Beyond the ground state: accelerating Dynamical Mean-Field Theory with quantum computers

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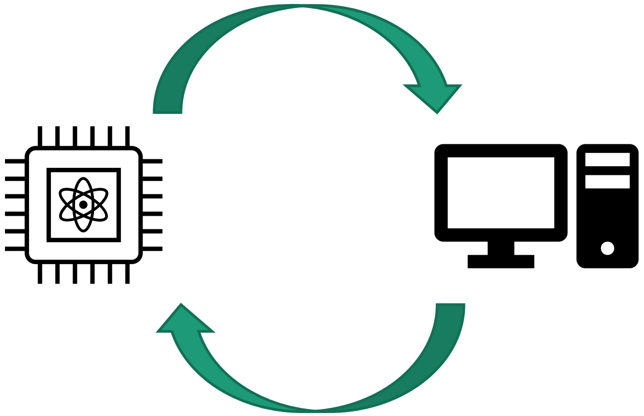
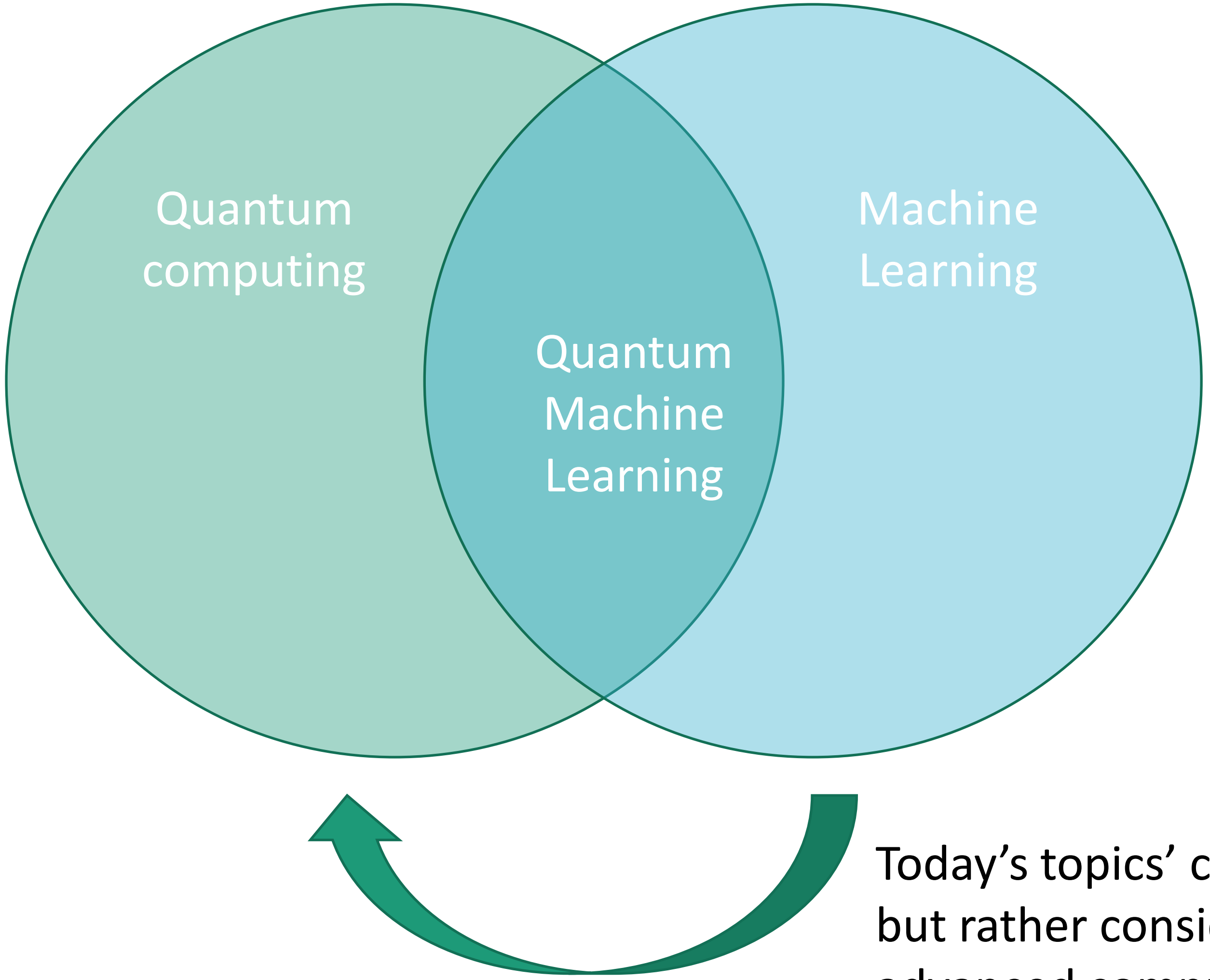
GDR IAMAT Spring School @Roscoff, April 2023





Today’s topics’ connection to ML,
but rather consider the school is about
advanced computing schemes for materials!

Overview

I. Scope: impurity solving with a quantum computer for DMFT calculations

II. Quantum computing 101

- Paradigms
- Circuit model
- Gate model
- Measuring observables

III. Tackling a quantum many-body problem with a quantum computer

- Encoding
- Measuring Green’s functions: a black-box circuit

IV. Ground state preparation

- A quick word about adiabatic state preparation
- Variational Quantum Eigensolver

V. Time-evolving on a chip: trotterization algorithm

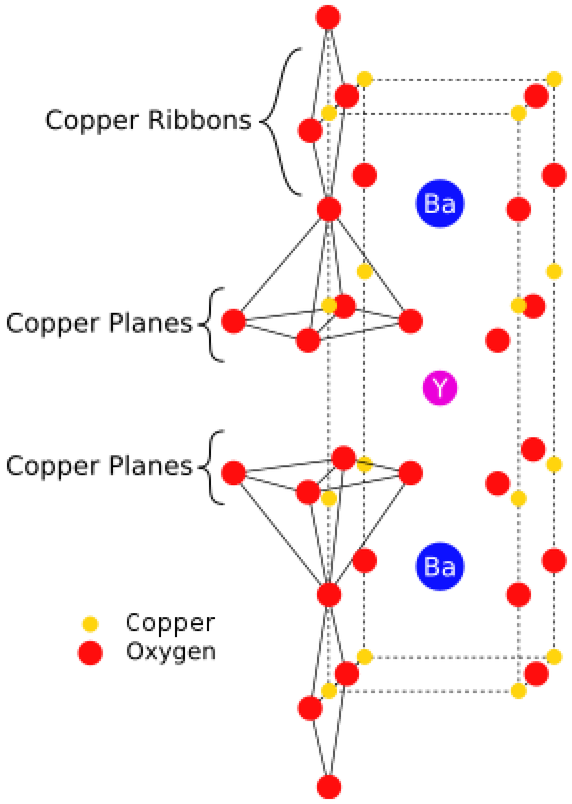
VI. Hardware noise

- Noise sources
- Modelization: example of the depolarizing model
- Error mitigation

I. Scope: impurity solving with a quantum computer for DMFT calculations

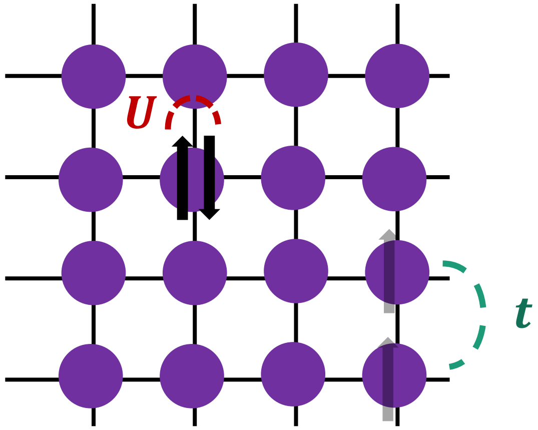
What is DMFT? How can quantum computers enter the game?

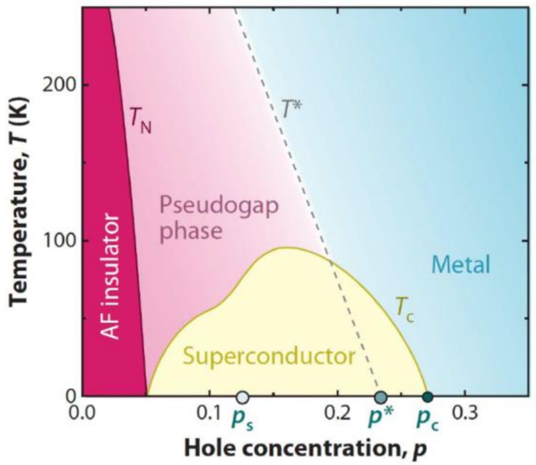
Strongly-correlated materials' spherical cow: Hubbard model



Construct abstract model capturing competition between localization and itinerancy

$$H_{Hub} = \boldsymbol{U}\sum_{i} n_{i\uparrow}n_{i\downarrow} - \mu\sum_{i,\sigma} n_{i\sigma} - \boldsymbol{t}\sum_{\langle i,j,\sigma\rangle} c_{i\sigma}^{\dagger}\, c_{j\sigma}$$

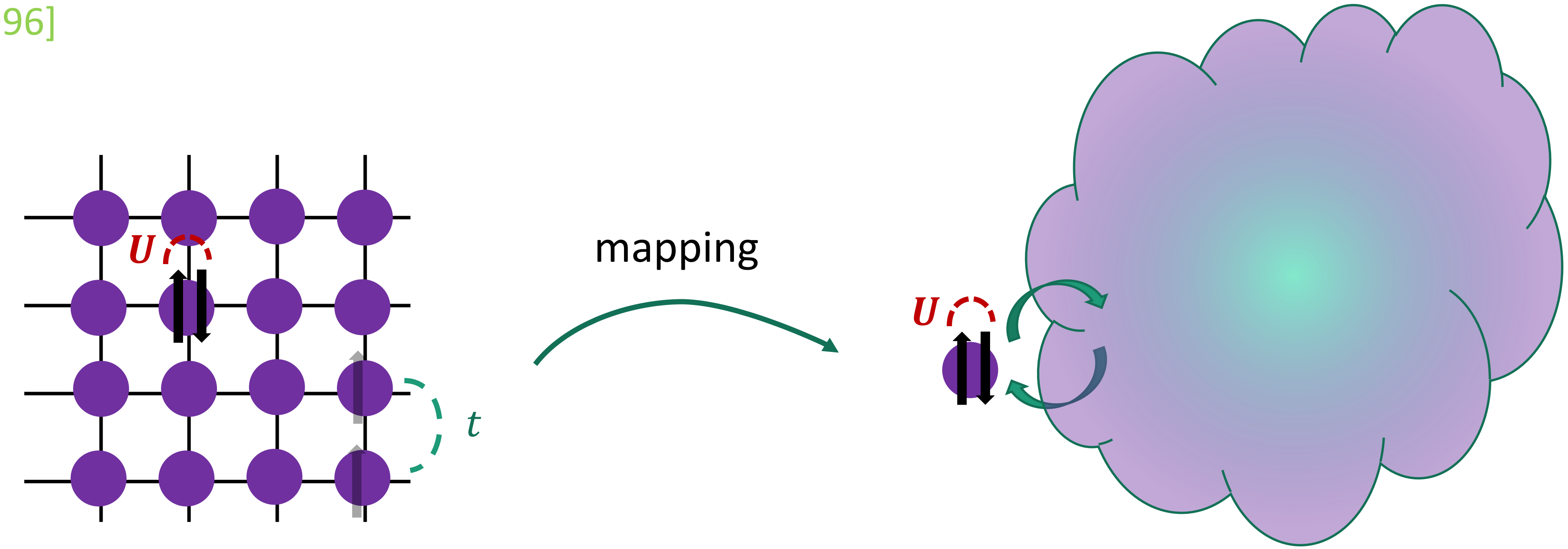




Rich phase diagrams! But extremely complicated to solve….

Dynamical Mean-Field Theory (DMFT) approach: go back to an atomic picture!

