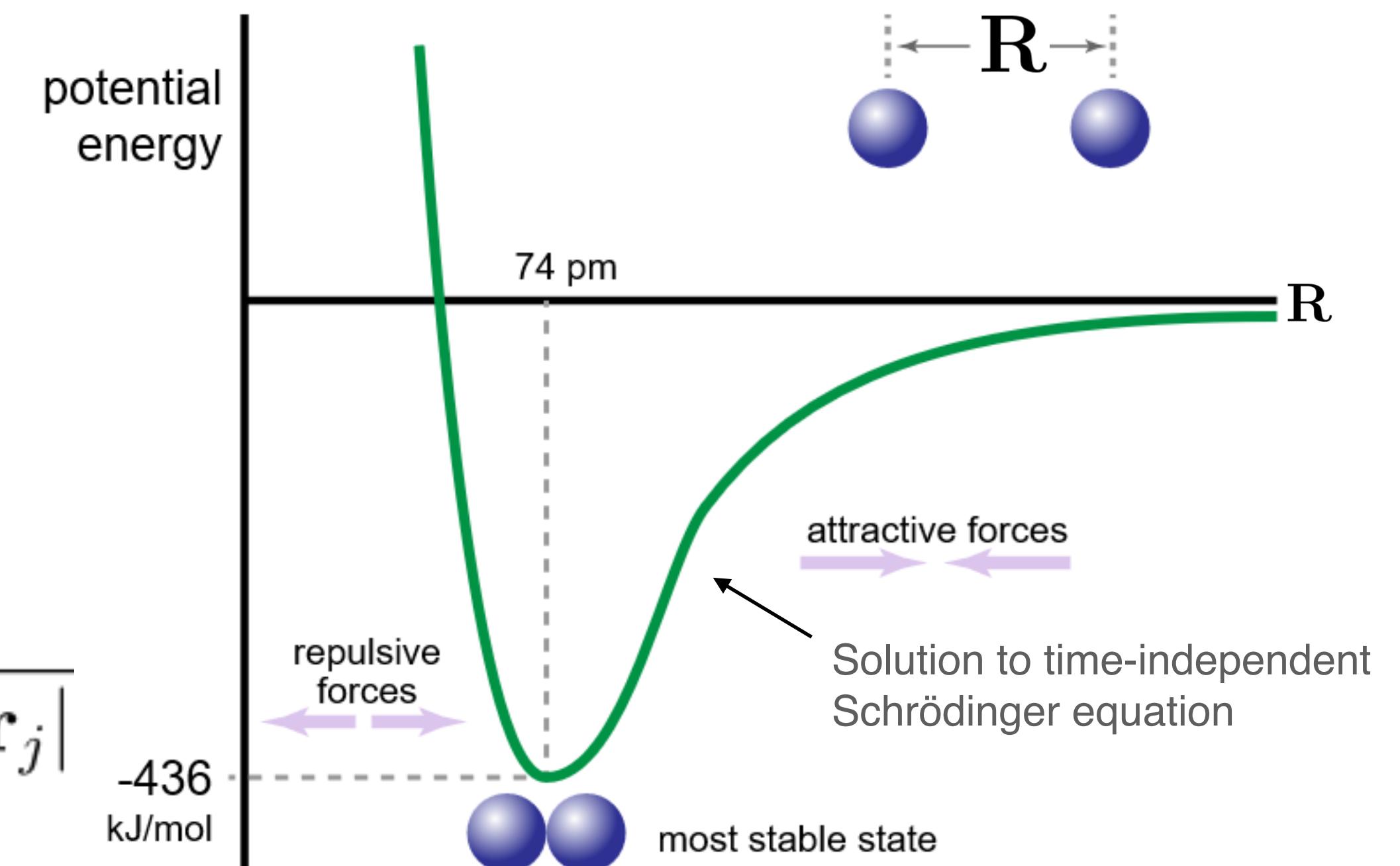
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Well-known from QM theory
Efficient classical representation

High-dimensional vector
in Hilbert space



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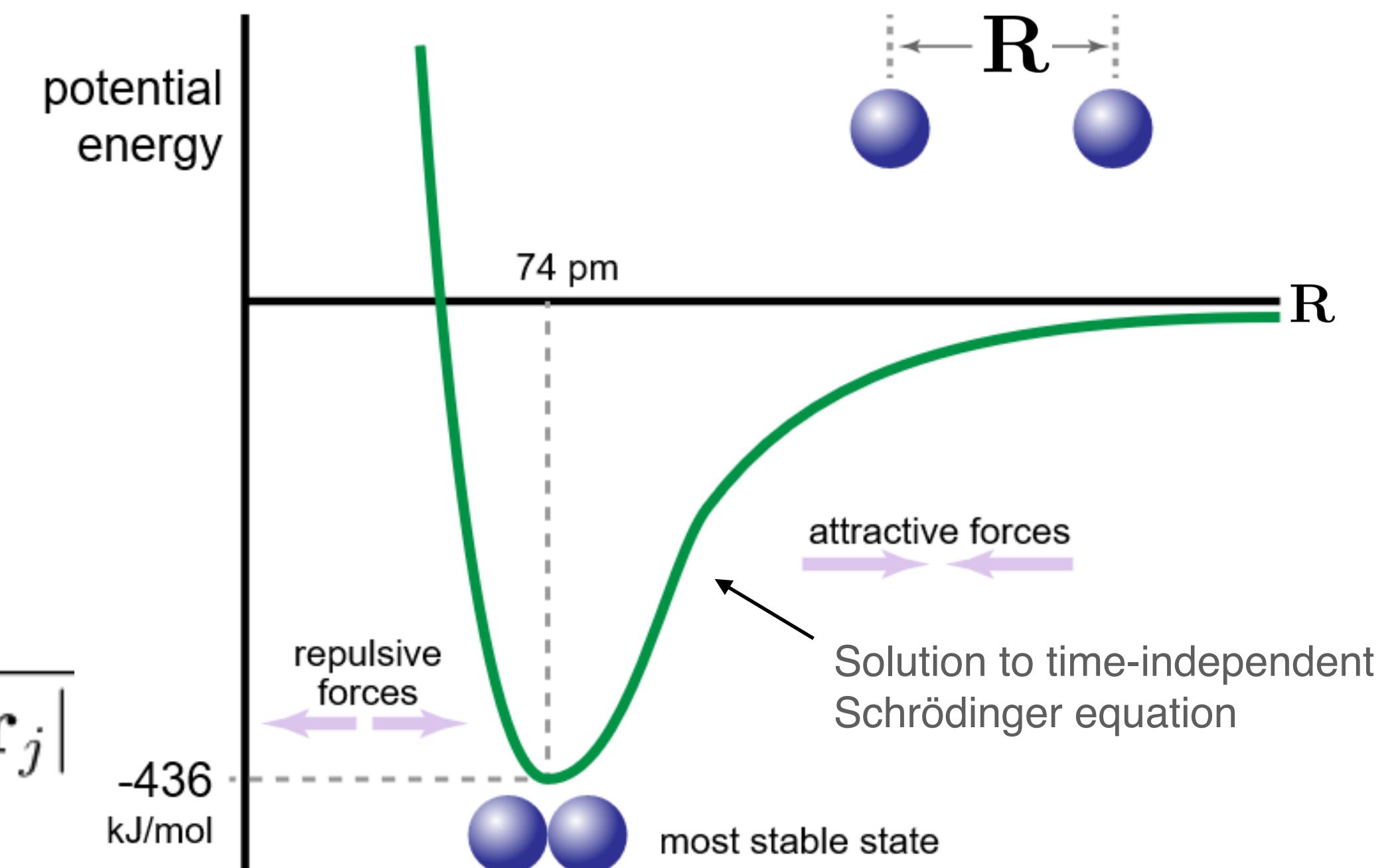
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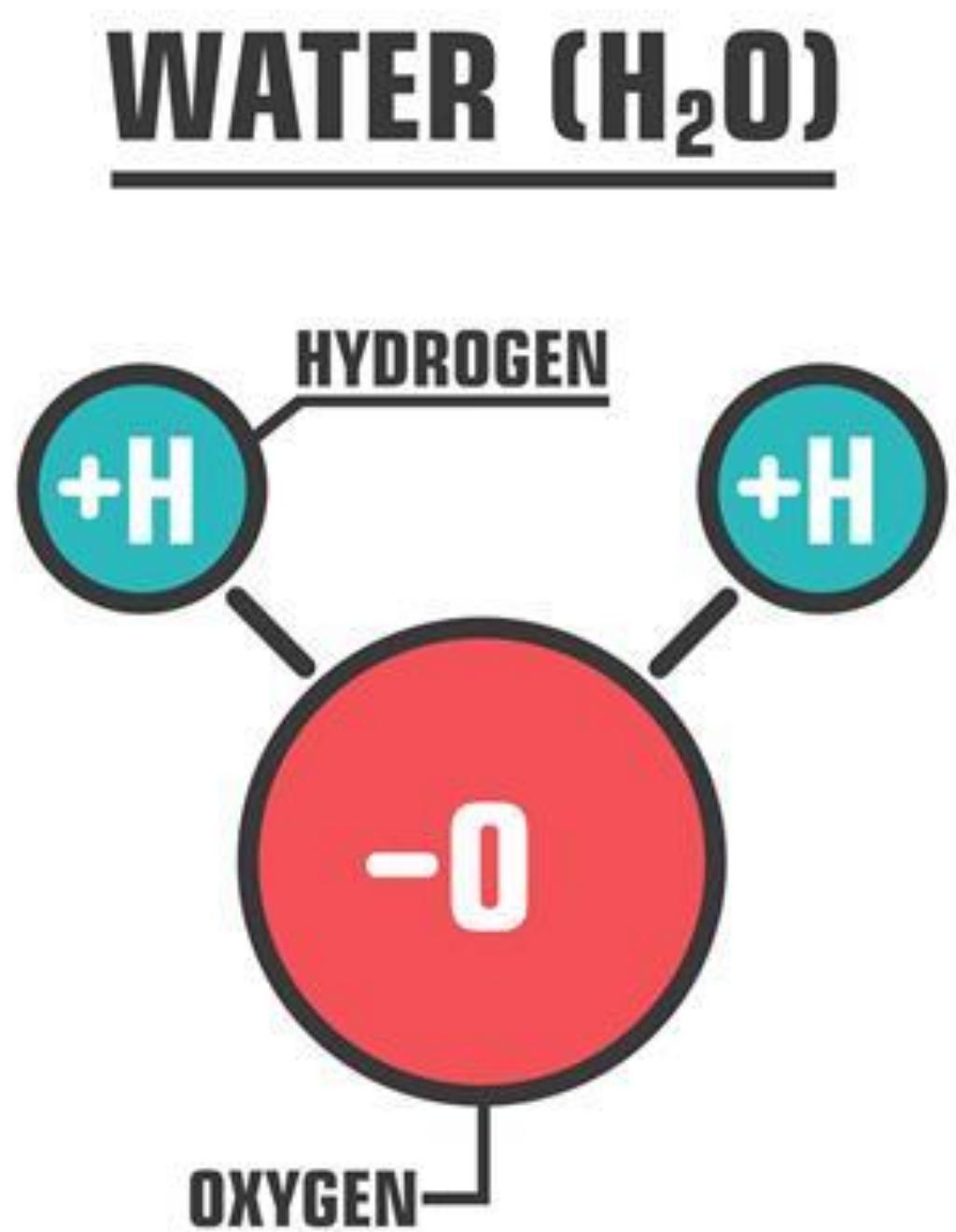
Well-known from QM theory
Efficient classical representation

High-dimensional vector
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Why is this difficult?

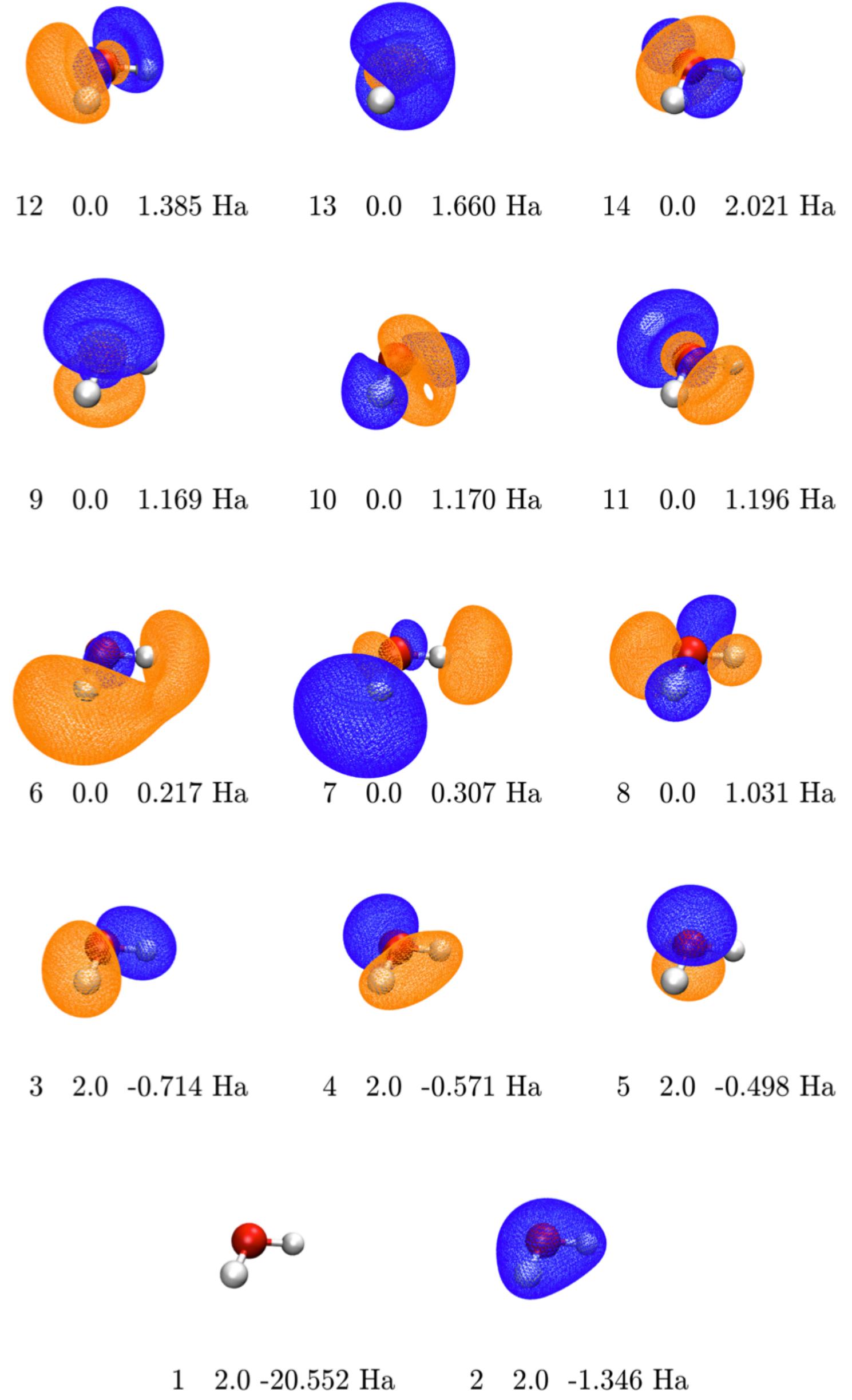
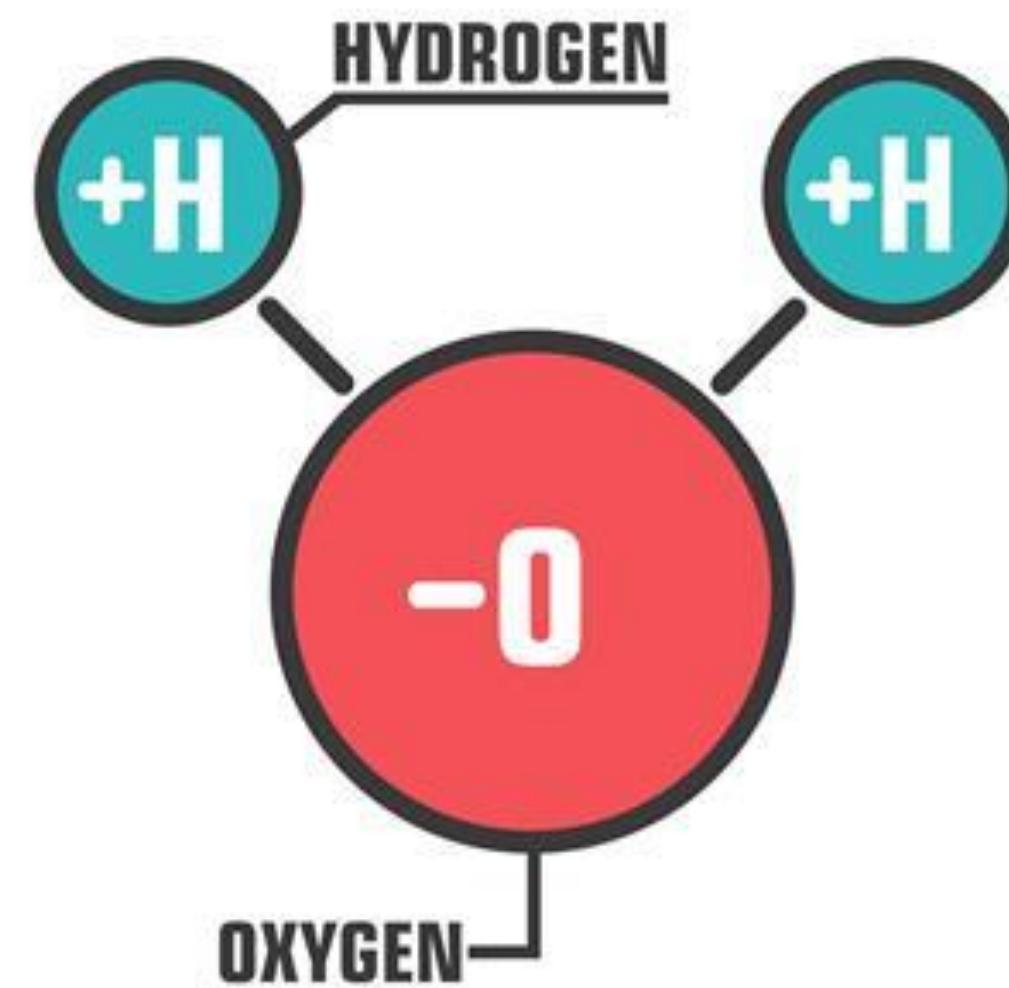
Dimensionality of many-body QM



Why is this difficult?

