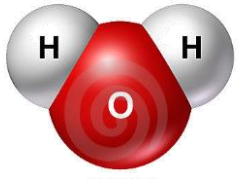
Quantum computing and quantum information

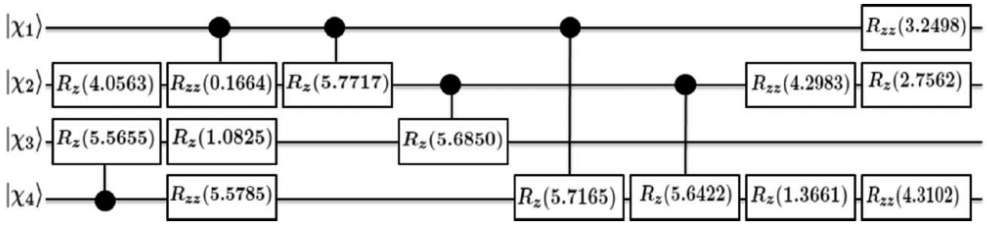
KAIS GROUP

Main themes

arXiv:1004.2242 [cs.NE]
arXiv:1009.5625 [quant-ph]
arXiv:1307.7220 [quant-ph]
arXiv:1302.1946 [quant-ph]
arXiv:1302.0579 [quant-ph]
…

Quantum algorithms. In particular for quantum chemistry



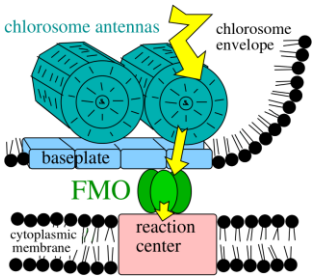


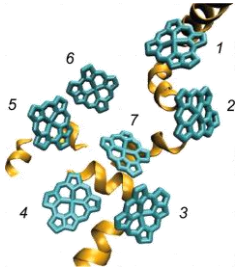
Molecular Hamiltonian

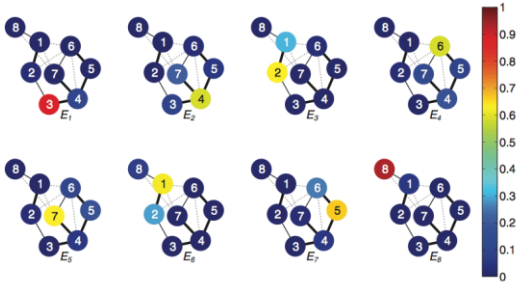
Quantum circuit

arXiv:1502.00671 [physics.bio-ph]
arXiv:1408.3556 [physics.bio-ph]
arXiv:1204.5262 [physics.chem-ph]

Entanglement for complex chemical and biological systems

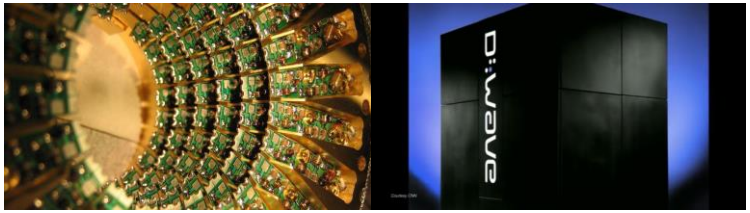




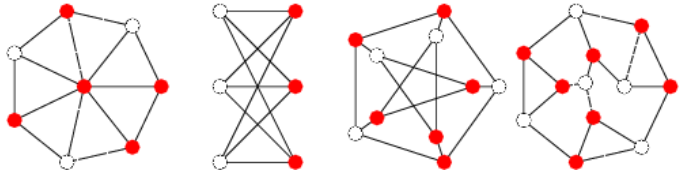


Adiabatic quantum algorithms for quantum simulation and more

arXiv:1311.2555 [quant-ph]
arXiv:1310.1933 [quant-ph]

