

# Quantum chemistry on near-term devices

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

# Quantum computing is evolving very quickly

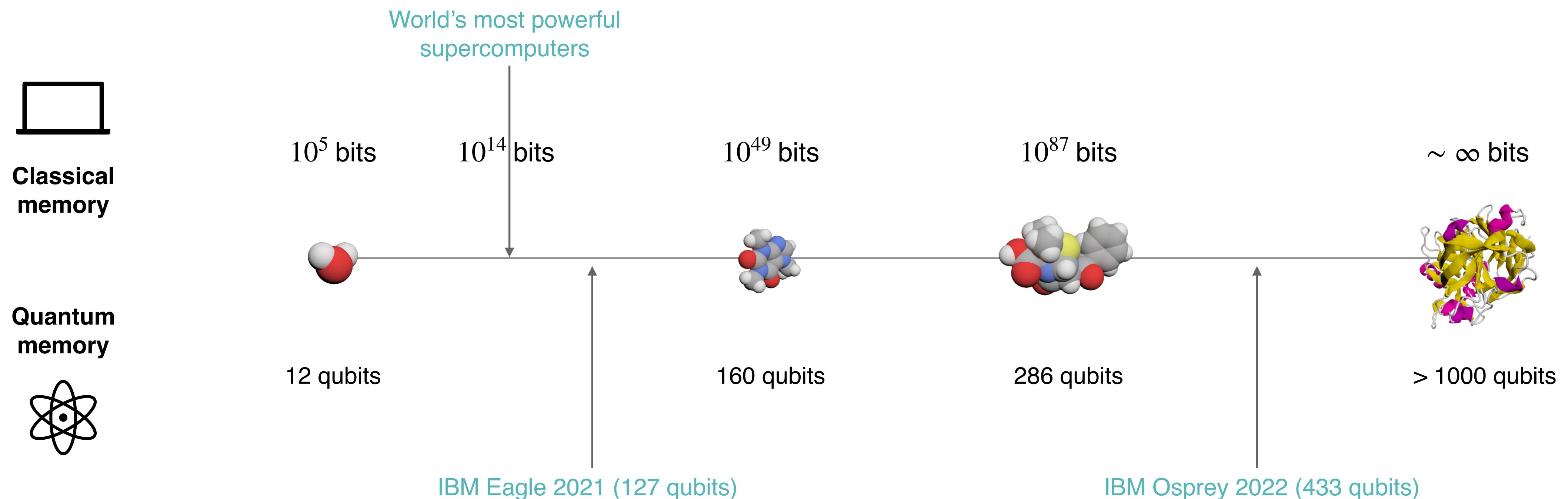


Billions are being invested

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

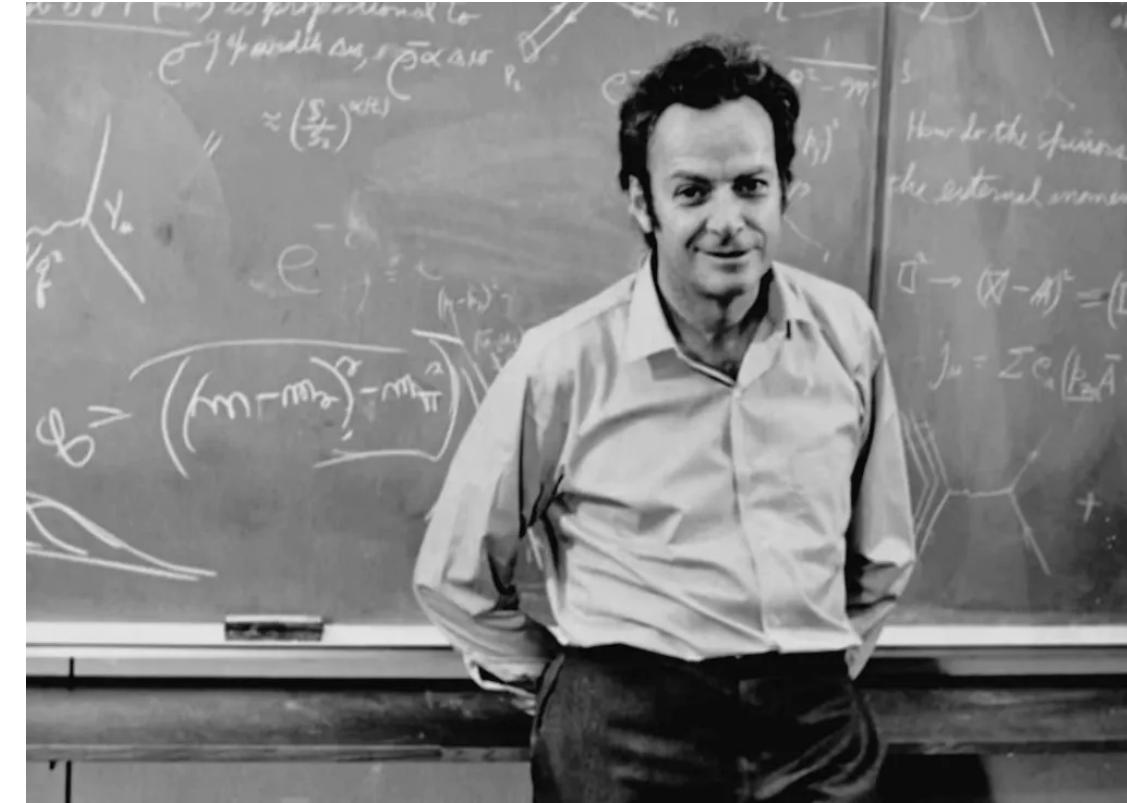


# The origins of quantum computing

Simulating quantum physics



Yuri Manin  
1980



Richard Feynman  
1982

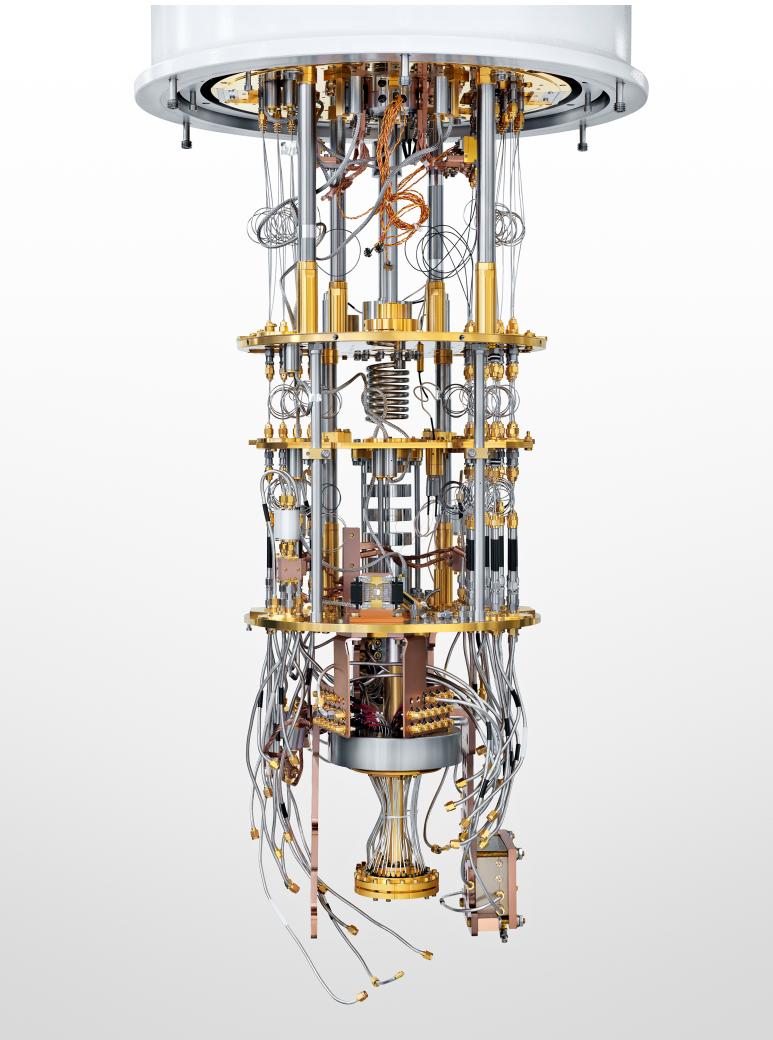
Simulating some quantum mechanical effects  
on a classical computer is unfeasible



Use a quantum one!

# Using a quantum computer

As a quantum physics simulator

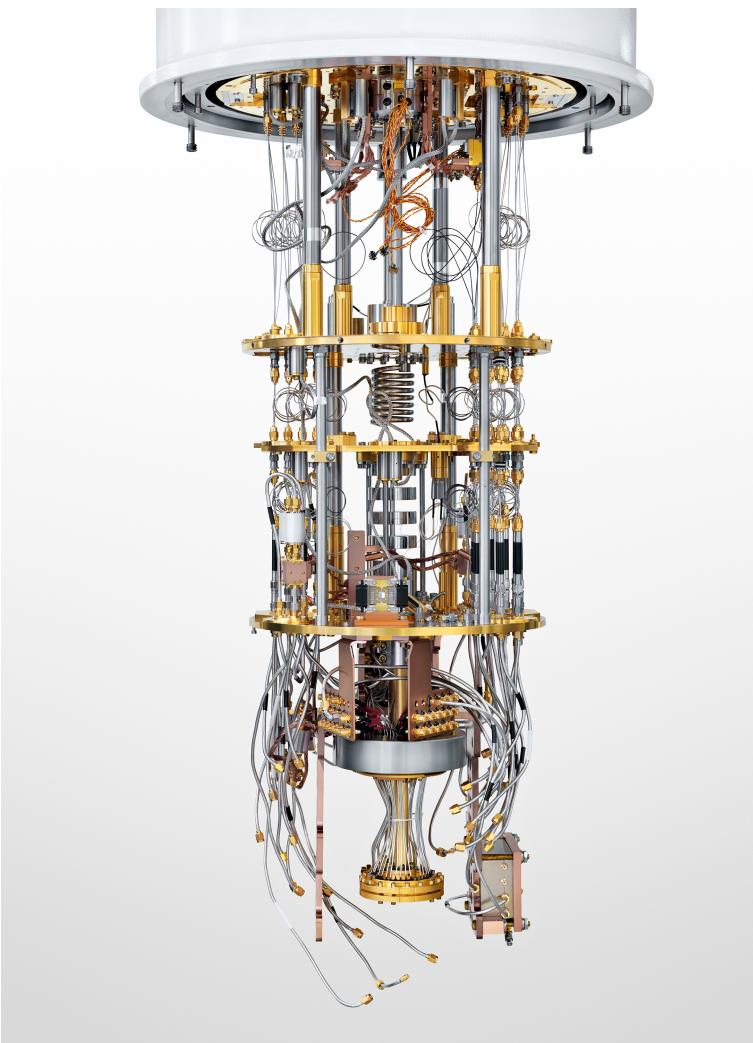


Arbitrary state of its quantum bits (qubits)

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

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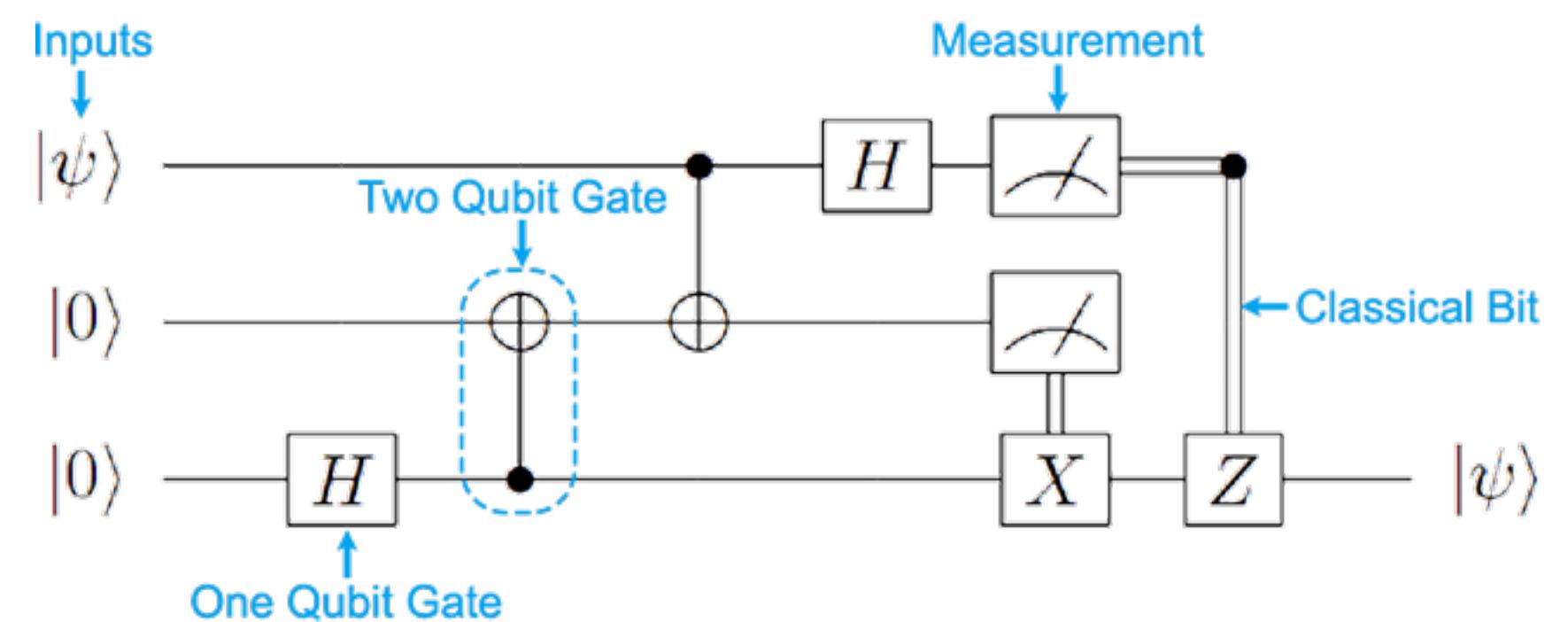
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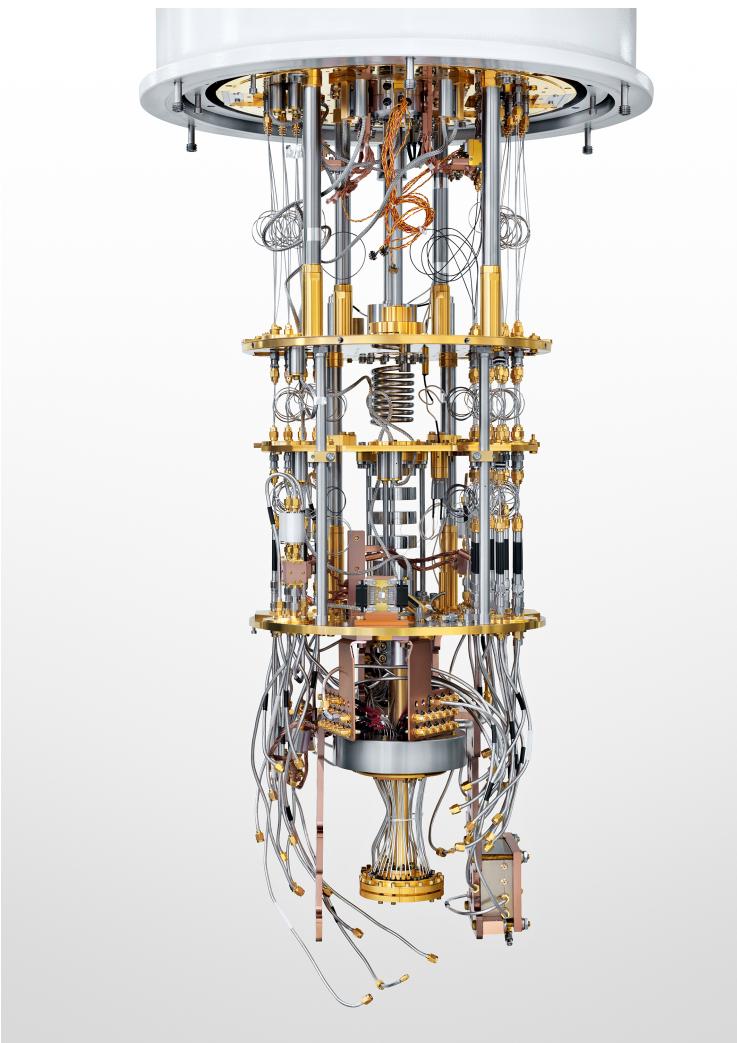
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A universal quantum computer can solve problems beyond quantum simulation (e.g. factorisation)



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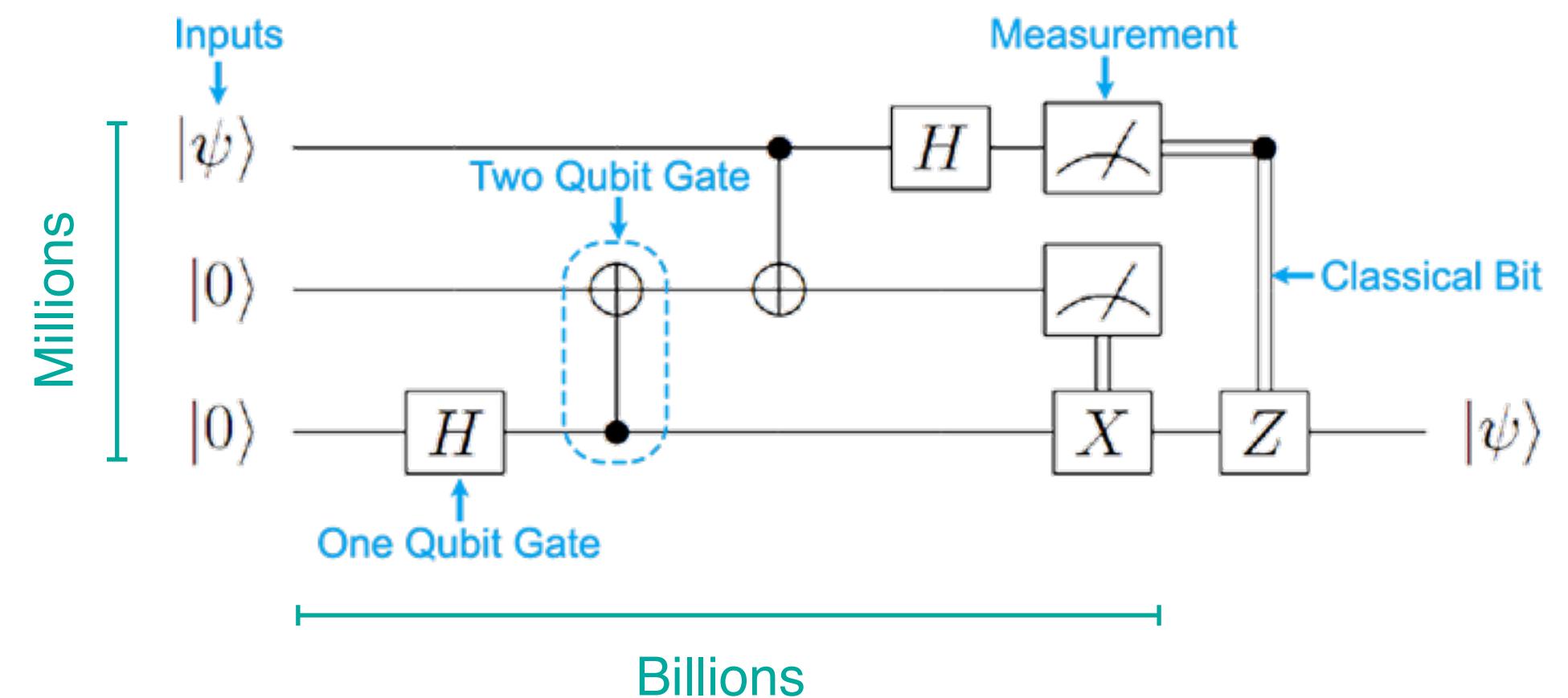
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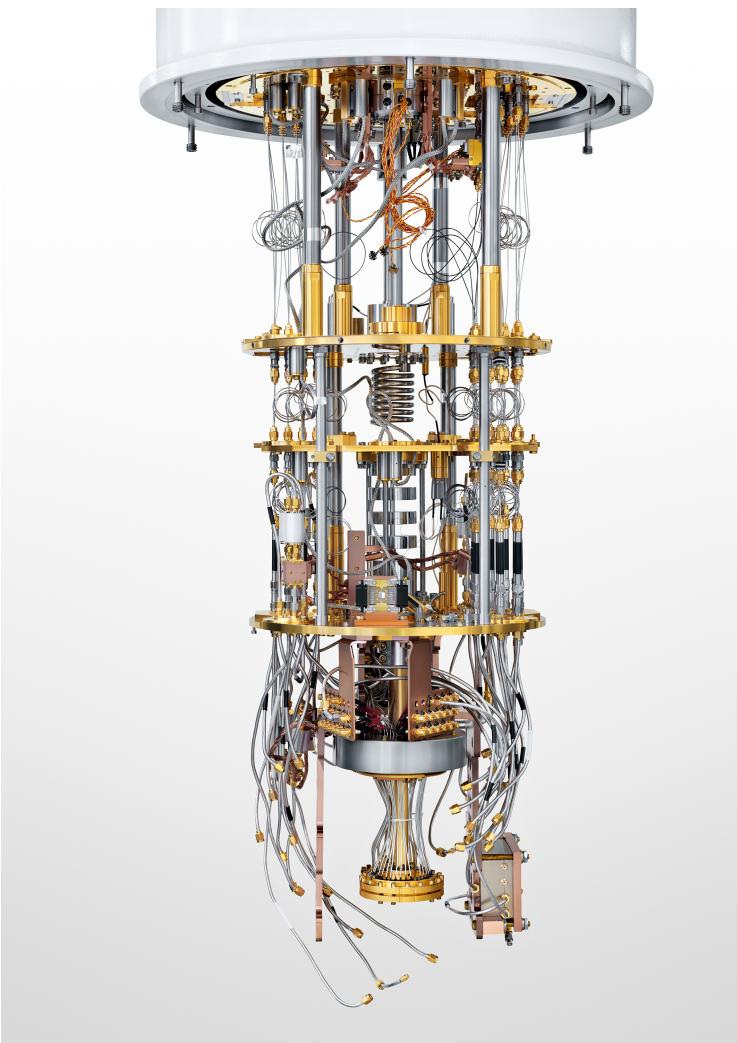
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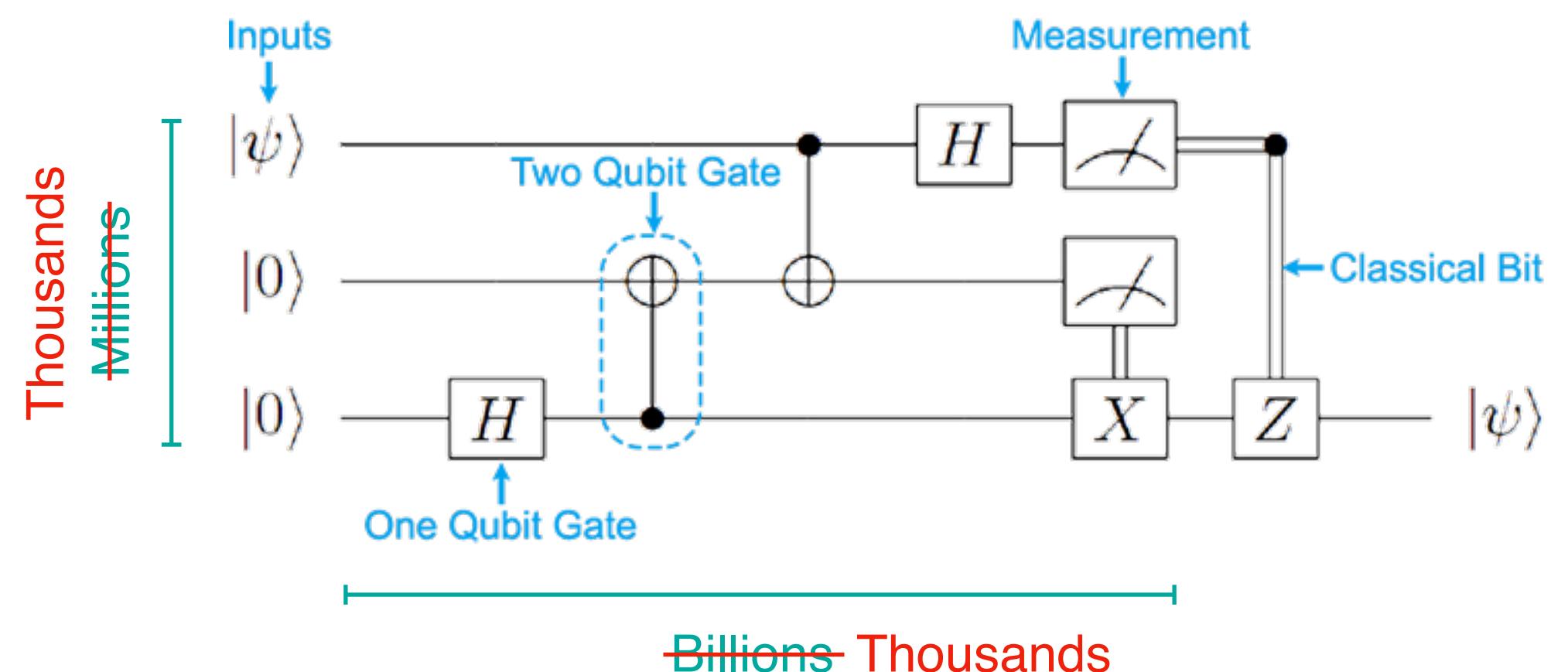
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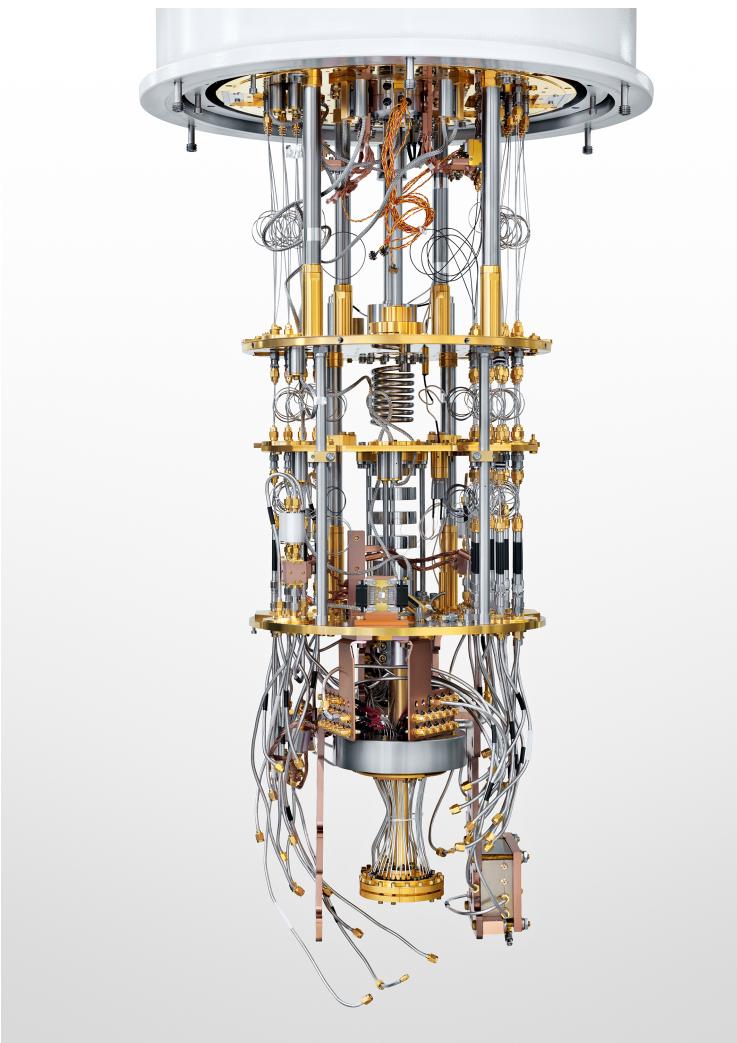
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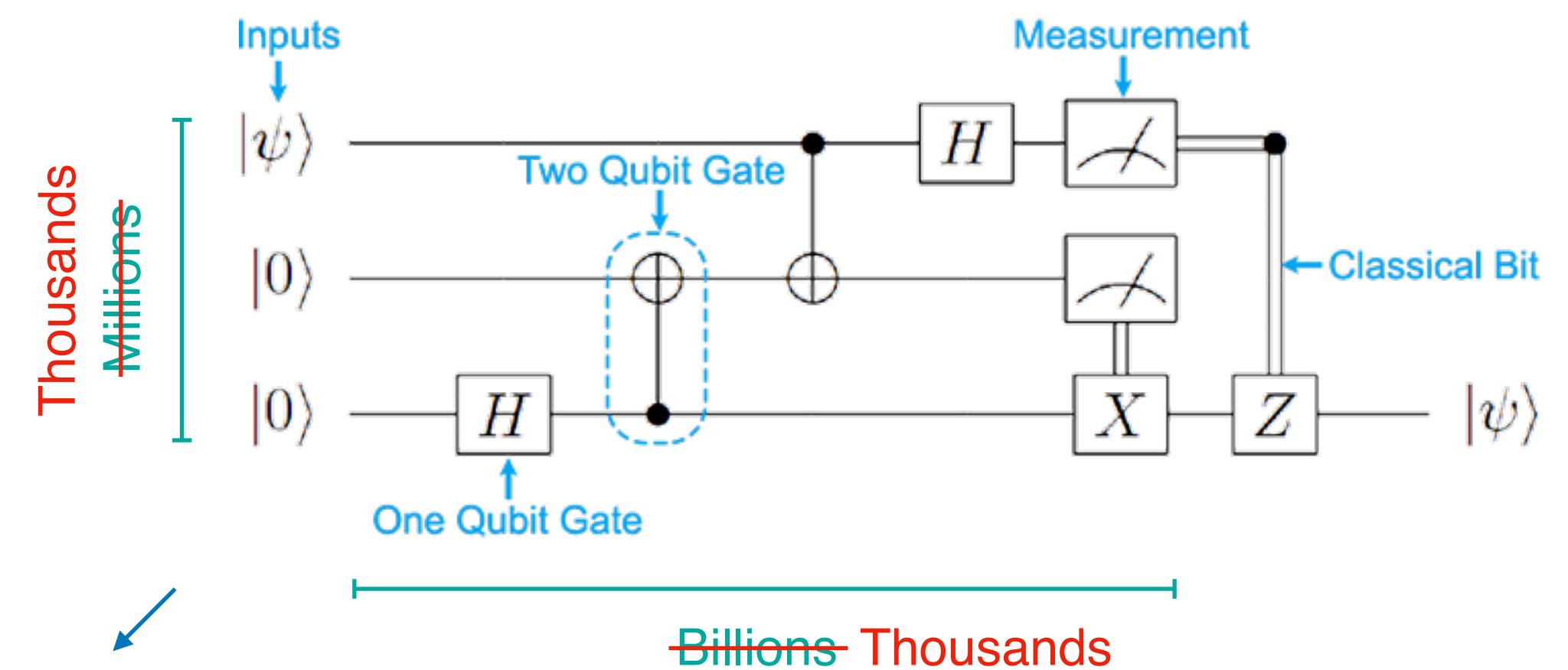
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We are in the era of the Noisy Intermediate-Scale Quantum computers:  
soon useful for simulation!

