

uroCC National

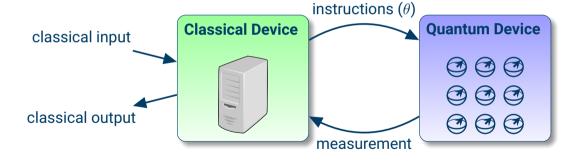


#ENCCS

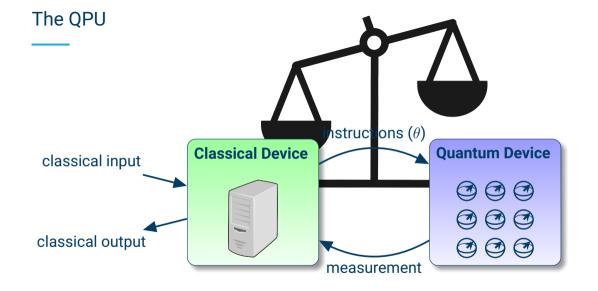
Variational quantum algorithms

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The QPU



1



Variational Principle

Given:

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- an observable $A = \sum_{i} \lambda_{i} \ket{\psi_{i}} \bra{\psi_{i}}$

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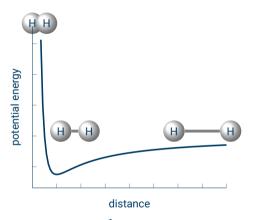
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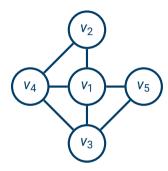
Idea:

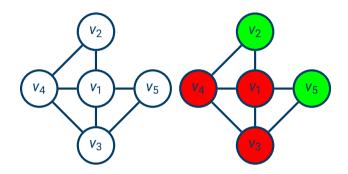
• Encode problem in λ_{\min}

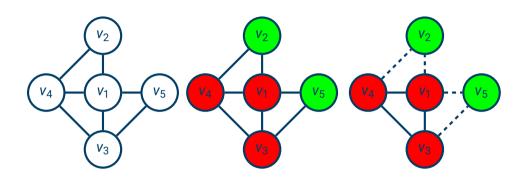
Quantum Chemistry

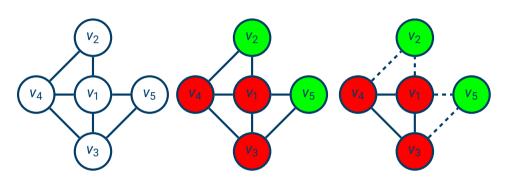


$$H(x) = \sum_{p,q} h_{p,q}(x) a_p^{\dagger} a_q + \frac{1}{2} \sum_{p,q,r,s} h_{p,q,r,s}(x) a_p^{\dagger} a_q^{\dagger} a_r a_s + h_{\text{nuc}}$$
 (2)









$$H = \sum_{i,j} a_{i,j} Z_i Z_j + \sum_i b_i Z_i$$
 (3)

Express problem as ground state of Hamiltonian

$$H_{j,k} = \text{diag}(+1, -1, -1, +1) = Z_j \otimes Z_k, \quad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$
 (4)

Observe that, e.g.,

•
$$H_{i,k} |00\rangle = +1|00\rangle$$
,

•
$$H_{i,k} |01\rangle = -1 |01\rangle$$
,

•
$$H_{i,k} |10\rangle = -1 |10\rangle$$
,

•
$$H_{j,k} |11\rangle = +1 |11\rangle$$

Global continuous optimization problem

original problem

 $Hamiltonian \rightarrow$

minimize $\mathsf{cost}(\theta) = \langle \phi(\theta) | A | \phi(\theta)
angle$

Different ansätze: $|\phi(\theta)\rangle = \textit{U}(\theta)\,|0
angle$

Example Ansatz

Using 2p parameters $\gamma=\gamma_1,\ldots,\gamma_p$, $\beta=\beta_1,\ldots,\beta_p$, prepare state

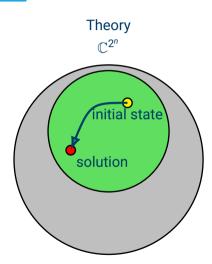
$$|\Psi(\gamma,\beta)\rangle = U_{B_p}U_{C_p}\dots U_{B_1}U_{C_1}|+\rangle^{\otimes n}, \qquad (5)$$

where the operators have the explicit form

$$U_{B_{I}} = e^{-i\beta_{I}H_{B}} = \prod_{j=1}^{n} e^{-i\beta_{I}\sigma_{x}^{j}},$$

$$U_{C_{I}} = e^{-i\beta_{I}H_{C}} = \prod_{(j,k)\in E} e^{-i\gamma_{I}w_{j,k}H_{i,j}},$$
(6)

Expressability of Ansatz



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