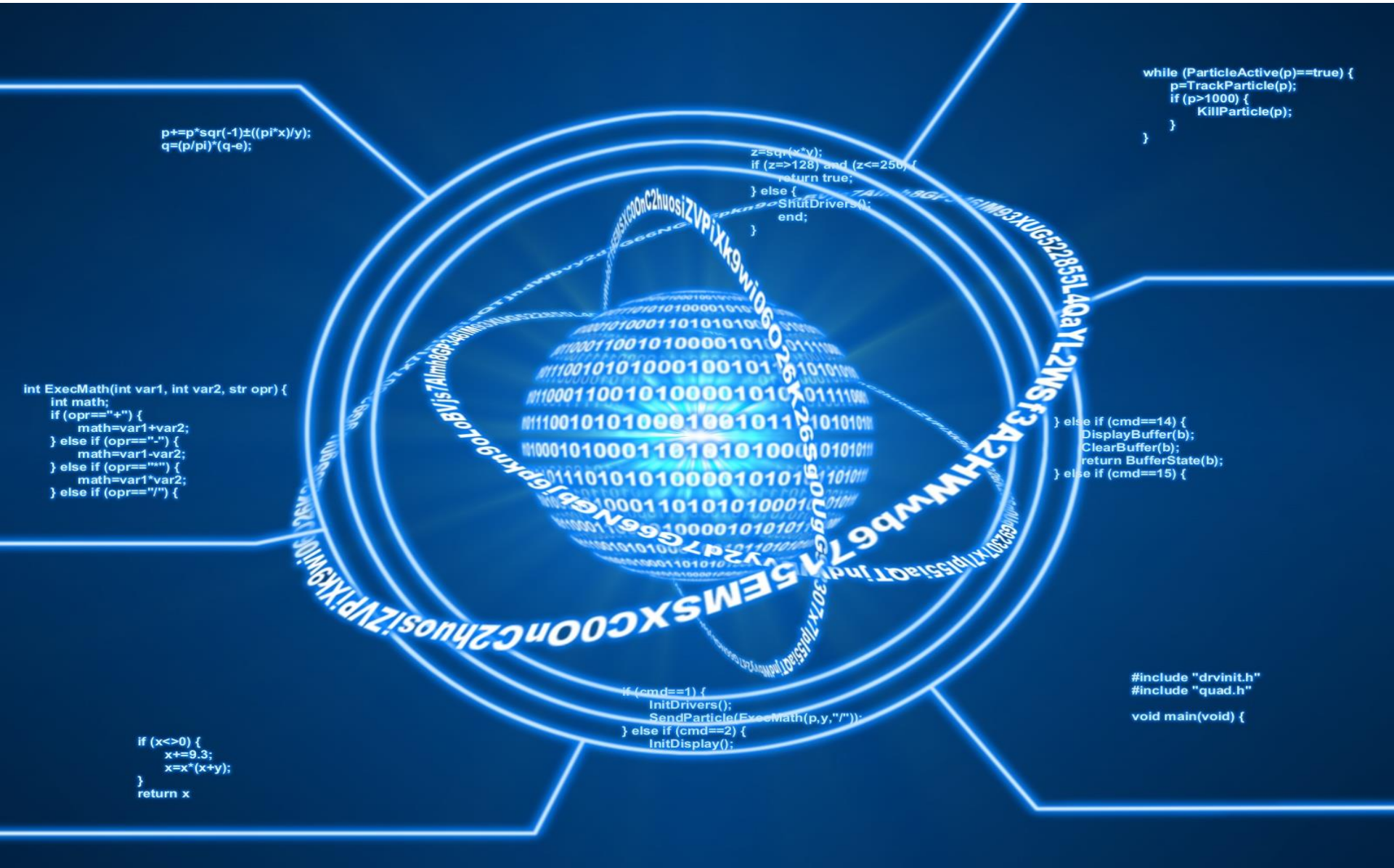


Adiabatic quantum device (quantum annealer)



Hard Optimization problems +2 papers in progress

Quantum algorithms



Quantum algorithms

Main applications of quantum computing:

- Hidden abelian subgroup problem (Shor's alg., exponential speedup)
- Unstructured search (Grover's, quadratic speedup)
- **Quantum simulation** (exponential speedup)

  e.g. quantum chemistry: exact diagonalization

Need **thousands of qubits** to surpass classical computation
arXiv:quant-ph/0205095

Classical: maximum 50 ~ 60 orbitals
Quantum: need to handle 50 ~ 100 orbitals at least to surpass classical

⇒ Need **50 ~ 100 qubits**

Quantum simulation is one of the most promising near-term applications for quantum computation that could demonstrate significant advantage over classical algorithms.

Google IBM Microsoft

Quantum simulation

Goal: simulate properties of quantum systems

1) Dynamic properties: time evolution e^{-iHt} for a given Hamiltonian *H*

2) Static properties: for example the ground state of a given *H*

$U = e^{-iHt}$ — Gate decomposition → $U' = U_m U_{m-1} \dots U_2 U_1$

Target unitary — Elementary gate sequence

Gate decomposition schemes:

- Trotter-Suzuki
- Solovay-Kitaev
- Taylor Series
- …
- **Heuristic approach**

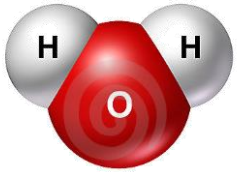
Group leaders optimization algorithm
[Daskin, Kais, *JCP*, 2011; *Mol. Phys., 2011*]

Input: Gate set, target unitary *U* and error ε

Output: Gate sequence *U'* such that

$$\|U - U'\| \leq \varepsilon$$

Quantum simulation of molecular Hamiltonians



Molecular Hamiltonian

$$H = \sum_{i,j} h_{ij} a_i^\dagger a_j + \frac{1}{2} \sum_{i,j,k,l} h_{ijkl} a_i^\dagger a_j^\dagger a_k a_l$$

Second-quantized form

J-W

$$H = \sum_{i,\alpha} h_\alpha^i \sigma_\alpha^i + \sum_{ij\alpha\beta} h_{\alpha\beta}^{ij} \sigma_\alpha^i \sigma_\beta^j + \cdots$$

Qubit Hamiltonian
(sum of tensor products of Pauli matrices)

$$U = e^{-iHt}$$

Target unitary

Jordan-Wigner transform

$$a_j \to \left(\prod_{k=1}^{j-1} -\sigma_z^k \right) \sigma_-^j = (-1)^{j-1} \sigma_z^1 \sigma_z^2 .... \sigma_z^{j-1} \sigma_-^j$$

$$a_j^\dagger \to \left(\prod_{k=1}^{j-1} -\sigma_z^k \right) \sigma_+^j = (-1)^{j-1} \sigma_z^1 \sigma_z^2 .... \sigma_z^{j-1} \sigma_+^j .$$

Gate decomposition scheme

$U = e^{-iHt}$ — Gate decomposition → $U' = U_m U_{m-1} \dots U_2 U_1$

Target unitary — Elementary gate sequence

Rephrase gate decomposition as an **optimization** problem:

$$\min_{U'} \left| 1 - \left[\alpha \cdot \frac{1}{N} \mathbf{Tr}\left(U' U^{\dagger}\right) + \frac{\beta}{\text{Cost}} \right] \right|$$

U' is a sequence of gates from a user-defined elementary gate set

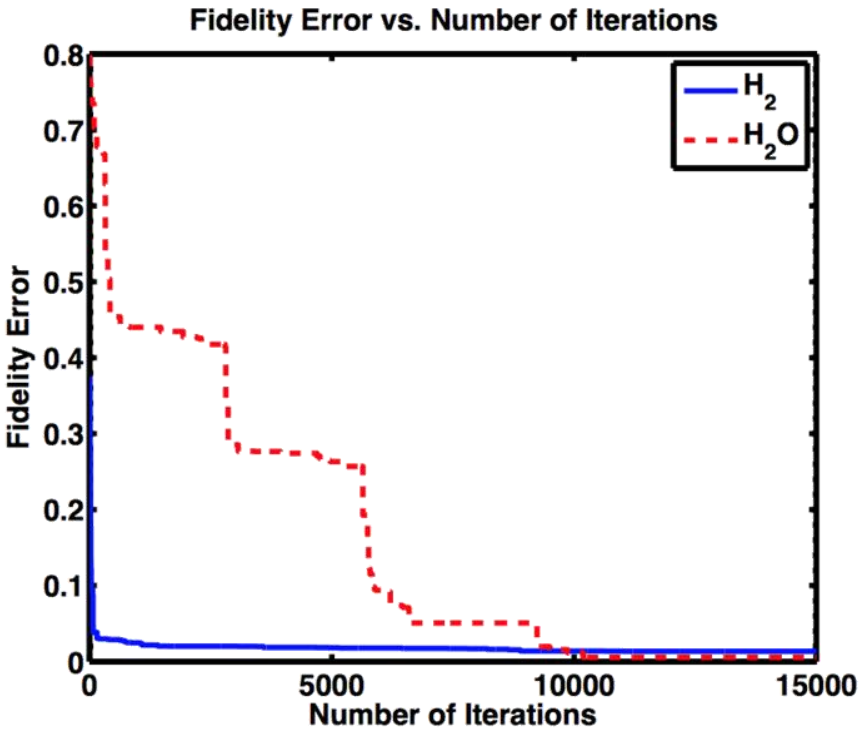
$\frac{1}{N} \mathbf{Tr}\left(U' U^{\dagger}\right)$ is the correctness of the circuit *U'*