[Georges, 1996]



$$H_{Hub} = U \sum_{i} n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i,\sigma} n_{i\sigma} - t \sum_{\langle i,j,\sigma \rangle} c^{\dagger}_{i\sigma} c_{j\sigma}$$

$$H_{emb} = \overset{\text{local, correlated part}}{\boxed{U n_{0\uparrow} n_{0\downarrow} - \mu(n_{0\uparrow} + n_{0\downarrow}}})$$

$$+ \underset{\text{hybridization}}{\boxed{\sum_{p>1,\sigma} V_p (c^{\dagger}_{0\sigma} c_{p\sigma} + hc)}} + \underset{\text{uncorrelated 'bath'}}{\boxed{\sum_{p} \epsilon_p (n_{p\uparrow} + n_{p\downarrow})}}$$

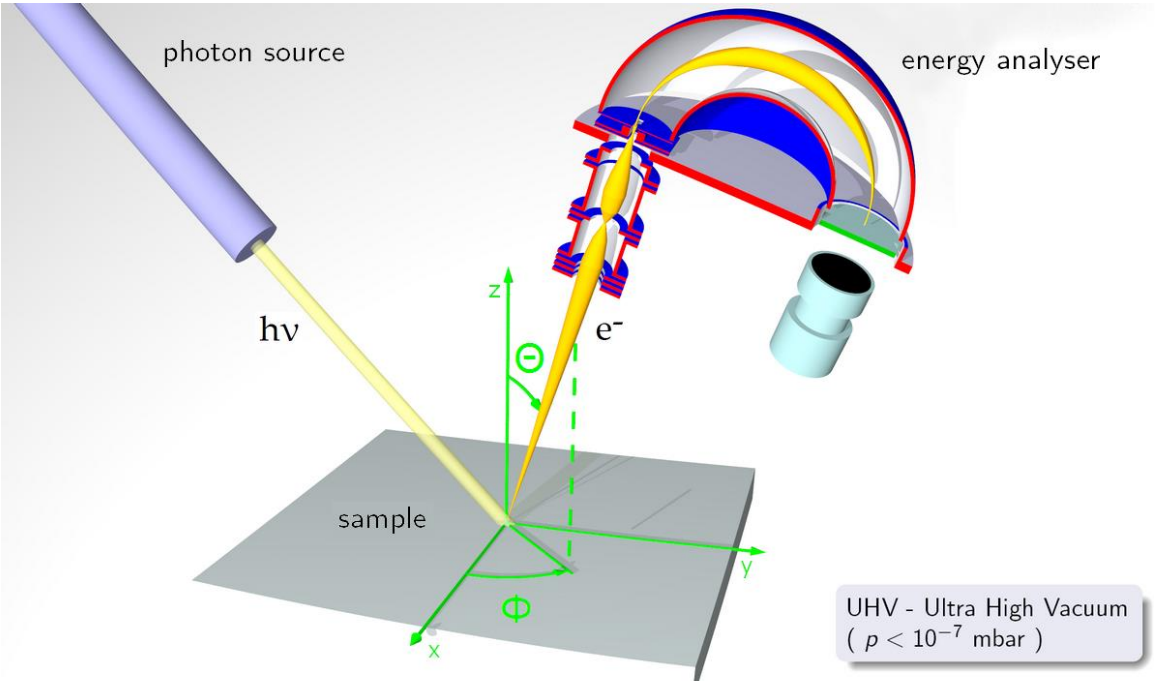
😗 Mapping??

Simpler, but still many-body!

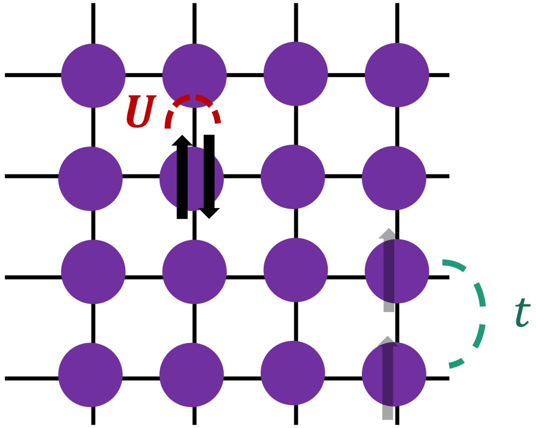
Dynamical Mean-Field Theory (DMFT) approach: go back to an atomic picture!

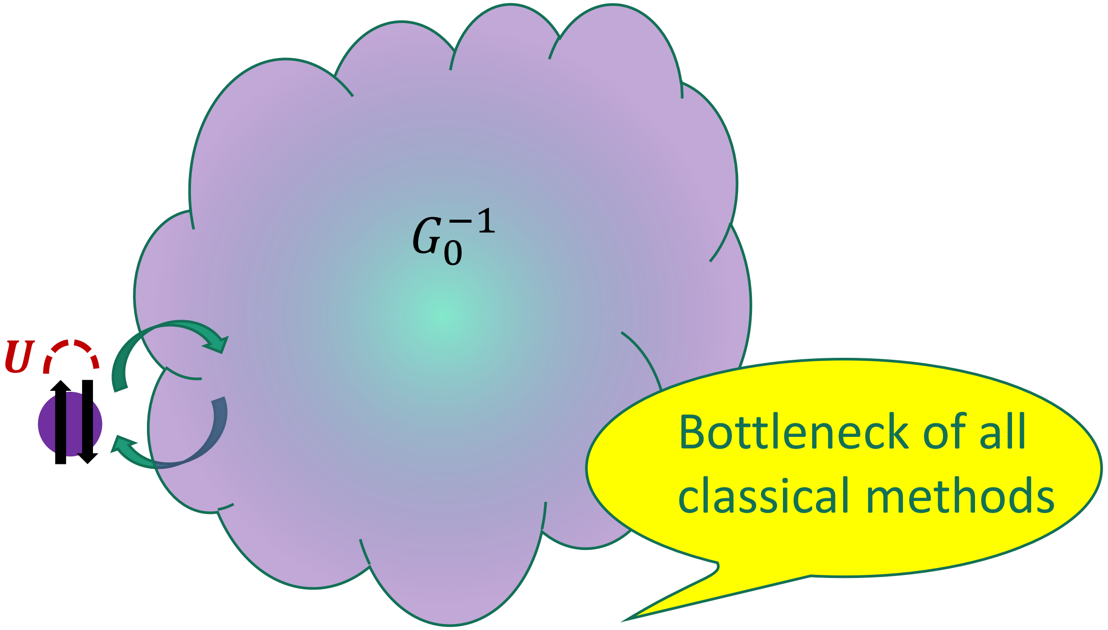
Crucial quantity to explore local degrees of freedom: **local Green's function**
(describes propagation of electrons and holes in the medium)

Relates to Angle-Resolved PhotoEmission Spectroscopy (ARPES) experiments



Dynamical Mean-Field Theory (DMFT) algorithm





Bottleneck of all classical methods

DMFT approximation:

$$\Sigma_{loc}(\omega, \boldsymbol{k}) \leftarrow \Sigma_{imp}(\omega)$$

Dyson equation → self-consistency

$$G_0^{-1} = \Sigma_{imp} + G_{loc}^{-1}[\Sigma_{imp}]$$

$$\xrightarrow{G_0^{-1}}$$

$$\xleftarrow{\Sigma_{imp}}$$

Solve impurity model = compute (TF of)

$$G_{imp}(t) = -i\langle\psi_0|T d_0\,(t) d_0^\dagger|\psi_0\rangle$$

Dyson equation:

$$\Sigma_{imp}(\omega) = G_0^{-1} - G_{imp}^{-1}$$

…then, what about solving the impurity model with a quantum computer?

- Qubits: lean towards discrete, Hamiltonian-based approach (as opposed to diagrammatic)
- Requires to deal with embedded Hamiltonian → electronic structure Hamiltonian, very sparse:

$$H = \sum h_{pq} c_p^\dagger c_q + \frac{1}{2} \sum h_{pqrs} \, c_p^\dagger c_q^\dagger c_r c_s$$

→ Up to $O(n^4)$ terms, manageable!

- Qubit registers can store the wavefunction without an exponential cost, and (as we'll see) implement time evolution. At least from textbook quantum **to resort to a quantum computer**!!*

Quantum computing with and for many-body physics

Thomas Ayral [a,1], Pauline Besserve [b,1,3], Denis Lacroix [c,2], Edgar Andrés Ruiz Guzman [d,2]

[1] Atos Quantum Lab, 78340 Les Clayes-sous-Bois, France
[2] Université Paris-Saclay, CNRS/IN2P3, IJCLab, 91405 Orsay, France
[3] Centre de Physique Théorique, 91120 Palaiseau, France

*no obvious exponential bottleneck to be seen anywhere ☺

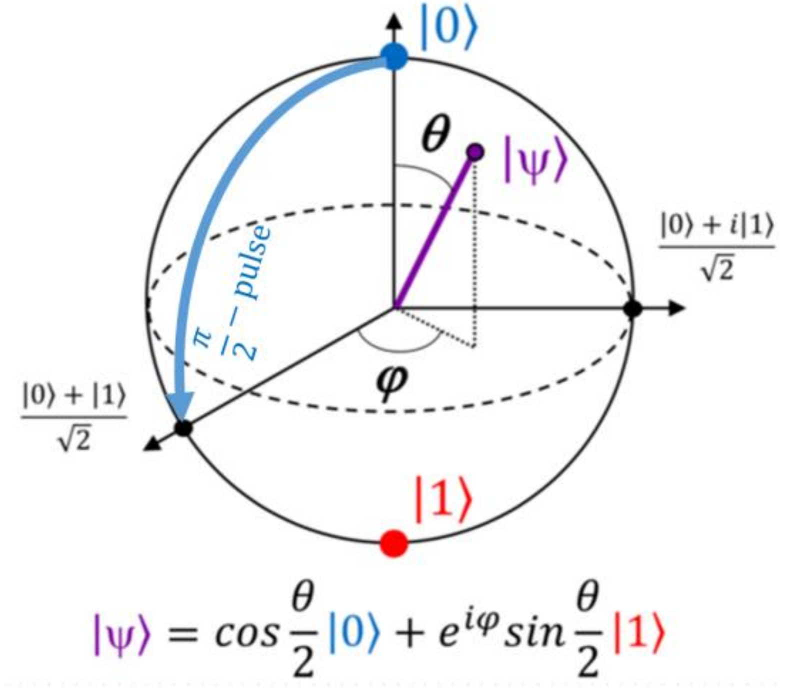
- Looking for a review about QC for many-body problems? arxiv:2303.04850

II. Quantum computing 101

How to compute with a quantum device?

The quantum bit (qubit)

Bloch sphere representation:



$$|\psi\rangle = cos\frac{\theta}{2}|0\rangle + e^{i\varphi}sin\frac{\theta}{2}|1\rangle$$

(image: Jazaeri et al, 2019)

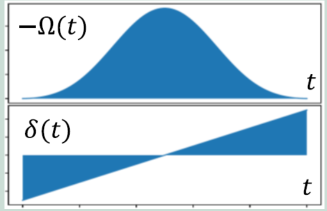
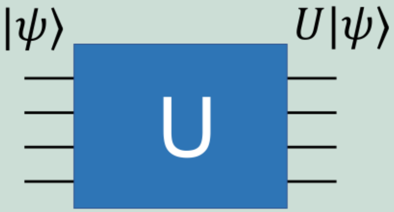
n qubits → 2^n **bitstrings** $\underbrace{|00\ldots0\rangle, |00\ldots1\rangle, \ldots, |11\ldots1\rangle}_{\textbf{computational basis}\text{ states}}$

There are several ways to create and manipulate qubits.

