

# Quantum Chemistry on Quantum Computers

## #6 Adiabatic Quantum Algorithms

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# Adiabatic theorem

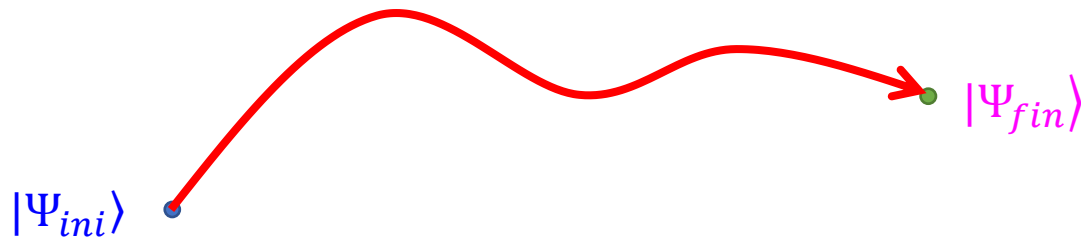
Assume that the system is in the eigenstate of a time-dependent Hamiltonian  $H(t)$  at  $t = 0$ .

The time evolution is governed by the Schrödinger equation:

$$i \frac{\partial |\Psi(t)\rangle}{\partial t} = H(t) |\Psi(t)\rangle$$

If the variation of Hamiltonian  $H(t)$  is sufficiently slow, the system is approximately in the eigenstate of  $H(t)$  at  $t > 0$ .

$$H(t) = (1 - s(t))H_{ini} + s(t)H_{fin}$$



$$H_{ini} |\Psi_{ini}\rangle = E_{ini} |\Psi_{ini}\rangle$$

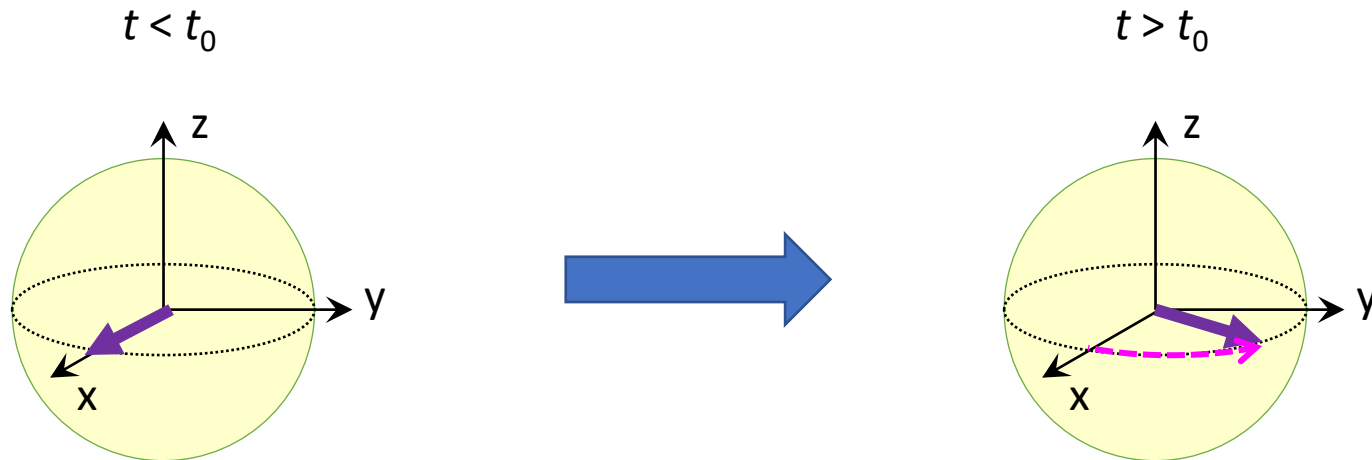
# The simplest example: One qubit system

$$H_{ini} = -\frac{\omega}{2}X \quad \text{Ground state of } H_{ini} \text{ is } |\Psi_0^{(ini)}\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \text{ with } E_0^{(ini)} = -\frac{\omega}{2}$$

$$H_{fin} = -\frac{\omega}{2}Z \quad \text{Ground state of } H_{fin} \text{ is } |\Psi_0^{(fin)}\rangle = |0\rangle \text{ with } E_0^{(fin)} = -\frac{\omega}{2}$$

At time  $t = 0$ , the system is in the ground state of  $H_{ini}$ .

What happens if the Hamiltonian suddenly changes from  $H_{ini}$  to  $H_{fin}$  at time  $t = t_0$ ?



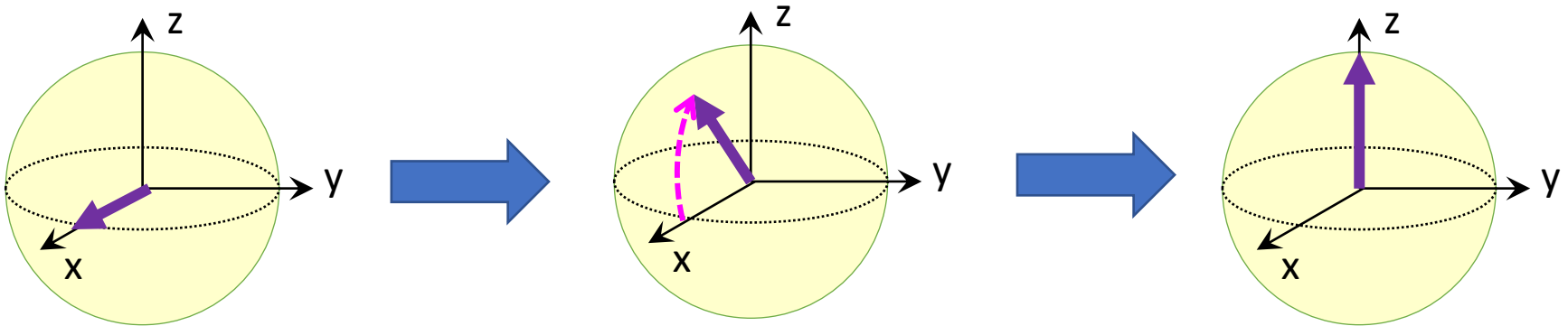
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At time  $t = 0$ , the system is in the ground state of  $H_{ini}$ .

