ICGM

Institut Charles Gerhardt Montpellier

CHEMISTRY: MOLECULES TO MATERIALS

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Introduction to Quantum Computation

Part 2

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December 12, 2022

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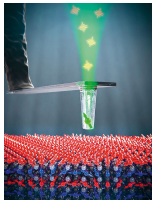
Quantum Communication

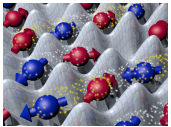
Secured transmissions

Quantum Sensors



Better sensitivity and resolution

Quantum Simulation

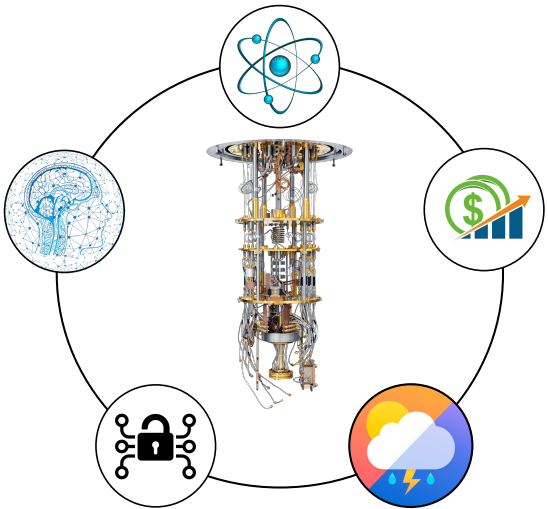


Chemical reaction and material properties

Quantum Computing

Powerful calculations

Applications of Quantum Computing



Electronic Structure Problem

Electronic structure problem

The Hamiltonian of a molecule composed of M nuclei and N electrons reads

$$\hat{H} = -\sum_i \frac{\hbar^2}{2m_e}\nabla_i^2 - \sum_I \frac{\hbar^2}{2M_I}\nabla_I^2 - \sum_{i,I} \frac{e^2}{4\pi\epsilon_0}\frac{Z_I}{|\mathbf{r}_i - \mathbf{R}_I|} + \frac{1}{2}\sum_{i\neq j} \frac{e^2}{4\pi\epsilon_0}\frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} + \frac{1}{2}\sum_{I\neq J} \frac{e^2}{4\pi\epsilon_0}\frac{Z_I Z_J}{|\mathbf{R}_i - \mathbf{R}_j|}$$

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Born-Oppenheimer approximation ($M_I > 1000 m_e$), nuclei are treated as stationary and decoupled with the dynamics of the electrons. In atomic units:

$$\hat{H} = -\sum_i \frac{\nabla_i^2}{2} - \sum_{i,I} \frac{Z_I}{|\mathbf{r}_i - \mathbf{R}_I|} + \frac{1}{2}\sum_{i\neq j} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}$$

We want to solve the time-dependent non-relativistic Schrödinger equation,

$$\hat{H}\,|\Psi_n\rangle = E_n\,|\Psi_n\rangle$$

Second quantization

In practice, one works with N basis functions $\{\phi_p(\mathbf{x}_i)\}$ (spin-orbitals) where $\mathbf{x}_i$ is the spatial and spin coordinate of the i-th electron, $\mathbf{x}_i = (\mathbf{r}_i, s_i)$. We project the Hamiltonian onto this basis such that

$$\hat{H} = \sum_{pq} h_{pq} \hat{a}_p^\dagger \hat{a}_q + \frac{1}{2} \sum_{pqrs} \langle pq|sr\rangle \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_r \hat{a}_s$$

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where

$$\begin{aligned} h_{pq} &= \int \mathrm{d}\mathbf{x} \phi_p^*(\mathbf{x}) \left(-\frac{\nabla^2}{2} - \sum_I \frac{Z_I}{|\mathbf{r} - \mathbf{R}_I|} \right) \phi_q(\mathbf{x}) \\ \langle pq|sr\rangle &= \iint \mathrm{d}\mathbf{x}_1 \mathbf{x}_2 \, \phi_p^*(\mathbf{x}_1) \phi_q^*(\mathbf{x}_2) \frac{1}{|\mathbf{x}_1 - \mathbf{x}_2|} \phi_s(\mathbf{x}_1) \phi_r(\mathbf{x}_2) \end{aligned}$$