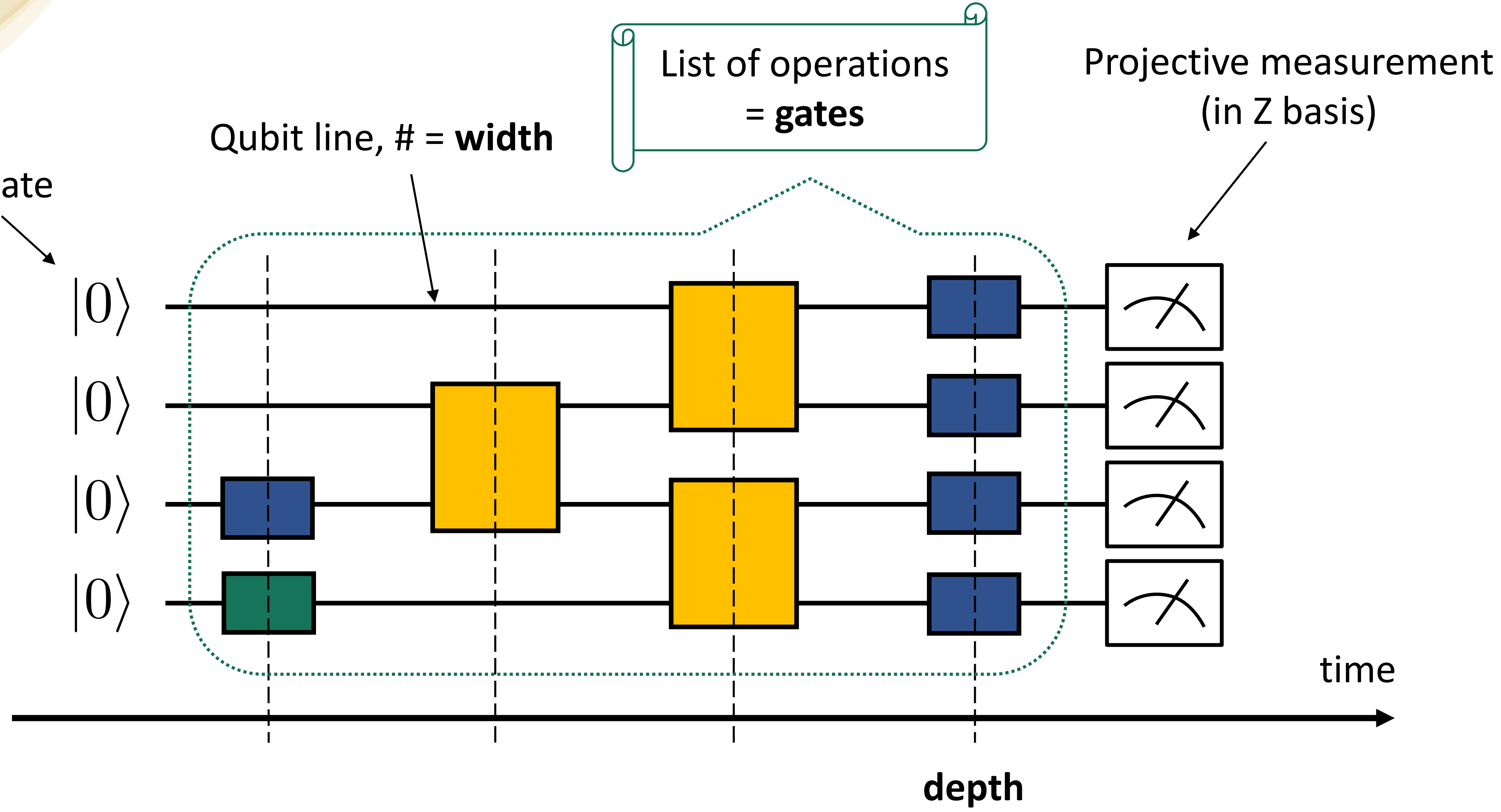
II.1. Paradigms

Consider…

With…

Analog QC / Simulator	**Digital / Universal QC**	**Emulator**
Schrödinger time evolution $Te^{-i\int H_{res}(t)dt}$ under some resource Hamiltonian H_{res} with tunable control fields 	Any unitary evolution 	Testing of algorithmic strategies on a classical supercomputer
Ultracold atoms, Rydberg atoms, spin qubits…	Superconducting qubits, trapped ions…	Atos' *Quantum Learning Machine*

II.2. Circuit model



List of operations = **gates**

Projective measurement (in Z basis)

Qubit line, # = **width**

Initial state

$|0\rangle$

$|0\rangle$

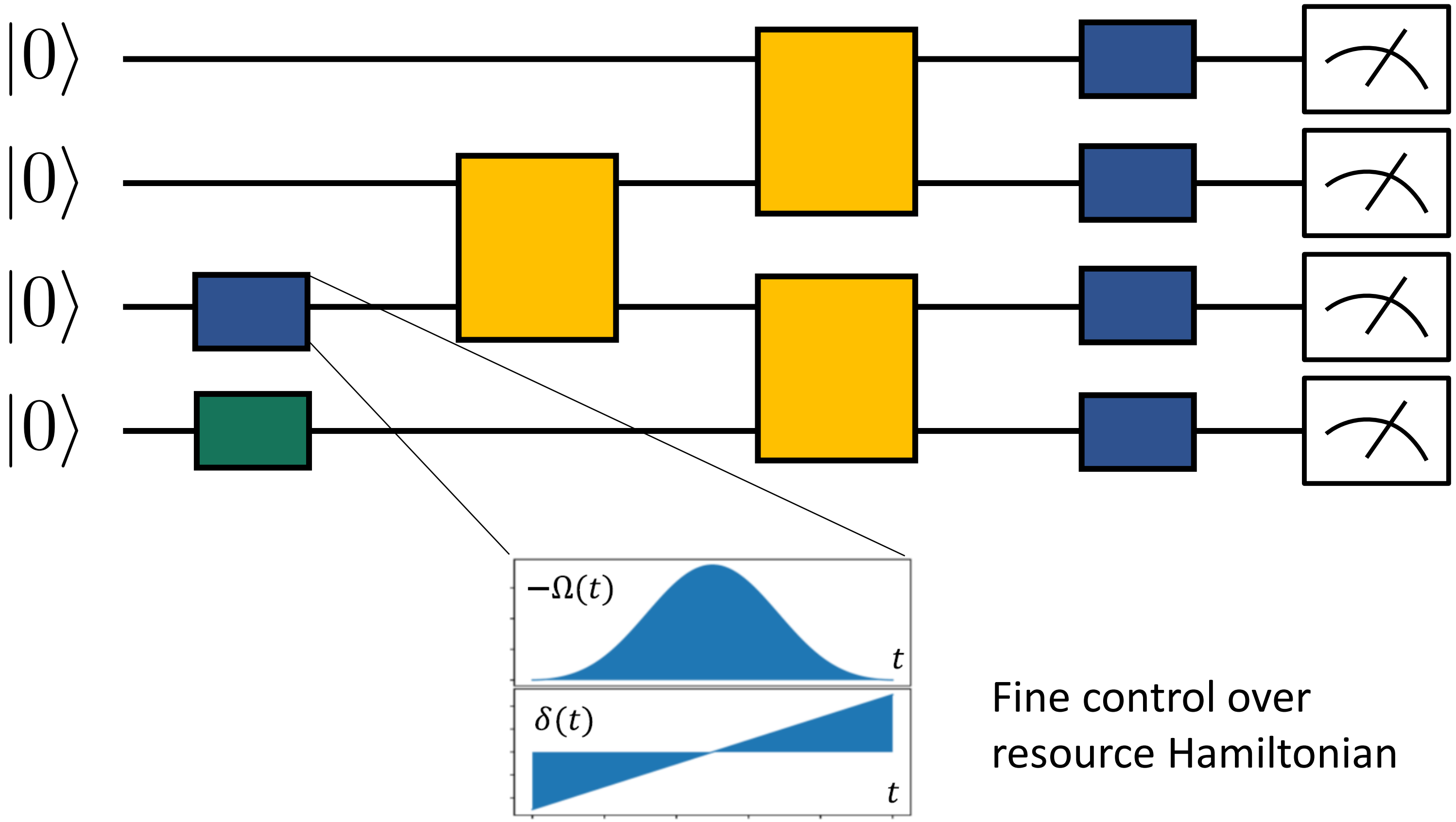
$|0\rangle$

$|0\rangle$

time

depth

II.3. Gate model



Fine control over
resource Hamiltonian

II.3. Gate model

$$|0\rangle \rightarrow \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad |1\rangle \rightarrow \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Pauli gates:

$$\boxed{X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = |0\rangle\langle 1| + |1\rangle\langle 0|} \qquad Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Logical NOT gate!

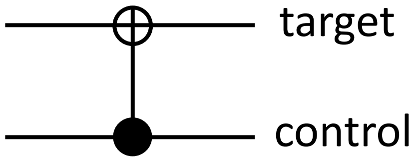
Pauli rotations:

$$RX(\theta) = e^{-\frac{i\theta}{2}X} = \cos\left(\frac{\theta}{2}\right) I - i \sin\left(\frac{\theta}{2}\right) X, \qquad RY(\theta) = \cdots$$

Hadamard gate:

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

What about gates on more qubits?



C(ontrolled)- **NOT** gate

		control	
		0	1
target	0	00	11
	1	10	01

? No more-qubit gates?

✓ Any unitary can be decomposed onto single and two-qubit gates (albeit with possibly exp #)

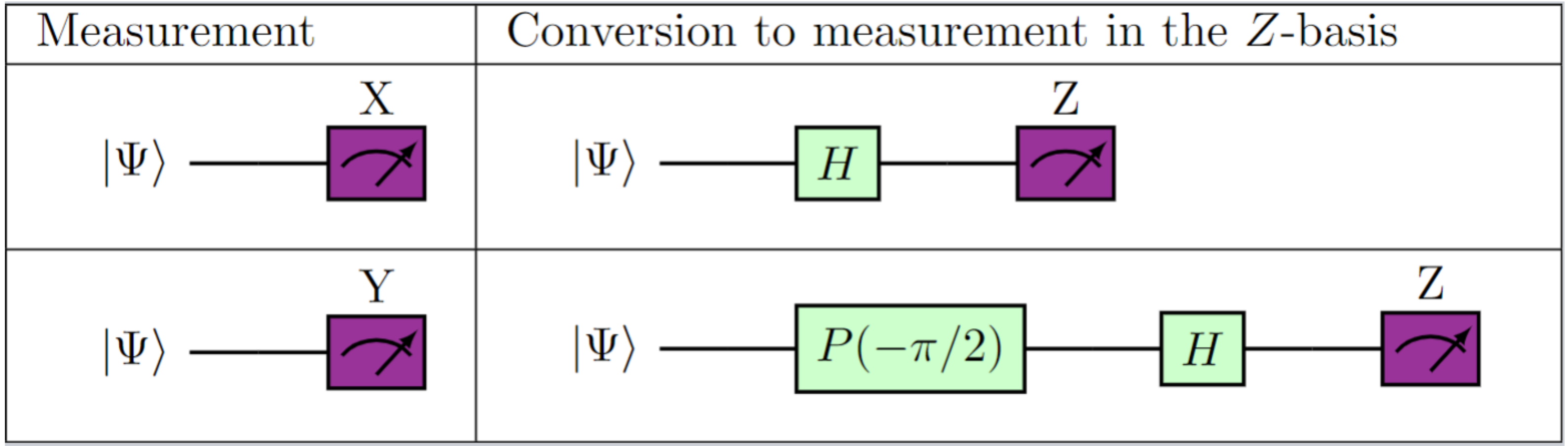
II.4. Measuring observables

Observable = Hermitian operator $O = O^\dagger$ so that $\langle\psi|O|\psi\rangle \in \mathbb{R}$
Decomposes as $O = \sum_k \lambda_k P_k$, P_k : **Pauli word** $\sigma^1\sigma^2 \ldots \sigma^N$, $\sigma^j \in \{I, X, Y, Z\}$
Example: number operator (counts #1's in bitstring)

$$\hat{N} = \frac{1}{2}\left(I - \sum_i I \otimes I \otimes \cdots \otimes Z_i \otimes I \otimes \cdots \otimes I\right) = \frac{1}{2}(I - \sum_i Z_i)$$

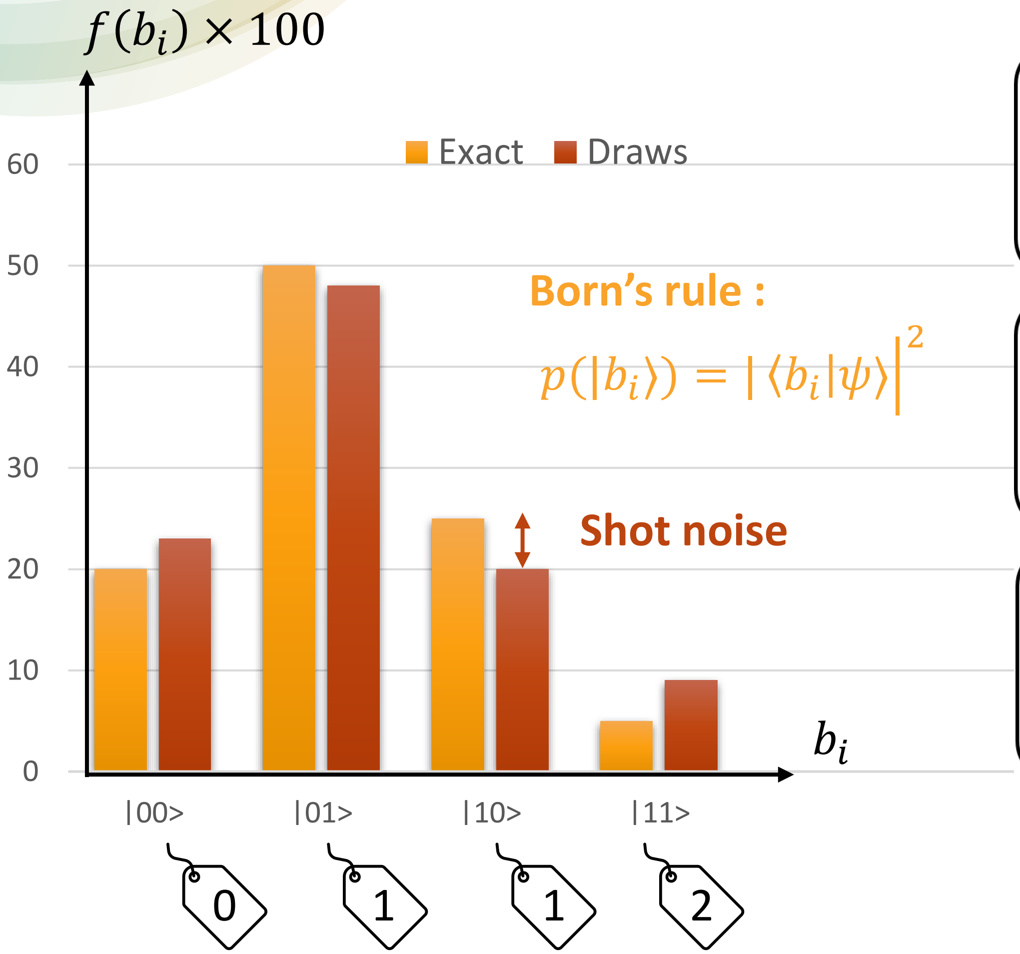
Qubits are measured in the Z basis: $|0\rangle \to +1, |1\rangle \to -1$