Cost is a user-defined function that decides the cost of each elementary gate

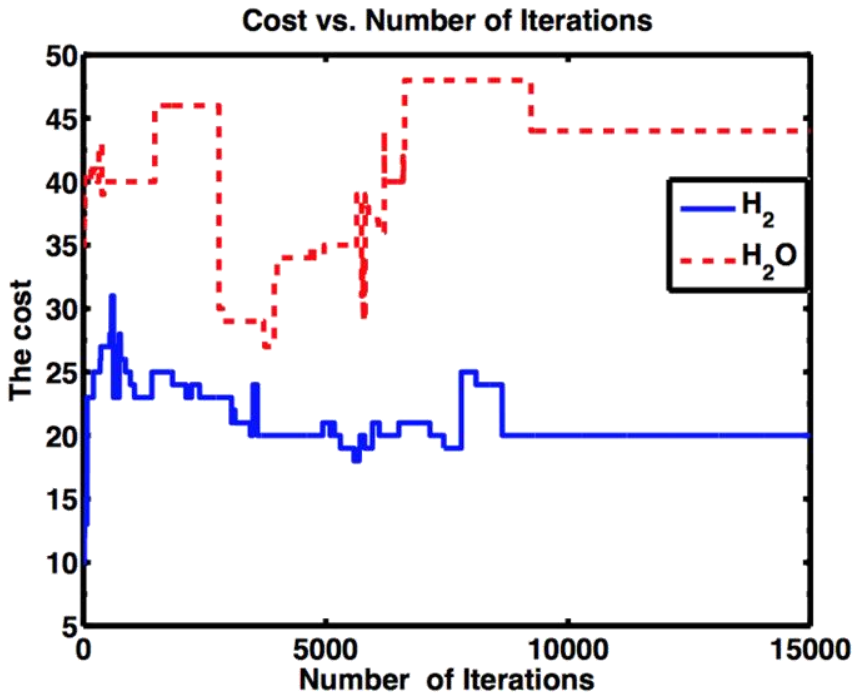
The heuristic algorithm strive to find a globally optimized gate sequence with respect to the gate set and cost function assigned by the user.

A. Daskin and S. Kais, ***Mol. Phys***. 109, 761 (2011).

Gate decomposition: numerics



(a) The evolution of the fidelity error.

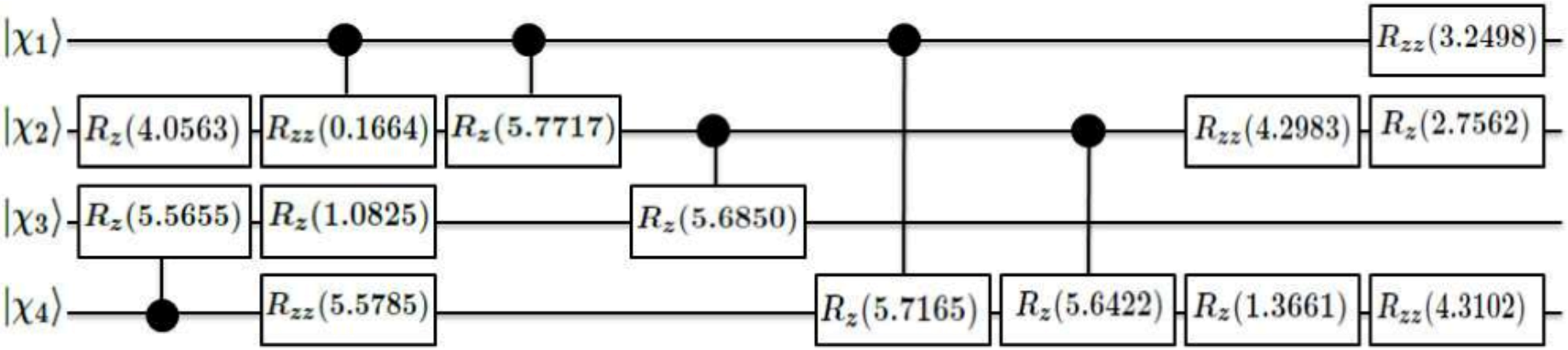


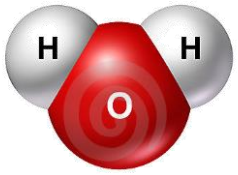
(b) The evolution of the cost.

FIG. 11: The evolutions of the cost and the error in the optimization for the exponentials of the Hamiltonians of the water and the hydrogen molecules.

A. Daskin and S. Kais. ***J. Chem. Phys.*** 134, 144112 (2011).

Example: H_2O molecule





Molecular Hamiltonian → Second-quantized form → J-W → Qubit Hamiltonian (sum of tensor products of Pauli matrices) → Target unitary → Quantum circuit

More quantum algorithms…

Quantum circuit schemes

Quantum circuits for solving linear systems arXiv:1110.2232 [quant-ph]

Quantum algorithm for solving Poisson equation (collaboration with Joseph Traub at Columbia U.) arXiv:1207.2485 [quant-ph]

Quantum algorithm for multiple network alignment arXiv:1307.7220 [quant-ph]

Universal quantum circuit scheme for finding complex eigenvalues arXiv:1302.0579 [quant-ph]