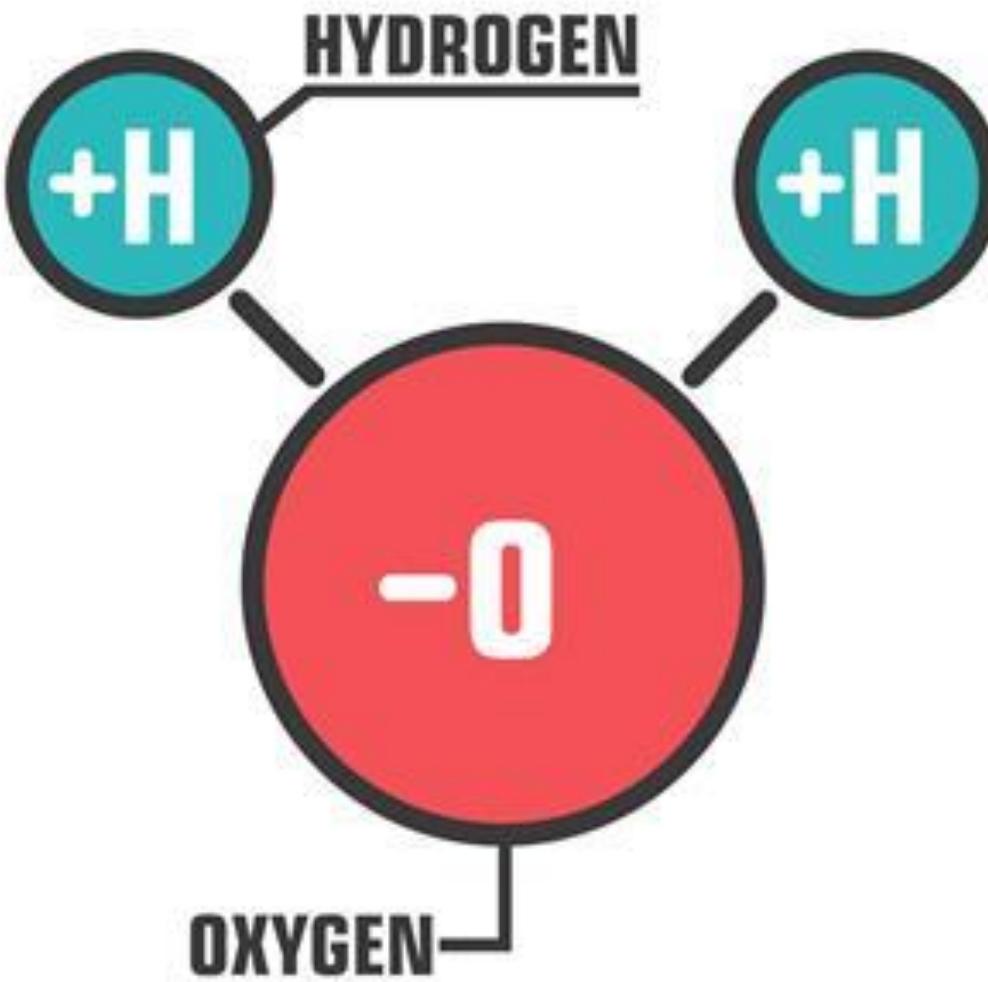
# Variational Quantum Eigensolver

# (General) problem statement

Molecular ground-state energy

- Composition of the molecule is given

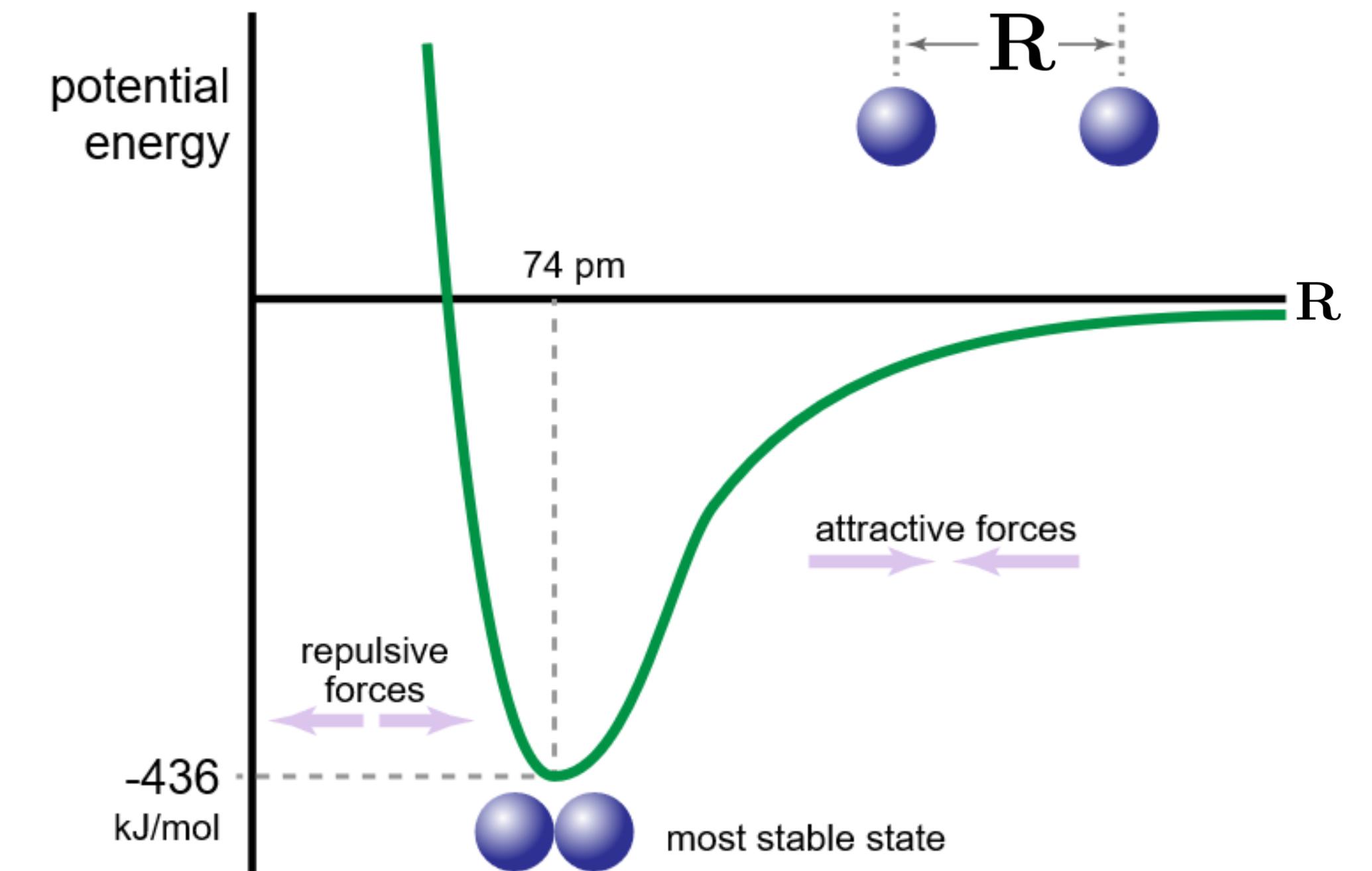
**WATER ( $H_2O$ )**



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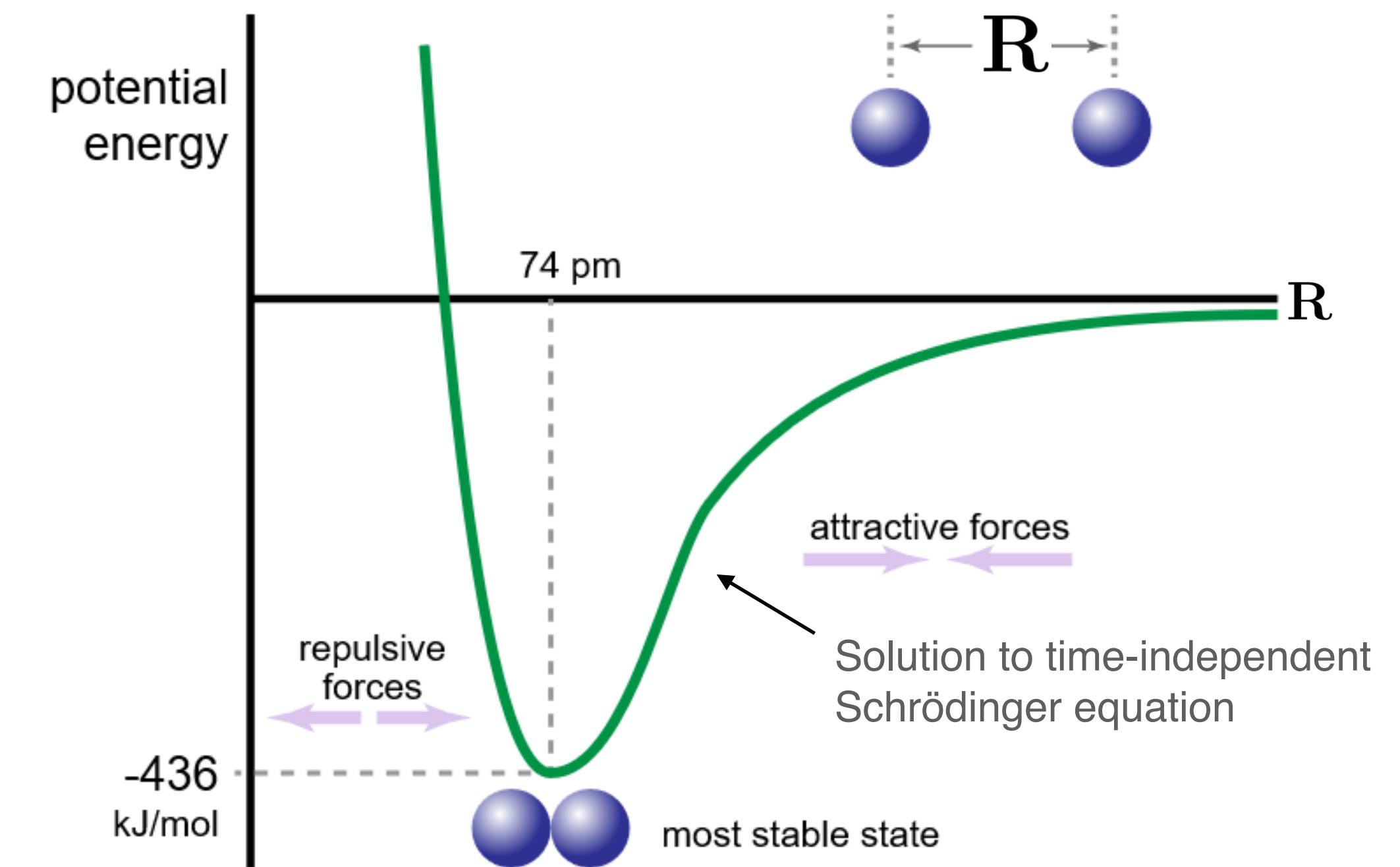
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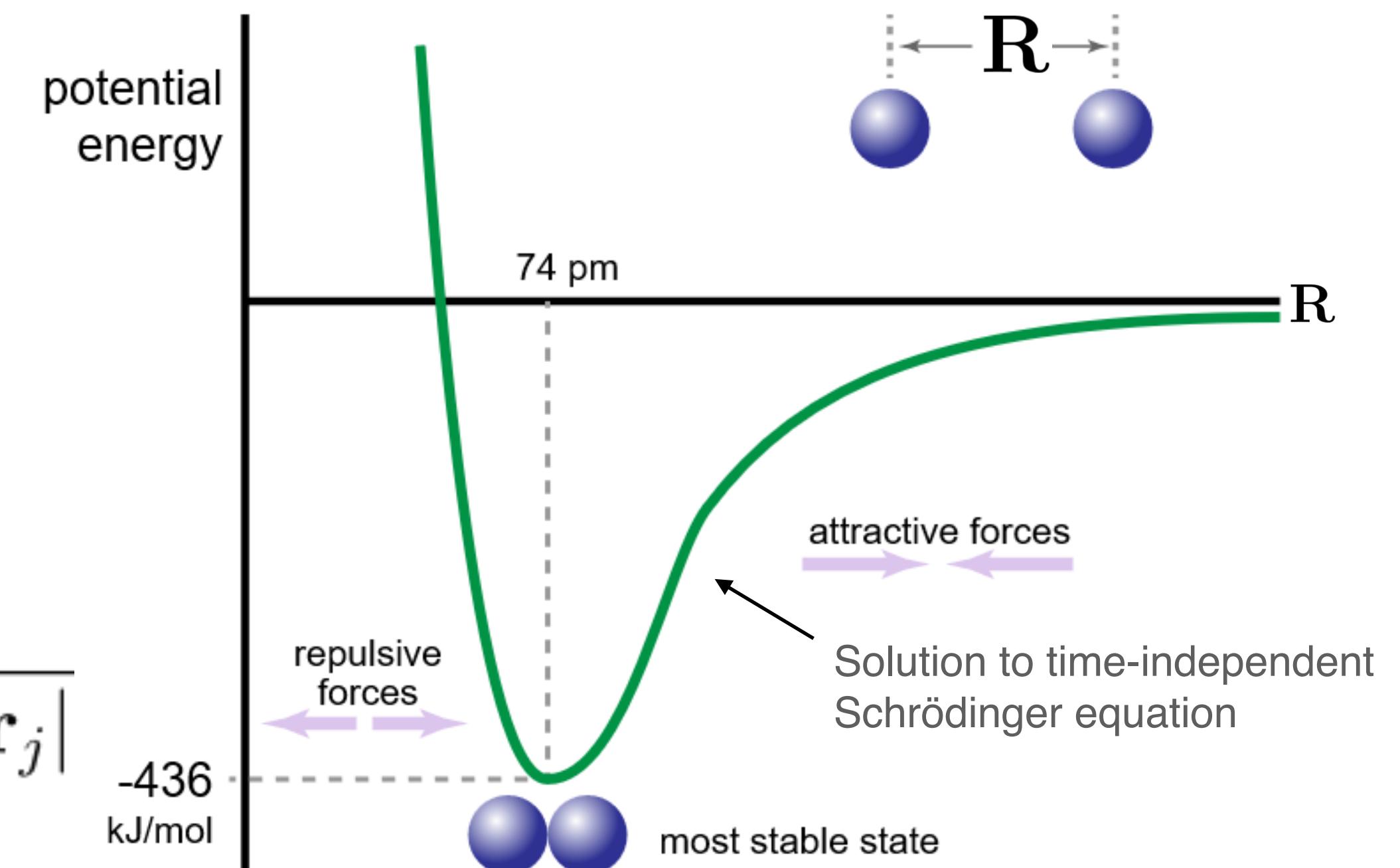


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$$\hat{H}_e = -\frac{1}{2} \sum_i \nabla_i^2 - \sum_i \sum_{\alpha} \frac{Z_{\alpha}}{|\mathbf{R}_{\alpha} - \mathbf{r}_i|} + \frac{1}{2} \sum_{i \neq j} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}$$
$$\hat{H}_e |\Psi\rangle = E |\Psi\rangle$$



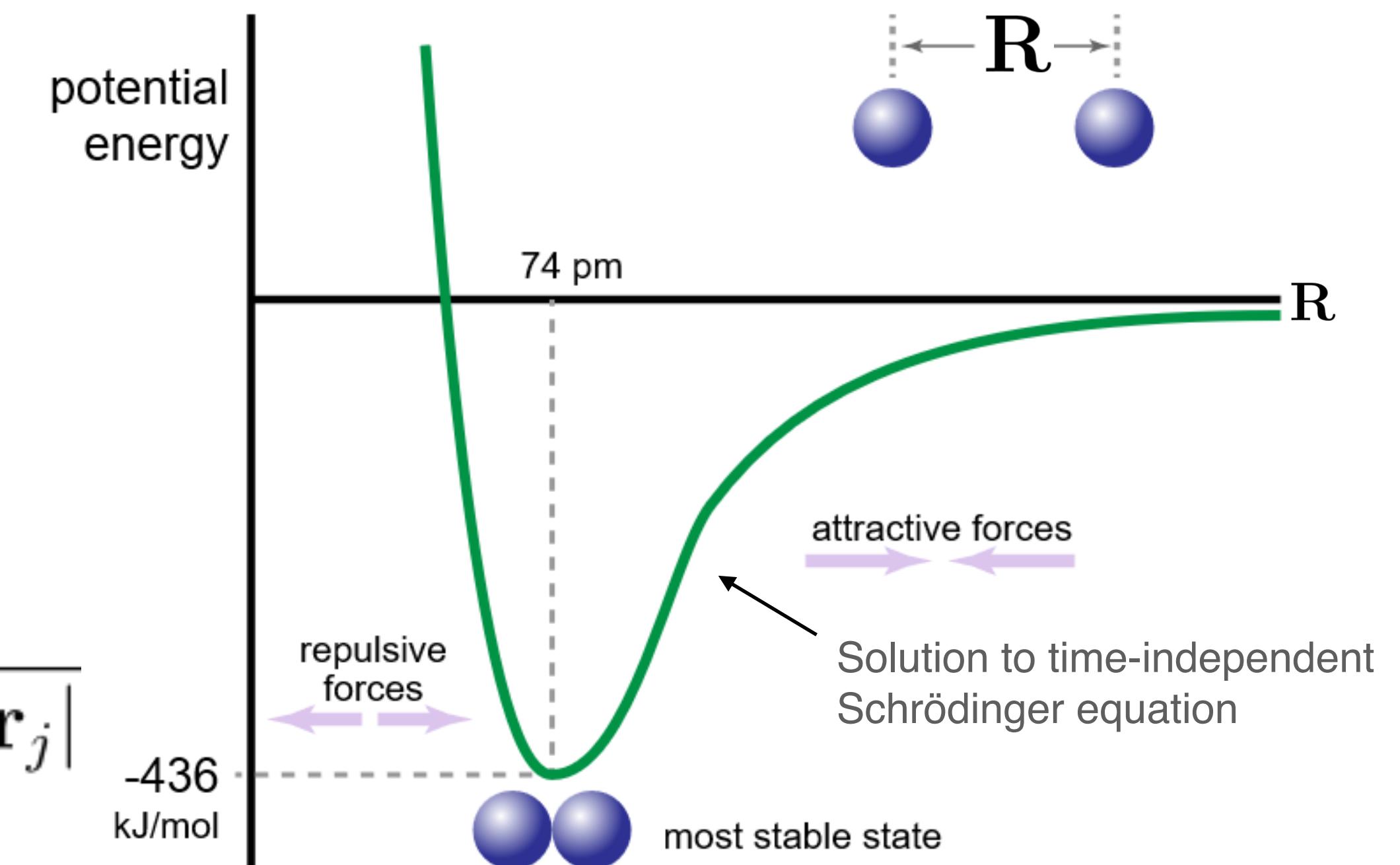
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High-dimensional vector  
in Hilbert space



