Quantum Chemistry & Quantum Computing

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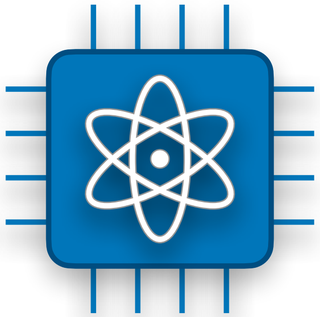
iC Institut de Chimie de Strasbourg UMR 7177

Summary

I) From quantum computing to quantum chemistry

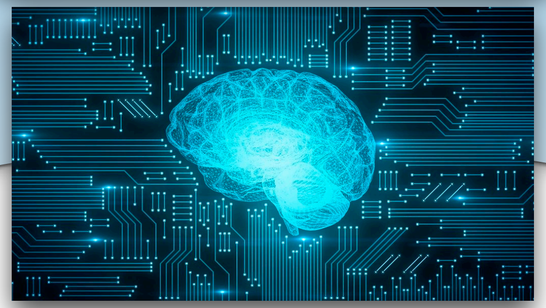
Quantum

Computing



I) From quantum computing to quantum chemistry

Machine Learning



Quantum Computing

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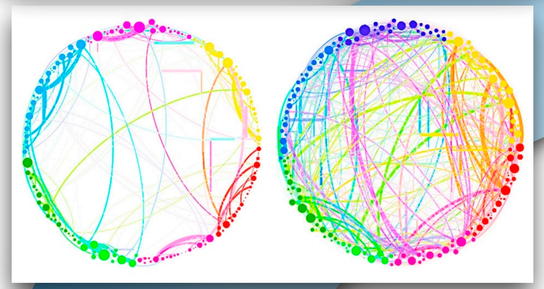
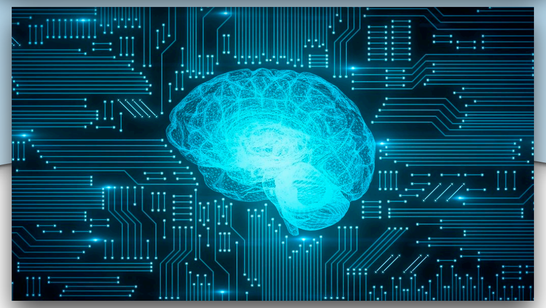
Big Data





Quantum Computing

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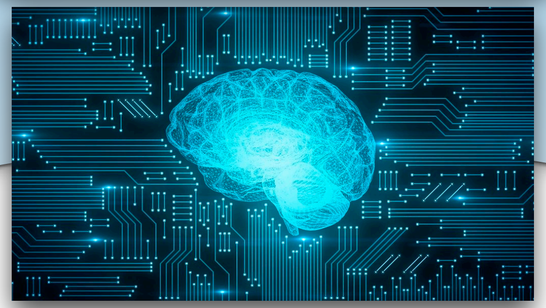

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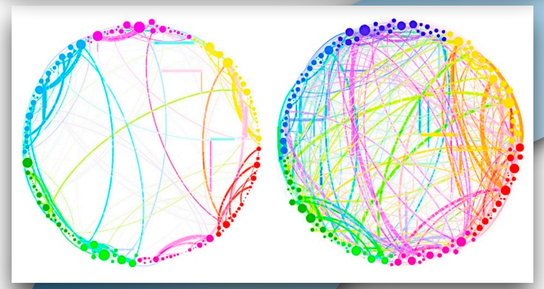
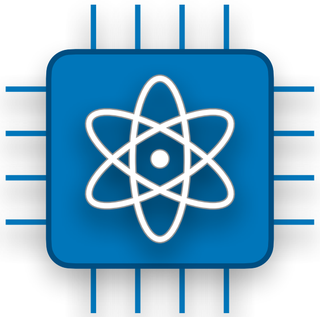


Quantum Computing



Cryptography

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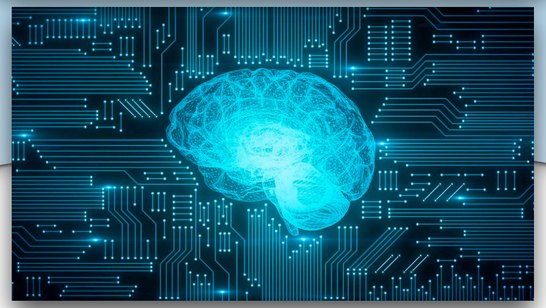
Machine Learning



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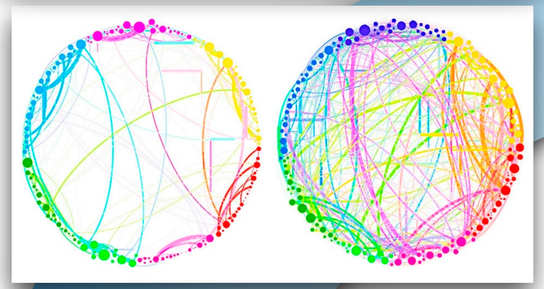

Quantum Computing

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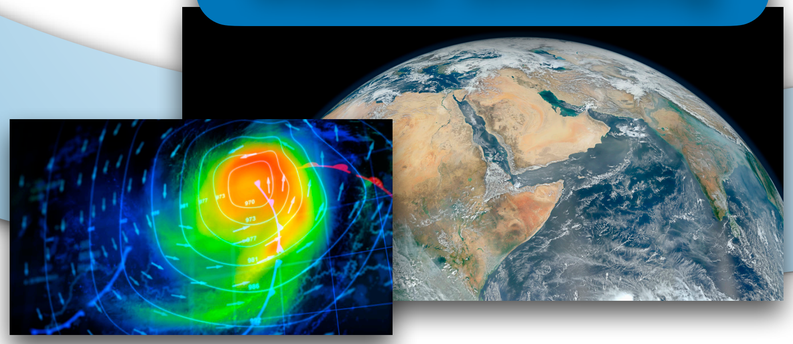
Weather forecasting



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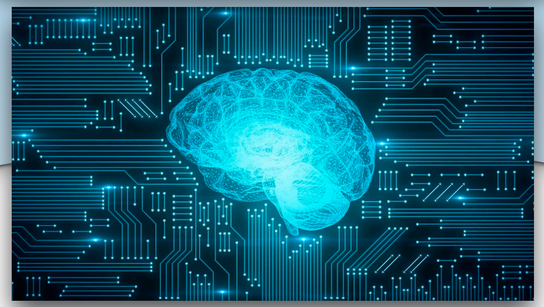
Machine Learning



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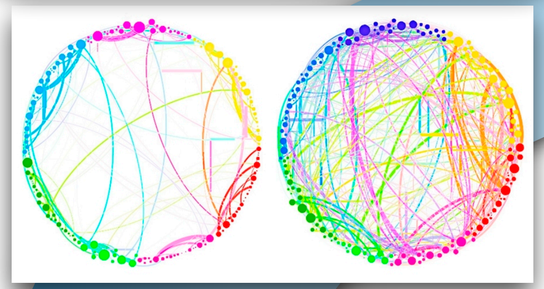

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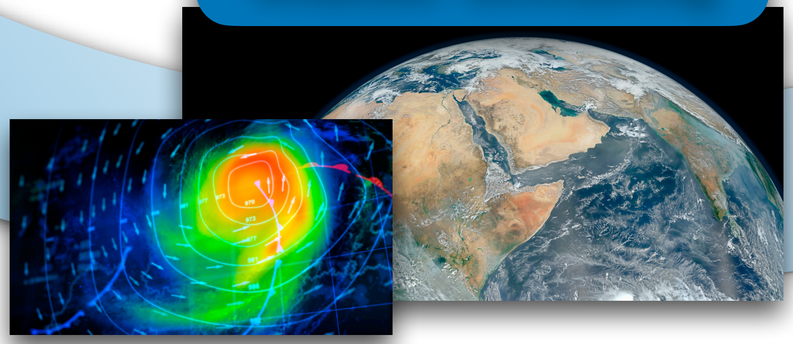
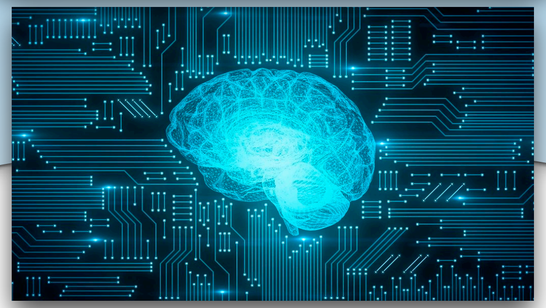


Financial Modelling

I) From quantum computing to quantum chemistry

Machine Learning



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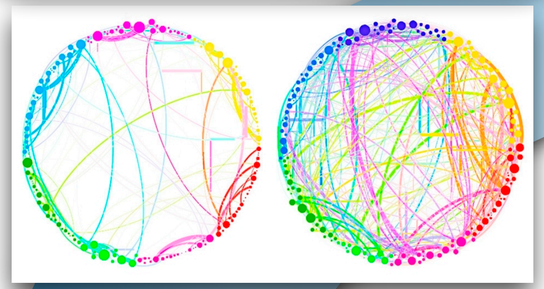
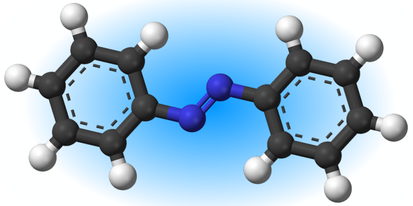
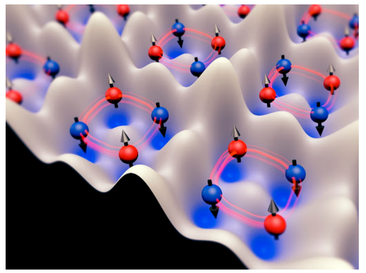


Complex physical systems

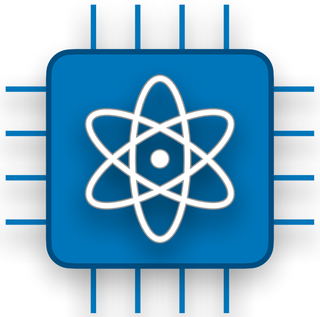
Quantum chemistry





Condensed matter physics

Quantum Computing



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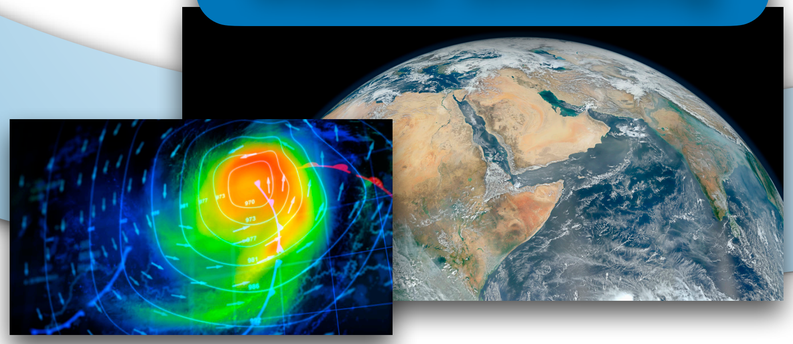

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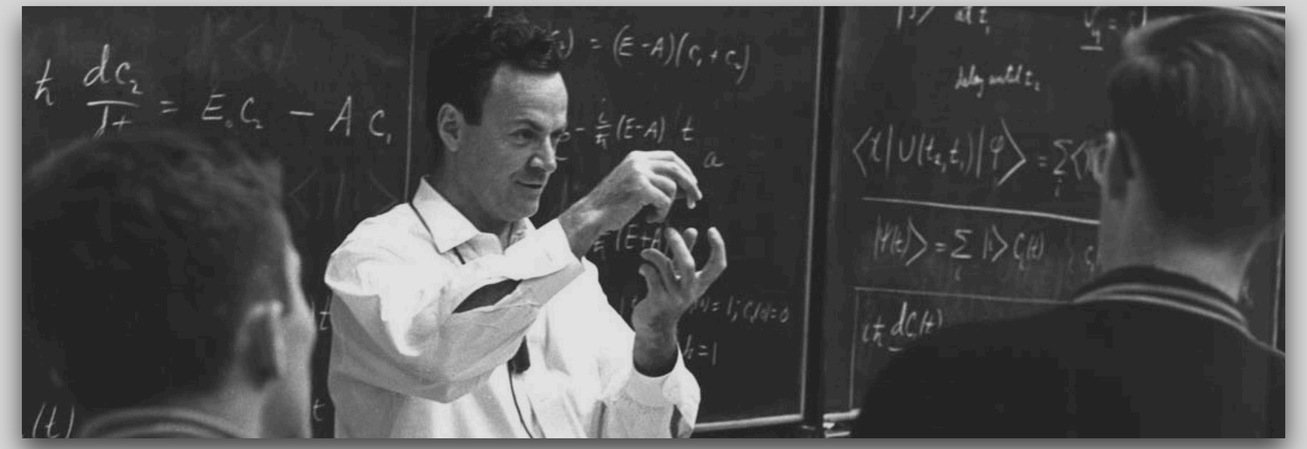
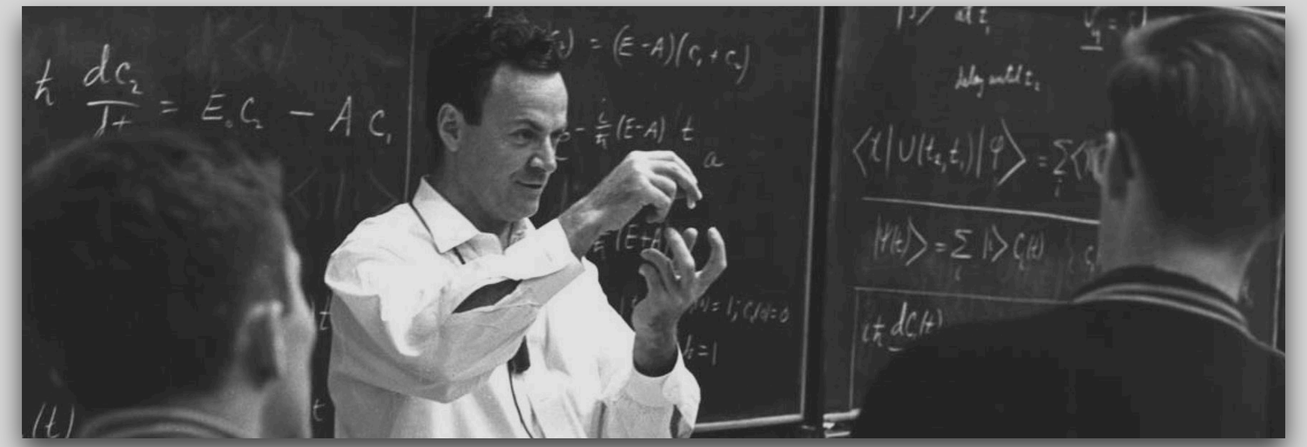


-Richard P. Feynman

"Nature (e.g. atoms, molecules ...) isn't classical and if you want to make a simulation of nature, you'd better make it quantum mechanical."

I) From quantum computing to quantum chemistry



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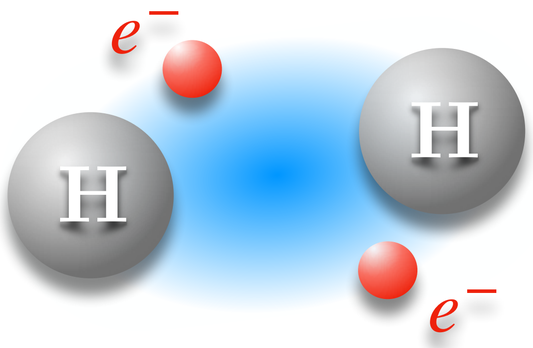

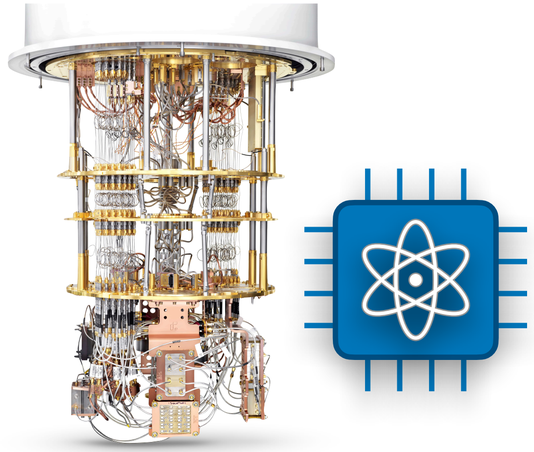

Quantum Computer

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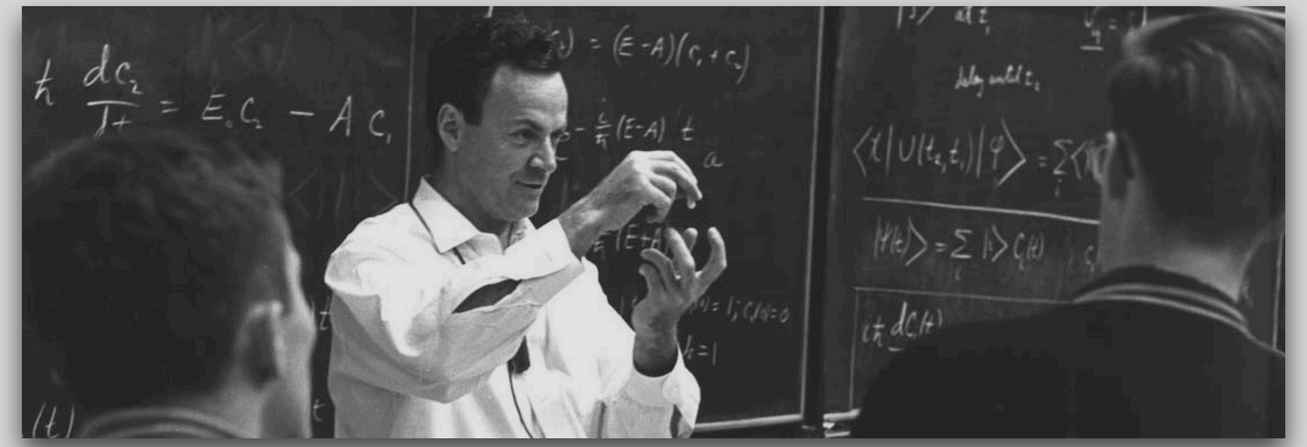

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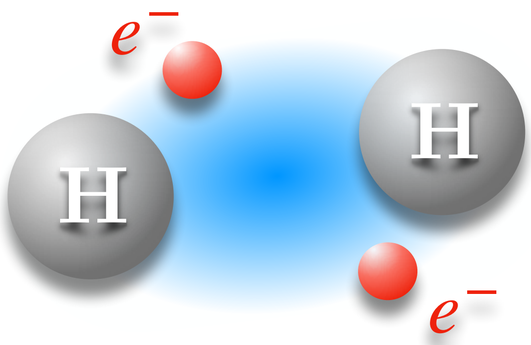

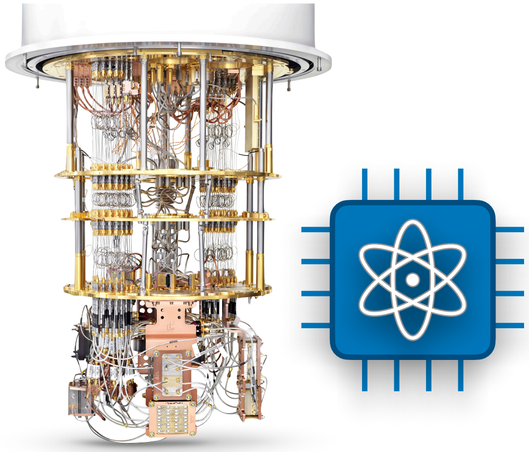

Quantum Computer

VS.

Classical Computer

Classical Computer

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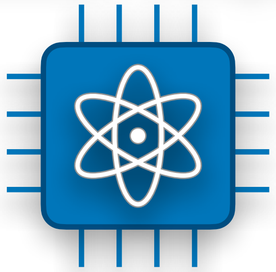
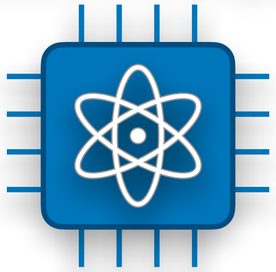
Quantum Computer



I) From quantum computing to quantum chemistry

	Unit of Information	Basic Logic	Prog. Langage
Classical Computer 			
VS.			
Quantum Computer 			

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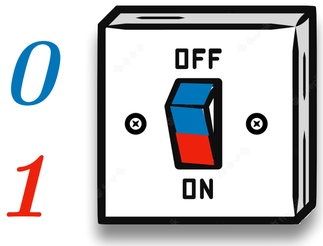
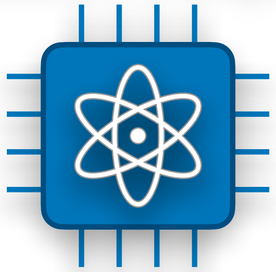
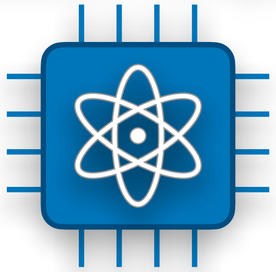
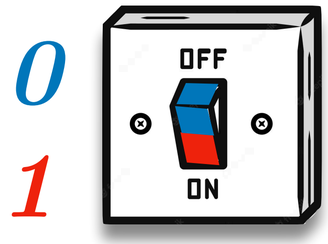
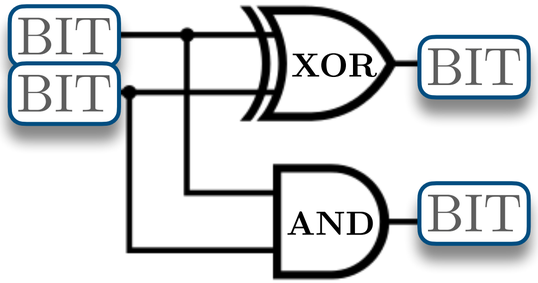
	Unit of Information	Basic Logic	Prog. Langage
Classical Computer 	The Bit 		
VS.			
Quantum Computer 			

I) From quantum computing to quantum chemistry

	Unit of Information	Basic Logic	Prog. Langage
Classical Computer  *VS.* *Quantum Computer* 	The Bit 	Logical circuit 	

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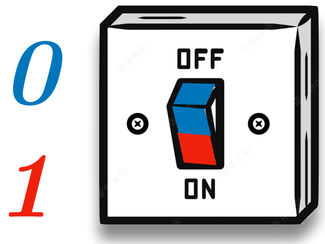
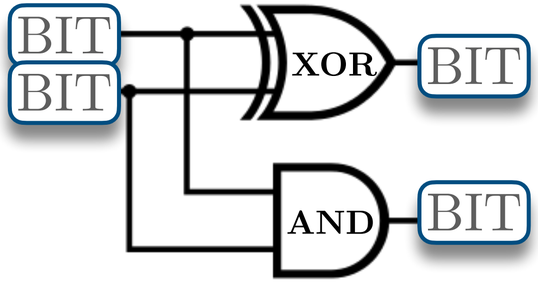
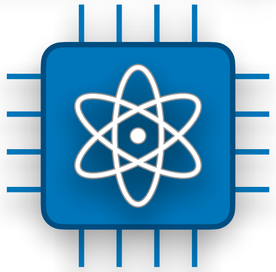
Classical Computer 	The Bit 	Logical circuit 	Fortran, C, Python ... 
VS.			
Quantum Computer 			

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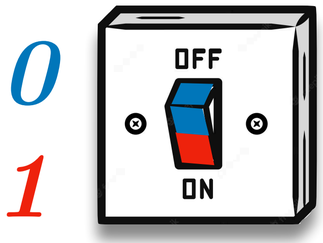
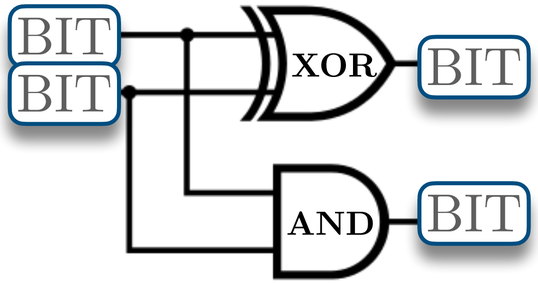
Classical Computer 	The Bit 	Logical circuit 	Fortran, C, Python ... 
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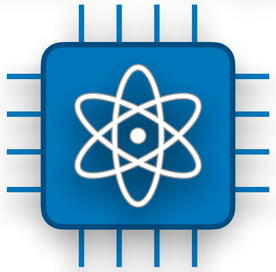
Quantum Computer 	The Qubit  $\|Q\rangle = c_0\|0\rangle + c_1\|1\rangle$		

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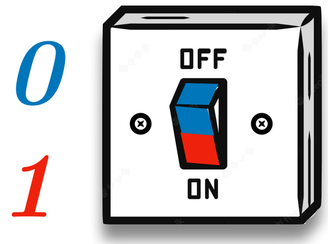
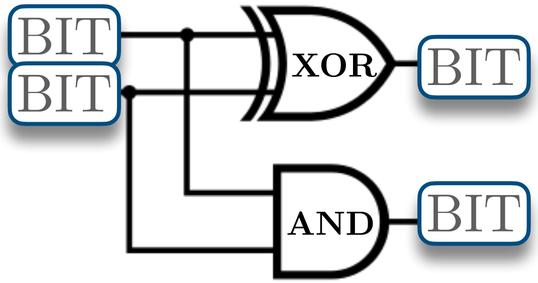
Classical Computer 	The Bit 	Logical circuit 	Fortran, C, Python ... 
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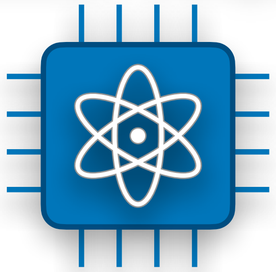
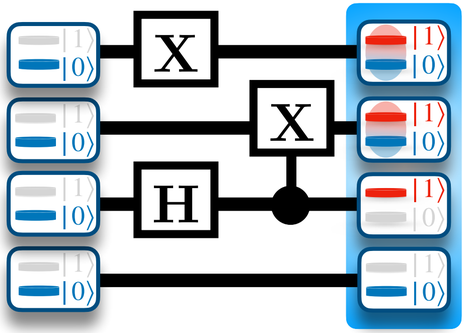
Quantum Computer 	The Qubit  $\|Q\rangle = c_0\|0\rangle + c_1\|1\rangle$	Quantum Circuit 	

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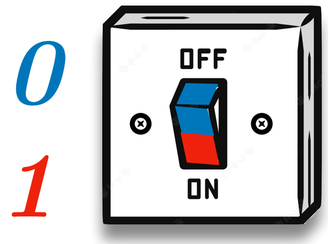
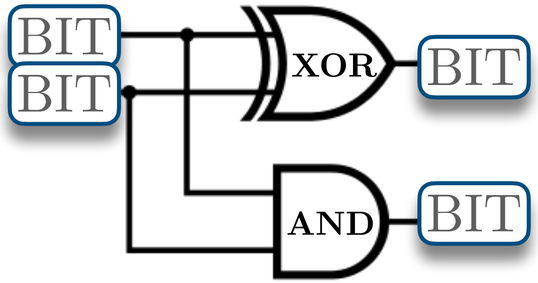
Classical Computer 	The Bit 	Logical circuit 	Fortran, C, Python ... 
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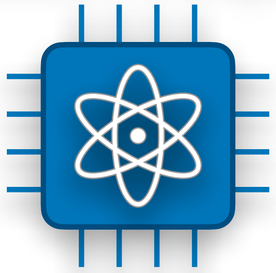
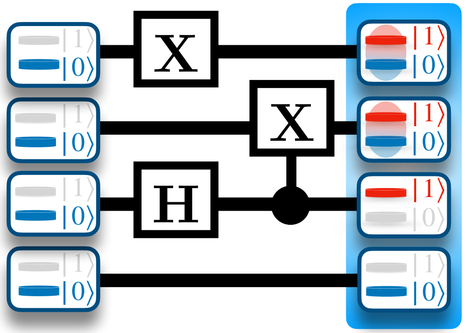
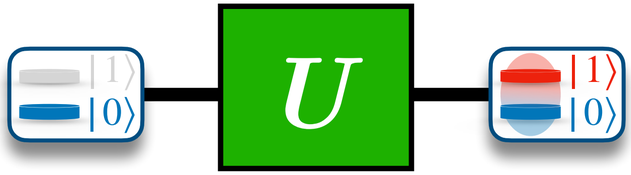
Quantum Computer 	The Qubit  $\|Q\rangle = c_0\|0\rangle + c_1\|1\rangle$	Quantum Circuit 	Quantum Physics ! (Unitary Transformations) 

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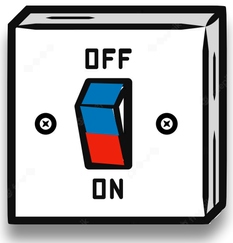
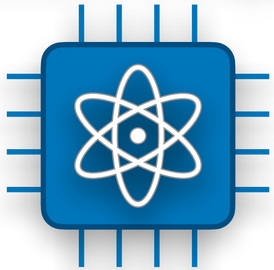
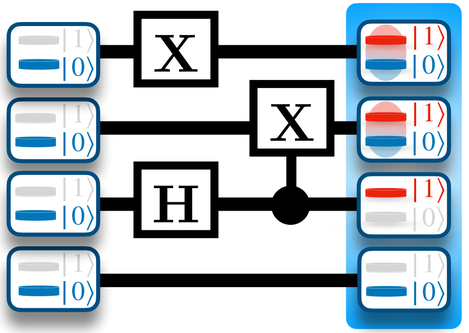
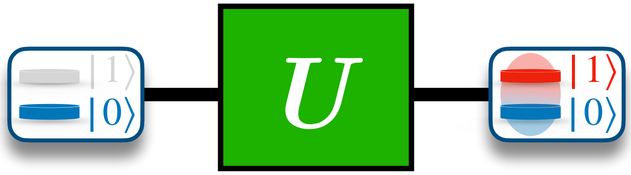
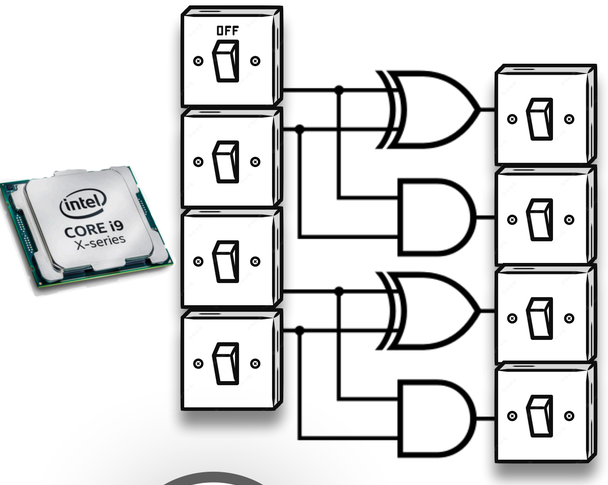
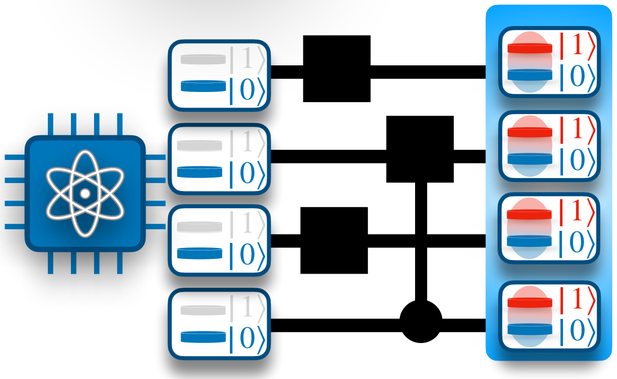
	 	0 1 	
Quantum Computer	The Qubit	Quantum Circuit	Quantum Physics ! (Unitary Transformations)
	  $\|Q\rangle = c_0\|0\rangle + c_1\|1\rangle$		

QUESTION Why a Quantum computer is more powerful than a classical one ?

ANSWER How to encode/manipulate information in Qubits vs. Bits



VS.