Experimental collaborations

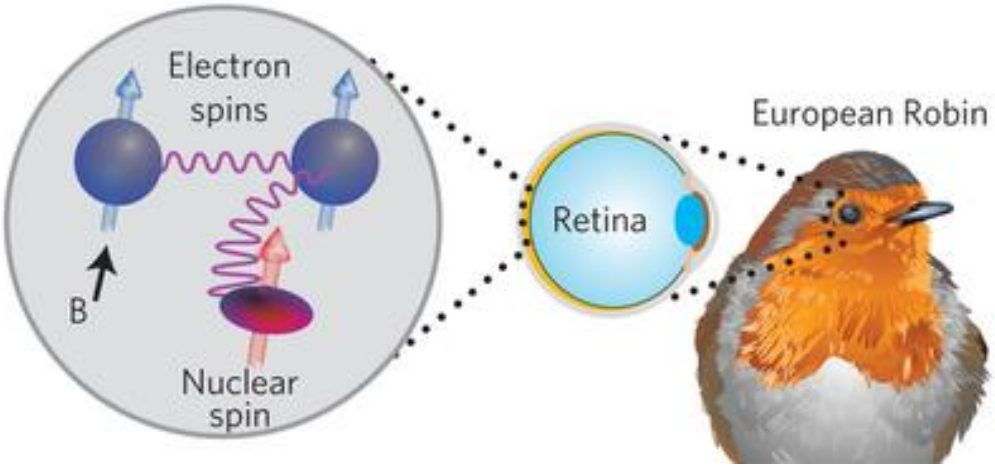
Experimental realization on NMR (collaboration with Jiangfeng Du at Univ. Sci. Tech. China) arXiv:1302.1946 [quant-ph]

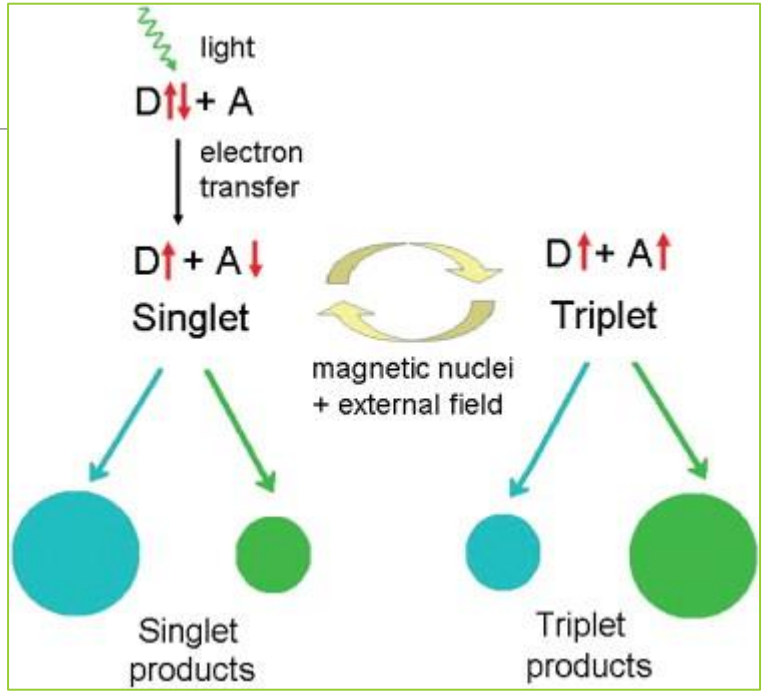
Entanglement and coherence in biological and chemical systems

