PHYSICS REBOOTCAMP
QUANTUM INFORMATION BOOTCAMP VENEZUELA
2022

QUANTUM ALGORITHMS

A very short introduction

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A very short introduction….

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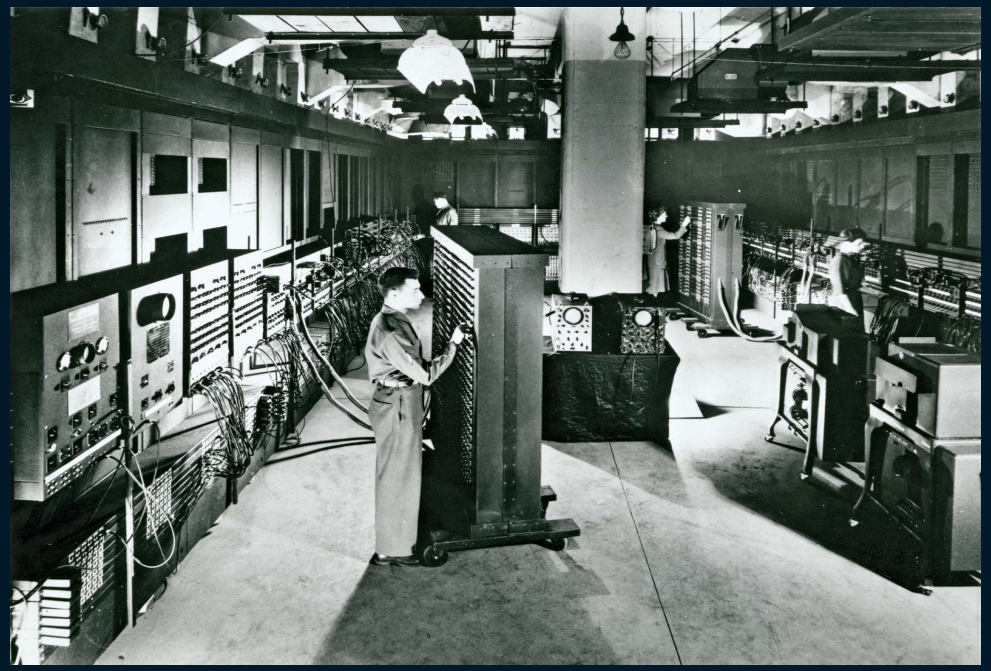
B

C



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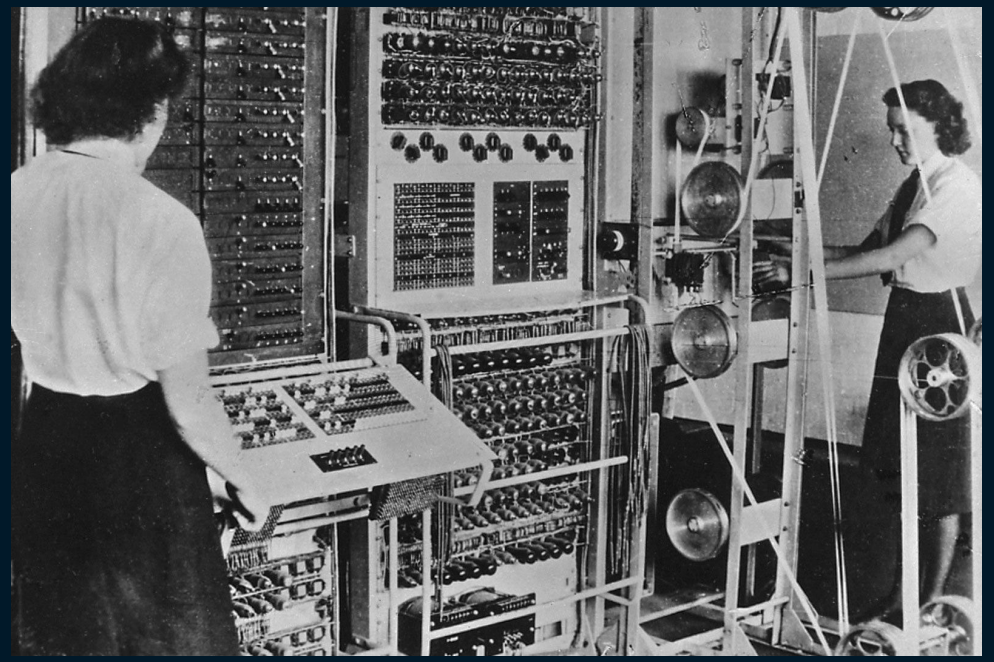
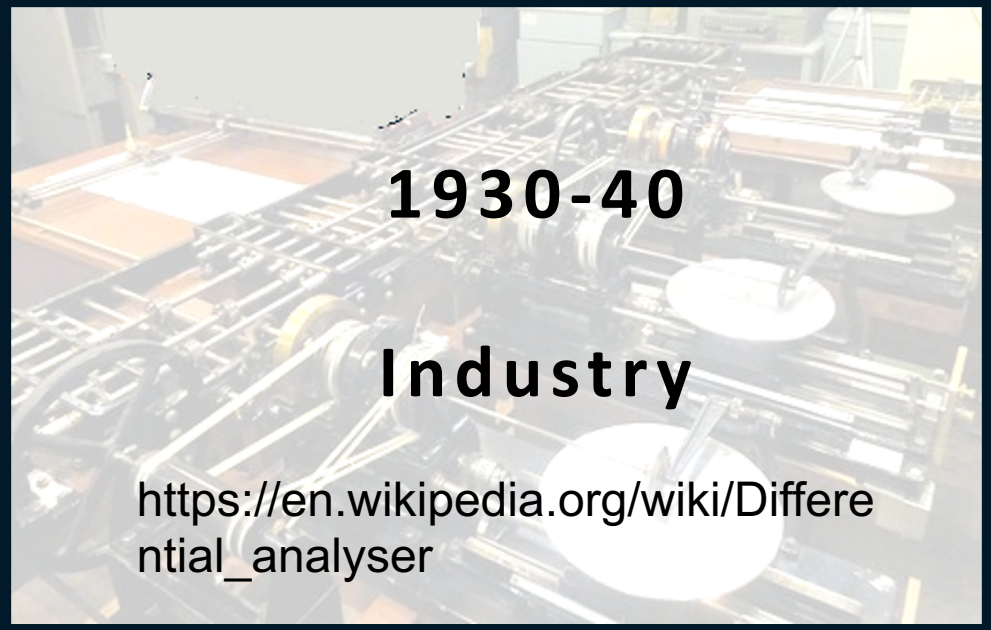