Measurement in X or Y basis: small gate overhead



II.4. Measuring observables

Easy case: Pauli words commute



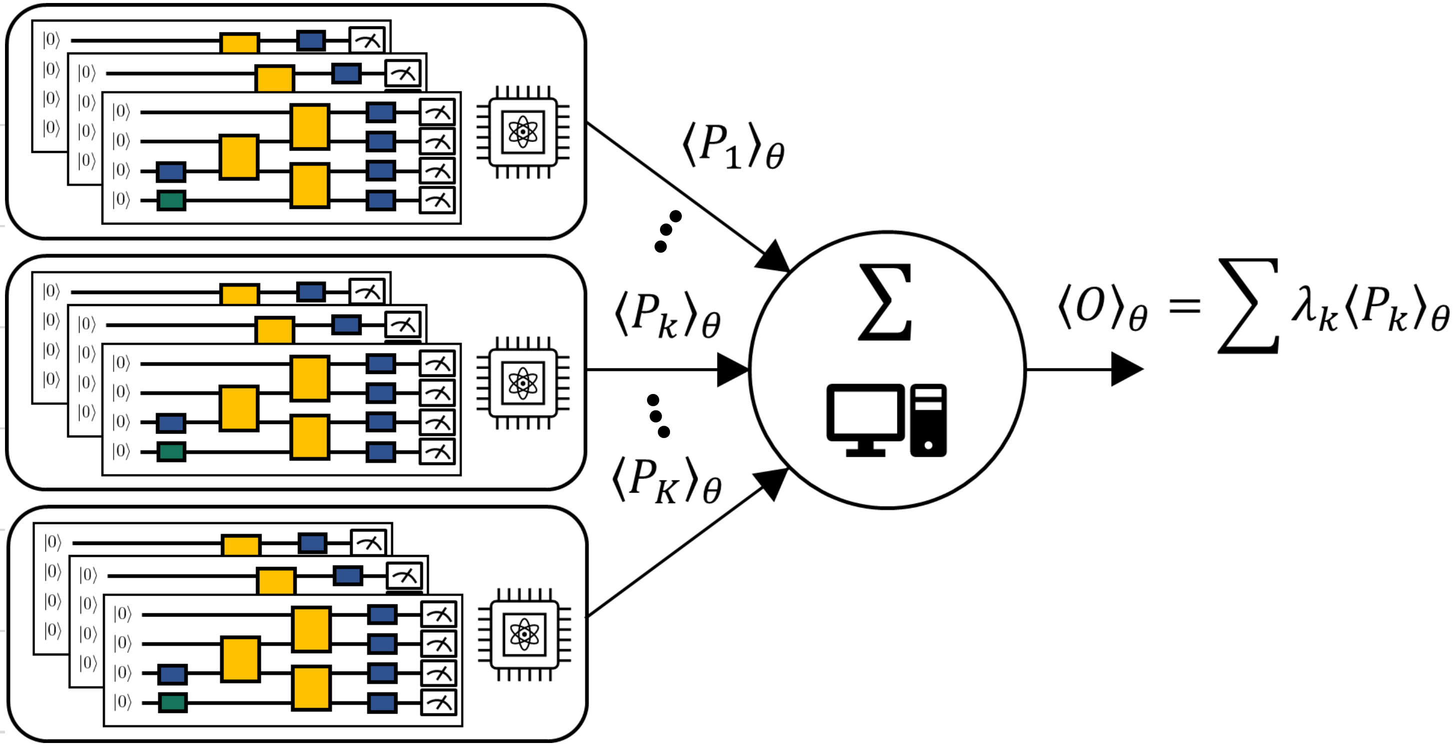
Born's rule :

$$p(|b_i\rangle) = |\langle b_i|\psi\rangle|^2$$

Shot noise

$$\langle \hat{N} \rangle = \sum f(b_i) \times$$

Most general case: averaging over Pauli words' expectation values



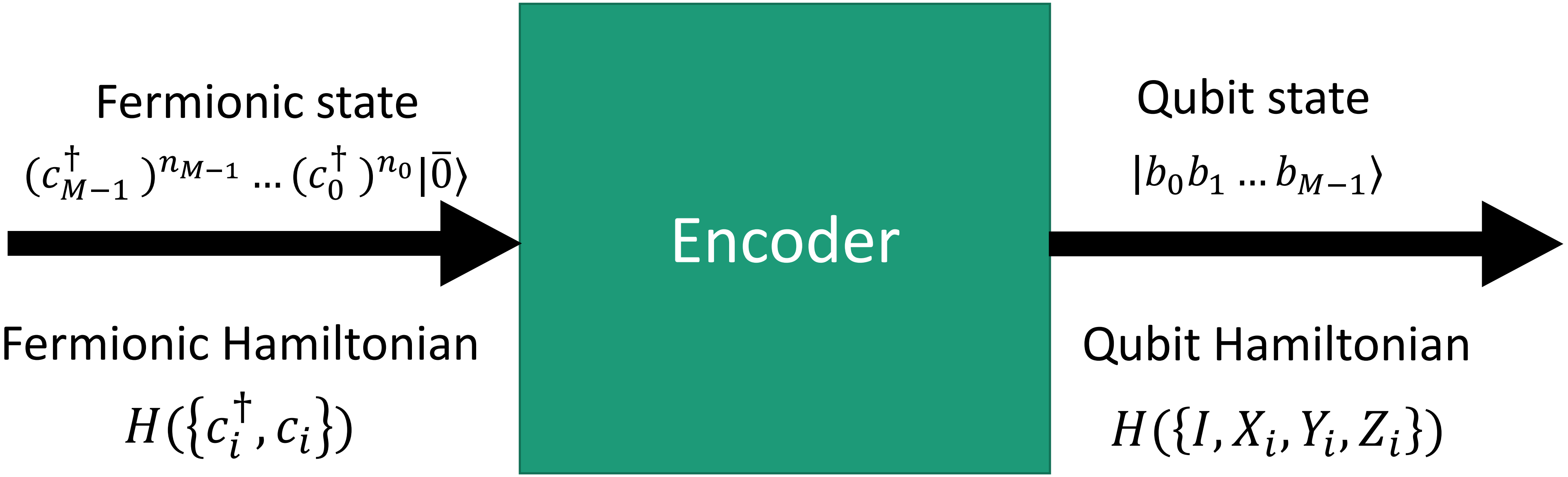
$$\langle O \rangle_\theta = \sum \lambda_k \langle P_k \rangle_\theta$$

Remark: very naive
(typically, k-locality → some Pauli strings commute)

III. Tackling a quantum many-body problem with a quantum computer

How to represent fermionic systems with qubit states? How to measure fermionic Hamiltonians?

III.1. Encoding



Fermionic state

$(c_{M-1}^{\dagger})^{n_{M-1}} \ldots (c_0^{\dagger})^{n_0}|\bar{0}\rangle$

Fermionic Hamiltonian

$H(\{c_i^{\dagger}, c_i\})$

Encoder

Qubit state

$|b_0 b_1 \ldots b_{M-1}\rangle$

Qubit Hamiltonian

$H(\{I, X_i, Y_i, Z_i\})$

III.1. Encoding

- Spin-orbitals (SO): empty or filled with one electron, qubits: 0 or 1
- Most straightforward encoding: empty → 0, filled → 1, namely: $n_i = b_i$ (**Jordan-Wigner,** drawback: lose locality, see below)
- What about anti-commutation relations?

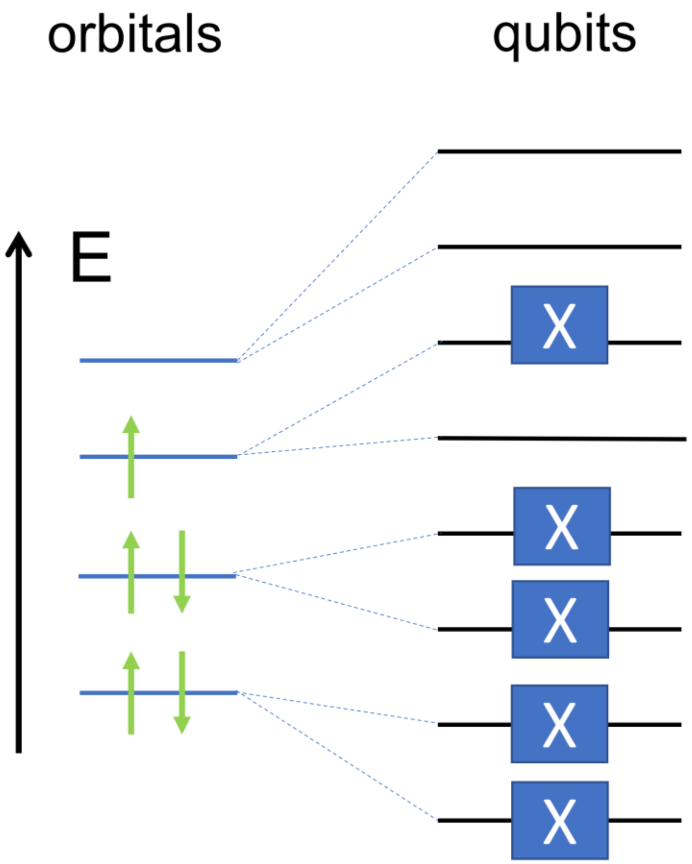
$$\{c_p^\dagger, c_q\} = \delta_{pq} I$$
$$\{c_p, c_q\} = 0$$

$$\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

$$c_p^\dagger \to Z_0 \otimes Z_1 \otimes \cdots \otimes Z_{p-1} \otimes \boxed{\frac{1}{2}\left(X_p - iY_p\right)} \otimes I_{p+1} \otimes \cdots \otimes I_n$$

Enforce ACR

Ladder operator → deal with local occupancy



(X gate=NOT gate: $X|0\rangle = |1\rangle$)

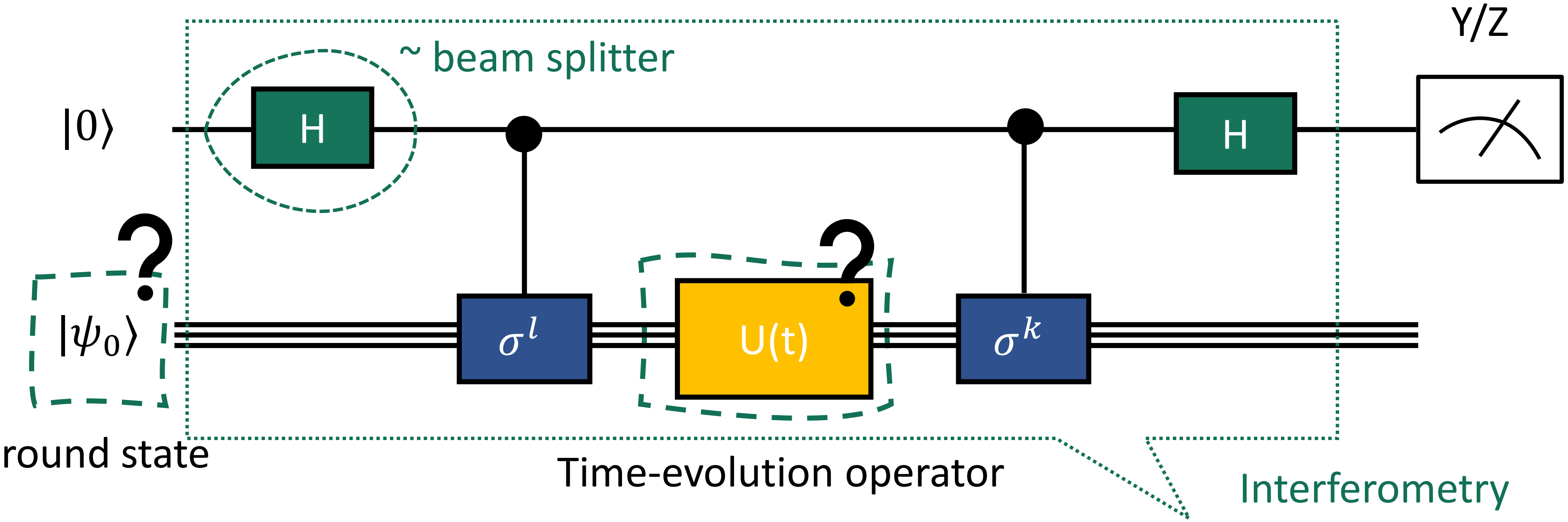
III.2. Measuring Green’s functions: a black-box circuit