Coherent energy transfer in photosynthetic systems

Avian compass

Radical pair mechanism for avian compass



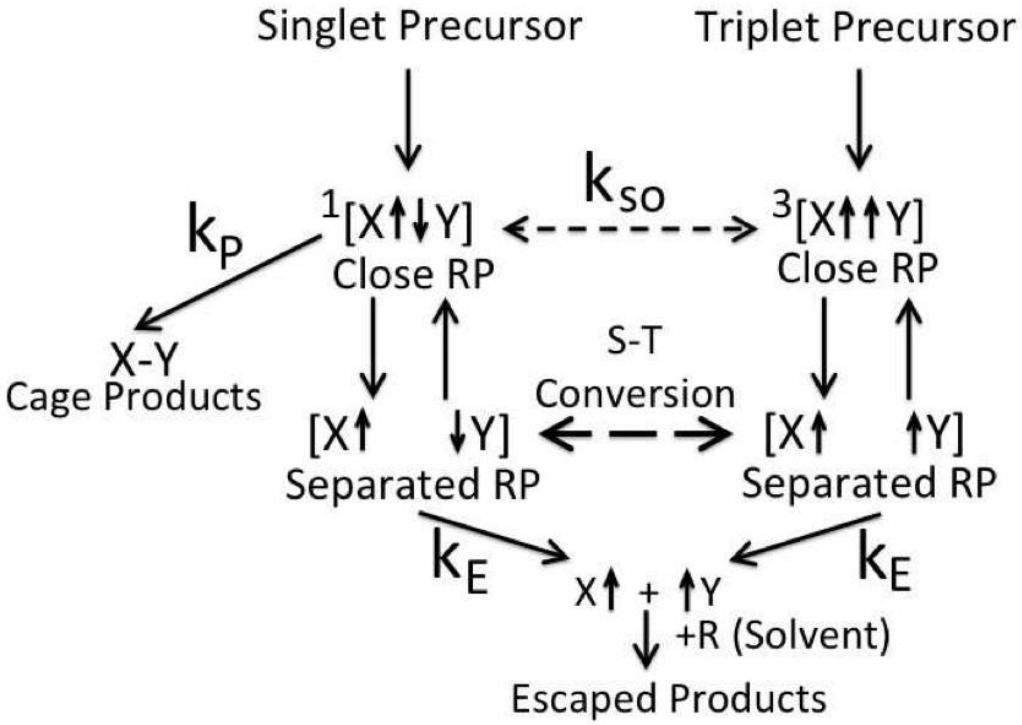


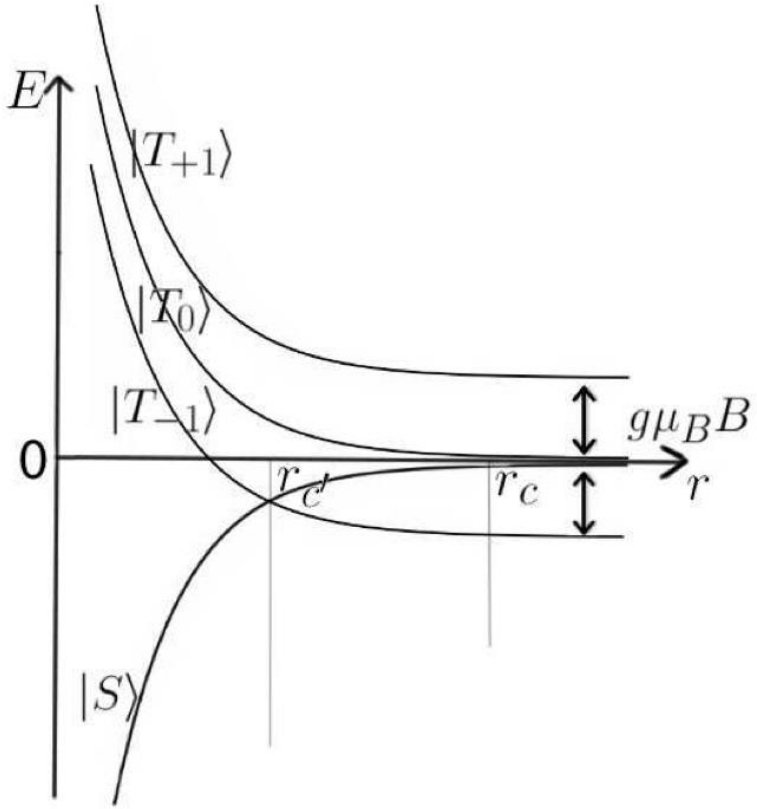
External magnetic field *B* alternates the state of a weakly coupled radical pair

S-T Conversion influenced by **Zeeman effect** and **hyperfine interaction**

Inspired applications: synthetic donor-bridge-acceptor compass, chemical compass using magnetic nanostructures

Radical pair mechanism

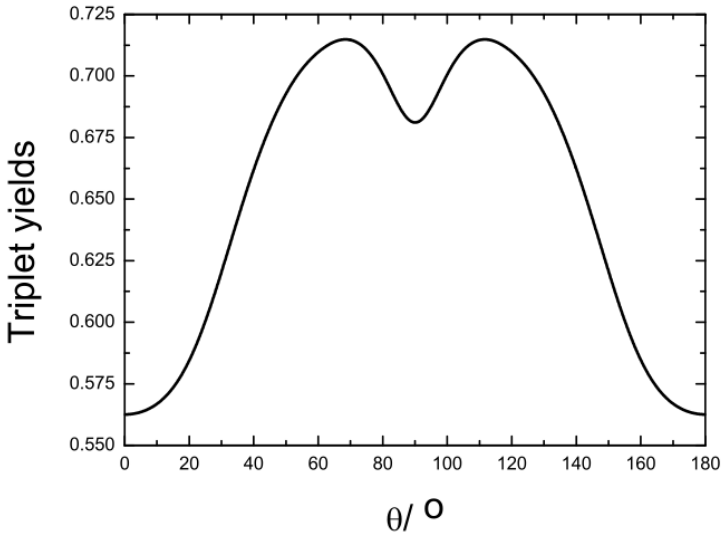




Radical pair mechanism: numerics

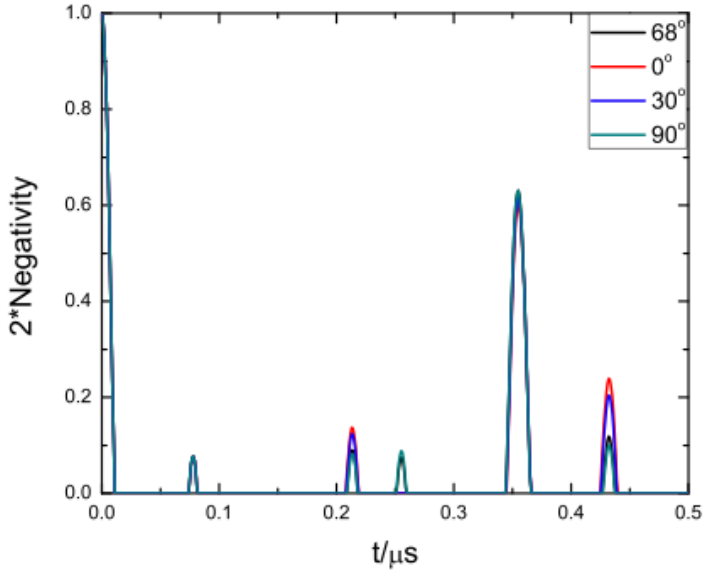
Quantum entanglement measured by **Negativity**

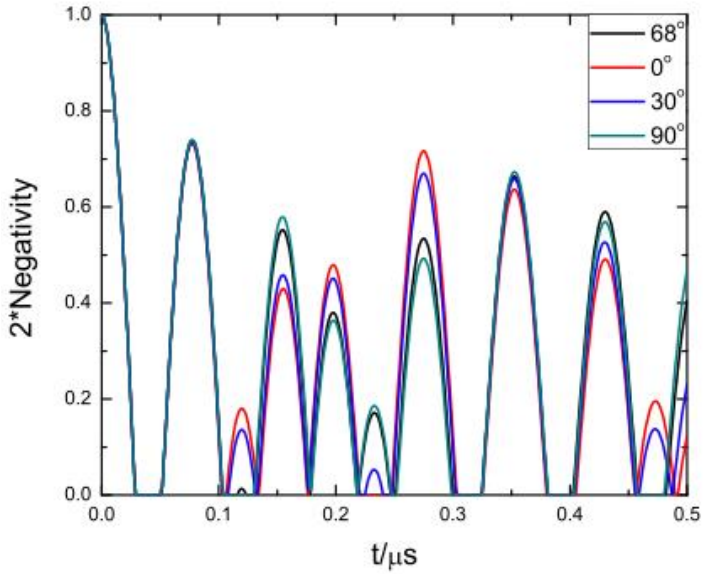
1. Yields dependent on angle;
2. Entanglement dependent on angle if hyperfine coupling is **anisotropic**.



$$\widehat{A_1^b} = \begin{pmatrix} 10\mathrm{G} & 0 & 0 \\ 0 & 10\mathrm{G} & 0 \\ 0 & 0 & 4\mathrm{G} \end{pmatrix},$$