200 b.c.

Astronomy

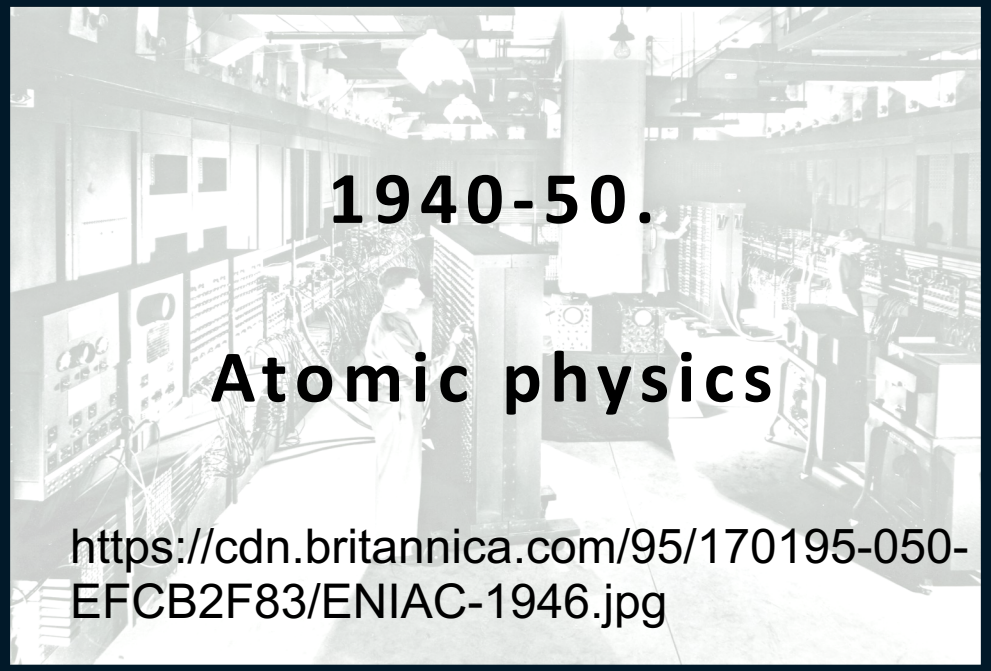
https://www.techeblog.com/antikythera-mechanism-ancient-computer-greece/



1930-40

Industry

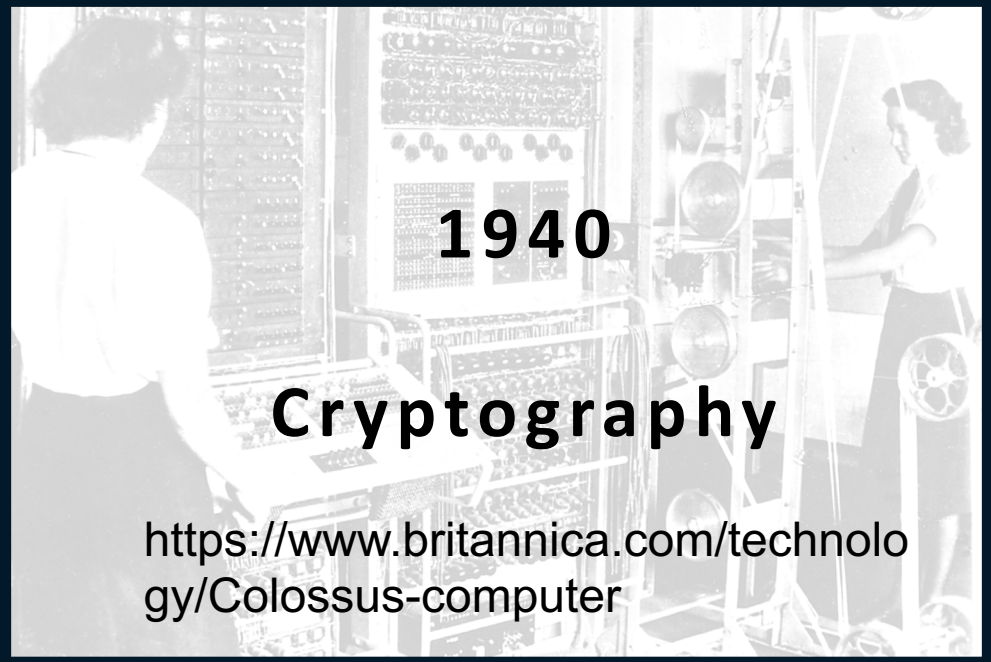
https://en.wikipedia.org/wiki/Differential_analyser