Dimensionality of many-body QM

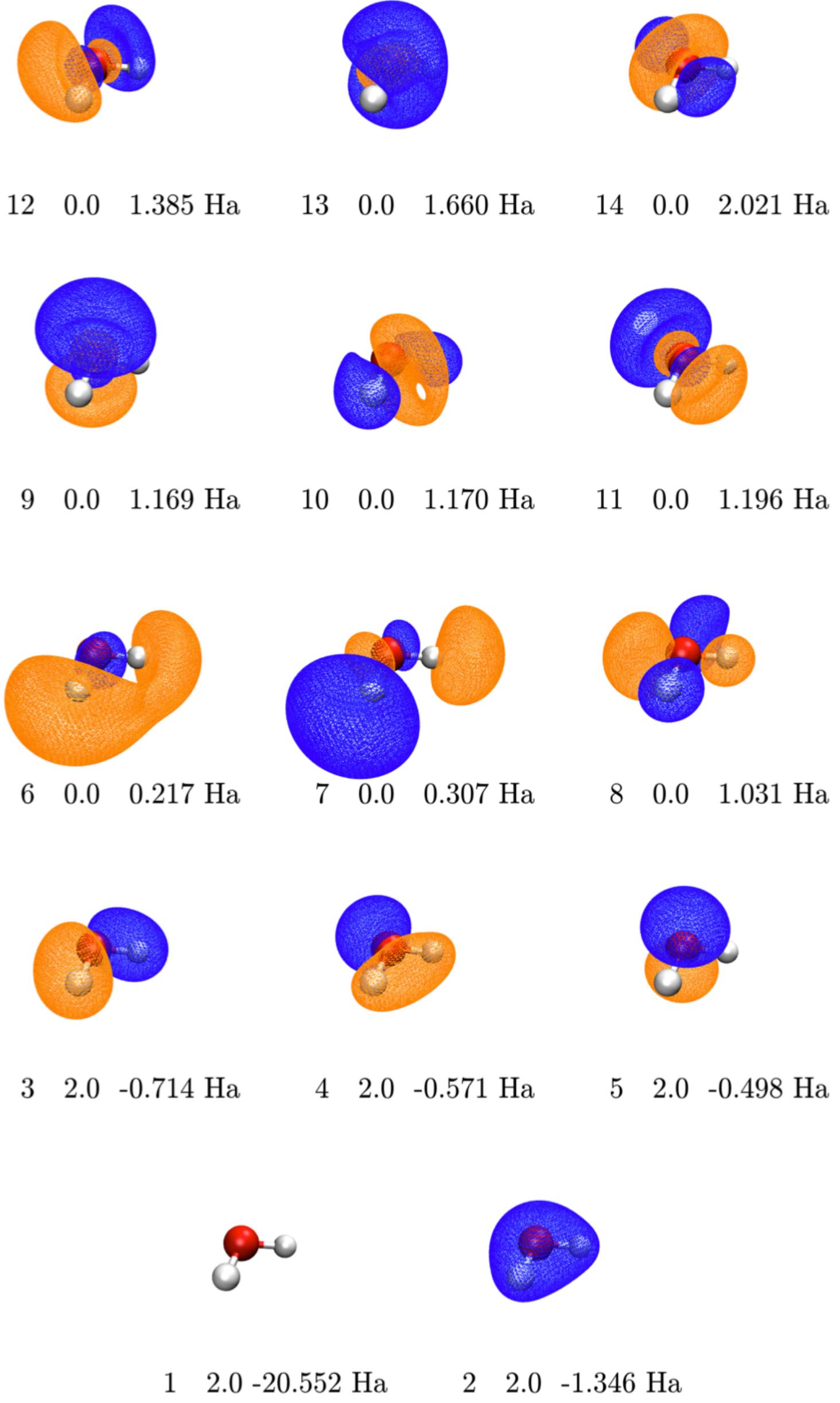
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$$|\Psi\rangle = |f_1 f_2 \dots f_M\rangle$$



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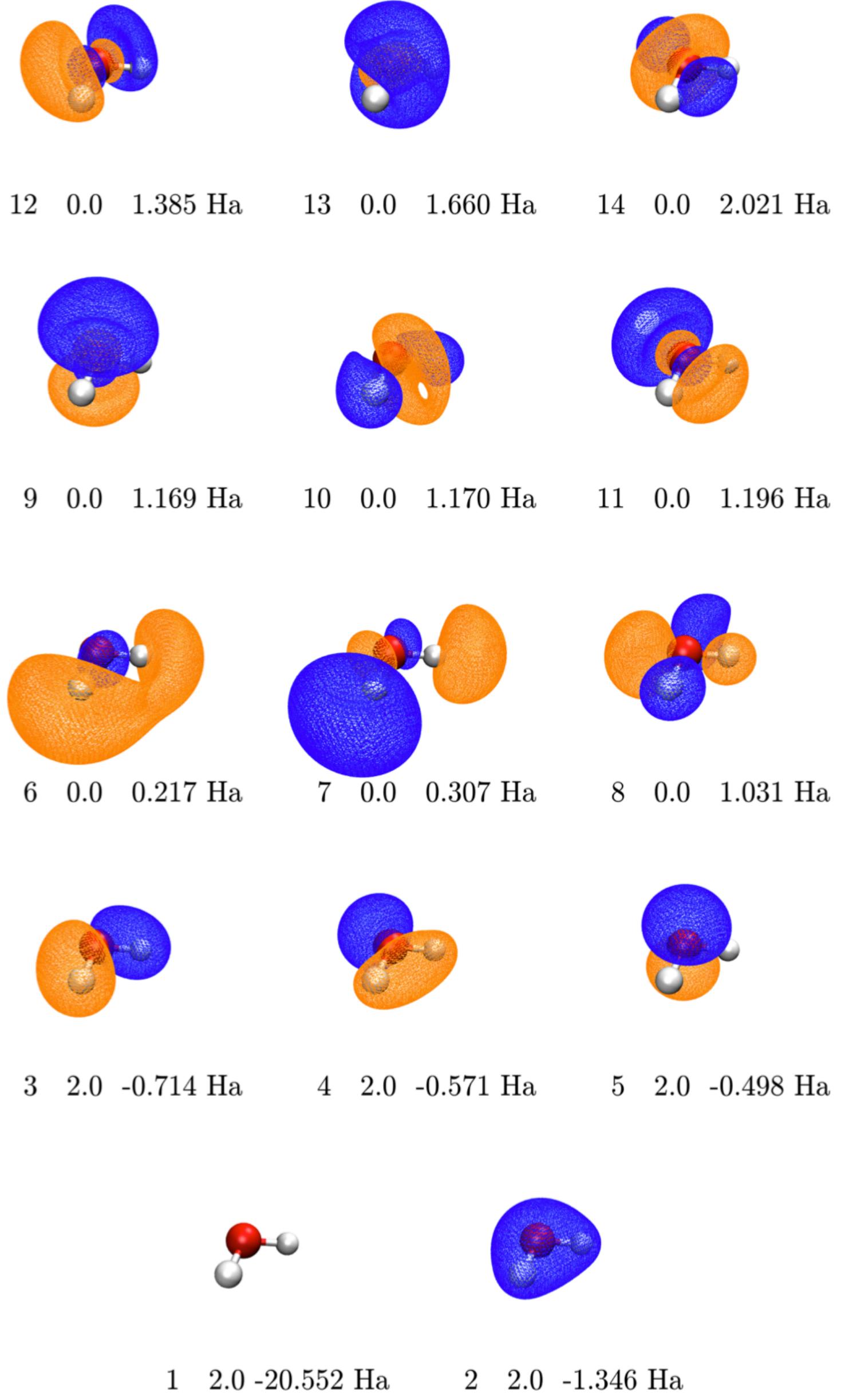
As many positions
as spin-orbitals



$$|\Psi\rangle = |f_1 f_2 \dots f_M\rangle$$



Equal to 1 if spin-orbital occupied
Otherwise 0



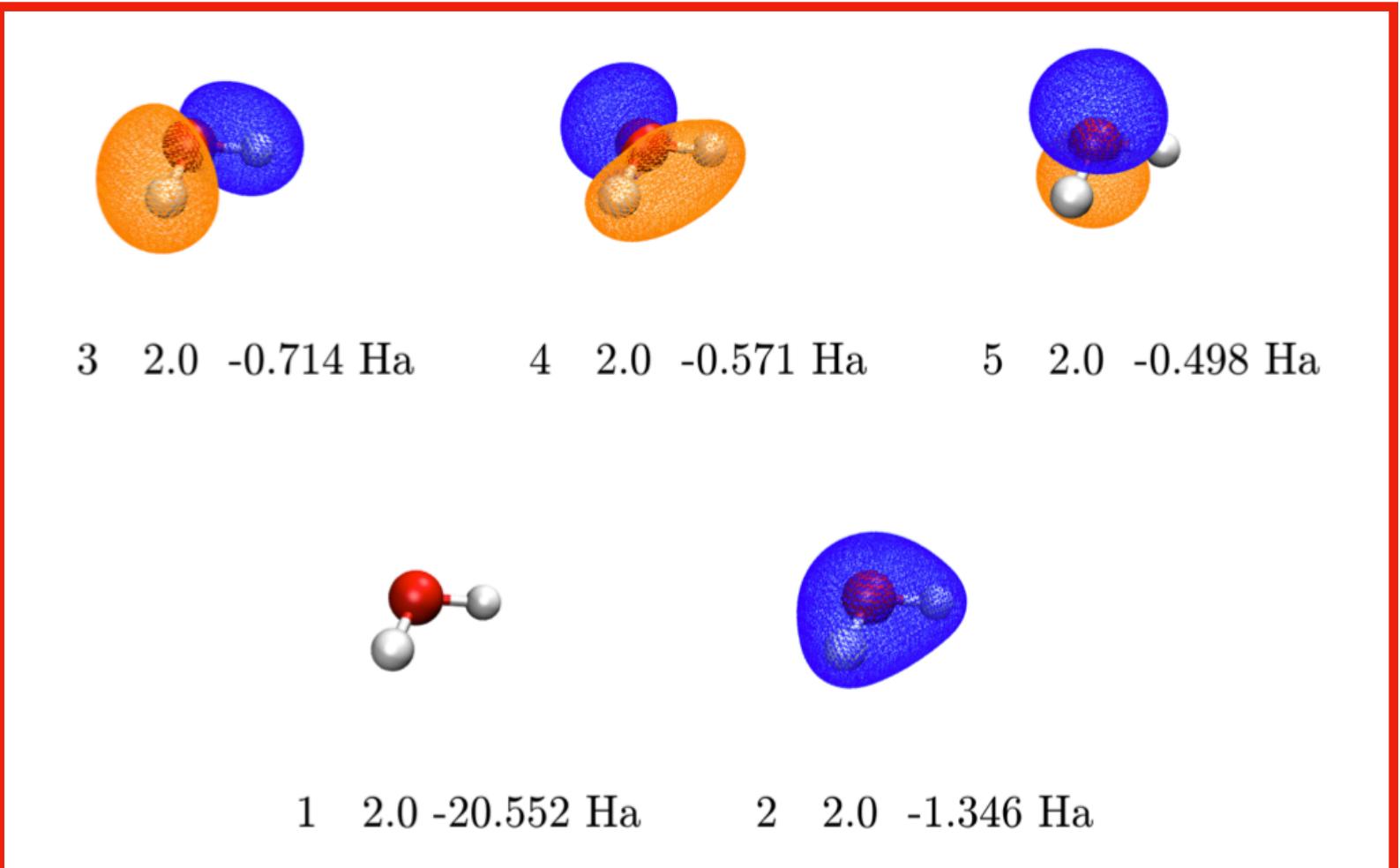
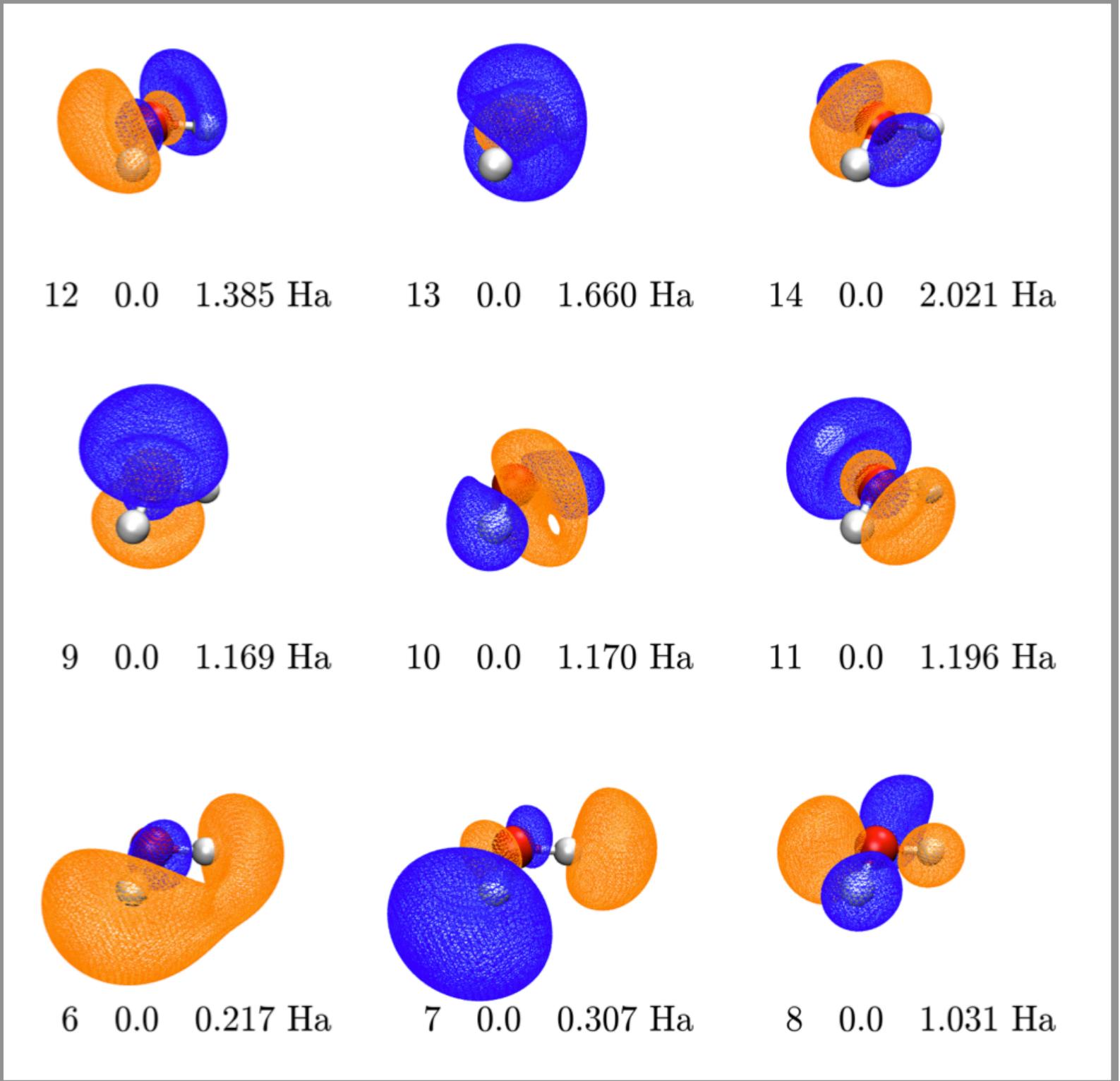
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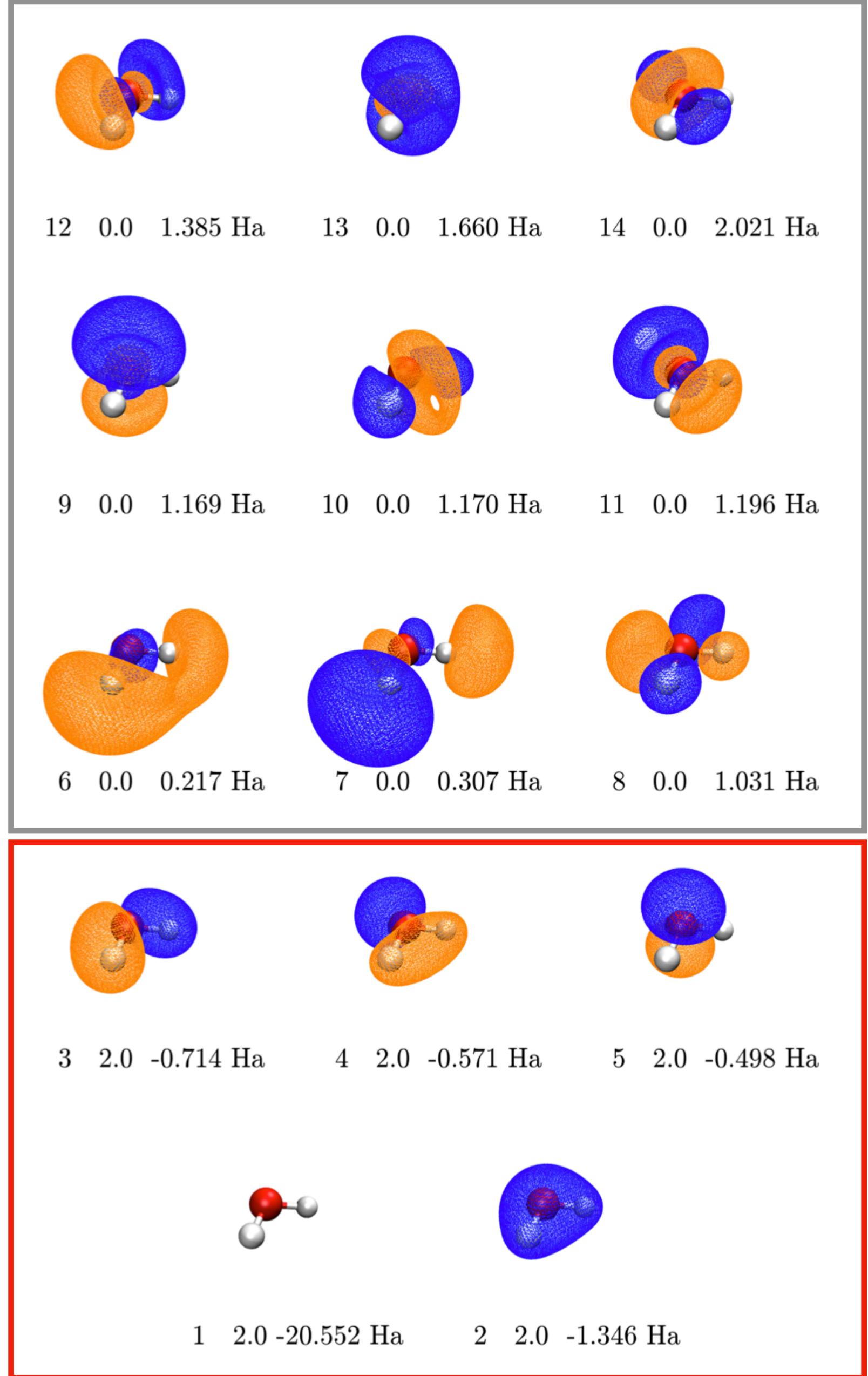
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$$|\Psi\rangle = |1 \dots 1 \boxed{0} \dots 0\rangle$$



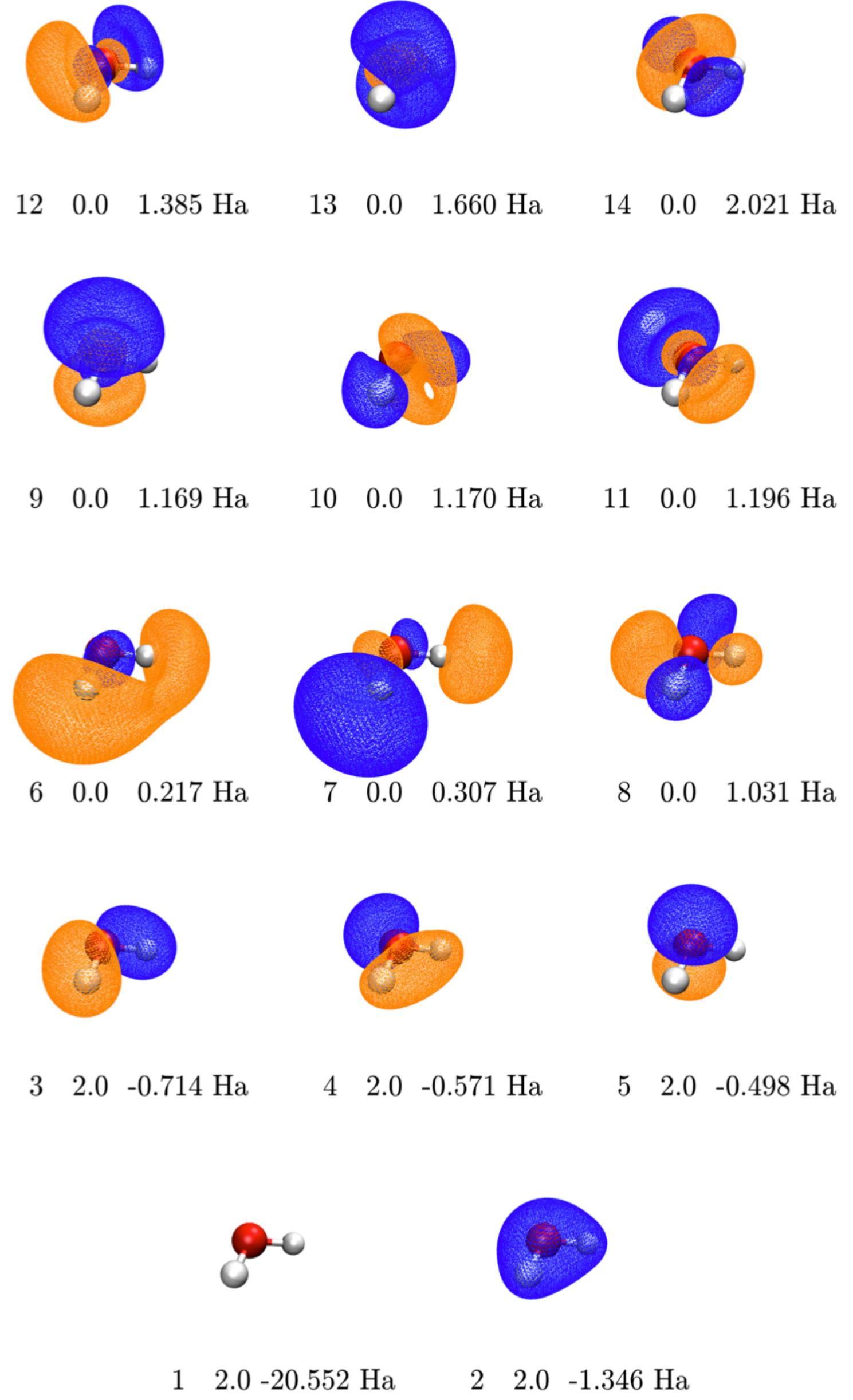
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Dimensionality of many-body QM