Green’s functions elements of the form $\langle\psi_0|c_p(t)c_q^\dagger|\psi_0\rangle$

Heisenberg representation: $c_p(t) = U(t)^\dagger c_p U(t)$, with $U(t) = e^{-iHt}$

Jordan-Wigner encoding: $c_p^\dagger \sim \frac{1}{2}\left(X_p - iY_p\right)$

Needed: $C_{kl} \equiv \langle\psi_0|U(t)^\dagger\sigma^k\ U(t)\sigma^l\ |\psi_0\rangle$, accessible as $\langle Z_0\rangle + i\langle \mathrm{Y}_0\rangle$ where 0 labels the **ancillary qubit** of the following circuit:



~ beam splitter

Ground state

Time-evolution operator

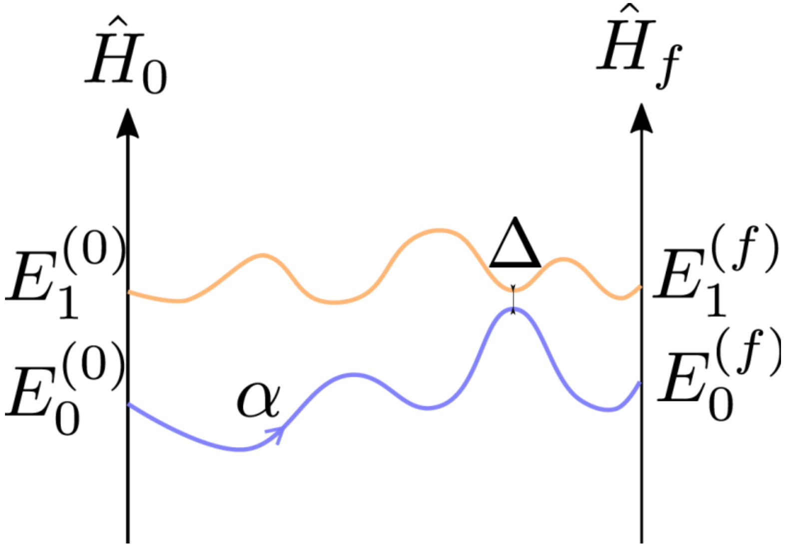
Interferometry experiment!

IV. Ground state preparation

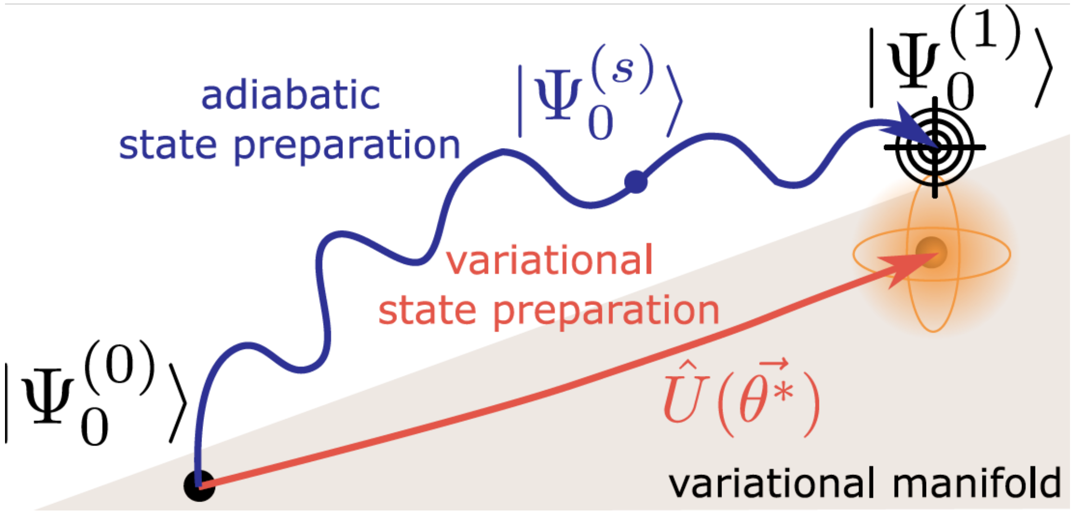
How do I put my qubit register in the state representing my target ground state?

IV.1. A word on adiabatic state preparation

- Theoretical guarantee to attain GS within time-evolution under interpolation Hamiltonian if $\mathrm{T} > 1/\Delta^2$: **adiabatic theorem**
- Exists as a digital (=gate-based) algorithm (incurs massive gate count, not reviewed here)
- But, important insight: putting gates mirroring terms of the Hamiltonian in a quantum circuit should lead to the GS
- Can't we find a 'diabatic shortcut' to the GS?



$$\alpha = \alpha(t), \alpha(0) = 0, \alpha(T) = 1$$
$$H_\alpha = \alpha H_f + (1-\alpha) H_0$$

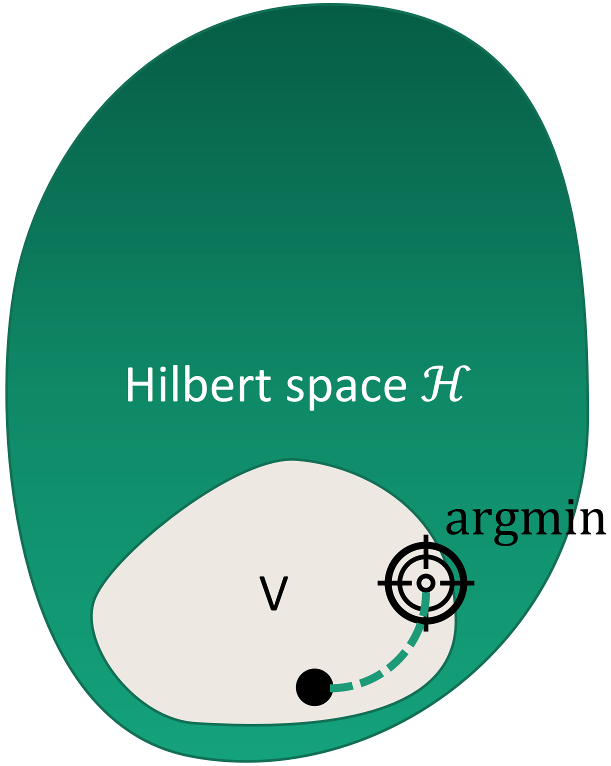


IV.2. Variational Quantum Eigensolver

[Peruzzo, 2014]

- Starting point: **Rayleigh-Ritz principle** (as seen in F. Vicentini's talk)$|\psi_0\rangle = \mathrm{argmin}_{|\psi\rangle\in\mathcal{H}} \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}$

- Hilbert space is huge, and GS have structure… → **explore small, relevant subspace**:



$$\mathrm{argmin}_{|\psi\rangle\in\mathrm{V}} \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} = \sim |\psi_0\rangle$$

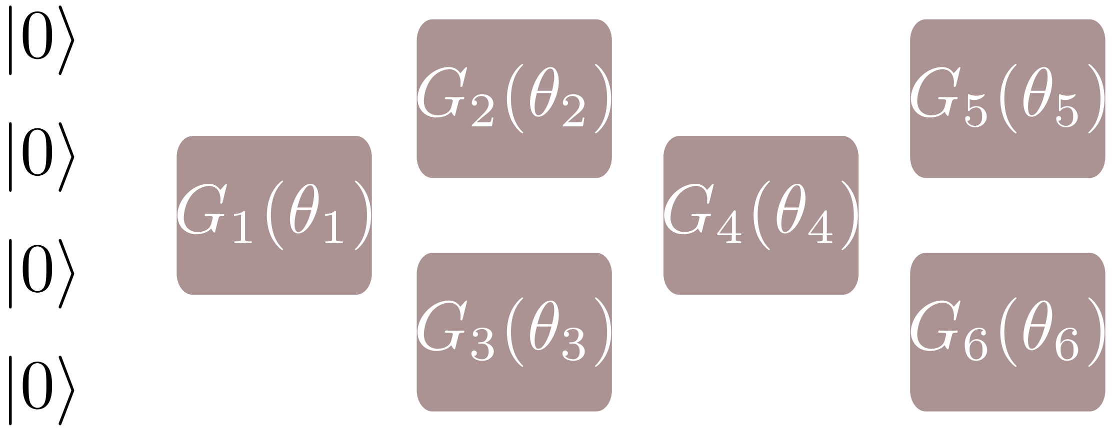
IV.2. Variational Quantum Eigensolver

VQE recipe for GS preparation:

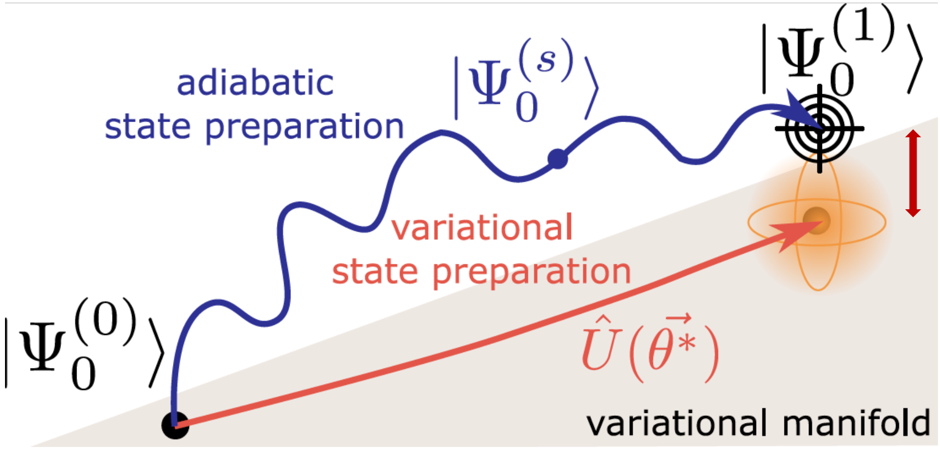
Select **variational** manifold (of physical states $\langle\psi(\boldsymbol{\theta})|\psi(\boldsymbol{\theta})\rangle = 1$) and find **optimal parametrization**

$$|\psi(\boldsymbol{\theta}^*)\rangle = \mathrm{argmin}_{\boldsymbol{\theta}} \langle\psi(\boldsymbol{\theta})|H|\psi(\boldsymbol{\theta})\rangle$$

Define search space with parametrized quantum circuit:



Comes with intrinsic expressivity:

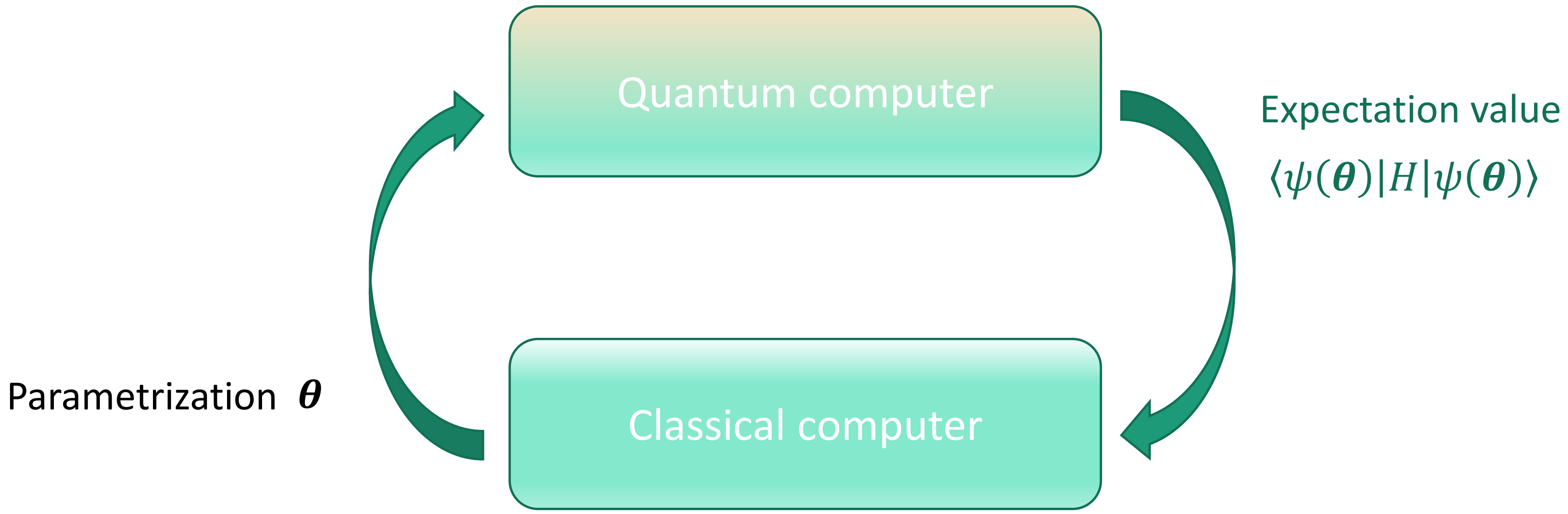


…but can accomodate capabilities of your QC!