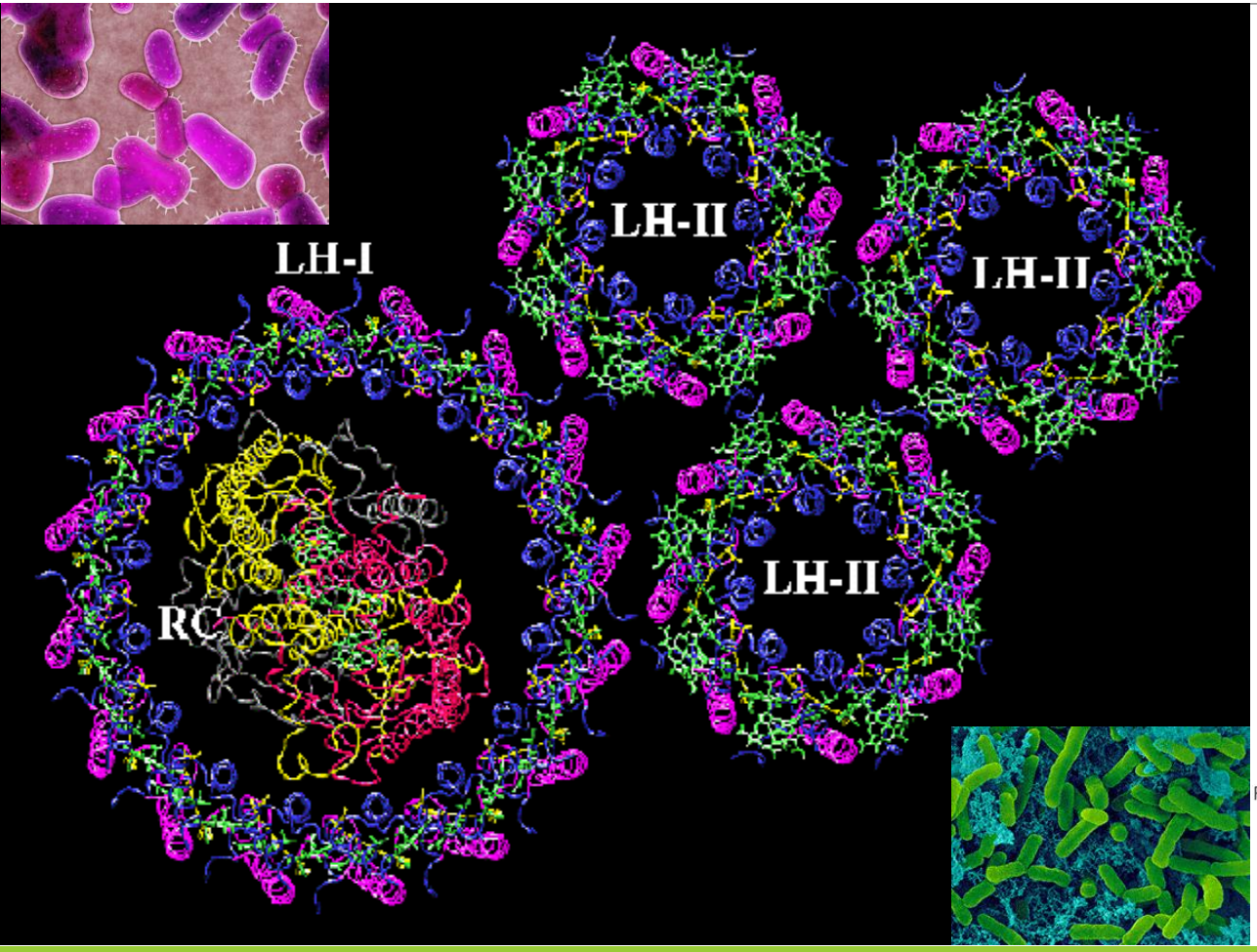
$$\widehat{A_2^b} = \begin{pmatrix} 5\mathrm{G} & 5\mathrm{G} & 0 \\ 0 & 5\mathrm{G} & 0 \\ 0 & 0 & 5\mathrm{G} \end{pmatrix},$$

