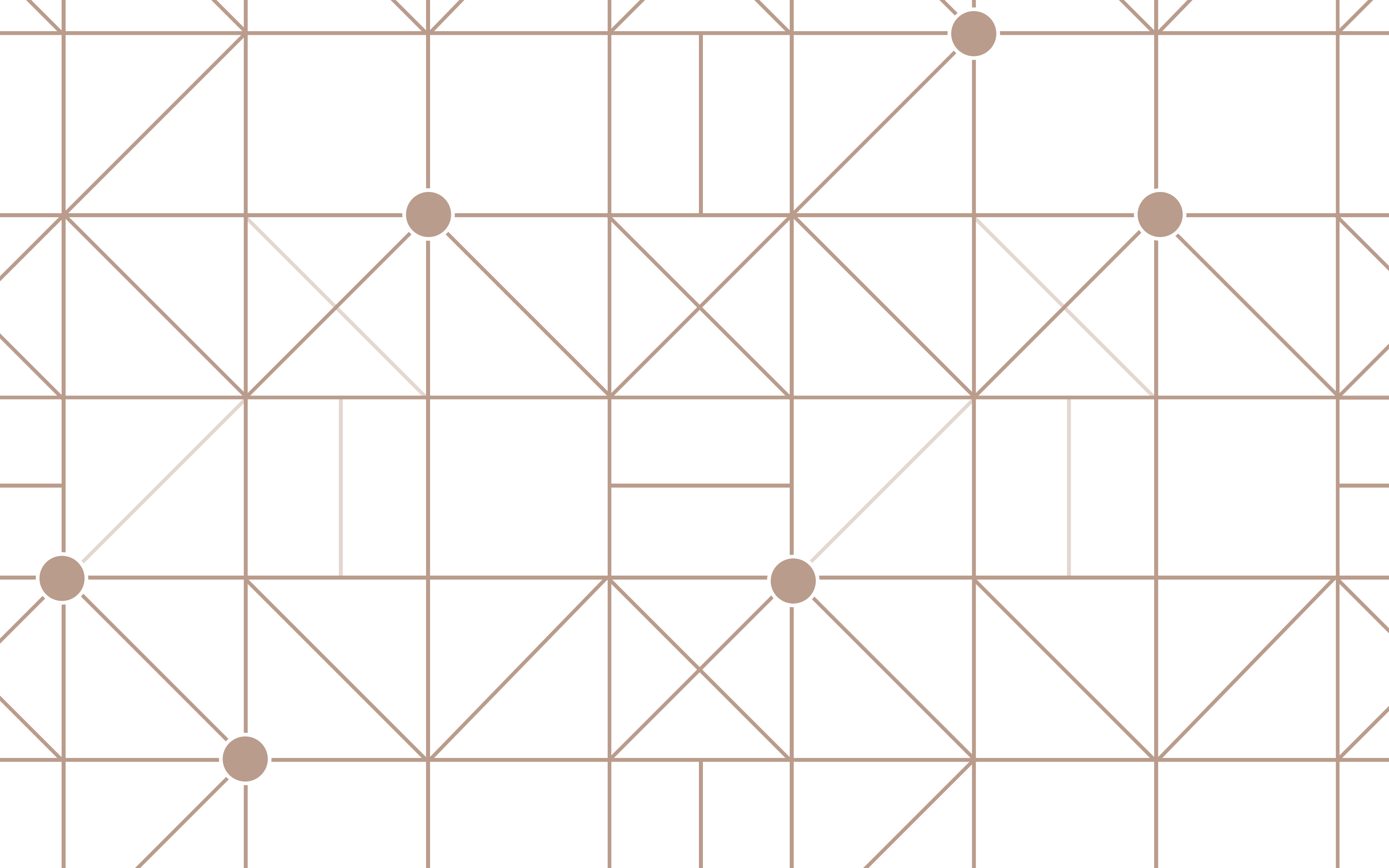


Variational Quantum Eigensolver
(VQE)