IV.2. Variational Quantum Eigensolver

Goal: find optimal parametrization $|\psi(\boldsymbol{\theta}^*)\rangle = \mathrm{argmin}_{\boldsymbol{\theta}} \langle\psi(\boldsymbol{\theta})|H|\psi(\boldsymbol{\theta})\rangle$

Optimization of a **cost function** $\mathbb{R}^n \to \mathbb{R}$: evaluation of cost on QC, parameters update with classical computer



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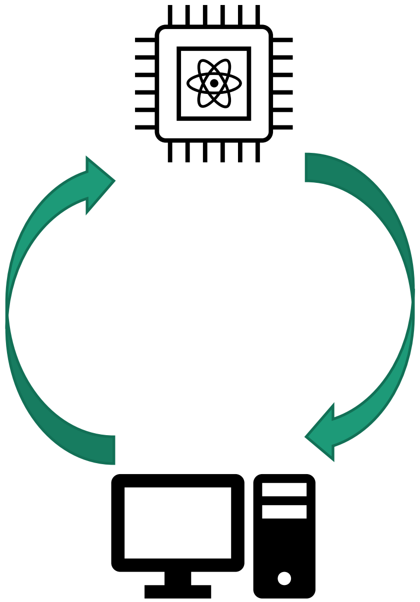
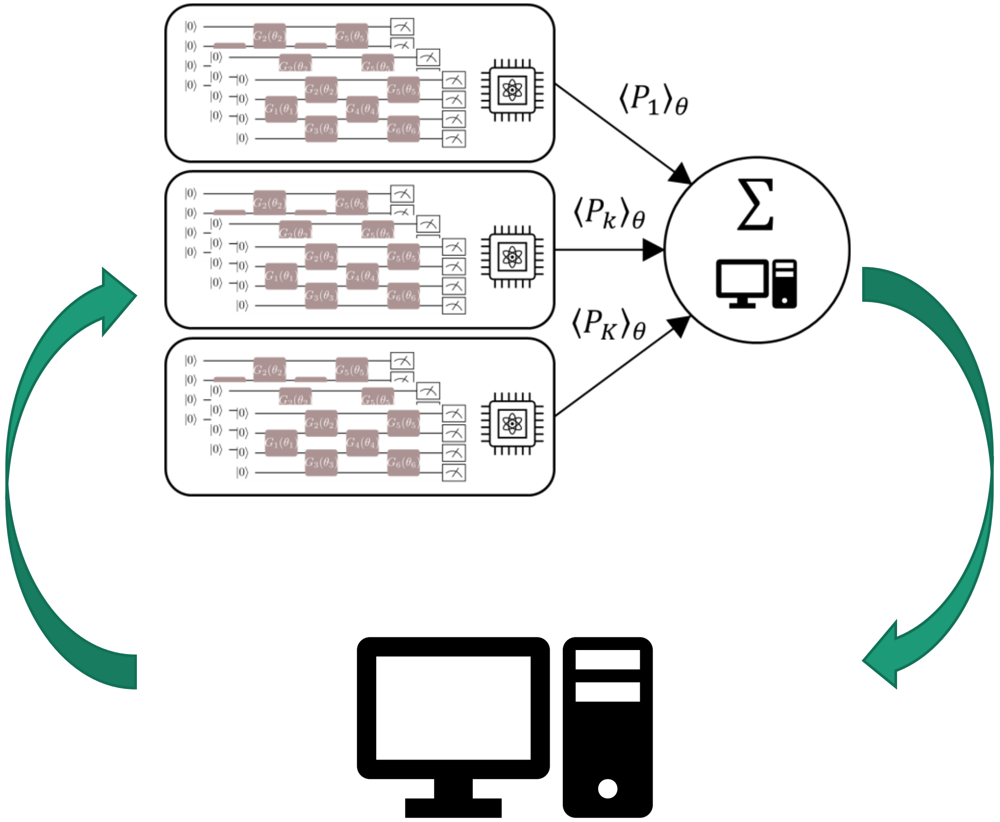


QPU/CPU hybridization

IV.2. Variational Quantum Eigensolver

Actually, remember that cost function evaluation is already hybrid! Putting things together:



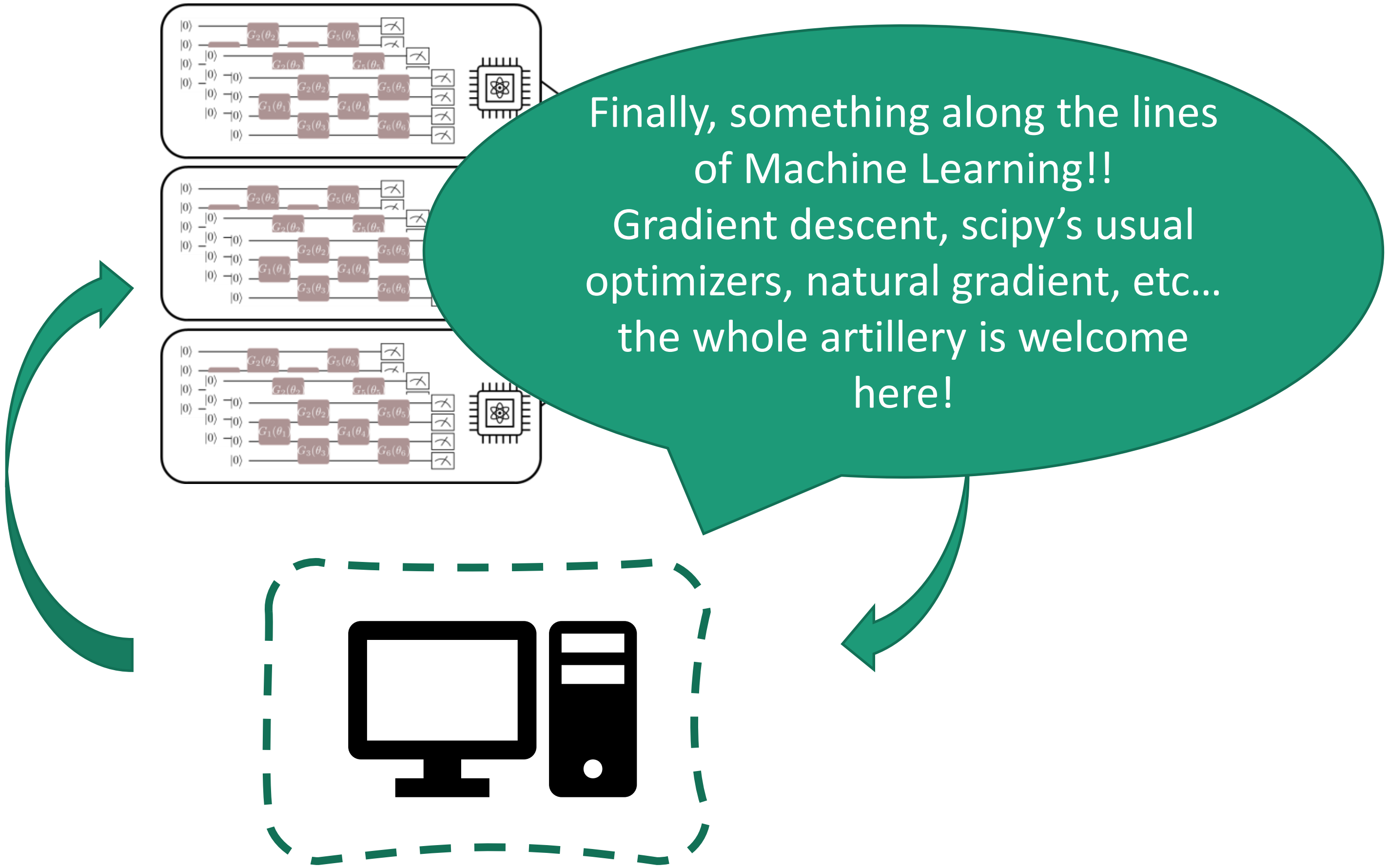
Expectation value

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

Parametrization $\boldsymbol{\theta}$

IV.2. Variational Quantum Eigensolver

Actually, remember that cost function evaluation is already hybrid! Putting things together:



Finally, something along the lines of Machine Learning!! Gradient descent, scipy’s usual optimizers, natural gradient, etc… the whole artillery is welcome here!

Parametrization $\boldsymbol{\theta}$

IV.2. Variational Quantum Eigensolver

Which circuits for fermionic ground states?

Two main classes:

Type of circuit	Physically-motivated	Hardware-efficient
Expressivity	✓	buildable
Noise resilience	✗	✓
Optimization	✓	✗ (Barren plateaus due to lack of structure)
Examples	« Low-Depth Circuit Ansatz » Elaborating upon free-fermions states preparation [Dallaire-Demers, 2018]	Stacking layers of dressed CNOT

⇧

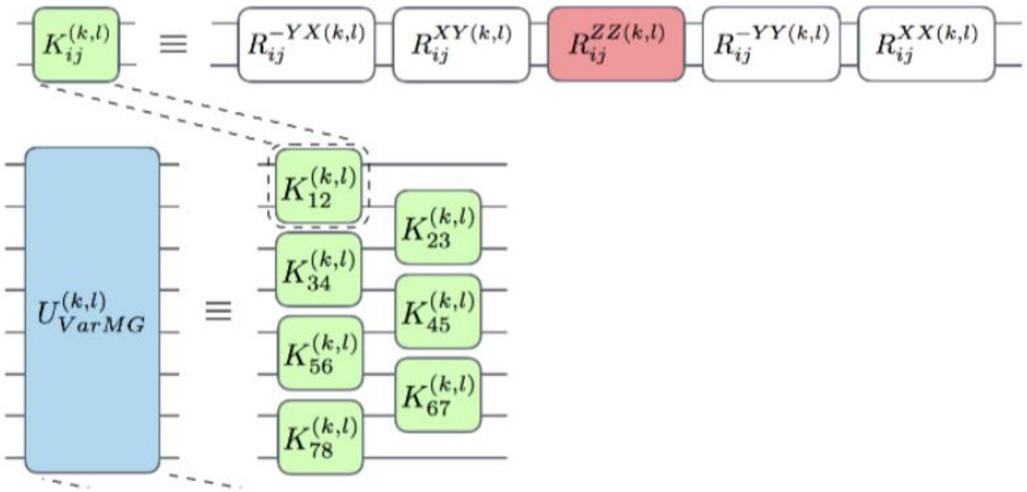
Echoes Filippo's talk: importance of using knowledge of the physics of your system!

IV.2. Variational Quantum Eigensolver

« Low-Depth Circuit Ansatz » elaborating upon free-fermions states preparation: gold standard for fermionic states preparation (but too deep for noisy QC)

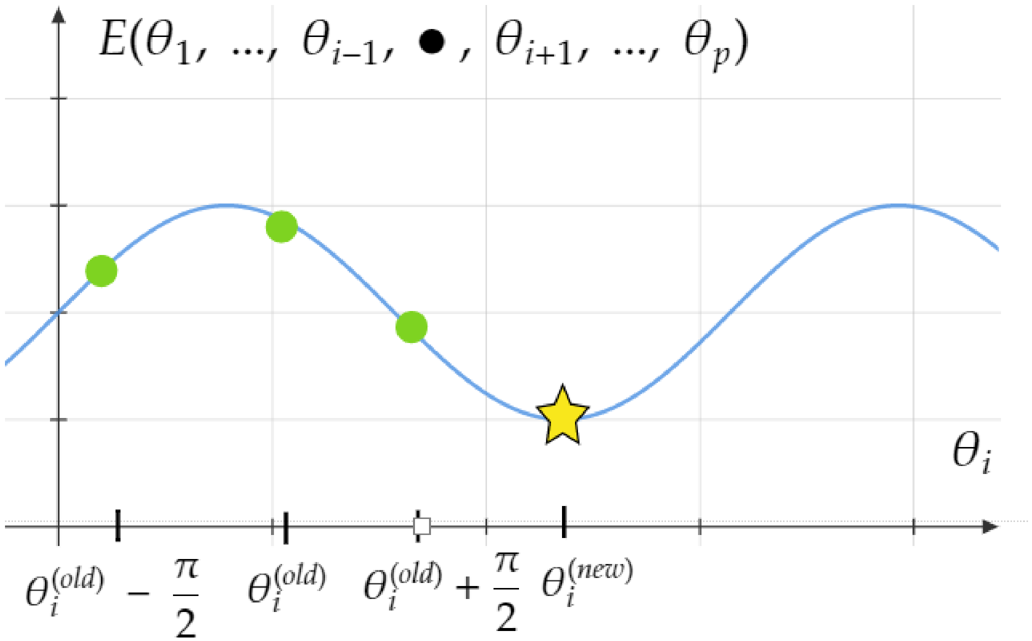
Based on preparation of GS of uncorrelated fermionic Hamiltonians

Generalizes to correlated states thanks to addition of R_{ZZ} gates (+ stacking of identical parametrized routines)



IV.2. Variational Quantum Eigensolver

A nice **shot-noise resilient** optimization algorithm proposed by ML/QC people [Ostaszewski, 2019]: **Rotosolve**



- Applies to specific circuits only (CNOT and rotations-based are eligible)
- Based on analytical formula for the gradient (**parameter-shift rule**)

→ **Local optimal update rule**:

$$\theta_i^{(new)} = f\left(E\left(\theta_i^{(old)}\right), E\left(\theta_i^{(old)} - \frac{\pi}{2}\right), E\left(\theta_i^{(old)} + \frac{\pi}{2}\right)\right)$$

- Global minimization of loss function by cycling through all the parameters until stopping criterion is met.