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and the creation and annihilation operators fulfill the fermionic anticommutation rules,

$$\{\hat{a}_p, \hat{a}_q^\dagger\} = \hat{a}_p \hat{a}_q^\dagger + \hat{a}_q^\dagger \hat{a}_p = \delta_{pq}, \qquad \{\hat{a}_p, \hat{a}_q\} = \{\hat{a}_p^\dagger, \hat{a}_q^\dagger\} = 0.$$

Slater determinants

A Slater determinant is a many-body wavefunction written as an antisymmetrized product of single electron basis functions $\{\phi_p(\mathbf{x}_i)\}$,

$$\Phi(\mathbf{x}_1 \cdots \mathbf{x}_{N_e}) = \frac{1}{\sqrt{N_e}} \begin{vmatrix} \phi_1(\mathbf{x}_1) & \phi_2(\mathbf{x}_1) & \cdots & \phi_N(\mathbf{x}_1) \\ \phi_1(\mathbf{x}_2) & \phi_2(\mathbf{x}_2) & \cdots & \phi_N(\mathbf{x}_2) \\ . & . & . & . \\ . & . & . & . \\ . & . & . & . \\ \phi_1(\mathbf{x}_{N_e}) & \phi_2(\mathbf{x}_{N_e}) & \cdots & \phi_N(\mathbf{x}_{N_e}) \end{vmatrix} \equiv |f_N, f_{N-1}, \cdots, f_2, f_1\rangle \equiv |f\rangle\,, \quad f_i \in \{0,1\}$$

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The second quantized formalism consists in manipulating those *occupation vectors* (determinants) which form a complete many-body basis of the problem Hilbert space, i.e.

$$|\Psi_n\rangle = \sum_f c_{fn} |f\rangle$$

There are $\binom{N}{N_e}$ many Slater determinants !

Electronic Structure Problem on QC

2nd Quantized Fermion Encodings

Jordan–Wigner encoding

Direct mapping between the *occupation of an orbital* and the state of the qubit:

$$|\psi_{\text{qubit}}\rangle = \alpha\,|0\rangle + \beta\,|1\rangle\,, \quad |0\rangle \leftrightarrow \text{empty}, \quad |1\rangle \leftrightarrow \text{occupied}$$

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N-qubit register can generate a quantum state superposition of $2^N > \binom{N}{N_e}$ bitstrings:

$$|\Psi_{\text{qubit}}\rangle = \sum_{q=0}^{2^N-1} c_q\,|q\rangle \longleftrightarrow |\Psi_n\rangle = \sum_{f}^{\binom{N}{N_e}} c_{fn}\,|f\rangle$$

where the integer value of q is associated to the bitstring corresponding to this integer.

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where the integer value of q is associated to the bitstring corresponding to this integer.

Obviously, one can map $|\Psi_n\rangle$ as a *superposition* of *all the bitstrings that contains exactly* N_e *ones and* $N - N_e$ *zeros*,

$$|f_N, f_{N-1}, \cdots, f_2, f_1\rangle \to |q_N, q_{N-1}, \cdots, q_2, q_1\rangle\,, \qquad q_p = f_p \in \{0, 1\}$$

Jordan–Wigner encoding

Qubit mappings of the creation and annihilation operators:

$$\hat{a}_p^\dagger = \left(\bigotimes_{i=p+1}^{N} I_i\right) \otimes Q_p^\dagger \otimes \left(\bigotimes_{i=1}^{p-1} Z_i\right), \quad \hat{a}_p = \left(\bigotimes_{i=p+1}^{N} I_i\right) \otimes Q_p \otimes \left(\bigotimes_{i=1}^{p-1} Z_i\right)$$

where $Q^\dagger = |1\rangle\langle 0| = \dfrac{X - iY}{2}$, $Q = |0\rangle\langle 1| = \dfrac{X + iY}{2}$, and the string of Z operators enforces the exchange anti-symmetry of fermions.

The string of Z operators means that it takes $\mathcal{O}(N)$ qubit operations to apply a fermionic operator.