What happens if the Hamiltonian slowly changes from  $H_{ini}$  to  $H_{fin}$ ?



# Adiabatic quantum computing

Quantum Computation by Adiabatic Evolution

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MIT CTP # 2936 [quant-ph/0001106](#)

*“The evolution of the quantum state is governed by a **time-dependent Hamiltonian** that interpolates between an initial Hamiltonian, whose ground state is easy to construct, and a final Hamiltonian, whose ground state encodes the satisfying assignment.”*

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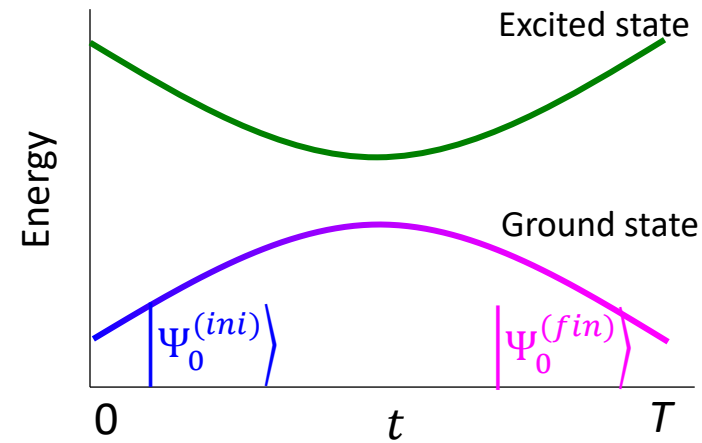
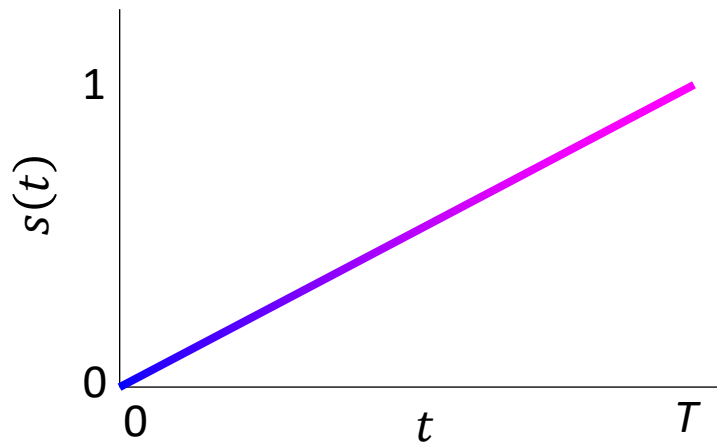
## Adiabatic Quantum Computation Is Equivalent to Standard Quantum Computation\*

*“Adiabatic computational model and the conventional quantum computation model are polynomially equivalent.”*

Dorit Aharonov†  
Wim van Dam†  
Julia Kempe§  
Zeph Landau¶  
Seth Lloyd||  
Oded Regev§

# Adiabatic quantum computing

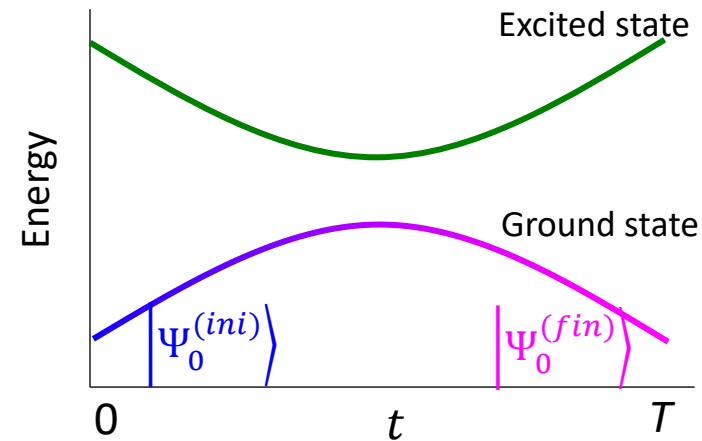
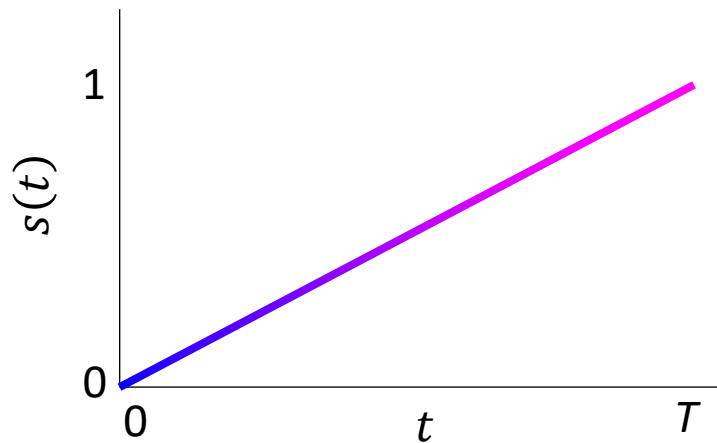
$$H(t) = (1 - s(t))H_{ini} + s(t)H_{fin}$$



- $H_{fin}$ : Hamiltonian of the problem we want to solve.
- $H_{ini}$ : Initial Hamiltonian of which ground state can be prepared easily.
- $[H_{ini}, H_{fin}] \neq 0$ . If two Hamiltonians commute, they have simultaneous eigenfunctions.
- Start from  $|\Psi_0^{(ini)}\rangle$ . Change the schedule function  $s(t) = t/T$  slowly.
- If the variation of the Hamiltonian  $H(t)$  is slow enough, we can obtain the ground state of  $H_{fin}$  at time  $t = T$ .