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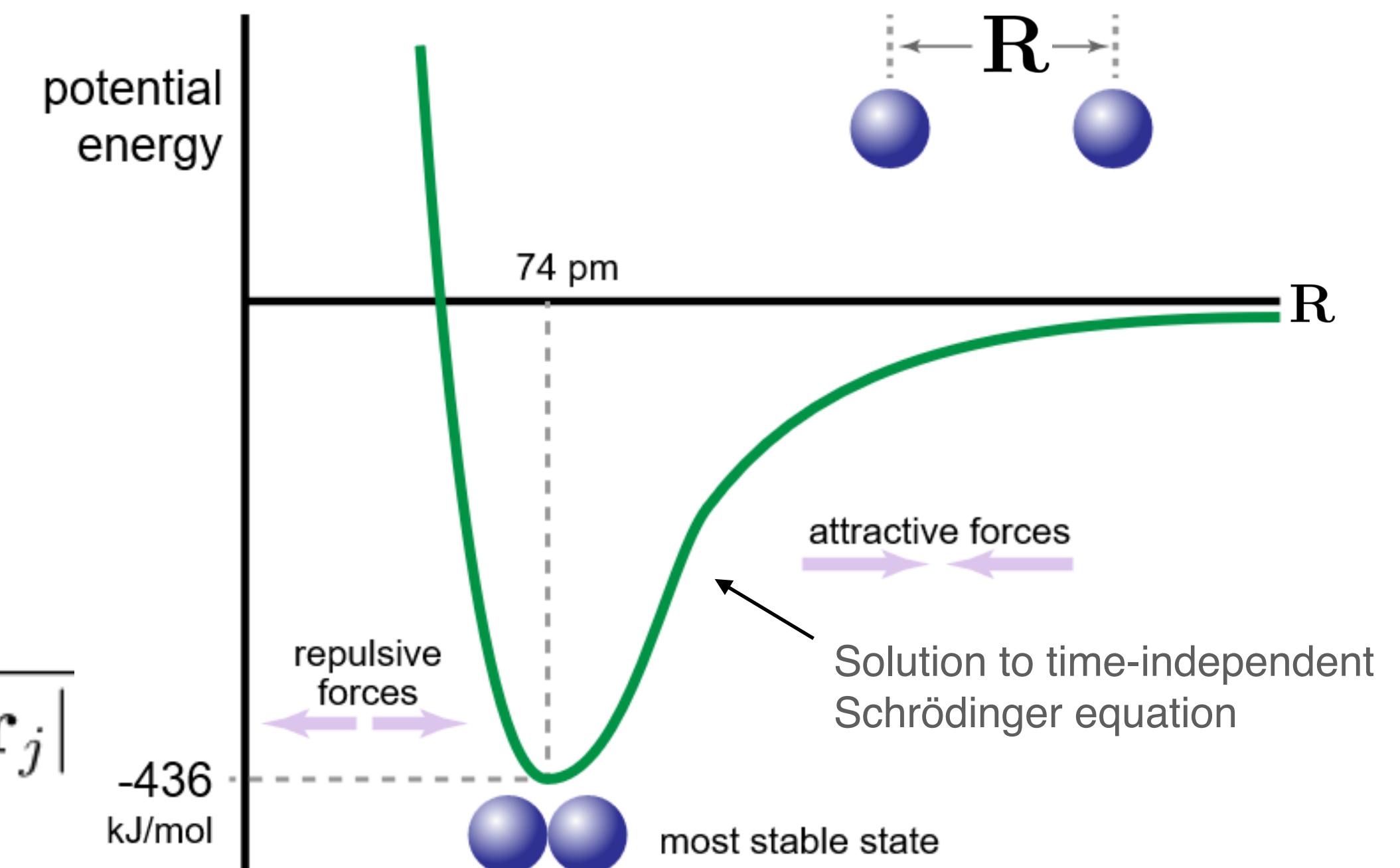
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Well-known from QM theory  
Efficient classical representation

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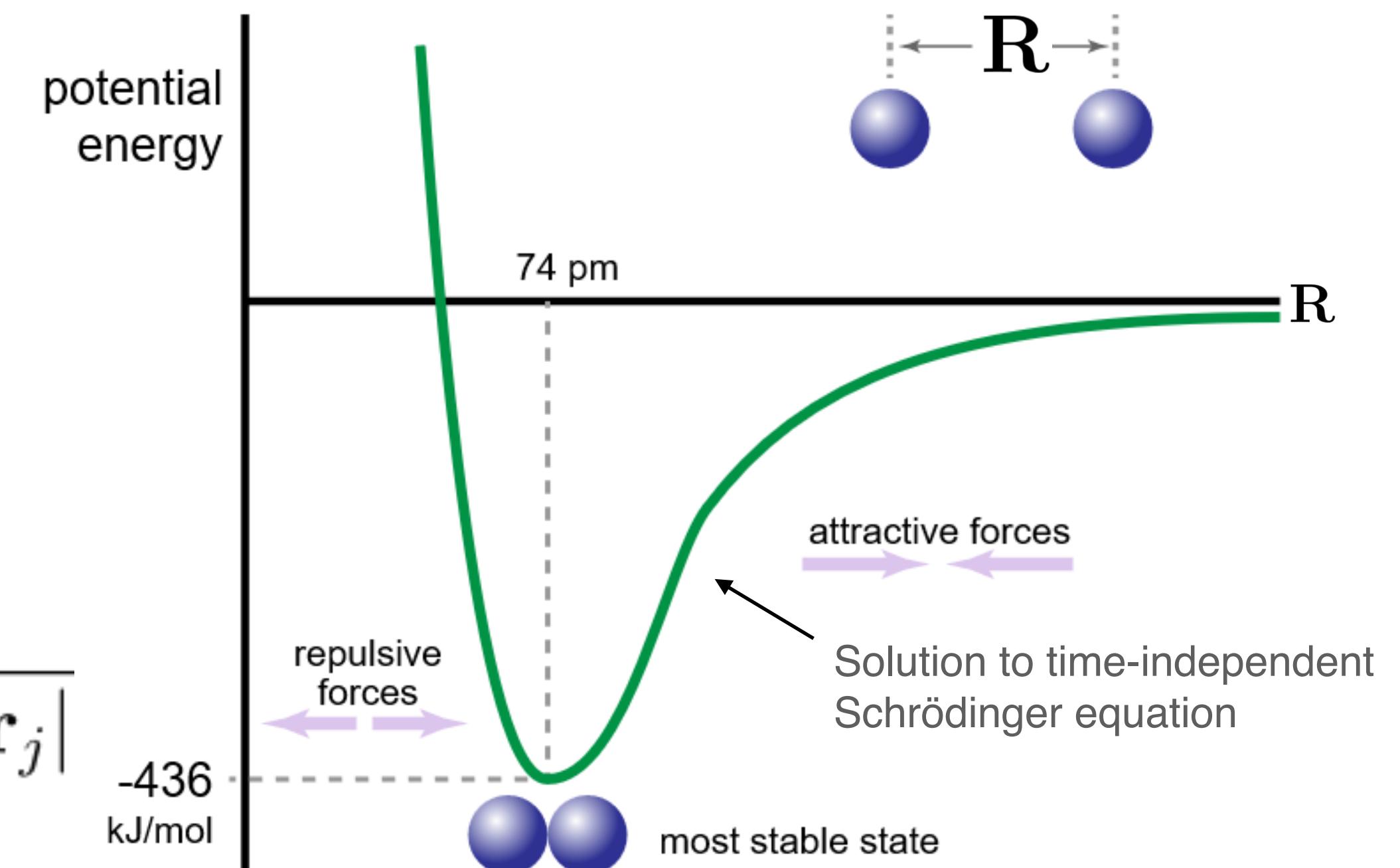
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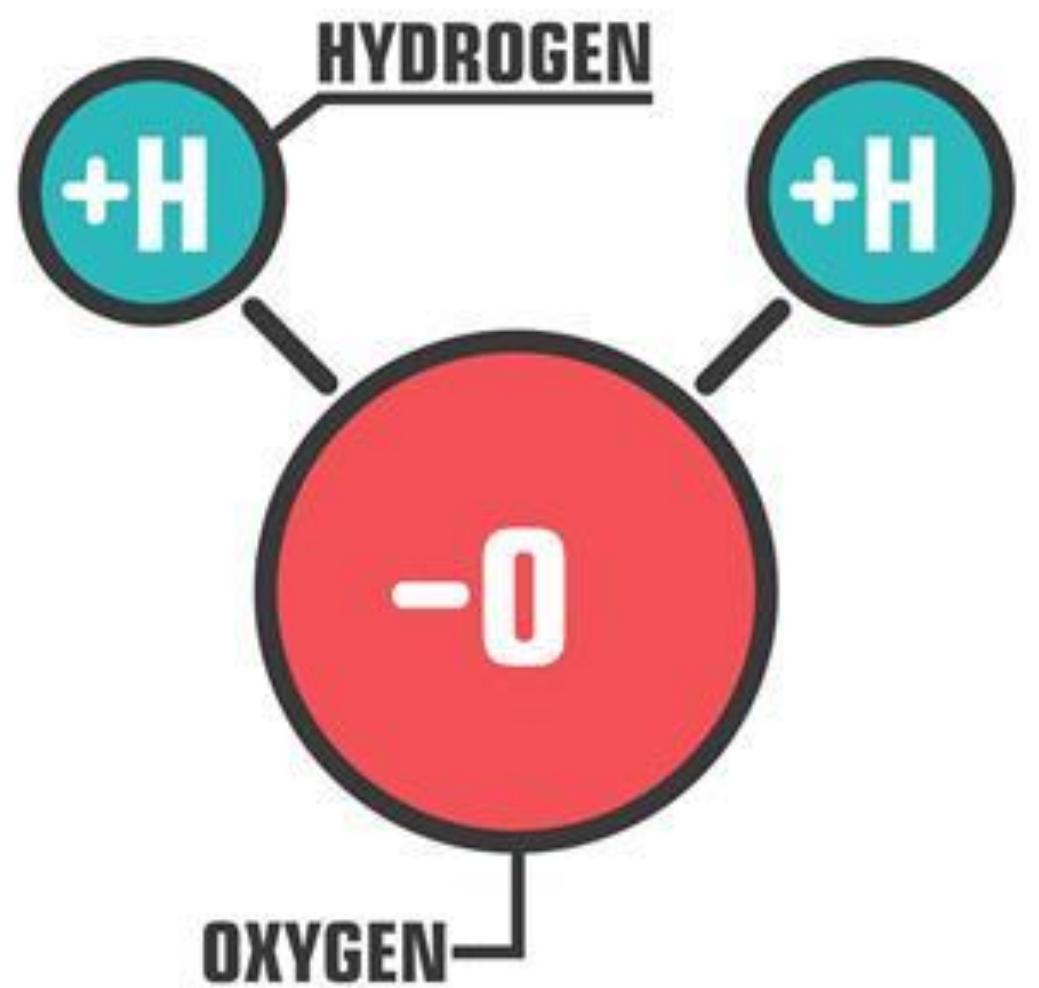
High-dimensional vector  
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# Why is this difficult?

Dimensionality of many-body QM

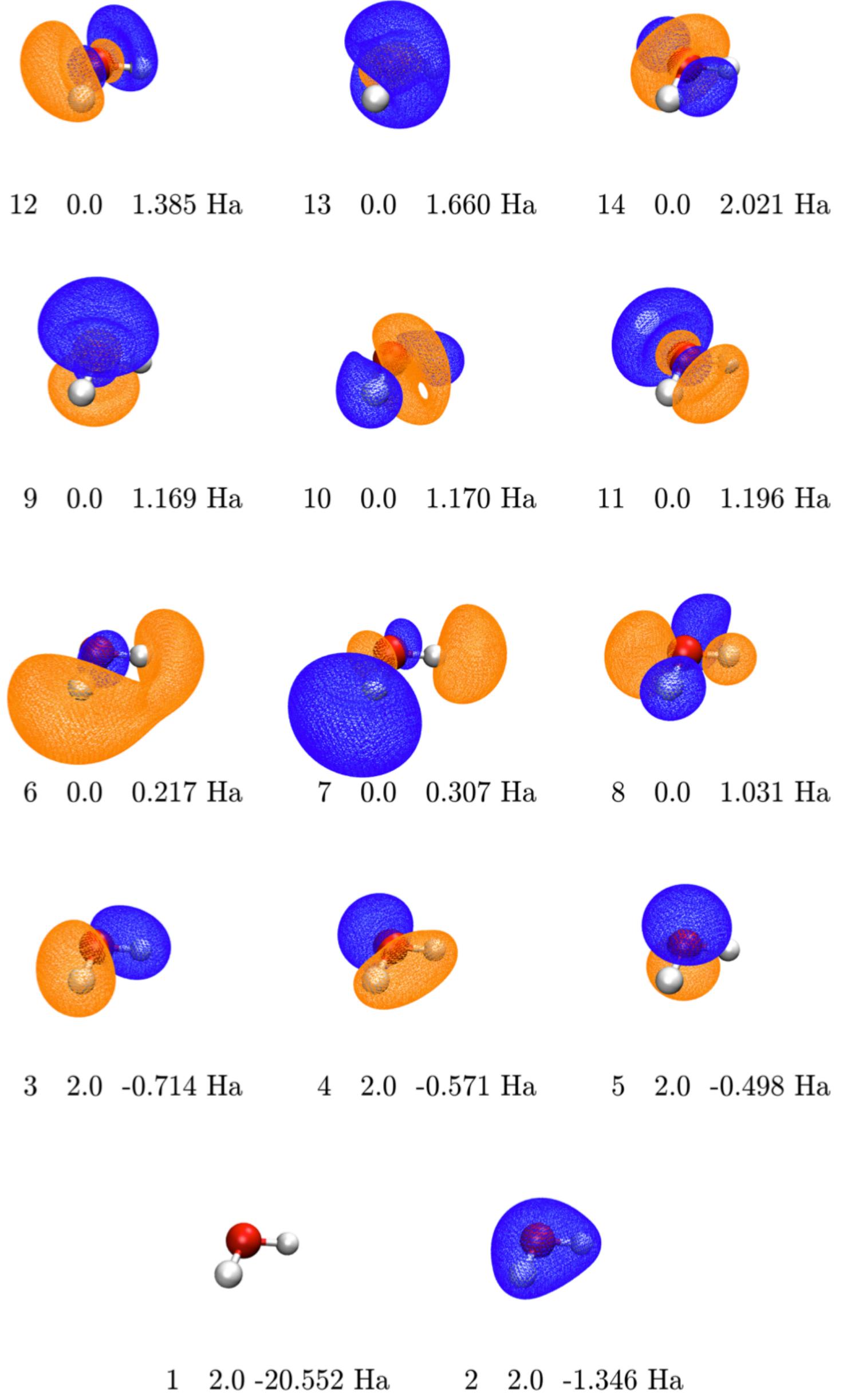
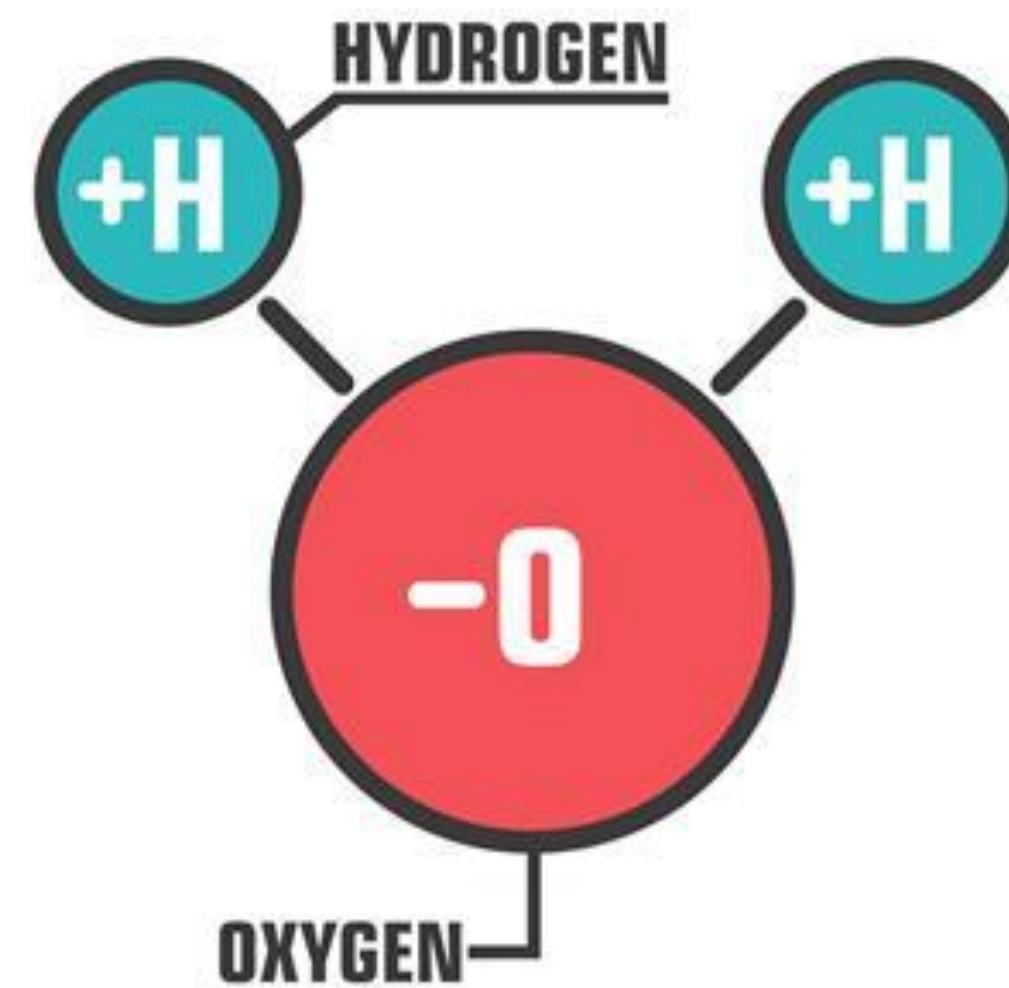
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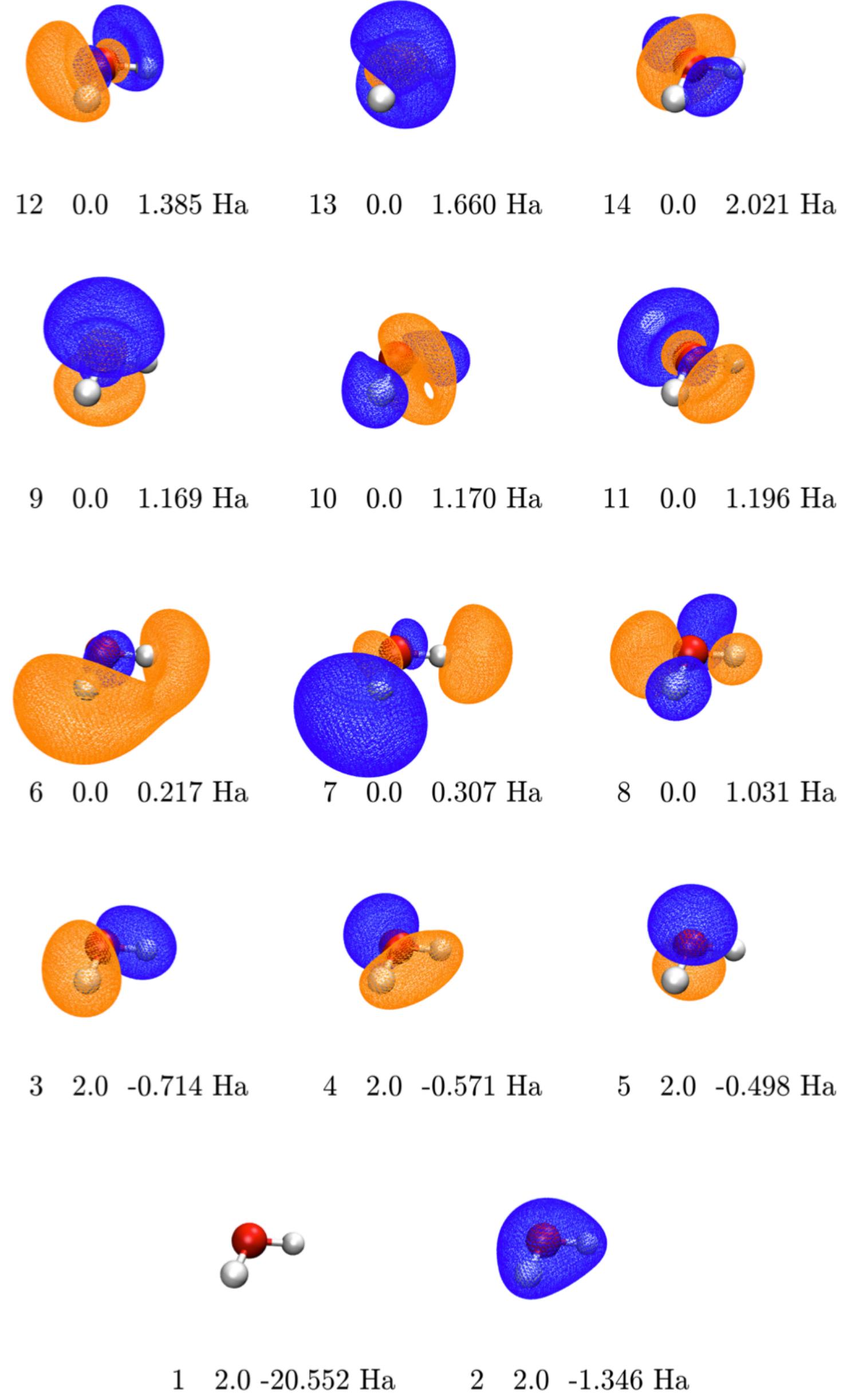
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$$|\Psi\rangle = |f_1 f_2 \dots f_M\rangle$$



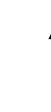
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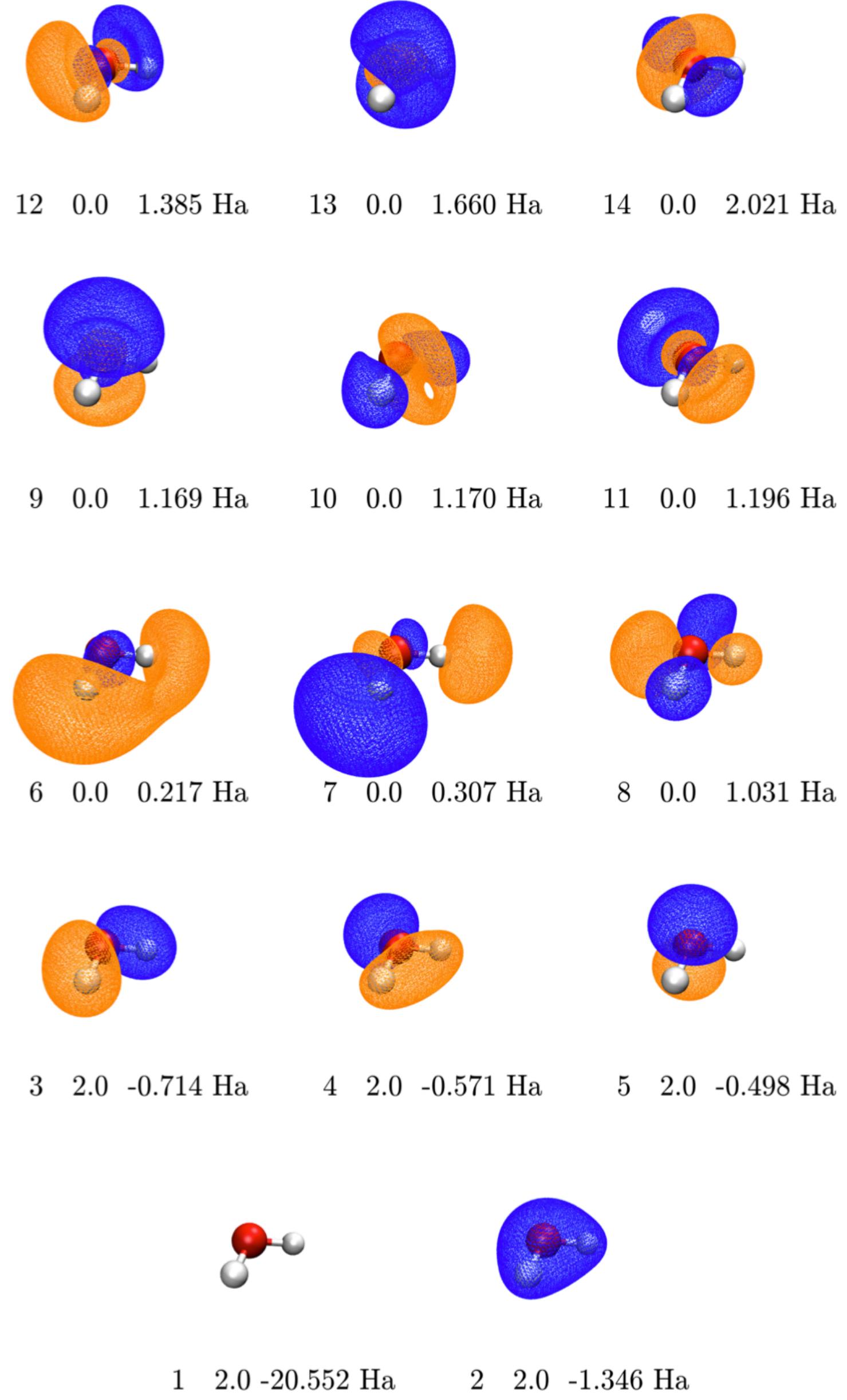
As many positions  
as spin-orbitals