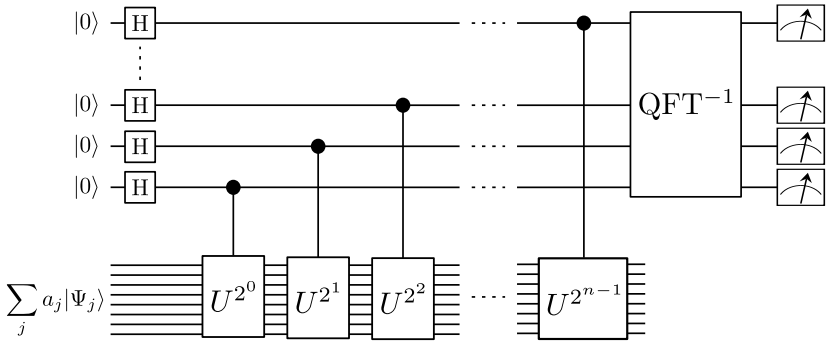
Electronic Structure Problem on QC

Quantum Algorithms

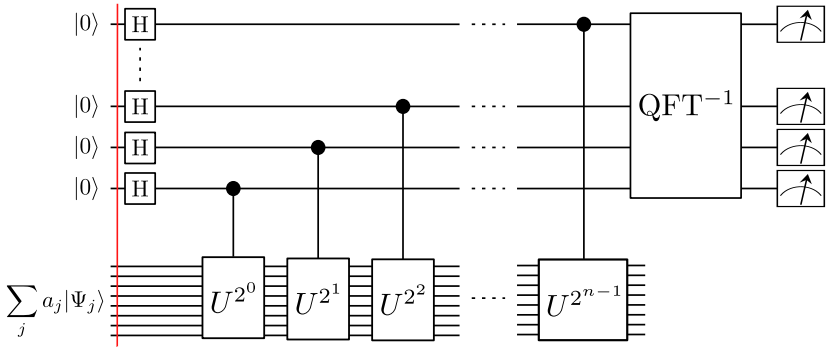
Quantum Phase Estimation

Quantum Phase Estimation

- **Phase estimation**: $E_j t$ of $U = e^{i\hat{H}t}$ with $e^{i\hat{H}t}|\Psi_j\rangle = e^{iE_j t}|\Psi_j\rangle$
- **Two qubit registers**: one encoding the state and the other composed of ancilla qubits
- **Initial state**: non-zero overlap with the eigenstates, $|\Phi\rangle = \sum_j a_j |\Psi_j\rangle$

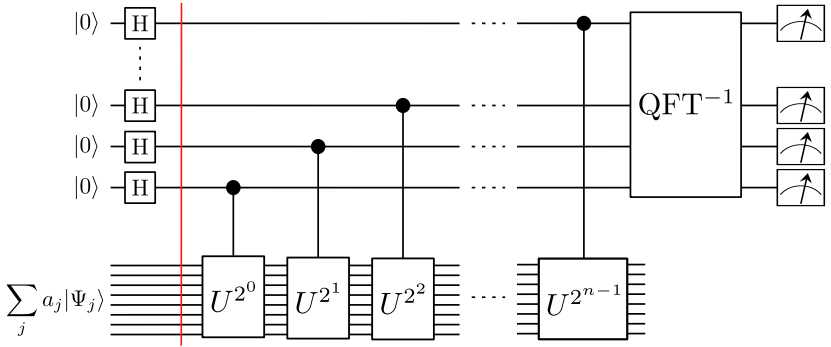


Quantum Phase Estimation



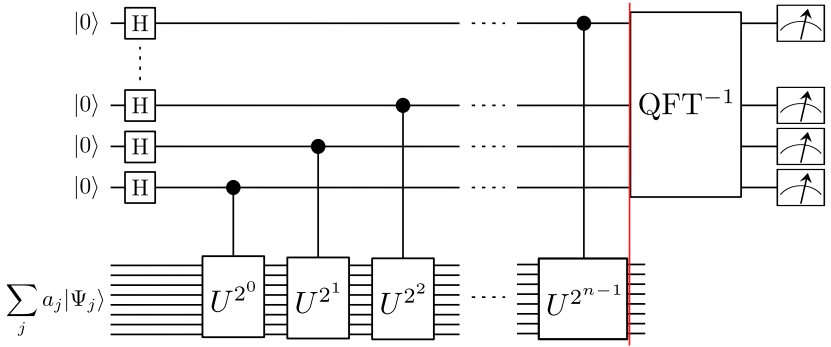
$$|0\rangle^{\otimes n} \otimes \sum_j a_j \, |\Psi_j\rangle$$