Superposition principle: states are linear combinations of basis states



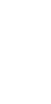
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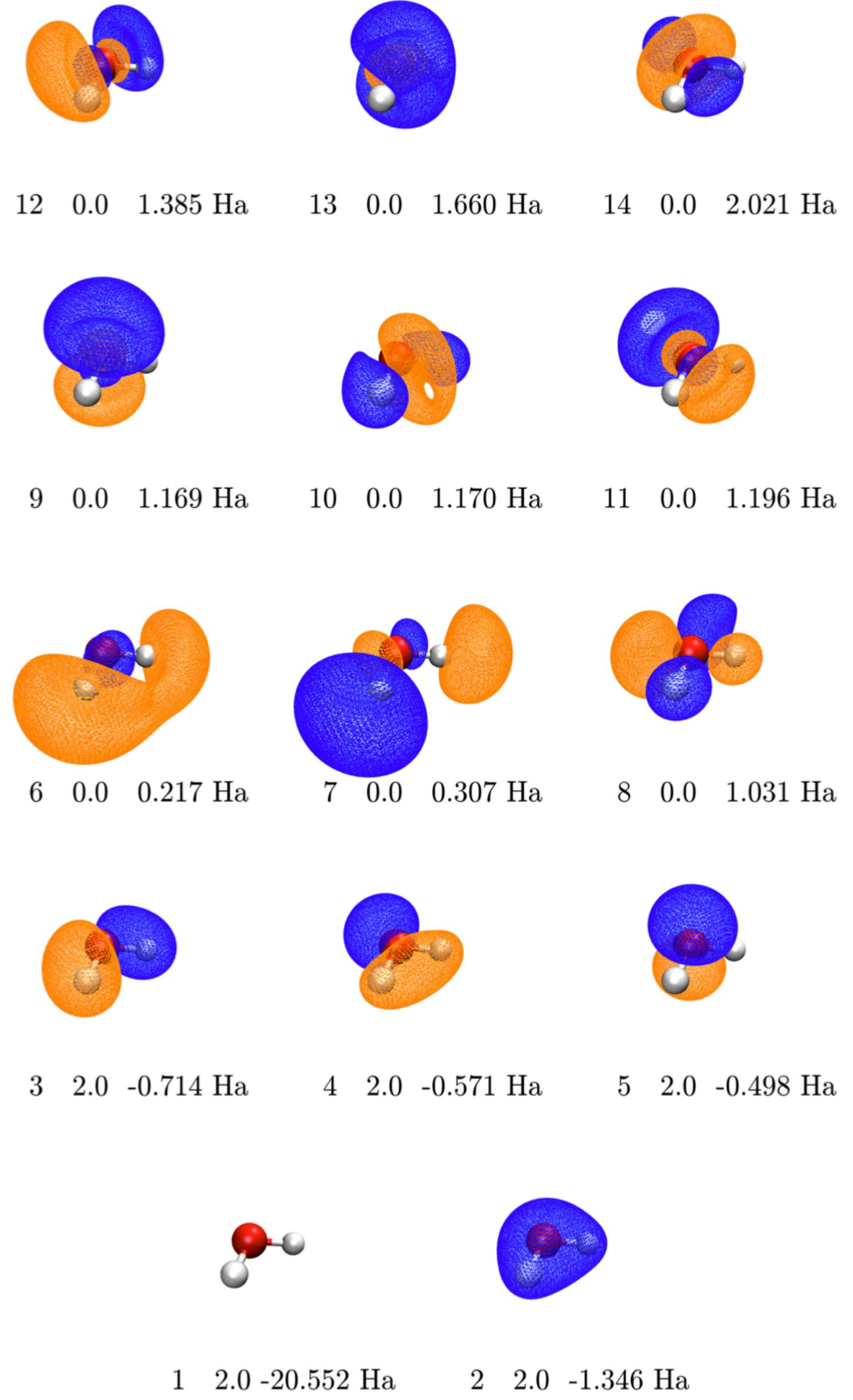
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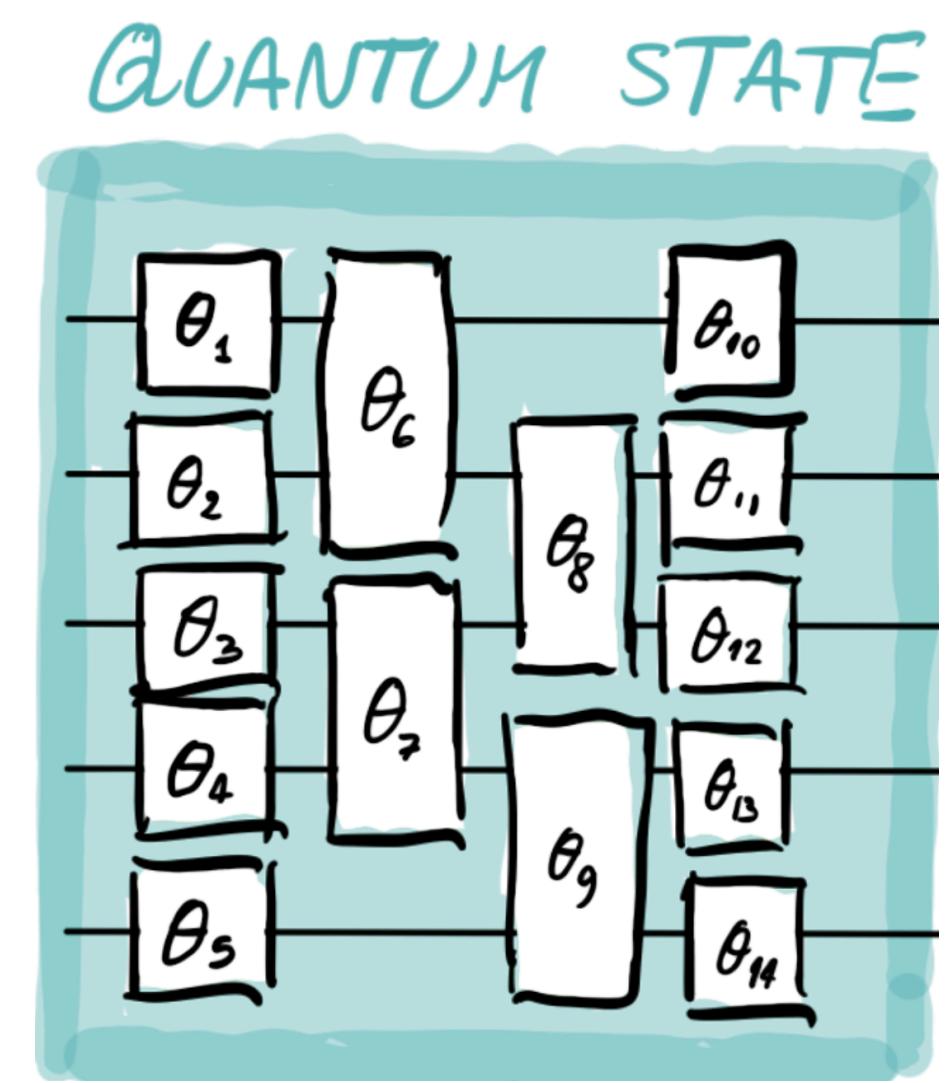
The dimensionality of state space is **classically** intractable



Solving the problem

The Variational Quantum Eigensolver

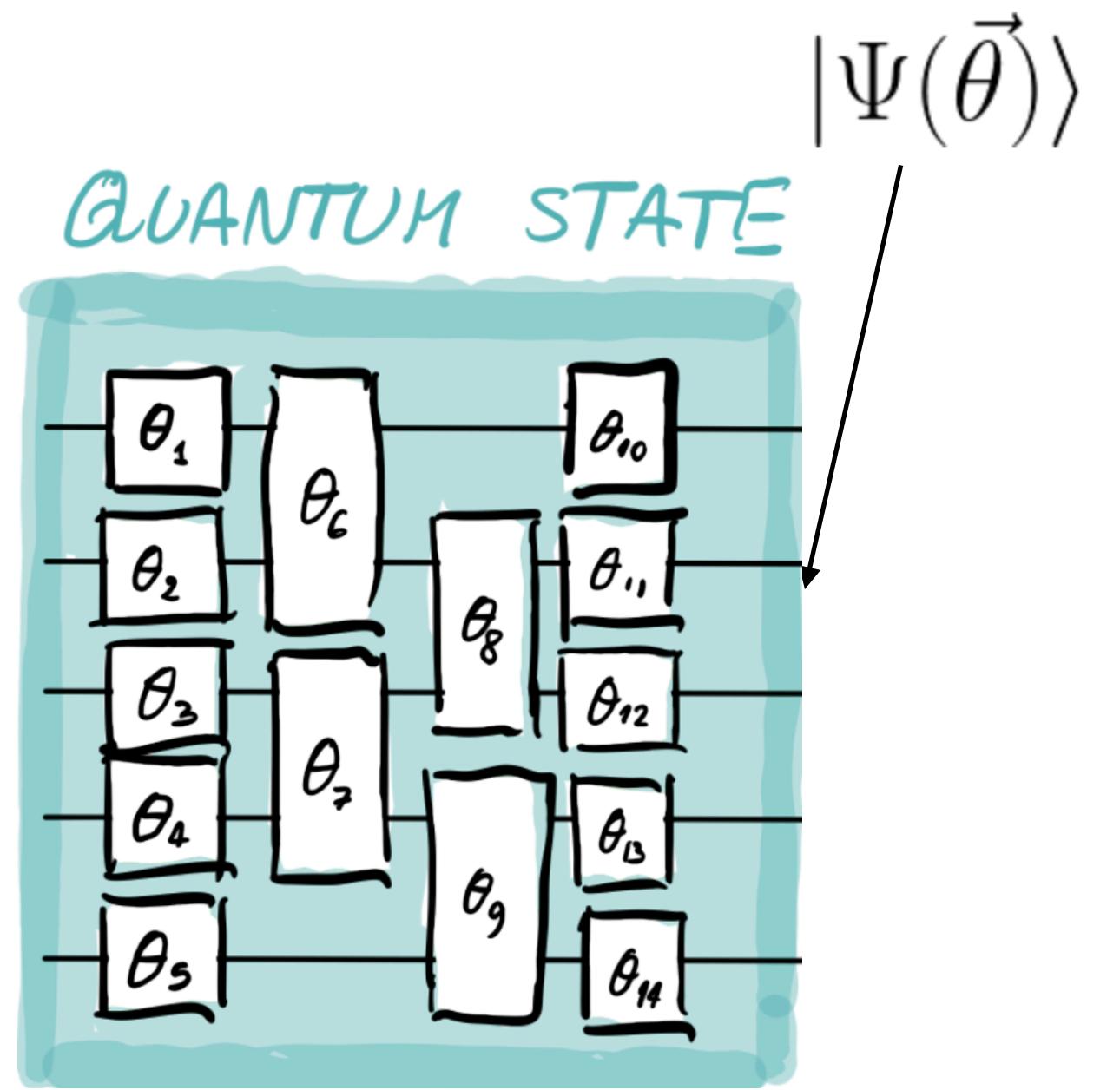
- Prepare *some* quantum state using a so-called variational form (ansatz)



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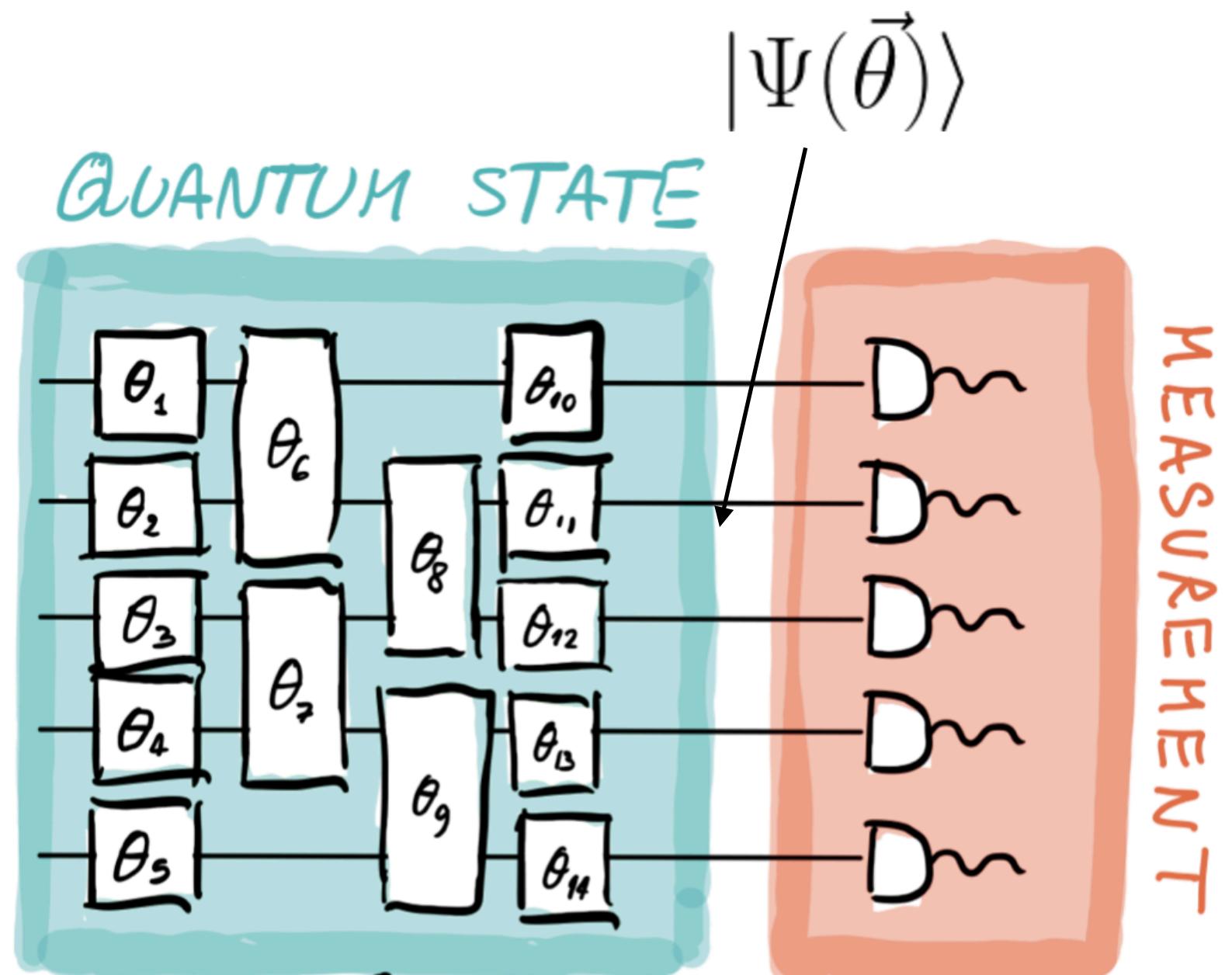
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Solving the problem

The Variational Quantum Eigensolver

- Prepare *some* quantum state using a so-called variational form (ansatz)
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- For each value of the parameters the resulting state has some mean energy

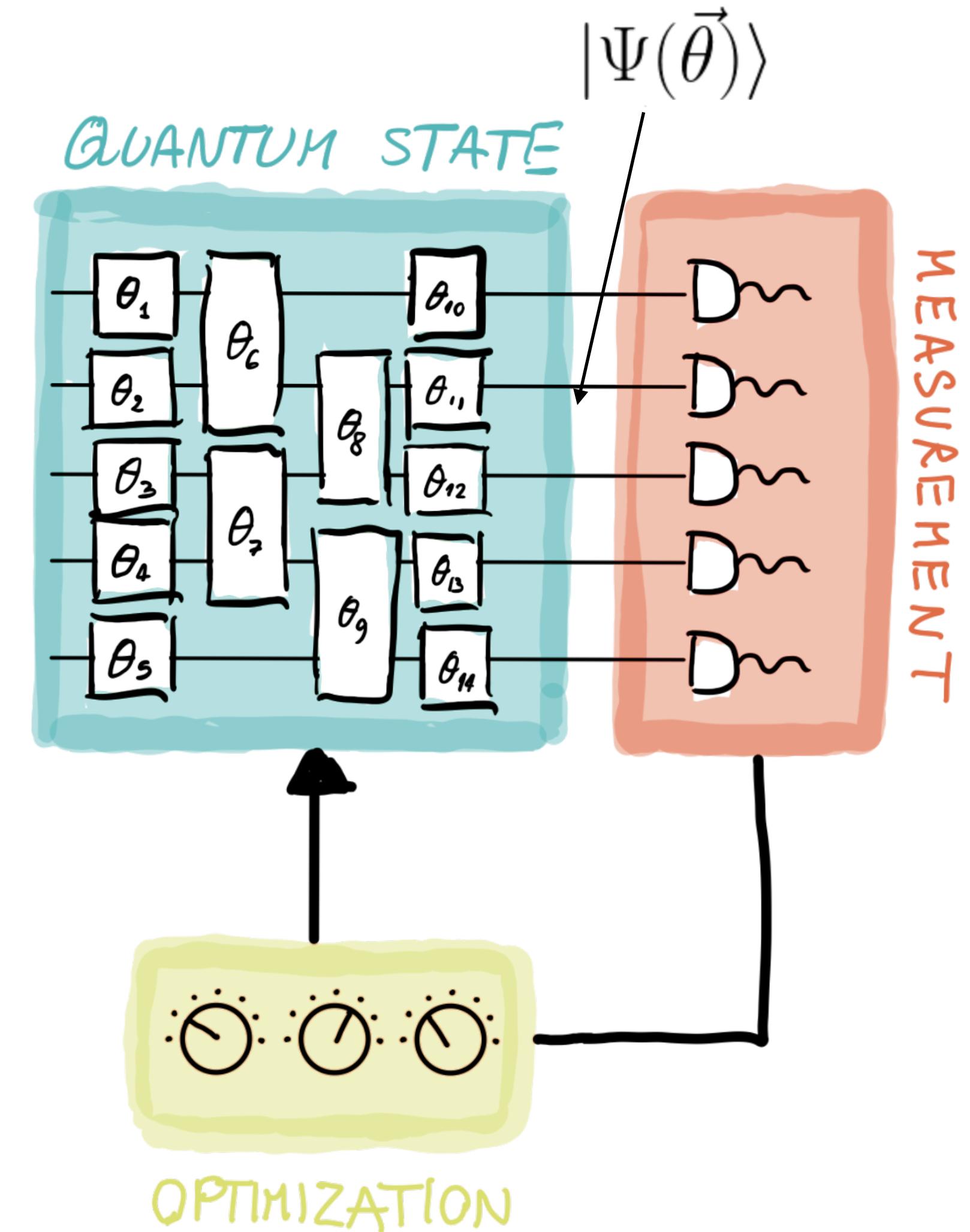


$$\langle E \rangle = \langle \Psi(\vec{\theta}) | \hat{H}_e | \Psi(\vec{\theta}) \rangle \geq E_{\text{ground}}$$