# Adiabatic quantum computing

$$H(t) = (1 - s(t))H_{ini} + s(t)H_{fin}$$



$$\max_{s \in [0,1]} \frac{|\langle \Psi_j(s) | \partial_s H(s) | \Psi_0(s) \rangle|}{|E_j(s) - E_0(s)|^2} \ll T$$

\* This equation is approximate in the sense that it does not result in strict inequality.

Roughly speaking,  $T$  must be lengthened inversely proportional to the **square of the energy gap** between the ground and the excited states.

## An example: Factorization of 21

$$21 = x \times y \quad \begin{aligned} x &= (I_0 - Z_0) + 1 \\ y &= 2(I_1 - Z_1) + (I_2 - Z_2) + 1 \end{aligned}$$

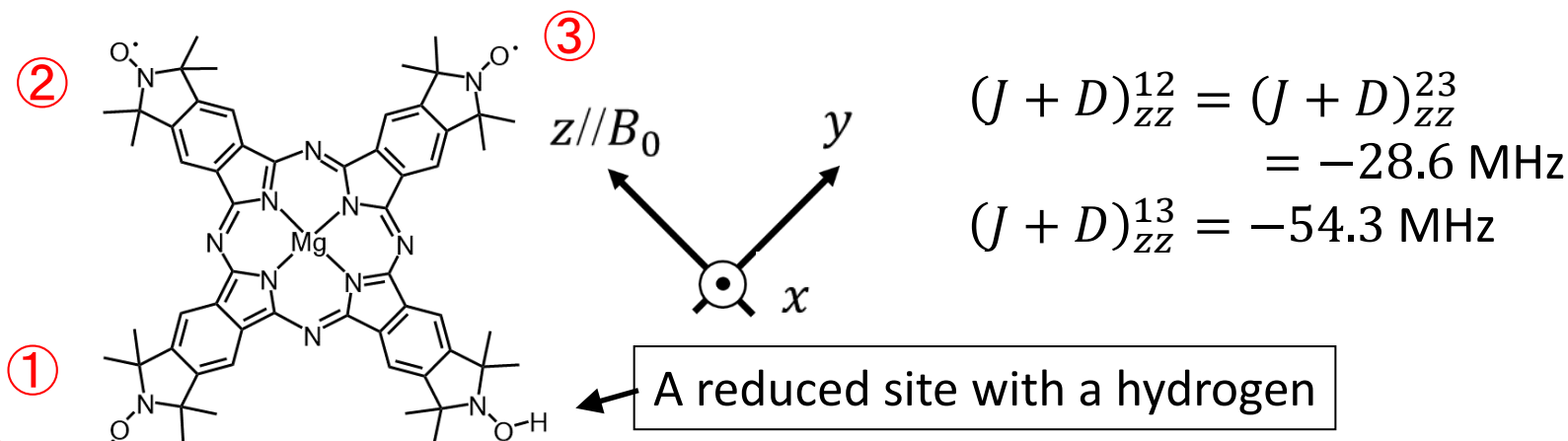
$$H_{fin} = (21 - xy)^2$$

$$\approx 84Z_0 + 88Z_1 + 44Z_2 - 20Z_0Z_1 - 10Z_0Z_2 - 20Z_1Z_2 - 16Z_0Z_1Z_2$$

$$H_{ini} = 30X_0 + 30X_1 + 30X_2$$

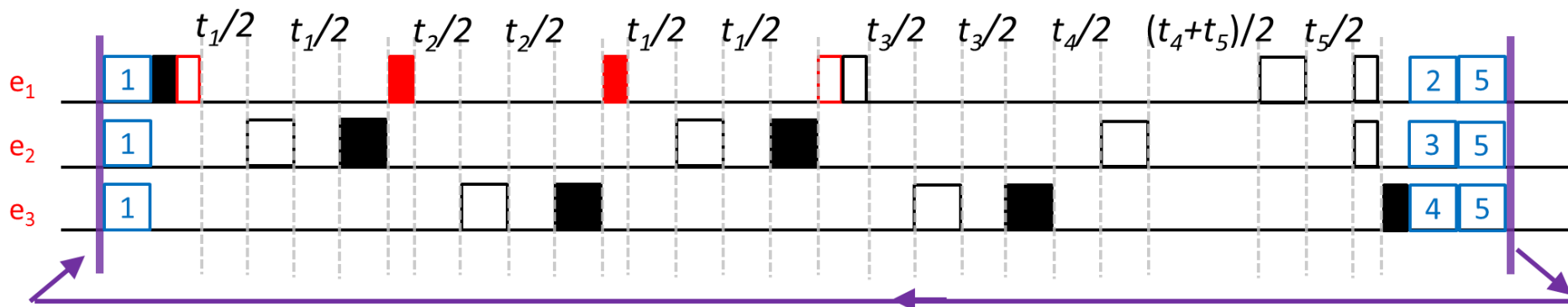
This problem can be implemented by using 3 qubit systems:

### 3e system (phthalocyanine) system



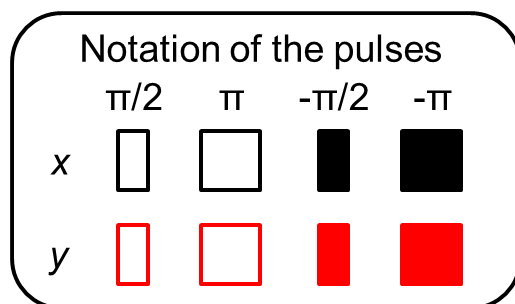


# An example: Factorization of 21



Repeat five times (changing  $n = 1$  to 5)

$$\ln (J + D)_{zz}^{12}, (J + D)_{zz}^{23}, (J + D)_{zz}^{13} < 0$$



- 1 : x-axis,  $30(1-S_n)\tau$
- 2 : y-axis,  $168S_n\tau$
- 3 : y-axis,  $176S_n\tau$
- 4 : y-axis,  $88S_n\tau$
- 5 : x-axis,  $30(1-S_n)\tau + \pi/2$