Quantum Phase Estimation



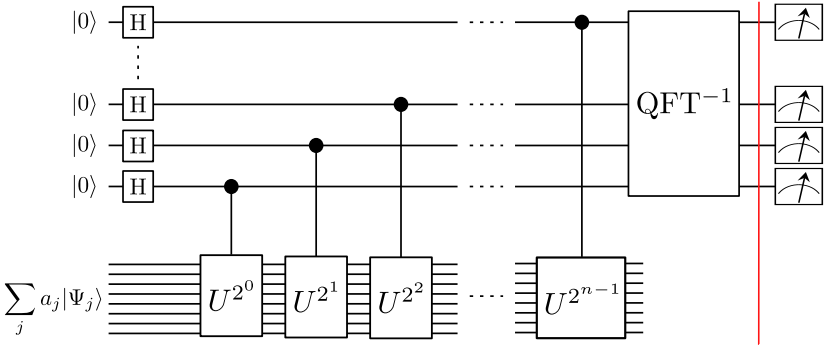
$$\underbrace{\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes \cdots \otimes \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)}_{n \text{ times}} \otimes \sum_j a_j |\Psi_j\rangle$$

Quantum Phase Estimation



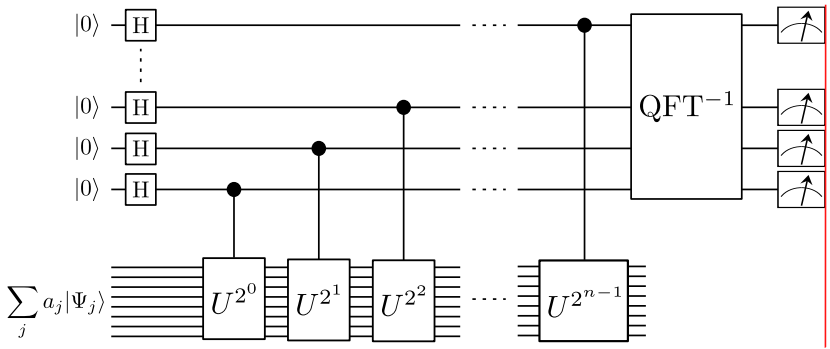
$$\frac{1}{\sqrt{2^n}}\sum_j a_j(|0\rangle+e^{iE_j 2^{n-1}t}|1\rangle)\otimes(|0\rangle+e^{iE_j 2^{n-2}t}|1\rangle)\otimes\cdots\otimes(|0\rangle+e^{iE_j 2t}|1\rangle)\otimes|\Psi_j\rangle = \frac{1}{\sqrt{2^n}}\sum_j a_j \sum_{k=0}^{2^n-1} e^{iE_j kt}|\Psi_j\rangle$$

Quantum Phase Estimation



$$\frac{1}{\sqrt{2^n}}\sum_j a_j \sum_{k=0}^{2^n-1} e^{iE_j kt}|\Psi_j\rangle \xrightarrow{\mathsf{QFT}^{-1}} \sum_j a_j \left|\tilde{E}_j t\right\rangle |\Psi_j\rangle$$

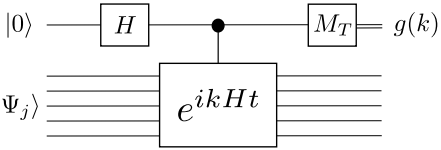
Quantum Phase Estimation



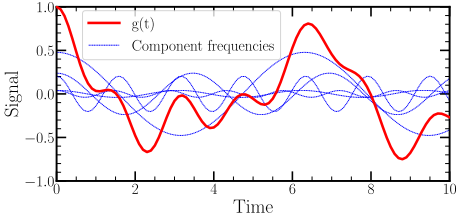
One measures the value of the phase $\tilde{E}_j t$ (as a binary fraction on the ancilla register), i.e. an approximation of $E_j t$ with n bits of accuracy, with probability $|a_j|^2 = |\langle\Phi|\Psi_j\rangle|^2$. The system register collapses to the eigenstate $|\Psi_j\rangle$.