Solving the problem

The Variational Quantum Eigensolver

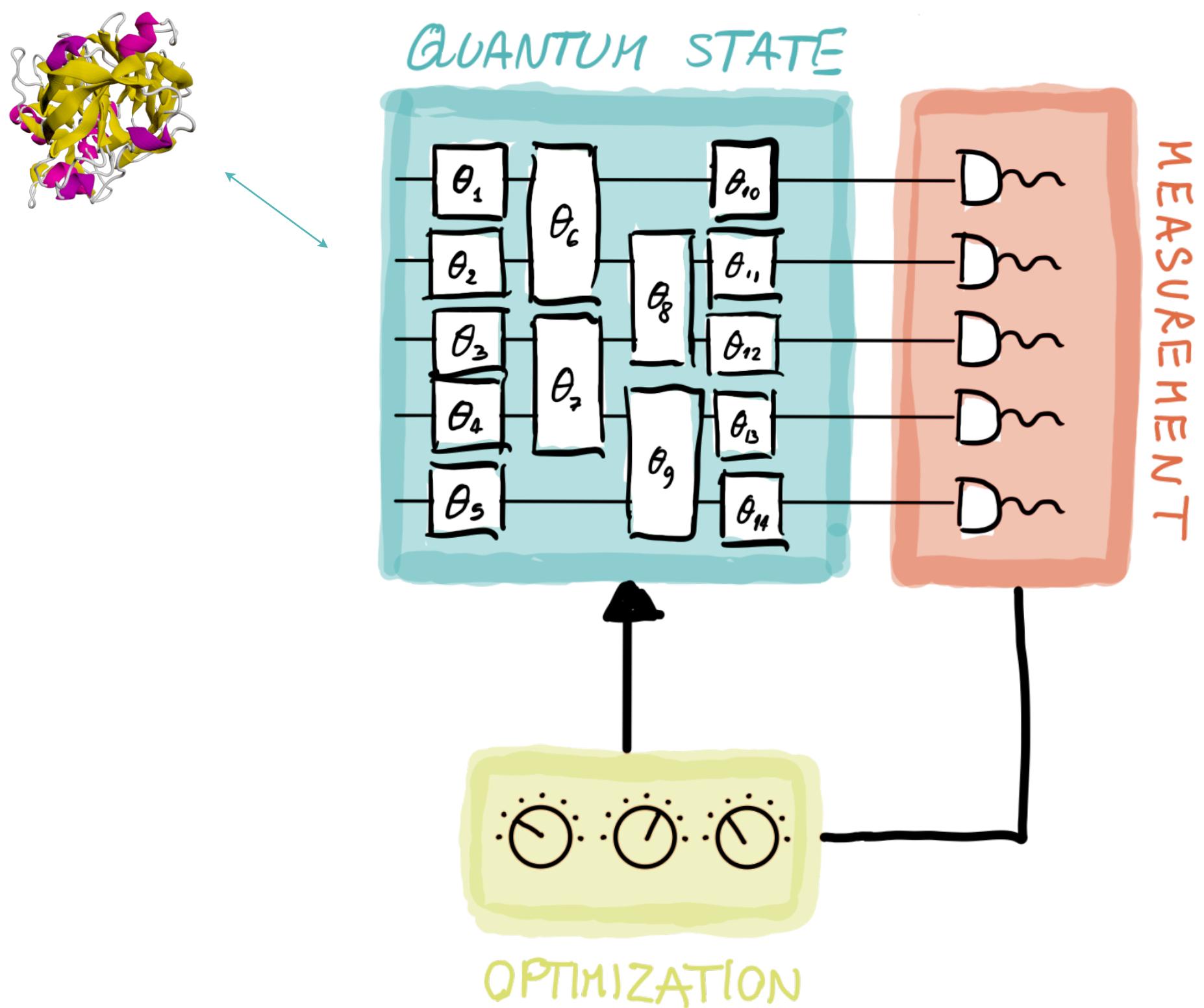
- Prepare *some* quantum state using a so-called variational form (ansatz)
- Gates in the ansatz have free parameters
- For each value of the parameters the resulting state has some mean energy
- Find the ground state variationally, that is, minimising over the parameters



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Quantum chemistry in the near term

The variational quantum eigensolver

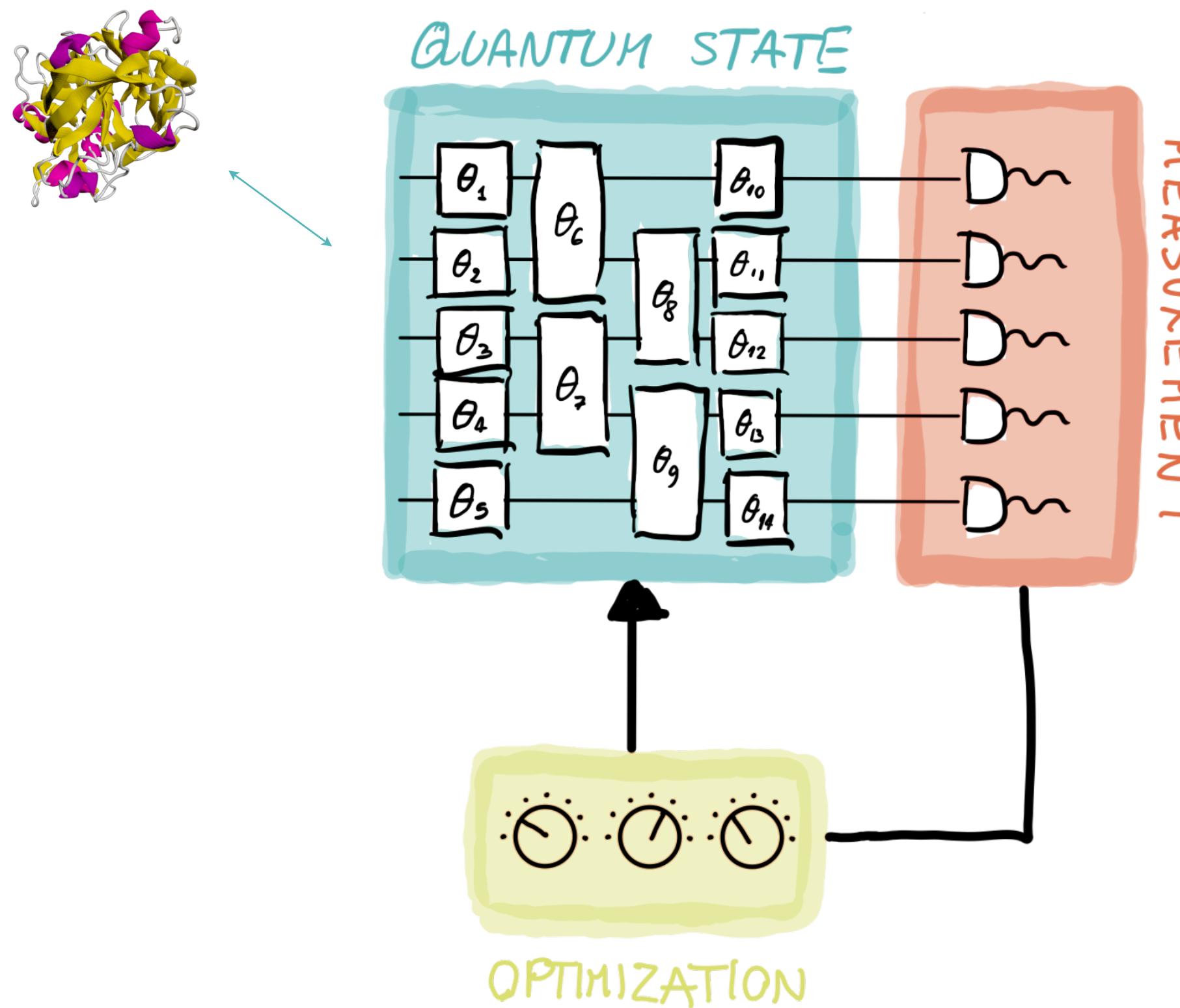


Challenges

- Hilbert space is a big space
- Quantum computers are error-prone
- Not many qubits available
- Simulations can be time-consuming

Quantum chemistry in the near term

The variational quantum eigensolver



Challenges

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Identifying challenges towards practical quantum advantage through resource estimation:
the **measurement roadblock** in the variational quantum eigensolver

Jérôme F. Gonthier,¹ Maxwell D. Radin,¹ Corneliu Buda,²
Eric J. Doskocil,² Clena M. Abuan,³ and Jhonathan Romero¹

¹Zapata Computing, Inc., 100 Federal St., Boston, MA 02110, USA

Molecule	H ₂ O	CO ₂	CH ₄	CH ₄ O	C ₂ H ₆	C ₂ H ₄	C ₂ H ₂	C ₂ H ₆ O	C ₃ H ₈	C ₃ H ₆	C ₃ H ₄
N _{el}	8	16	8	14	14	12	10	20	20	18	16
N _q	104	208	104	182	182	156	130	260	260	234	208
K · 10 ⁻³	1.9	16	1.6	8.4	8.5	6.6	3.1	24	16	23	18
M · 10 ⁻⁹	3.9	32	3.2	17	17	13	6.2	48	31	46	36
t (days)	2.3	39	1.9	18	18	12	4.6	71	47	62	44

33 TABLE IV. Estimated runtimes t in days for a single energy evaluation using the number of measurements M from extrapolated

State preparation

in a VQE simulation

- Borrow from the coupled cluster (CC) method in computational chemistry

$$|\text{CC}\rangle = e^{\hat{T}}|0\rangle \quad \hat{T} = \sum_k \hat{T}_k = \sum_k \frac{1}{(k!)^2} \left(\sum_{i_1 \dots i_k} \sum_{a_1 \dots a_k} t_{a_1 \dots a_k}^{i_1 \dots i_k} a_{a_1}^\dagger a_{a_k}^\dagger a_{i_k} \cdots a_{i_1} \right)$$

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- Use its ***unitary variant***

$$|\text{UCC}\rangle = e^{\hat{T} - \hat{T}^\dagger}|0\rangle$$

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- Use its ***unitary variant***

$$|\text{UCC}\rangle = e^{\hat{T} - \hat{T}^\dagger}|0\rangle$$

- ***Truncated*** to single and double excitations

$$\hat{T} = \hat{T}_1 + \hat{T}_2$$

- Apply in ***Trotterized form***

Measuring the energy

in a VQE simulation

- The Hamiltonian is given as a linear combination of Pauli strings

$$\hat{H}_e = \sum c_{\mathbf{k}} \hat{P}_{\mathbf{k}} \quad \leftarrow \text{ Each term is a product of local operators} \quad P_{\mathbf{k}} = \bigotimes_{i=1}^N \sigma_{k_i}^{(i)}$$

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$$|\Psi\rangle = \sum_{\vec{f}} \alpha_{\vec{f}} |f_1 f_2 \dots f_M\rangle \quad \rightarrow \quad \langle \Psi | \hat{H}_e | \Psi \rangle = \sum c_{\mathbf{k}} \langle \Psi | \hat{P}_{\mathbf{k}} | \Psi \rangle$$

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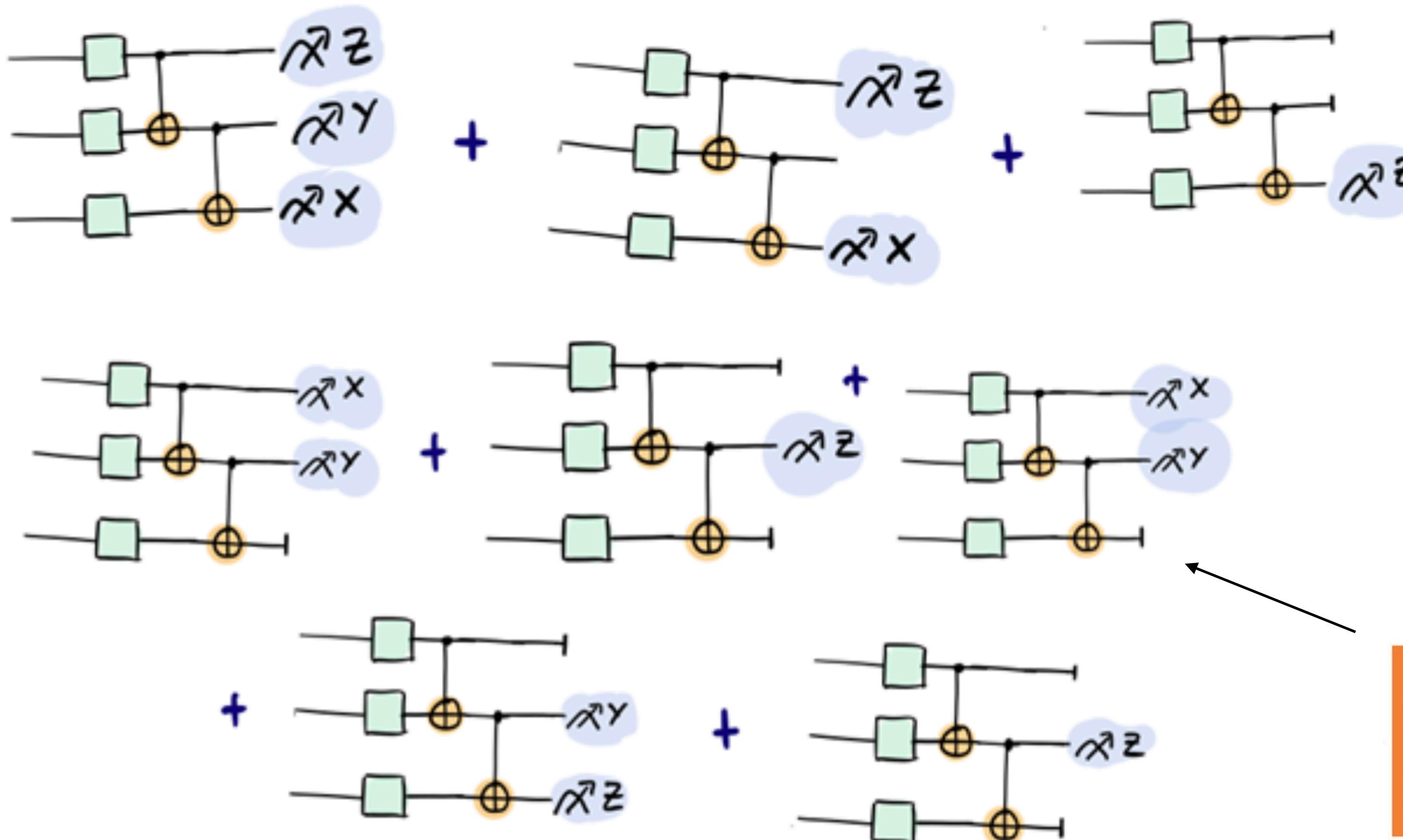


Cannot even write down
on a classical computer

Easy on a quantum computer: only
requires measuring Pauli strings

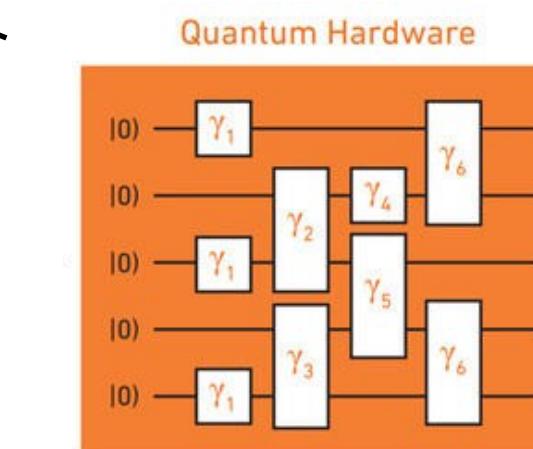
(Specific) problem statement

Measurement cost in VQE



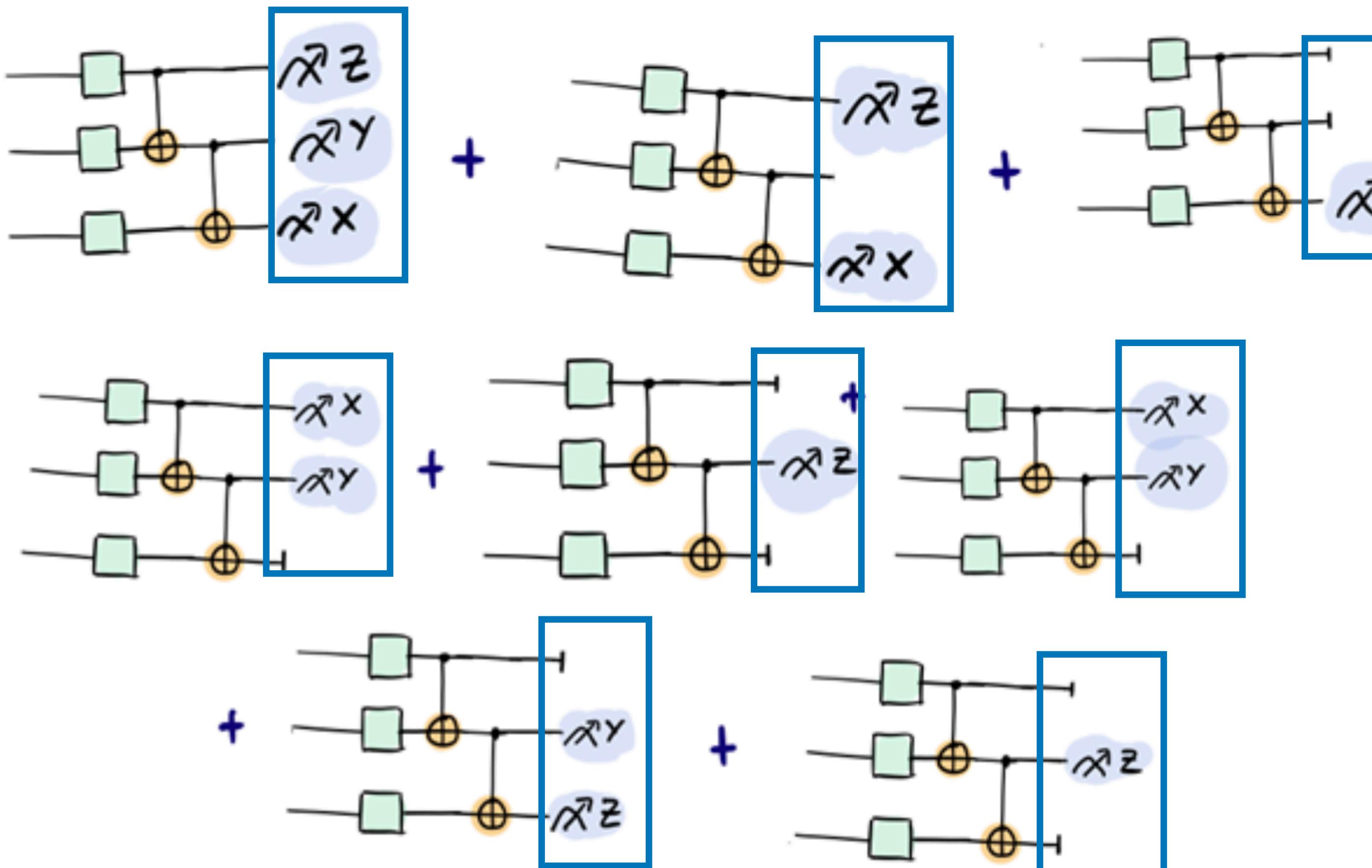
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Every Pauli string evaluated
independently through repeated
measurements