1940-50.

Atomic physics

https://cdn.britannica.com/95/170195-050-EFCB2F83/ENIAC-1946.jpg



1940

Cryptography

https://www.britannica.com/technology/Colossus-computer

Deutsh-Jozsa Algorithm

Deutsh-Jozsa Algorithm

The problem consists in a boolean function f(x1,x2,...xn) with “n” INPUTS only capable of two specific behaviors: a balanced function and a constant function.

f(x1,x2,…,xn) is balanced if 50% of the OUTPUT is the value “1” and 50% the value “0”

f(x1,x2,...xn) is constant if 100% of the OUTPUT is the value “1” or 100% is the value “0”

For a function of n boolean INPUTS the total number of different evaluations for the function is: 2^n.

In the best case the function should only be evaluated TWICE to determine that is a balanced function.

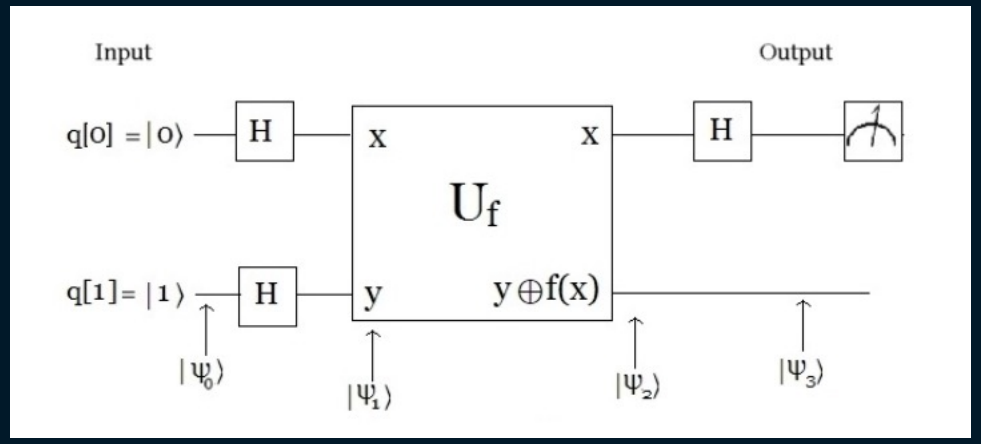
In the worst case the function should be evaluated $2^{n-1} + 1$ times to determine if the function is constant.

Deutsh-Jozsa Algorithm

If n is “big enough” the number of iterations can reach unmanageable numbers

For n=30 the number of iterations is 536870912 (around half a million iterations).

The algorithm of Deutsh (for only one control qubit) consists in the following quantum circuit:



Deutsh-Jozsa Algorithm

The algorithm starts with a “control” qubit in the “0” state and the “target” qubit in the state “1”

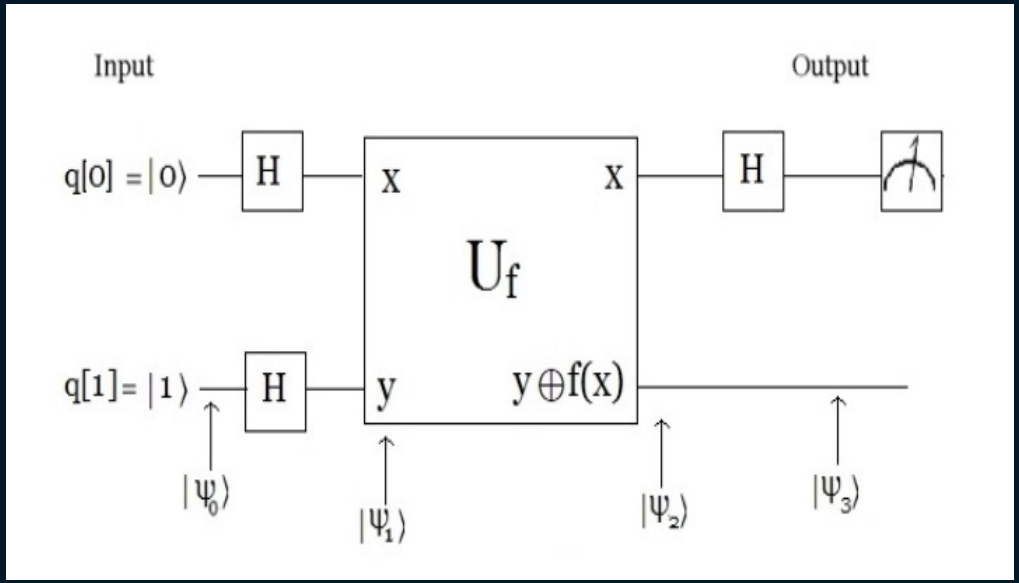
$$|\Psi_0\rangle = |0\rangle_c |1\rangle_t$$