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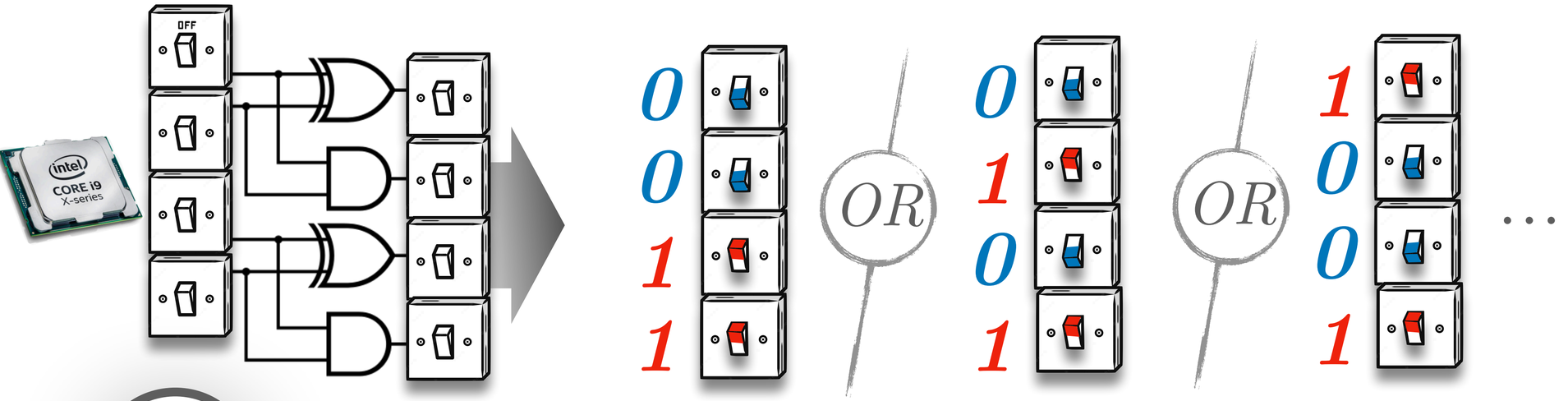
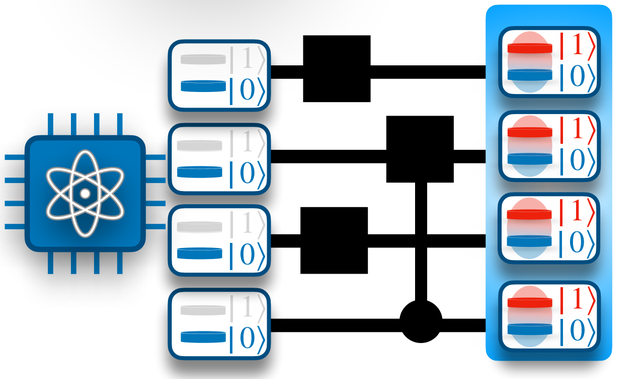


VS.



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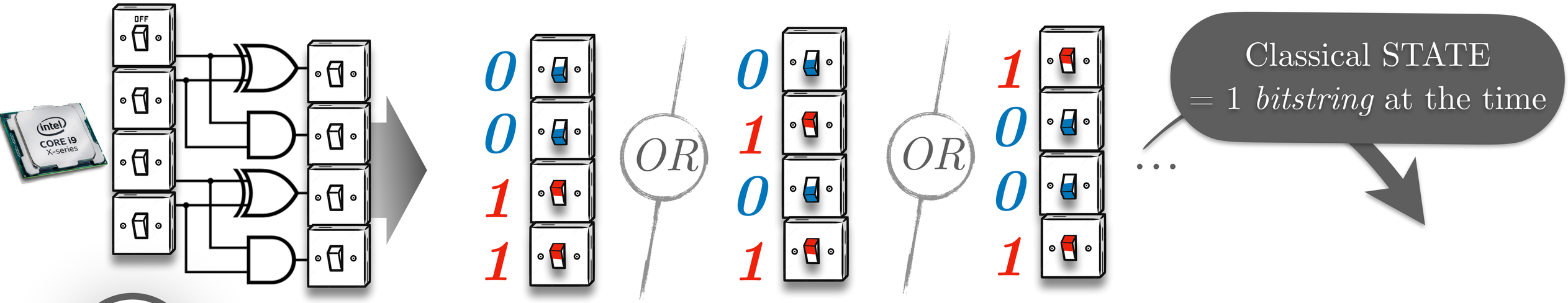
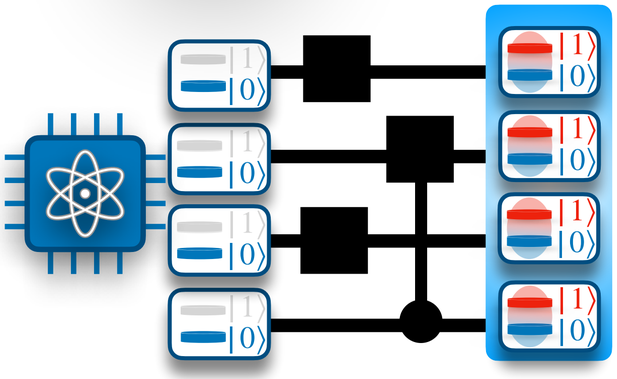


VS.



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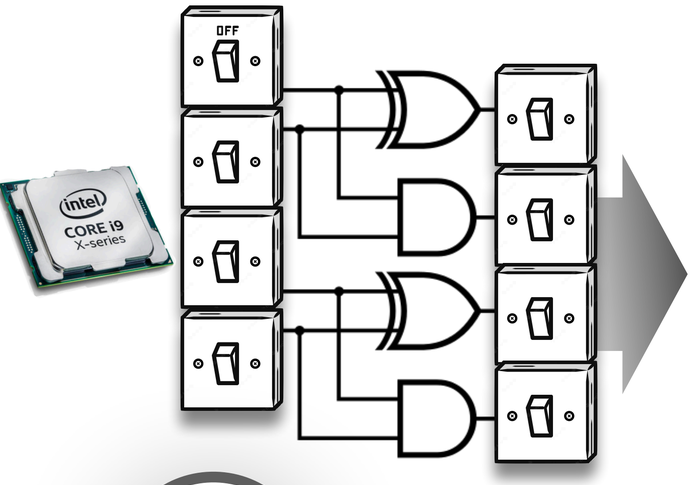
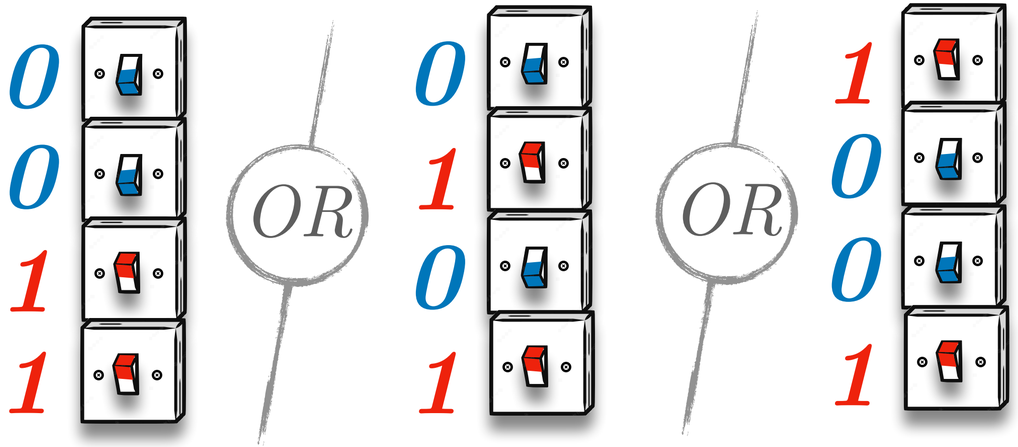


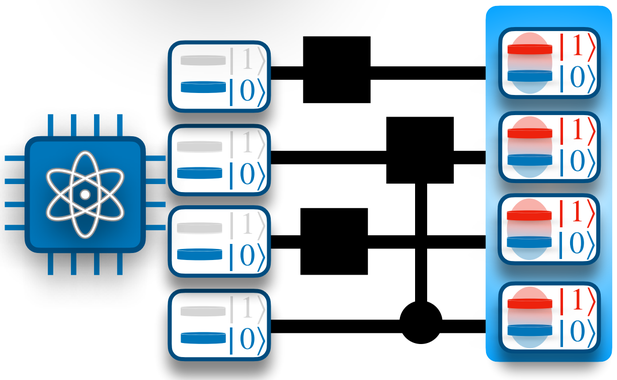


...

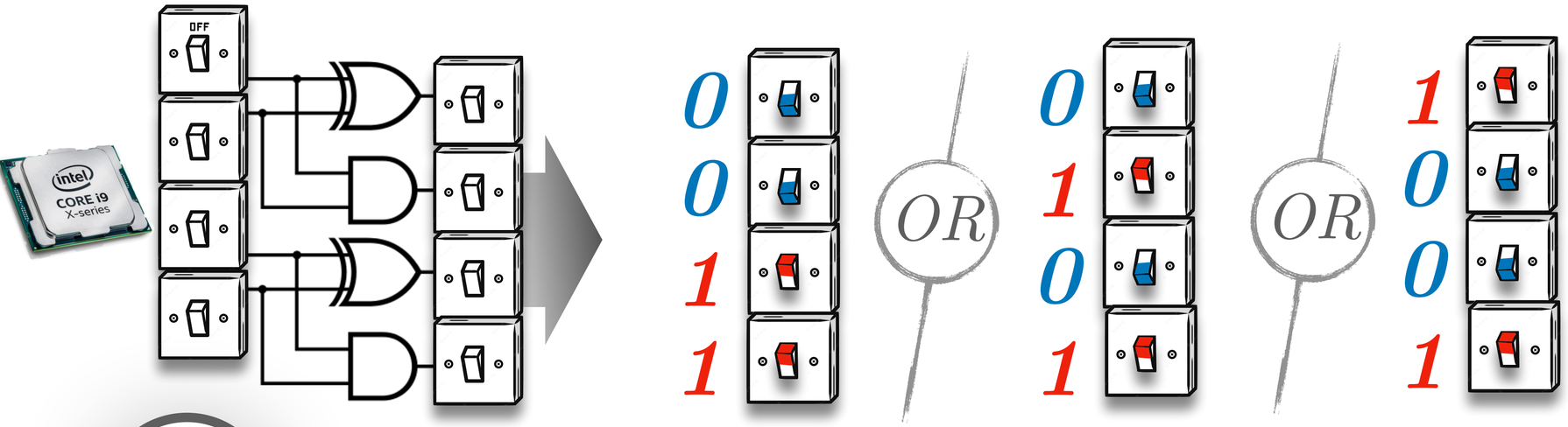
Classical STATE
= 1 *bitstring* at the time

2^N accessible *Bitstrings*

VS.



ANSWER How to encode/manipulate information in Qubits vs. Bits



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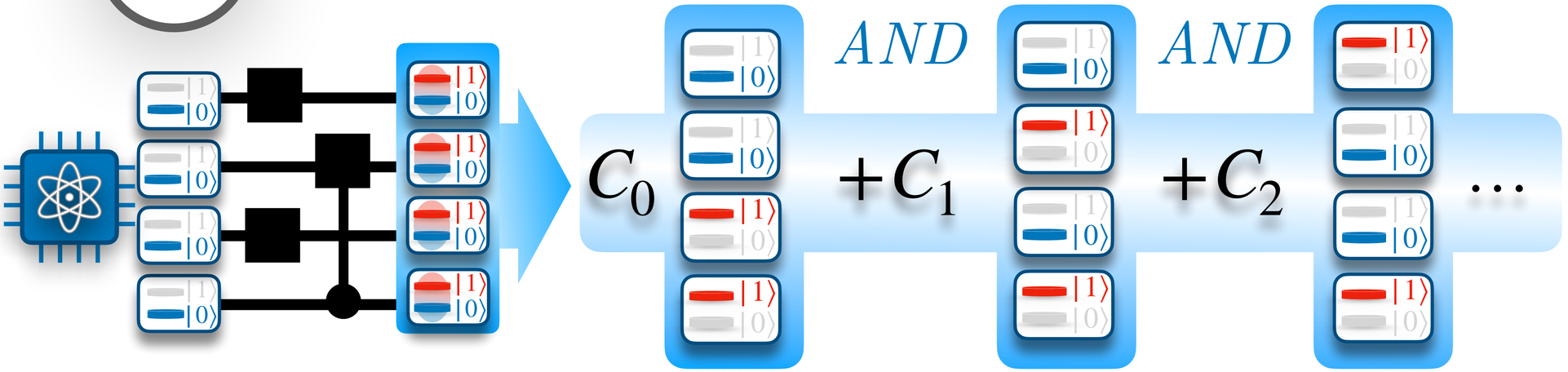
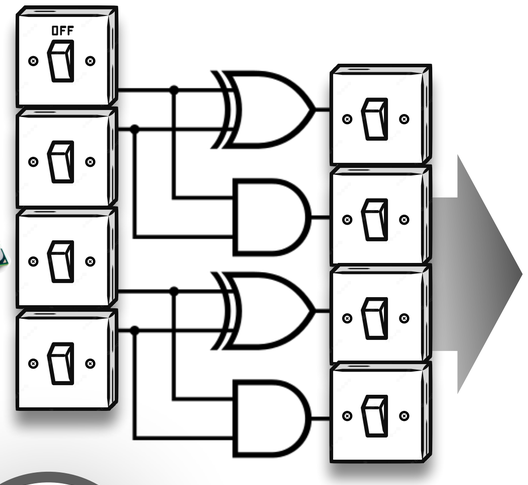
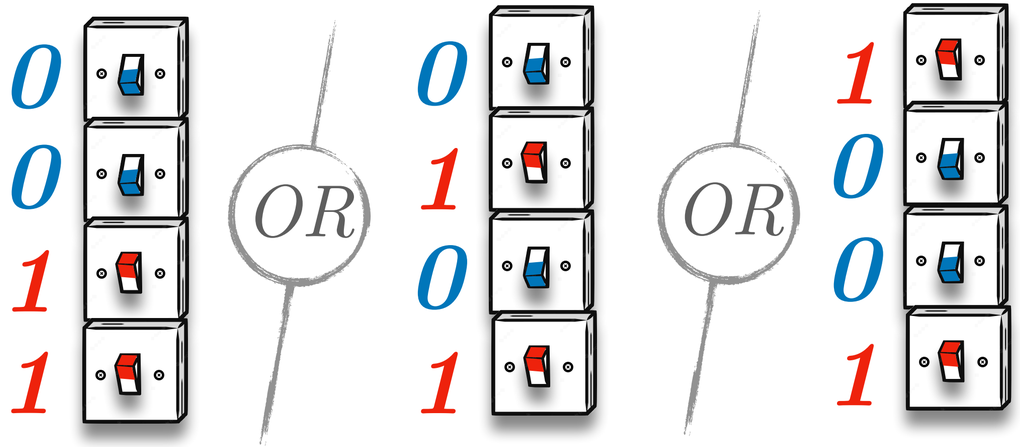


ANSWER How to encode/manipulate information in Qubits vs. Bits





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= 1 *bitstring* at the time

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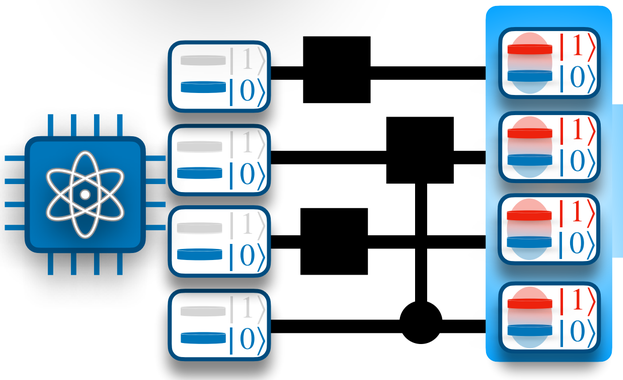
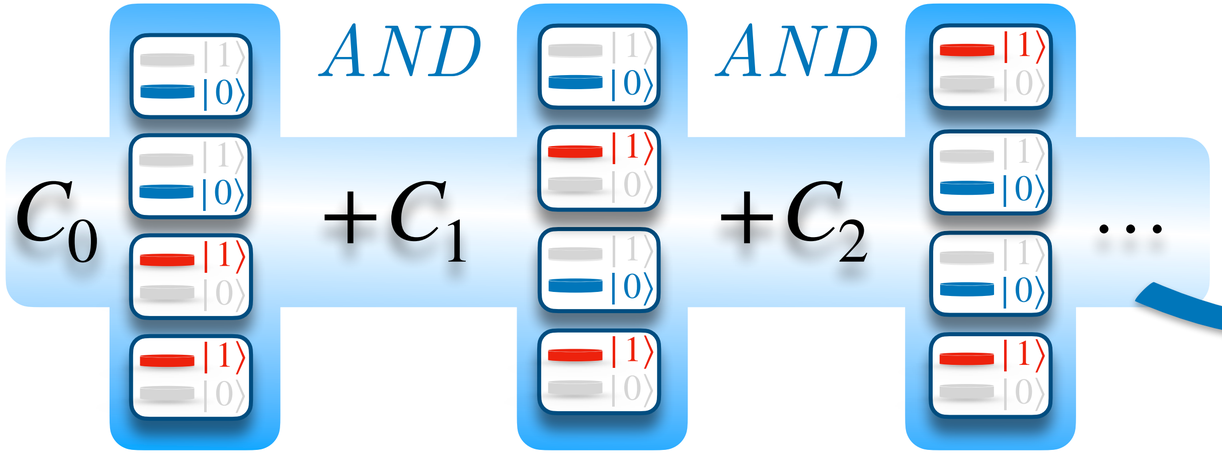
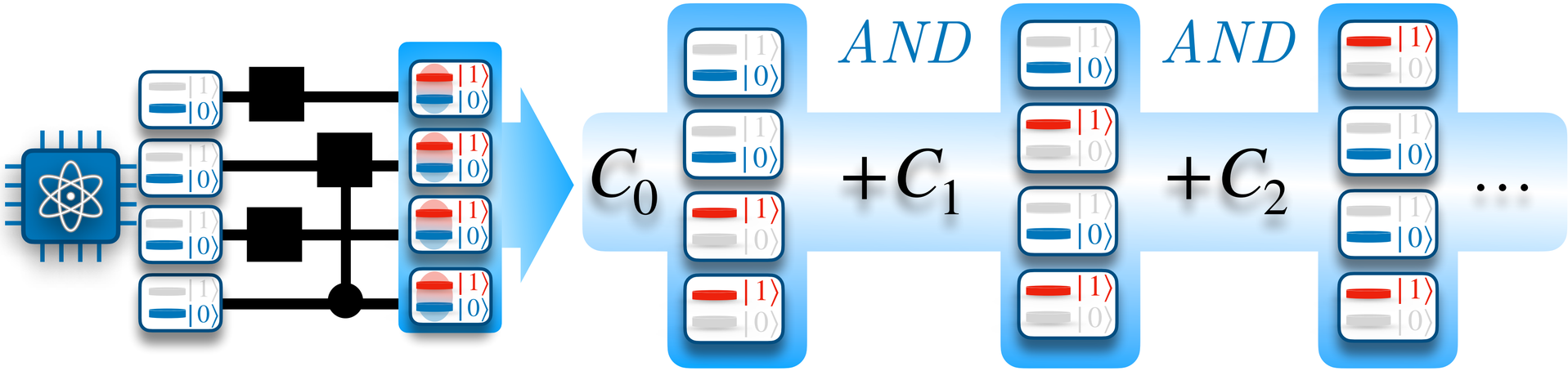




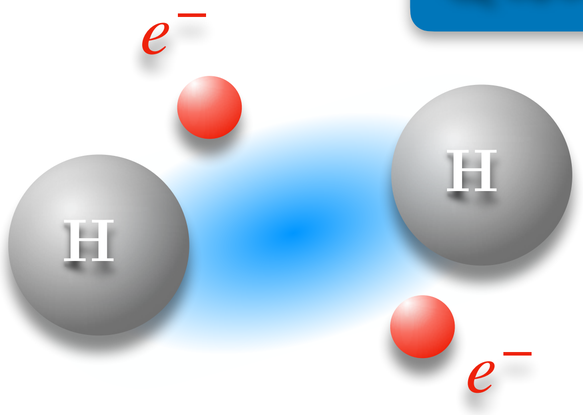
$|\Psi_{\text{Qubits}}\rangle = 2^N$ *bistrings* simultaneously

Exemple of Full Quantum Superposition



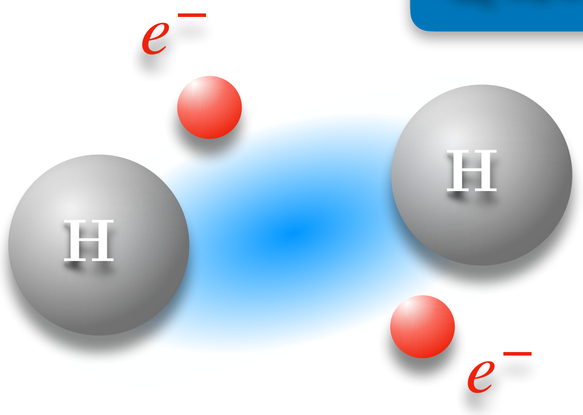
Let's build a quantum circuit !

Quantum Chemistry



$$\hat{H}\,|\Psi_k\rangle = E_k\,|\Psi_k\rangle$$

Quantum Chemistry



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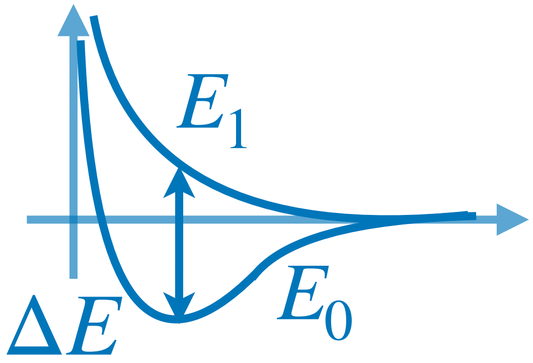
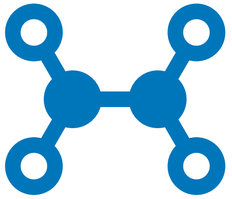


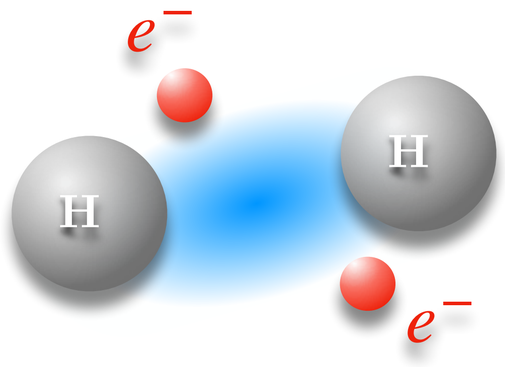
Potential Energy Surfaces

$$\frac{dE}{dR}$$

Nuclear Forces (Energy dervatives)

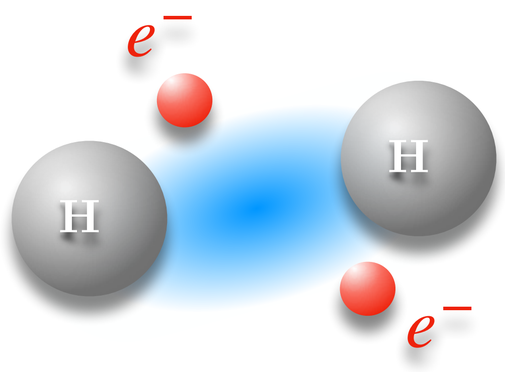


Stable Molecular Geometries



Electronic structure Hamiltonian
(Born-Oppenheimer approximation)

$$H = \sum_{pq}^{N_o} h_{pq} \sum_{\sigma}^{\{\uparrow,\downarrow\}} \hat{a}^\dagger_{p\sigma} \hat{a}_{q\sigma} + \frac{1}{2} \sum_{pqrs}^{N_o} g_{pqrs} \sum_{\sigma,\tau}^{\{\uparrow,\downarrow\}} \hat{a}^\dagger_{p\sigma} \hat{a}^\dagger_{r\tau} \hat{a}_{s\tau} \hat{a}_{q\sigma}$$



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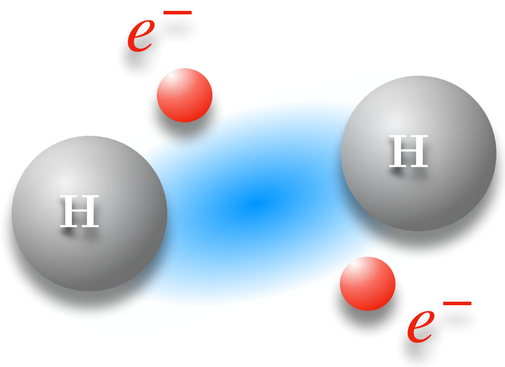
With 1- and 2-electron integrals

$$h_{pq} = \int \phi_p^*(\mathbf{r}_i)\left(-\frac{1}{2}\nabla^2_{\mathbf{r}_i} - \sum_{A=1}^{N_a}\frac{Z_A}{|\mathbf{r}_i - \mathbf{R}_A|}\right)\phi_q(\mathbf{r}_i)\mathrm{d}\mathbf{r}_i$$

$$g_{pqrs} = \iint \phi_p^*(\mathbf{r}_i)\phi_r^*(\mathbf{r}_j)\frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}\phi_q(\mathbf{r}_i)\phi_s(\mathbf{r}_j)\mathrm{d}\mathbf{r}_i\ \mathrm{d}\mathbf{r}_j$$



$$H|\Psi_0\rangle = E_0|\Psi_0\rangle$$

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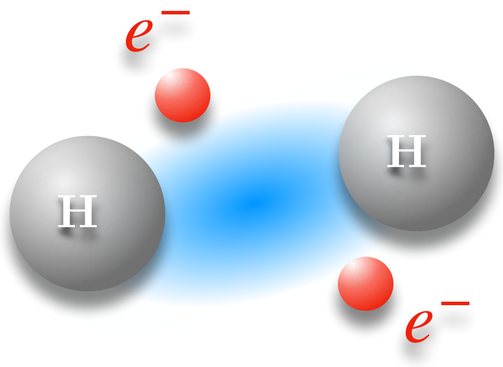

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Mean-Field Approach
(Hartree-Fock)

Single Configuration
Approximation

$$|\Psi_0\rangle \approx |\Phi_{HF}\rangle$$

Electronic structure Hamiltonian
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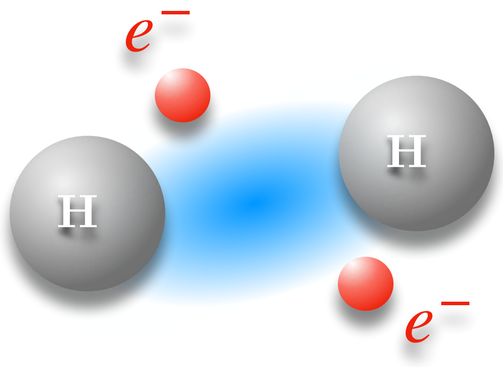

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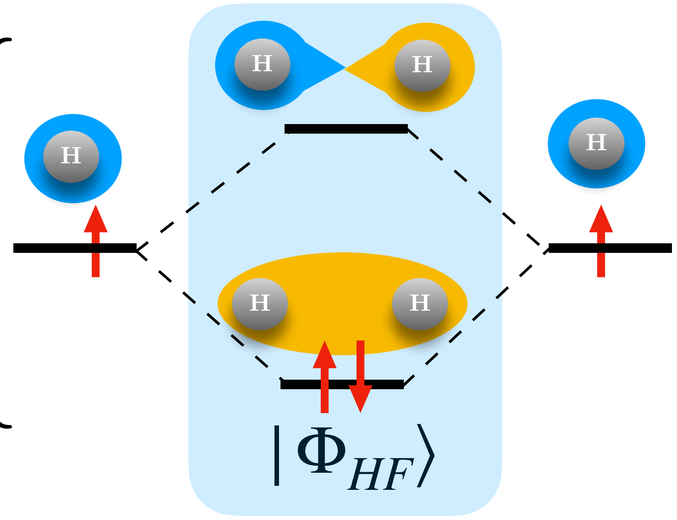
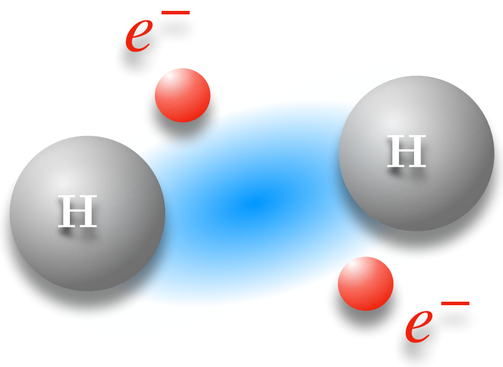
Mean-Field Approach
(Hartree-Fock)

Single Configuration Approximation

$$|\Psi_0\rangle \approx |\Phi_{HF}\rangle$$

Molecular Orbitals





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Mean-Field Approach
(Hartree-Fock)

Single Configuration Approximation

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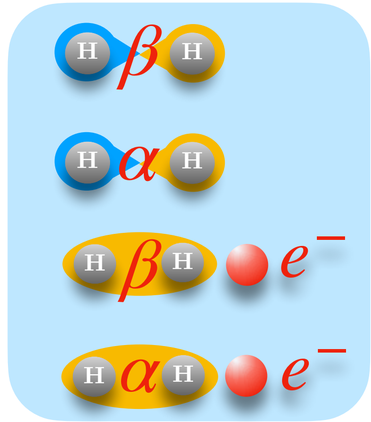
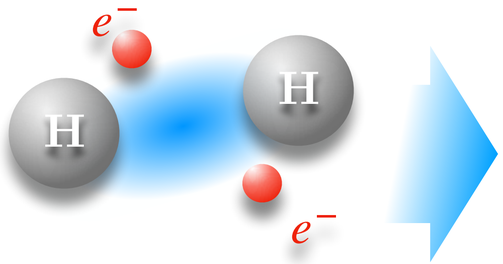
Spin-Orbitals



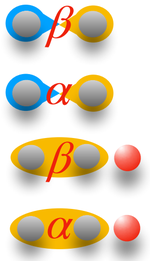
0
0
1
1

$$|\Phi_{HF}\rangle = |1100\rangle$$

Beyond Hartree-Fock: Full Configuration Interaction

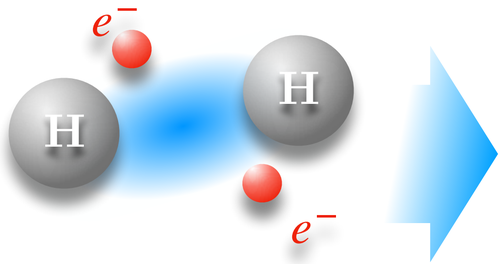


$$|\Psi_0^{FCI}\rangle =$$



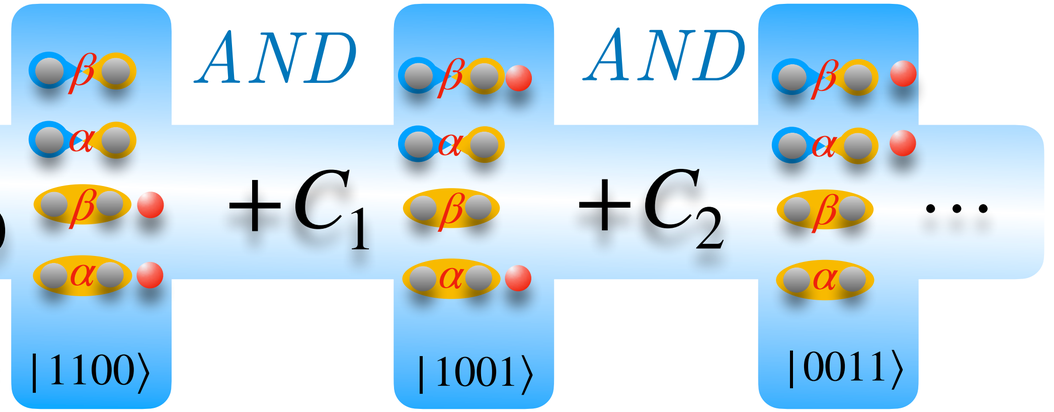
$$H|\Psi_0\rangle = E_0|\Psi_0\rangle \qquad |\mathrm{HF}\rangle = |1100\rangle$$

Beyond Hartree-Fock: Full Configuration Interaction



$$H|\Psi_0\rangle = E_0|\Psi_0\rangle$$

$$|\Psi_0^{FCI}\rangle = C_0|\mathrm{HF}\rangle + C_1|1001\rangle + C_2|0011\rangle + \cdots$$



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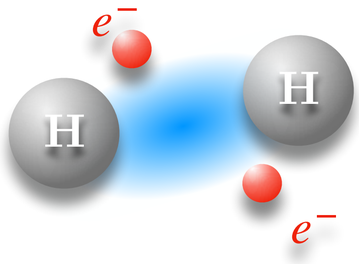

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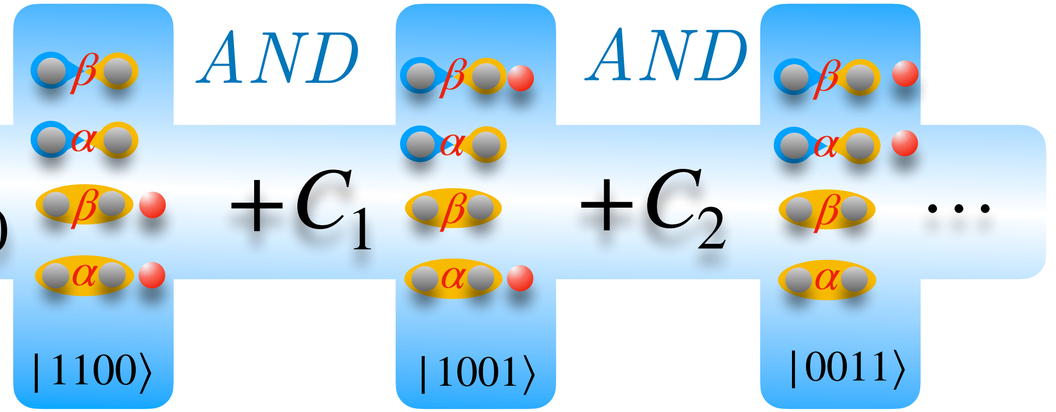
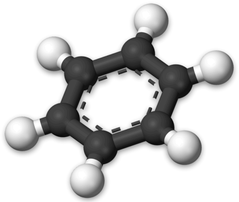
$$|\Psi_0^{FCI}\rangle = C_0|\mathrm{HF}\rangle + C_1|1001\rangle + C_2|0011\rangle + \cdots$$

$$|\mathrm{HF}\rangle = |1100\rangle$$

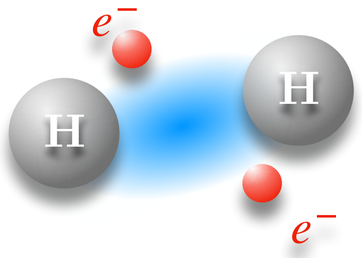


Problem:
FCI = Expensive!