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Measurement cost in VQE



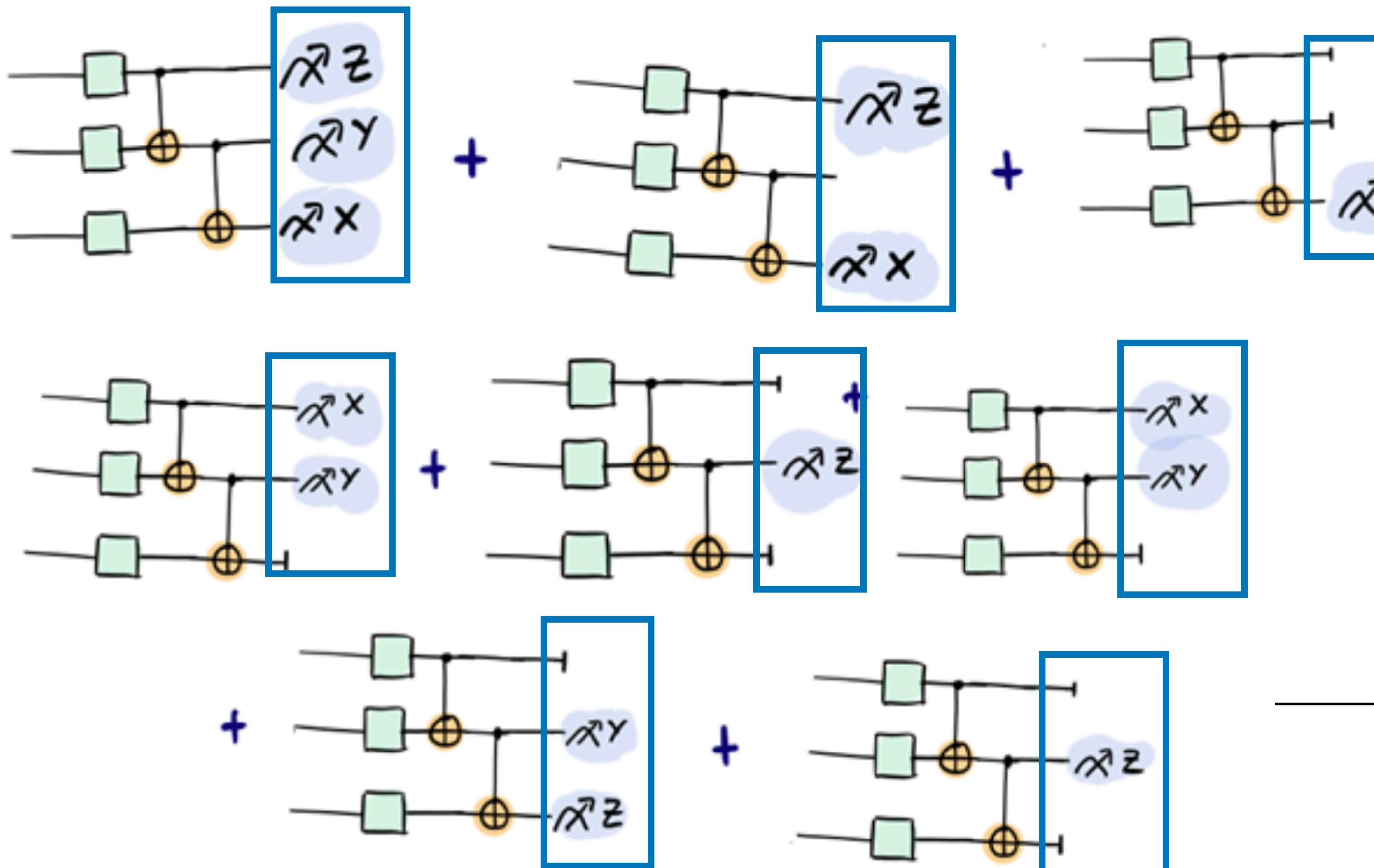
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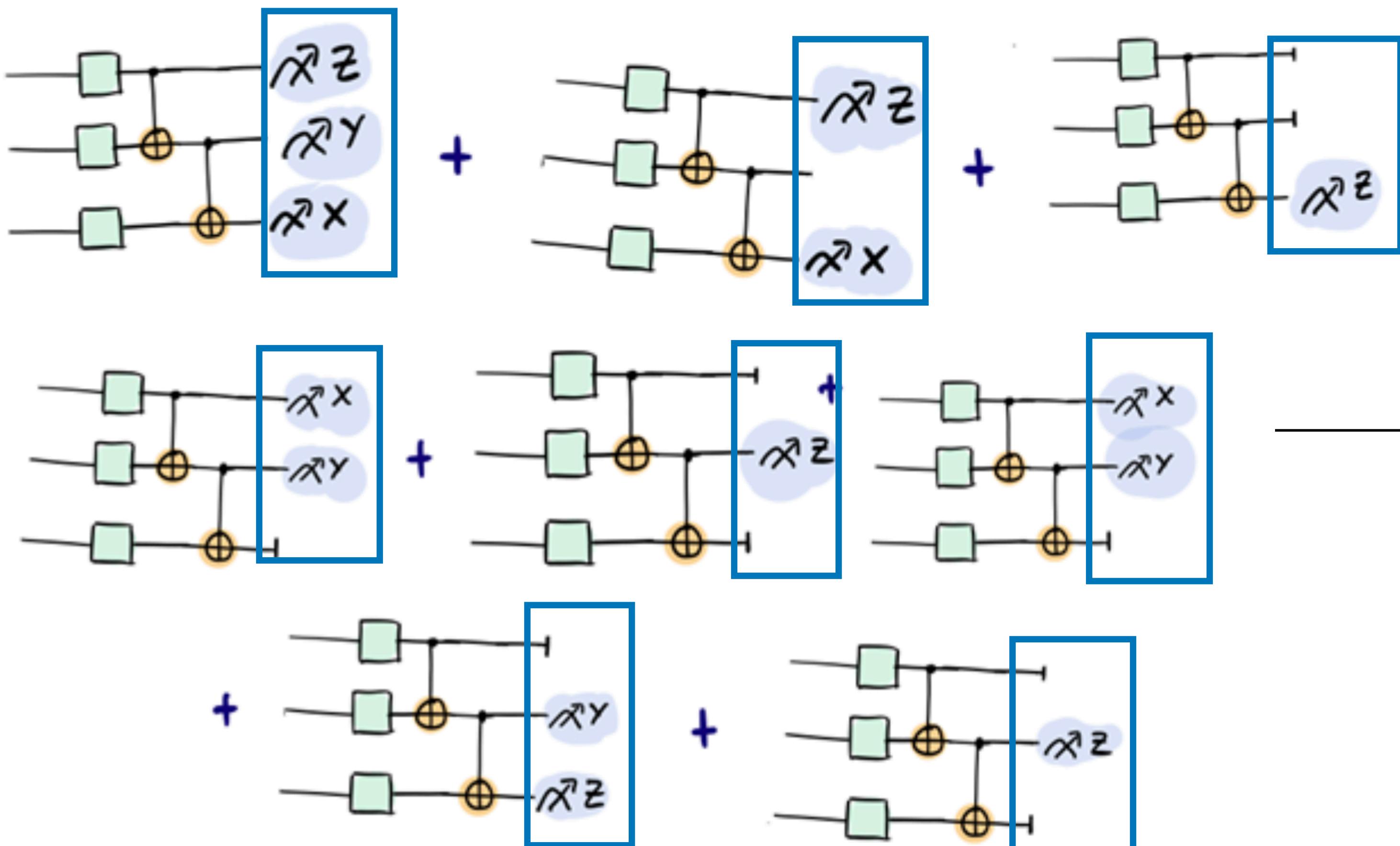


Every Pauli string evaluated independently through repeated measurements

Repeat each many times to estimate the mean $\langle \Psi | \hat{P}_k | \Psi \rangle$

(Specific) problem statement

Measurement cost in VQE



$$\langle \Psi | \hat{H}_e | \Psi \rangle = \sum c_k \langle \Psi | \hat{P}_k | \Psi \rangle \sim O(N^4)$$

Every Pauli string evaluated independently through repeated measurements

Repeat each many times to estimate $\langle \Psi | \hat{P}_k | \Psi \rangle$

Estimation error:

$$\epsilon = \sqrt{\sum_k |c_k|^2 \text{Var}(P_k)/S_k}$$

Number of shots needed to reach given precision: $S = O(N^{5/6})$

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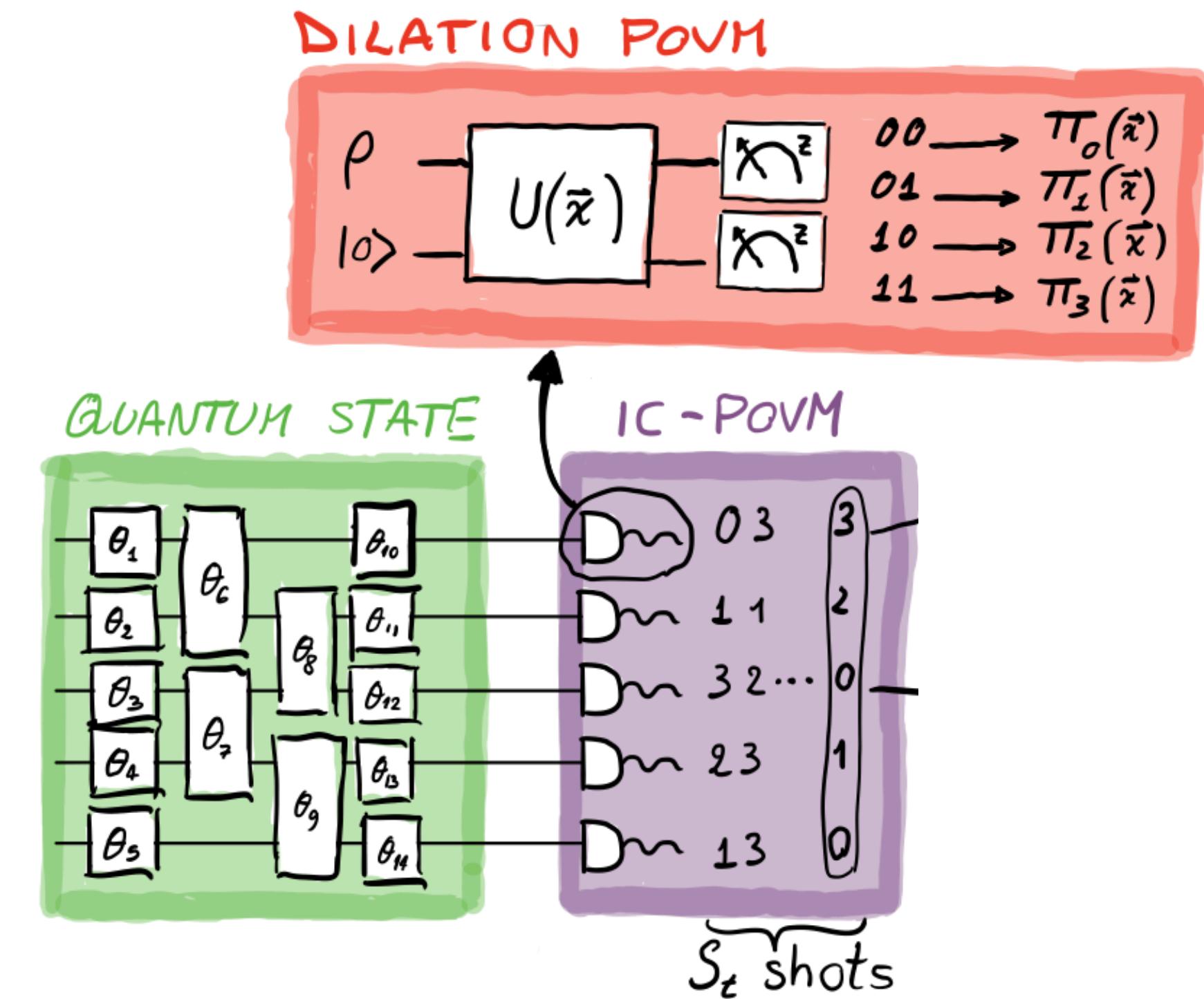
Informationally Complete Measurements

Tackling the measurement problem

with generalised measurements

Using generalised quantum measurements

- Add ancillary qubit in a known state
- Apply a two-qubit transformation
- Measure both in the computational basis



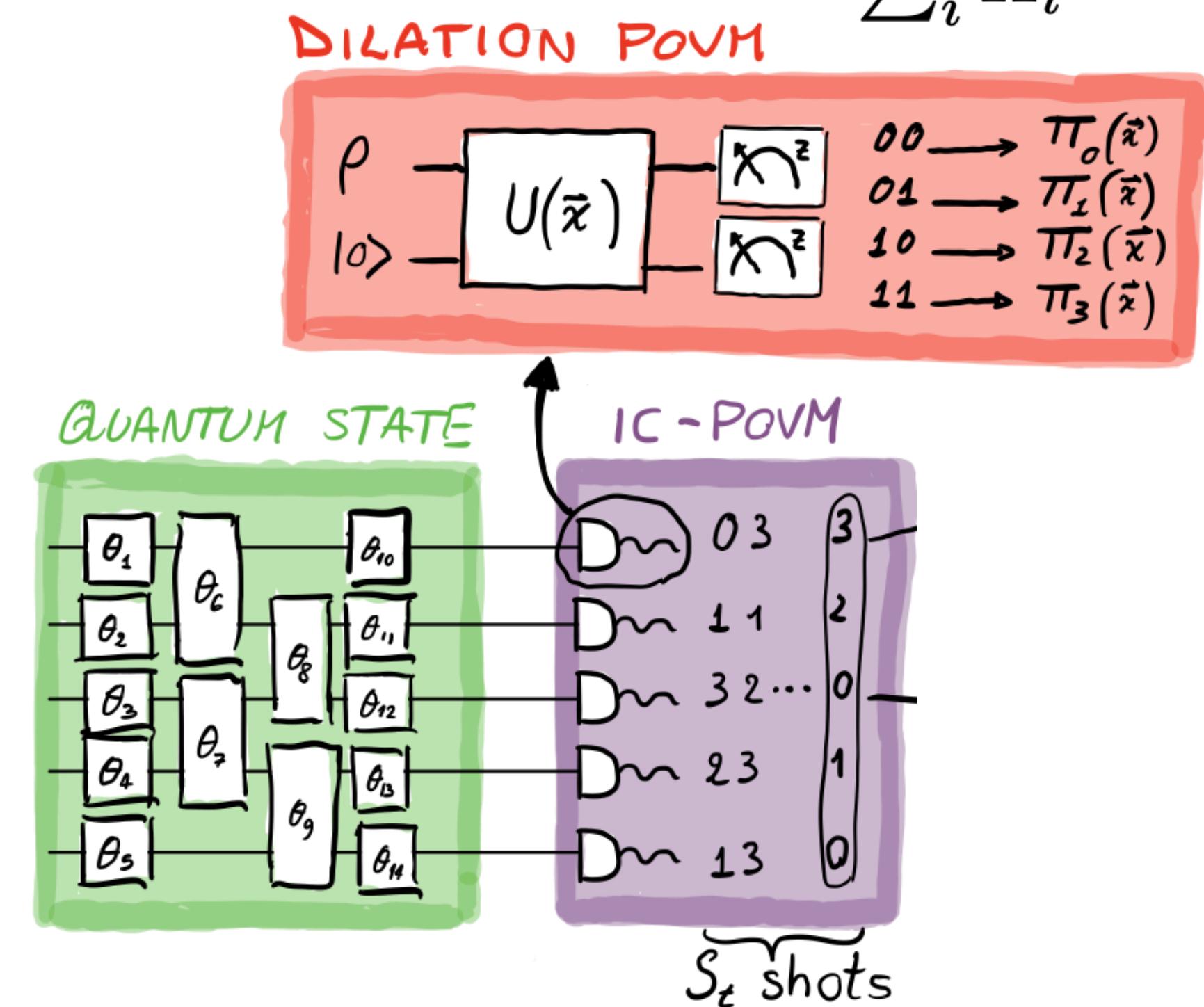
Tackling the measurement problem

with generalised measurements

Using generalised quantum measurements

- Add ancillary qubit in a known state
- Apply a two-qubit transformation
- Measure both in the computational basis

$$\begin{aligned}\Pi_i &> 0 \\ \sum_i \Pi_i &= \mathbb{I}\end{aligned}$$



Probability of outcome \mathbf{m} : $\text{Tr}[\rho \Pi_{\mathbf{m}}]$ where $\Pi_{\mathbf{m}} = \bigotimes_{i=1}^N \Pi_{m_i}^{(i)}$

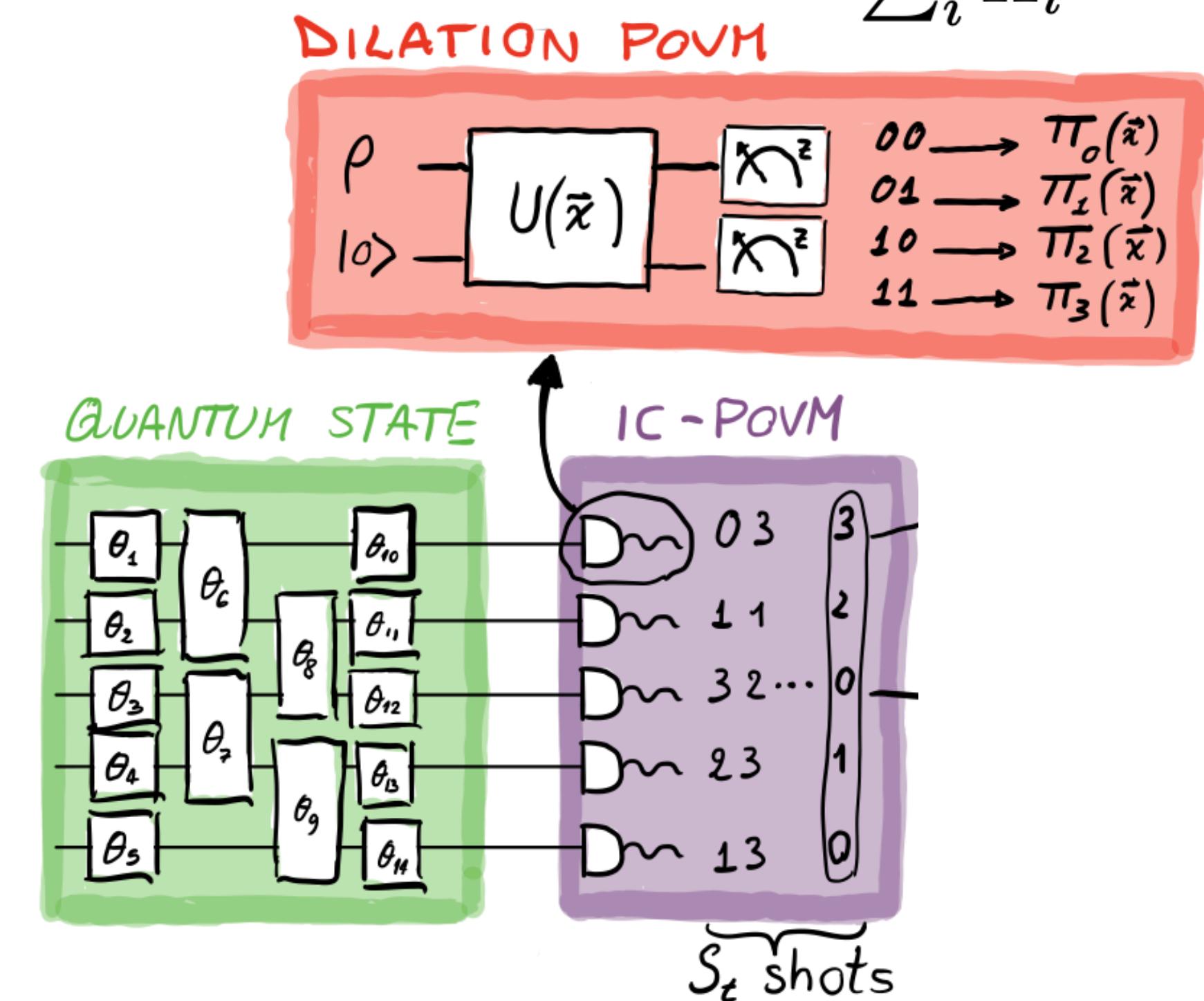
Tackling the measurement problem

with generalised measurements

Using generalised quantum measurements

- Add ancillary qubit in a known state
- Apply a two-qubit transformation
- Measure both in the computational basis
- Outcomes are **informationally complete**, so not measuring only the energy