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



Equal to 1 if spin-orbital occupied  
Otherwise 0



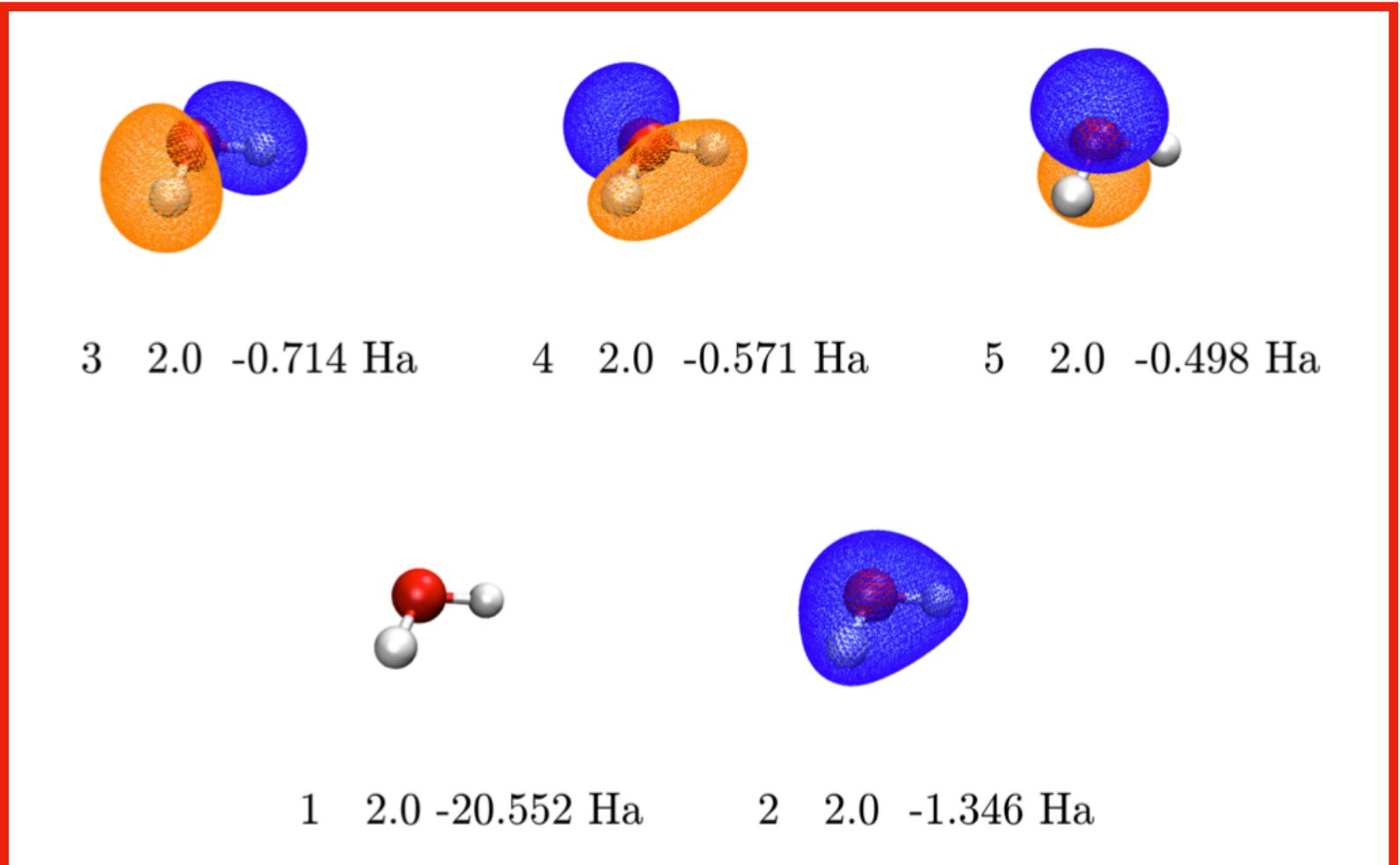
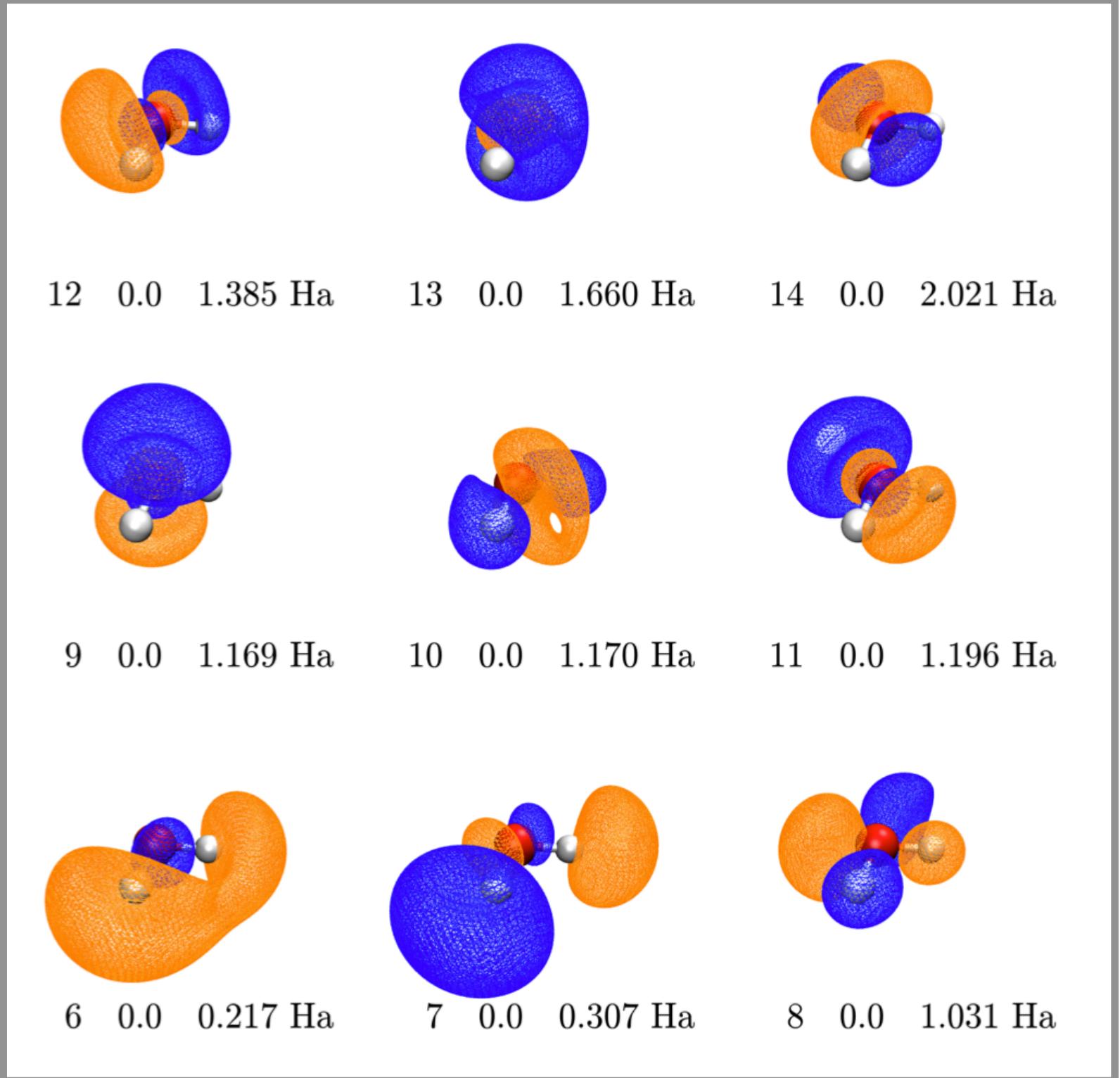
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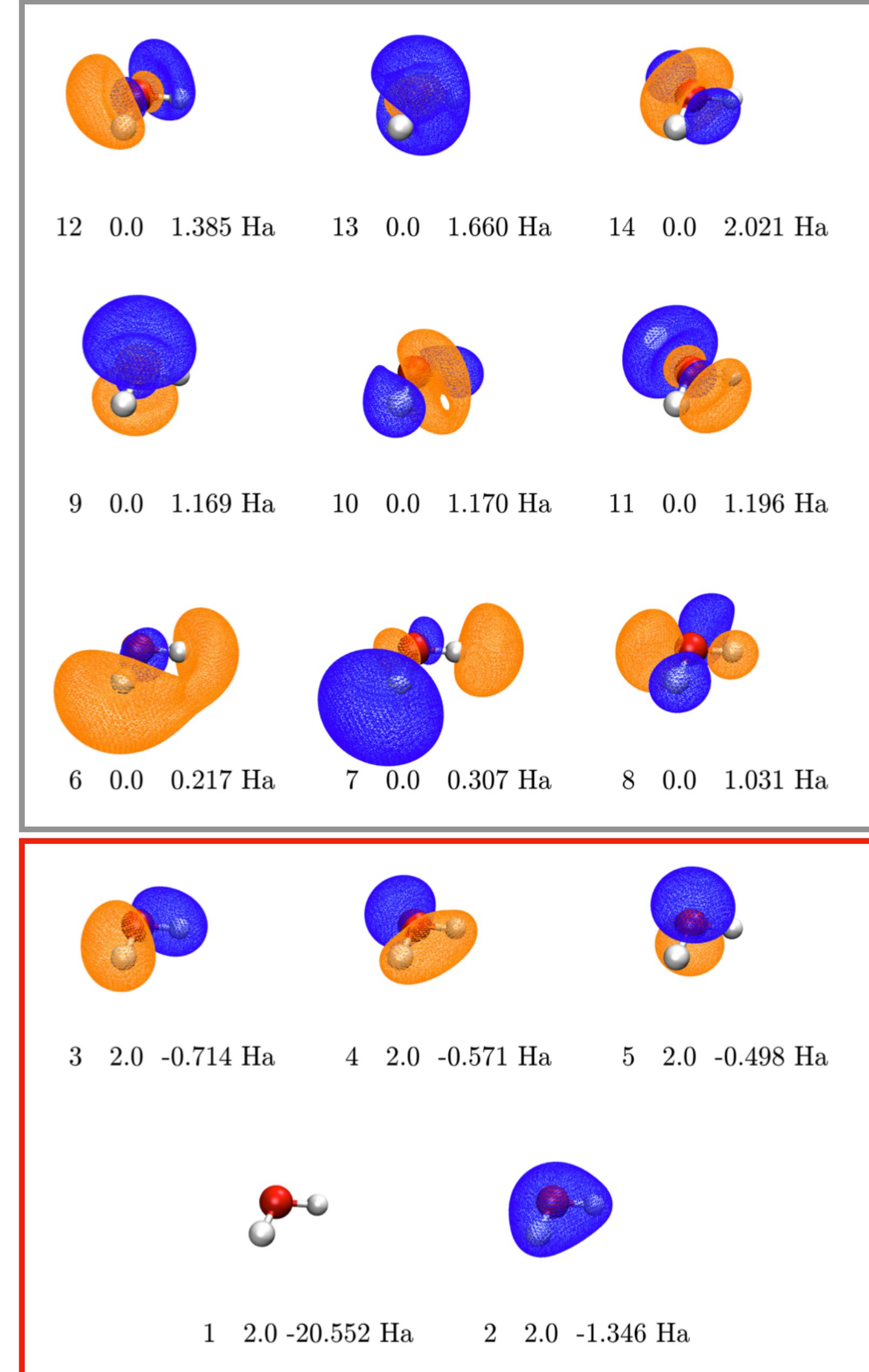
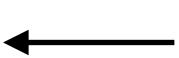
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$$|\Psi\rangle = |1 \dots 1 \boxed{0} \dots 0\rangle$$



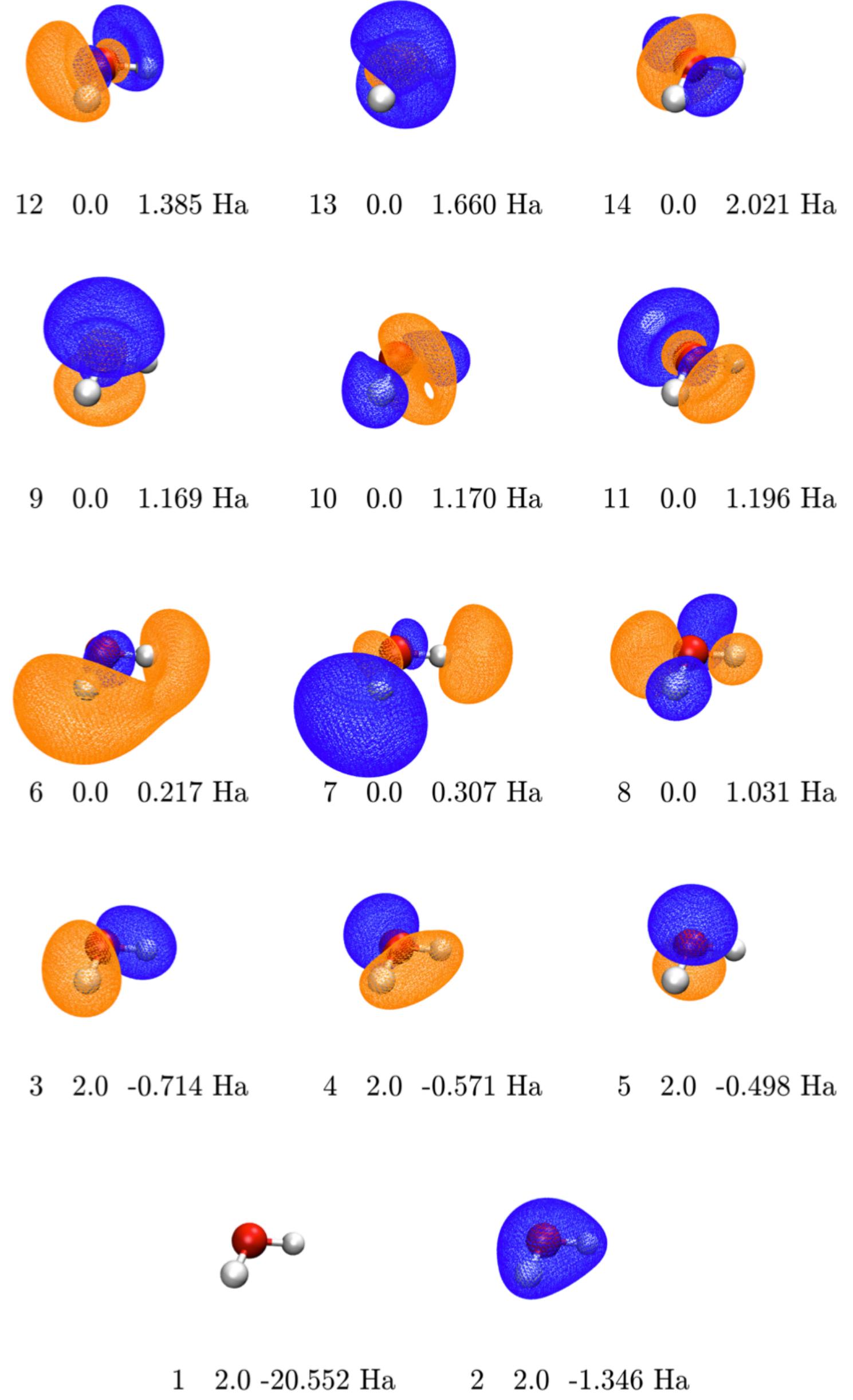
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Superposition principle: states are linear combinations of basis states



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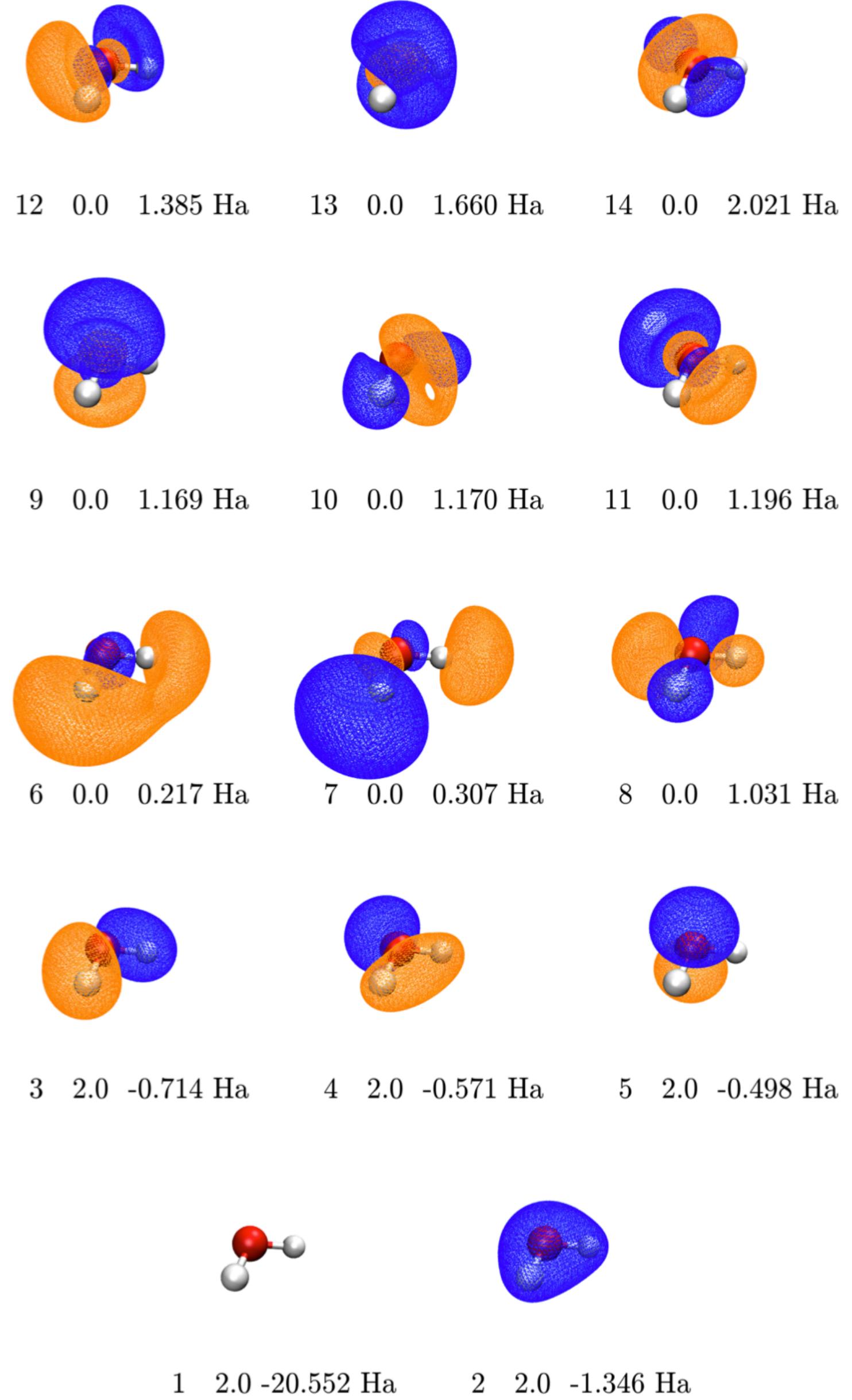
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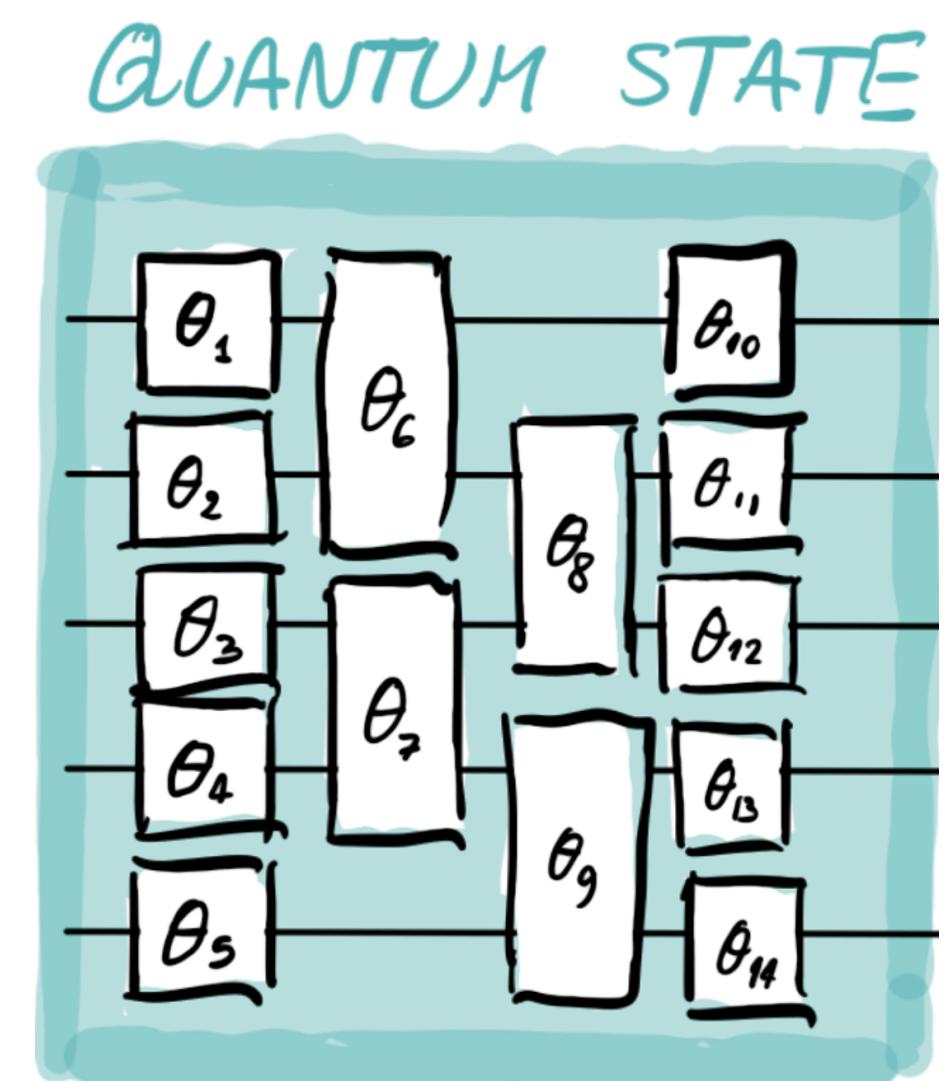
The dimensionality of state space is **classically** intractable



# Solving the problem

## The Variational Quantum Eigensolver

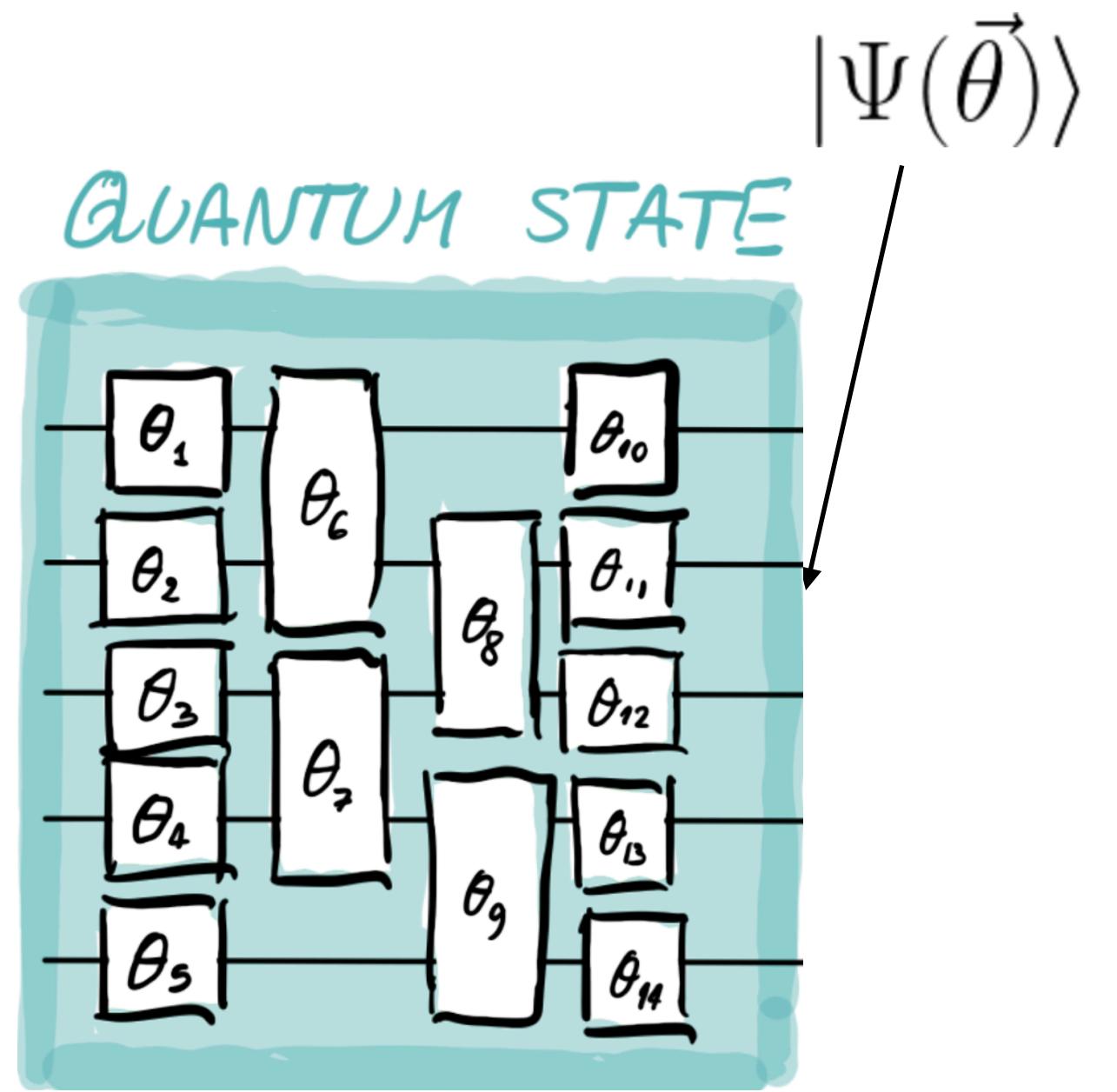
- Prepare *some* quantum state using a so-called variational form (ansatz)