Benzene $N_{CONF} \sim 10^{19}$



Beyond Hartree-Fock: Full Configuration Interaction



$$H|\Psi_0\rangle = E_0|\Psi_0\rangle$$

$$|\Psi_0^{FCI}\rangle = C_0|\mathrm{HF}\rangle + C_1|1001\rangle + C_2|0011\rangle + \cdots \quad (AND)$$

$$|\mathrm{HF}\rangle = |1100\rangle$$

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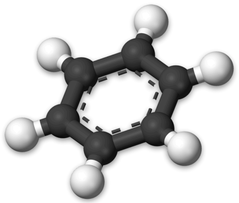

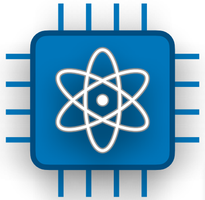

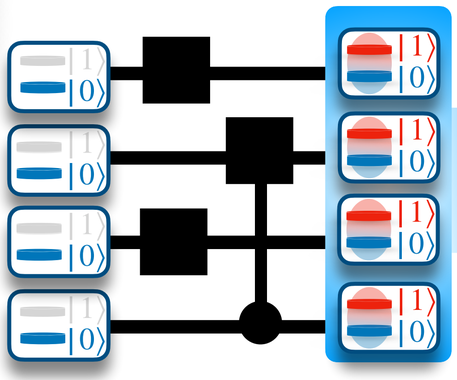

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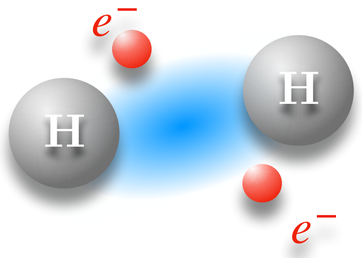

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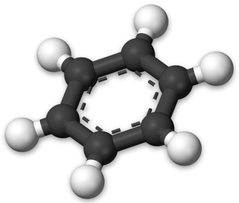

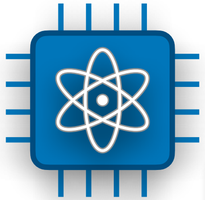

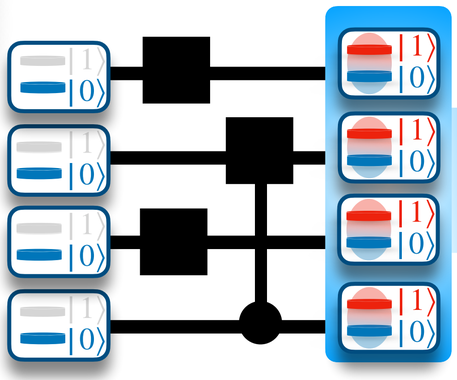

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AND *AND*

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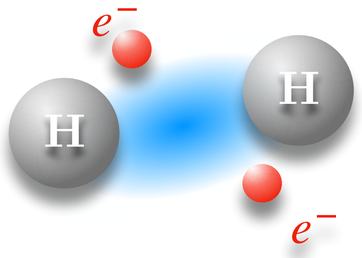

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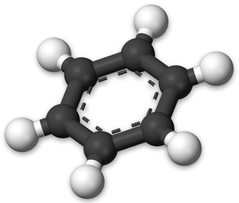
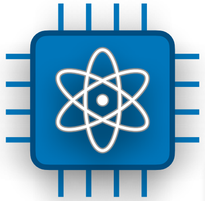
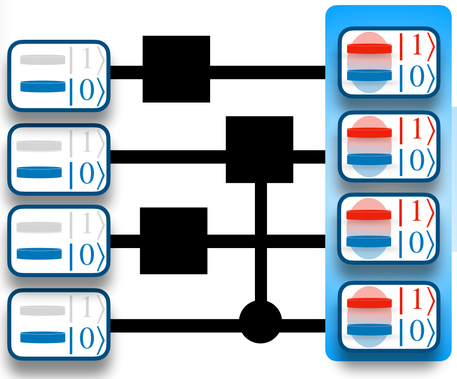






$$C_0 + C_1 + C_2 + \cdots$$

AND *AND*

HOW TO
Connect
Both Worlds?

II) Electronic Structure on a Quantum Computer

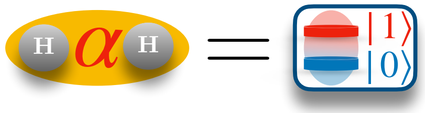
-Richard P. Feynman

"Nature (e.g. atoms, molecules ...) isn't classical and if you want to make a simulation of nature, you'd better make it quantum mechanical."

Jordan-Wigner Mapping (Fermion to qubit)

Jordan-Wigner Mapping (Fermion to qubit)

1-to-1 Physical Correspondence

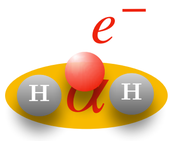


=

Jordan-Wigner Mapping (Fermion to qubit)

1-to-1 Physical Correspondence

Occupied spinorbital



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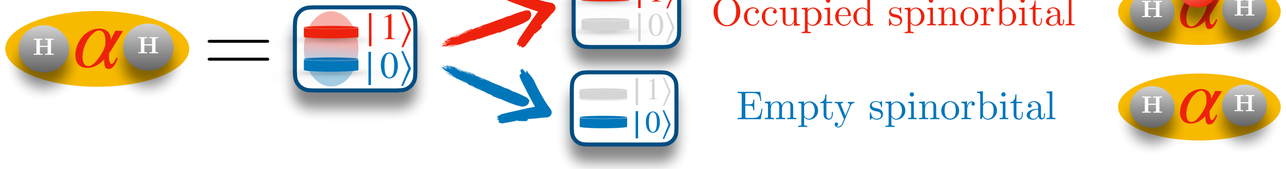

Occupied spinorbital

Empty spinorbital

Jordan-Wigner Mapping (Fermion to qubit)

1-to-1 Physical Correspondence

Translation of Fermionic Algebra

Pauli Operators

$$X = |0\rangle\langle 1| + |1\rangle\langle 0|$$

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Creating 1 electron
in the qubit/spinorbital *"p"*

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Ensuring fermionic anti-symmetry

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Ensuring fermionic anti-symmetry

What Possibilities ?

- We can express fermionic operators (products of $\hat{a}^\dagger/\hat{a}$) in Qubit algebra

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$\bigotimes_{q=0}^{p-1} Z_q$: Ensuring fermionic anti-symmetry

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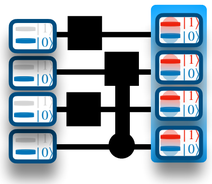
- We can encode fermionic unitaries in a quantum circuit

$$\exp(\hat{T} - \hat{T}^\dagger)$$
$$\exp(-it\hat{H})$$



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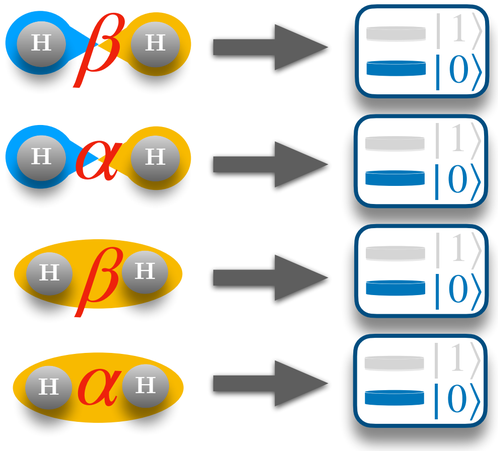
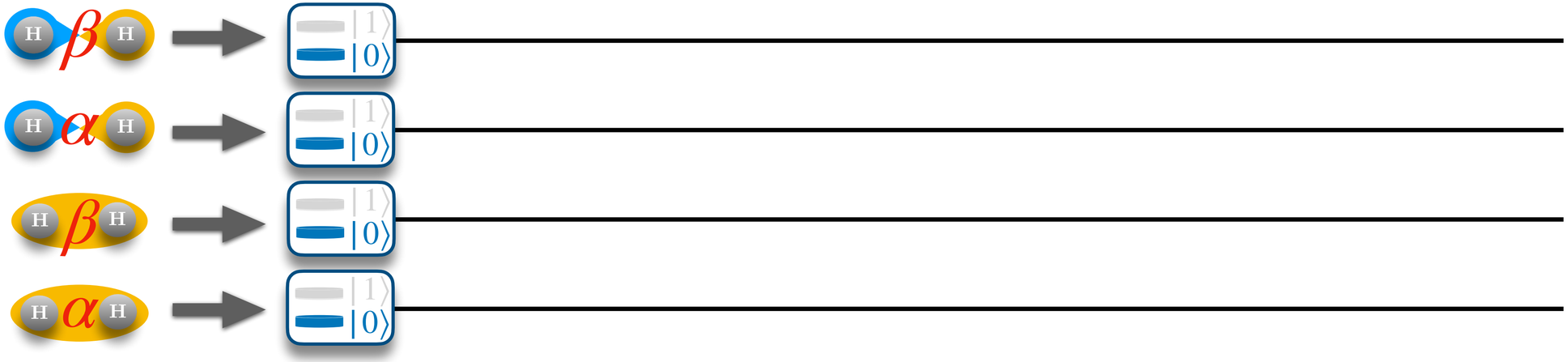


II) Electronic structure on a Quantum Computer

Jordan-Wigner mapping



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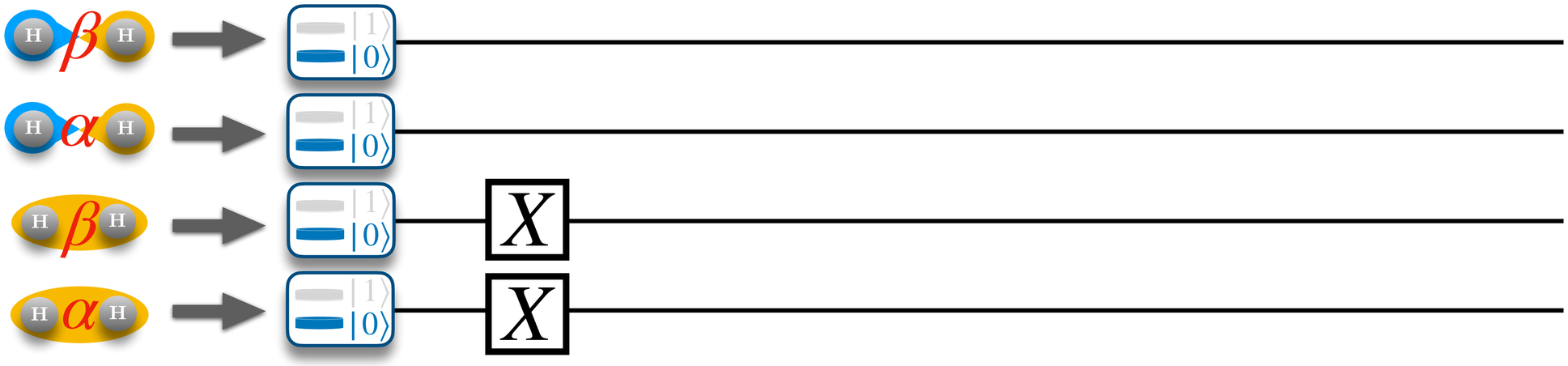

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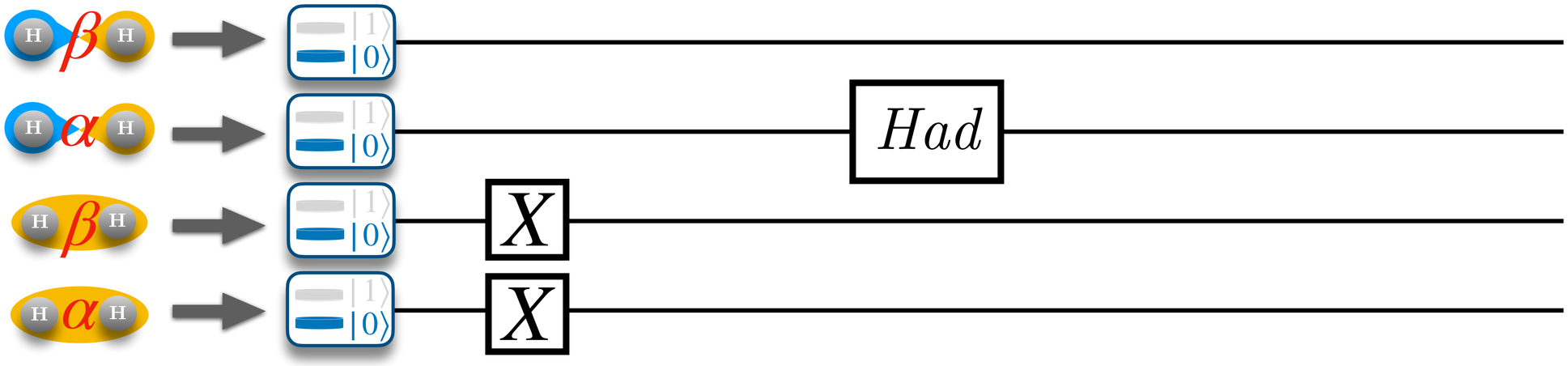

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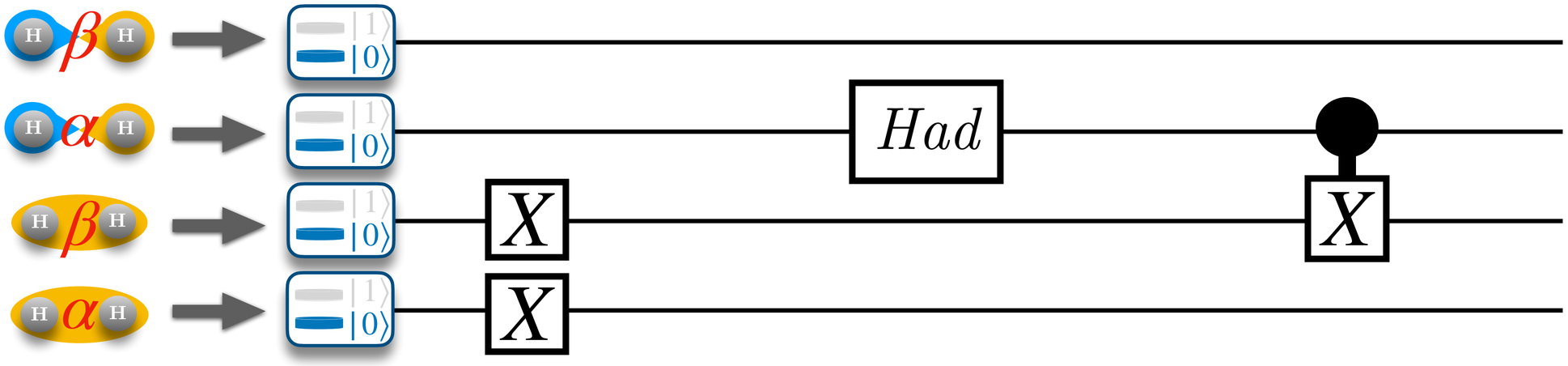
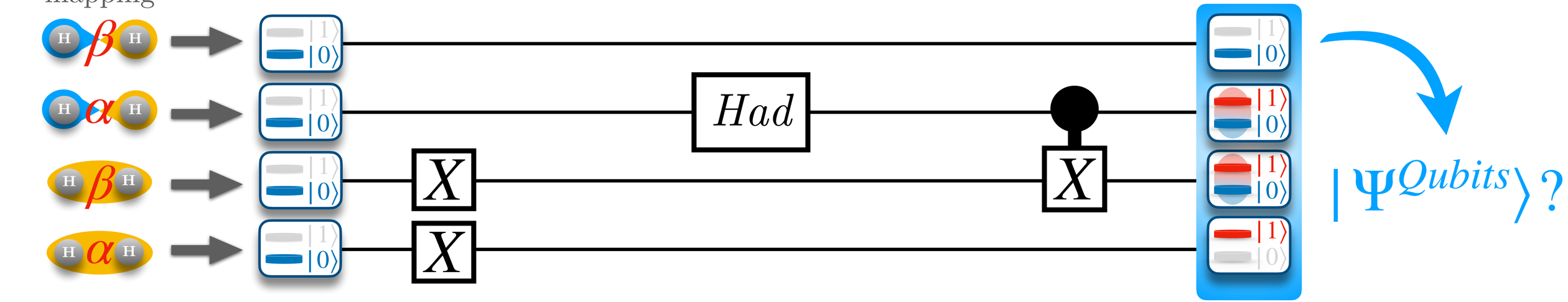


QUESTION What is the final state of the qubit register (i.e. the molecule)?



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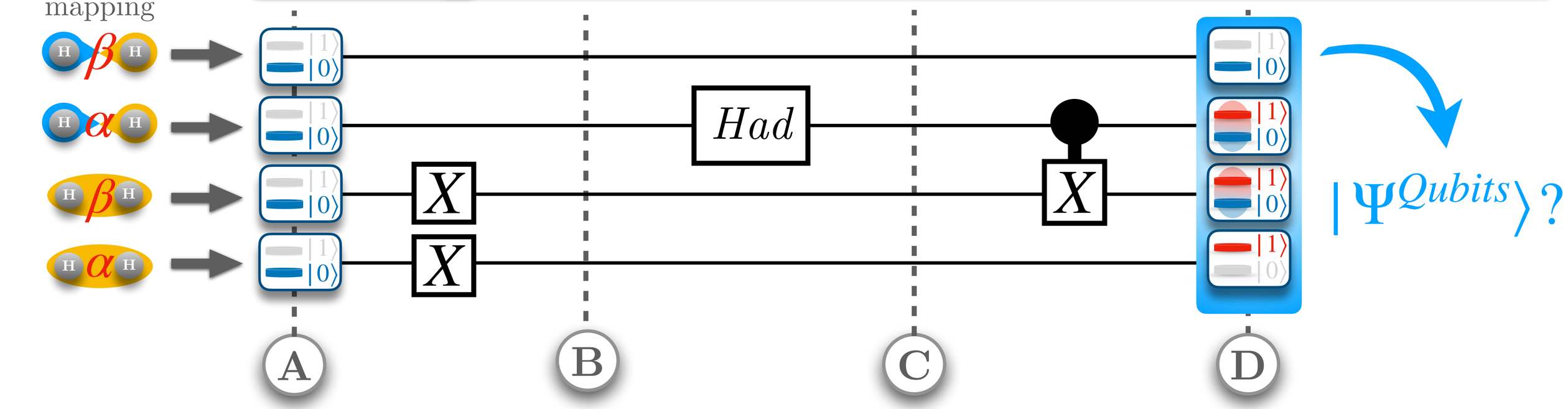

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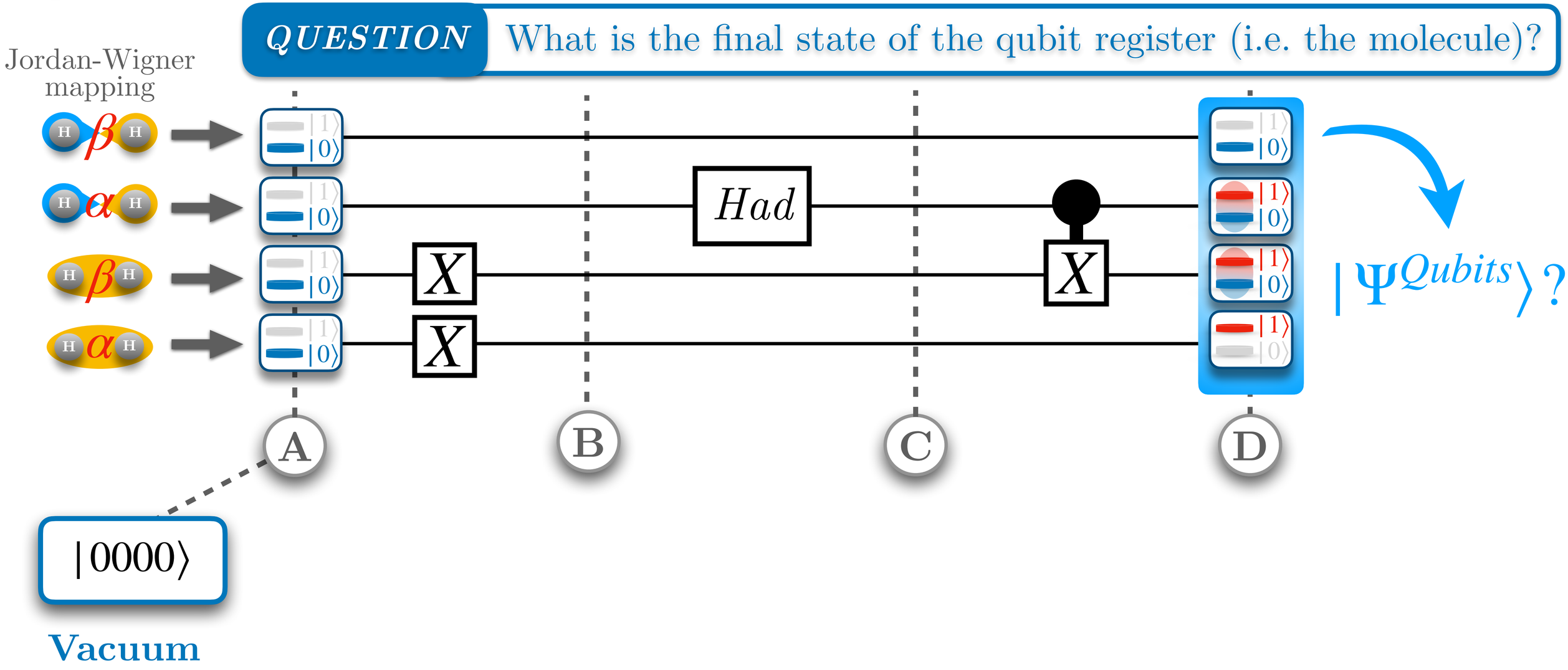

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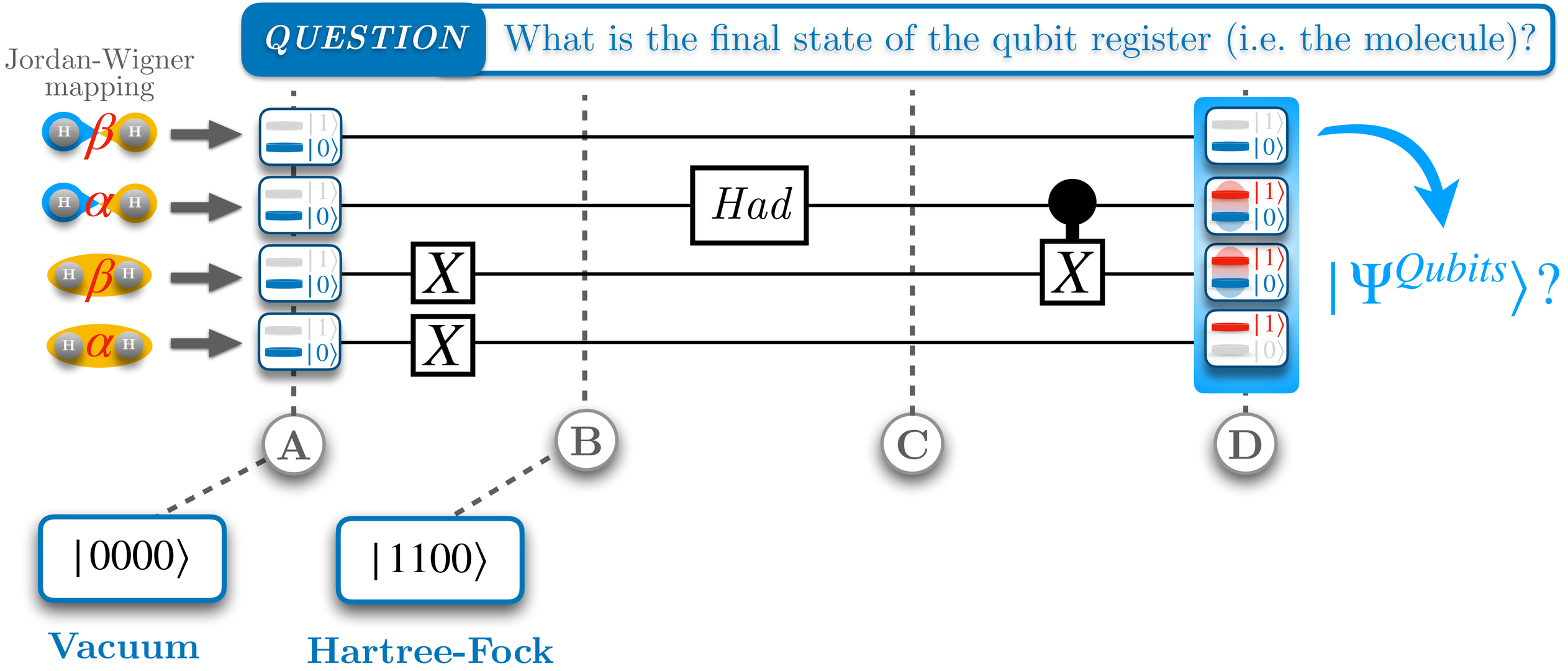

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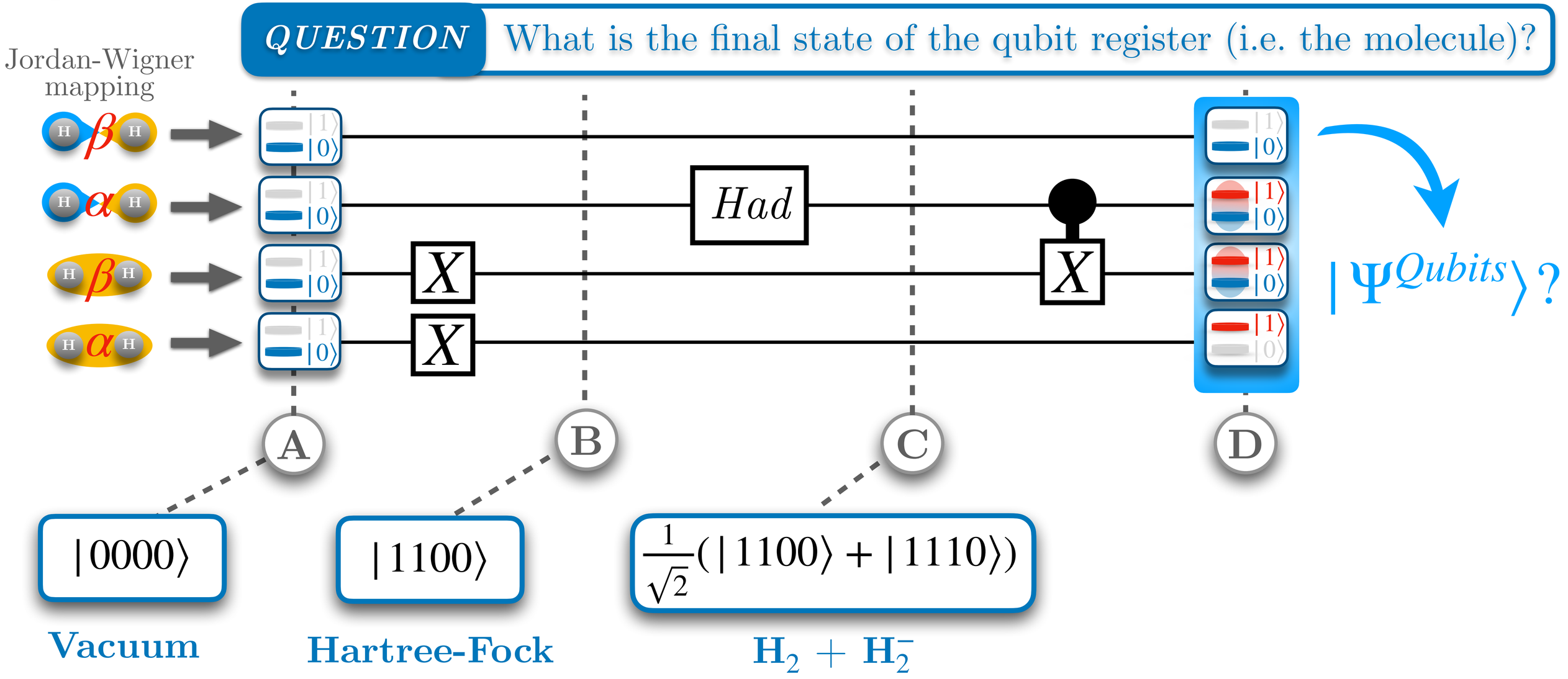

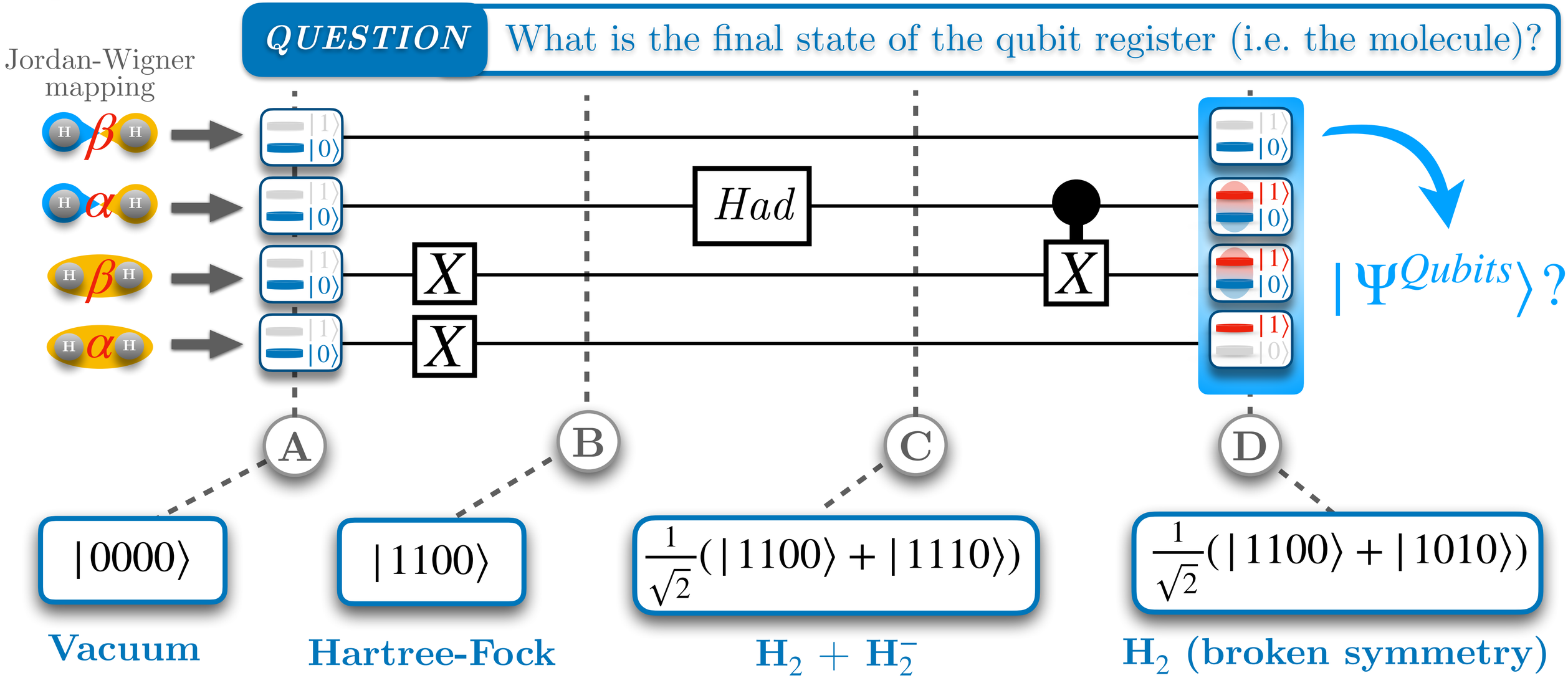
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Jordan-Wigner mapping
H β H
H α H
H β H
H α H
|1⟩
|0⟩
X
X
Had
X
|Ψ^Qubits⟩ ?
A
B
C
D
|0000⟩
|1100⟩
1/√2 (|1100⟩ + |1110⟩)
1/√2 (|1100⟩ + |1010⟩)
Vacuum
Hartree-Fock
H2 + H2−
H2 (broken symmetry)