$$\begin{aligned}\Pi_i &> 0 \\ \sum_i \Pi_i &= \mathbb{I}\end{aligned}$$



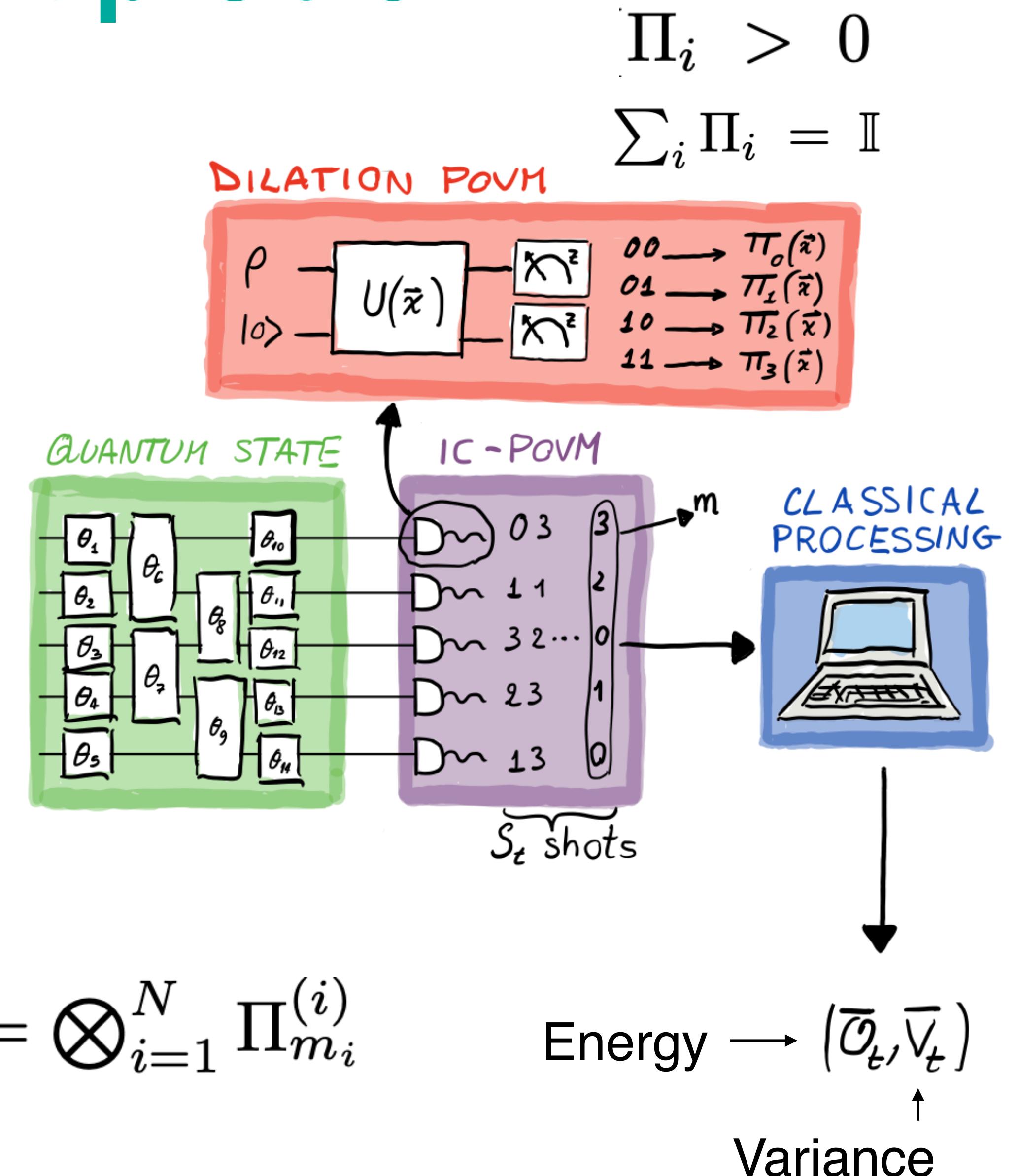
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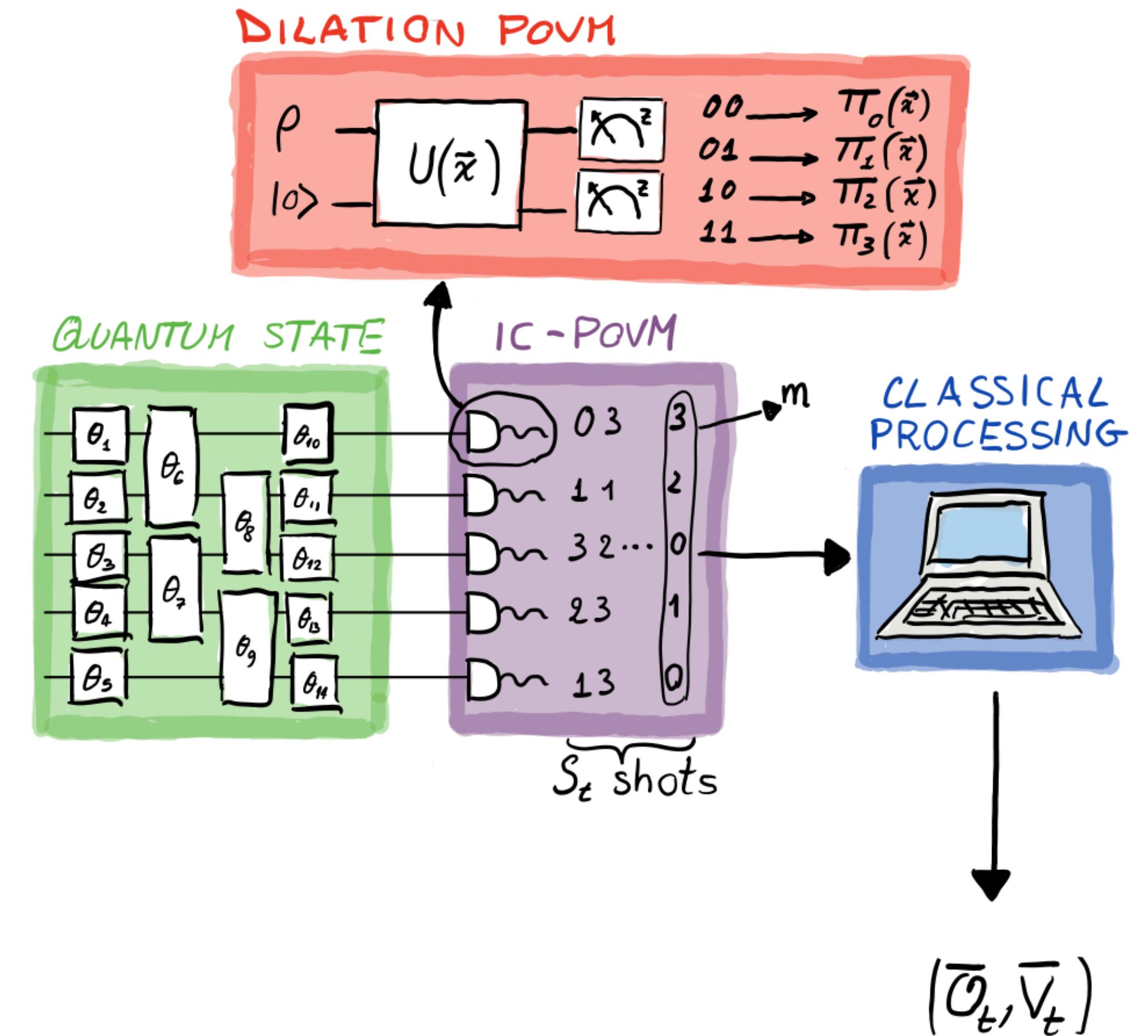
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Tackling the measurement problem

with adaptive generalised measurements

Optimising measurements on the fly

- Qubit-ancilla interaction is parametrised

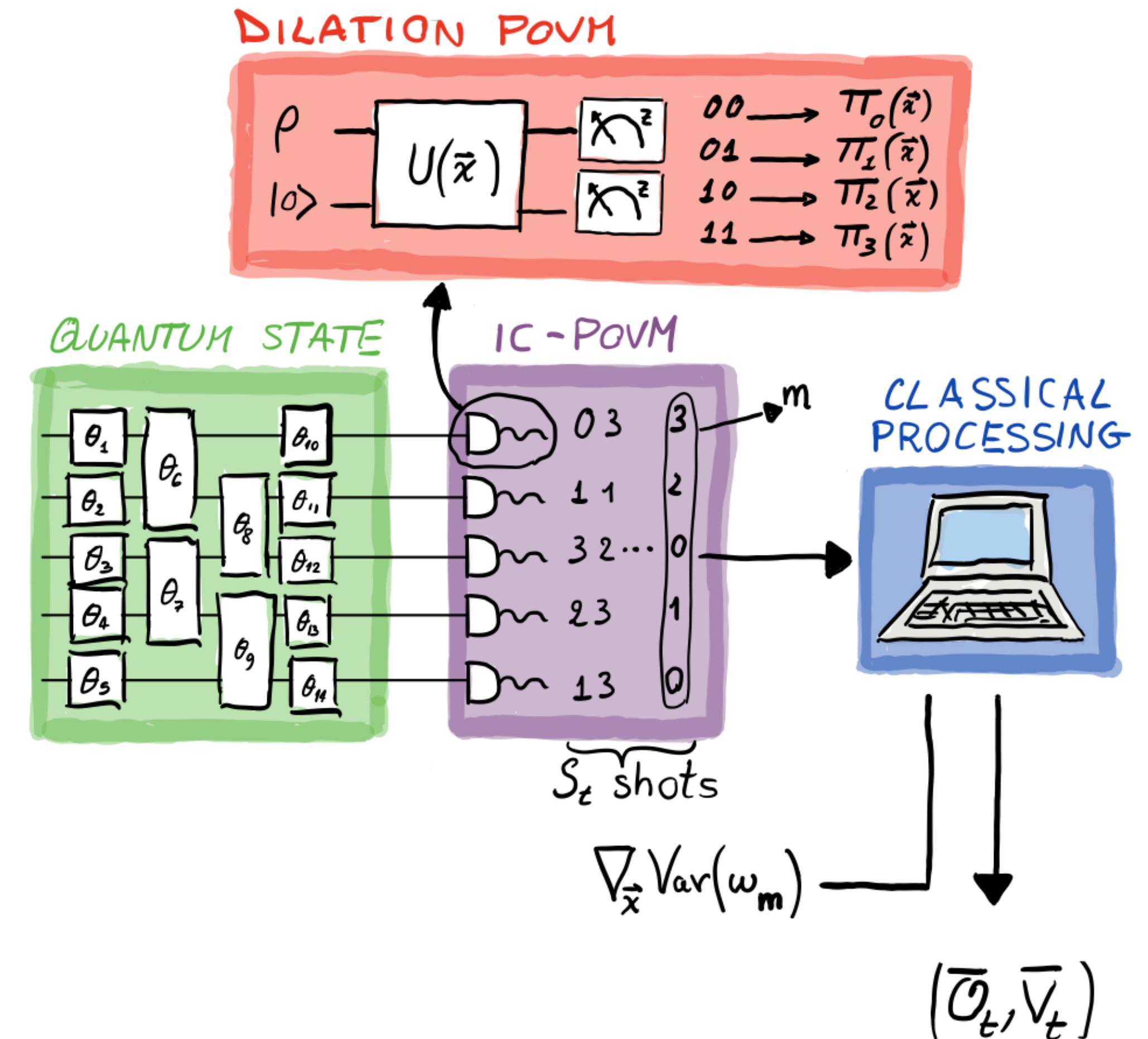


Tackling the measurement problem

with adaptive generalised measurements

Optimising measurements on the fly

- Qubit-ancilla interaction is parametrised
- Can use informationally complete data to calculate gradient of measurement error

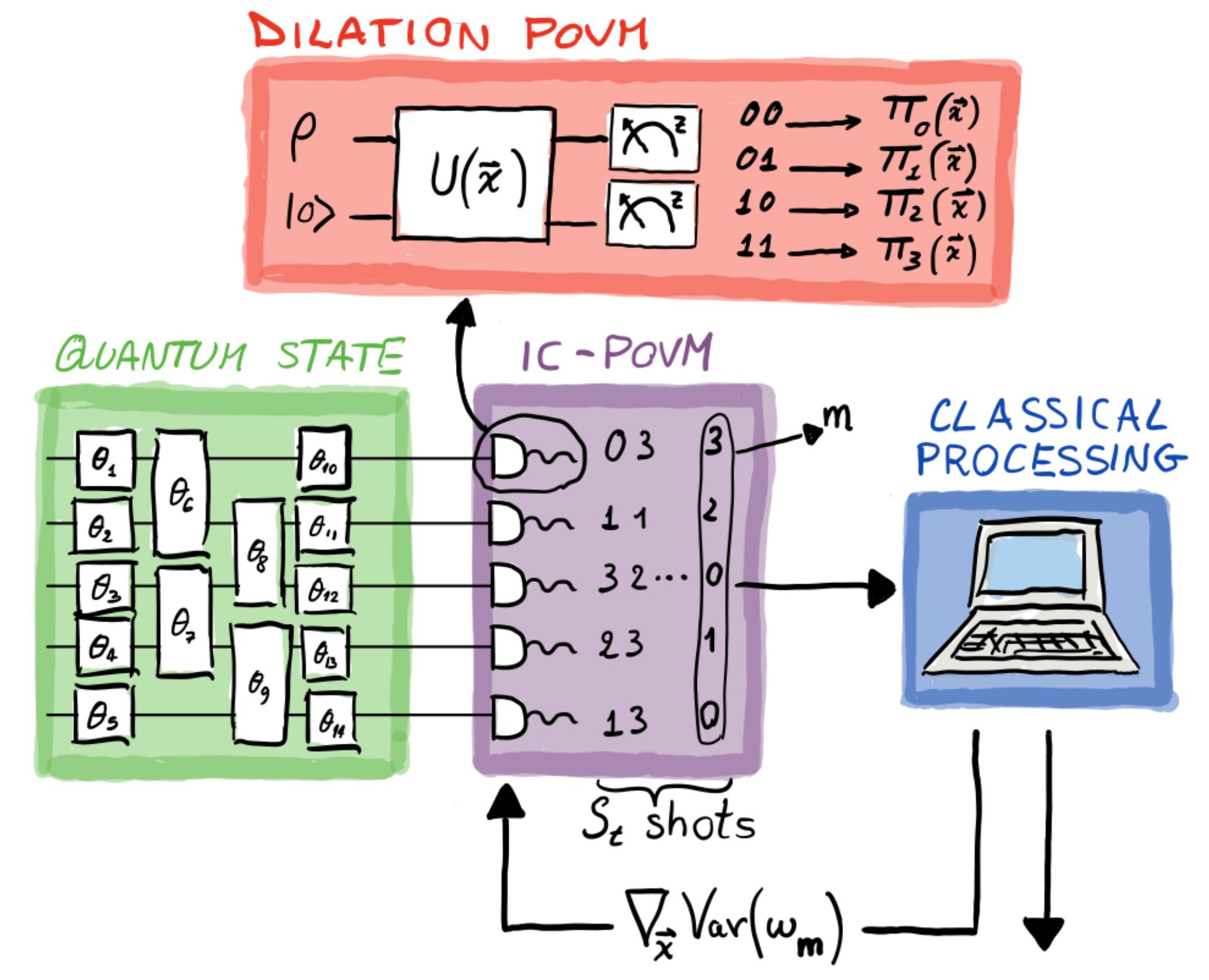


Tackling the measurement problem

with adaptive generalised measurements

Optimising measurements on the fly

- Qubit-ancilla interaction is parametrised
- Can use informationally complete data to calculate gradient of measurement error
- At every iteration, we use a better POVM than in the previous one



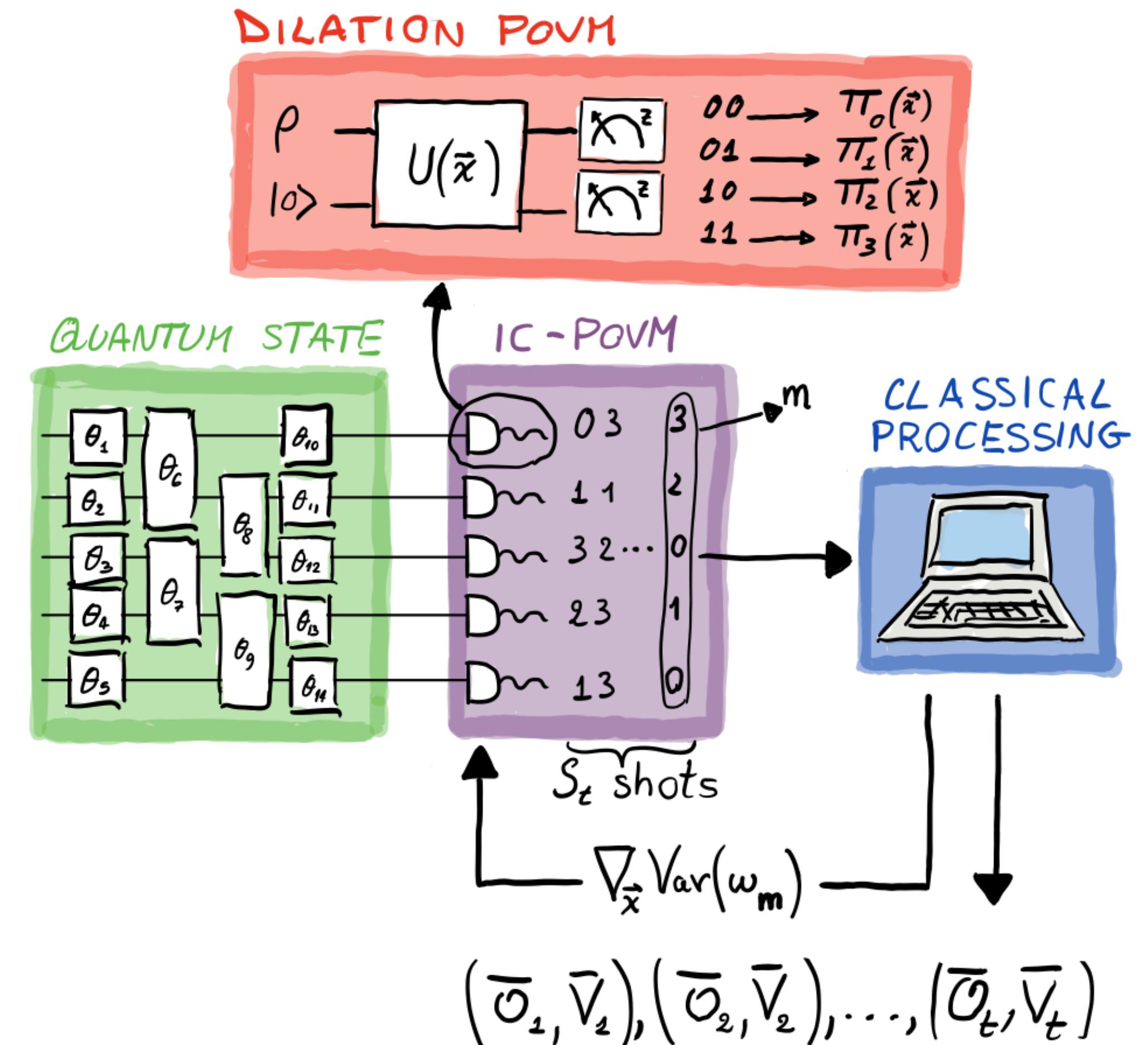
$$(\bar{O}_t, \bar{V}_t)$$

Tackling the measurement problem

with adaptive generalised measurements

Optimising measurements on the fly

- Qubit-ancilla interaction is parametrised
- Can use informationally complete data to calculate gradient of measurement error
- At every iteration, we use a better POVM than in the previous one
- We produce many estimators of the mean with different statistical error