# Solving the problem

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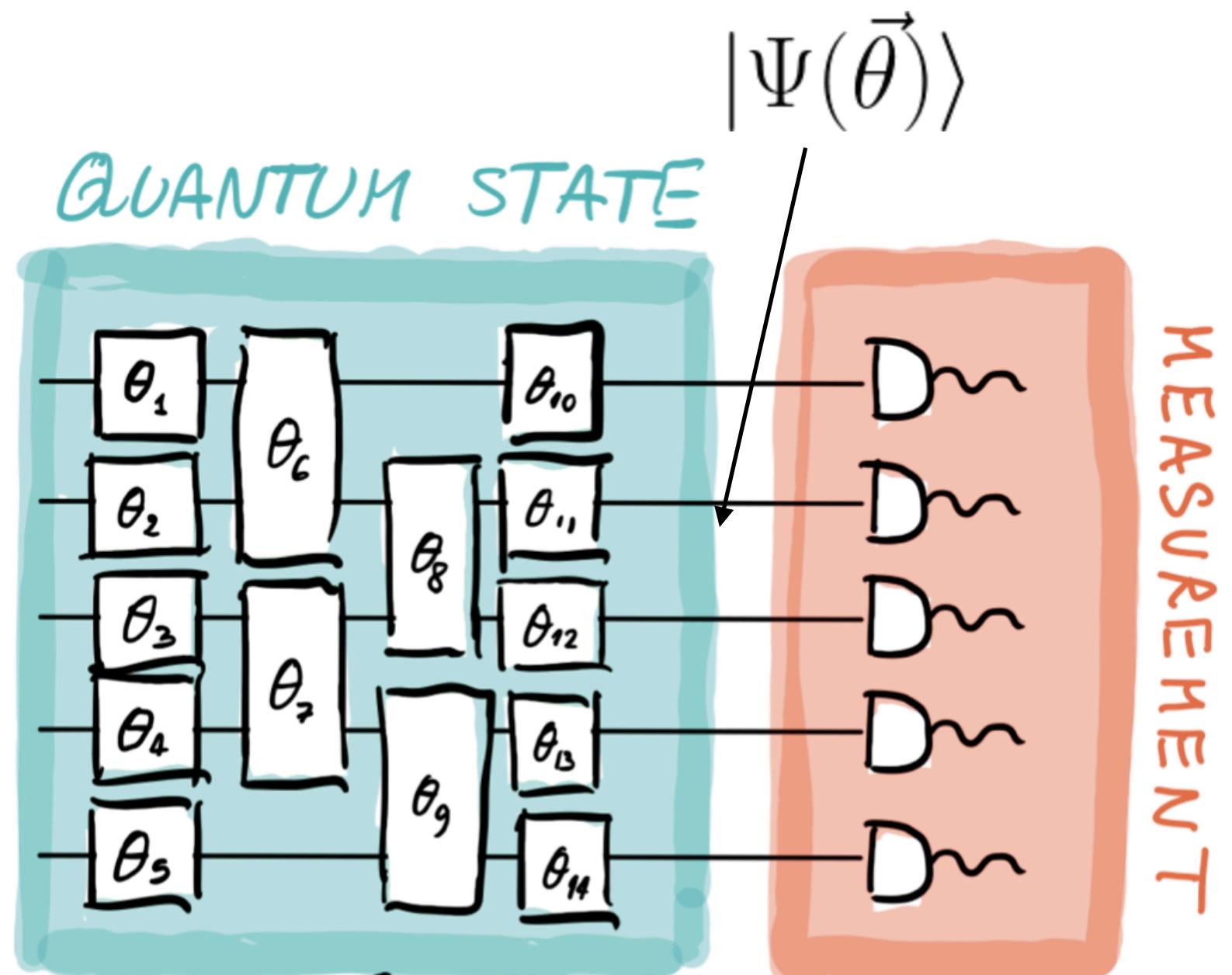
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# Solving the problem

## 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

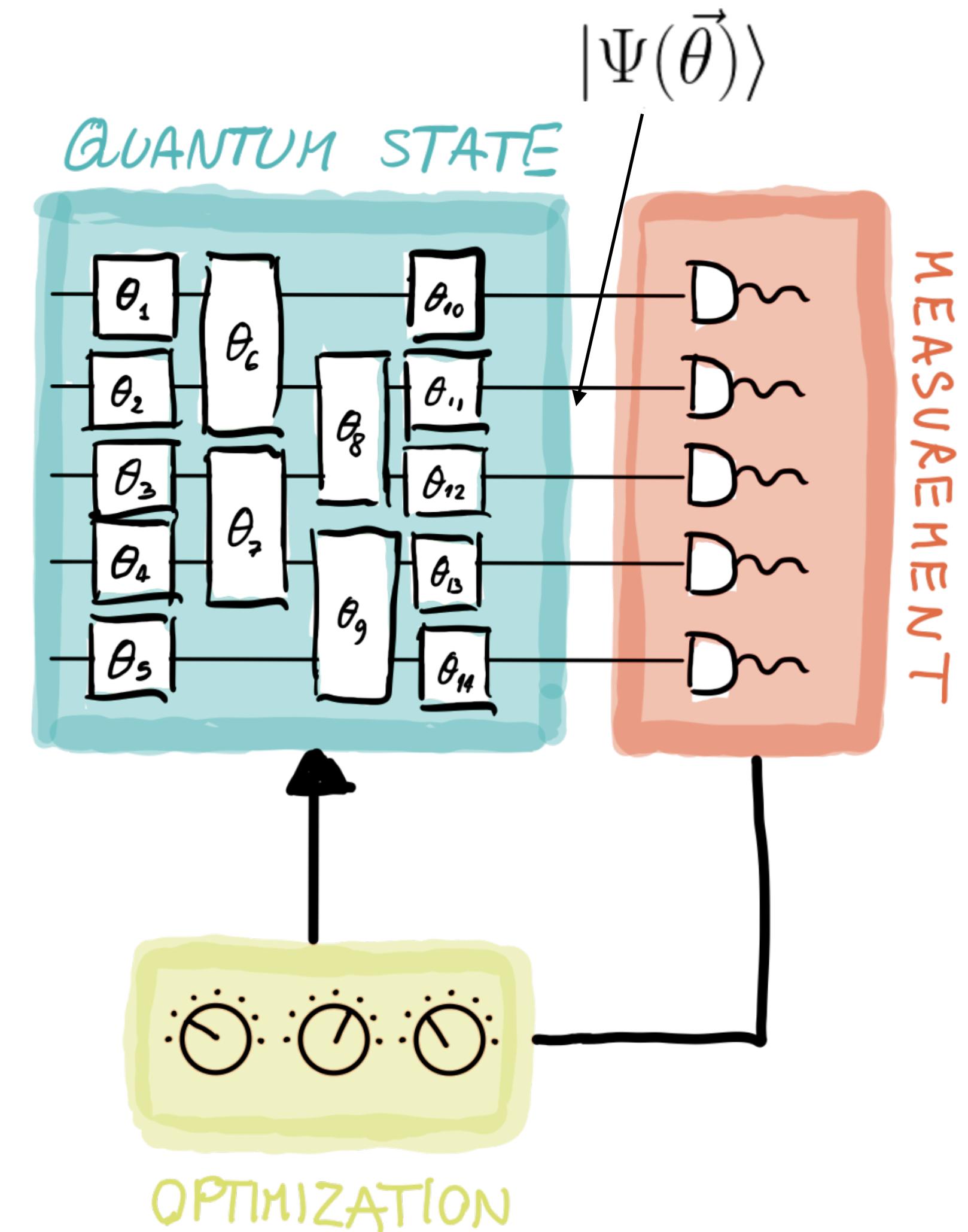


$$\langle E \rangle = \langle \Psi(\vec{\theta}) | \hat{H}_e | \Psi(\vec{\theta}) \rangle \geq E_{\text{ground}}$$

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## The Variational Quantum Eigensolver

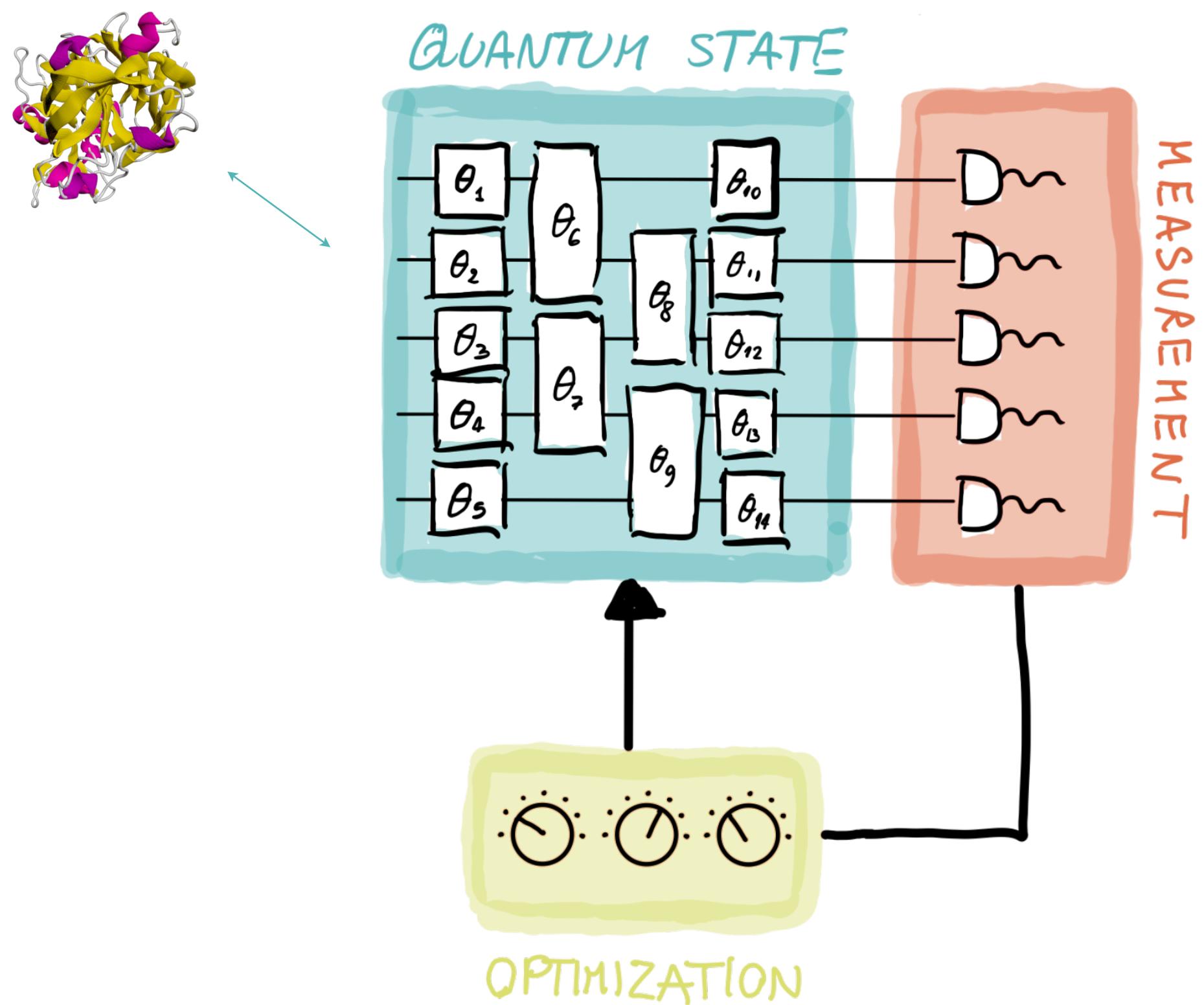
- Prepare *some* quantum state using a so-called variational form (ansatz)
- Gates in the ansatz have free parameters
- For each value of the parameters the resulting state has some mean energy
- Find the ground state variationally, that is, minimising over the parameters



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# Quantum chemistry in the near term

## The variational quantum eigensolver

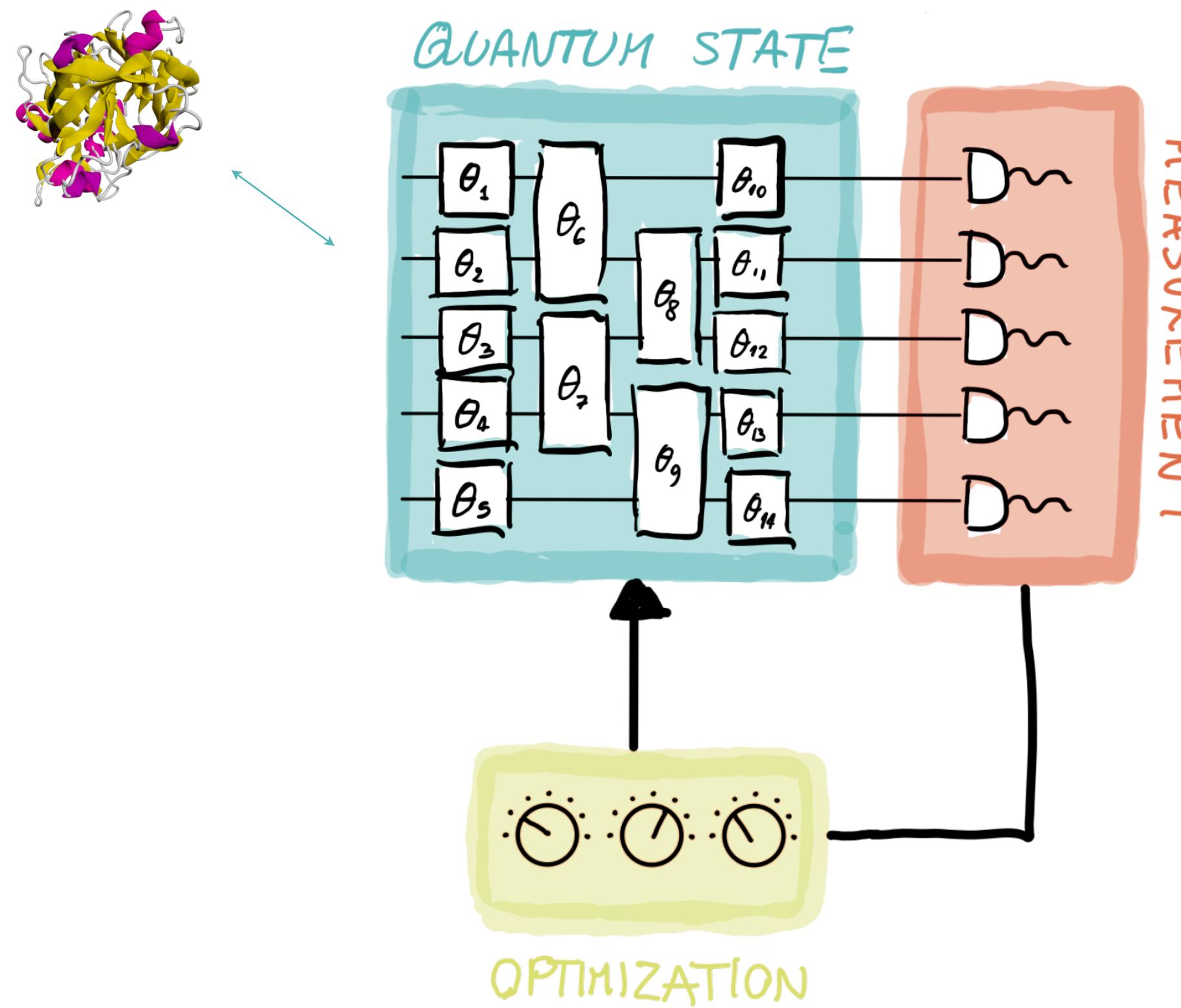


### Challenges

- 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



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

Jérôme F. Gonthier,<sup>1</sup> Maxwell D. Radin,<sup>1</sup> Corneliu Buda,<sup>2</sup>  
Eric J. Doskocil,<sup>2</sup> Clena M. Abuan,<sup>3</sup> and Jhonathan Romero<sup>1</sup>

<sup>1</sup>Zapata Computing, Inc., 100 Federal St., Boston, MA 02110, USA

Molecule	H <sub>2</sub> O	CO <sub>2</sub>	CH <sub>4</sub>	CH <sub>4</sub> O	C <sub>2</sub> H <sub>6</sub>	C <sub>2</sub> H <sub>4</sub>	C <sub>2</sub> H <sub>2</sub>	C <sub>2</sub> H <sub>6</sub> O	C <sub>3</sub> H <sub>8</sub>	C <sub>3</sub> H <sub>6</sub>	C <sub>3</sub> H <sub>4</sub>
N <sub>el</sub>	8	16	8	14	14	12	10	20	20	18	16
N <sub>q</sub>	104	208	104	182	182	156	130	260	260	234	208
K · 10 <sup>-3</sup>	1.9	16	1.6	8.4	8.5	6.6	3.1	24	16	23	18
M · 10 <sup>-9</sup>	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

31 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

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

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

- 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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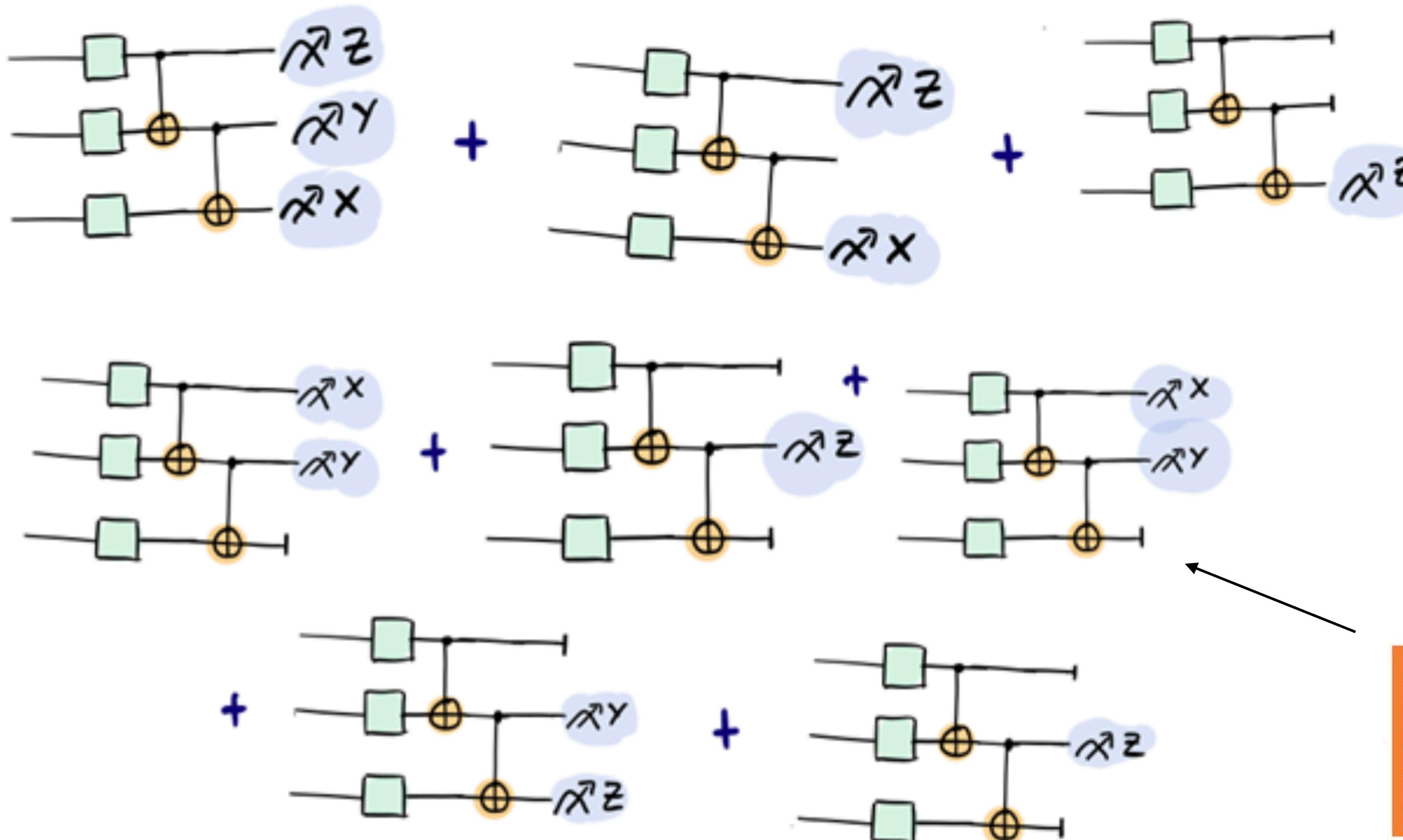


Cannot even write down  
on a classical computer

Easy on a quantum computer: only  
requires measuring Pauli strings

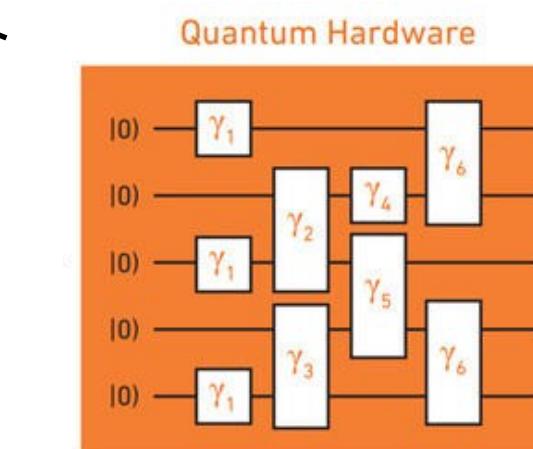
# (Specific) problem statement

Measurement cost in VQE



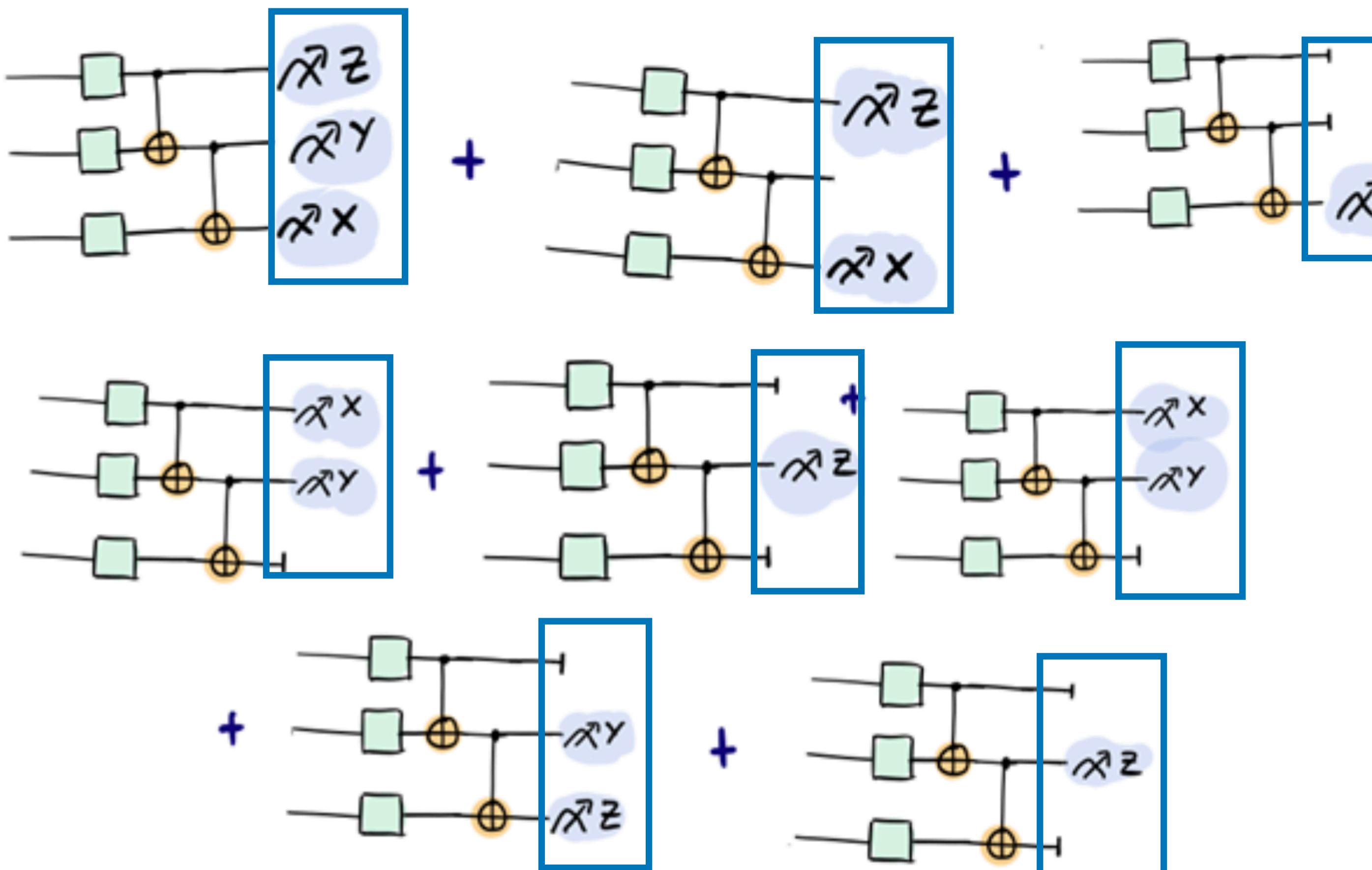
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Every Pauli string evaluated  
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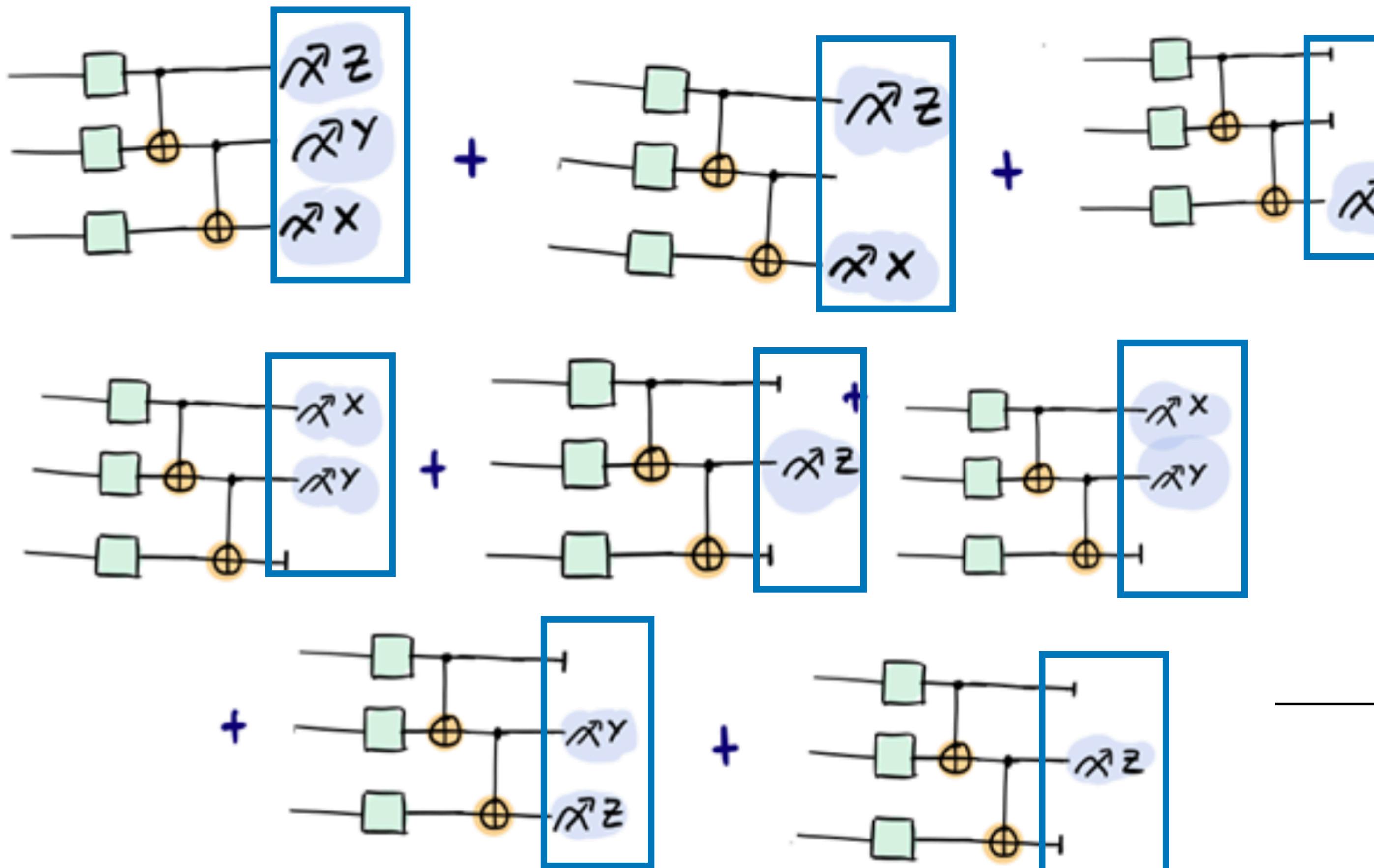
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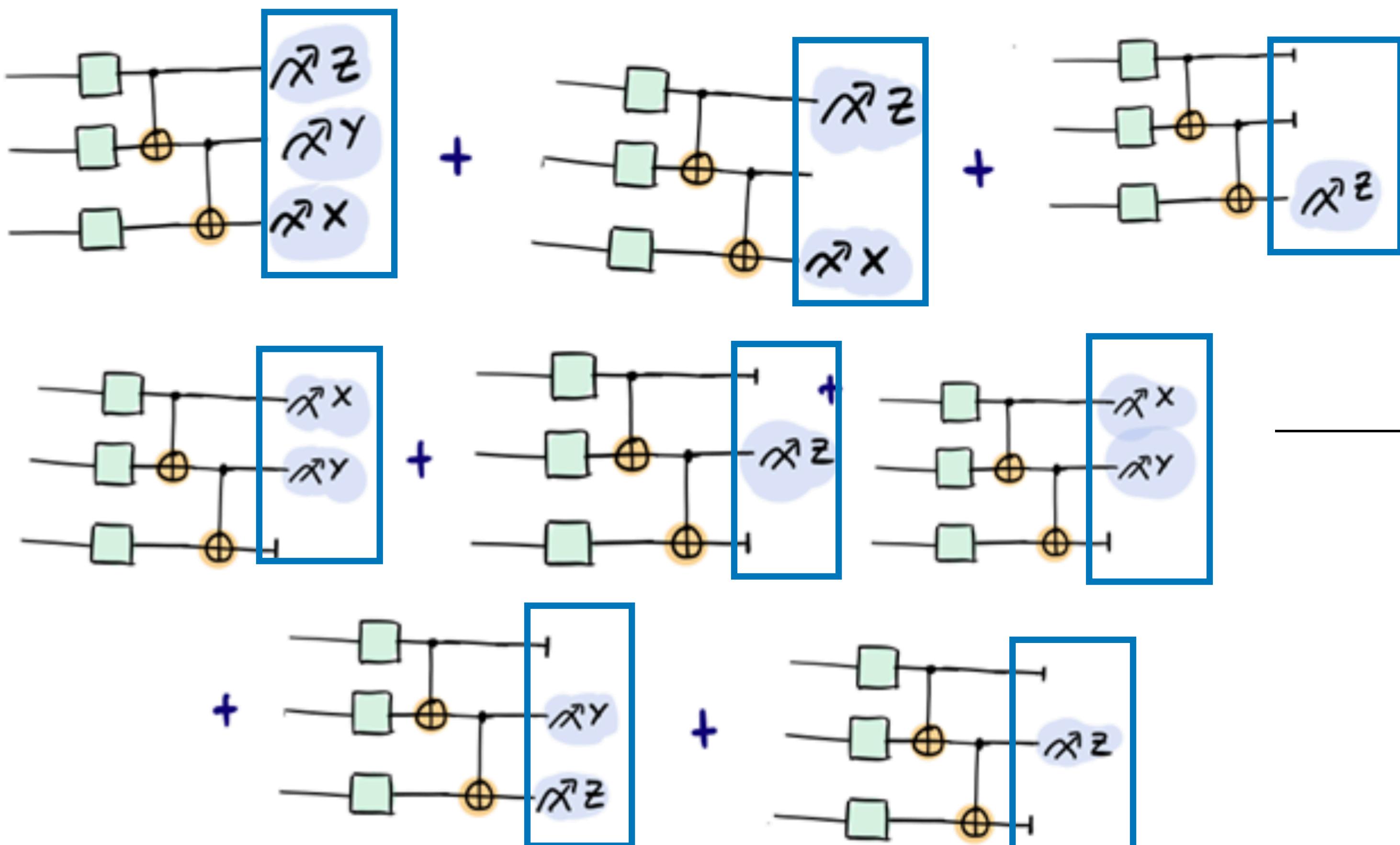