Single-ancilla Quantum Phase Estimation

Single-ancilla Quantum Phase Estimation



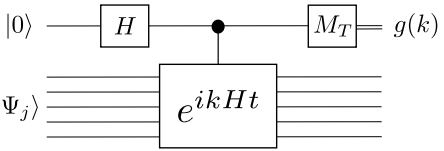
$$|\Phi\rangle = \sum_j a_j |\Psi_j\rangle$$

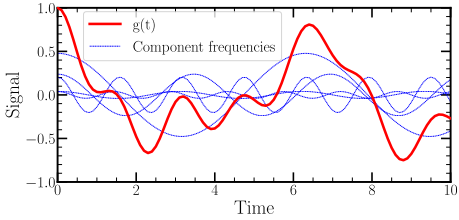


$$\sum_j a_j |\Psi_j\rangle \otimes \frac{1}{\sqrt{2}} \left(|0\rangle + e^{ikE_j t} |1\rangle\right)$$

Single-ancilla Quantum Phase Estimation

$$|\Phi\rangle = \sum_j a_j |\Psi_j\rangle$$





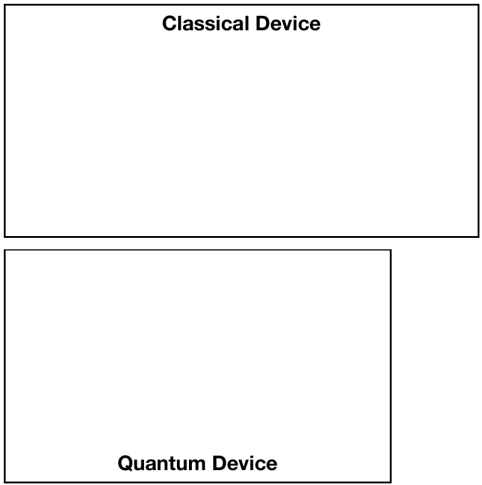
$$\sum_j a_j |\Psi_j\rangle \otimes \frac{1}{\sqrt{2}}\left(|0\rangle + e^{ikE_j t}|1\rangle\right) \xrightarrow{\text{Tomography gate } M_T} g(k) = \sum_j |a_j|^2 e^{ikE_j t}$$

- Imprint multiple E_j as frequencies of an ancilla qubit ('phase kickback').
- Extract in postprocessing like identifying notes in a chord.

Variational Quantum Eigensolver

Peruzzo *et al.*, Nature Communication (2014)

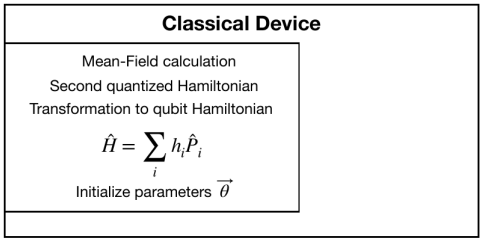
Variational Quantum Eigensolver



Variational principle:

$$E_0 = \min_{\vec{\theta}} \langle \Psi(\vec{\theta}) | \hat{H} | \Psi(\vec{\theta}) \rangle$$

Variational Quantum Eigensolver



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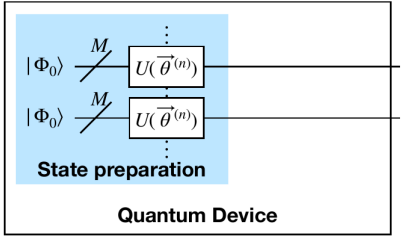
Variational Quantum Eigensolver

Classical Device

Mean-Field calculation
Second quantized Hamiltonian
Transformation to qubit Hamiltonian

$$\hat{H} = \sum_i h_i \hat{P}_i$$

Initialize parameters $\vec{\theta}$



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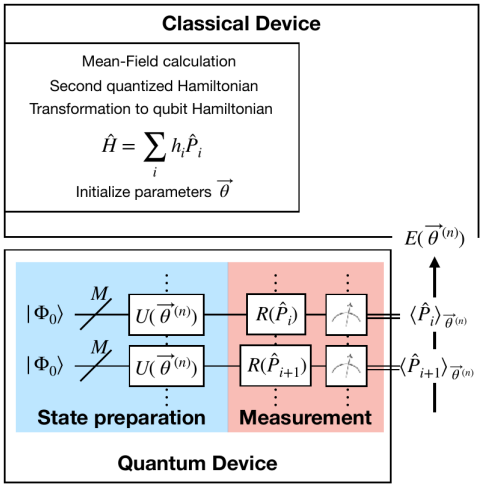
$$|\Psi(\vec{\theta})\rangle = U(\vec{\theta}) |\Phi_0\rangle$$