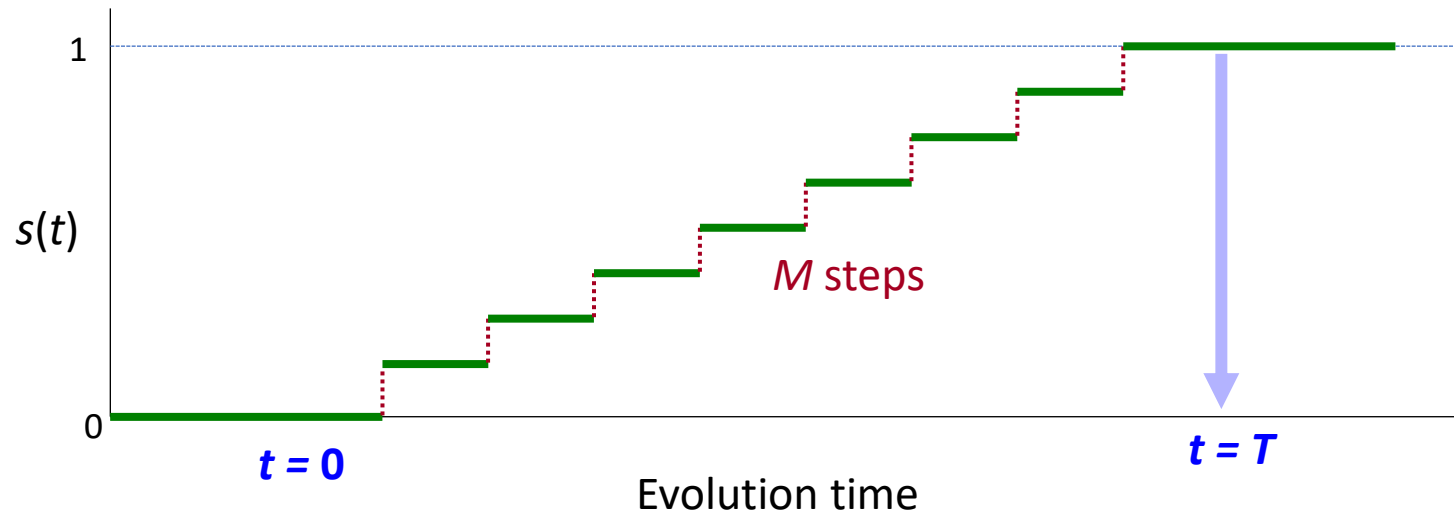
Analytical operation time in the 3e system

$$a_n = 0.028\hbar(n/5)^2$$

$t_1 / s$	$t_2 / s$	$t_3 / s$	$t_4 / s$	$t_5 / s$
$-\pi\hbar/(D_{zz}+J)^{13}$	$-64a_n/(D_{zz}+J)^{12}$	$-80a_n/(D_{zz}+J)^{12}$	$-40a_n/(D_{zz}+J)^{13}$	$-80a_n/(D_{zz}+J)^{23}$

# Adiabatic state preparation

$$H(t) = (1 - s(t))H_{\text{HF}} + s(t)H_{\text{Full-CI}}$$

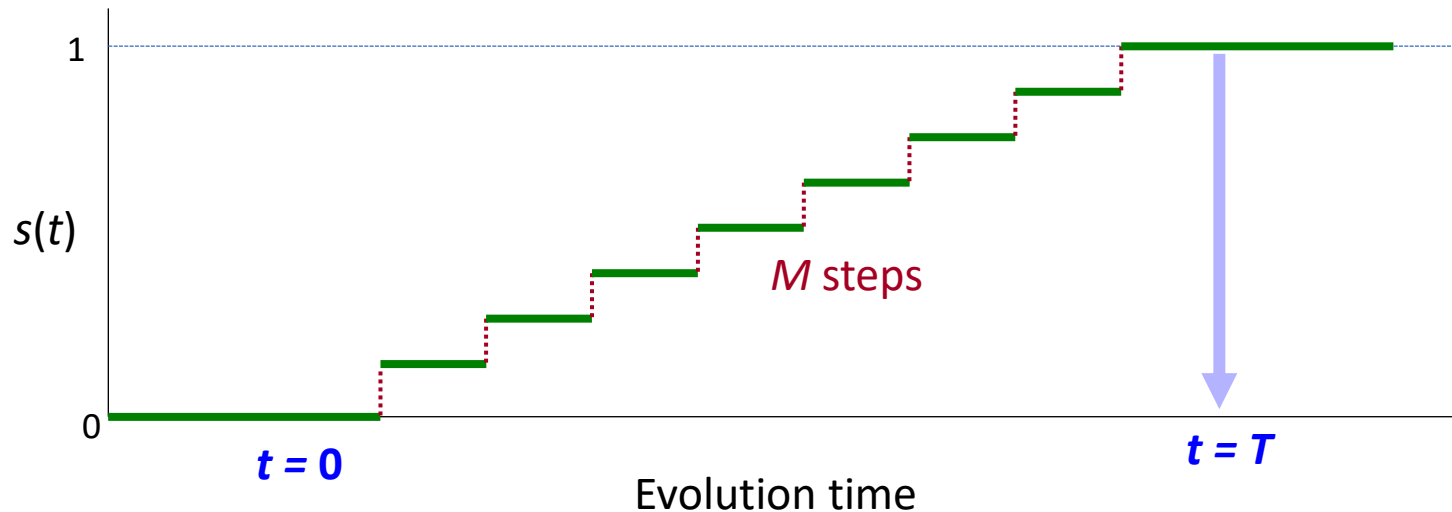


```
time_for_each_step = total_evolution_time/M
```

```
for m in range(M+1):  
    s = m/M  
    hamiltonian = (1-s)*h_hf + s*h_full_ci  
    time_evolution_operator = exp(-i*hamiltonian*time_for_each_step)  
    |asp_next> = time_evolution_operator * |asp_current>
```