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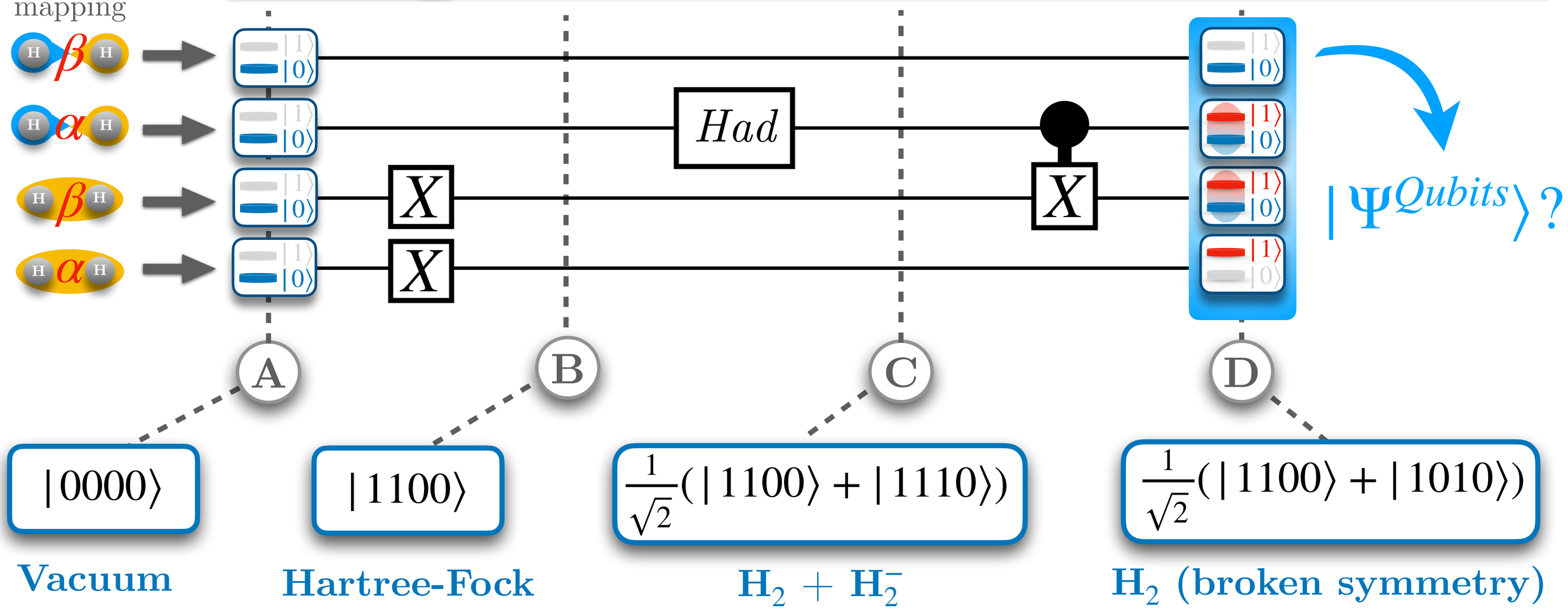

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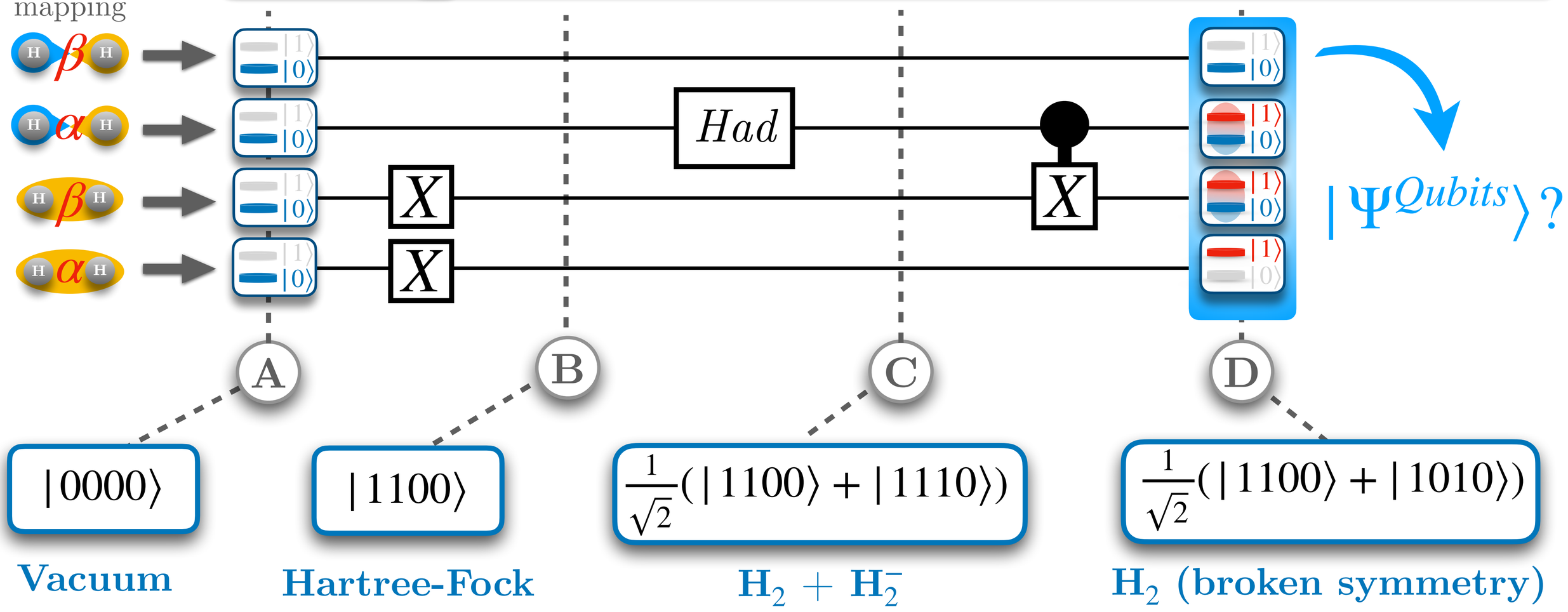

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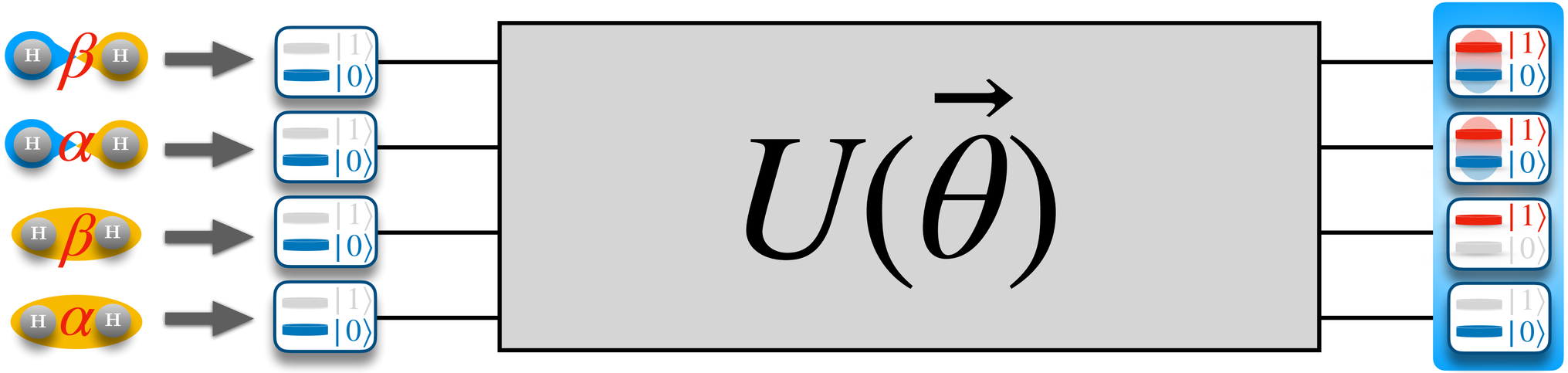
$$\langle \hat{a}_0^\dagger \hat{a}_0 \rangle \longrightarrow \frac{1}{2}\langle 1 - Z_0 \rangle = 1$$

II) Electronic structure on a Quantum Computer



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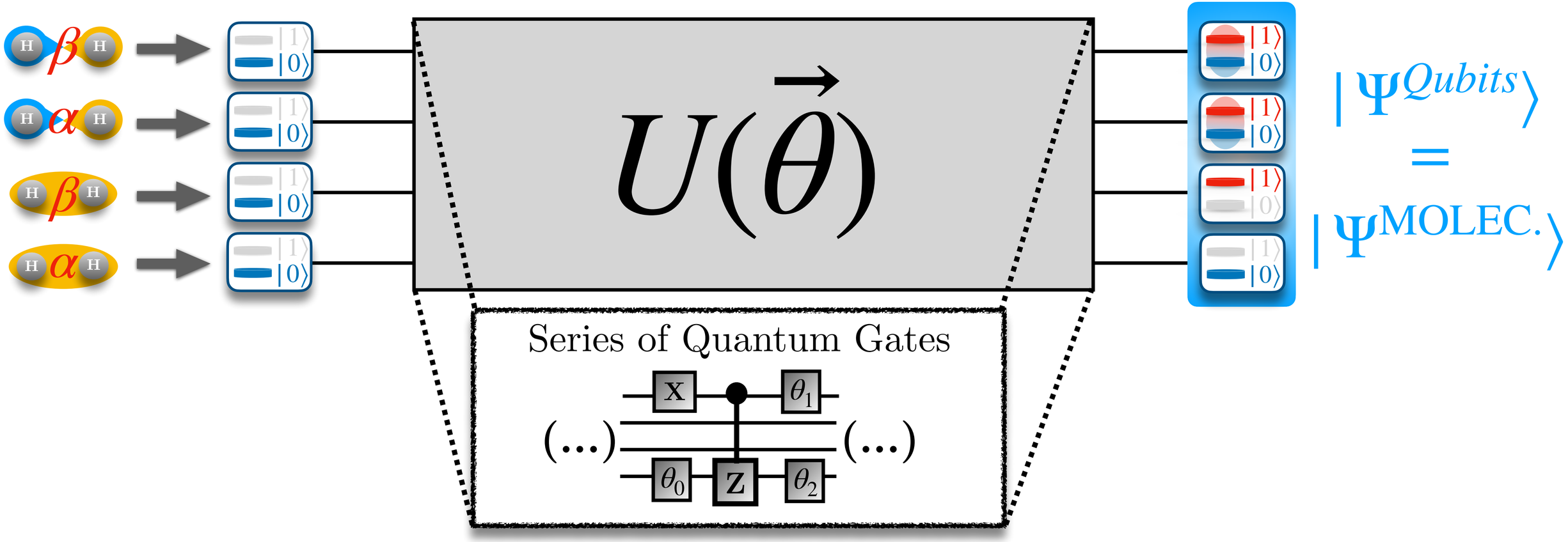

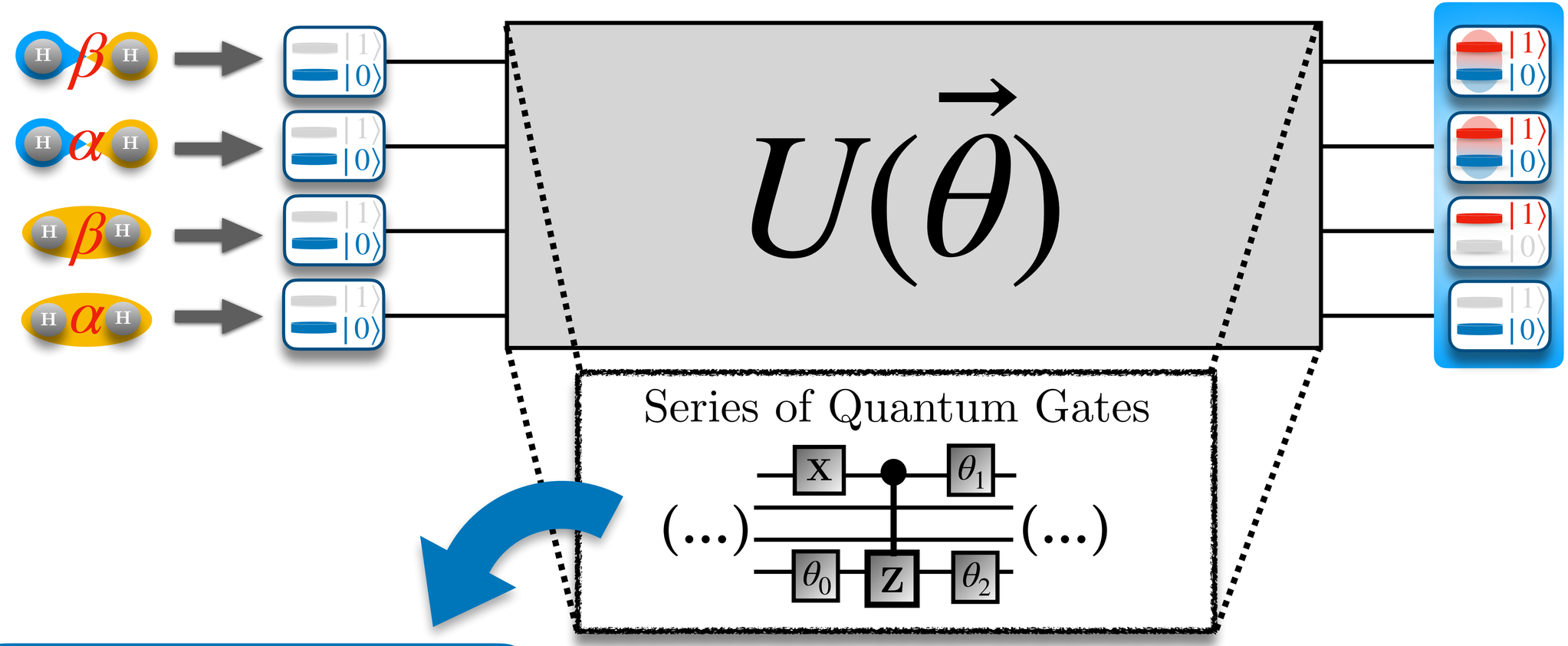

$$|\Psi^{Qubits}\rangle = |\Psi^{MOLEC.}\rangle$$

Near Term Era

Hardware limitations

Variational Quantum Eigensolver

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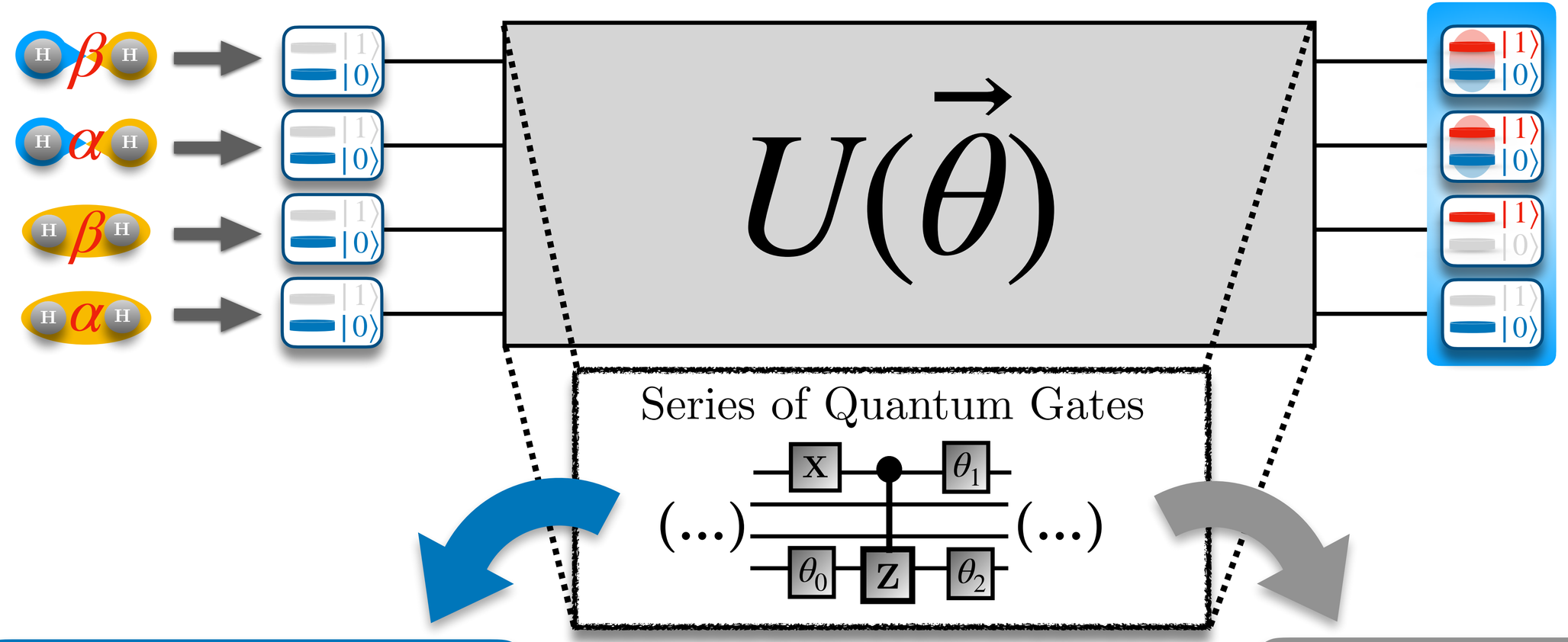

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Near Term Era

Hardware limitations

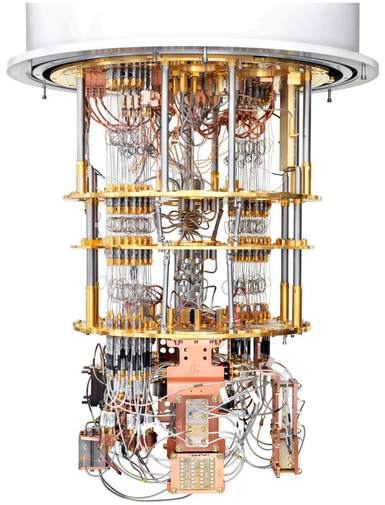
Variational Quantum Eigensolver

Fault Tolerant Era

No Hardware limitations

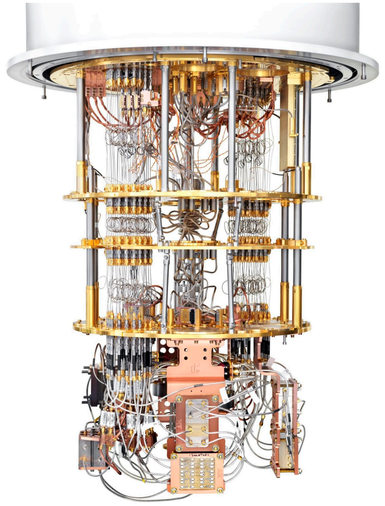
Quantum Phase Estimation

III) Near Term Era:
Variational Quantum Eigensolver



Emerging quantum computers are "NISQ" devices.

(NISQ : Noisy Intermediate-Scale Quantum)



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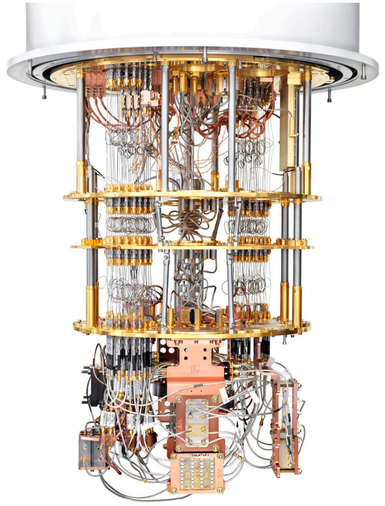

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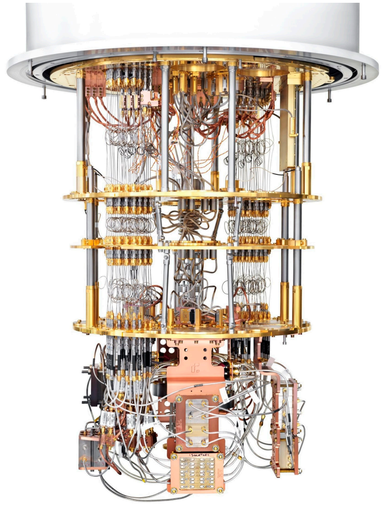
$N_{qubits} \sim 10$

III) Near Term Era: Variational Quantum Eigensolver



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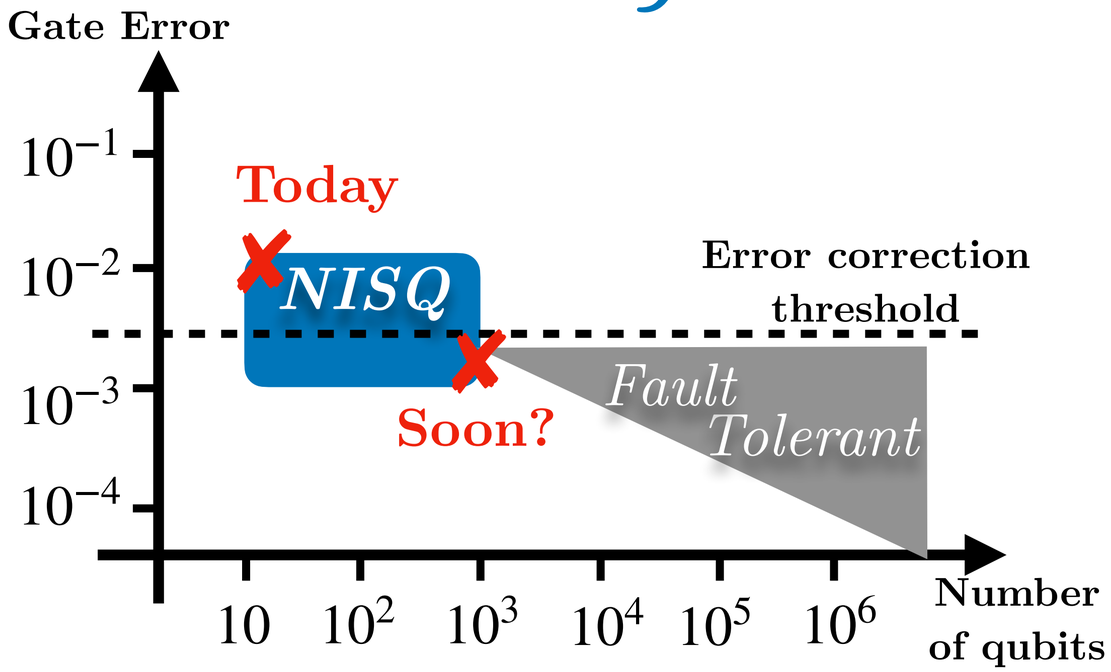

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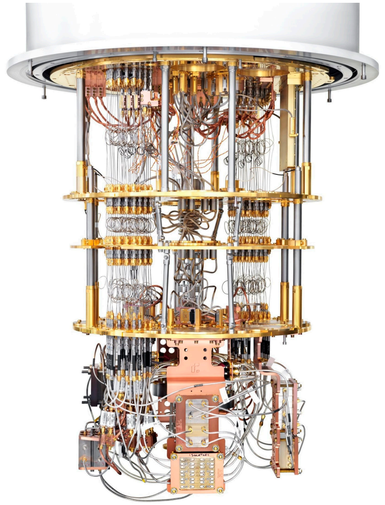

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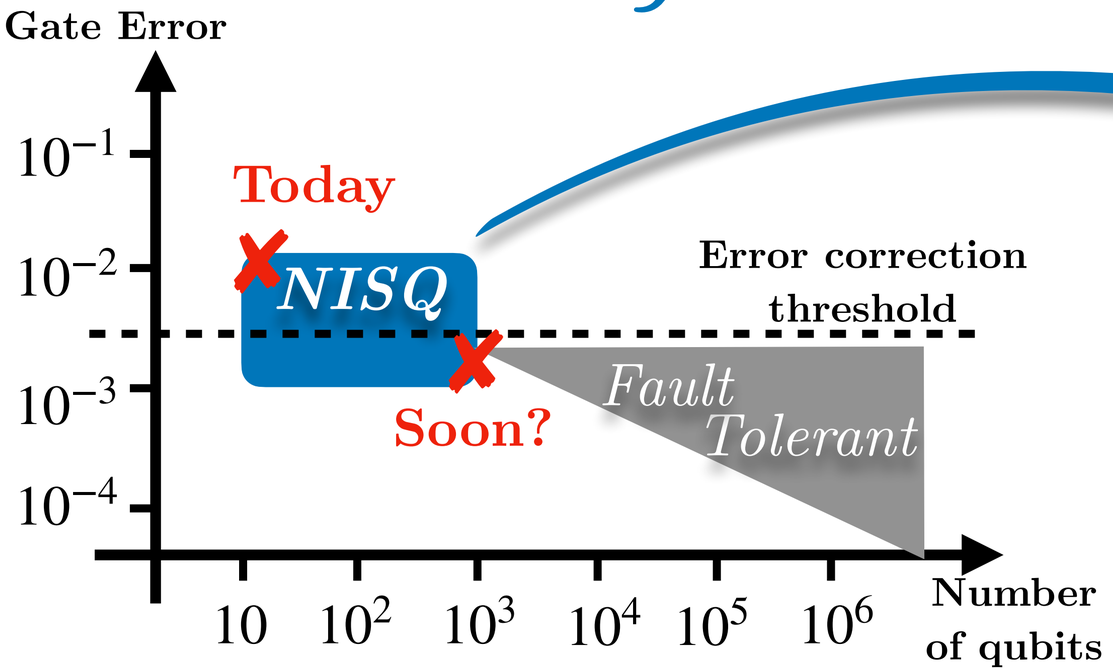
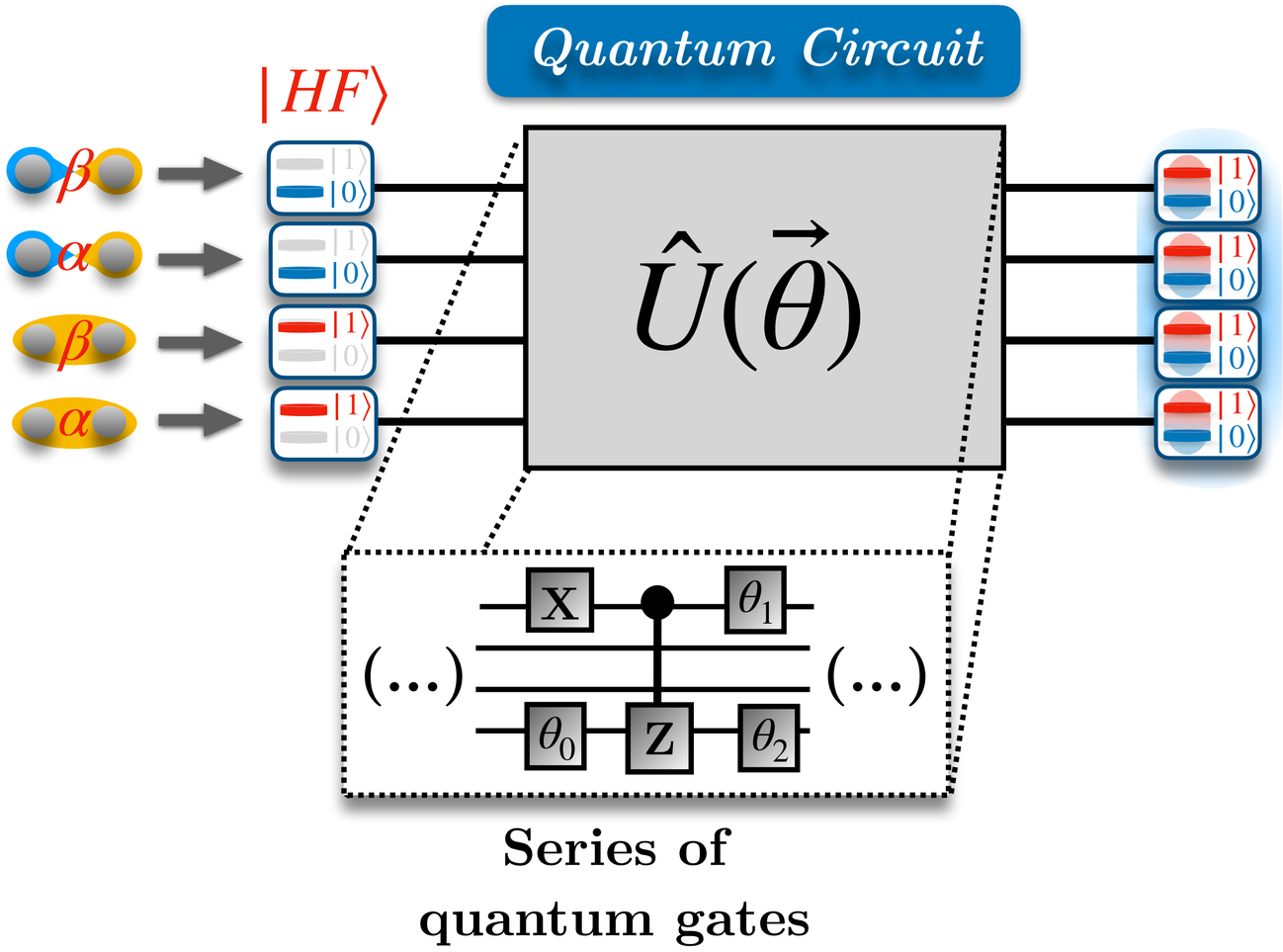


NISQ algorithms

- Based on **a few qubits and quantum gates.**
- Pretty resistant to the **noise effects**.
- ***Exponentially*** **fewer resources to store information**

VQE: Variational Quantum Eigensolver



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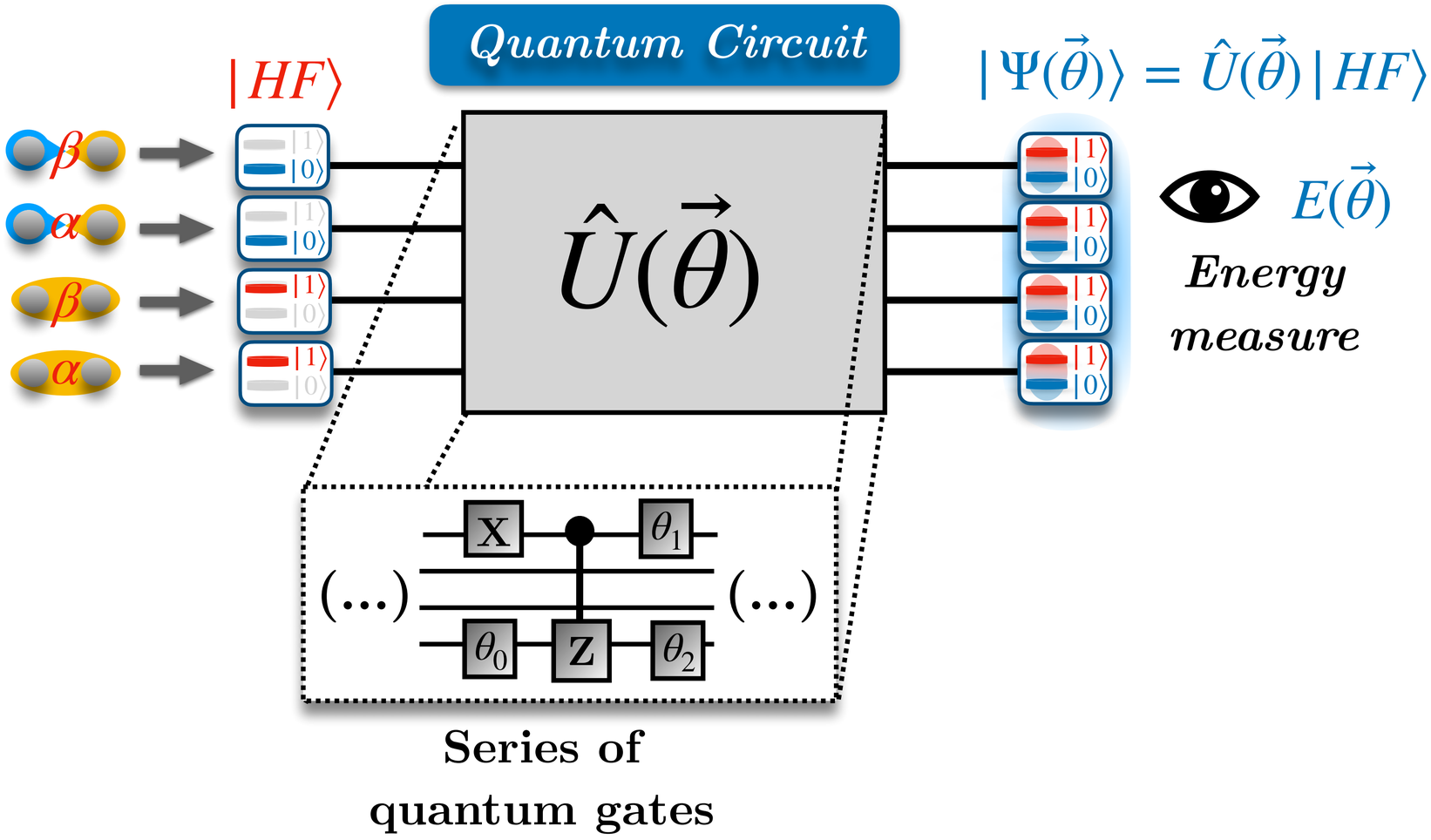