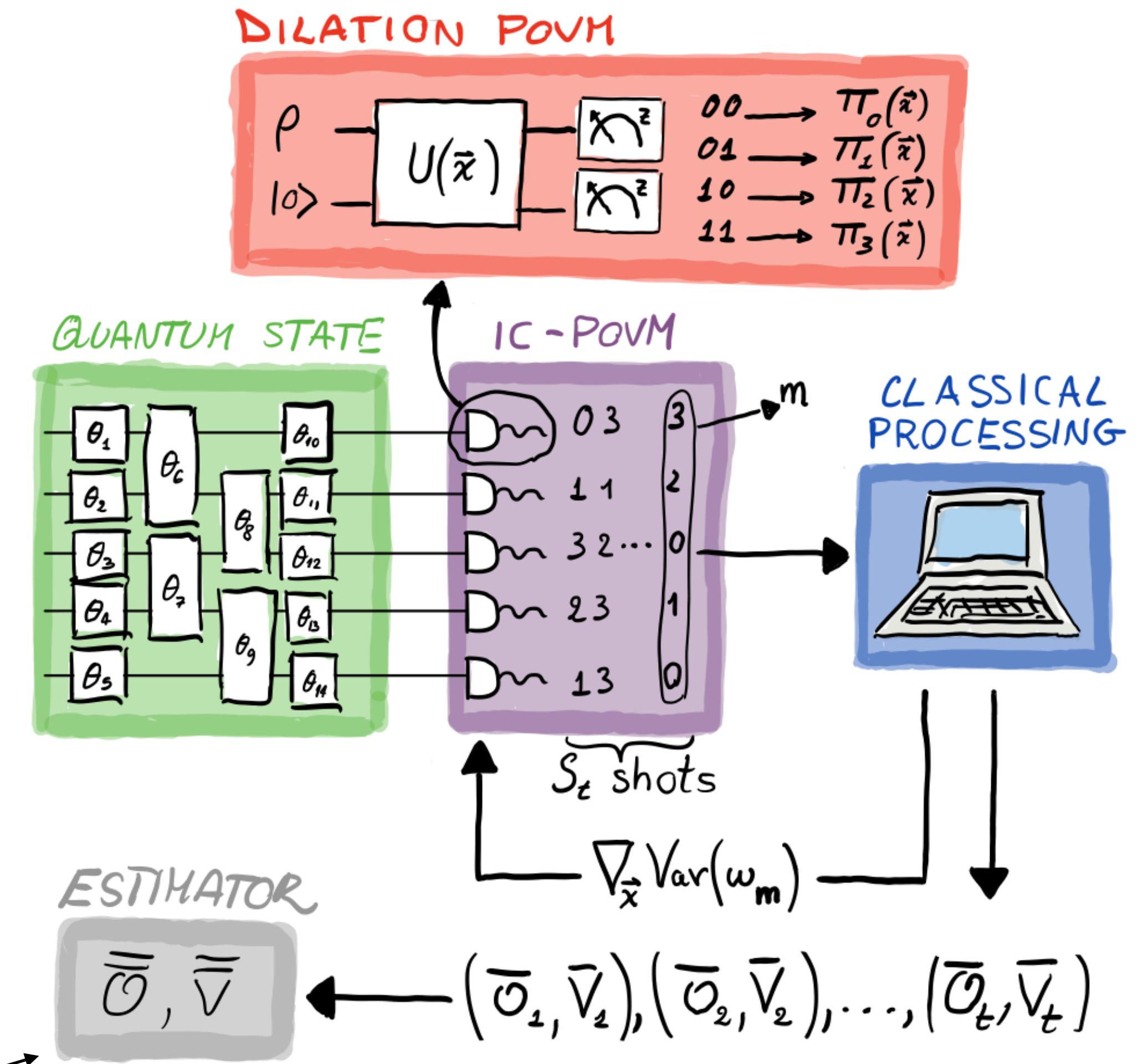


Tackling the measurement problem

with adaptive generalised measurements

Optimising measurements on the fly

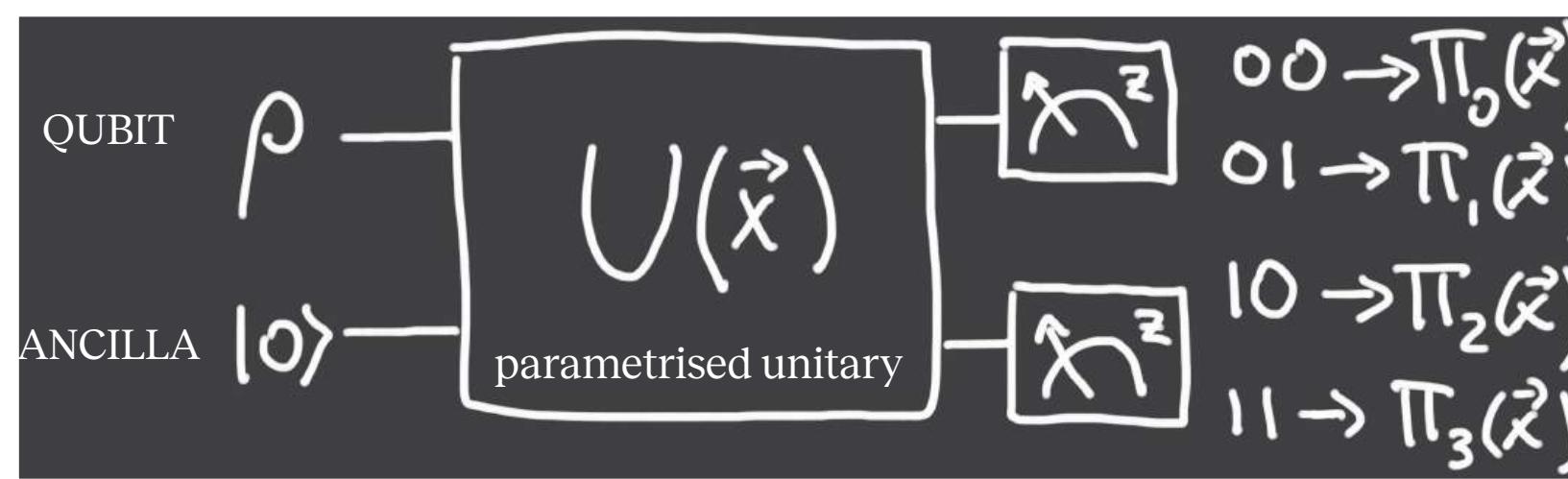
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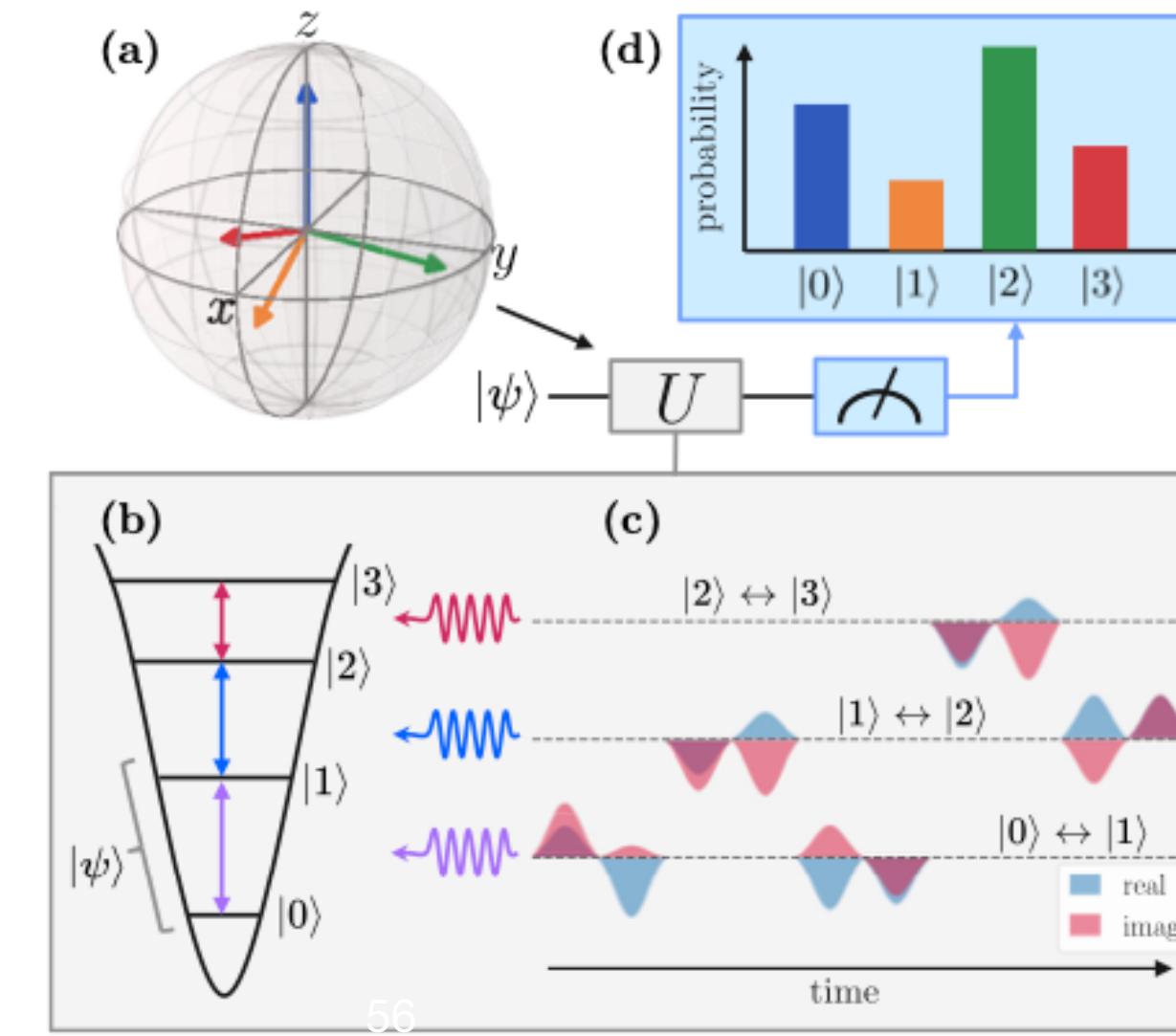
POVM implementations

1. Dilation POVM [García-Pérez et al. PRX Quantum 2, 040342 (2021)]
2. Physical dilation POVM [Fischer et al. PRR 4 (2022)]
3. Randomized unitaries [Glos et al., arXiv:2208.07817]

[1]

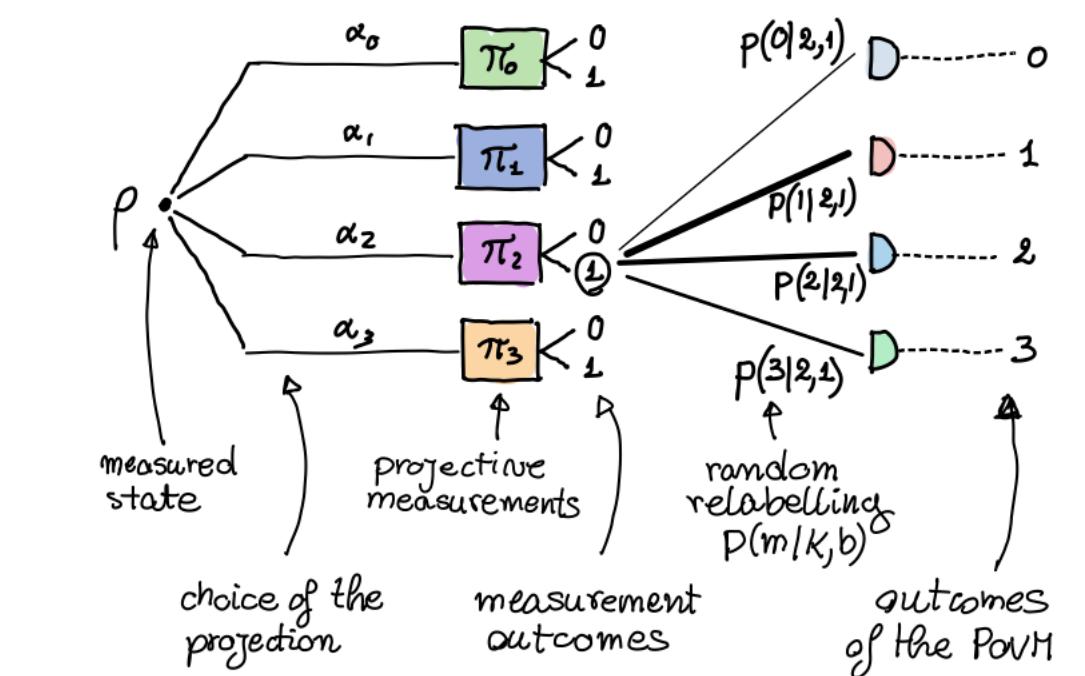


[2]



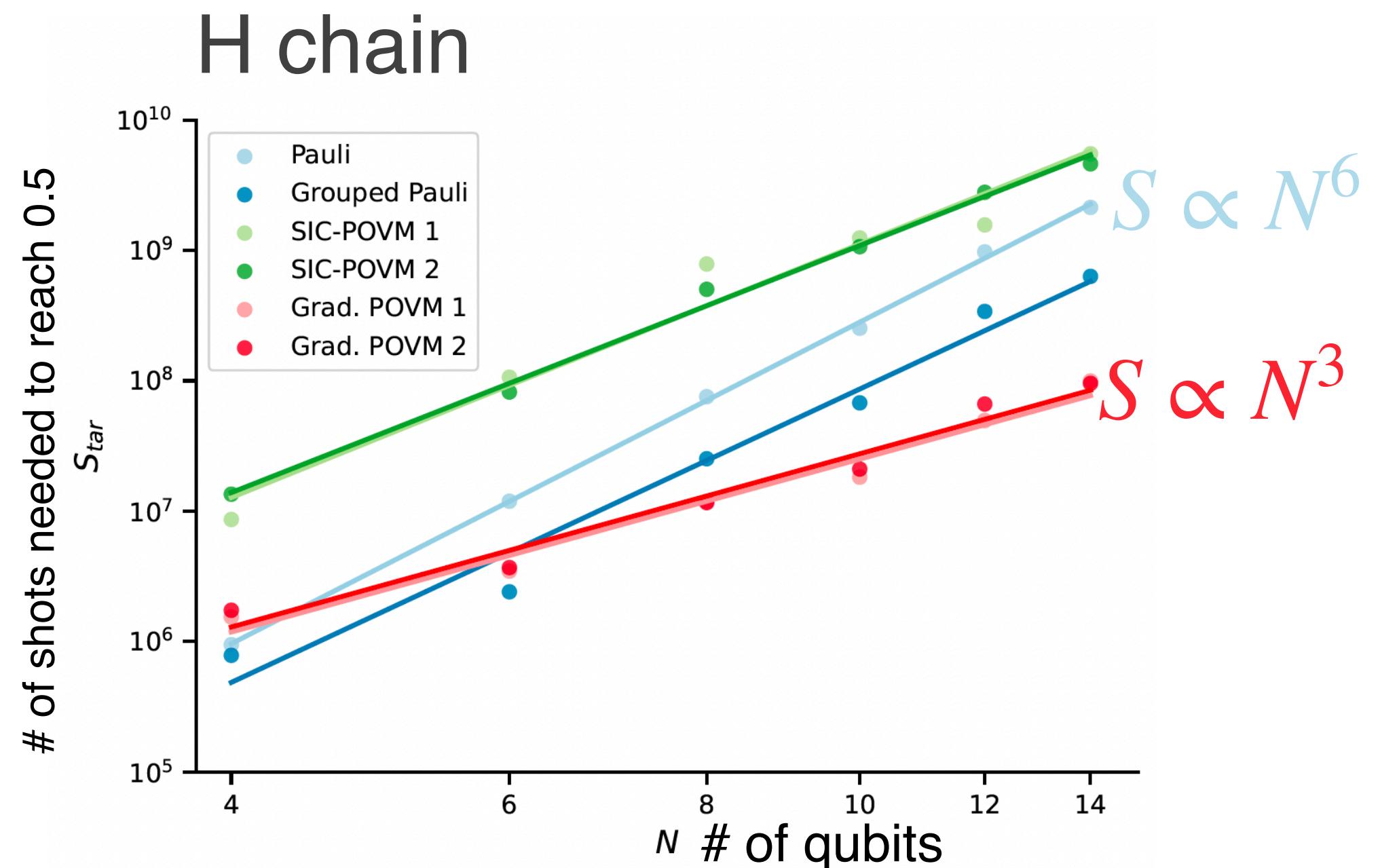
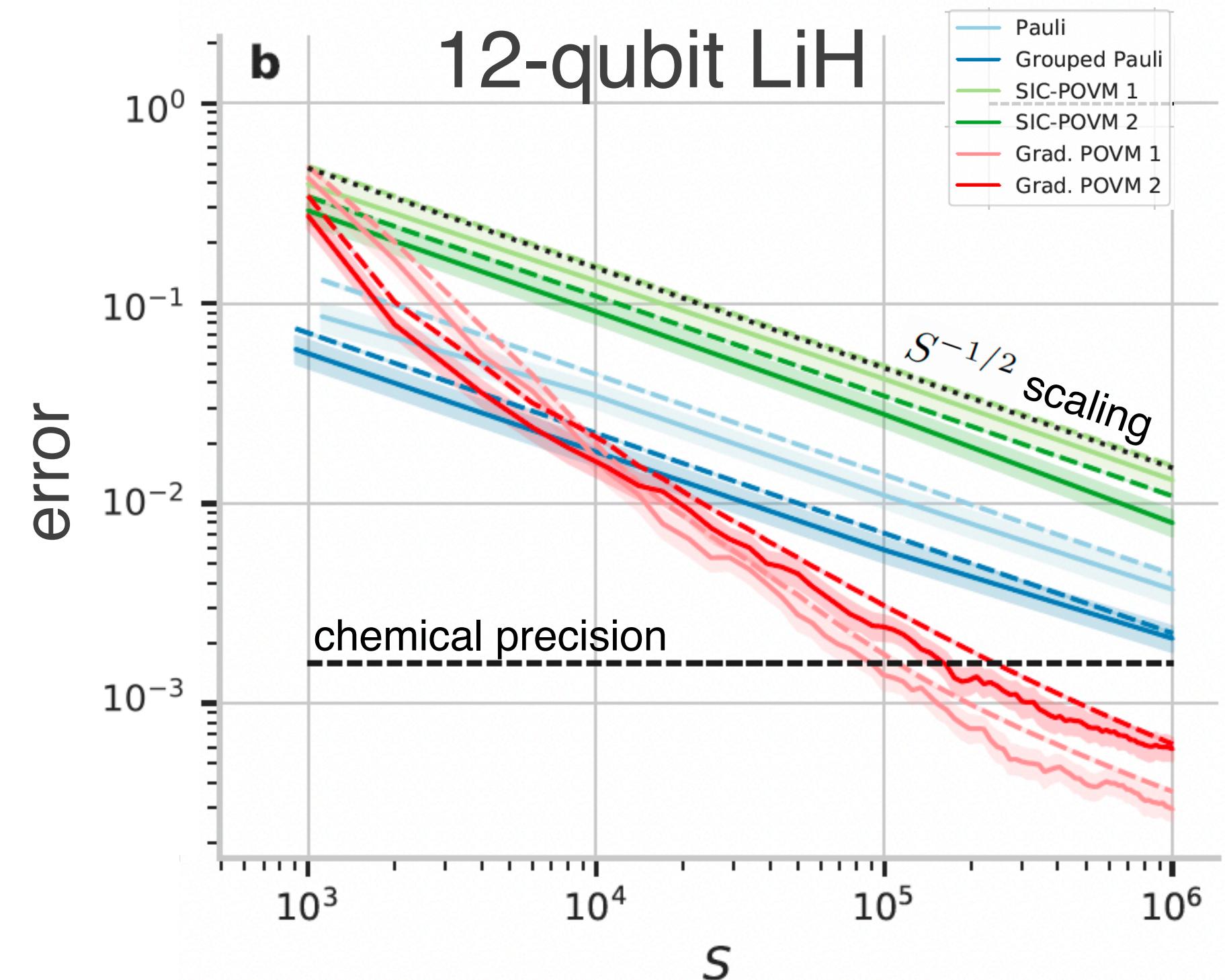
56

[3]



Benefits of IC-POVMs

- Can be adapted to improve estimation precision for a given state and observable
- Provide better scaling of the number of measurements vs number of qubits
- Allow to estimate other observables with the same data:
 - RDMs
 - Commutators
 - Noise mitigation