hybrid

QPU

classical

Variational theorem

Hermitian operator $H = H^{+}$

$\hat{H} \rightarrow$ Hamiltonian

$H|\Phi\rangle = E|\Phi\rangle$

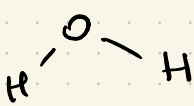
eigenvec

energy of system

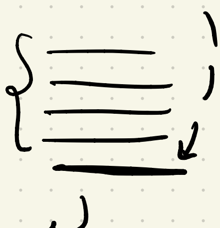
eigenval

$|\Phi\rangle \rightarrow$ parameters θ

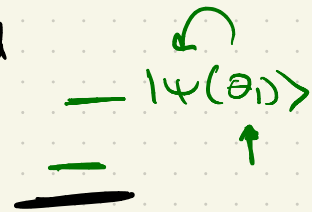
$|\Phi\rangle = |\Psi(\theta)\rangle$



excited states



lowest eigenvalue $\leftarrow$ ground state optimal approx of the ground state

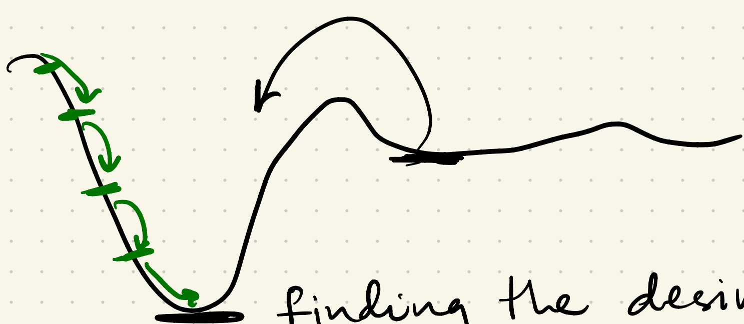


$|\Phi_0\rangle \rightarrow$ optimal / lowest eigenvec, $\lambda_0 \rightarrow$ eigenval

is the one that minimizes the expectation value of H

$$\boxed{\langle \hat{H} \rangle = \langle \Psi(\theta) | \hat{H} | \Psi(\theta) \rangle \geq \lambda_0}$$

Practically: find the "right" θ, to get close as possible to λ_0



finding the desired λ_0

Hybrid algorithm → classical

- optimize our parameters

↓

Quantum

- set up + define problem
- test possible solution

Algorithm:

1. Initialize the problem
   - default state $|00\ldots00\rangle$
   - classical + quantum state
   - application-specific ref state

entangled? TwoLocal? QML → ZZFeatureMap

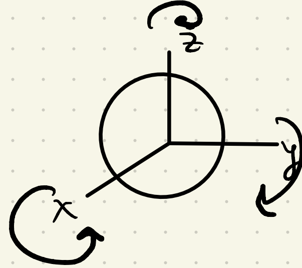
2. Prepare ansatz → parametrized quantum circuit
   - application specific
   - variatiational ansatz
   - ansatzes on the fly

QAOA

UCCSD ansatz

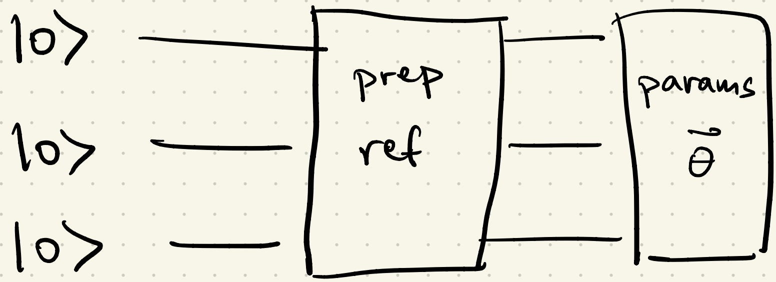
HE

$$R_x(\theta) = \begin{bmatrix} \cos \theta/2 & -i\sin \theta/2 \\ -i\sin \theta/2 & \cos \theta/2 \end{bmatrix}$$



$$R_y(\theta) = \begin{bmatrix} \cos \theta/2 & -\sin \theta/2 \\ \sin \theta/2 & \cos \theta/2 \end{bmatrix}$$

$$R_z(\theta) = \begin{bmatrix} e^{-i\theta/2} & 0 \\ 0 & e^{i\theta/2} \end{bmatrix}$$



③ Cost function

↳ what are we trying to minimize

- nature of function
- measurement strategy
- primitives

- errors!