Then a Hadamard gate is applied to each qubit

$$\Psi_1\rangle = H|\Psi_0\rangle = H_c|0\rangle_c H_t|1\rangle_t = \frac{1}{2}(|0\rangle + |1\rangle)_c(|0\rangle - |1\rangle)_t$$

Here both qubits enter a gate called “oracle” (Uf) as INPUTS and this gate results in the control qubit not modified and the target qubit modified depending on the value of the control qubit via the boolean function f(x)

$$|\Psi_2\rangle = U_f|\Psi_1\rangle = \frac{1}{2}(|0\rangle + |1\rangle)_c)(|0 \bigoplus f(x)\rangle - |1 \bigoplus f(x)\rangle)_t$$



Deutsh-Jozsa Algorithm

With some manipulation is possible to write the output states as function of the initial states and the value of the function:

$$|\Psi_2\rangle = \frac{1}{2}(|0\rangle+|1\rangle)_c)(|0 \bigoplus f(x)\rangle - |1 \bigoplus f(x)\rangle)_t = \frac{1}{2}(-1)^{f(0)}\,|0\rangle_c\,(|0\rangle-|1\rangle)_t + (-1)^{f(1)}\,|1\rangle_c\,(|0\rangle-|1\rangle)_t$$

Then finally a Hadamar gate is applied in the control qubit:

$$|\Psi_3\rangle = H_c\,|\Psi_2\rangle = \frac{1}{2}((-1)^{f(0)}H_c\,|0\rangle_c\,(|0\rangle - |1\rangle)_t + (-1)^{f(1)}H_c\,|1\rangle_c\,(|0\rangle - |1\rangle)_t$$

Then again with some manipulation we can see the following result:

$$|\Psi_3\rangle = \frac{1}{2}((\frac{(-1)^{f(0)} + (-1)^{f(1)}}{\sqrt{2}})\,|0\rangle_c + (\frac{(-1)^{f(0)} - (-1)^{f(1)}}{\sqrt{2}})\,|1\rangle_c\,(|0\rangle - |1\rangle)_t$$

Deutsh-Jozsa Algorithm

Then is possible to measure the control qubit with and determine what kind of function is f(x).

Is also possible to generalize the result to n control qubits with a simmilar procedure and get the following result for the Probability of the system in the base state:

$$\left| \frac{1}{2^n} \sum_{x=0}^{2^n-1} (-1)^{f(x)} \right|^2$$

If the function is constant the probability of measure the base state is 1, if the function is balanced the probability of measure this state is 0.