References

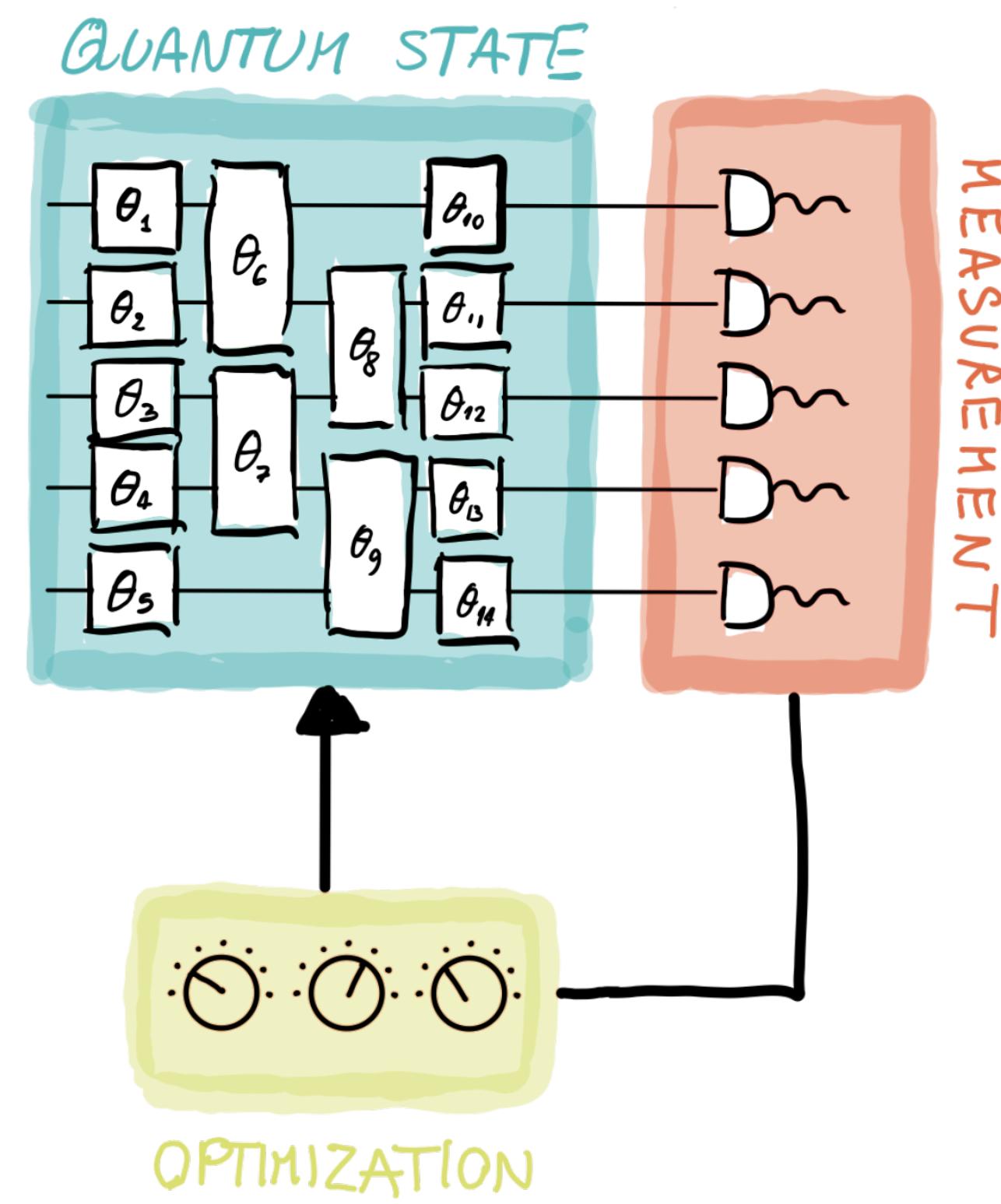
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Advanced State Preparation Techniques

Ansatz preparation

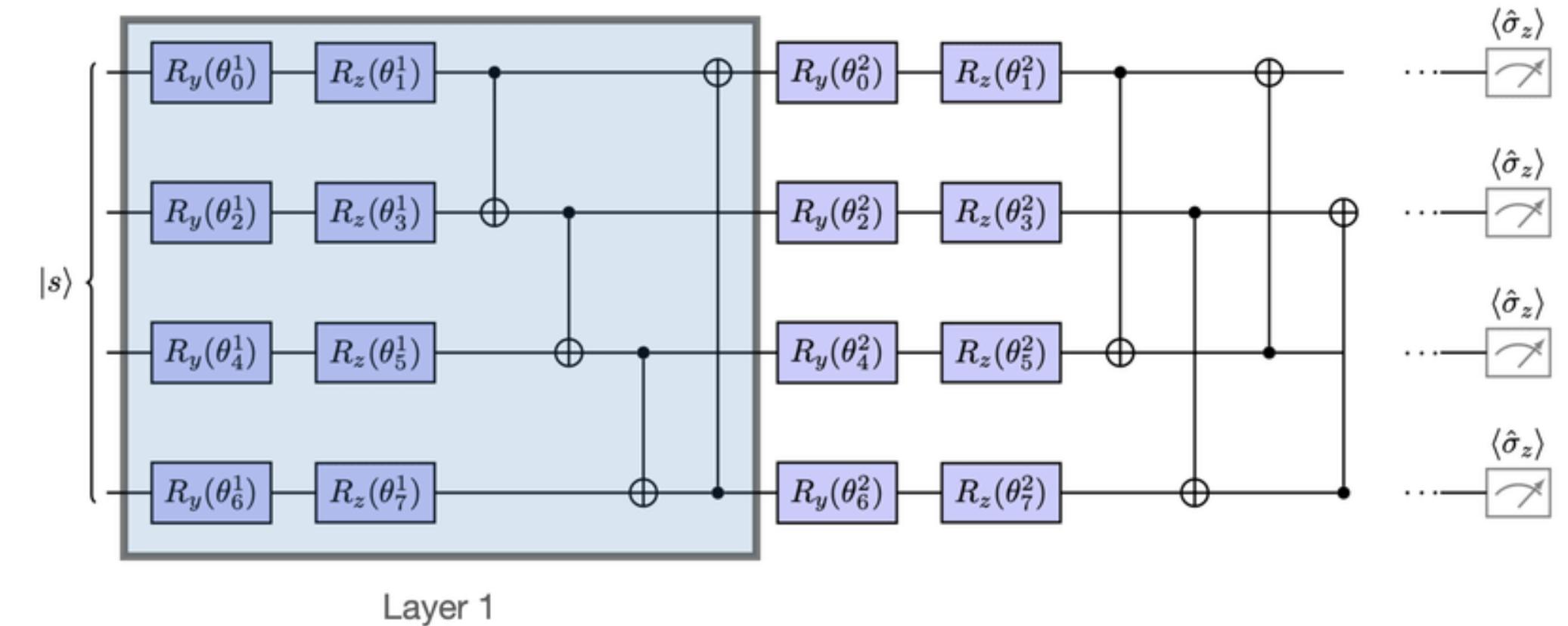
Efficient representation of state

- Design a quantum circuit, which efficiently covers a part of Hilbert space that contains the target quantum state
- Things to consider
 - Expressibility
 - Optimisability
 - Scalability
 - Depth
 - Gate count
 - Hardware layout
 - Native gate set



Ansatz types

- Hardware efficient Ansatz
 - Expressible circuits, but too much -> Hard to optimize
 - Barren plateaus -> Finding gradient direction requires very precise measurements
- Unitary Coupled-Cluster Singles and Doubles (UCCSD)
 - Chemically inspired, ansatz consists of fermionic single and double excitations
 - Long circuits
 - Fail to simulate largest correlations, too many parameters and gate ordering not optimal

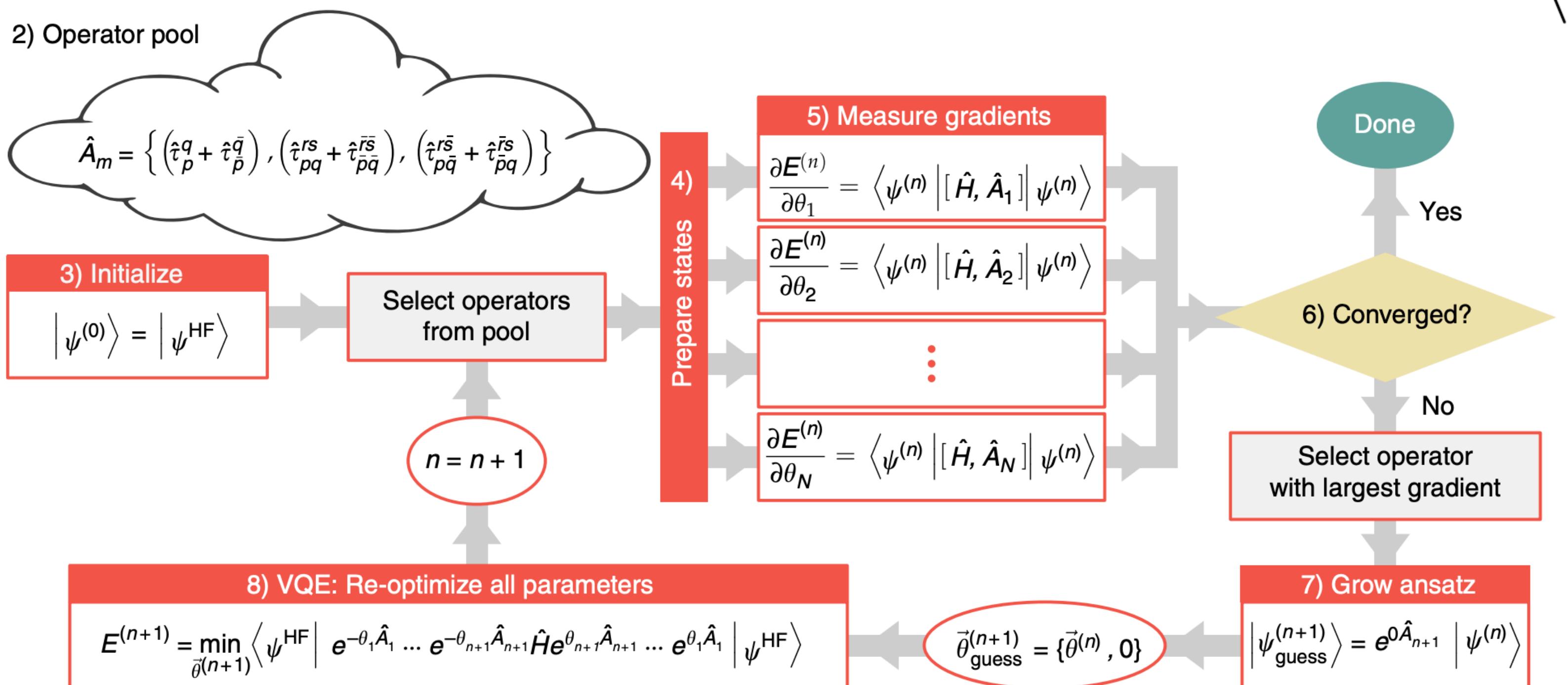


$$\begin{aligned}\hat{\tau}_p^q &= a_q^\dagger a_p - a_p^\dagger a_q \\ \hat{\tau}_{rs}^{pq} &= a_p^\dagger a_q^\dagger a_r a_s - a_s^\dagger a_r^\dagger a_q a_p\end{aligned}$$

Adaptive Ansätze

- Adaptively build a problem-tailored ansatz
 - Expressive enough to contain the ground state
 - Not too expressive to make it easily optimisable
- Operators chosen by their energy gradient

$$\begin{aligned}\left. \frac{\partial E}{\partial \theta_i} \right|_{\theta_i=0} &= \left[\frac{\partial}{\partial \theta_i} \left\langle \psi^{(n)} \left| e^{-\theta_i A_i} H e^{\theta_i A_i} \right| \psi^{(n)} \right\rangle \right] \Big|_{\theta_i=0} \\ &= \left\langle \psi^{(n)} \left| [H, A_i] \right| \psi^{(n)} \right\rangle\end{aligned}$$



Gates in ADAPT

- Fermionic single and double excitations
 - Chemical motivation -> Good convergence
 - Hardware implementations are deep (Jordan-Wigner mapping has efficient implementations)
- Qubit Excitation Based (QEB) operators (only Jordan-Wigner)
 - Remove Z-chains -> More hardware-efficient in all-to-all connectivity
 - Negligible effect on convergence for small molecules
- q-ADAPT
 - Split generators into separate terms
 - More parameters, but more hardware-efficient

$$A_{ik}(\theta) = e^{\theta T_{ik}} = \exp \left[\theta(a_i^\dagger a_k - a_k^\dagger a_i) \right] \text{ and}$$

$$A_{ijkl}(\theta) = e^{\theta T_{ijkl}} = \exp \left[\theta(a_i^\dagger a_j^\dagger a_k a_l - a_k^\dagger a_l^\dagger a_i a_j) \right]$$

$$A_{ik}(\theta) = \exp \left[i \frac{\theta}{2} (X_i Y_k - Y_i X_k) \prod_{r=i+1}^{k-1} Z_r \right] \text{ and}$$

$$A_{ijkl}(\theta) = \exp \left[i \frac{\theta}{8} (X_i Y_j X_k X_l + Y_i X_j X_k X_l + Y_i Y_j Y_k X_l + Y_i Y_j X_k Y_l - X_i X_j Y_k X_l - X_i X_j X_k Y_l - Y_i X_j Y_k Y_l - X_i Y_j Y_k Y_l) \prod_{r=i+1}^{j-1} Z_r \prod_{r'=k+1}^{l-1} Z_{r'} \right].$$

$$A_{ijkl,1}(\theta_1) = \exp(i\theta_1 X_i Y_j X_k X_l)$$

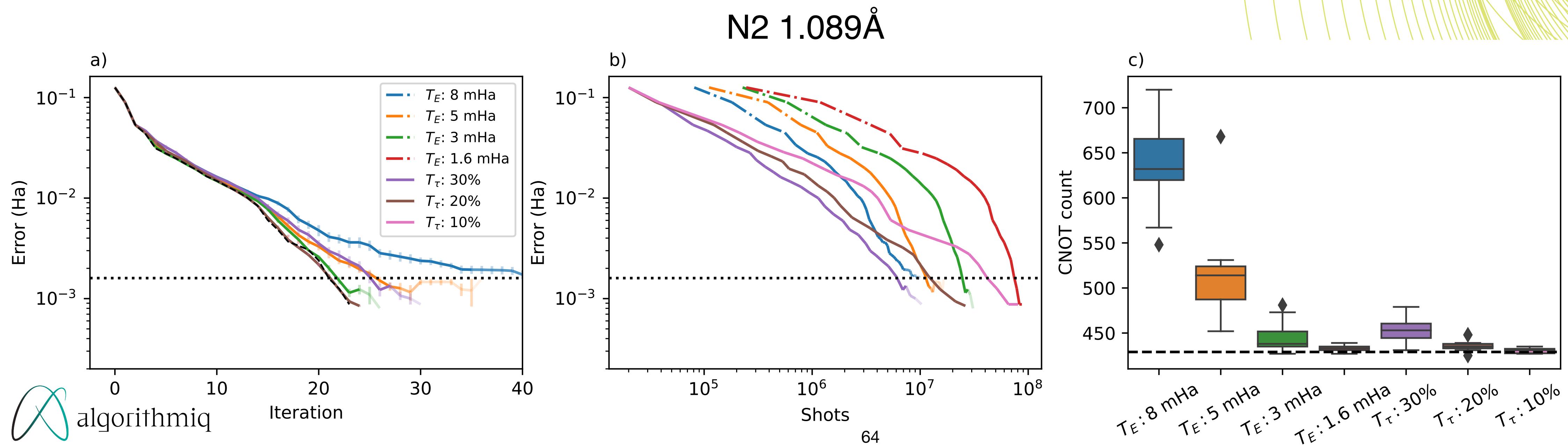
$$A_{ijkl,2}(\theta_2) = \exp(i\theta_2 Y_i X_j X_k X_l)$$

:

Main limitation of ADAPT

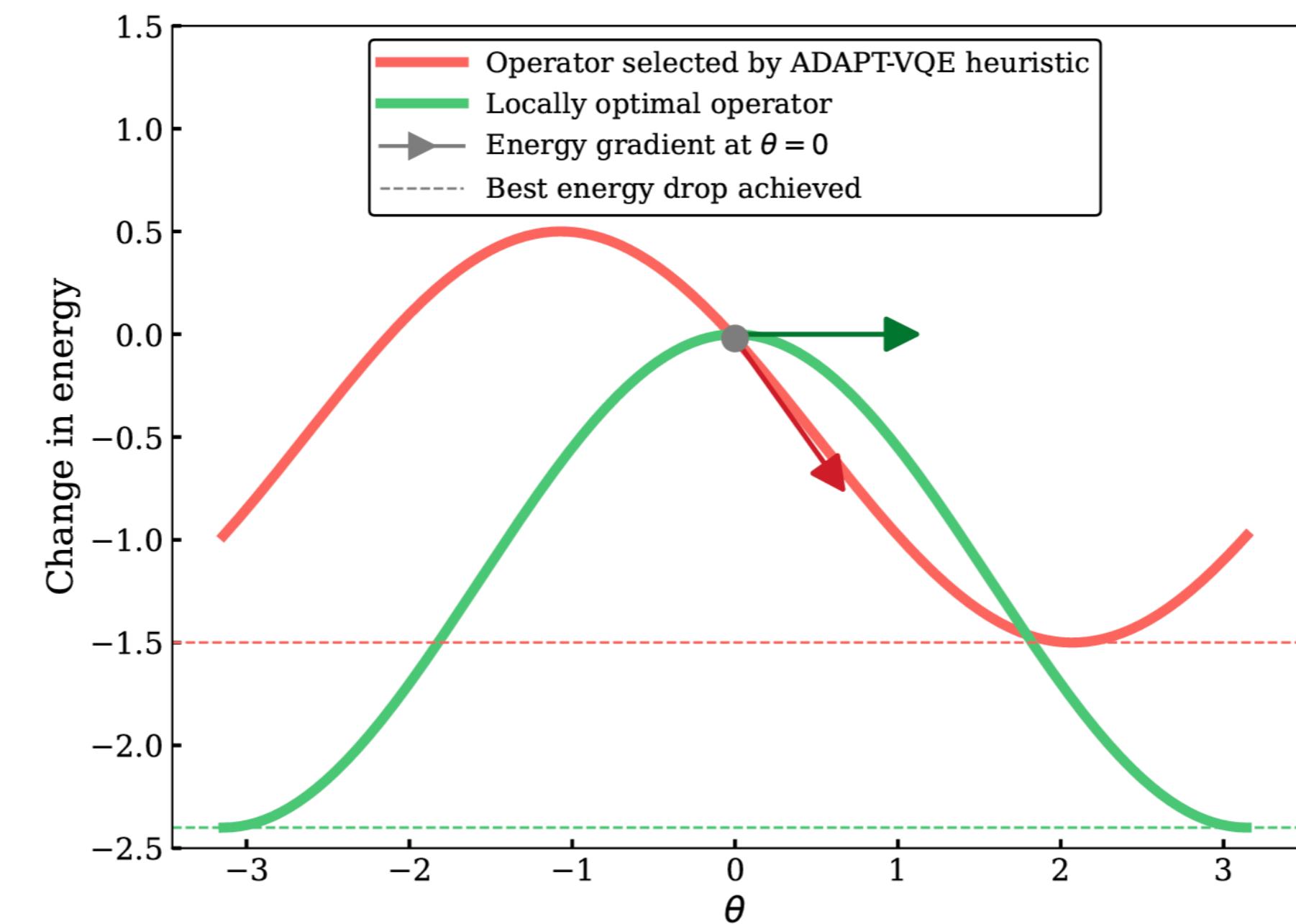
Measurement overhead

- To find the operator with the highest gradient, one needs to measure a commutator for each operator in the operator pool
- IC-POVMs solve the problem. Just measure the energy and use the same measurement data for the evaluations of the commutators.



Selection criteria

- Gradient selection is robust but not necessarily the most efficient
 - The gradient is measured at parameter 0.0, so low gradient doesn't necessarily mean small effect on energy.
 - Alternatively, select the operator which lowers the energy the most
- Use overlap selection and optimisation if the target state or an approximation of it is known
 - Not eas



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