# Adiabatic state preparation

$$H(t) = (1 - s(t))H_{\text{HF}} + s(t)H_{\text{Full-CI}}$$



## Types and sources of errors

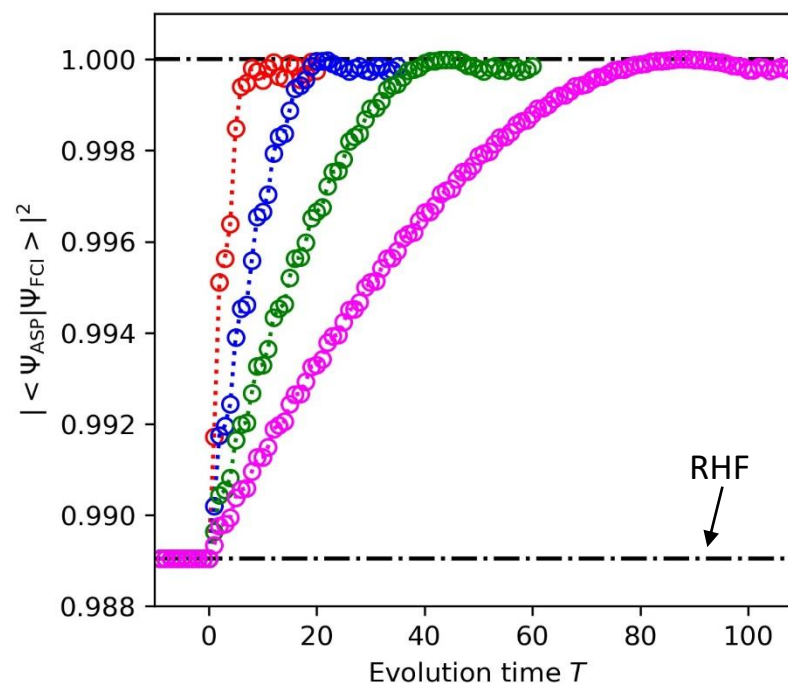
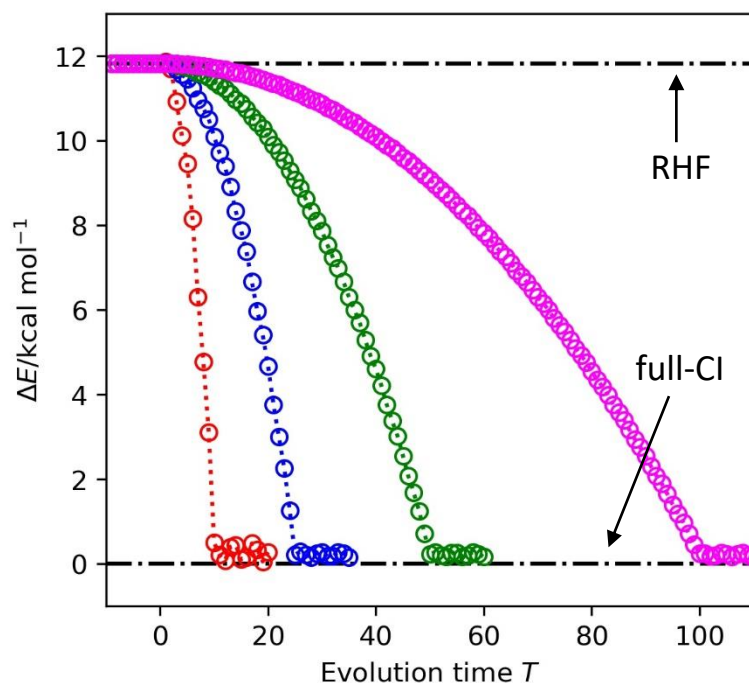
- 1) **Non-adiabaticity error** ...  $T$  is too short to follow the adiabatic path.
- 2) **Discretization error** ... Step number  $M$  is too small. Hamiltonian of the  $(m + 1)$ -th step is too different from that of the  $m$ -th.
- 3) **Trotter decomposition error** ...  $T/M$  is too long.
- 4) Decoherence, incomplete operations

# ASP examples: Evolution time dependence

$\text{H}_2$  molecule at  $R(\text{H-H}) = 0.7 \text{ \AA}$ , STO-3G basis set

Evolution time  $T = 10, 25, 50$ , and  $100$

Time for single Trotter step = 1.0



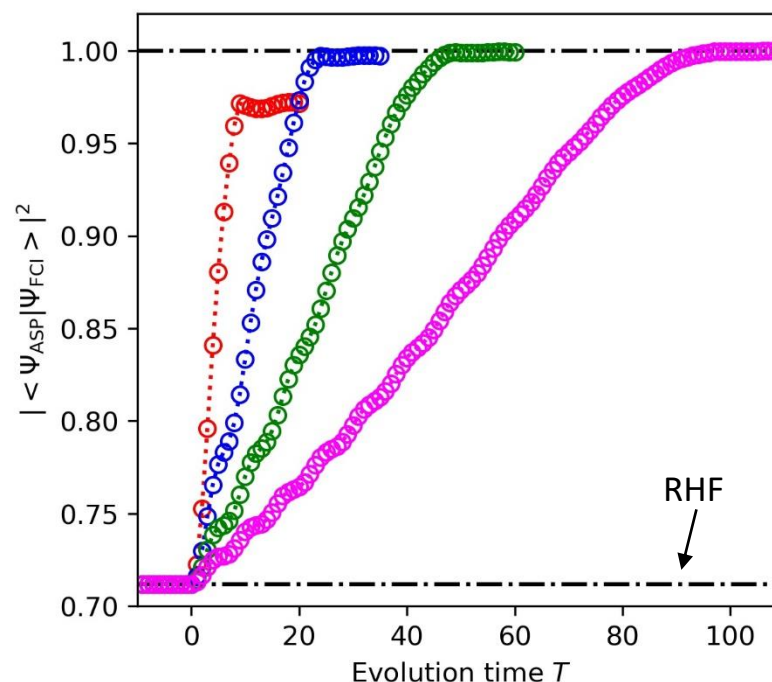
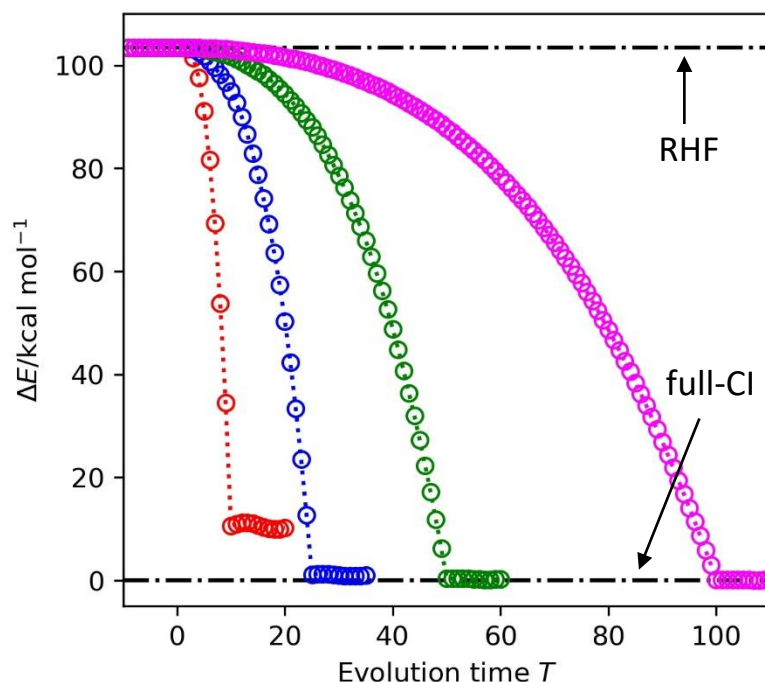
At  $R(\text{H-H}) = 0.7 \text{ \AA}$ , RHF wave function is a good approximation of the ground state. ASP converges quickly even for shorter evolution time.