Variational Quantum Eigensolver



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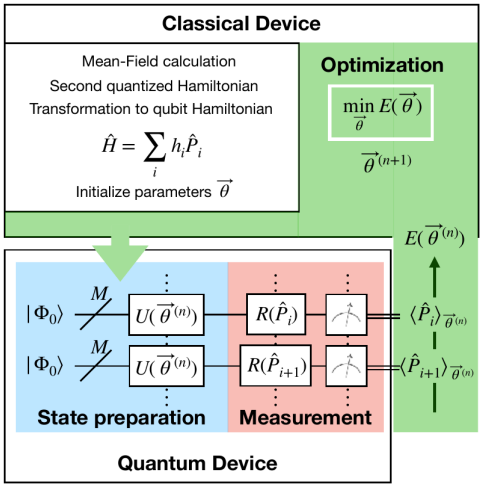
Measurement:

$$P\left(\sum_i m_i = 1 \bmod 2 \,\middle|\, R(\hat{P}) \right) = \frac{1}{2}\left(1 - \langle \hat{P} \rangle\right)$$

$$E(\vec{\theta}) = \sum_i h_i \langle \hat{P}_i \rangle_{\vec{\theta}}$$

Variational Quantum Eigensolver



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VQE Ansatz

There are mainly two types of ansatz, physically-inspired and hardware efficient.

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Hardware efficient: R_Y ansatz (Kandala *et al.*, Nature 2017)

$$\hat{U}(\boldsymbol{\theta}) \quad = \quad \prod_{m=1}^{M} R_{Y,m}(\theta_m^0) \prod_{n=1}^{N_L} \hat{U}_n^{\mathrm{ENT}}(\boldsymbol{\theta}^n)$$

for a number of layers N_L and a number of qubits M. The entanglement unitary blocks read

$$\hat{U}_n^{\mathrm{ENT}}(\boldsymbol{\theta}^n) = \prod_{m=1}^{M-1} \mathrm{CNOT}_{m(m+1)} \prod_{m=1}^{M} R_{Y,m}(\theta_m^n).$$

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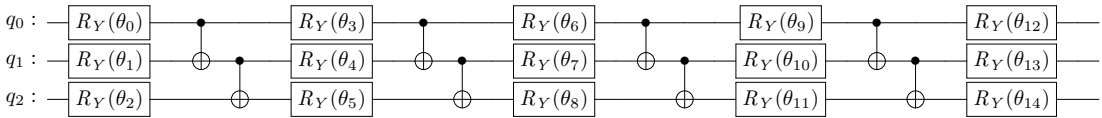

VQE Ansatz

Physically-inspired: Unitary Coupled Cluster ansatz

$$\hat{U}(\boldsymbol{\theta}) = e^{\hat{T}-\hat{T}^\dagger}, \quad \hat{T} = \hat{T}_1 + \hat{T}_2 + \cdots, \quad \hat{T}_1 = \sum_{pq} \theta_q^p \, \hat{a}_p^\dagger \hat{a}_q, \quad \hat{T}_2 = \sum_{pqrs} \theta_{rs}^{pq} \, \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_s \hat{a}_r$$

VQE Ansatz

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Applying Jordan–Wigner (assuming $q > p > s > r$):

$$\theta_q^p \left(\hat{a}_p^\dagger \hat{a}_q - \text{h.c.} \right) = \frac{i\theta_q^p}{2} \bigotimes_{k=q+1}^{p-1} Z_k \left(Y_q X_p - X_q Y_p \right)$$

$$\theta_{rs}^{pq} \left(\hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_s \hat{a}_r - \text{h.c.} \right) = \frac{i\theta_{rs}^{pq}}{8} \bigotimes_{k=r+1}^{s-1} Z_k \bigotimes_{l=p+1}^{q-1} Z_l (\quad X_r X_s Y_q X_p + Y_r X_s Y_q Y_p + X_r Y_s Y_q Y_p + X_r X_s X_q Y_p$$

$$- \quad Y_r X_s X_q X_p - X_r Y_s X_q X_p - Y_r Y_s Y_q X_p - Y_r Y_s X_q Y_p)$$