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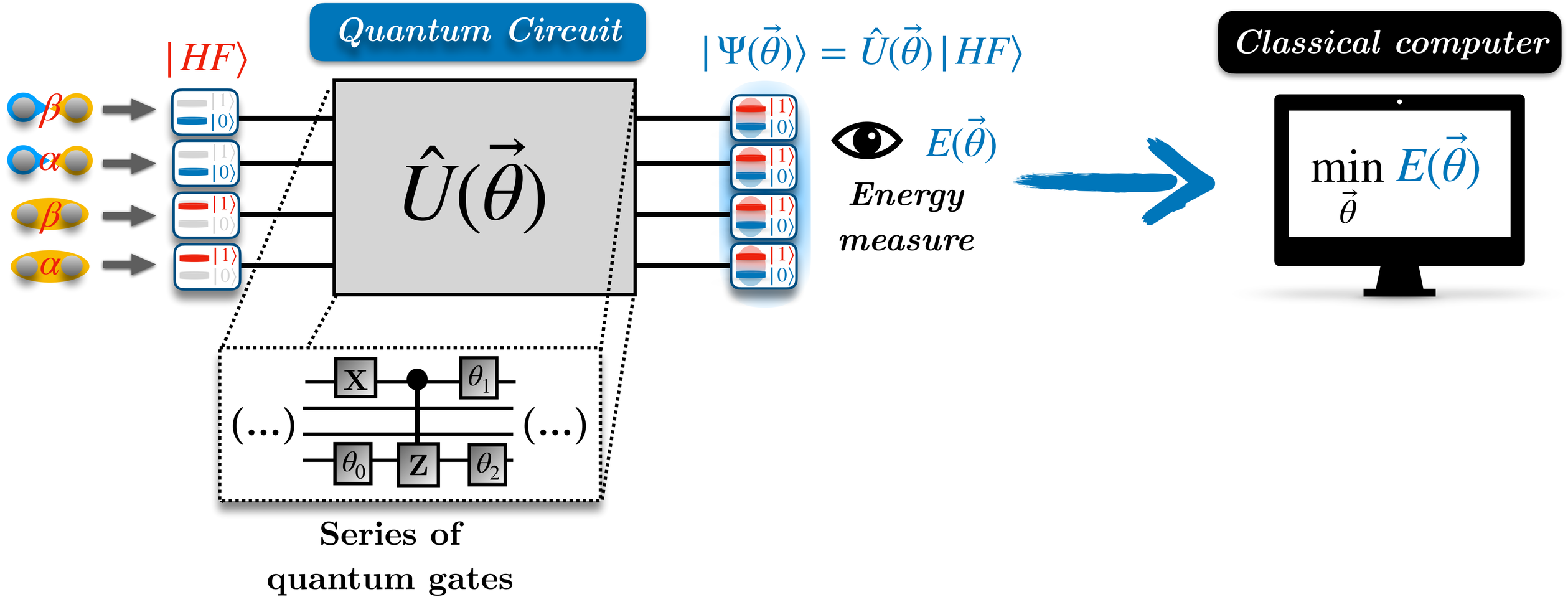

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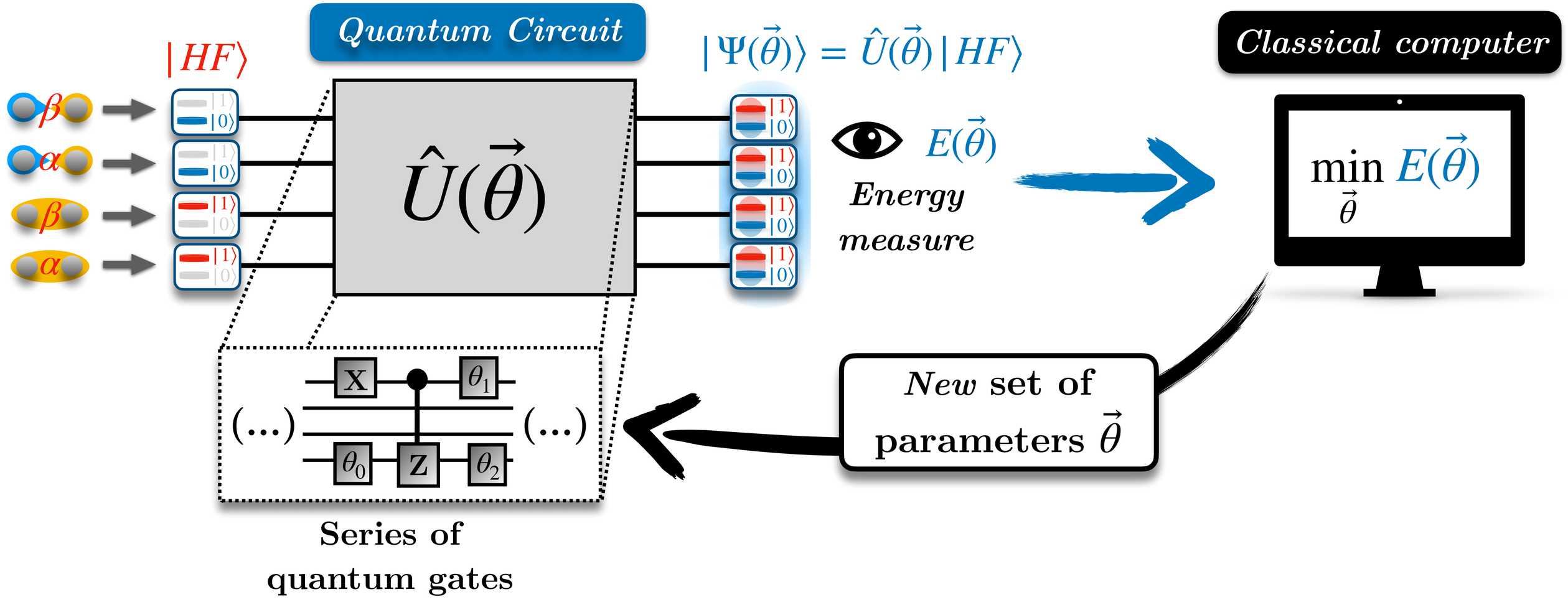

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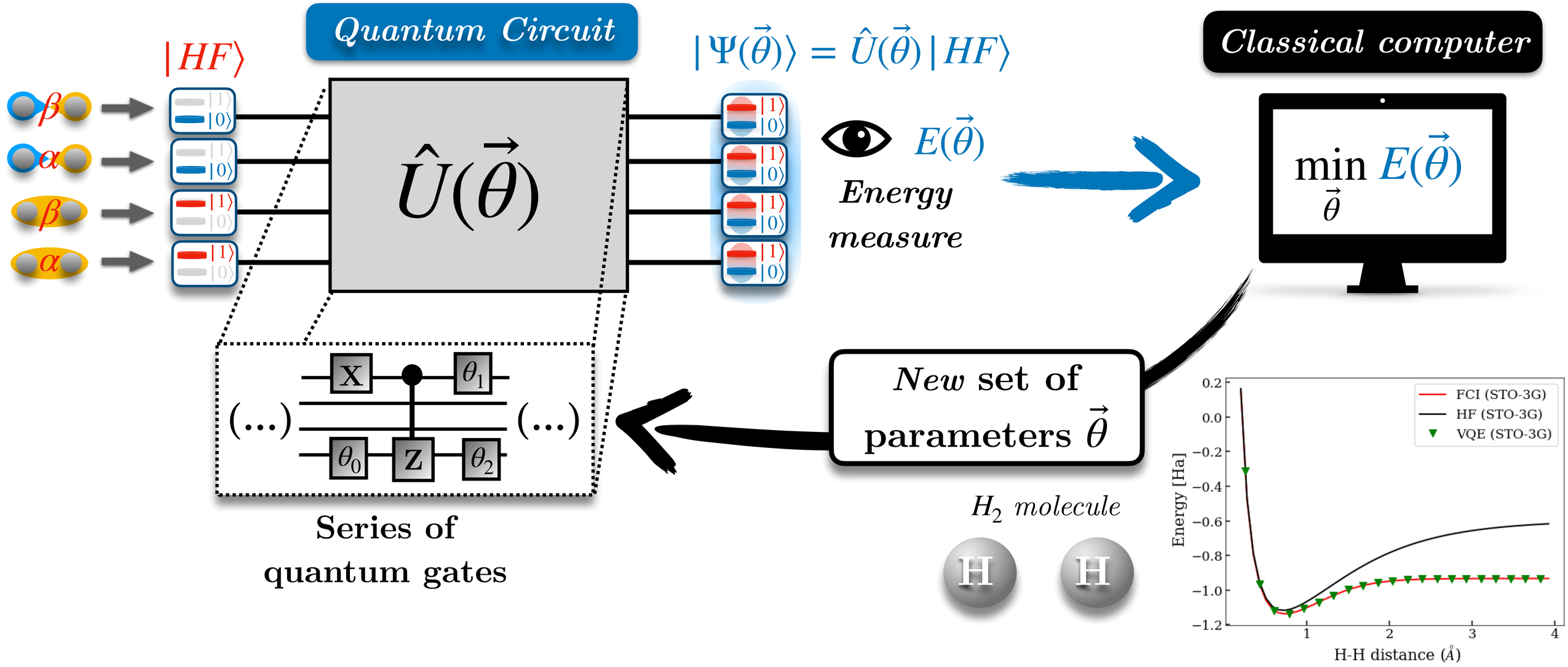
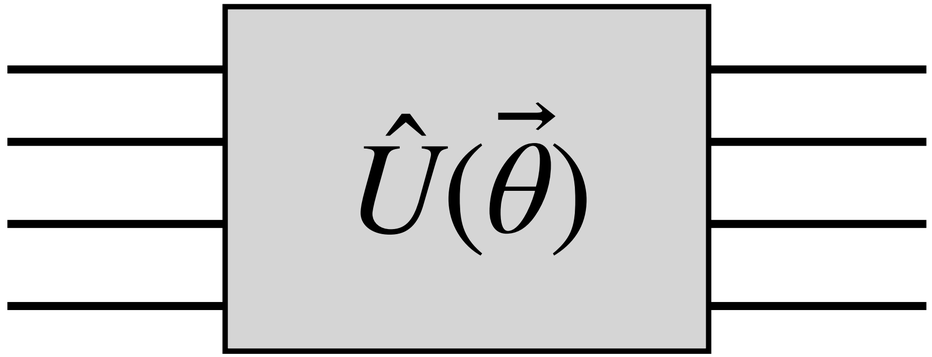
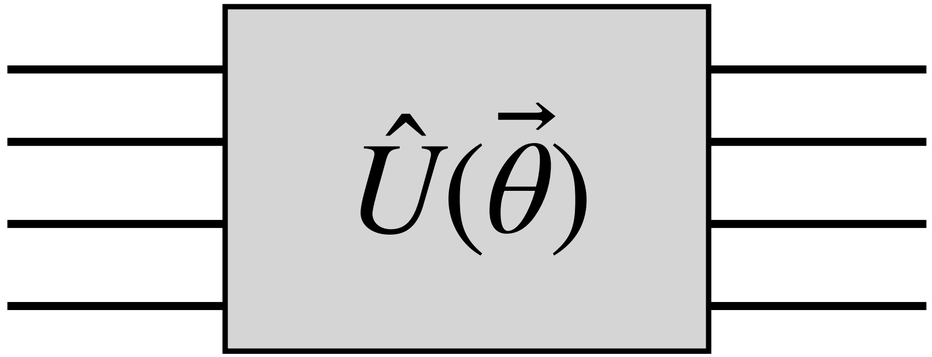




Which ansatze ?

How do we build them ?



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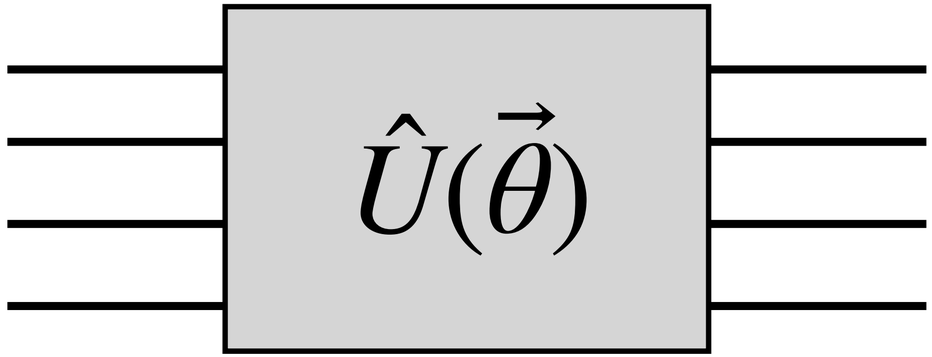
Hardware-efficient ansatz



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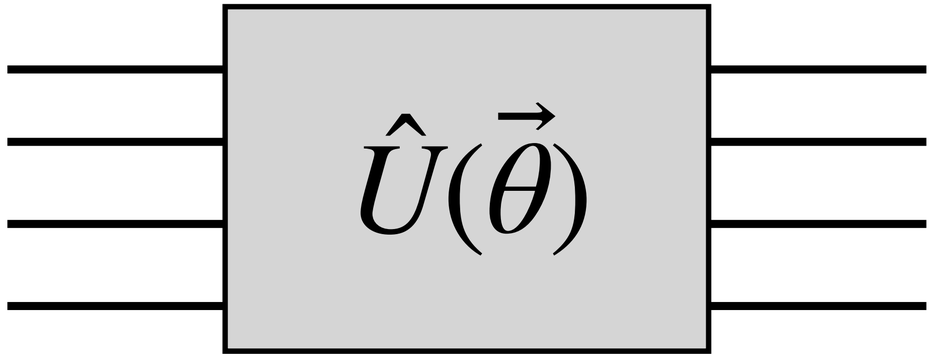

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Demo

Hardware-efficient ansatz

Kandala, Abhinav, et al. "Hardware-efficient variational quantum eigensolver for small molecules and quantum magnets." *Nature* 549.7671 (2017): 242-246.

Hardware-efficient ansatz

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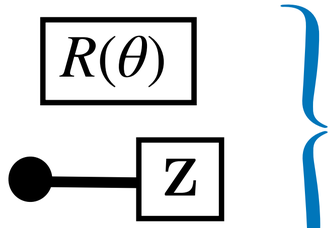

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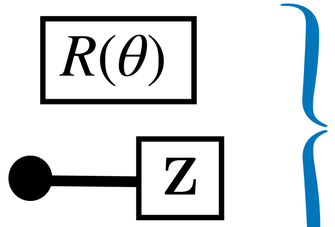

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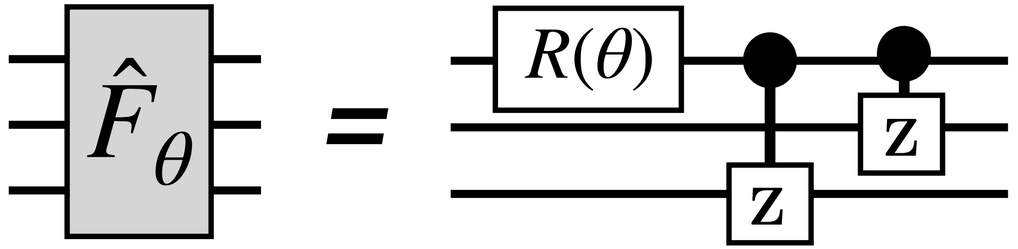

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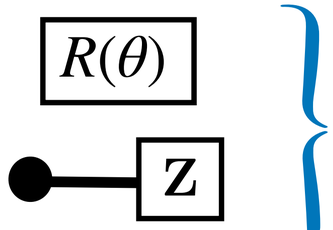

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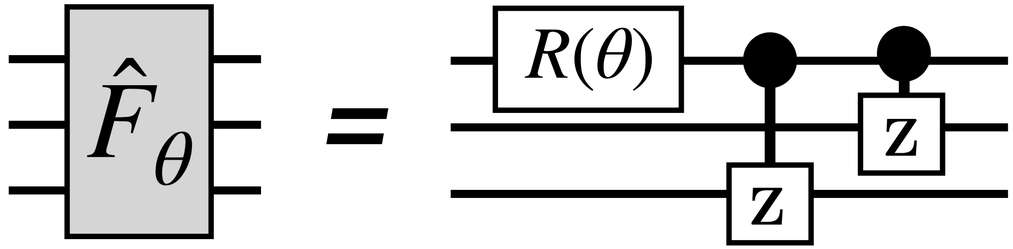

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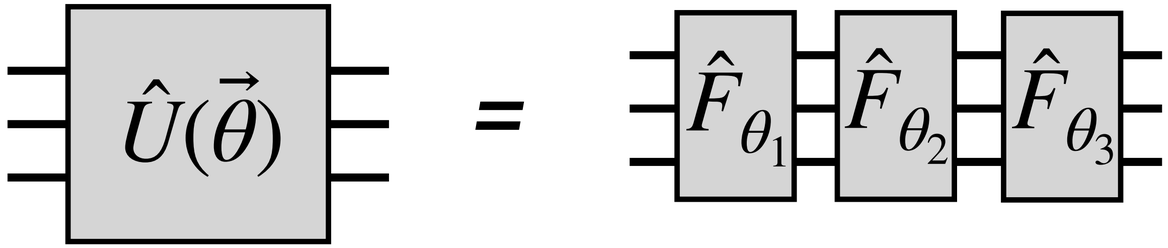

Repeated fragment

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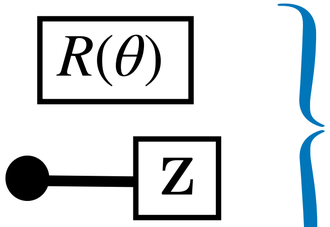

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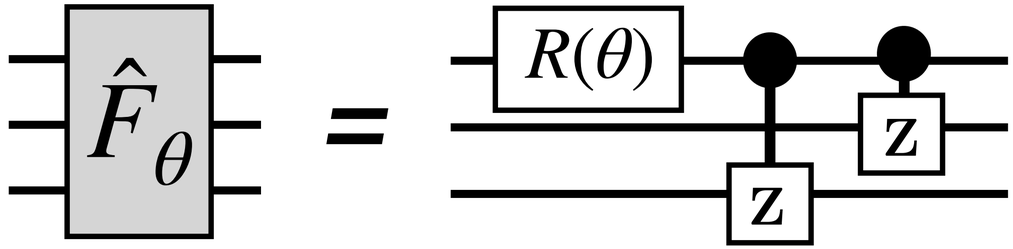

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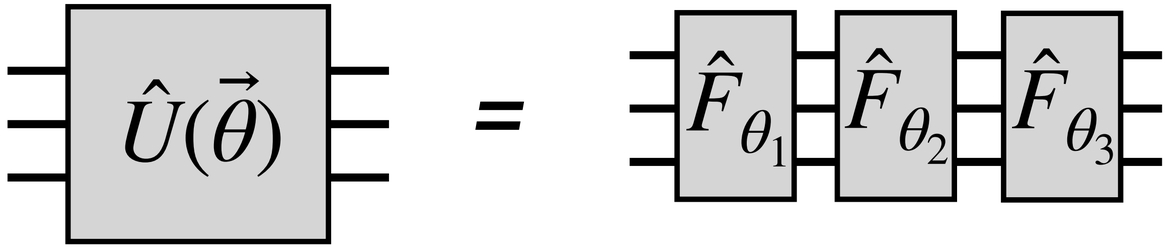

Repeated fragment

✓ **Not expensive**

✓ ✗ **May break symmetries**

✗ **Optimisation seems hard**

Unitary Coupled Cluster ansatz

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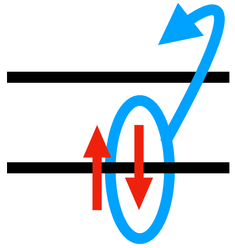

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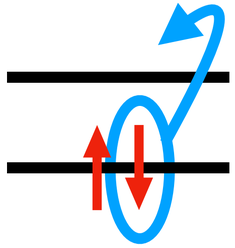

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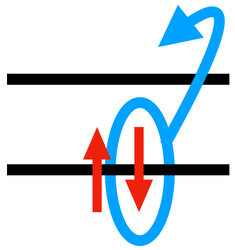

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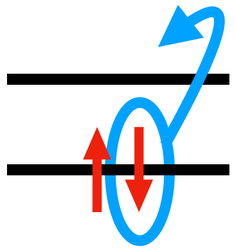

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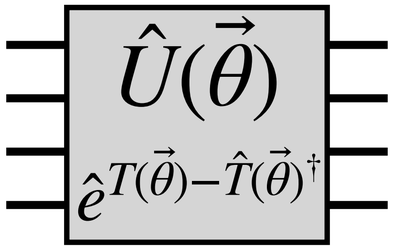

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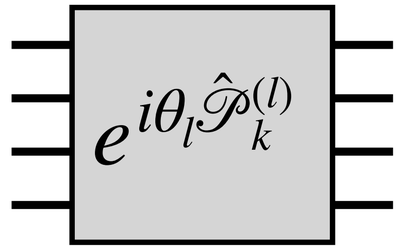

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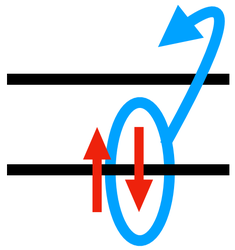

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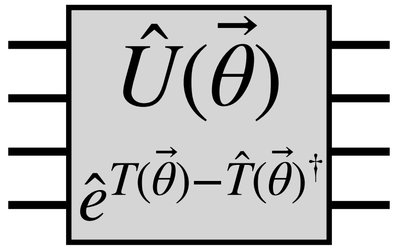

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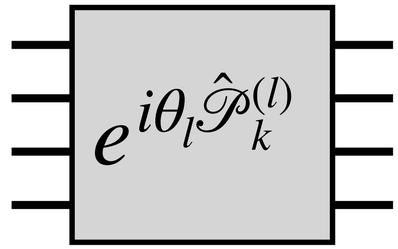
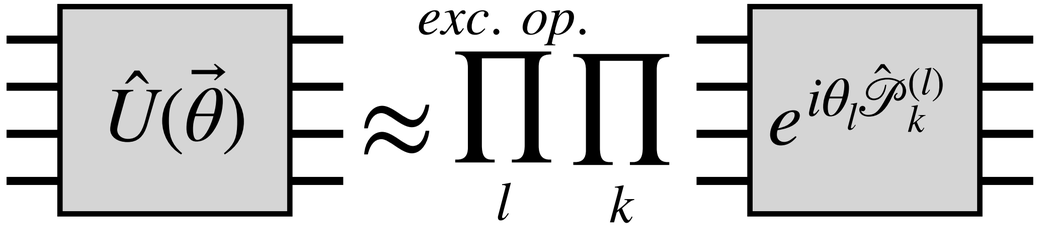


✓ ✗ **Polynomial cost** ✓ **Conserved number of particle** ✓ **Simpler to optimize**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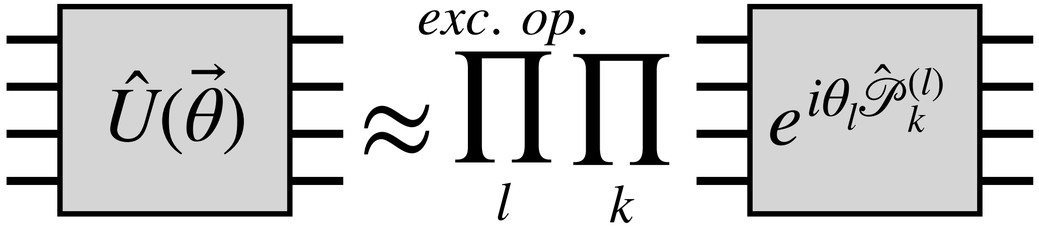

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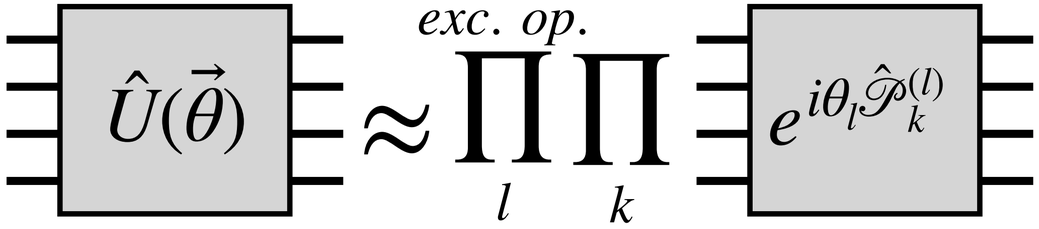
$$e^{-i\theta Z_A X_B} = \cos(\theta)\mathbf{1} - i\sin(\theta) Z_A X_B$$



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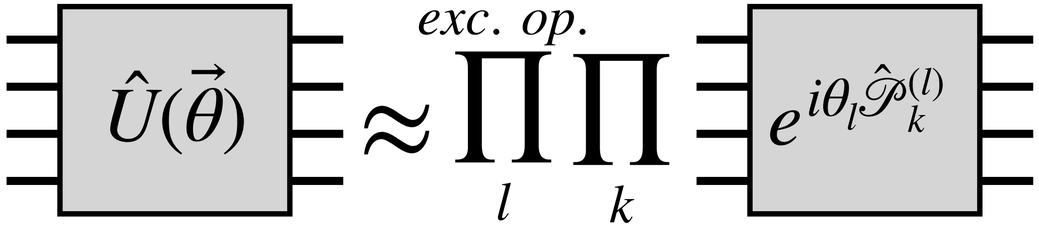
$$e^{-i\theta Z_q} = R_{Z_q}(2\theta) = \cos(\theta)\mathbf{1}_q - i\sin(\theta) Z_q$$

$$C^X_{qq'}\ Z_{q'}\ C^X_{qq'} = Z_q Z_{q'}$$

$$R_{Y_q}(\pi/2)\ Z_q\ R_{Y_q}(-\pi/2) = X_q$$



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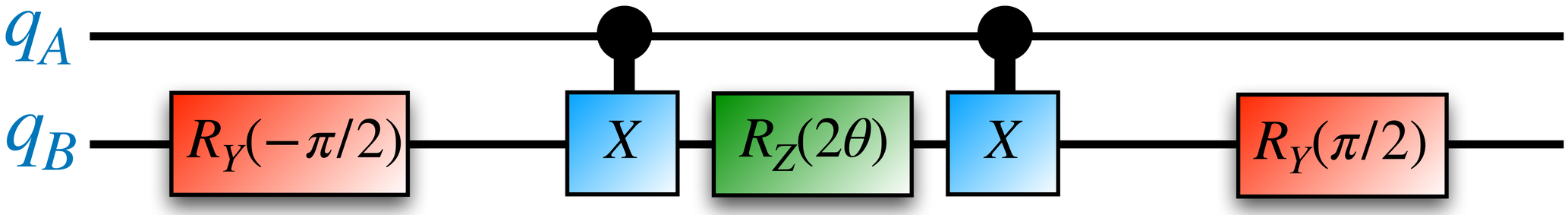

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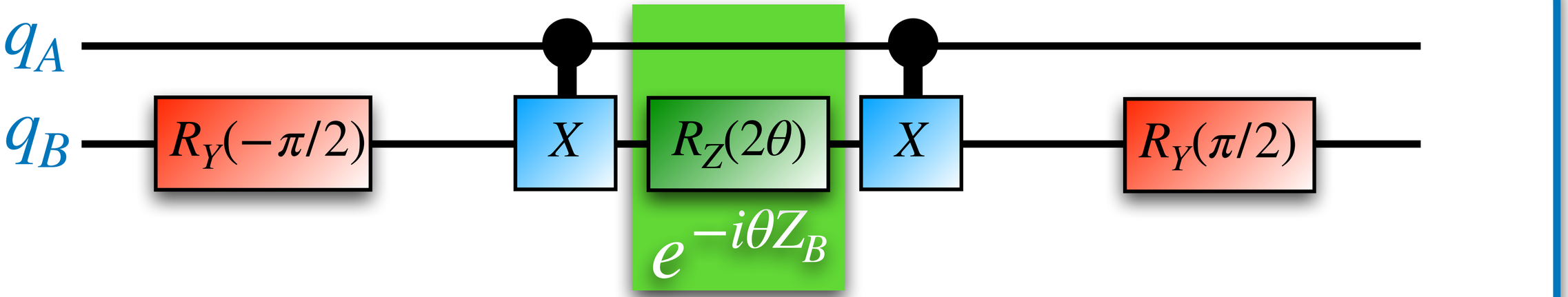

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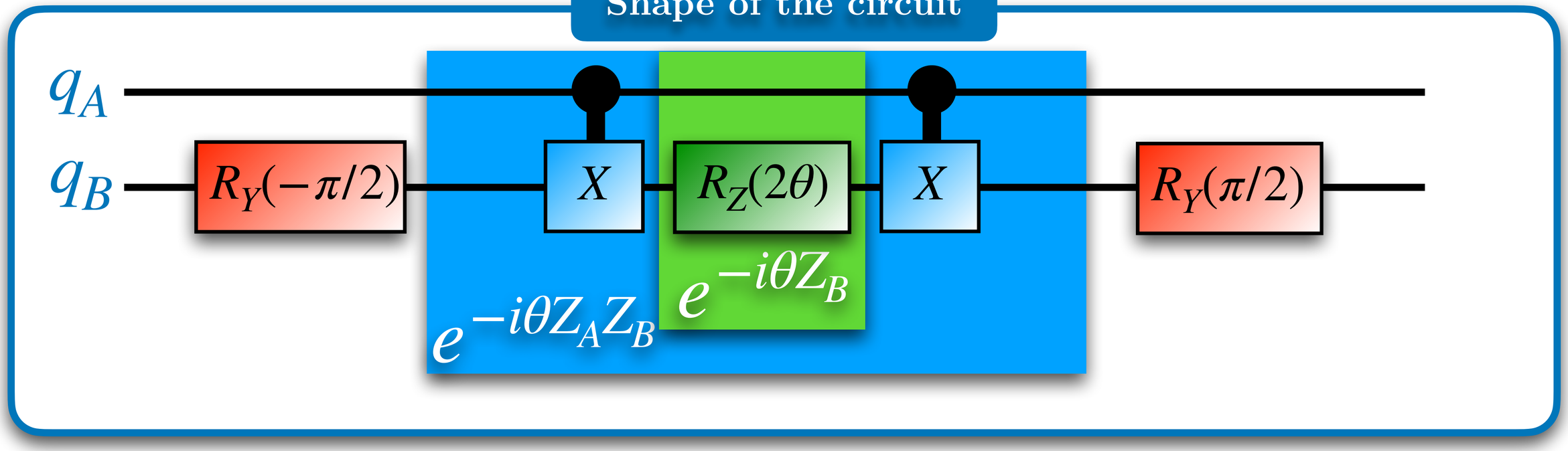

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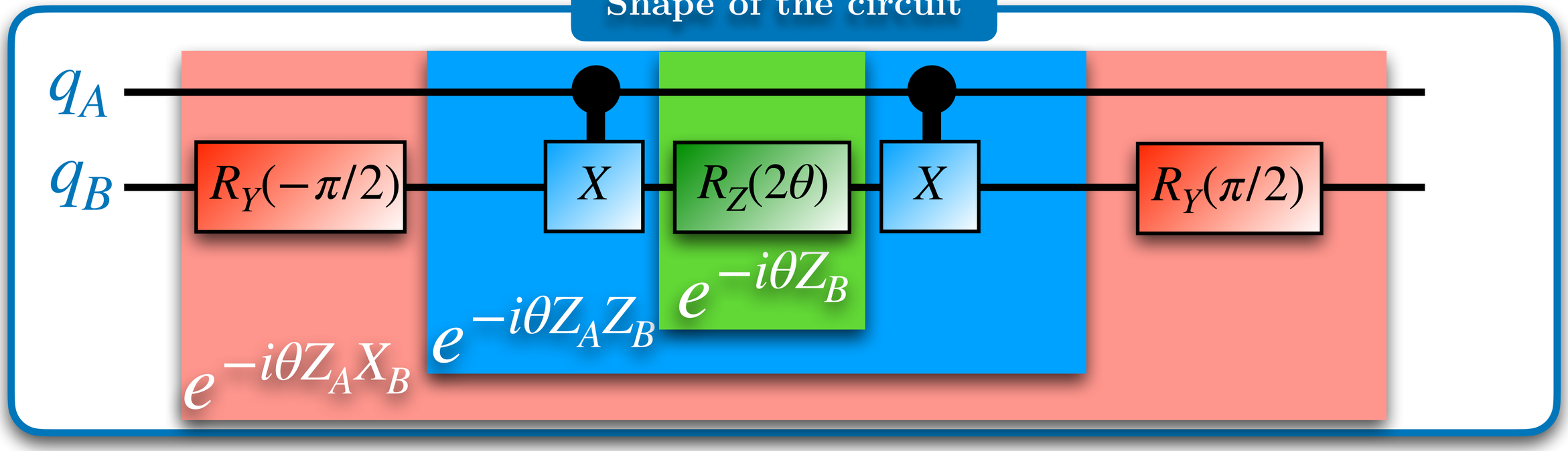

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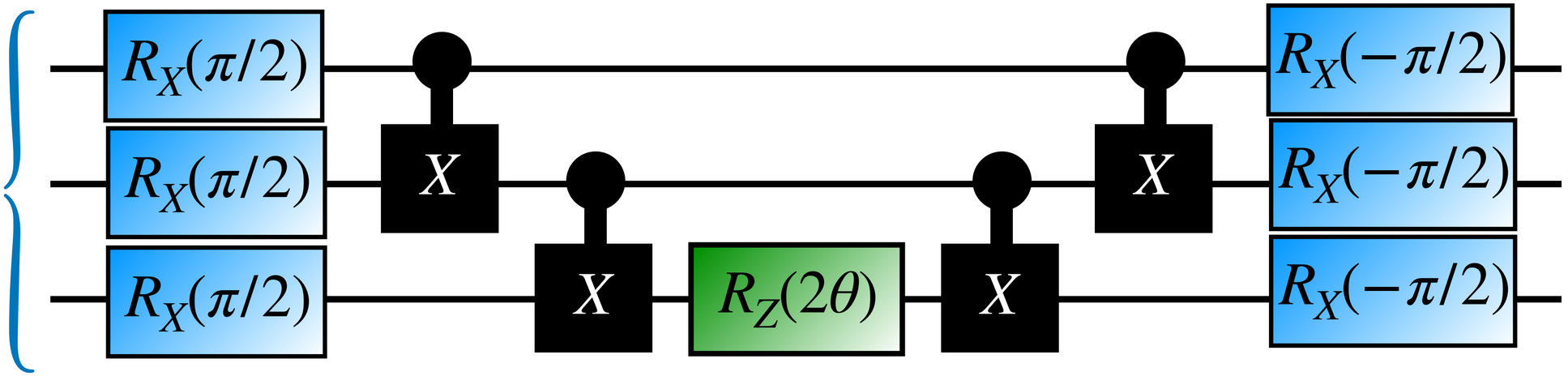