Variational Quantum Eigensolver Algorithm

The Variational Quantum Eigensolver algorithm
an overview

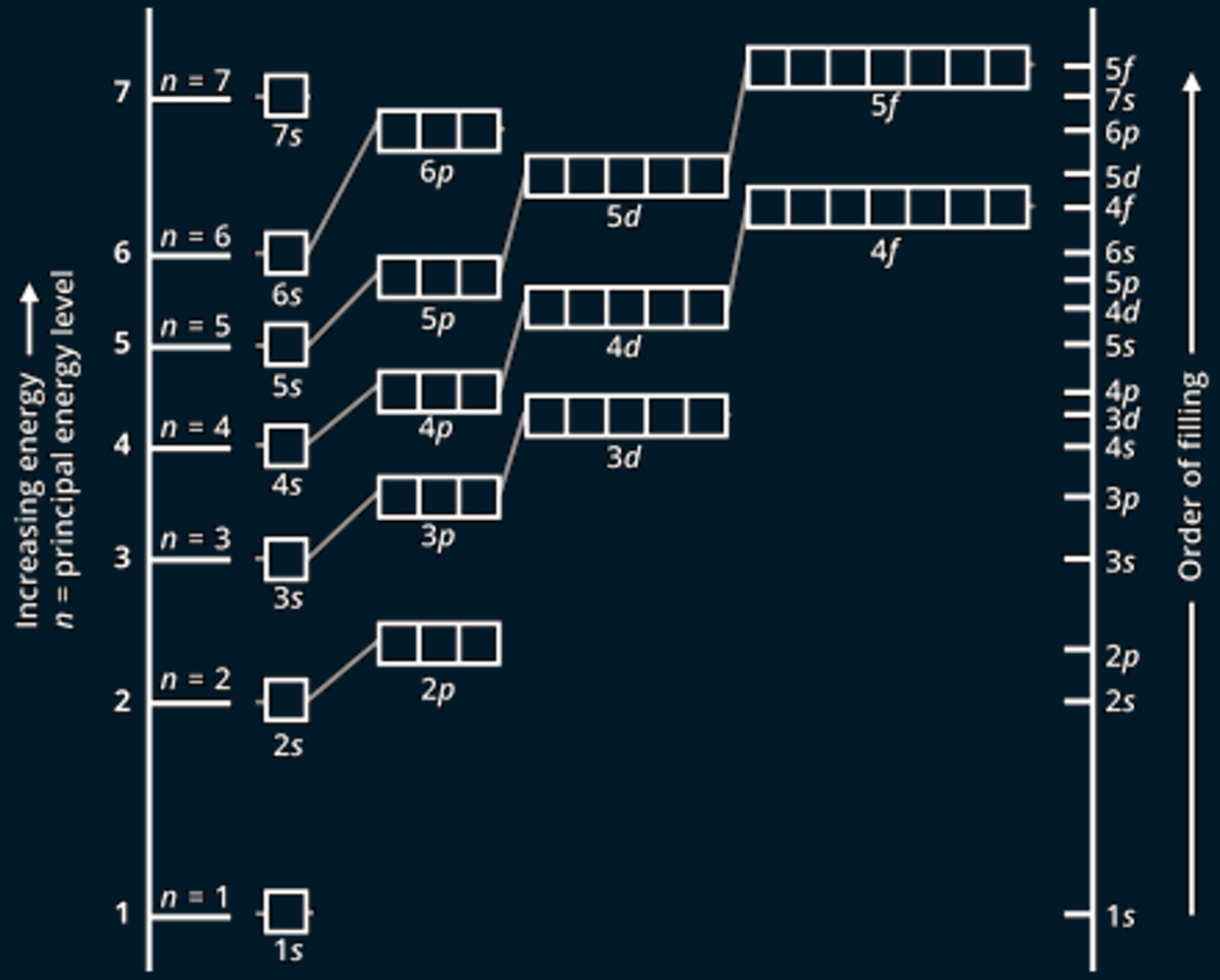
I. Electronic structure of matter

II. Second quantization

III. Variational methods

IV. VQE Algorithm

Electronic structure of matter



Z atomic number

A mass number

nlj subshell

Light Matter interaction (atomic, molecular level)

- Physical and chemical properties

Electronic structure of matter

N-electron-P nucleon Hamiltonian (atom):

$$\widehat{H}_{\text{tot}} = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\nabla_i^2 - \sum_{i=1}^{N}\sum_{l=1}^{P}\frac{Z_{ll}^2}{r_{il}} + \sum_{i=1}^{N}\sum_{j>i}^{N}\frac{e^2}{r_{ij}} + \sum_{l=1}^{P}\sum_{m>l}^{P}\frac{Z_l Z_m e^2}{r_{lm}} - \frac{\hbar^2}{2}\sum_{l=1}^{P}\frac{\nabla_l^2}{M_l} \qquad (1)$$

Using the Born-Oppenheimer approximation $\longrightarrow$ Electronic part separation

Second quantization results

$$\xi_{ij}(\mathbf{r}_1, \mathbf{r}_2) = \left[\phi_i(\mathbf{r}_1)\phi_j(\mathbf{r}_2) - \phi_i(\mathbf{r}_2)\phi_j(\mathbf{r}_1)\right]/\sqrt{2} \qquad (2)$$

Slater determinant
2-electron state function

$$\Phi(\mathbf{r}_1, \mathbf{r}_2) = \sum_{i>j=1}^{N_o} C_{ij}\xi_{ij}(\mathbf{r}_1, \mathbf{r}_2) \qquad (3)$$

Fock space

$$|\Phi\rangle = \sum_{\bar{n}} C_{\bar{n}}\left|n_1, n_2, \dots n_{N_o}\right\rangle, n_i = \{0,1\} \qquad (4)$$

Operators definition

$$\hat{a}_i^\dagger\left|n_1, \dots n_i, \dots n_{N_o}\right\rangle = \delta_{n_i 0}(-1)^{\sum_{j<i} n_j}\left|n_1, \dots (n_i + 1), \dots n_{N_o}\right\rangle$$

$$\hat{a}_i\left|n_1, \dots n_i, \dots n_{N_o}\right\rangle = \delta_{\mathrm{n}_i,}(-1)^{\sum_{j<1} n_j}\left|n_1, \dots (n_i - 1), \dots n_{N_o}\right\rangle \qquad (5)$$

$$\{\hat{a}_i^\dagger, \hat{a}_j\} = \delta_{ij}\{\hat{a}_i, \hat{a}_j\} = \{\hat{a}_i^\dagger, \hat{a}_j^\dagger\} = 0 \quad (6)$$