# ASP examples: Evolution time dependence

$\text{H}_2$  molecule at  $R(\text{H-H}) = 2.0 \text{ \AA}$ , STO-3G basis set

Evolution time  $T = 10, 25, 50$ , and  $100$

Time for single Trotter step = 1.0



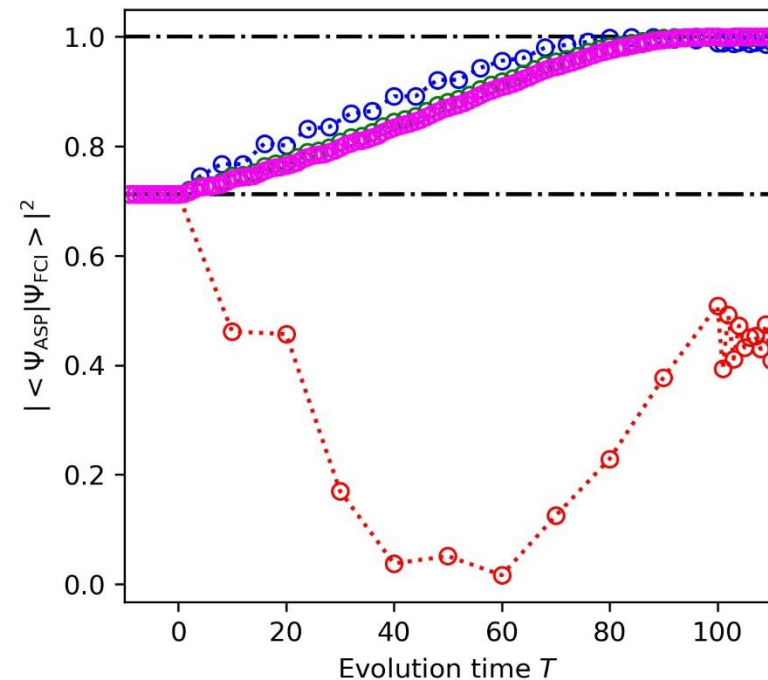
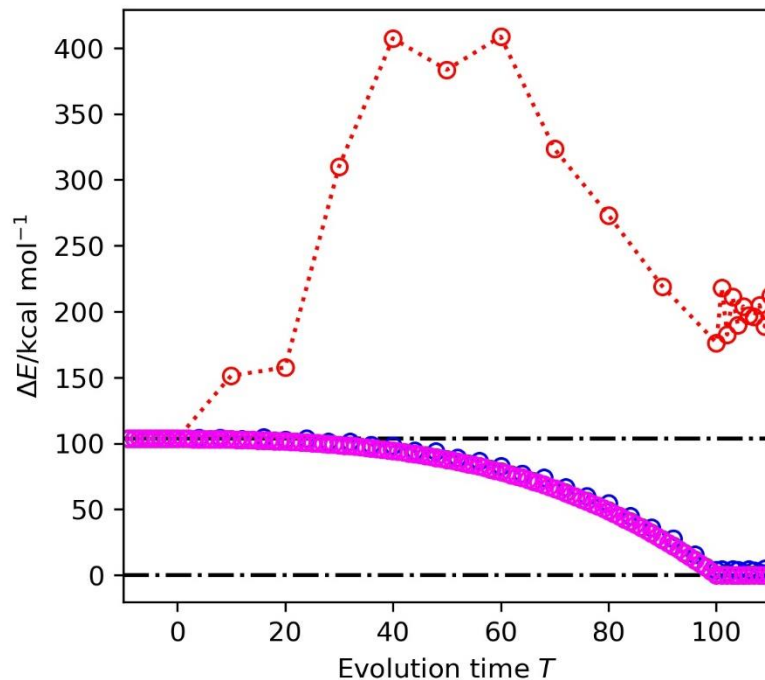
At  $R(\text{H-H}) = 2.0 \text{ \AA}$ , RHF wave function is not a good approximation of the ground state. The deviation from full-CI becomes larger for shorter evolution time  $T$ .

# ASP examples: Trotter slice dependence

$\text{H}_2$  molecule at  $R(\text{H-H}) = 2.0 \text{ \AA}$ , STO-3G basis set

Evolution time  $T = 100$  (Fixed)

Time for single Trotter step = 10, 4, 2, 1



Clearly, ASP fails if the evolution time for each step is short.