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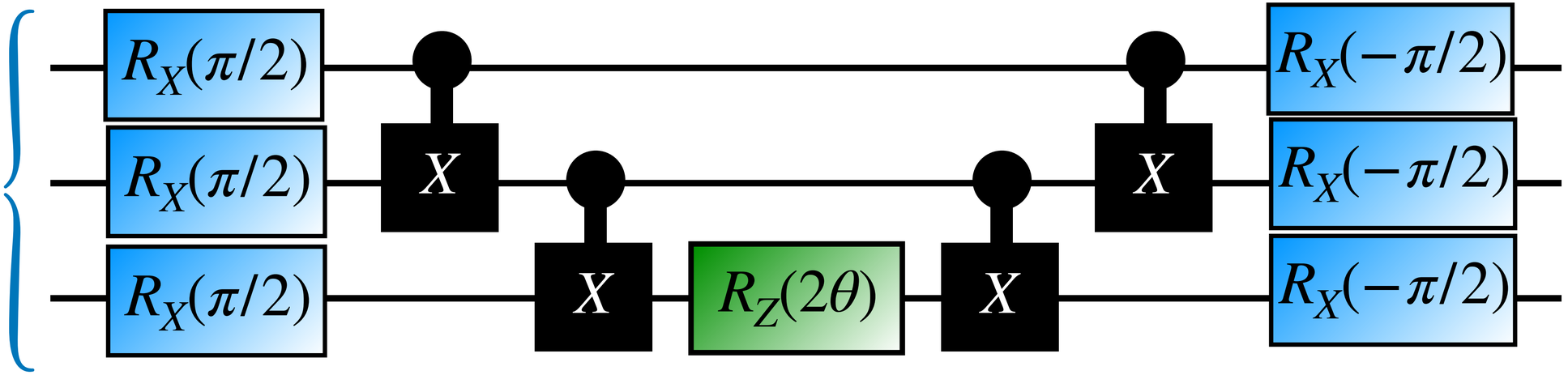

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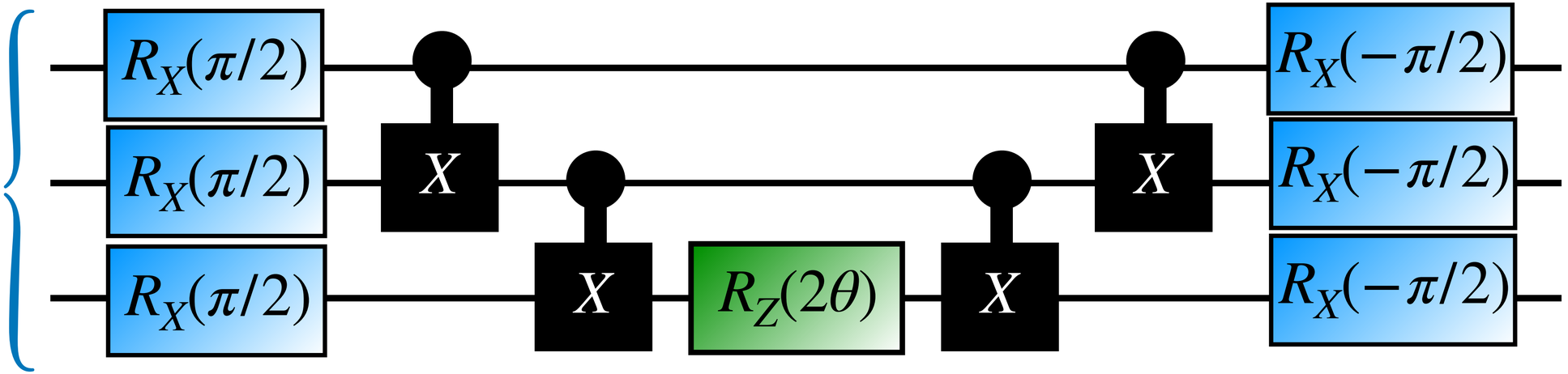

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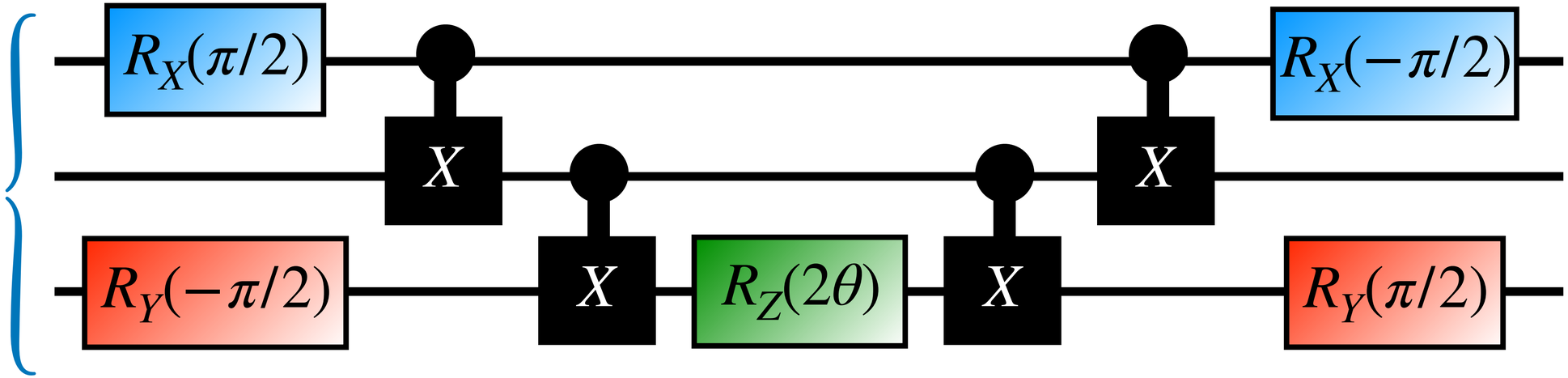
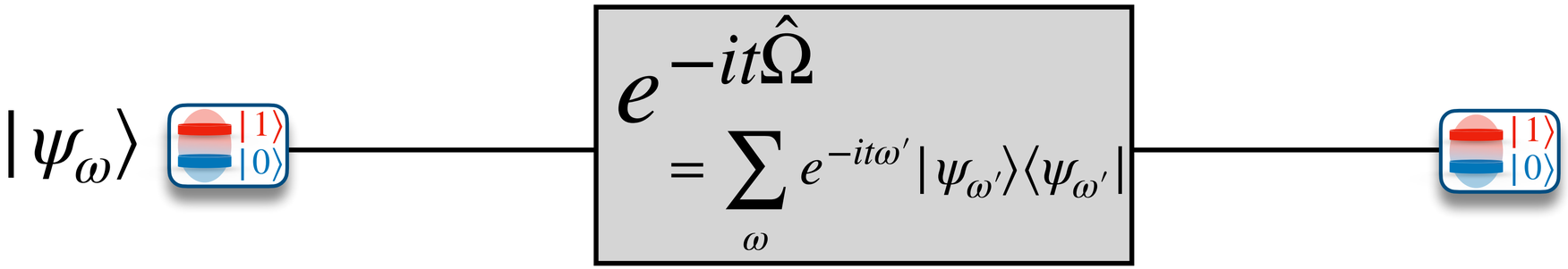


IV) Fault Tolerant Era: Quantum Phase Estimation

GOAL: we want to know ω



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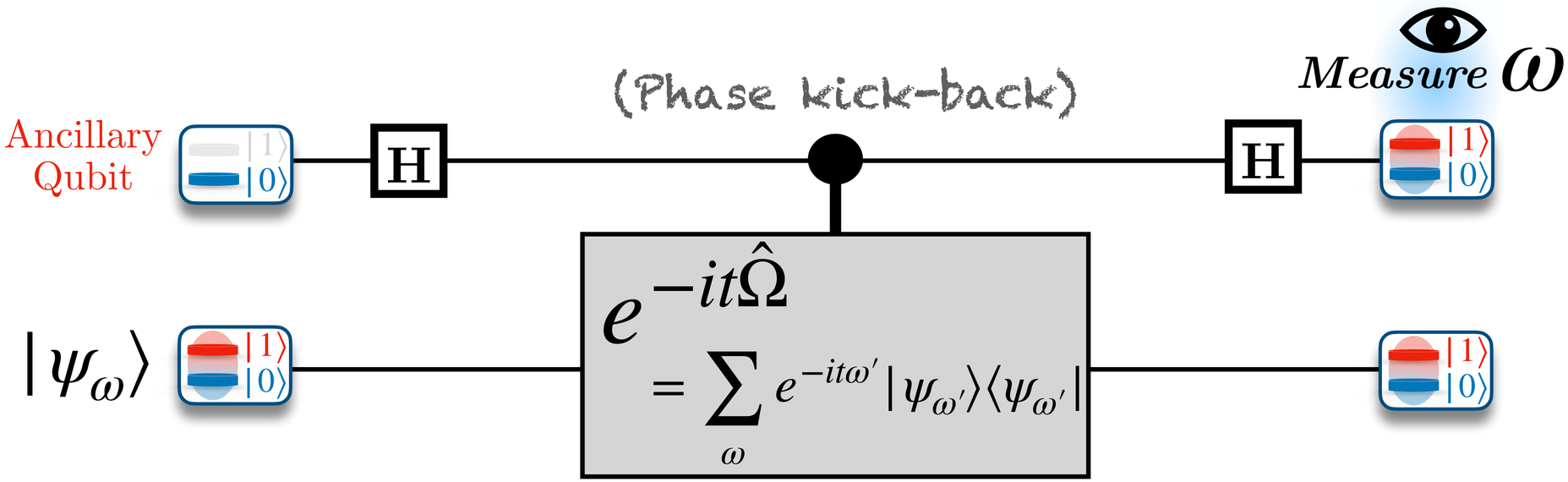

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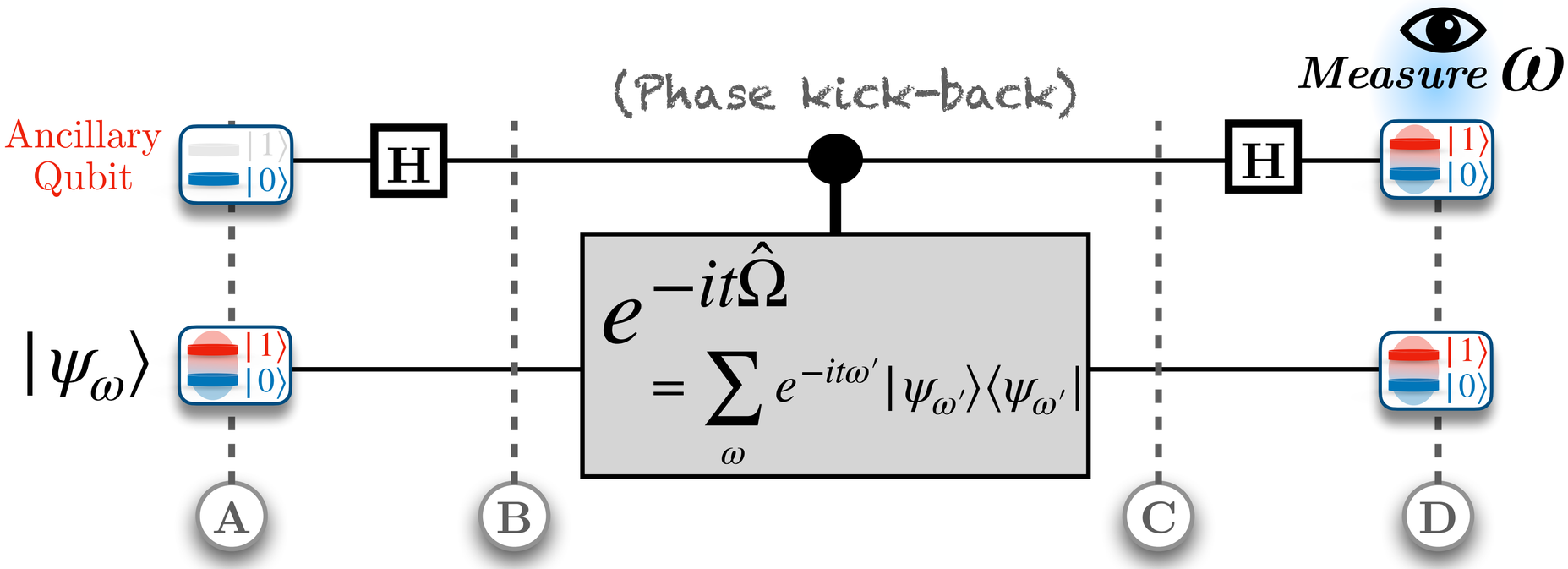

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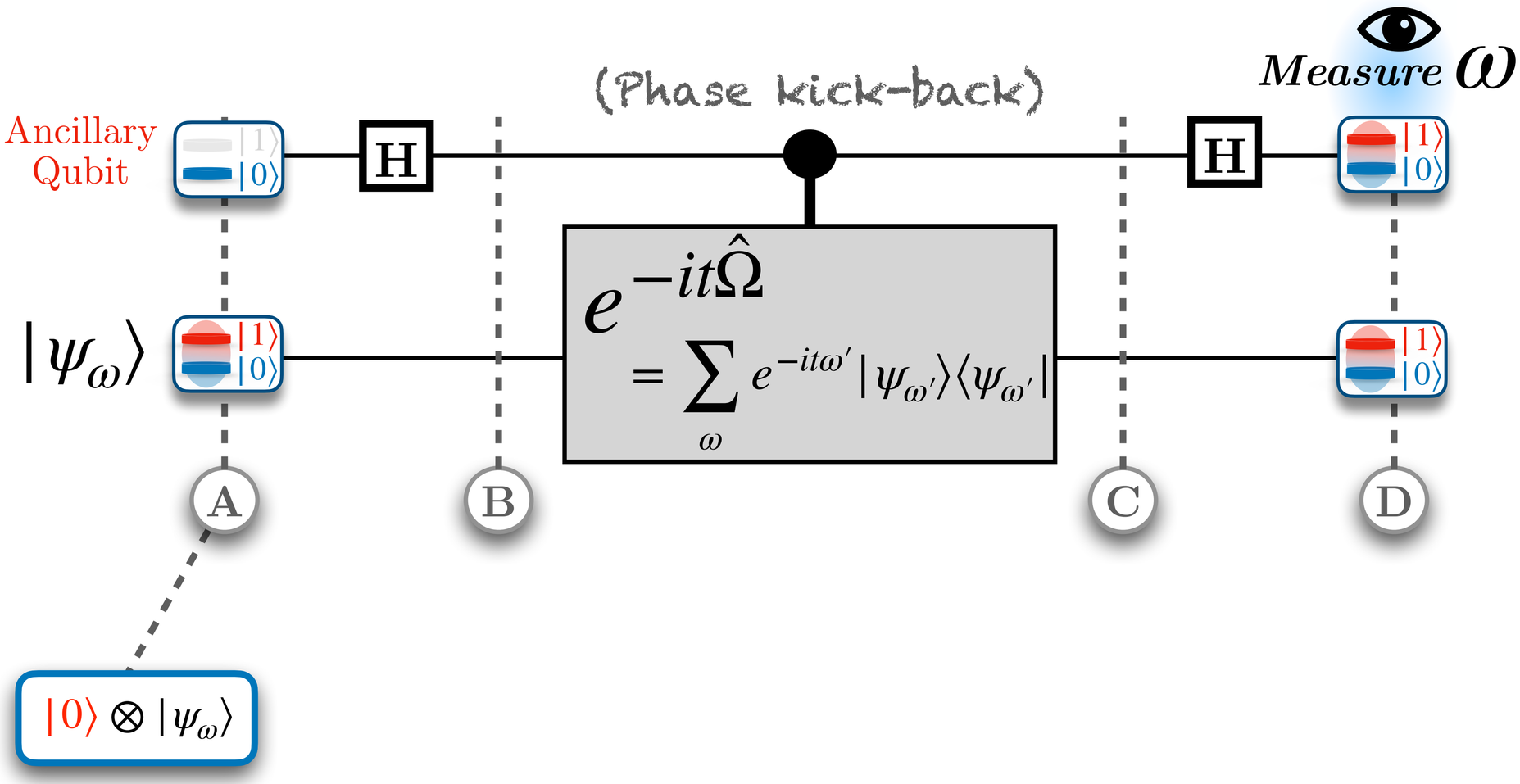

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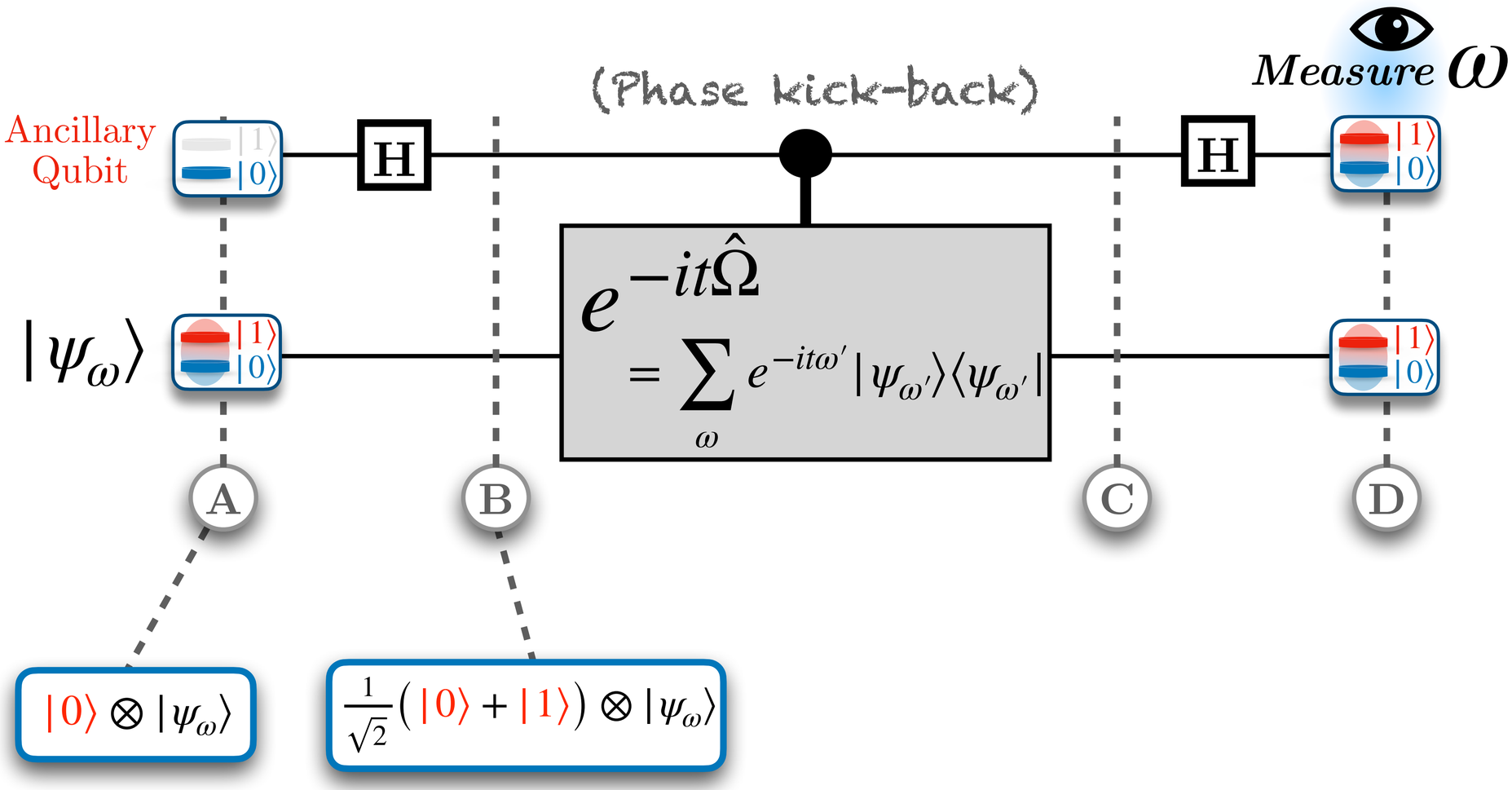

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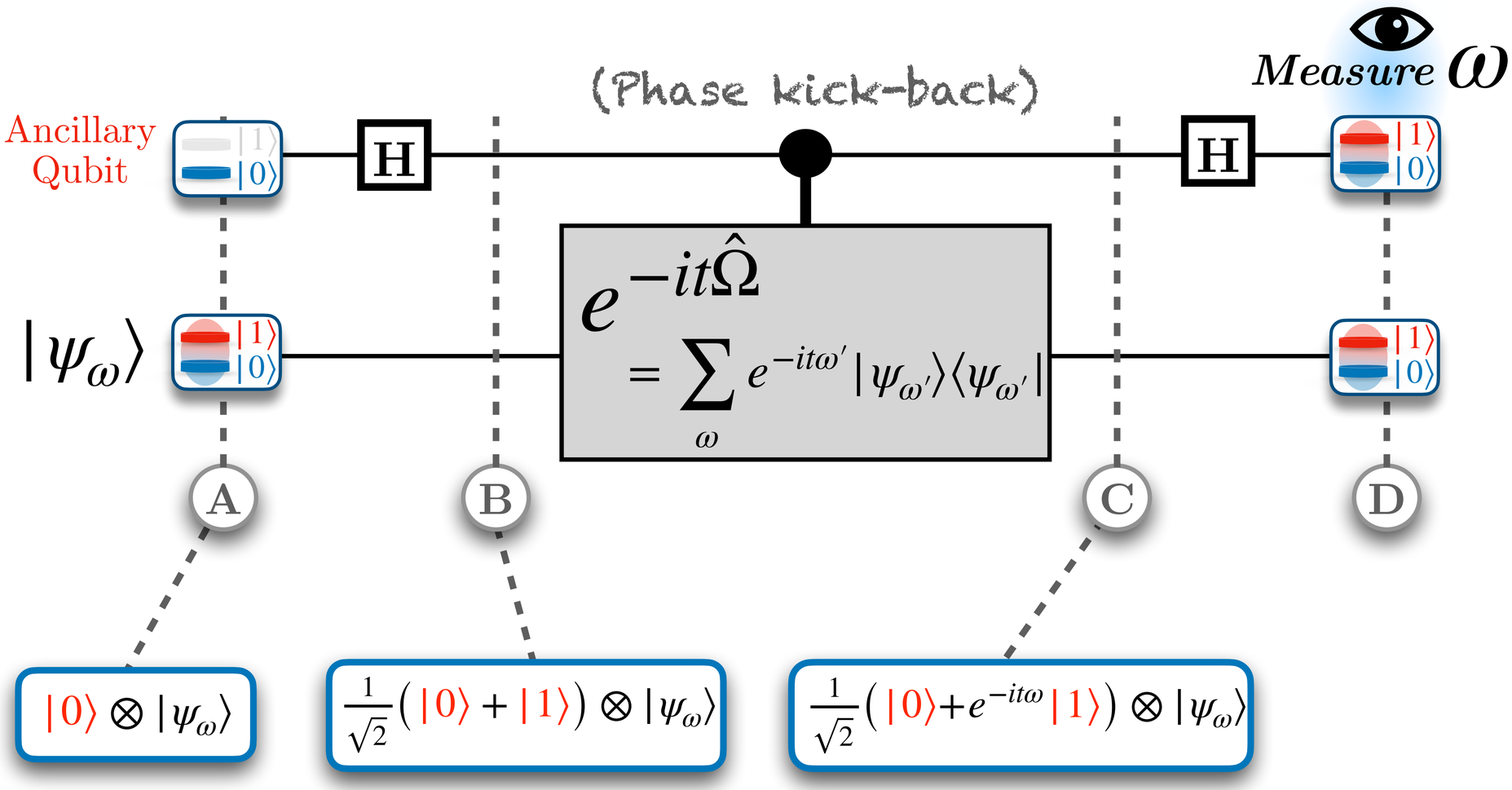

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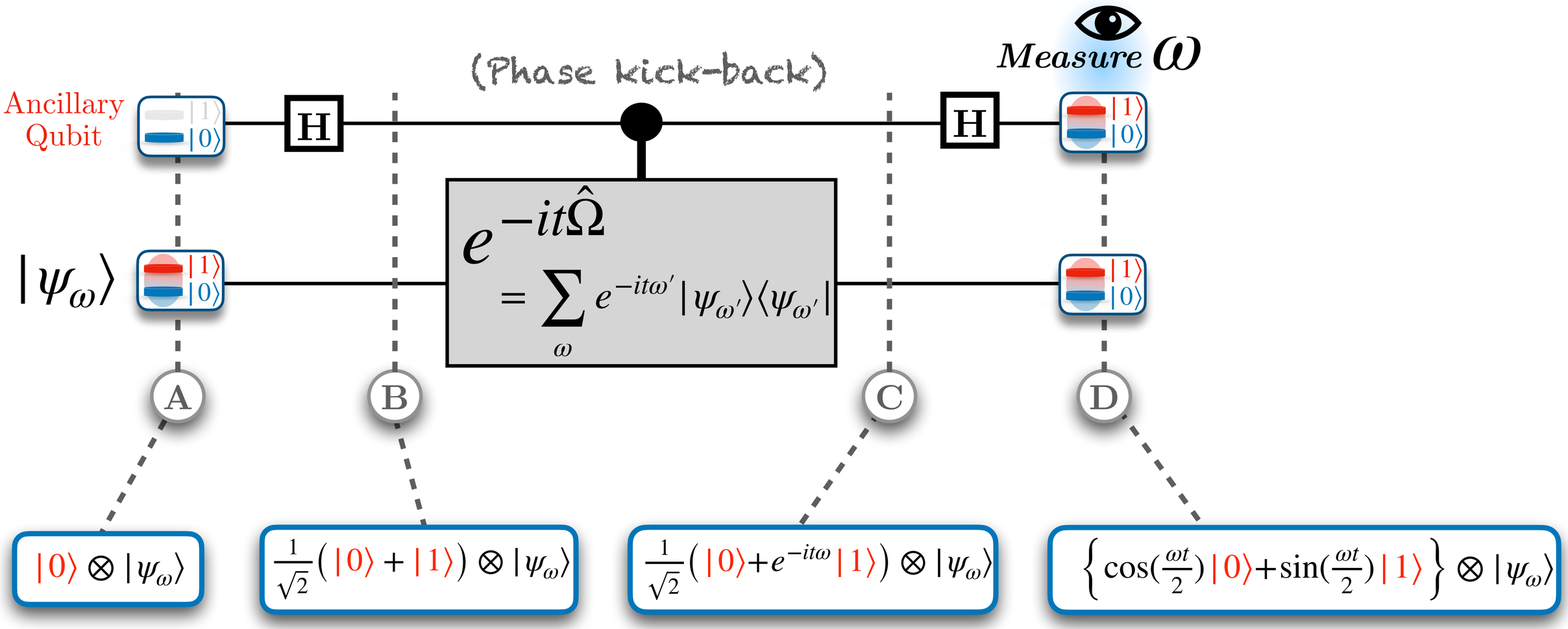

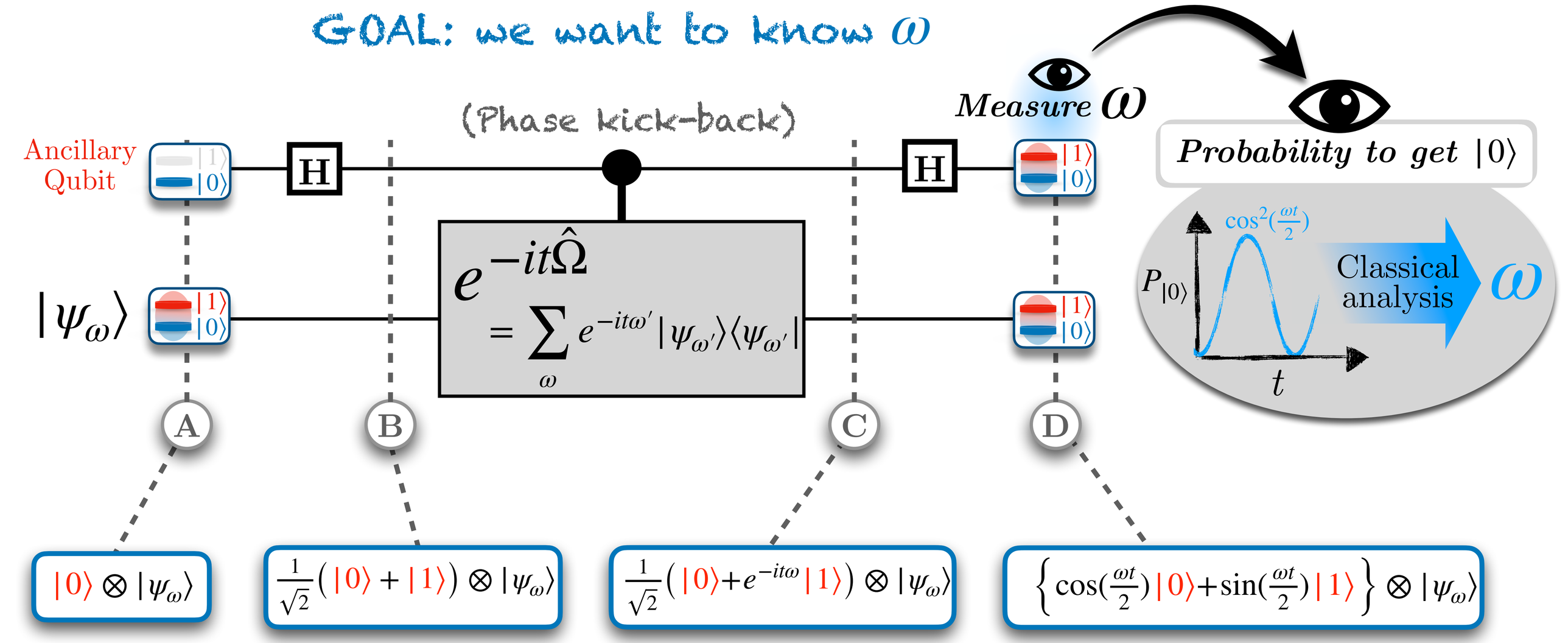
GOAL: we want to know ω
Measure ω
Probability to get $|0\rangle$
(Phase kick-back)
Ancillary Qubit
$|\psi_\omega\rangle$
H
H
$|1\rangle$
$|0\rangle$
$e^{-it\hat{\Omega}} = \sum_\omega e^{-it\omega'} |\psi_{\omega'}\rangle\langle\psi_{\omega'}|$
$\cos^2(\frac{\omega t}{2})$
$P_{|0\rangle}$
t
Classical analysis
ω
A
B
C
D
$|0\rangle \otimes |\psi_\omega\rangle$
$\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes |\psi_\omega\rangle$
$\frac{1}{\sqrt{2}}(|0\rangle + e^{-it\omega}|1\rangle) \otimes |\psi_\omega\rangle$
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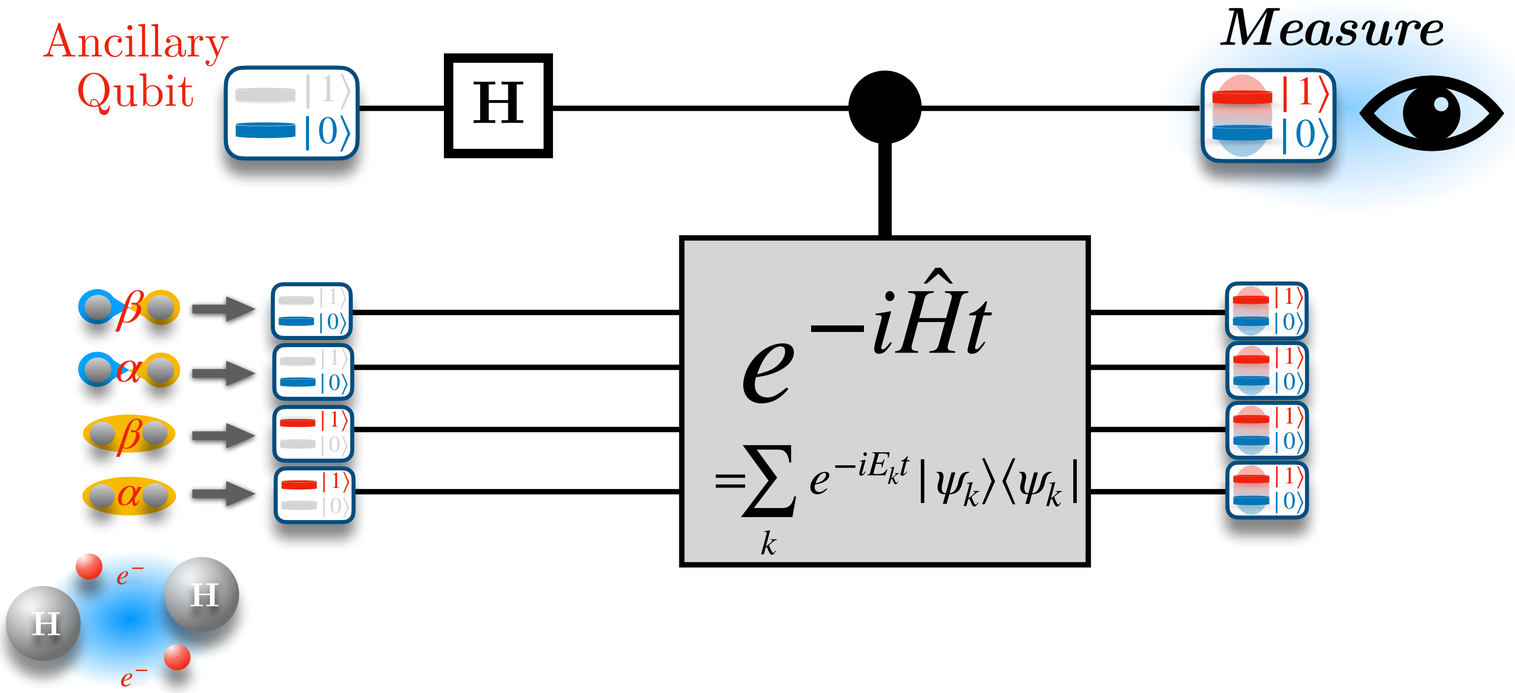
IV) Fault Tolerant Era: Quantum Phase Estimation