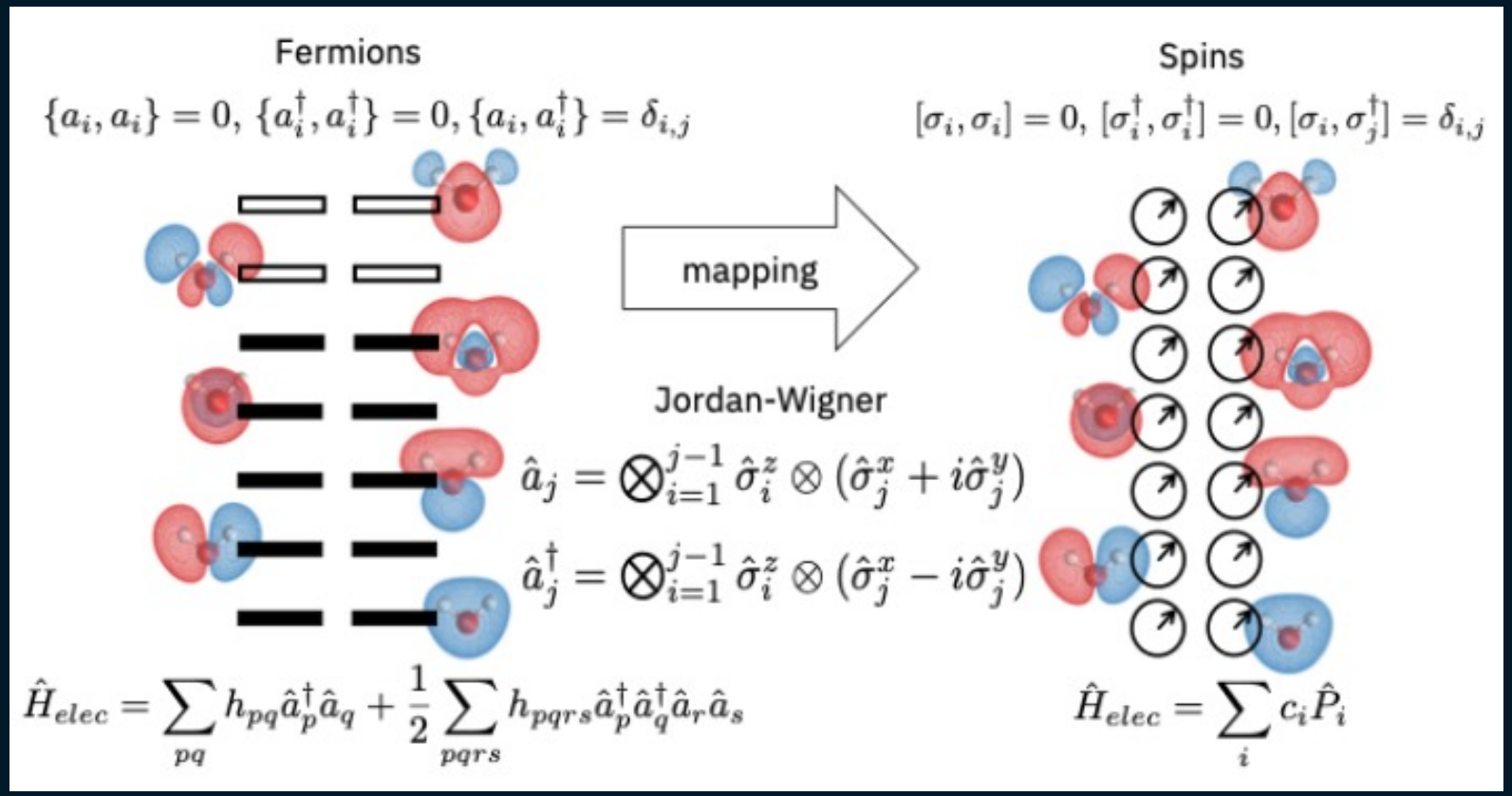
Algebra

$$\hat{H}_e = \sum_{pq} h_{pq}\hat{a}_p^\dagger \hat{a}_q + \sum_{pqrs} g_{pq,rs}\hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_r \hat{a}_s \quad (7)$$

Second quantization Hamiltonian

$$h_{pq} = \int \phi_p^*(r)\left(-\frac{1}{2}\nabla^2 - \sum_I \frac{Z_I}{R_I - r}\right)\phi_q(r)dr \quad (8)$$

$$h_{pqrs} = \int \frac{\phi_p^*(r_1)\phi_q^*(r_2)\phi_r(r_2)\phi_s(r_1)}{|r_1 - r_2|} dr_1 dr_2$$



Jordan Wigner Mapping

$|1100 > \rightarrow |\uparrow\uparrow\downarrow\downarrow>$

$\hat{a}_2|1100 >= (-1)|100 >$

$$\hat{a}_j \rightarrow \sigma_j^{(-)}$$

$$\hat{a}_j^\dagger \rightarrow \sigma_j^{(+)}$$

$$\sigma^{(z)}|\uparrow\rangle = -1|\uparrow\rangle$$

$$\hat{a}_j \rightarrow \sigma_j^{(-)} \otimes \sigma_{j-1}^{(z)} \cdots \otimes \sigma_1^{(z)}$$

$$\hat{a}_j^\dagger \rightarrow \sigma_j^{(+)} \otimes \sigma_{j-1}^{(z)} \cdots \otimes \sigma_1^{(z)} \qquad (9)$$