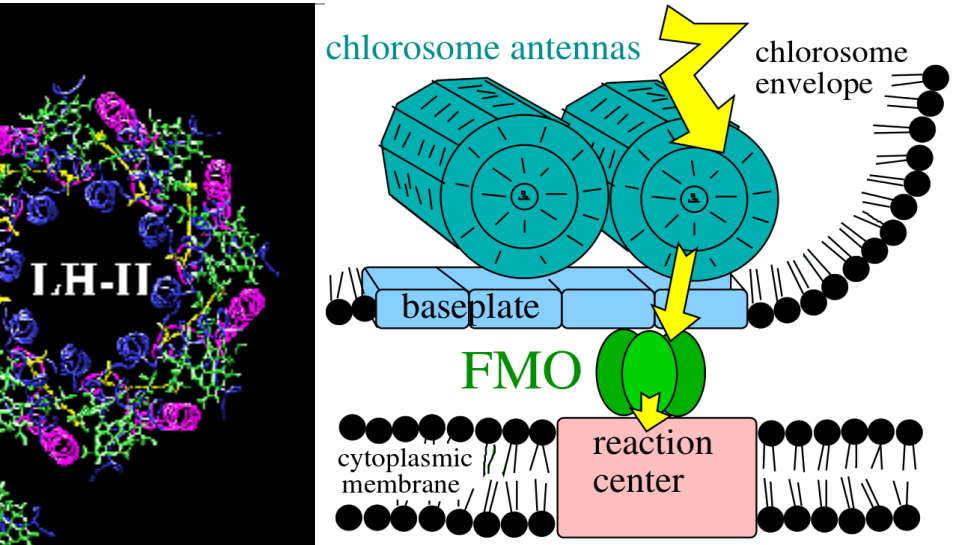


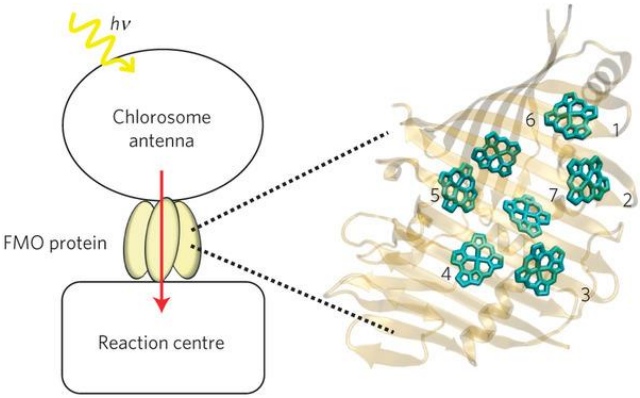


Y. Zhang, G. Berman, S. Kais. ***Int. J. Quant. Chem.***, 115, 15 (2015)

Entanglement and coherence in FMO and LH2 complex







S. Yeh, J. Zhu, S. Kais, ***J. Chem. Phys.*** 137, 084110 (2012); S. Yeh, S. Kais, arXiv:1408.3556v1 (2014)

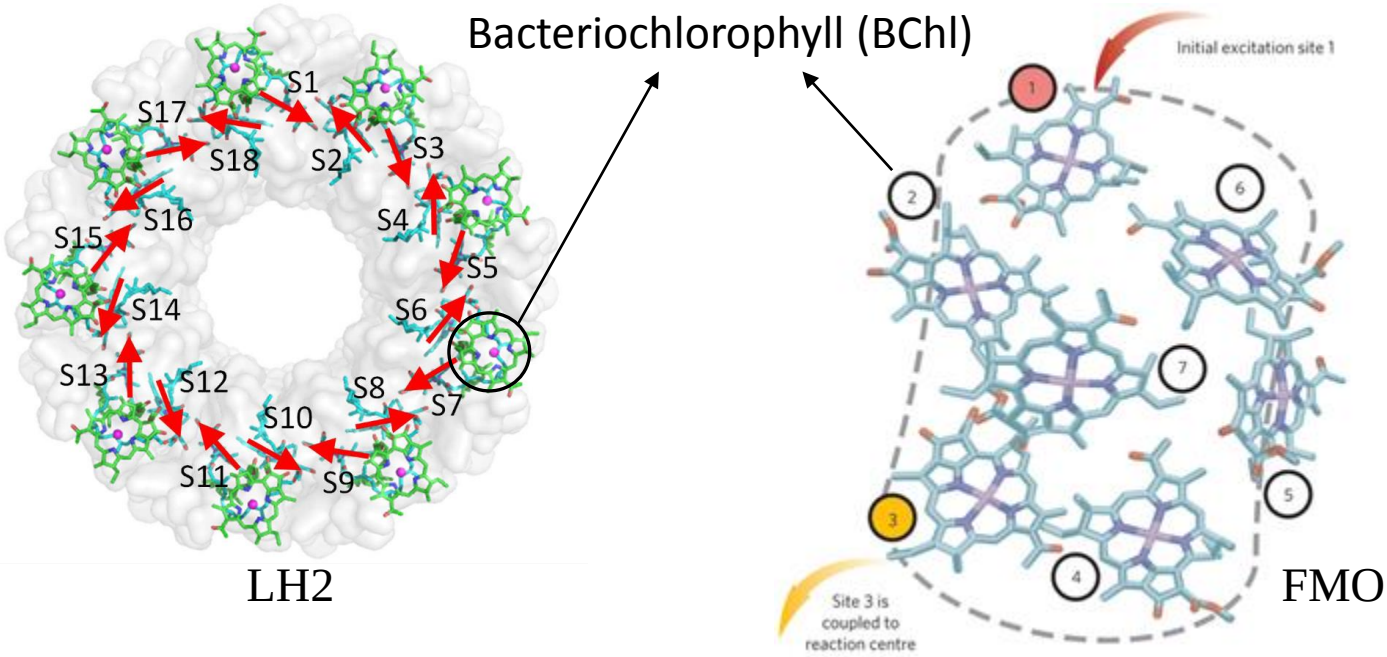
Model Hamiltonian

$$\mathcal{H}_S = \sum_{j=1}^{N} \varepsilon_j |j\rangle\langle j| + \sum_{j\neq k} J_{jk} \left(|j\rangle\langle k| + |k\rangle\langle j|\right)$$

$$\mathcal{H}_B = \sum_{j=1}^{N} \mathcal{H}_B^j = \sum_{j=1}^{N} \sum_{\xi=1}^{N_{jB}} \frac{P_{j\xi}^2}{2m_{j\xi}} + \frac{1}{2} m_{j\xi} \omega_{j\xi}^2 x_{j\xi}^2$$

$$\mathcal{H}_{SB} = \sum_{j=1}^{N} \mathcal{H}_{SB}^j = -\sum_{j=1}^{N} |j\rangle\langle j| \cdot \sum_{\xi} c_{j\xi} \cdot x_{j\xi} = -\sum_{j=1}^{N} \mathcal{V}_j \cdot F_j$$

$$\text{with } \mathcal{V}_j = |j\rangle\langle j| \text{ and } F_j = \sum_{\xi} c_{j\xi} \cdot x_{j\xi}$$



$\mathcal{H} = \mathcal{H}_S + \mathcal{H}_B + \mathcal{H}_{SB}$; system, bath, system-bath interaction

$\mathcal{H}_S$: 1-exciton and 2-exciton basis

$\mathcal{H}_B$: phonon bath

Numerical simulation

Simulation schemes

- Redfield equation — assumes $H_{SB} \ll H_S$
- Förster theory — assumes $H_{SB} \gg H_S$
- Hierarchical equation of motion (HEOM) — no requirements ✅

BChl coulomb coupling ≈ electron-bath coupling

➡ Scaled HEOM (Shi et al.)