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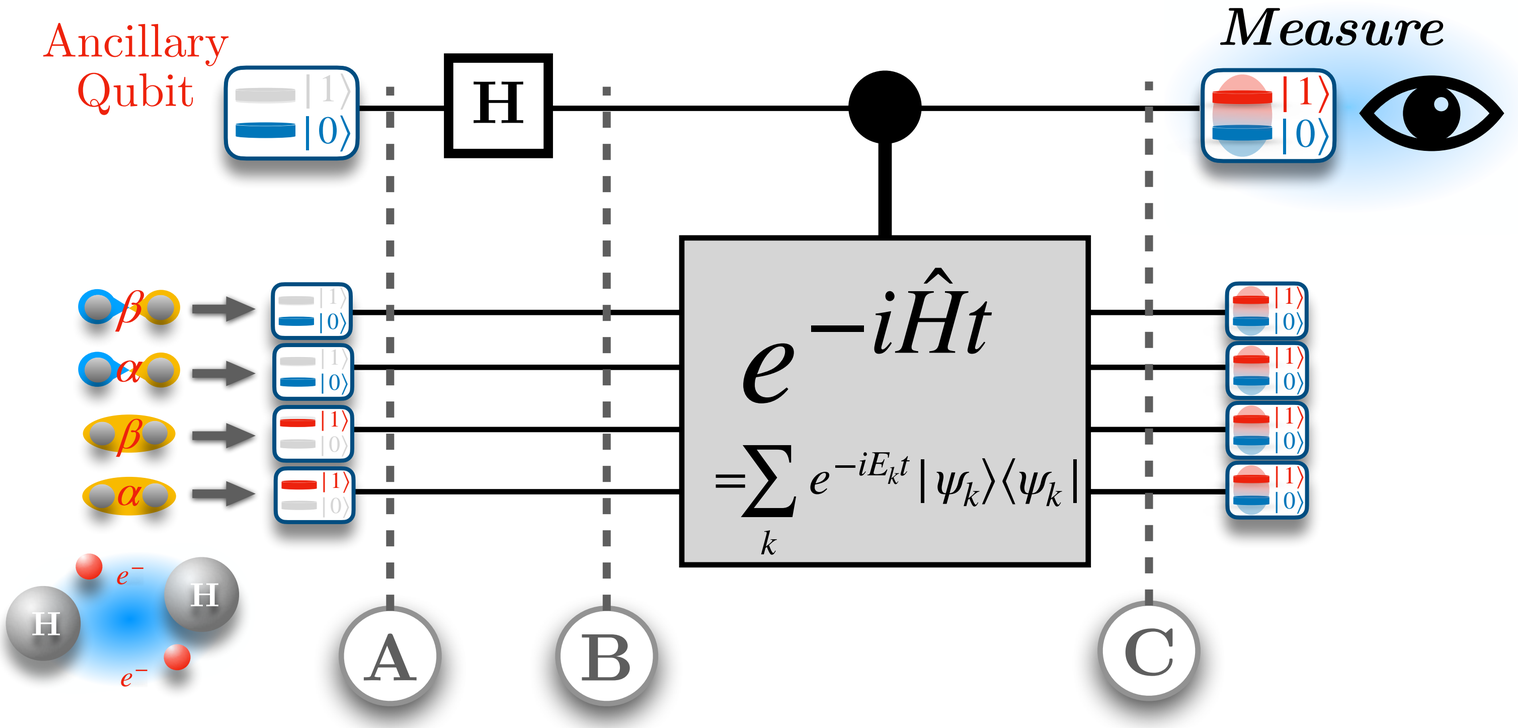

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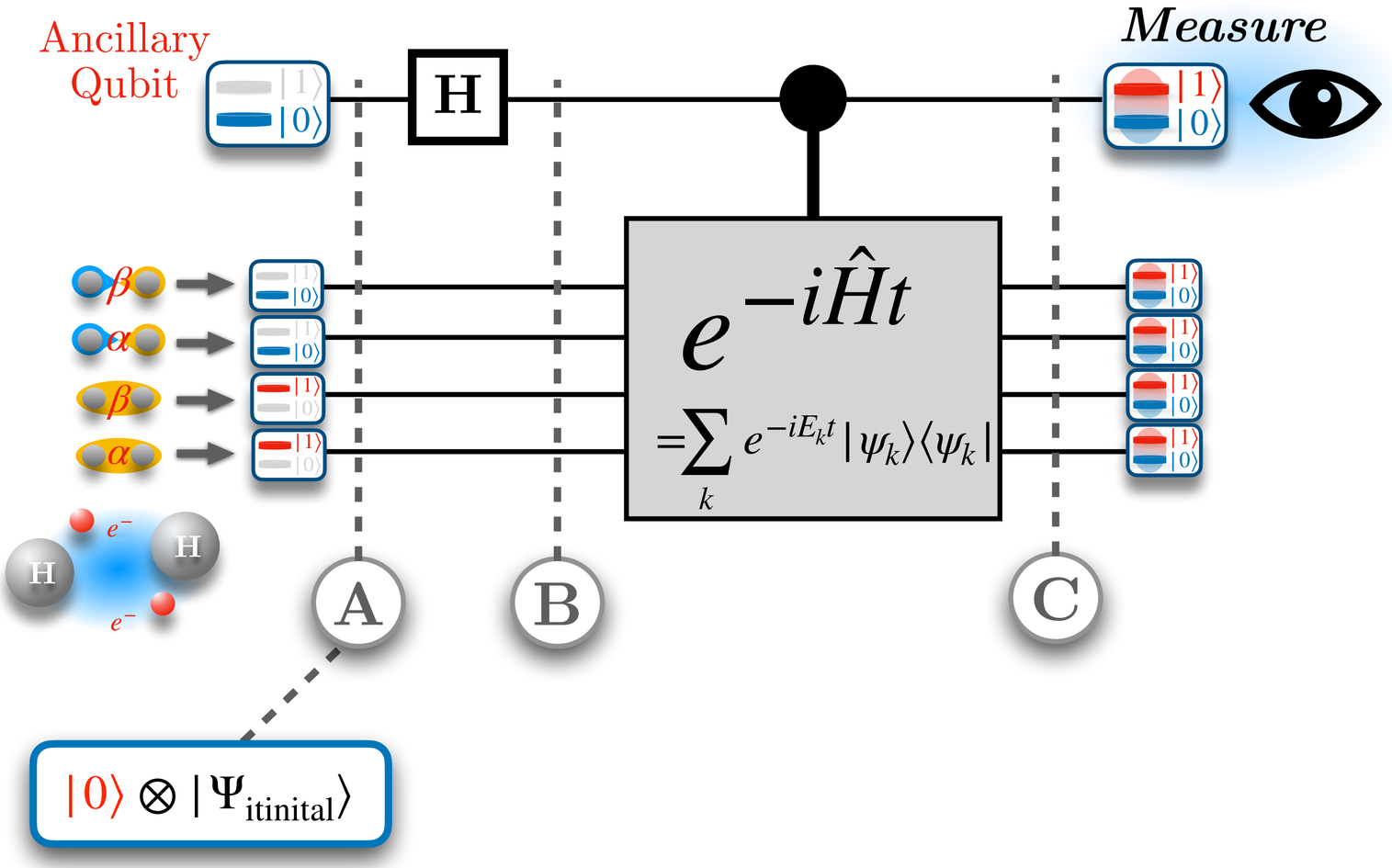

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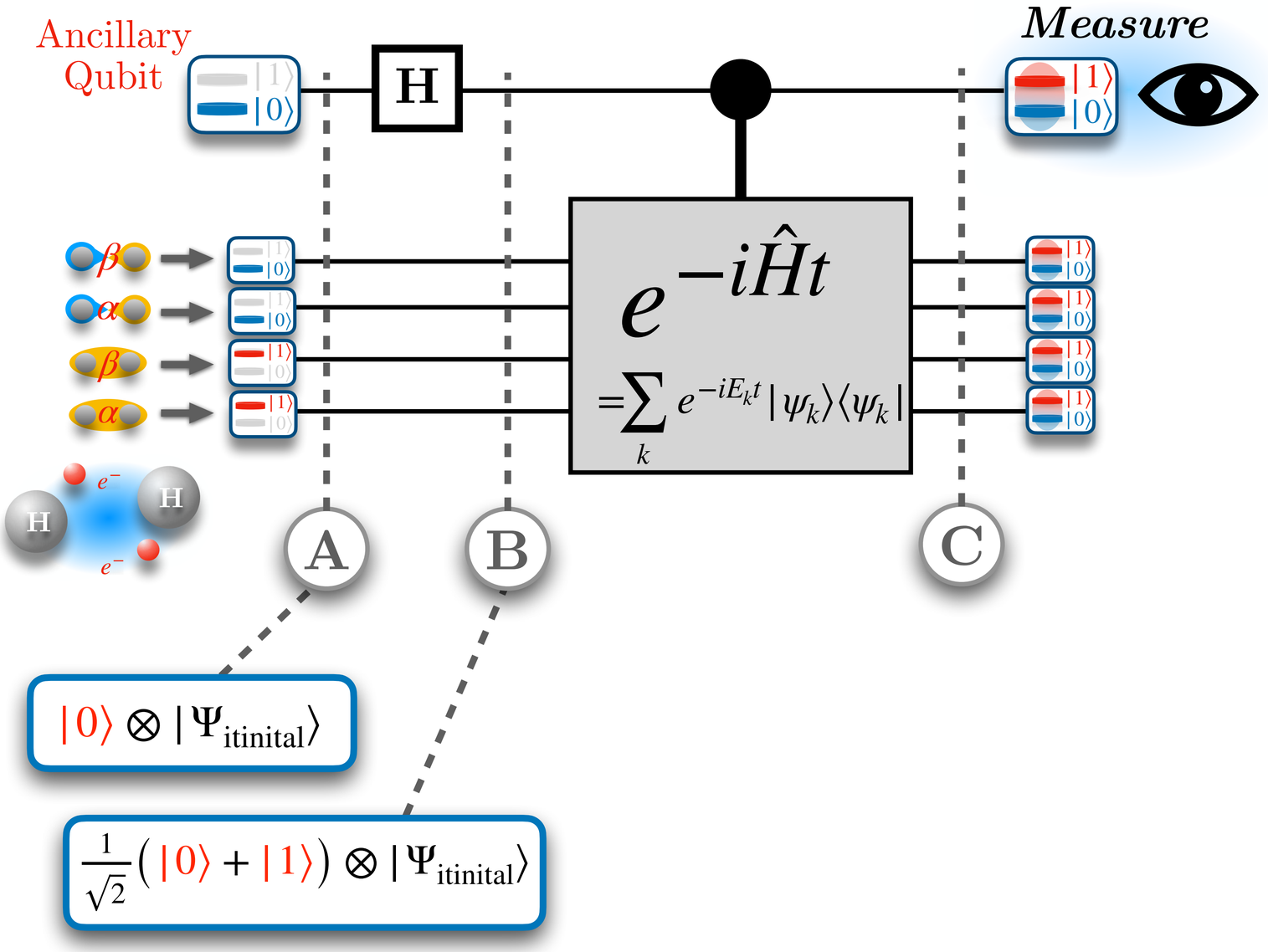

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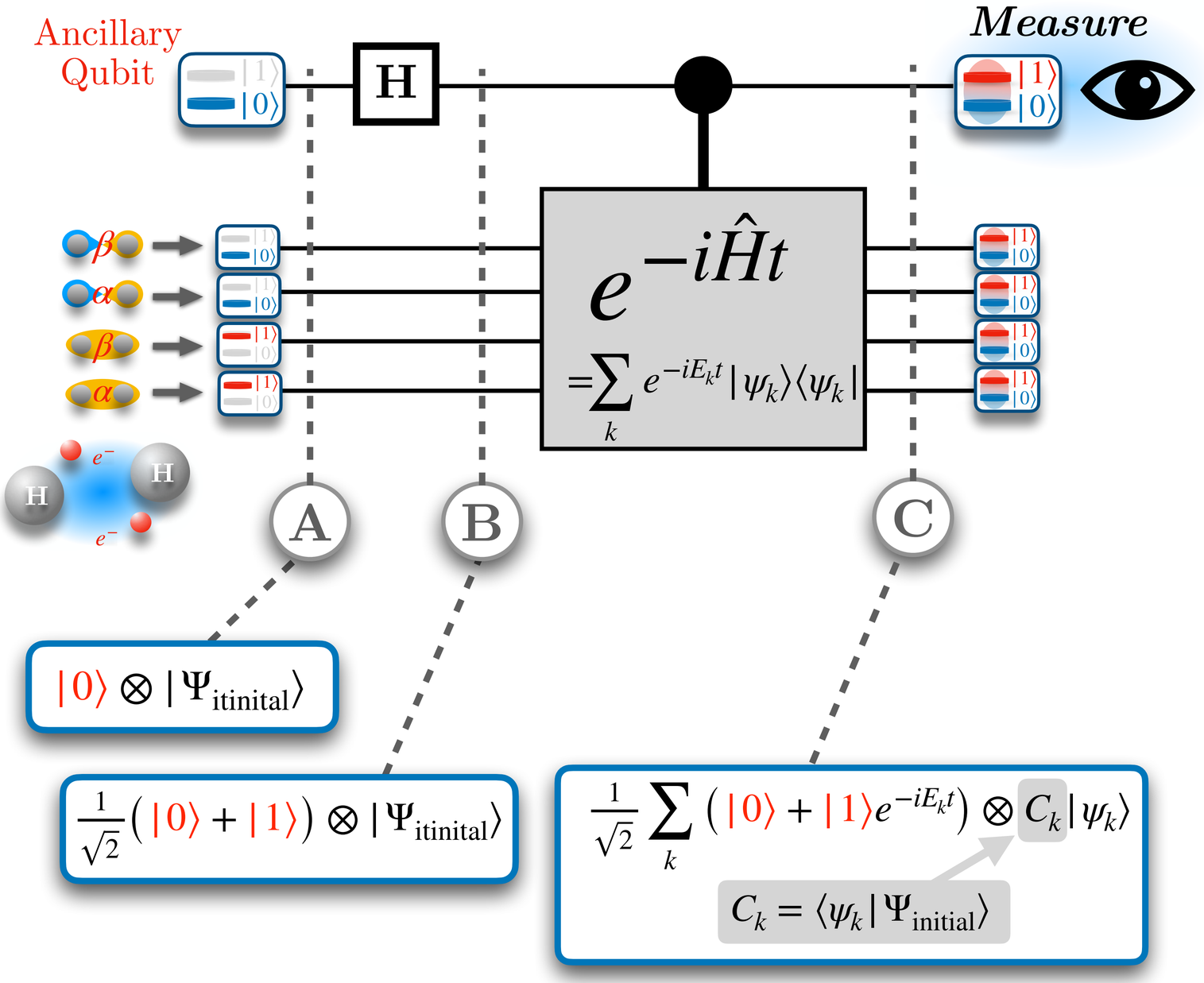

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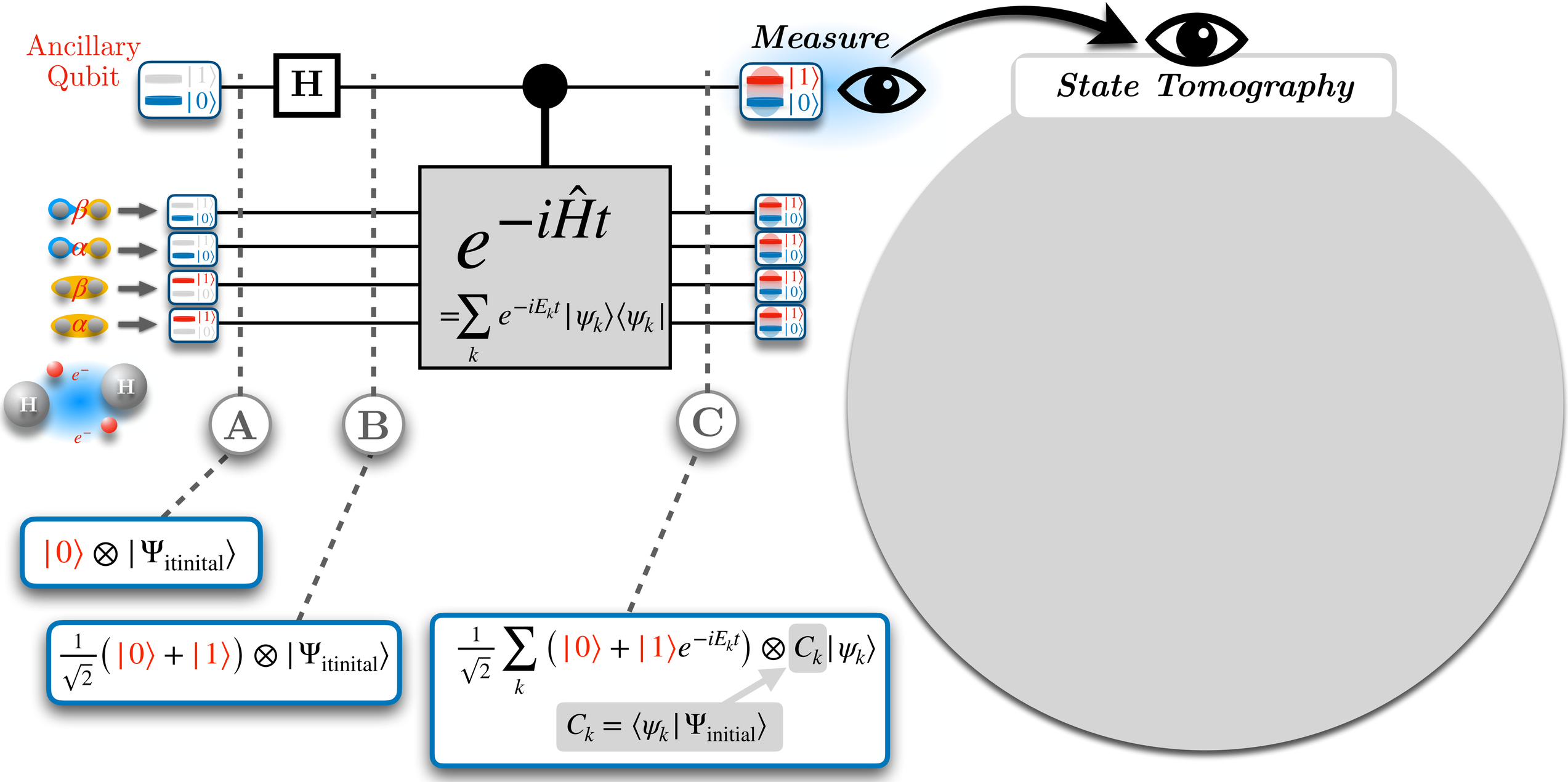

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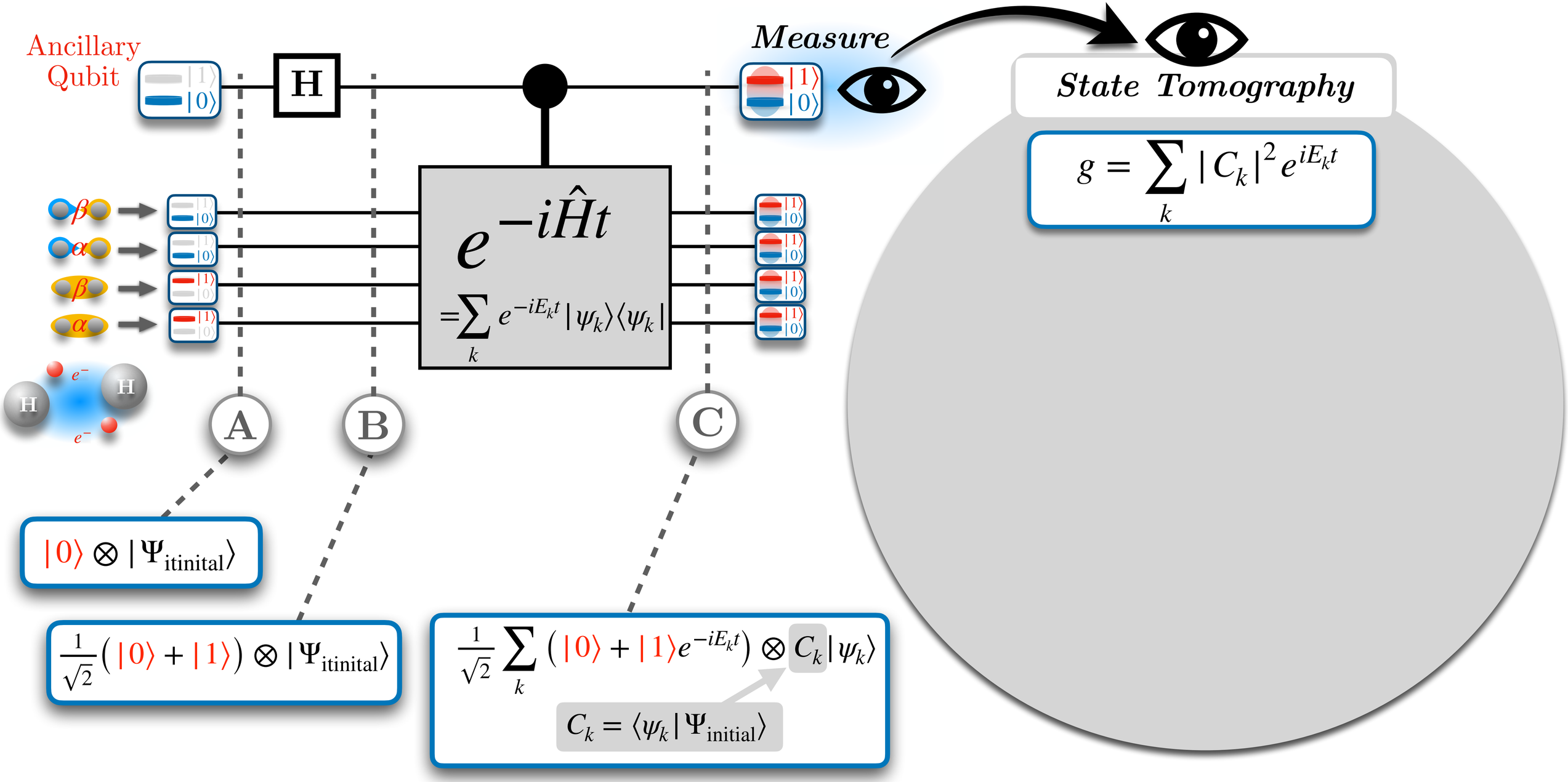

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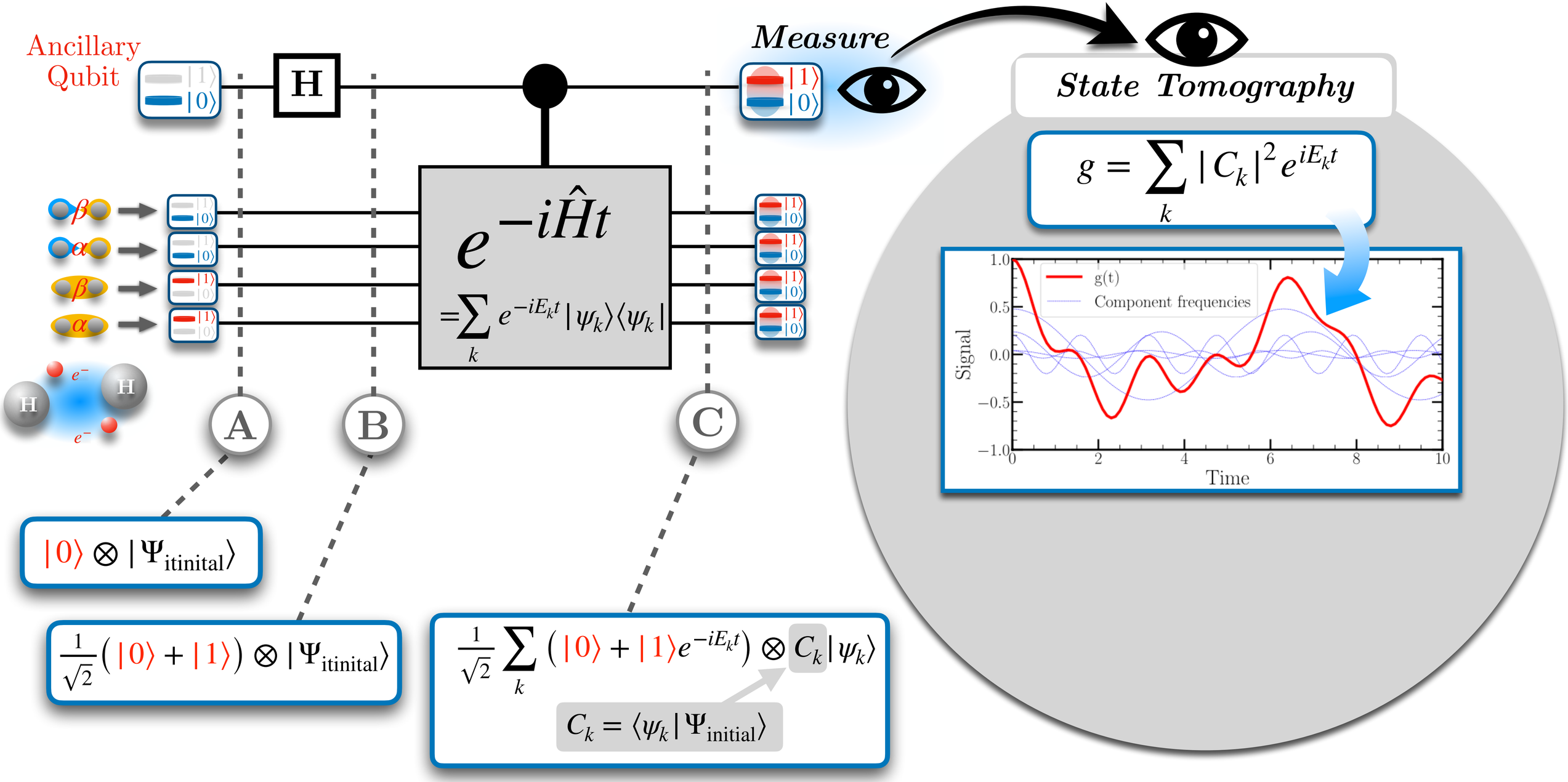

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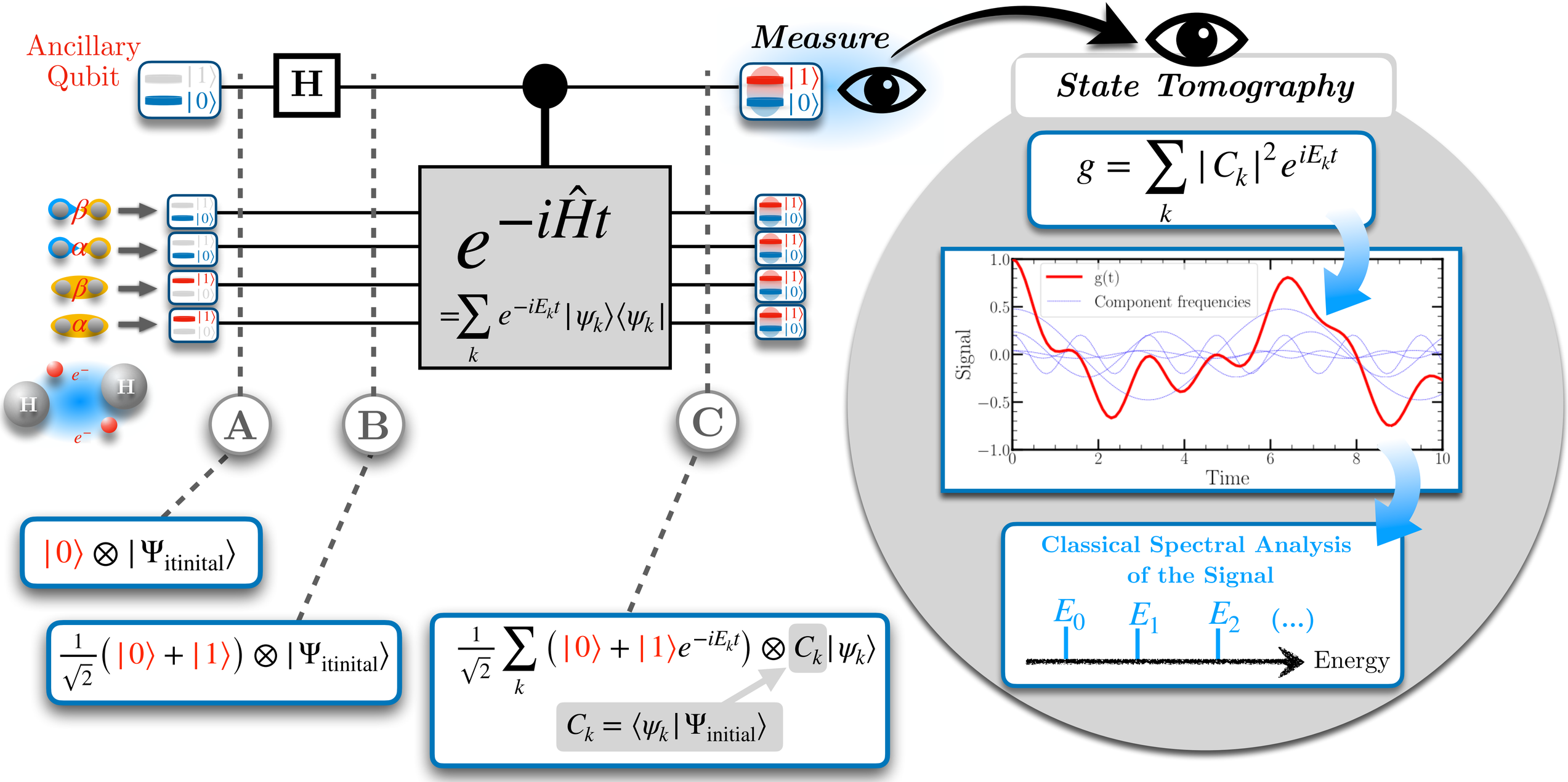

Conclusion

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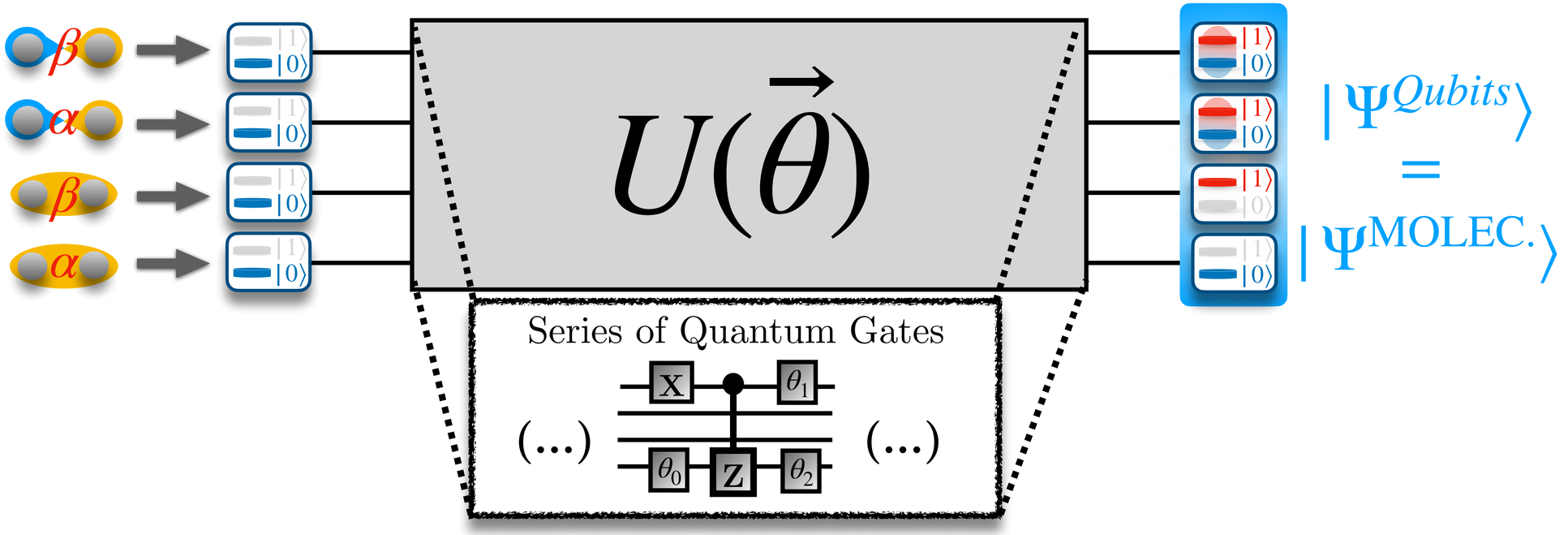