V. Time-evolving on a chip: trotterization algorithm

How do I implement time evolution with gates?

Trotterization

$H = \sum_j \alpha_j h_j$, $[h_j, h_k] \propto 1 - \delta_{jk}$

No general recipe to find gates implementing e^{-iHt}. Would be easier if we considered $e^{-i\alpha_j h_j t}$ ...

But, non commutativity of terms → $e^{-i(\sum_j \alpha_j h_j)t} \neq \prod_j e^{-i\alpha_j h_j t}$

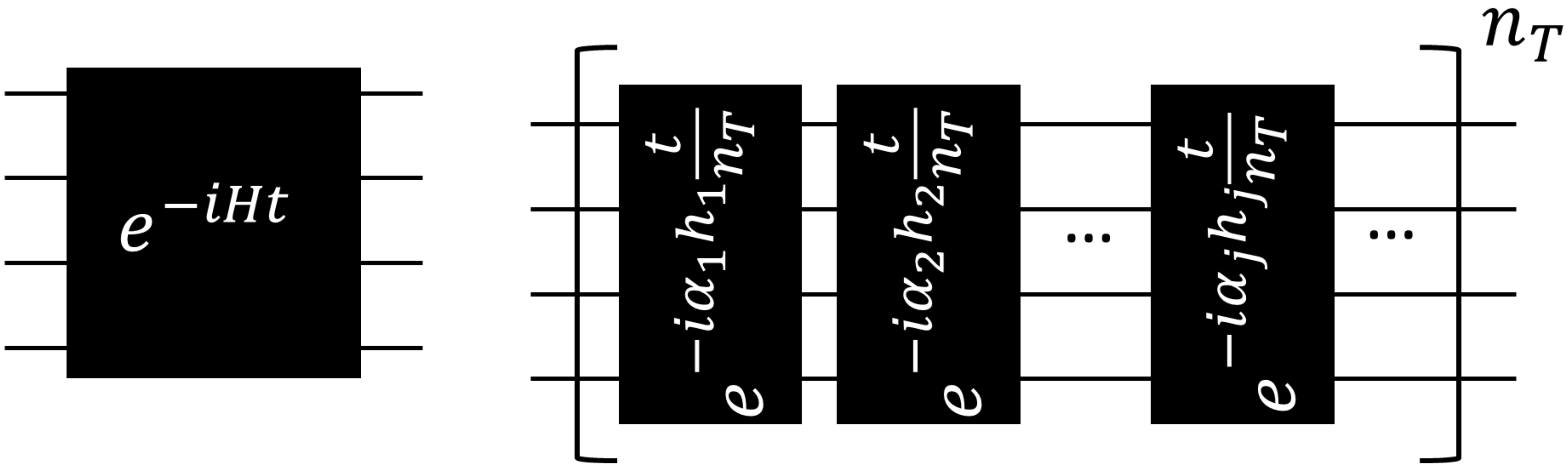
Actually, from BCH formula: $e^{t(A+B)} = e^{tA}e^{tB}e^{-\frac{t^2}{2}[A,B]}e^{\frac{t^3}{6}(2[B,[A,B]+[A,[A,B]])}...$

We learn that approximating exp. of sum with prod of exp is associated to an error $O(t^2)$ as $t \to 0$.
Nice because we can slice time: $e^{-iHt} = (e^{-iHt/n_T})^{n_T}$!
If n_T is big enough w.r.t t, we can approximate e^{-iHt} with the Lie-Trotter-Suzuki expansion (**trotterization**):

$$\boxed{e^{-iHt} \approx (\prod_j e^{-i\alpha_j h_j \frac{t}{n_T}})^{n_T}}$$

Trotterization circuit

Lie-Trotter-Suzuki expansion (**trotterization**): $e^{-iHt} \approx (\prod_j e^{-i\alpha_j h_j \frac{t}{n_T}})^{n_T}$

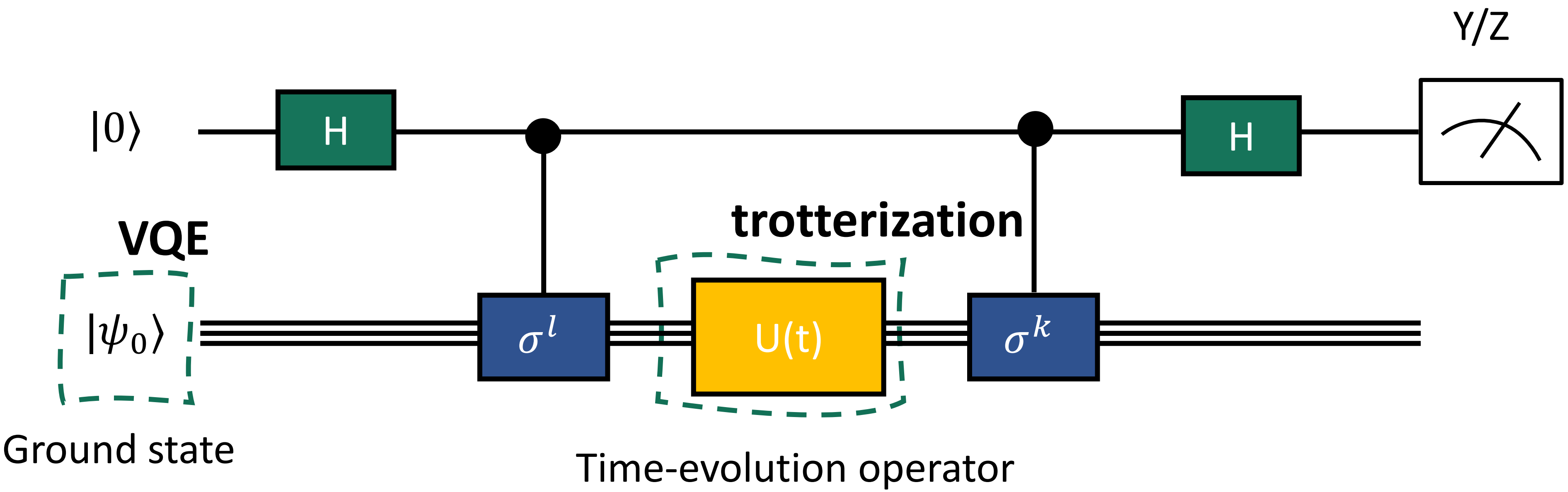


I haven't unpacked further what's in the boxes, but…

Electronic structure hamiltonians exhibit **k-locality**: terms of Hamiltonian act on at most k qubits. This can be shown to imply that the gate count of trotterized evolution is not exponential in the number of qubits.

Still, very large gate count. Linear scaling with t unavoidable in general (**no fast-forwarding theorem**).

OK, now you know all the ingredients to compute the impurity model's Green's function with a quantum computer!



VQE

trotterization

Ground state

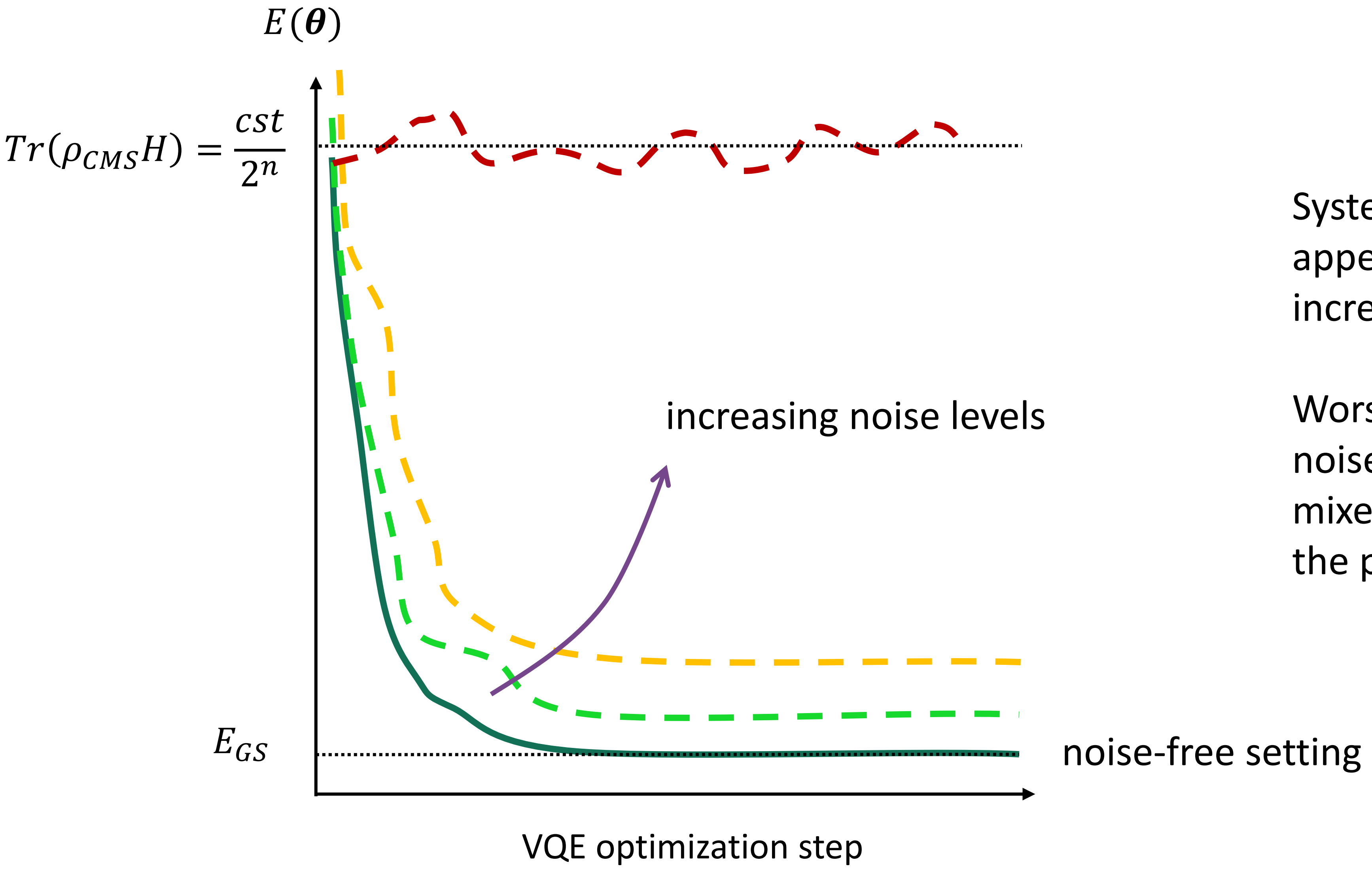
Time-evolution operator

But those are very noisy as for now…

VI. Hardware noise

How do imperfections of the device impact the results? How to model noise?