Circuit for the exponential of Pauli string

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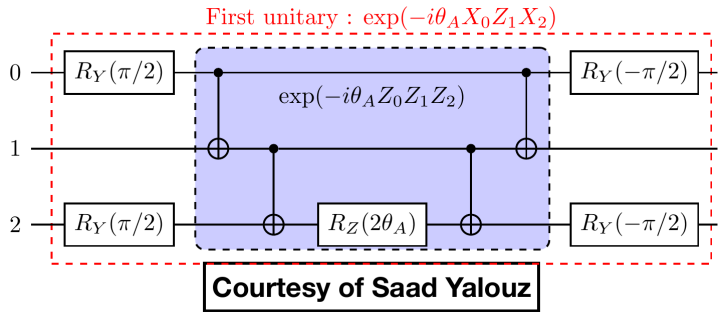
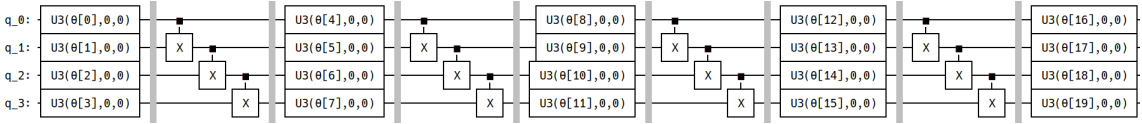
However, we know how to implement the exponential of a single Pauli string, so we can use (first-order) Trotter–Suzuki approximation:

$$e^{\sum_j \theta_j \hat{P}_j} \approx \prod_j e^{\theta_j \hat{P}_j}$$



VQE Ansatz

Ry (4 qubits, 4 layers, 19 parameters) $\mathcal{O}(N^2)$



VQE Ansatz

GUCCSD (4 qubits, 2 electrons, 9 parameters) $\mathcal{O}(N^4)$

Measuring the expectation value of a Hermitian operator

Measurements are usually supported in the computational basis $\{|j\rangle\}$ (measurement of the observable Z).

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The idea is to find the unitary which diagonalizes the Hermitian operator $\hat{P} = \hat{U}^\dagger\hat{\Lambda}\hat{U}$ with $\hat{\Lambda} = \mathrm{diag}(\lambda_1, \cdots, \lambda_n)$. Since $\hat{\Lambda}$ is diagonal, we have transformed the problem from one where we must perform a measurement in an arbitrary basis, to one where we simply measure in the computational basis:

$$\langle\Psi|\,\hat{P}\,|\Psi\rangle = \langle\Psi|\,\hat{U}^\dagger\hat{\Lambda}\hat{U}\,|\Psi\rangle = \left\langle\bar{\Psi}\right|\hat{\Lambda}\left|\bar{\Psi}\right\rangle = \sum_j \lambda_j|\langle\bar{\Psi}|j\rangle|^2, \quad \text{where}\left|\bar{\Psi}\right\rangle = \hat{U}\,|\Psi\rangle\,.$$

Measuring the energy

Remember that

$$\hat{H} = \sum_{pq} h_{pq} \hat{a}_p^\dagger \hat{a}_q + \frac{1}{2} \sum_{pqrs} \langle pq|sr\rangle \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_r \hat{a}_s = \sum_j h_j \hat{P}_j, \quad \text{with} \quad \hat{P}_j \in \{I, X, Y, Z\}^{\otimes N}$$

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The ground-state energy is determined by solving the Schrödinger equation $\hat{H}\,|\Psi_0\rangle = E_0\,|\Psi_0\rangle$, or equivalently:

$$\begin{aligned} E_0 = \langle \Psi_0 | \hat{H} | \Psi_0 \rangle &= \sum_{pq} h_{pq} \underbrace{\langle \Psi_0 | \hat{a}_p^\dagger \hat{a}_q | \Psi_0 \rangle}_{\text{1-RDM elements}} + \frac{1}{2} \sum_{pqrs} \langle pq|sr\rangle \underbrace{\langle \Psi_0 | \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_r \hat{a}_s | \Psi_0 \rangle}_{\text{2-RDM elements}} \\ &= \sum_j h_j \langle \Psi_0 | \hat{P}_j | \Psi_0 \rangle \end{aligned}$$

Hence, within VQE we measure the 1- and 2-RDM elements that are then multiplied by the electronic integrals to estimate the ground-state energy of the system.

QUIZZ

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Quantum implementation of a Functional-Free Density-Functional Theory

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