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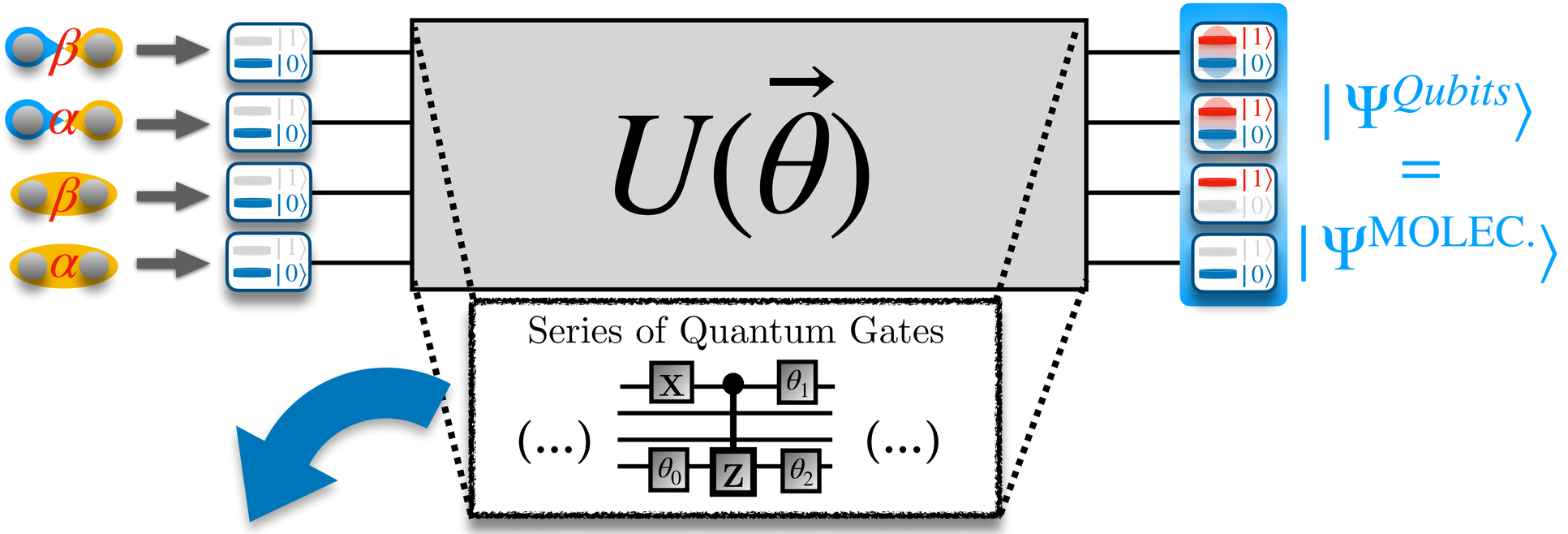
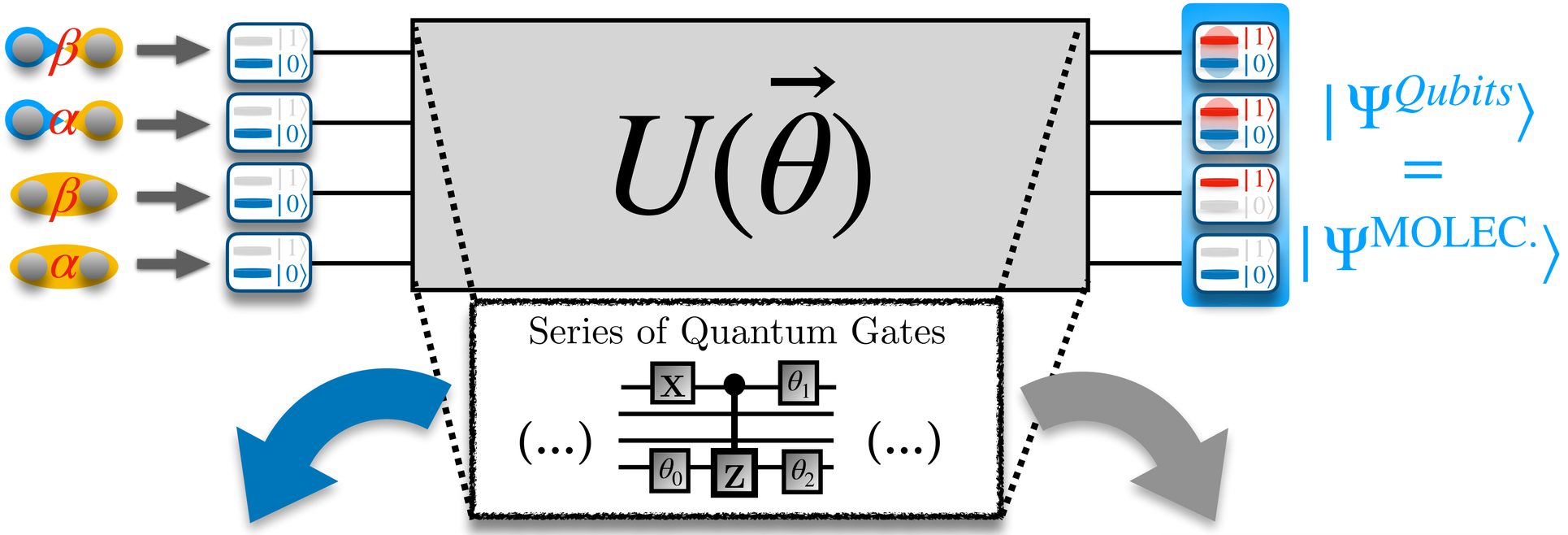


Near Term Era

Hardware limitations

Variational Quantum Eigensolver

Conclusion



Near Term Era

Hardware limitations

Variational Quantum Eigensolver

Fault Tolerant Era

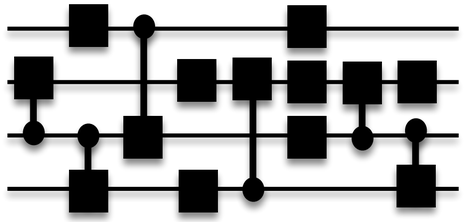
No Hardware limitations

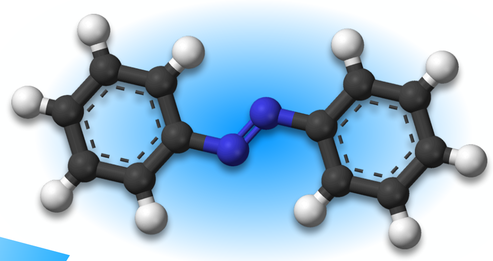
Quantum Phase Estimation

Announcement

PhD and Postdoc Opportunities coming soon in 2025 !!

Quantum Algorithm for Quantum Chemistry





$$H\Psi_k = E_k\Psi_k$$

⟨ LCQ | S ⟩
Laboratoire de Chimie Quantique de Strasbourg

ICGM
Institut Charles Gerhardt Montpellier

UMR5798
Laboratoire Ondes et Matière d'Aquitaine

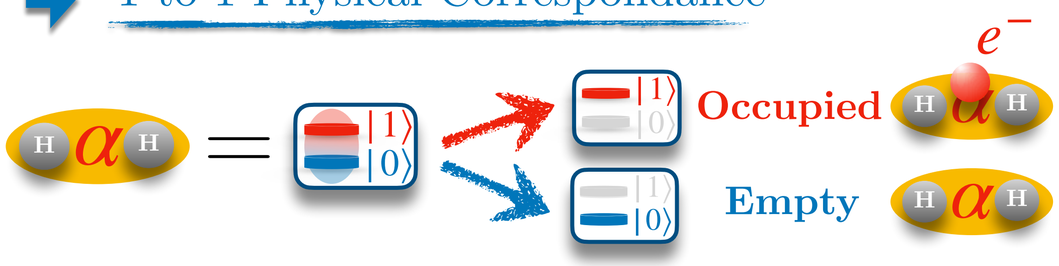
Contact us:

syalouz@unistra.fr or yalouzsaad@gmail.com

II) From quantum computing to chemistry

Jordan-Wigner Mapping

1-to-1 Physical Correspondance



Translation of Fermionic Algebra

Pauli Operators

$$X = |0\rangle\langle 1| + |1\rangle\langle 0|$$
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$$a_p^\dagger = \frac{X_p - iY_p}{2} \bigotimes_{q=0}^{p-1} Z_q$$

$|1_p\rangle\langle 0_p|$ — Create 1 electron in the spinorbital "p"

Fermionic anti-symmetry

$|\emptyset\rangle = |0000\rangle$ $\quad$ $|\Phi_{HF}\rangle = |1100\rangle$

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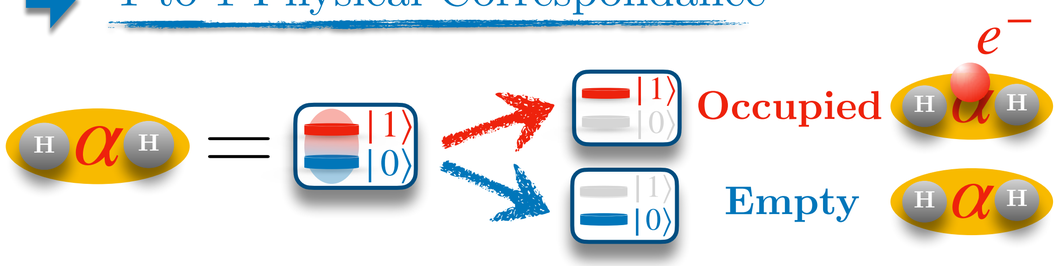

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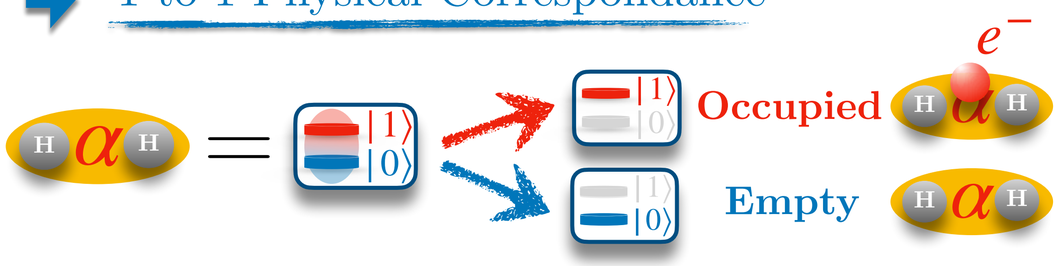

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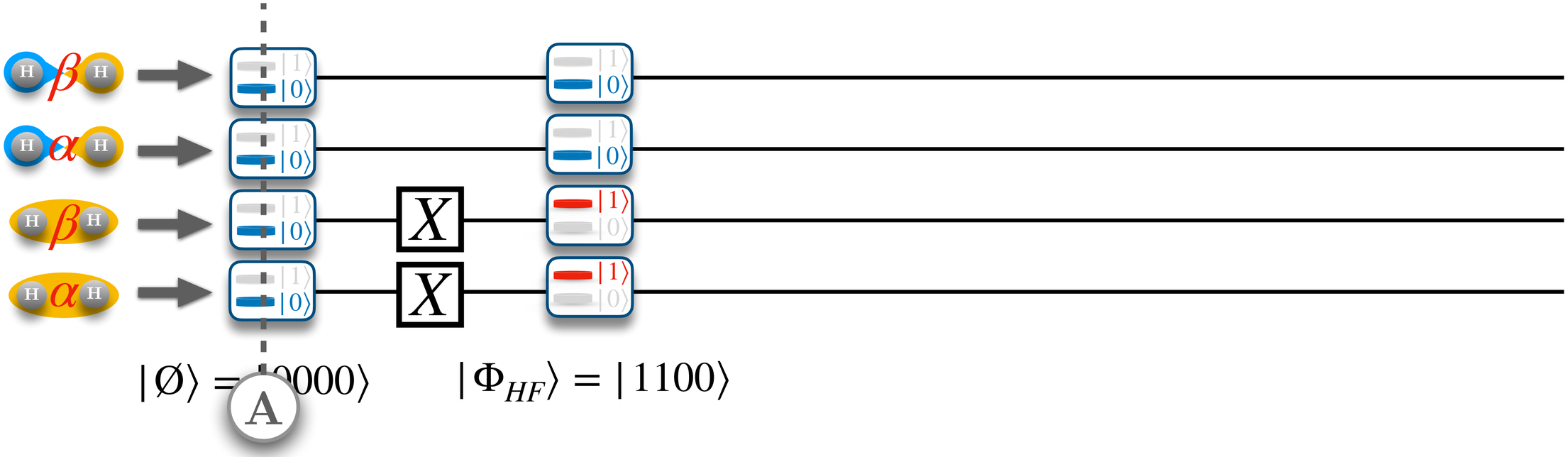

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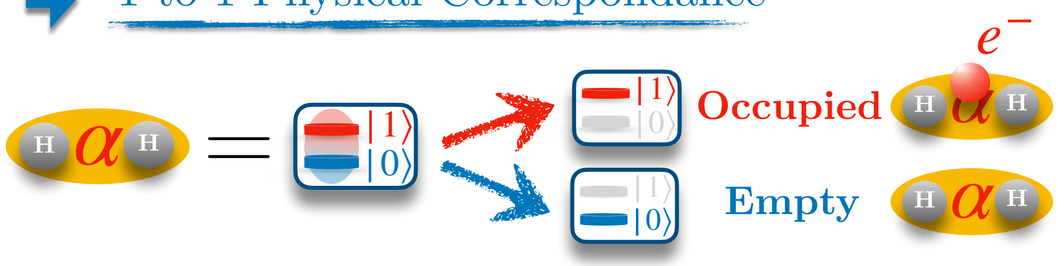

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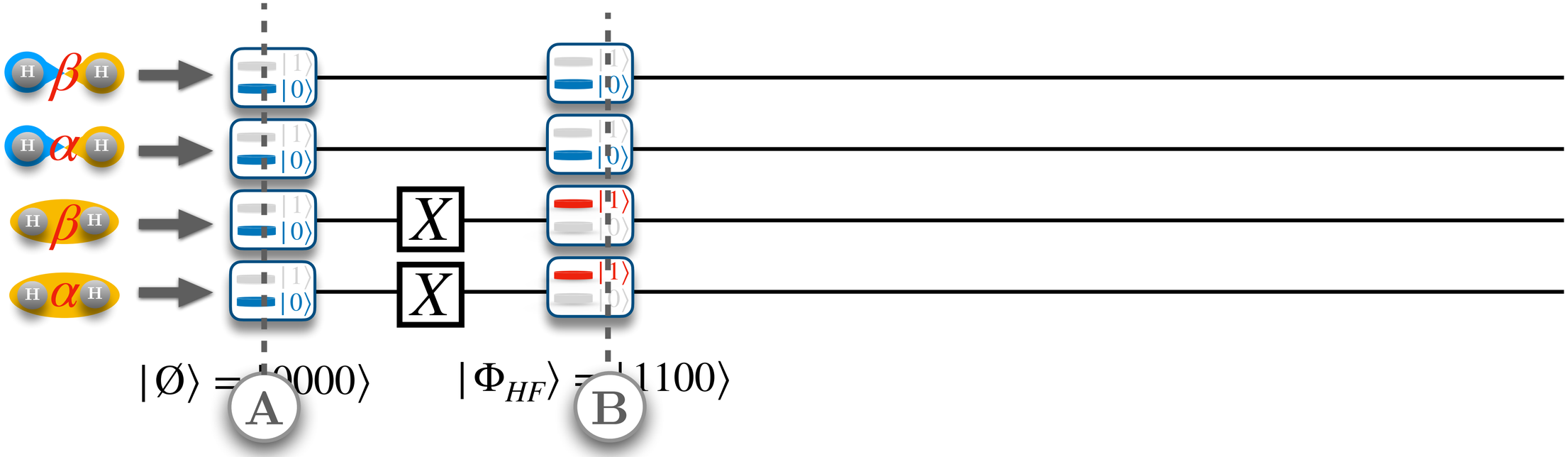

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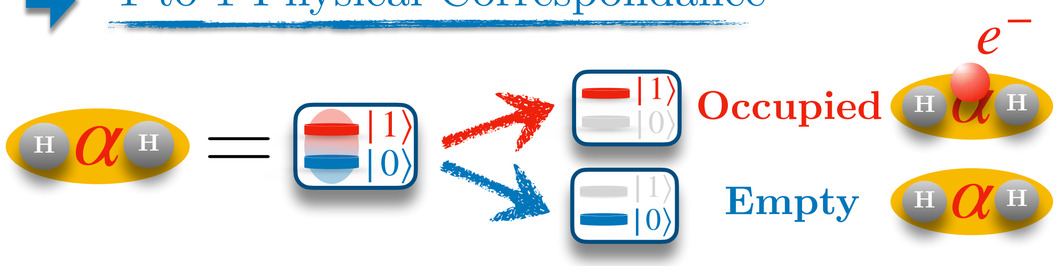
Jordan-Wigner Mapping

1-to-1 Physical Correspondance



Translation of Fermionic Algebra

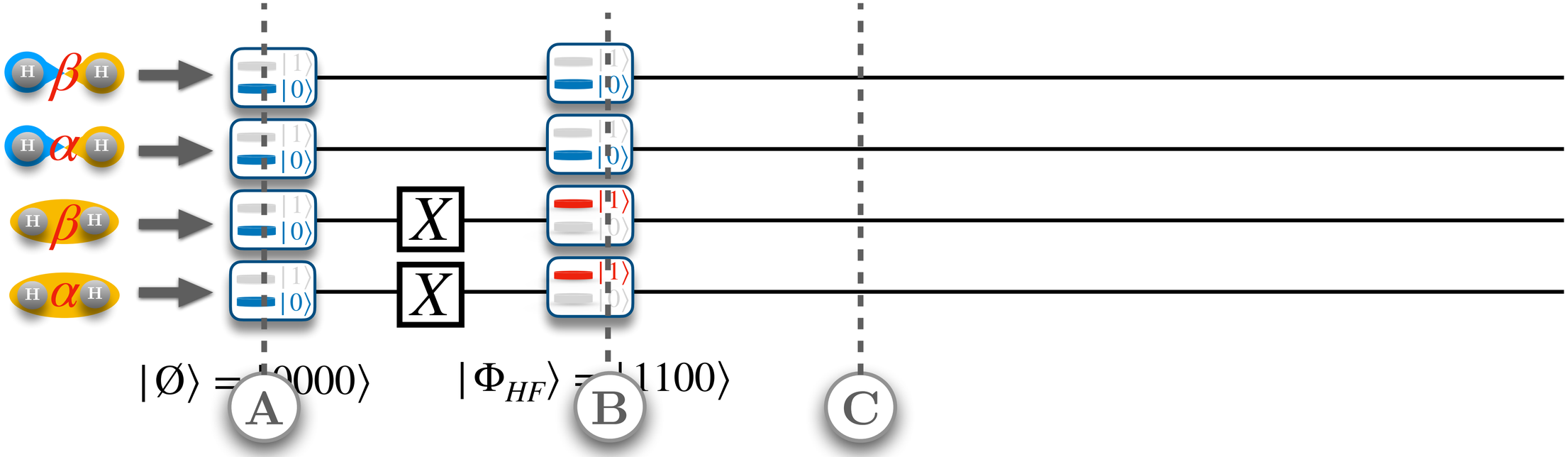
Pauli Operators

$$X = |0\rangle\langle 1| + |1\rangle\langle 0|$$
$$Y = -i|0\rangle\langle 1| + i|1\rangle\langle 0|$$
$$Z = |0\rangle\langle 0| - |1\rangle\langle 1|$$

$$a_p^\dagger = \frac{X_p - iY_p}{2} \bigotimes_{q=0}^{p-1} Z_q$$

$|1_p\rangle\langle 0_p|$ Create 1 electron in the spinorbital "p"

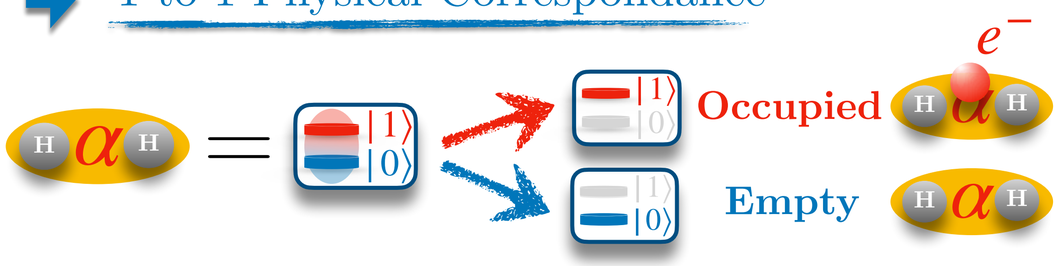
Fermionic anti-symmetry



II) From quantum computing to chemistry

Jordan-Wigner Mapping

1-to-1 Physical Correspondance



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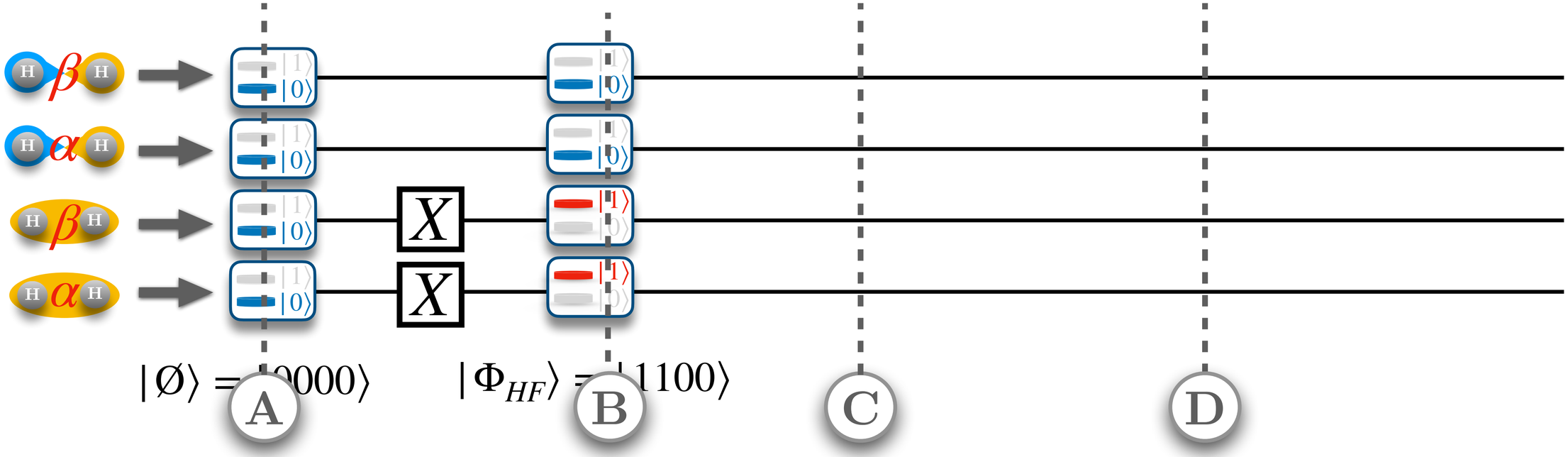
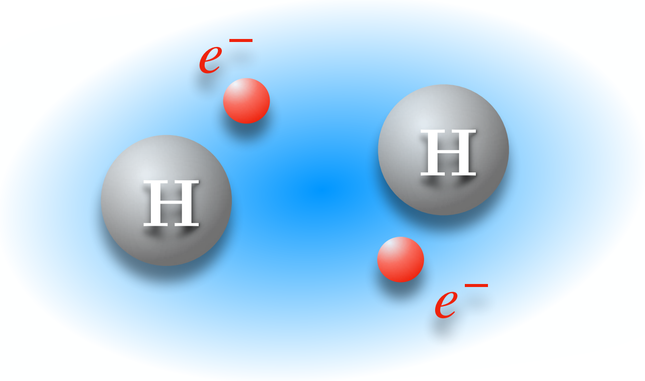


II) From quantum computing to chemistry

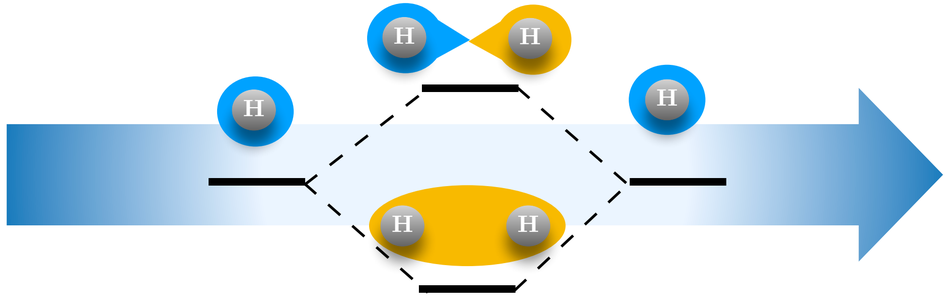
Electronic Structure Problem



$$H = \sum_{pq}^{N_o} h_{pq} \sum_{\sigma}^{\{\uparrow,\downarrow\}} \hat{a}^\dagger_{p\sigma}\hat{a}_{q\sigma} + \frac{1}{2}\sum_{pqrs}^{N_o} g_{pqrs} \sum_{\sigma,\tau}^{\{\uparrow,\downarrow\}} \hat{a}^\dagger_{p\sigma}\hat{a}^\dagger_{r\tau}\hat{a}_{s\tau}\hat{a}_{q\sigma} + E^{rep}_{nuc}$$

$$h_{pq} = \int \phi^*_p(\mathbf{r}_i)\left(-\frac{1}{2}\nabla^2_{\mathbf{r}_i} - \sum_{A=1}^{N_a}\frac{Z_A}{|\mathbf{r}_i - \mathbf{R}_A|}\right)\phi_q(\mathbf{r}_i)\mathrm{d}\mathbf{r}_i \qquad g_{pqrs} = \iint \phi^*_p(\mathbf{r}_i)\phi^*_r(\mathbf{r}_j)\frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}\phi_q(\mathbf{r}_i)\phi_s(\mathbf{r}_j)\mathrm{d}\mathbf{r}_i\,\mathrm{d}\mathbf{r}_j$$

Resolution: *Mean-Field Approach*



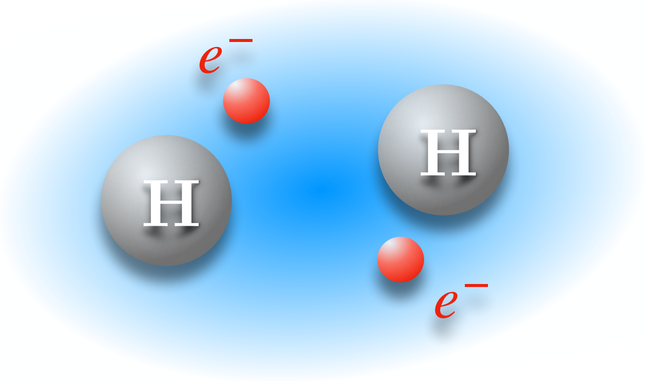
Single Configuration Approximation $|\Psi_0\rangle \approx |\mathrm{HF}\rangle$

Hartree-Fock calculation

$$|\phi_p\rangle = \sum_{\mu} C_{\mu p}\,|\mathrm{AO}_\mu\rangle$$

II) From quantum computing to chemistry

Electronic Structure Problem



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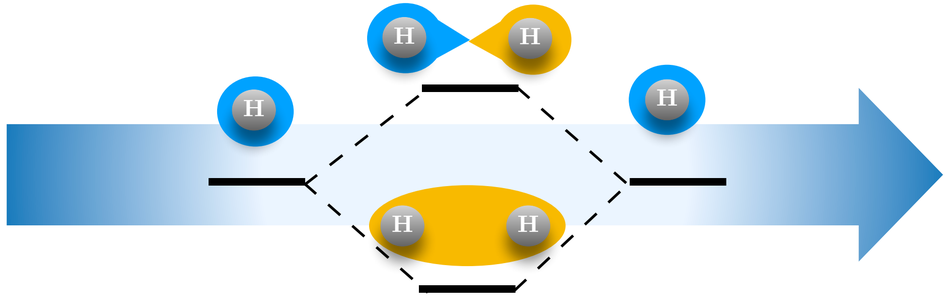

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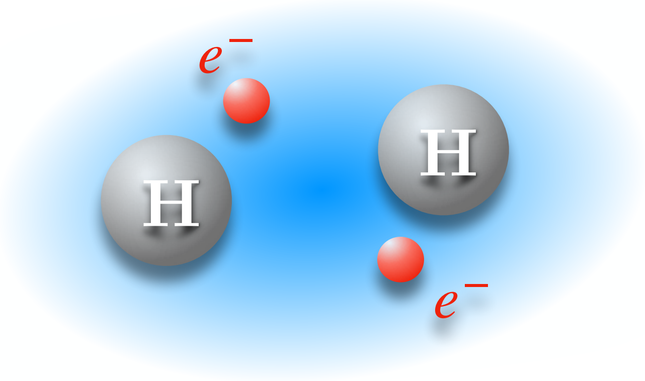
II) From quantum computing to chemistry

Electronic Structure Problem



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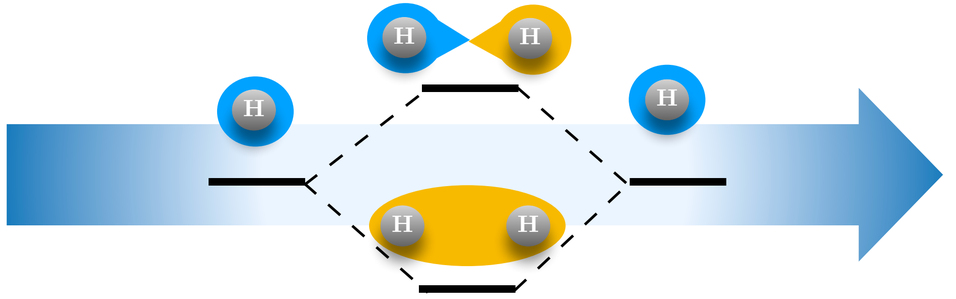

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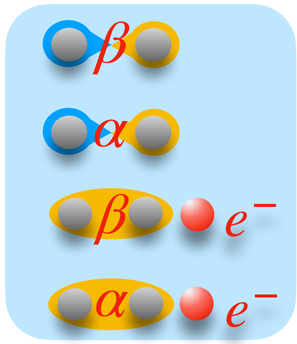
Spin-Orbitals

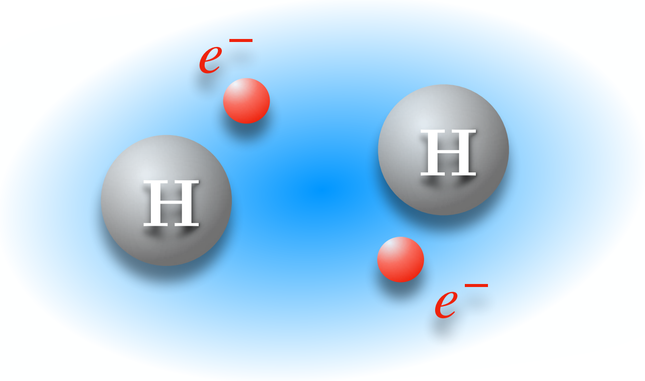


0
0
1
1

$|\mathrm{HF}\rangle = |1100\rangle$

II) From quantum computing to chemistry

Electronic Structure Problem



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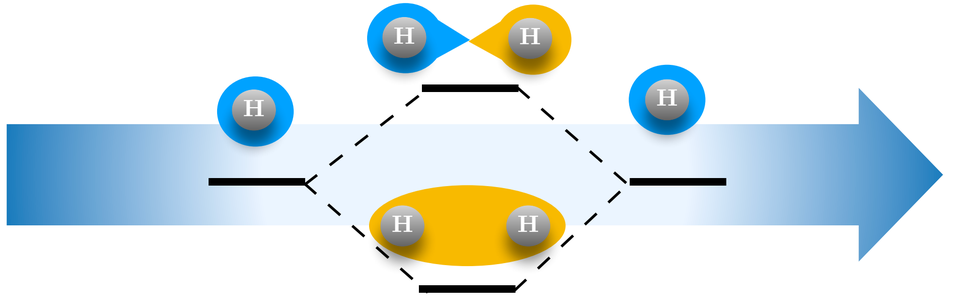

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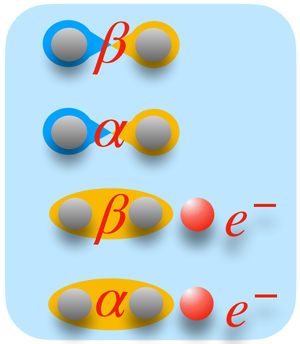

0
0
1
1

$|\mathrm{HF}\rangle = |1100\rangle$