# ASP with different initial Hamiltonian

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## Quantum Zeno approach for molecular energies with maximum commuting initial Hamiltonians

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<sup>2</sup>*C. N. Yang Institute for Theoretical Physics, State University of New York at Stony Brook, Stony Brook, New York 11794-3840, USA*

<sup>3</sup>*Institute for Advanced Computational Science, State University of New York at Stony Brook, Stony Brook, New York 11794-5250, USA*

Find the (approximate) maximal set of the Pauli operators by a greedy algorithm of which all Pauli operators in the set are commute to each other.

(Usually Pauli strings containing only Pauli-Z and  $I$  (identity) operators)



Use maximum commuting (MC) Hamiltonian as the initial Hamiltonian.

# Advantages and disadvantages of ASP

ASP is a technique to prepare correlated wave functions.

To calculate total energy or molecular properties, we have to perform QPE (for eigenvalues) or statistical sampling of measurement outcomes (for expectation values).

## Advantages

- We do not have to know the electronic structures of the target system in advance of the computation in detail.
- Polynomial computational cost against the system size, if the energy gap does not depends on the system size.

## Disadvantages

- If the energy gap between ground and excited states becomes exponentially small, we have to simulate exponentially long time evolution.
- Potentially unsuitable for strongly correlated systems.



# D-Wave quantum annealing machines



Photos and snapshots taken from D-Wave website:

<https://www.dwavesys.com/solutions-and-products/systems/>

$H_{ini}$ : Transverse magnetic field (Pauli-X only)

$H_{fin}$ : Ising Hamiltonian (Pauli-Z only)

	2000Q	Advantage	Advantage performance update
<b>Performance</b>			
Better Solutions (Satisfiability problems)	--	3x more often than 2000Q	23x more often than 2000Q
Time-To-Solution (3D lattice problems)	--	10x faster than 2000Q	2x faster than Advantage
<b>Annealing Quantum Processor Design</b>			
Qubits	2000+	5000+	5000+
Couplers	6000+	35000+	35000+
Couplers Per Qubit	6	15	15
<b>Topology</b>			
Graph	Chimera	Pegasus	Pegasus
Graph Size	C16	P16	P16
Connectivity	Degree 6	Degree 15	Degree 15
Lattice	8x8x8	15x15x12	15x15x12
Chain Length (for problem size n=64)	17	7	6

# Quantum chemical calculations on quantum annealer


THE JOURNAL OF  
PHYSICAL CHEMISTRY B

*J. Phys. Chem. B* **2018**, 122, 3384–3395.

Article

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## Electronic Structure Calculations and the Ising Hamiltonian

Rongxin Xia,<sup>†</sup> Teng Bian,<sup>†</sup> and Sabre Kais<sup>\*,†,§</sup> 

<sup>†</sup>Department of Physics, Purdue University, West Lafayette, Indiana 47907, United States

<sup>‡</sup>Department of Chemistry and Birck Nanotechnology Center, Purdue University, West Lafayette, Indiana 47907, United States

<sup>§</sup>Santa Fe Institute, 1399 Hyde Park Road, Santa Fe, New Mexico 87501, United States

$$H = \sum_{pq} h_{pq} a_p^\dagger a_q + \frac{1}{2} \sum_{pqrs} h_{pqrs} a_p^\dagger a_q^\dagger a_s a_r \quad \longrightarrow \quad H_q = \sum_k w_k P_k$$

*n*-qubit *k*-local Hamiltonian consisting of Pauli-X, Y, and Z operators



***rn*-qubit 2-local Hamiltonian  $H_q'$  consisting of only Pauli-Z operators**



*n*-qubit 2-local Hamiltonian consisting of Pauli-X, Y, and Z operators

# Quantum chemical calculations on quantum annealer


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$$\left\{ \begin{array}{l} X_j \rightarrow \frac{1 - Z_{jk}Z_{jl}}{2} S'(k)S'(l) \\ Y_j \rightarrow i \frac{Z_{jl} - Z_{jk}}{2} S'(k)S'(l) \\ Z_j \rightarrow i \frac{Z_{jk} + Z_{jl}}{2} S'(k)S'(l) \\ I_j \rightarrow \frac{1 + Z_{jk}Z_{jl}}{2} S'(k)S'(l) \end{array} \right.$$

$Z_{jk}$  is a Pauli-Z operator acting on the  $k$ -th ancillary qubit of the  $j$ -th original qubit.

The function  $S'(k)$  takes care of the sign of the state in the original Hilbert space.