Fermions to qubits mapping

Fermions

Ocupation

$$H_{\mathrm{e}} = \sum_{pq} h_{pq} \hat{a}_p^\dagger \hat{a}_q + \sum_{pqrs} g_{pq,rs} \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_r \hat{a}_s$$

$$|\Phi\rangle = \sum_{\bar{n}} C_{\bar{n}} \left| n_1, n_2, \dots n_{N_o} \right\rangle, n_i = \{0,1\}$$

$$|1,1,0,0\rangle = \hat{a}_1^\dagger \hat{a}_2^\dagger |0,0,0,0\rangle$$

Qubits

Orientarion

$$H_q = \sum_{i\alpha} h_i^{(\alpha)} \sigma_i^{(\alpha)} + \sum_{ij\alpha\beta} h_{ij}^{(\alpha\beta)} \sigma_i^{(\alpha)} \sigma_j^{(\beta)} + \cdots.$$

$$|\Phi\rangle = \sum_{\bar{\sigma}}^{2^{N_o}} C_{\bar{\sigma}} \left| \sigma_1^{(z)}, \sigma_2^{(z)}, \dots \sigma_{N_o}^{(z)} \right\rangle, \sigma_k^{(z)} = \{\uparrow, \downarrow\}$$

$$|\uparrow, \uparrow, \downarrow, \downarrow\rangle = \hat{\sigma}_1^{(+)} \hat{\sigma}_2^{(+)} \hat{\sigma}_1^{(z)} |\downarrow, \downarrow, \downarrow, \downarrow\rangle$$

VQR algorithm:

$$U = e^{it\hat{H}} \approx \prod_j U_j^{(g)} \quad (10)$$

Number of gates

$$U(\theta, T) = U_1(\theta)\mathrm{U}_2(T) \quad (11)$$

Successive parameters

$$\Pi_j e^{-iT_j(\mathbf{n},\boldsymbol{\sigma})_i}\left|\Phi_q(0)\right> = \left|\Phi_q(\mathbf{T})\right> \quad (12)$$

linear combination of orbitals

Variational principle

$$H_\mathrm{q}\left|\Phi_\mathrm{q}(\theta)\right\rangle = E_n\left|\Phi_\mathrm{q}(\theta)\right\rangle \quad (13)$$

Minimizing energy

$$E_0 = \frac{\left\langle \Psi\,(\theta)_0\middle|H_\mathrm{q}\middle|\Phi_\mathrm{q}(\theta)\right\rangle}{\left\langle \Phi_\mathrm{q}(\theta)\mid \Phi_\mathrm{q}(\theta)\right\rangle} \quad (14)$$

VQR algorithm:

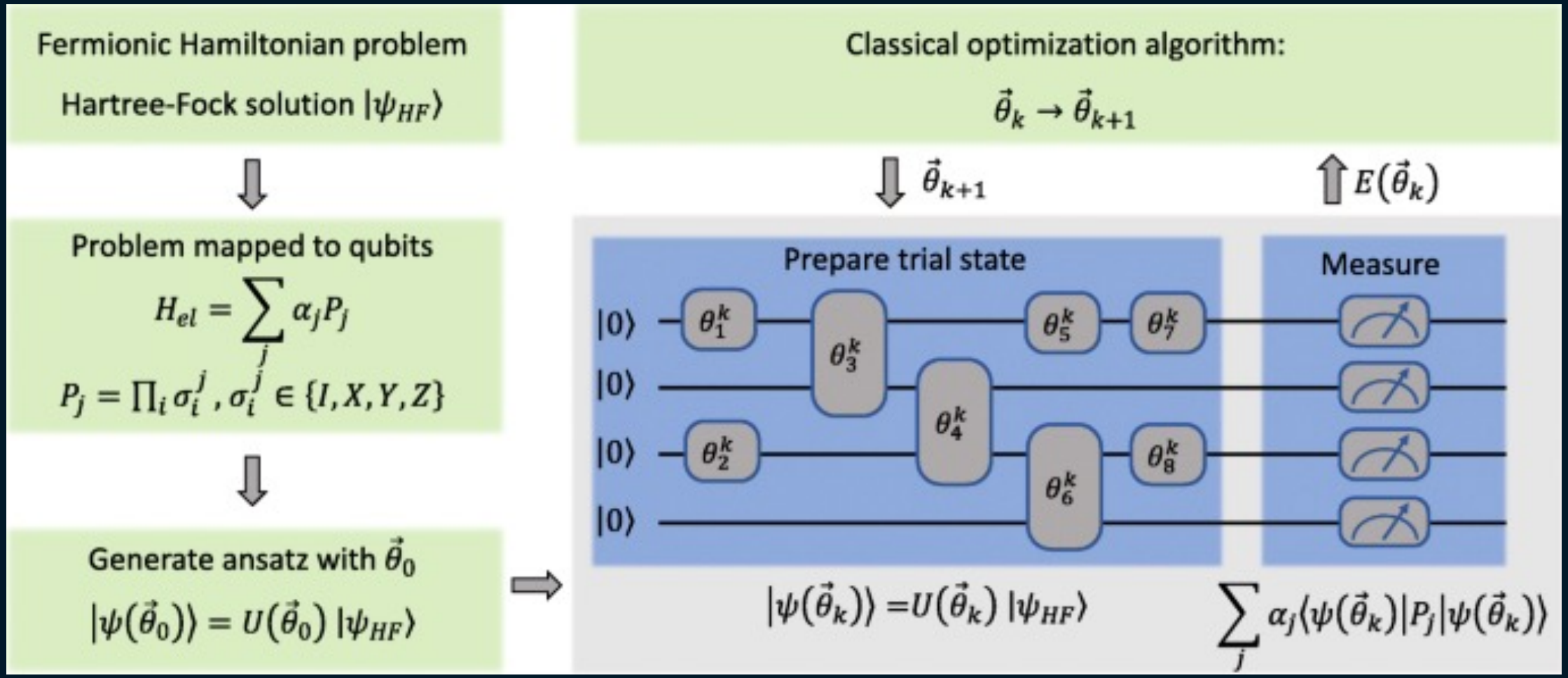


Figure: VQE diagram[1]

[1]https://media.springernature.com/lw685/springer-static/image/art%3A10.1186%2Fs41313-021-00032-6/MediaObjects/41313_2021_32_Fig1_HTML.png

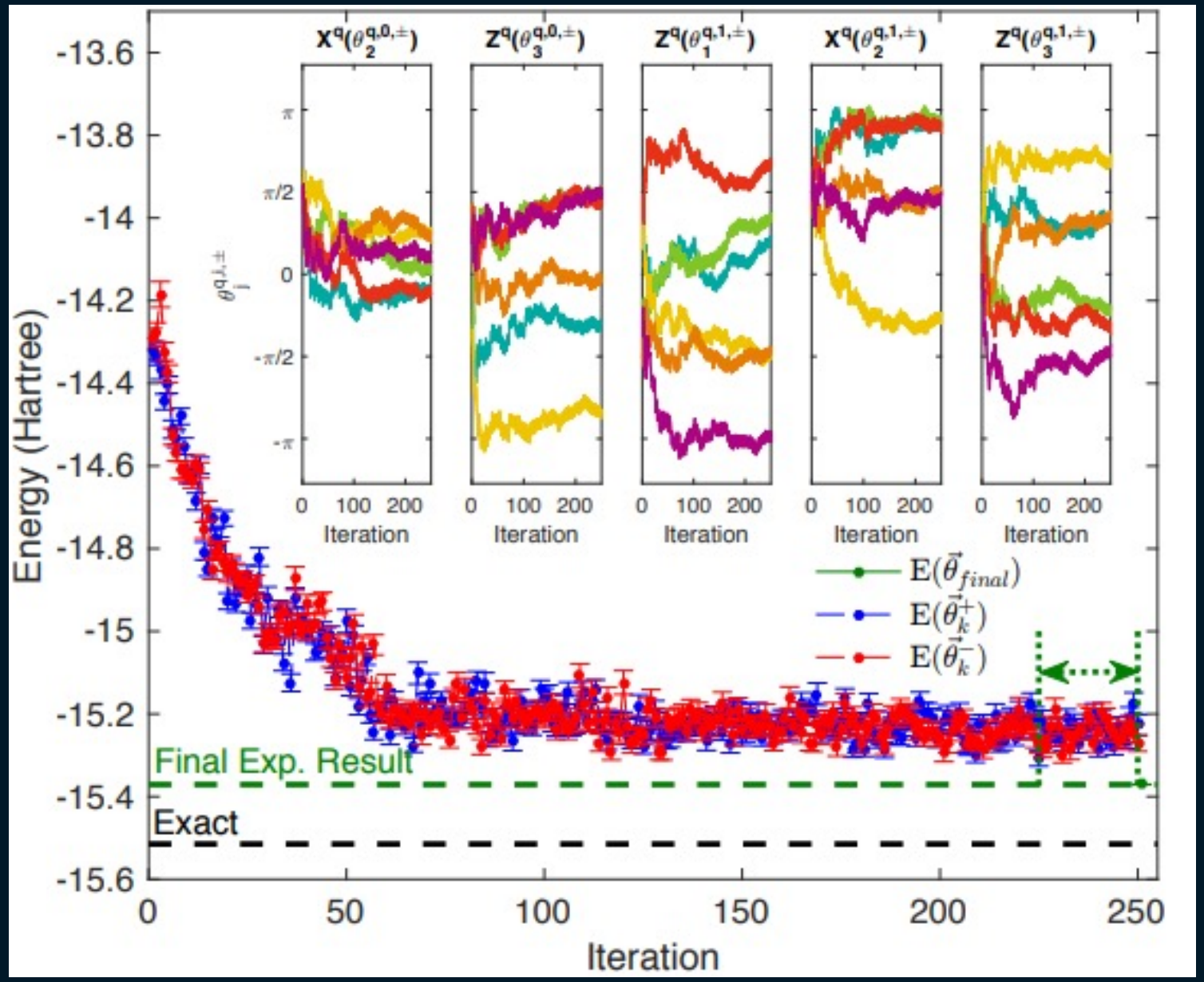


Figure 3. Energy minimization for the six-qubit Hamiltonian describing BeH2 at interatomic distance l = 1.7 A, plotted against the exact value (black dashed line).

https://arxiv.org/pdf/1704.05018.pdf