④ Optimize parameters

$\{\vec{\theta}\} \longrightarrow$ find $\{\theta_1^0, \theta_2^0, \dots \theta_n^0\}$

$\downarrow$ take a step

$\{\theta_1^1, \theta_2^1, \dots \theta_n^1\}$

$\downarrow$

$\{\theta_1^{opt}, \dots \theta_n^{opt}\}$

optimizers!

grad-based

↳ grad descent!

grad-free

bootstrapping

③ cost function

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

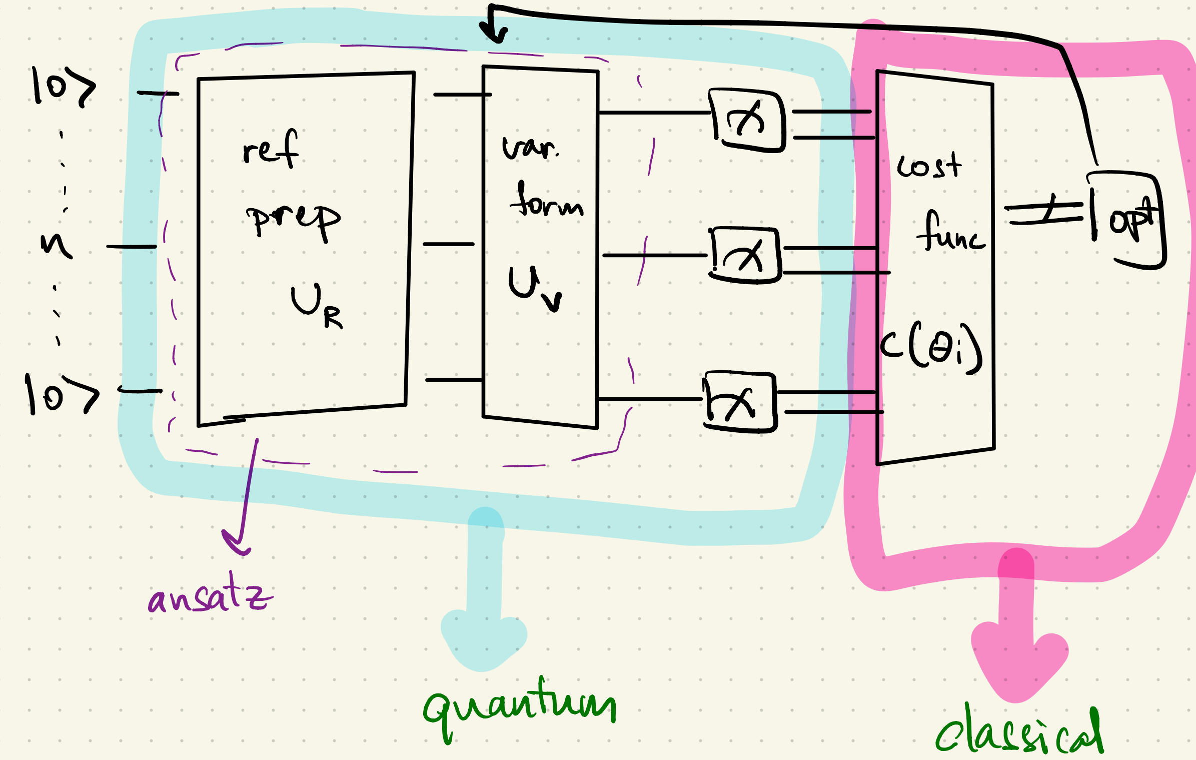
def cost func (θ, circ, ham, estimator):

return energy est.

computes the expectation value

also sampler

$p_k = |\langle k | \psi \rangle|^2$



VQE:

- prepare ref U_R

$$|0\rangle \xrightarrow{U_R} |\rho\rangle$$

- apply variational $U_v(\vec{\theta})$ to create ansatz $U_A(\vec{\theta})$

$$|\rho\rangle \longrightarrow U_v|\rho\rangle = |\psi(\vec{\theta})\rangle$$

- evaluate cost func

- optimize, pick a new θ_{i+1}
- repeat until convergence