# Quantum chemical calculations on quantum annealer

arXiv:1811.05256

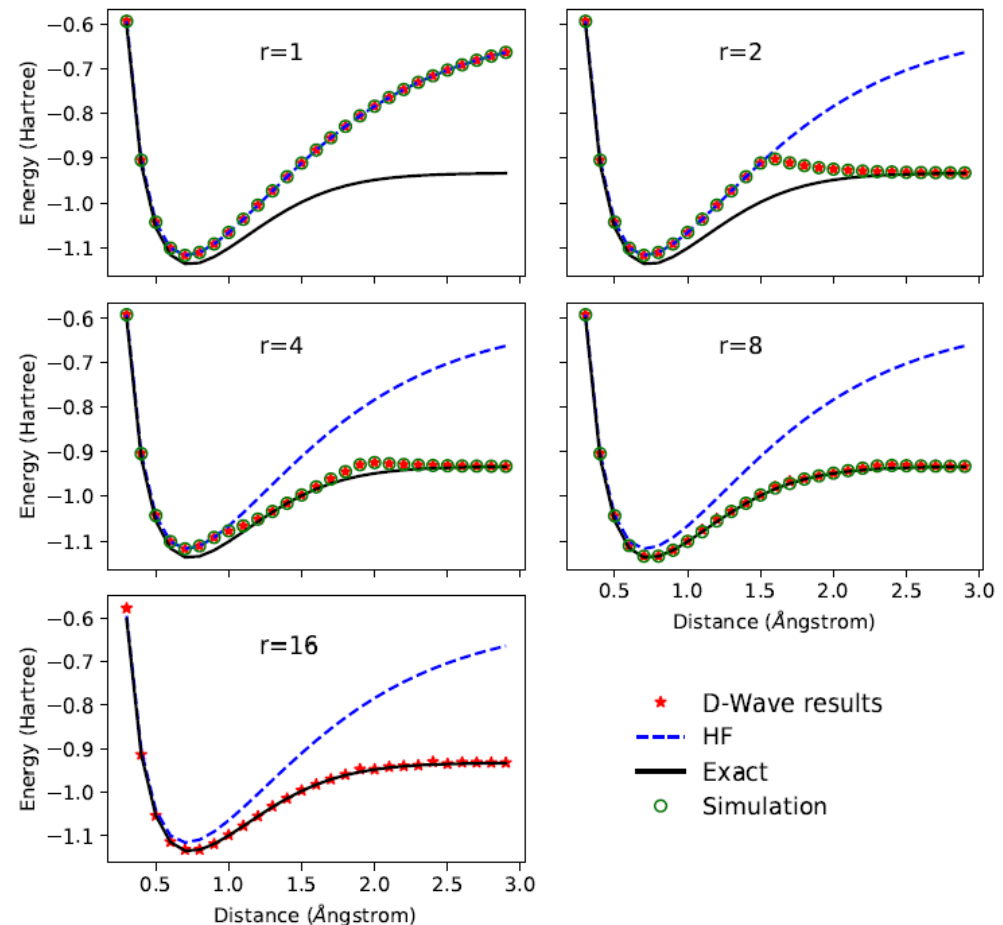
## Solving Quantum Chemistry Problems with a D-Wave Quantum Annealer

Michael Streif<sup>1</sup>, Florian Neukart<sup>2,3</sup>, and Martin Leib<sup>1</sup>

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<sup>2</sup> LIACS, Leiden University, Niels Bohrweg 1, 2333 CA Leiden, Netherlands

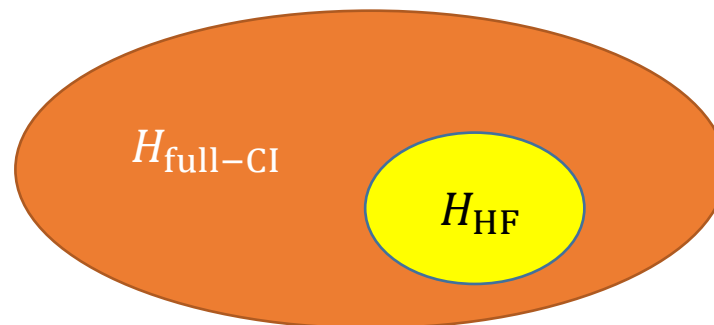
<sup>3</sup> Volkswagen Group of America, 201 Post Street, San Francisco, CA 94108, United States of America



# Differences between quantum annealing and ASP

$$H(t) = (1 - s(t))H_{\text{HF}} + s(t)H_{\text{Full-CI}}$$

	Quantum annealing on D-Wave machine	ASP
$H_{\text{ini}}$	$\sum_k c_k X_k$	$H_{\text{HF}}$ $= \sum_{p \in \text{Occ}} h_{pp} a_p^\dagger a_p$ $+ \sum_{p,q \in \text{Occ}} (h_{pqqp} a_p^\dagger a_q^\dagger a_q a_p + h_{pqpp} a_p^\dagger a_q^\dagger a_p a_q)$
$H_{\text{fin}}$	Ising	$H_{\text{full-CI}} = \sum_{p,q} h_{pq} a_p^\dagger a_q + \sum_{p,q,r,s} h_{pqrs} a_p^\dagger a_q^\dagger a_r a_s$

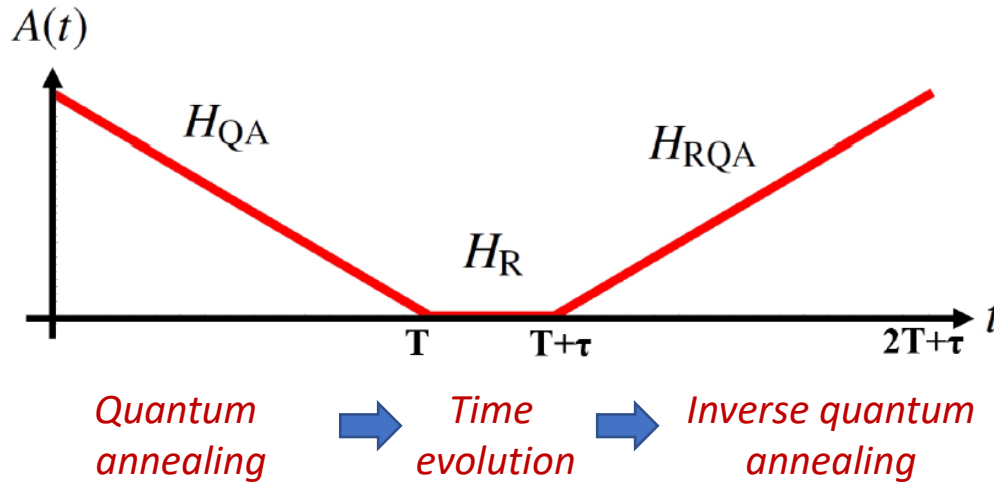


# Direct Calculation of Energy Gaps

$$H(t) = A(t)H_D + (1 - A(t))H_P$$

$$|\Psi(t = 0)\rangle = \frac{1}{\sqrt{2}} \left( |\Psi_0^{(D)}\rangle + |\Psi_1^{(D)}\rangle \right)$$

Superposition of **ground** and **excited** states



$$|\Psi(t = 2T + \tau)\rangle = \frac{1}{\sqrt{2}} \left( |\Psi_0^{(D)}\rangle + e^{-i\Delta E\tau - i\theta'} |\Psi_1^{(D)}\rangle \right)$$

Phase shift depends on the excitation energy

Projective measurements

Changing the evolution time  $\tau$

Fourier transformation