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Repeat each many times to  
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Measurement cost in VQE



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

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:  $S = O(N^{5/6})$

# References

- O'Malley, P. J. J.; Babbush, R.; Kivlichan, I. D.; Romero, J.; McClean, J. R.; Barends, R.; Kelly, J.; Roushan, P.; Tranter, A.; Ding, N.; Campbell, B.; Chen, Y.; Chen, Z.; Chiaro, B.; Dunsworth, A.; Fowler, A. G.; Jeffrey, E.; Lucero, E.; Megrant, A.; Mutus, J. Y.; Neeley, M.; Neill, C.; Quintana, C.; Sank, D.; Vainsencher, A.; Wenner, J.; White, T. C.; Coveney, P. V.; Love, P. J.; Neven, H.; Aspuru-Guzik, A.; Martinis, J. M. **Scalable Quantum Simulation of Molecular Energies**. *Phys. Rev. X*. 2016, 6, 031007. <https://doi.org/10.1103/PhysRevX.6.031007>.
- McArdle, S.; Endo, S.; Aspuru-Guzik, A.; Benjamin, S. C.; Yuan, X. **Quantum Computational Chemistry**. *Rev. Mod. Phys.* 2020, 92 (1), 015003. <https://doi.org/10.1103/revmodphys.92.015003>.
- Tilly, J.; Chen, H.; Cao, S.; Picozzi, D.; Setia, K.; Li, Y.; Grant, E.; Wossnig, L.; Rungger, I.; Booth, G. H.; Tennyson, J. **The Variational Quantum Eigensolver: A Review of Methods and Best Practices**. *Phys. Rep.* 2022, 986, 1–128. <https://doi.org/10.1016/j.physrep.2022.08.003>.
- Huggins, W. J.; McClean, J. R.; Rubin, N. C.; Jiang, Z.; Wiebe, N.; Whaley, K. B.; Babbush, R. **Efficient and Noise Resilient Measurements for Quantum Chemistry on Near-Term Quantum Computers**. *Npj Quantum Inf.* 2021, 7 (1), 1–9. <https://doi.org/10.1038/s41534-020-00341-7>.

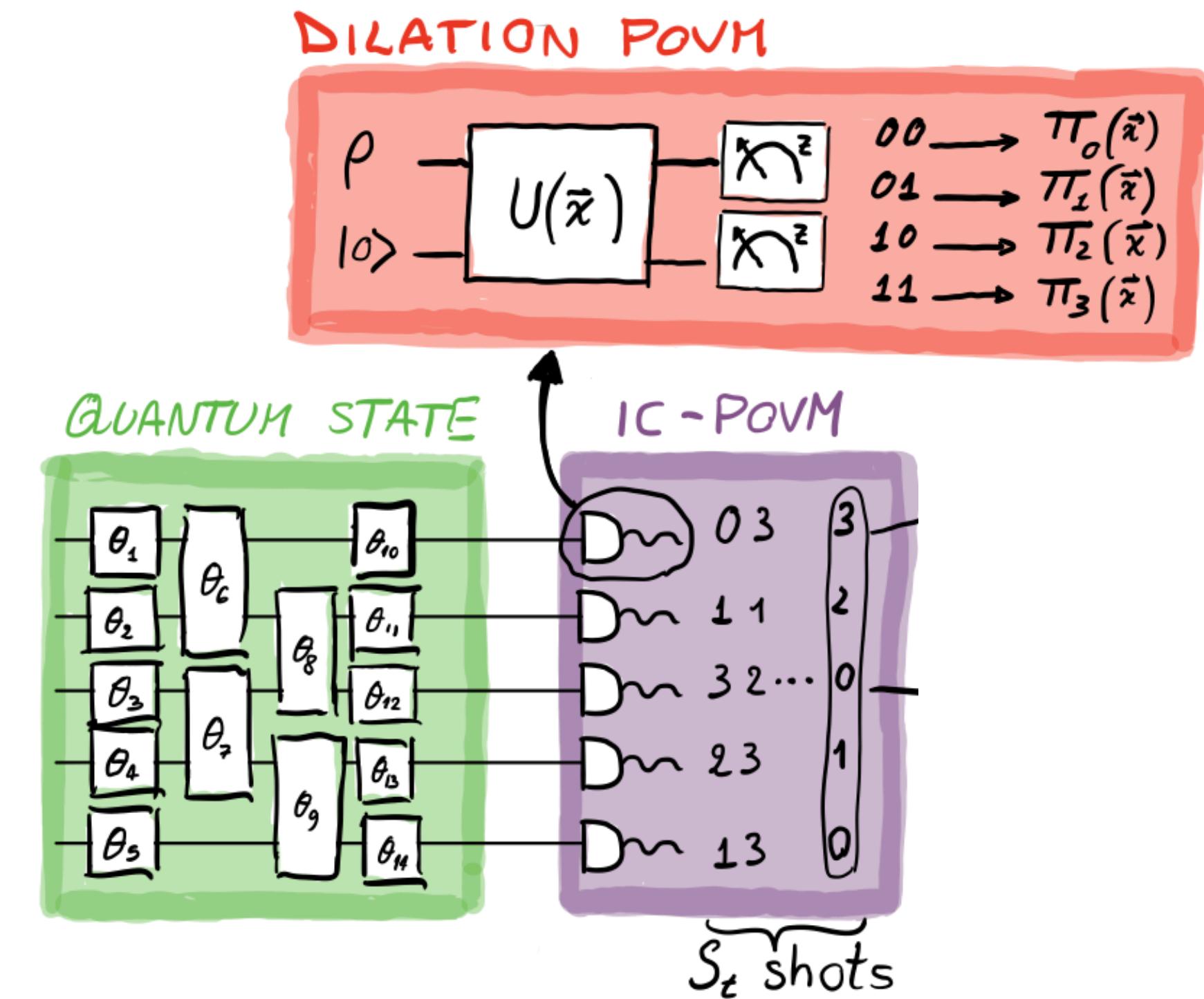
# Informationally Complete Measurements

# 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



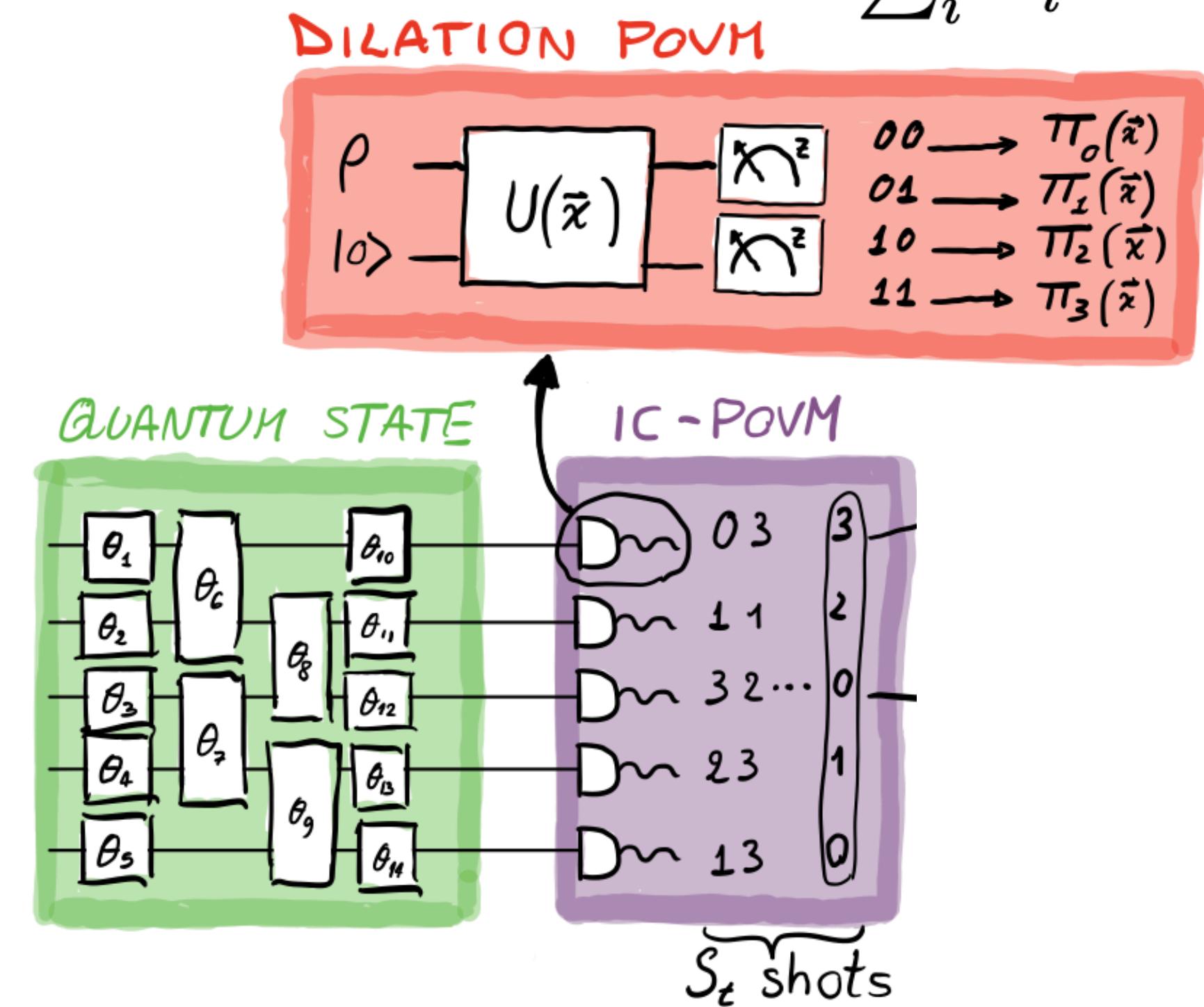
# Tackling the measurement problem

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  $\Pi_{\mathbf{m}} = \bigotimes_{i=1}^N \Pi_{m_i}^{(i)}$

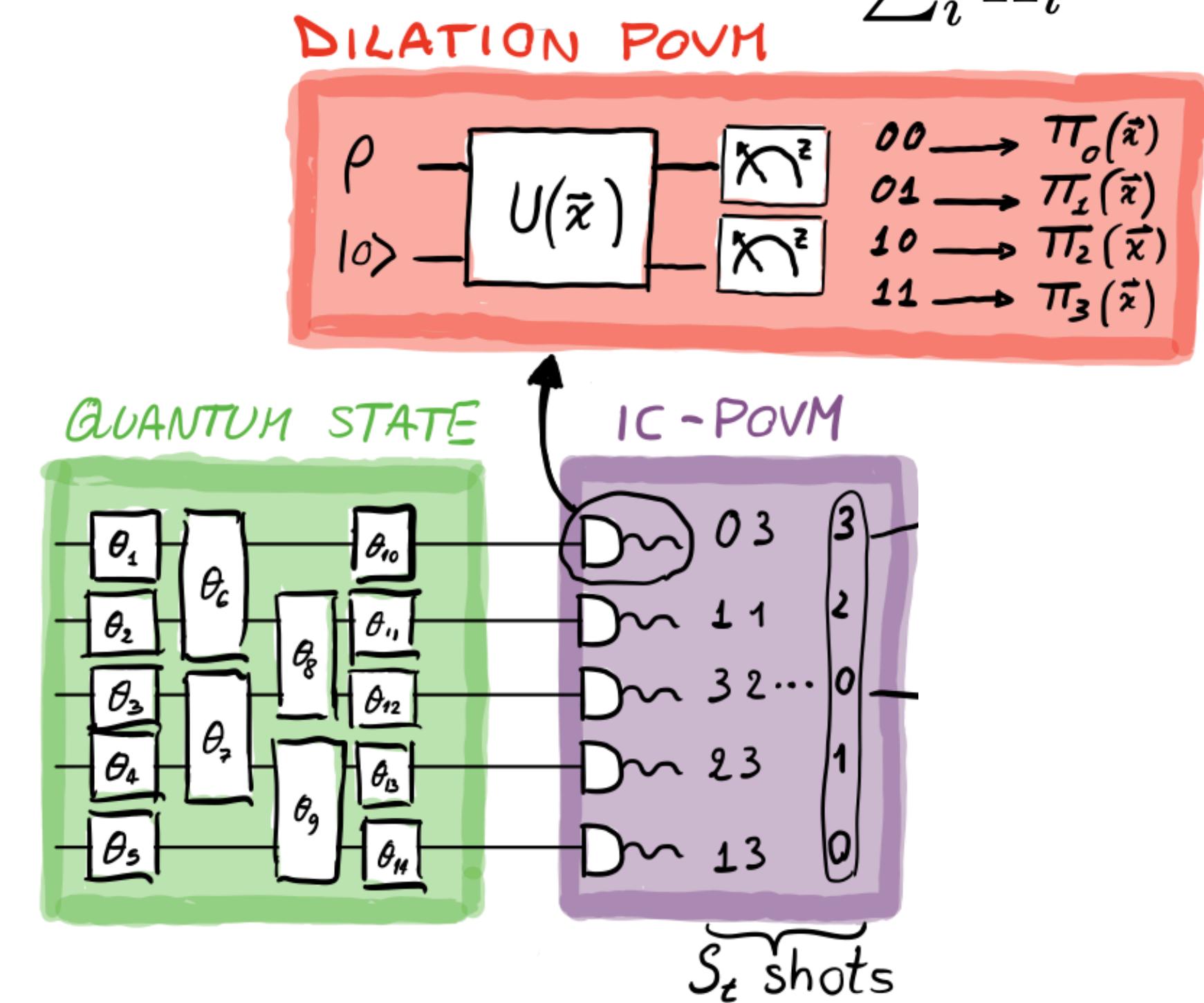
# Tackling the measurement problem

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

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



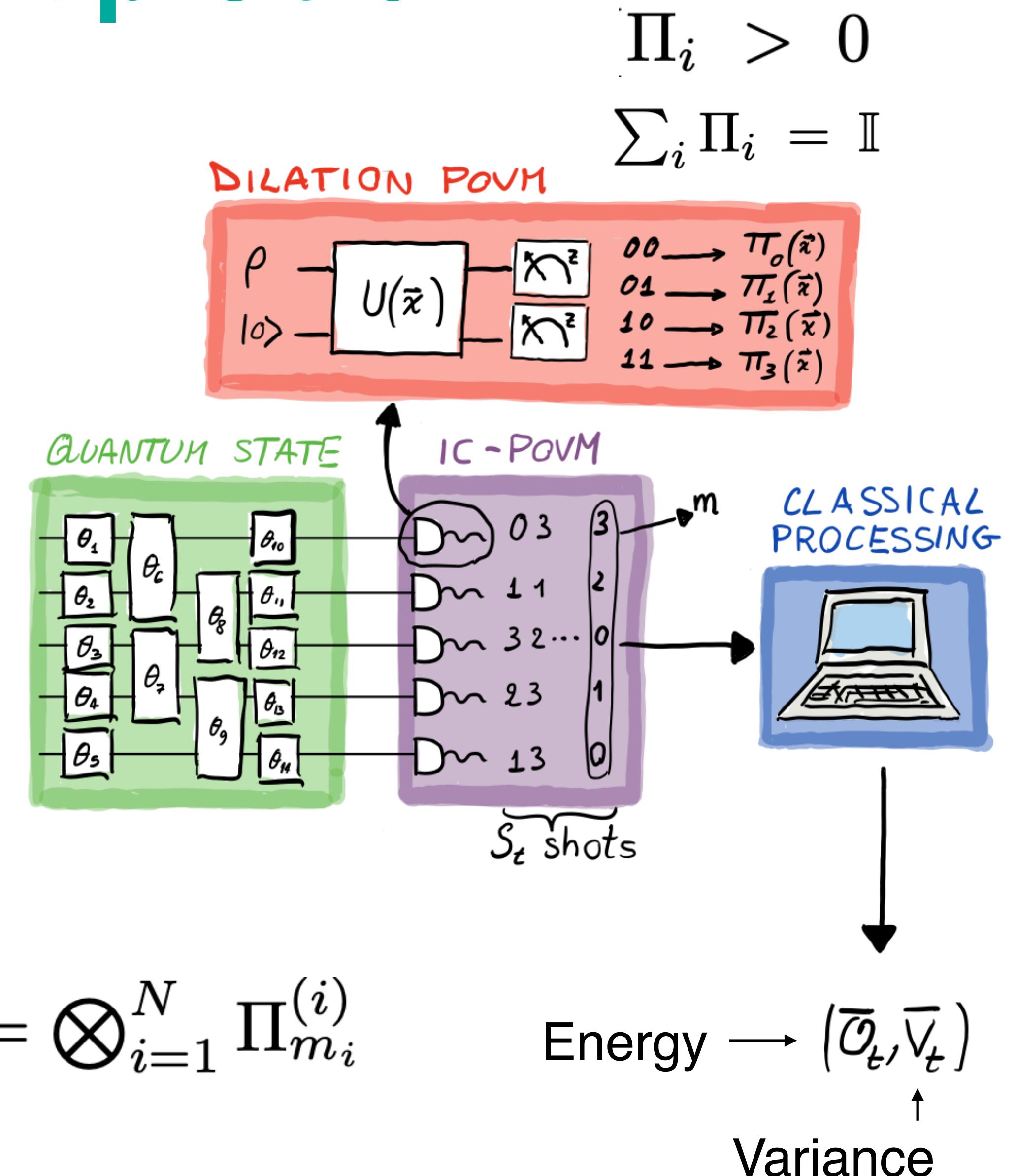
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Probability of outcome  $m$ :  $\text{Tr}[\rho \Pi_m]$  where  $\Pi_m = \bigotimes_{i=1}^N \Pi_{m_i}^{(i)}$