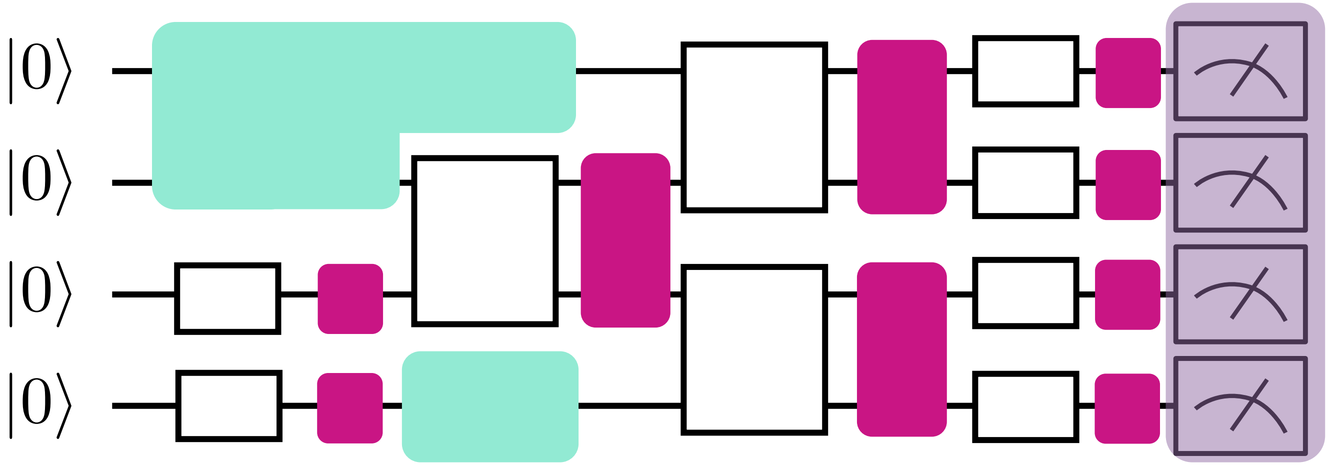
Effect of noise on VQE optimization of deep circuits



Systematic bias appears as noise increases.

Worst case: measure noise (get completely mixed state whichever the parametrization).

VI.1. Noise sources



- Idle noise (T_1, T_2) : relaxation $|1\rangle \rightarrow |0\rangle$, pure dephasing $|0\rangle + |1\rangle \rightarrow |0\rangle + e^{i\phi}|1\rangle$
- gates imperfections from imperfect control over tunable fields: represented as, eg, depolarizing noise (a Pauli gate randomly applies after the gate)
- Readout error: relaxation may occur during error as $t_{meas} \gg t_s, t_d$

VI.2. Modelization: example of the depolarizing model

Noise: $|\psi\rangle \rightarrow \rho = \sum_j p_j |\psi_j\rangle\langle\psi_j|$ (statistical mixture)

Model gate imperfections by adding Pauli operation/word at random after perfect gate applies

Noisy process is in all generality modelled through a quantum channel:

ε must be CPTP (Completely-Positive, Trace-Preserving) to be physical: → Kraus operators decomposition

$$\varepsilon(\rho) = \sum_k E_k \rho E_k^\dagger, \quad \sum_k E_k^\dagger E_k = I.$$

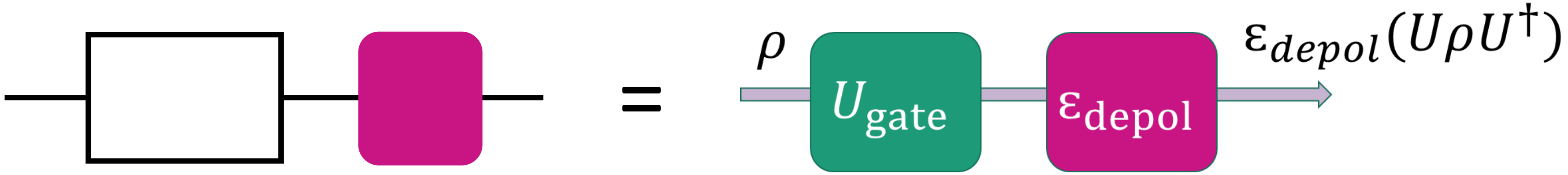
Formalism encompasses unitary (=noise-free) evolution: $\varepsilon(\rho) = U\rho U^\dagger$

VI.2. Modelization: example of the depolarizing model

Noise: $|\psi\rangle \rightarrow \rho = \sum_j p_j |\psi_j\rangle\langle\psi_j|$ (statistical mixture)

« Model gate imperfections by adding Pauli operation/word at random after perfect gate applies »

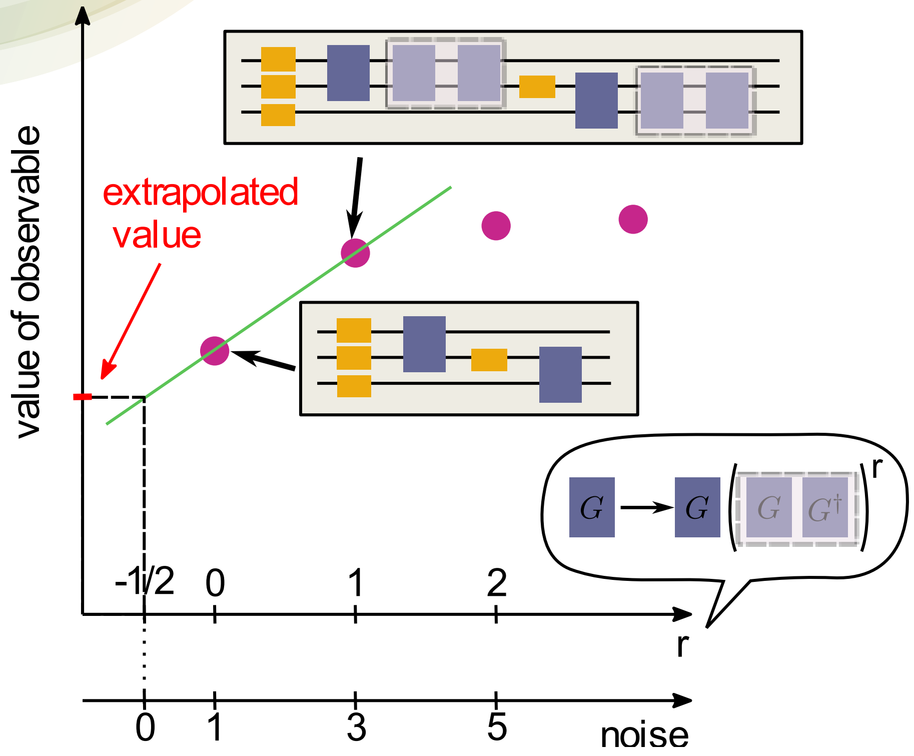
→ Single-qubit depolarizing channel reads: $\varepsilon_{\text{depol}}(\rho) = (1 - p)\rho + \frac{1}{3}p(X\rho X + Y\rho Y + Z\rho Z)$

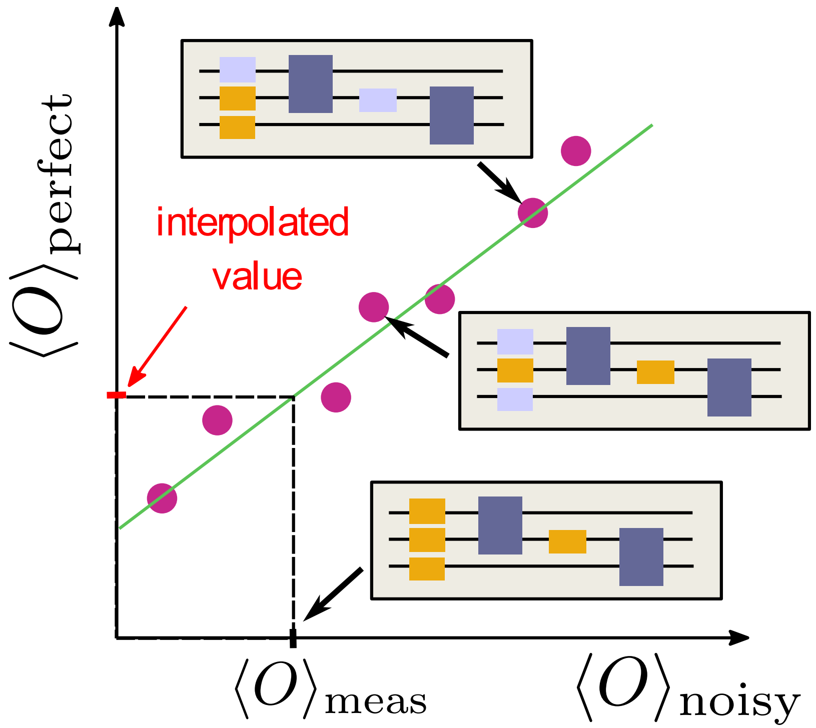


Two-qubit counterpart obtained as tensor product of such channels (but with higher value of depol.prob p!)

VI.3. Error mitigation

Examples of learning techniques to mitigate effect of gate noise on measured expectation value:





Zero-Noise Extrapolation: [Kandala, 2019]
Artificially inflate noise by duplicating noisy gates without changing logical function of circuit.

Clifford Data Regression: [Czarnik, 2021]
Train ansatz to associate measured observable to noisy counterpart by simulating resp. computing exactly the pair on training set of easy circuits similar to the target circuit.

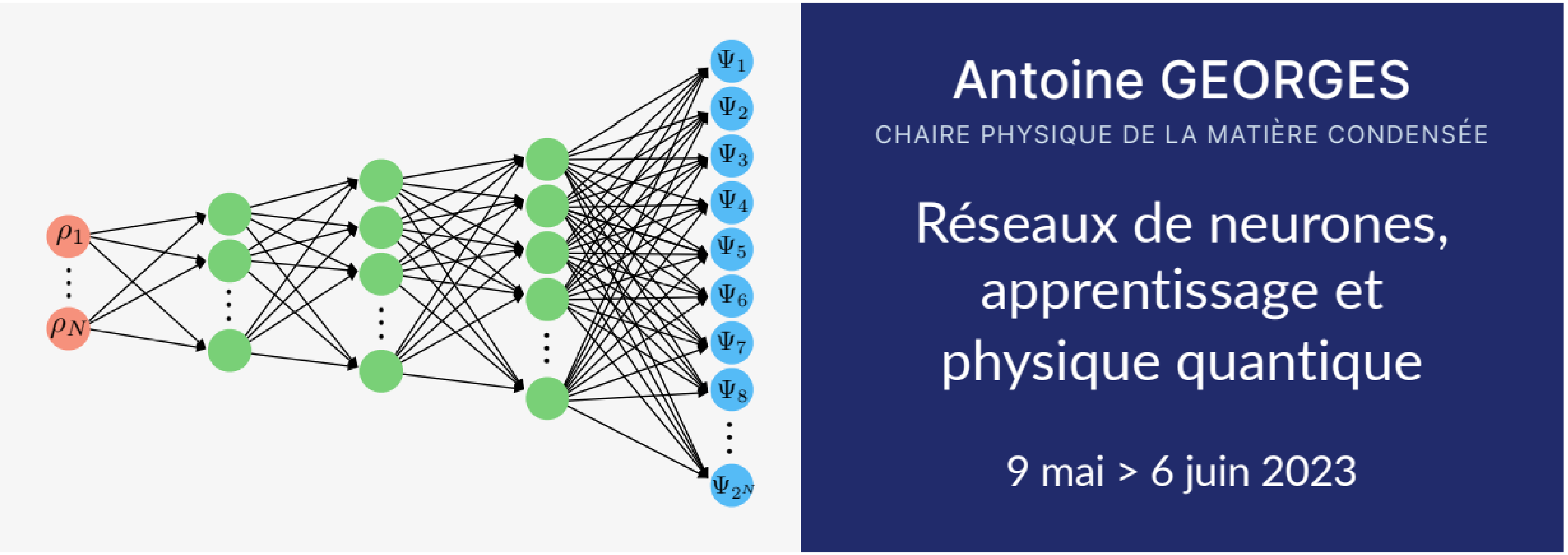
To wrap up…

- DMFT with a QC: compute GF of impurity model with QC
- Ground state preparation: variational method (VQE). Can be extended to reach excited states. Methods constructing the circuit on-the-fly were developed.
- Optimization still a classical task, benefitting from ML experience.
- Time-evolution: trotterization algorithm. Very deep circuits.
- Noise has a strong impact of the observables’ measured expectation values.
- Effect of gate imperfections can be mitigated, also borrowing techniques from ML
- Very active field!

Thank you for your attention!

Any questions?

Ad: upcoming lectures @Collège de France



Antoine GEORGES

CHAIRE PHYSIQUE DE LA MATIÈRE CONDENSÉE

Réseaux de neurones, apprentissage et physique quantique

9 mai > 6 juin 2023

Les applications des algorithmes d'apprentissage utilisant les réseaux de neurones profonds se sont considérablement développées récemment, avec des résultats souvent spectaculaires. La physique des systèmes quantiques complexes ne fait pas exception, avec de multiples applications qui constituent un nouveau champ de recherche. On peut citer par exemple la représentation et l'optimisation des fonctions d'onde de systèmes quantiques à grands nombre de degrés de liberté, la détermination de la fonction d'onde à partir de mesures (tomographie quantique) ou encore les applications à la structure électronique des matériaux comme la détermination de fonctionnelles de densité plus précises ou l'apprentissage de champs de forces pour accélérer les simulations de dynamique moléculaire. Le cours de cette année constituera une introduction à ce domaine pour les non spécialistes. Ce cours introductif sera complété par des séminaires présentant des développements récents et des recherches en cours.

Recordings (FR) and slides (ENG) will be put on CDF's website.