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

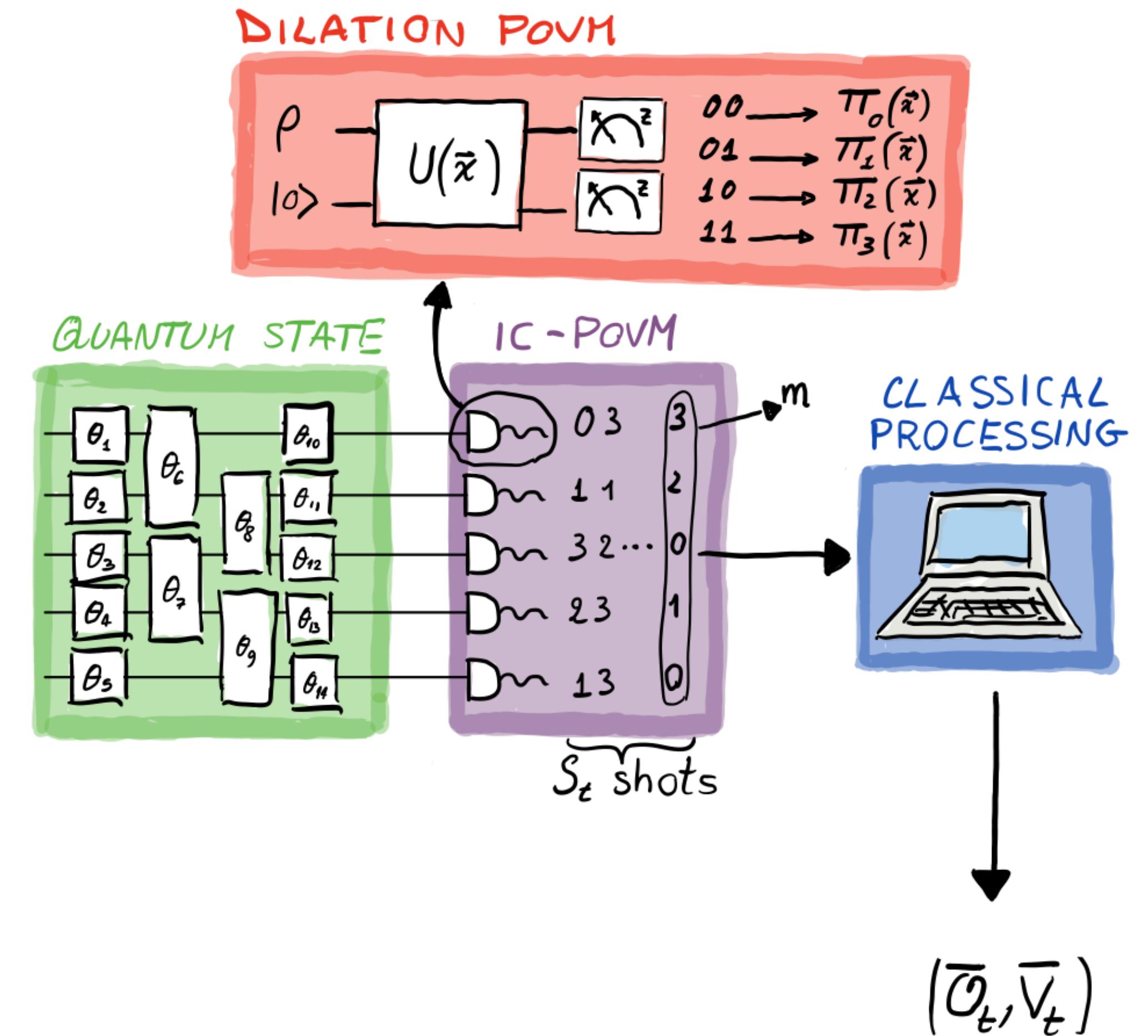
Variance  
↑

# Tackling the measurement problem

with adaptive generalised measurements

Optimising measurements on the fly

- Qubit-ancilla interaction is parametrised

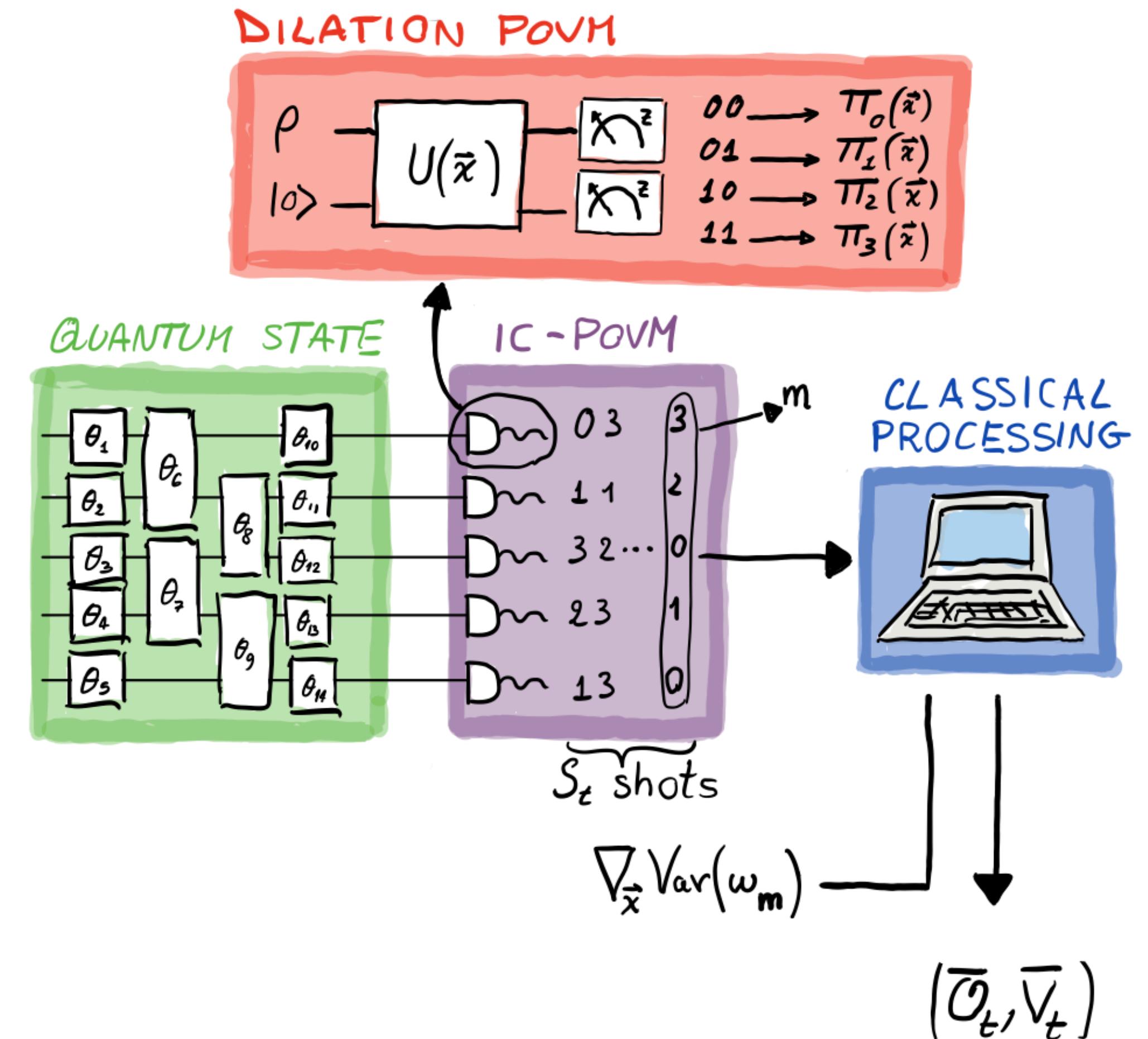


# Tackling the measurement problem

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

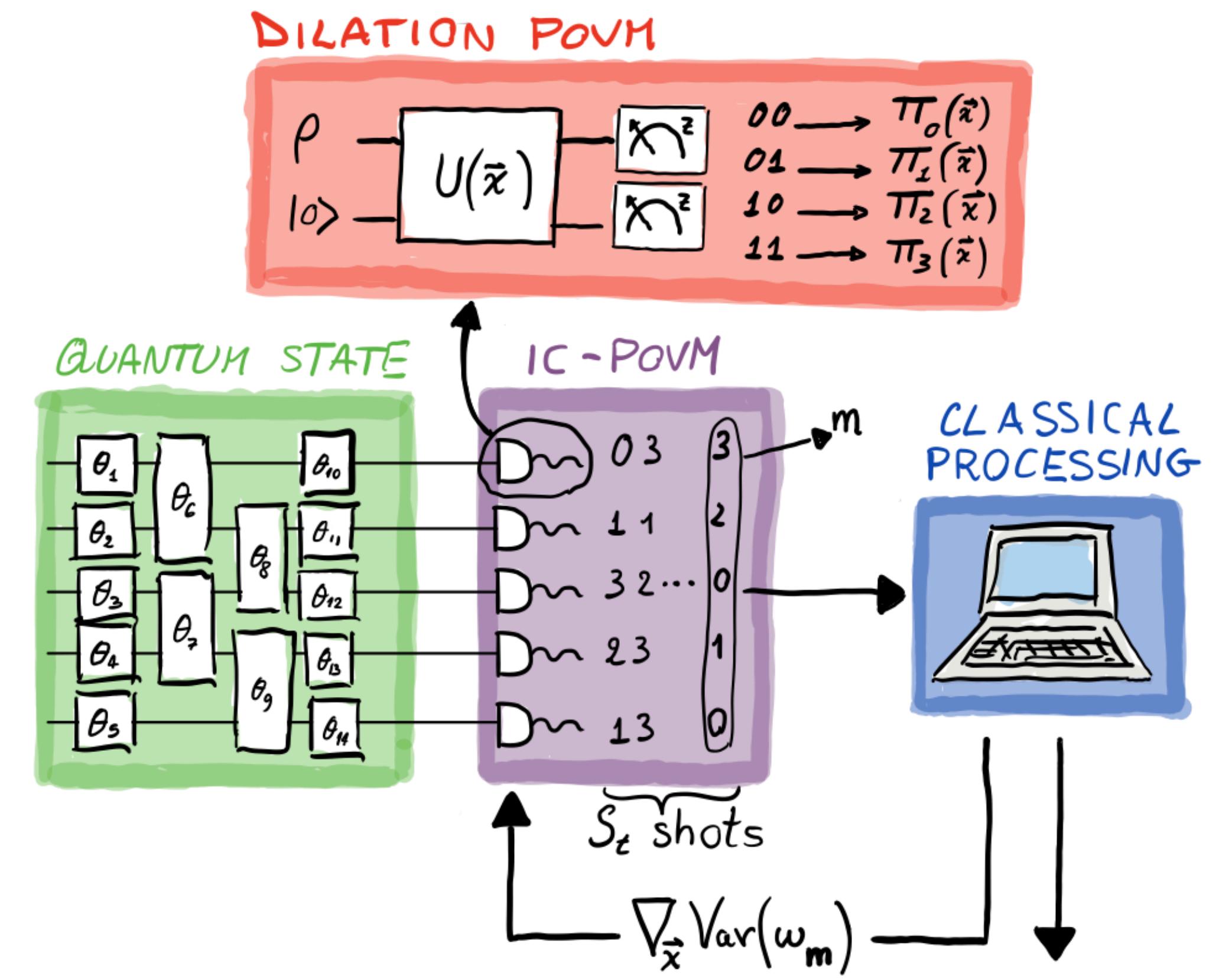


# Tackling the measurement problem

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



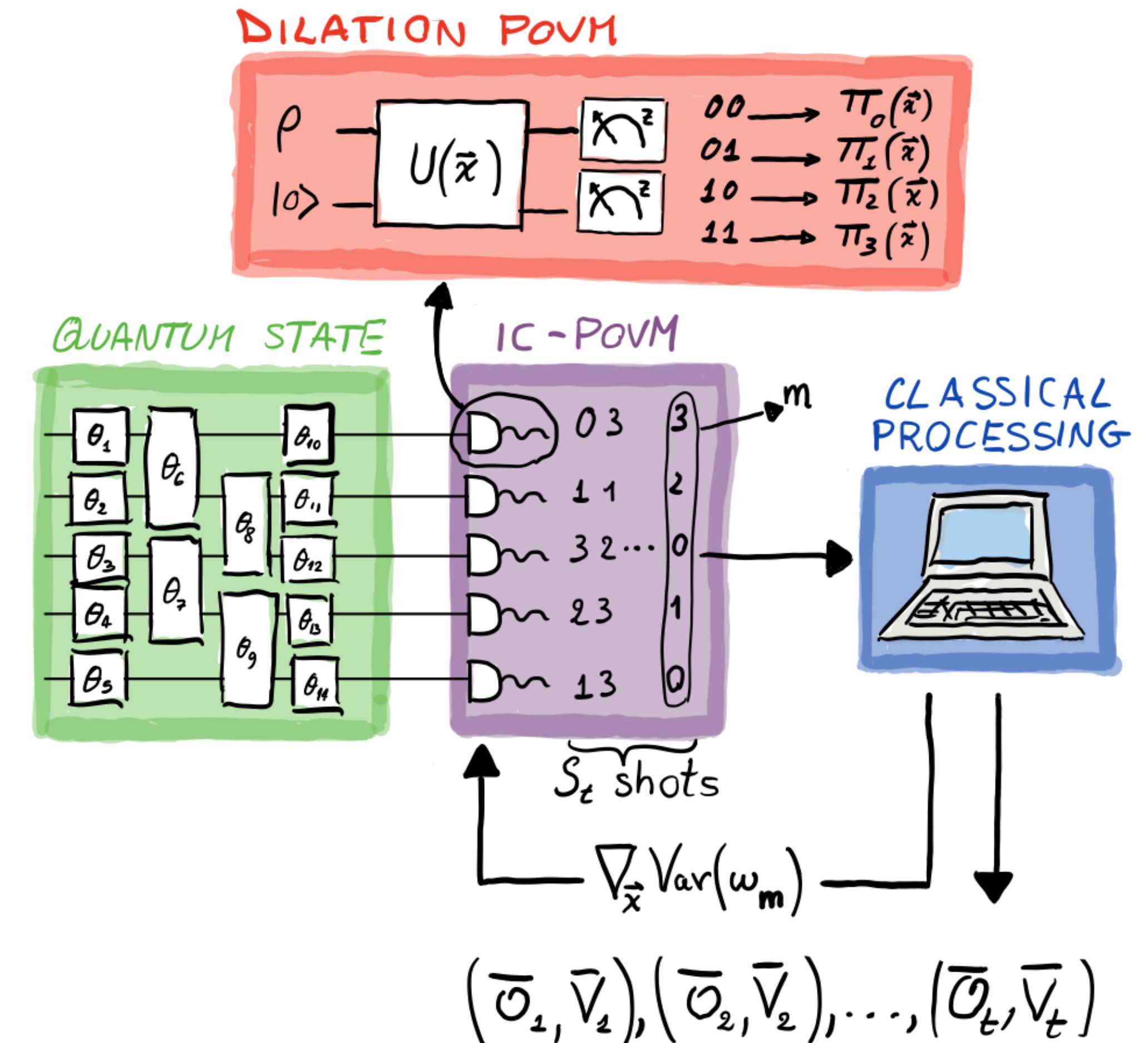
$$(\bar{O}_t, \bar{V}_t)$$

# 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

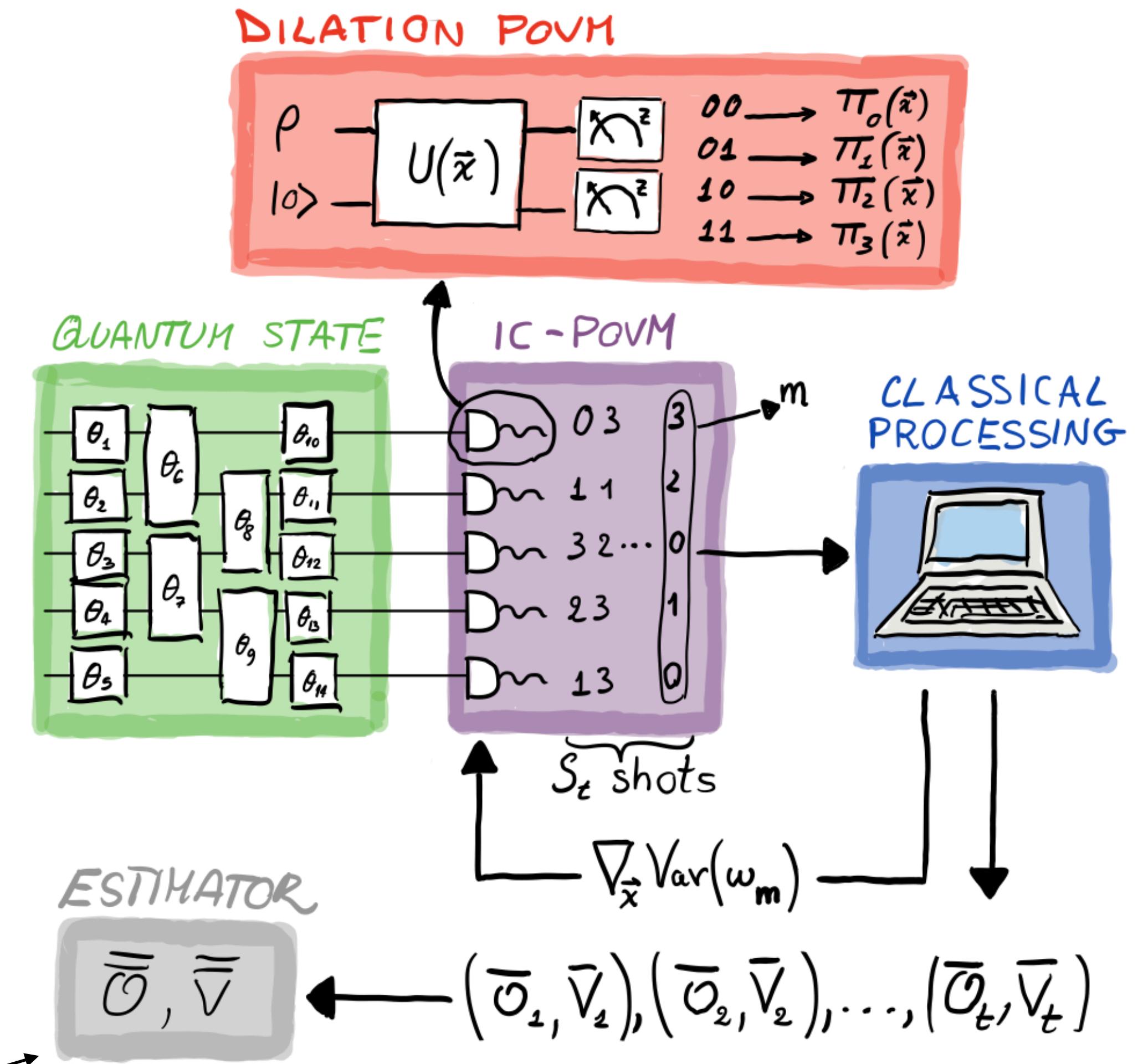


# Tackling the measurement problem

with adaptive generalised measurements

Optimising measurements on the fly

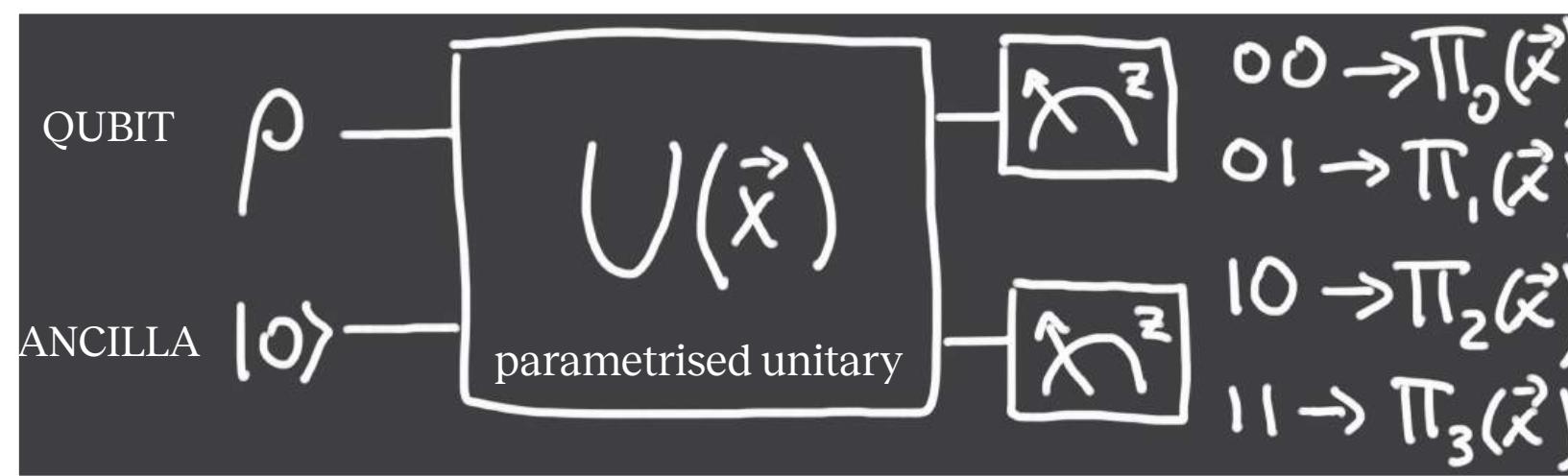
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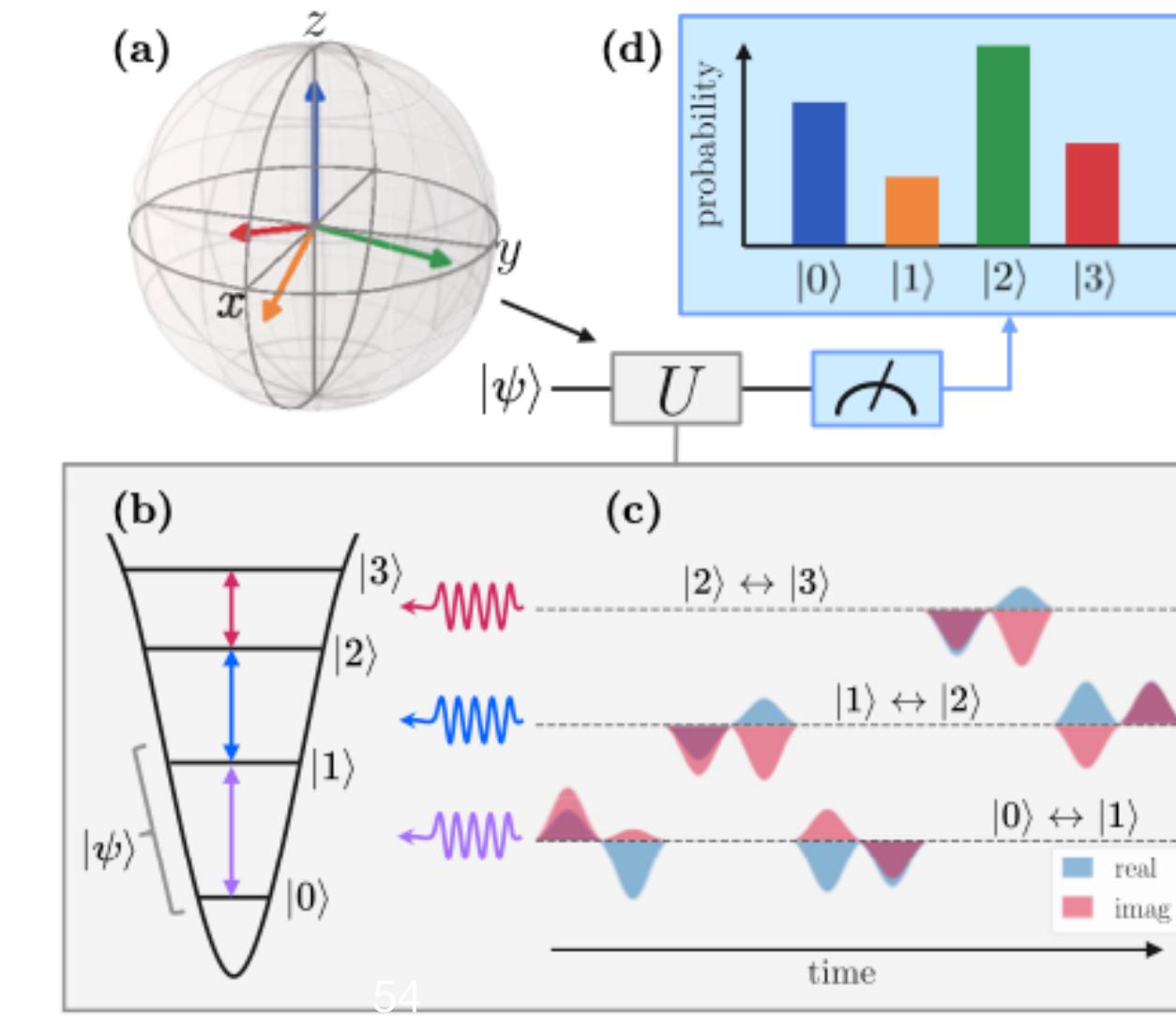
# POVM implementations

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]

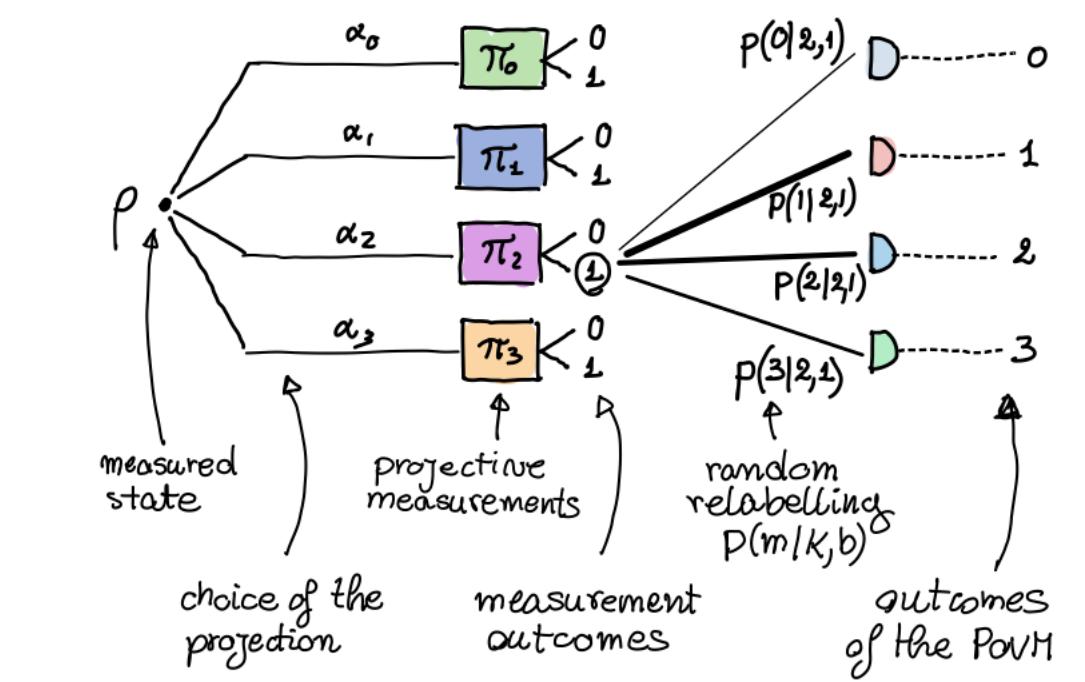


[2]



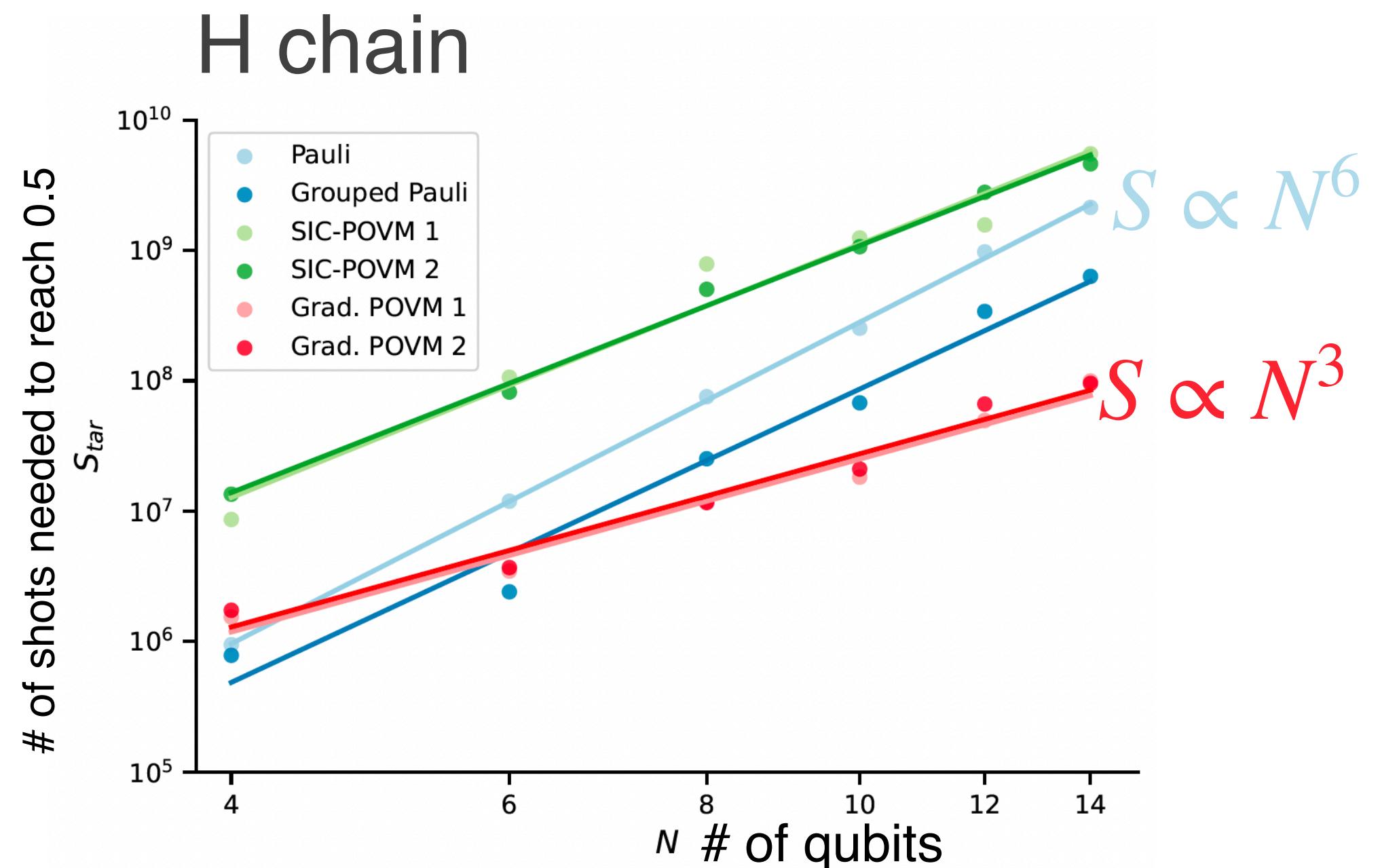
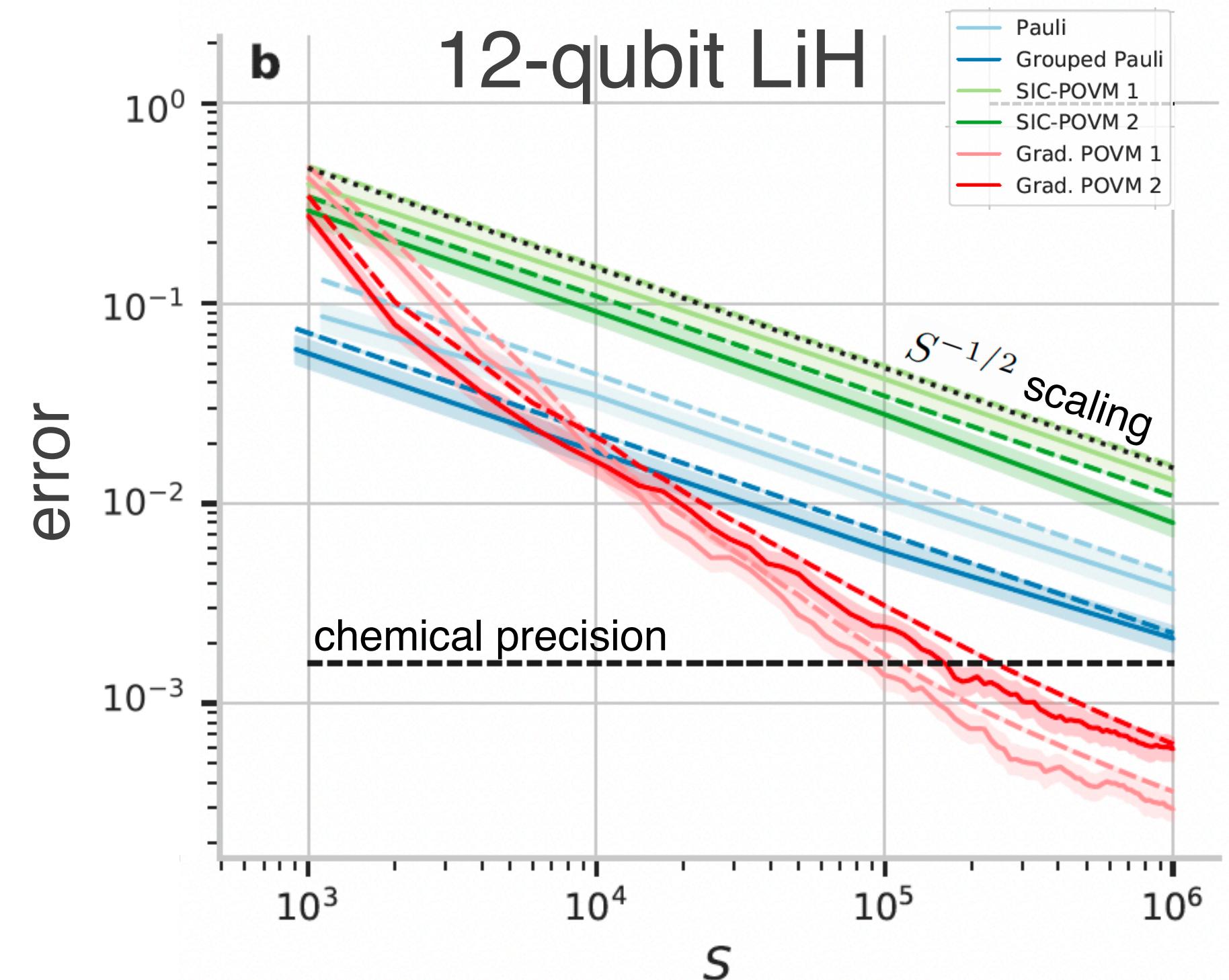
54

[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

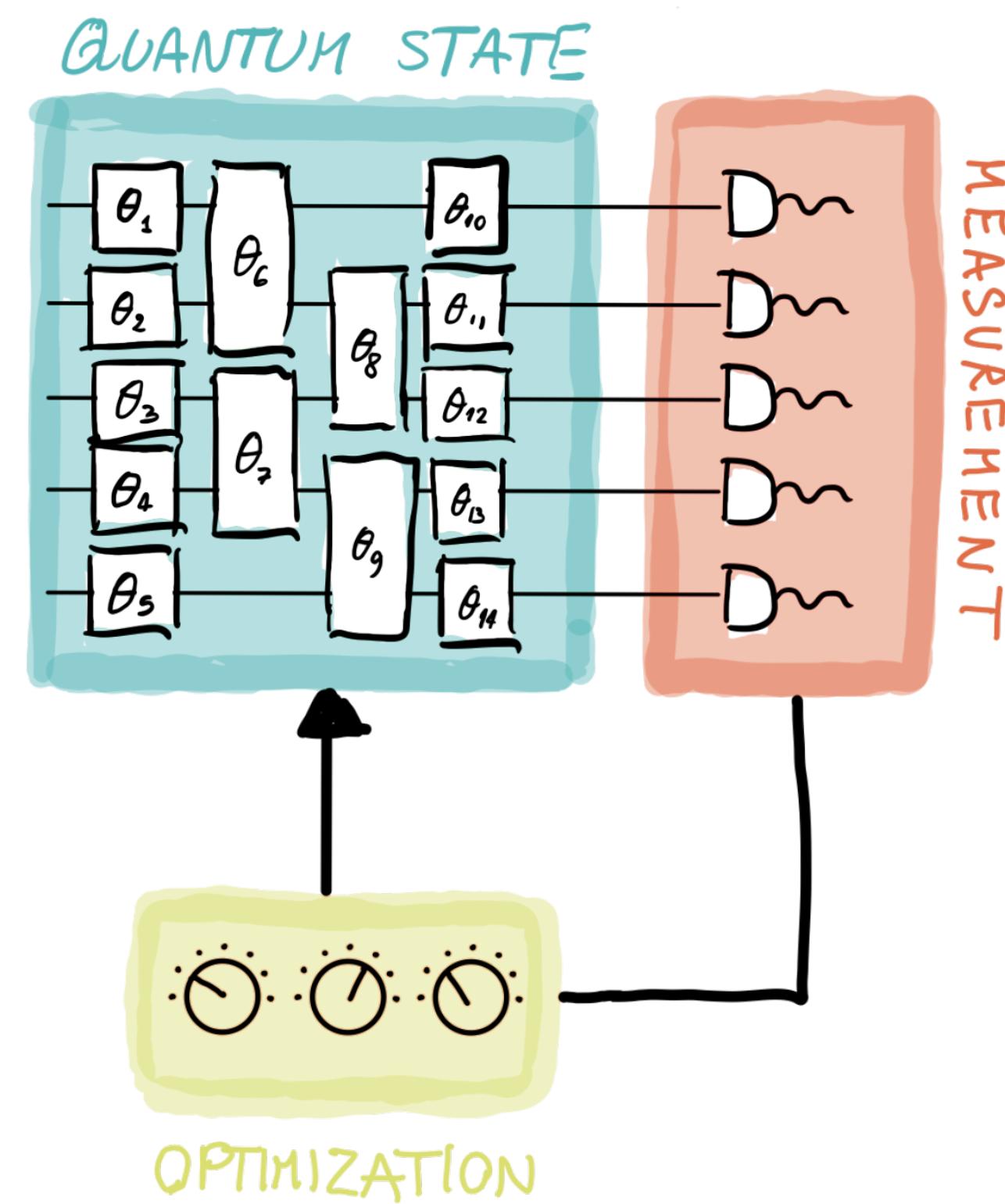
- García-Pérez, G.; Rossi, M. A. C.; Sokolov, B.; Tacchino, F.; Barkoutsos, P. K.; Mazzola, G.; Tavernelli, I.; Maniscalco, S. **Learning to Measure: Adaptive Informationally Complete Generalized Measurements for Quantum Algorithms.** PRX Quantum 2021, 2 (4), 040342. <https://doi.org/10.1103/PRXQuantum.2.040342>.
- Glos, A.; Nykänen, A.; Borrelli, E.-M.; Maniscalco, S.; Rossi, M. A. C.; Zimborás, Z.; García-Pérez, G. **Adaptive POVM Implementations and Measurement Error Mitigation Strategies for Near-Term Quantum Devices.** arXiv [quant-ph], 2022. <http://arxiv.org/abs/2208.07817>.
- Fischer, L. E.; Miller, D.; Tacchino, F.; Barkoutsos, P. K.; Egger, D. J.; Tavernelli, I. **Ancilla-Free Implementation of Generalized Measurements for Qubits Embedded in a Qudit Space.** Phys. Rev. Res. 2022, 4 (3), 033027. <https://doi.org/10.1103/physrevresearch.4.033027>.

# Advanced State Preparation Techniques

# Ansatz preparation

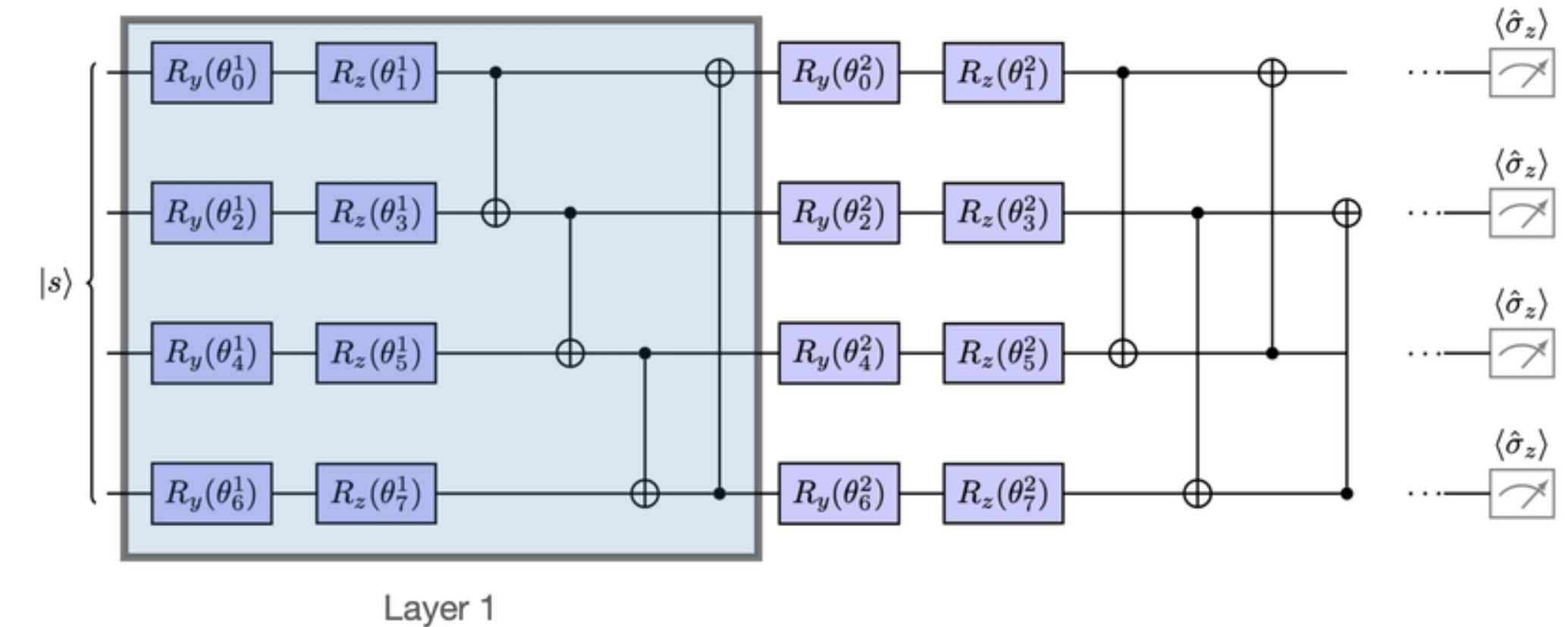
## Efficient representation of state

- 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

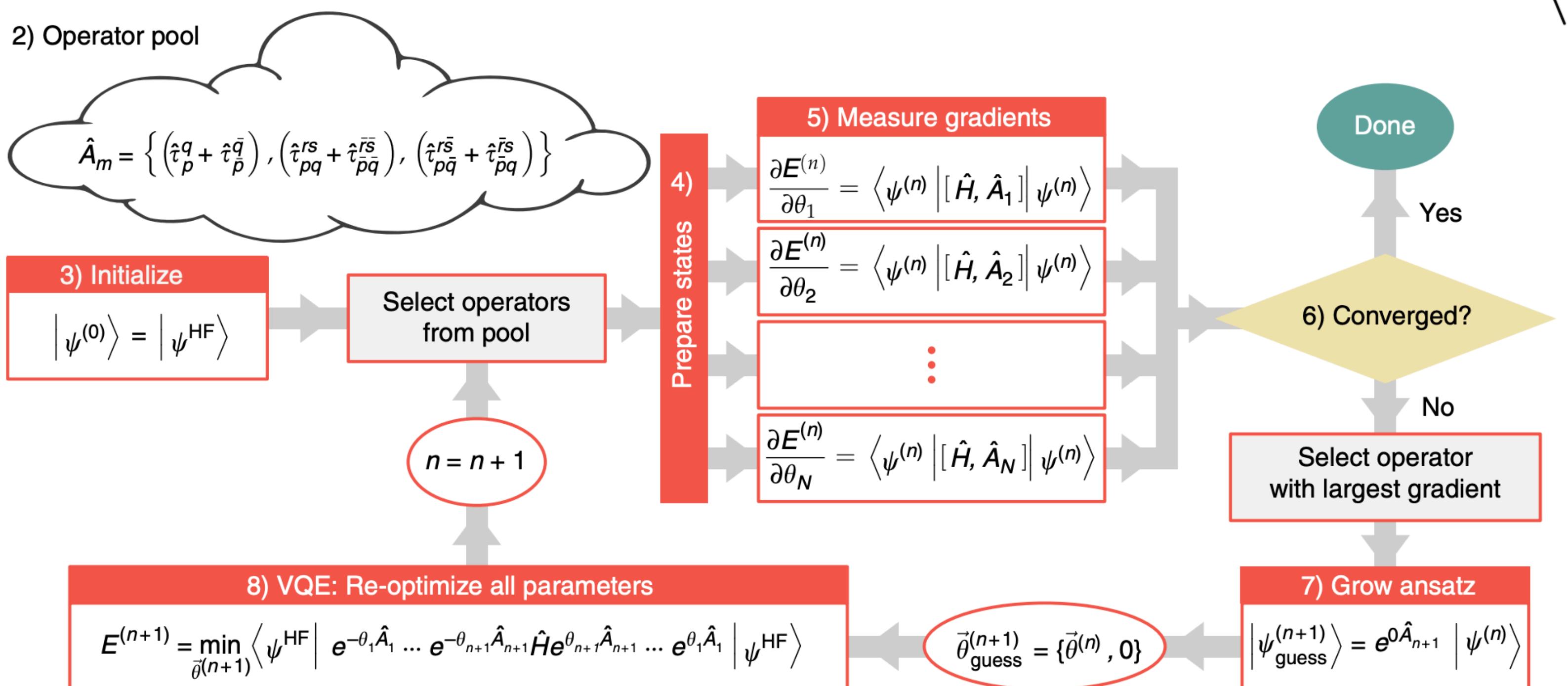


$$\begin{aligned}\hat{\tau}_p^q &= a_q^\dagger a_p - a_p^\dagger a_q \\ \hat{\tau}_{rs}^{pq} &= a_p^\dagger a_q^\dagger a_r a_s - a_s^\dagger a_r^\dagger a_q a_p\end{aligned}$$

# 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

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

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

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

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

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

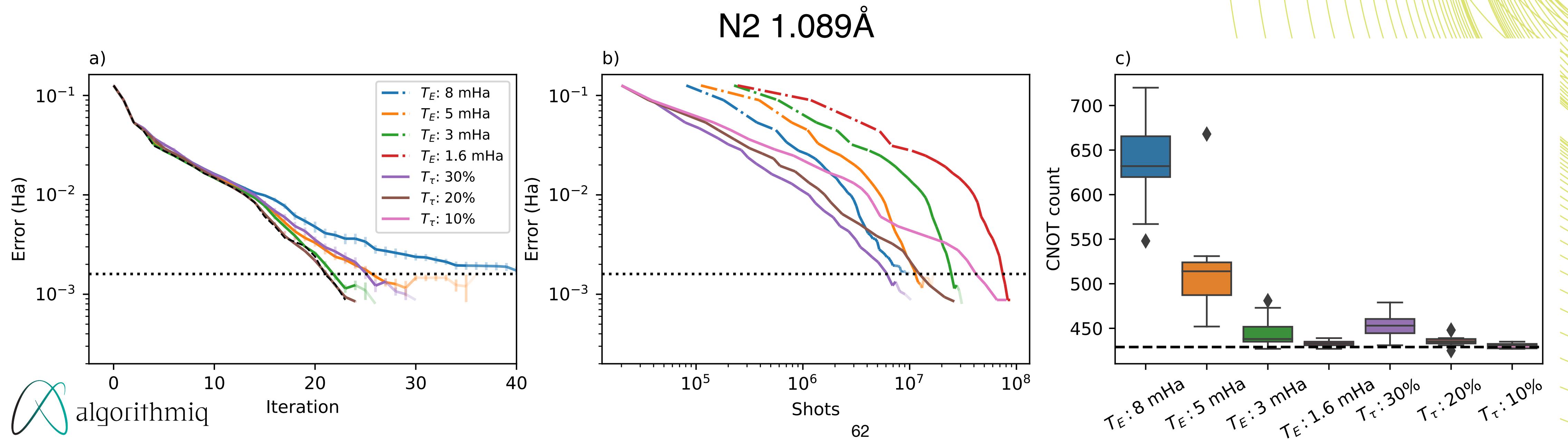
$$A_{ijkl,2}(\theta_2) = \exp(i\theta_2 Y_i X_j X_k X_l)$$

:

# Main limitation of ADAPT

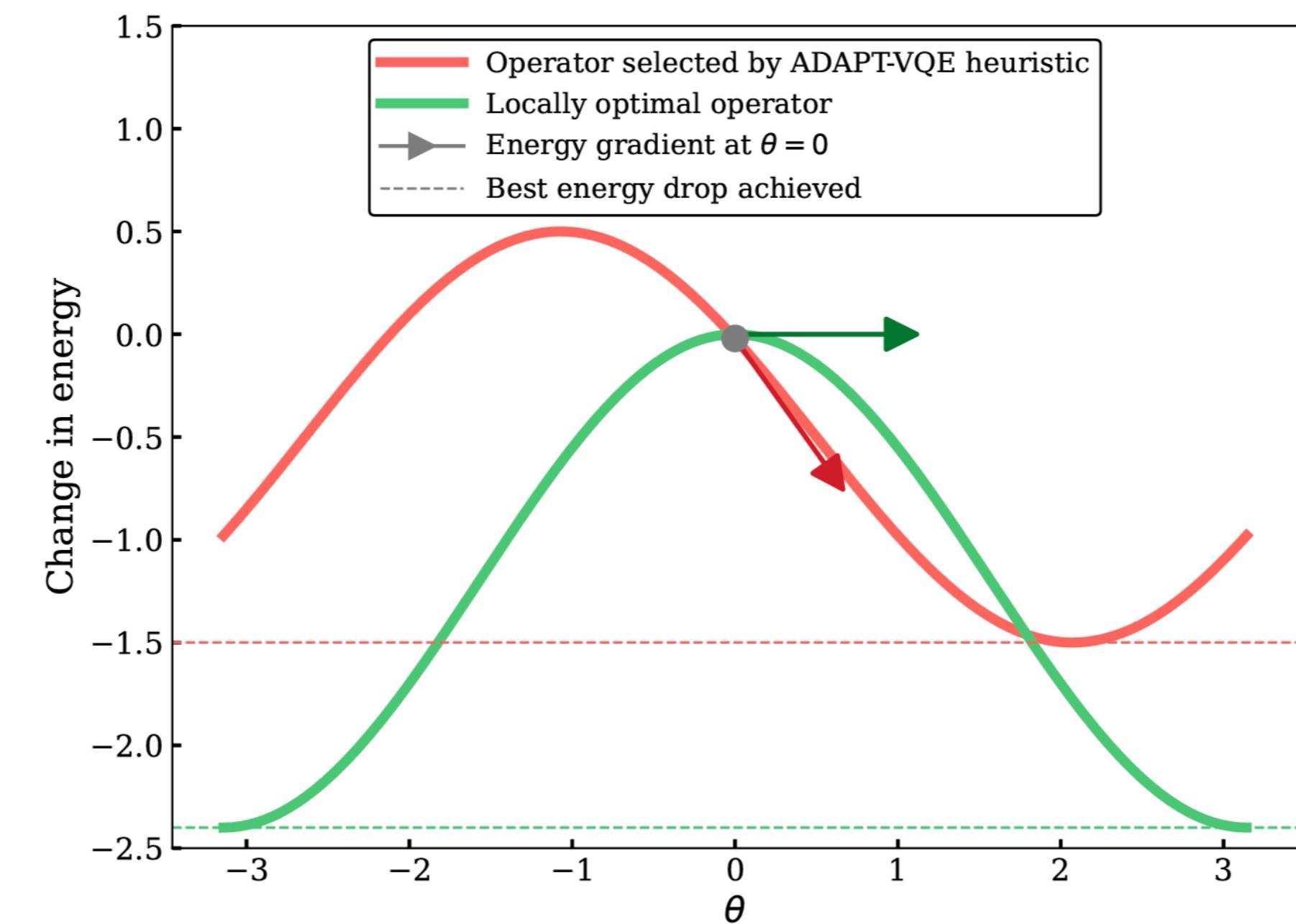
## Measurement overhead

- 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



# References

- Grimsley, H. R.; Economou, S. E.; Barnes, E.; Mayhall, N. J. **An Adaptive Variational Algorithm for Exact Molecular Simulations on a Quantum Computer.** Nat. Commun. 2019, 10 (1), 3007. <https://doi.org/10.1038/s41467-019-10988-2>.
- Tang, H. L.; Shkolnikov, V. O.; Barron, G. S.; Grimsley, H. R.; Mayhall, N. J.; Barnes, E.; Economou, S. E. **Qubit-ADAPT-VQE: An Adaptive Algorithm for Constructing Hardware-Efficient Ansätze on a Quantum Processor.** PRX quantum 2021, 2 (2), 020310. <https://doi.org/10.1103/prxquantum.2.020310>.
- Nykänen, A.; Rossi, M. A. C.; Borrelli, E.-M.; Maniscalco, S.; García-Pérez, G. **Mitigating the Measurement Overhead of ADAPT-VQE with Optimised Informationally Complete Generalised Measurements.** arXiv [quant-ph], 2022. <http://arxiv.org/abs/2212.09719>.
- Feniou, C.; Claudon, B.; Hassan, M.; Courtat, A.; Adjoua, O.; Maday, Y.; Piquemal, J.-P. **Greedy Gradient-Free Adaptive Variational Quantum Algorithms on a Noisy Intermediate Scale Quantum Computer.** arXiv [quant-ph], 2023. <http://arxiv.org/abs/2306.17159>.