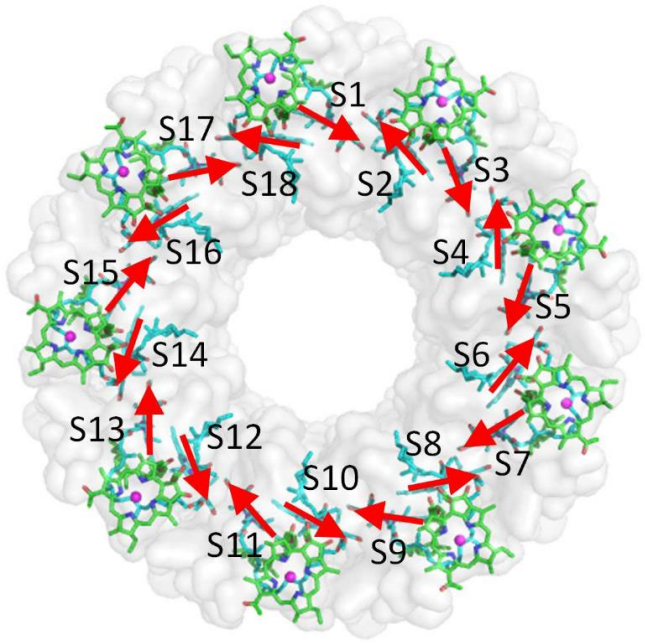
$$\frac{d}{dt}\rho_{\boldsymbol{n}} = -\frac{i}{\hbar}\left[\mathcal{H}_S,\ \rho_{\boldsymbol{n}}\right] - \sum_{j=1}^{N}\sum_{k=0}^{K} n_{jk}\nu_k \cdot \rho_{\boldsymbol{n}} - i\sum_{j=1}^{N}\sqrt{(n_{jk}+1)\,|c_k|}\left[\mathcal{V}_j,\ \sum_k \rho_{\boldsymbol{n}_{jk}^{+}}\right]$$

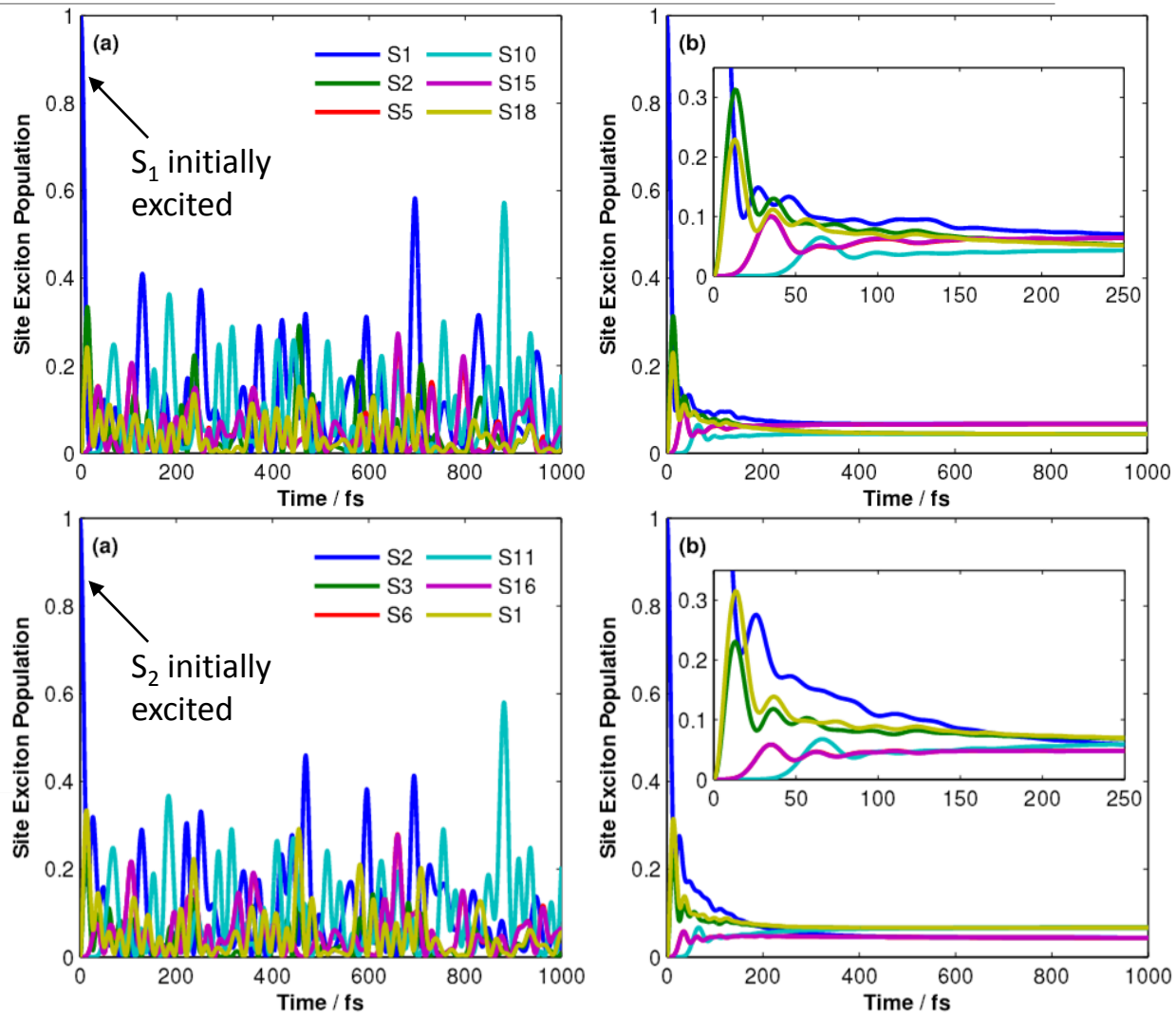
$$-\sum_{j=1}^{N}\sum_{m=K+1}^{\infty}\frac{c_{jm}}{\nu_{jm}}\cdot\left[\mathcal{V}_j,\ \left[\mathcal{V}_j,\ \rho_{\boldsymbol{n}}\right]\right] - i\sum_{j=1}^{N}\sum_{k=0}^{K}\sqrt{n_{jk}/|c_k|}\left(c_k\mathcal{V}_j\,\rho_{\boldsymbol{n}_{jk}^{-}} - c_k^{*}\rho_{\boldsymbol{n}_{jk}^{-}}\mathcal{V}_j\right)$$

We apply scaled HEOM on simulation of the dynamics of excitation energy transfer in LH2 and FMO complex

Q. Shi, L. P. Chen, G. J. Nan, R. X. Xu, Y. J. Yan, ***J. Chem. Phys.,*** 130, 084105 (2009)
J. Zhu, S. Kais, P. Rebentrost, and A. Aspuru-Guzik, ***J. Phys. Chem. B***, 115, 1531 (2011).
J. Zhu, S. Kais, A. Aspuru-Guzik, S. Rodriques, B. Brock, and P. J. Love, arXiv:1202.4519v1 (2012).

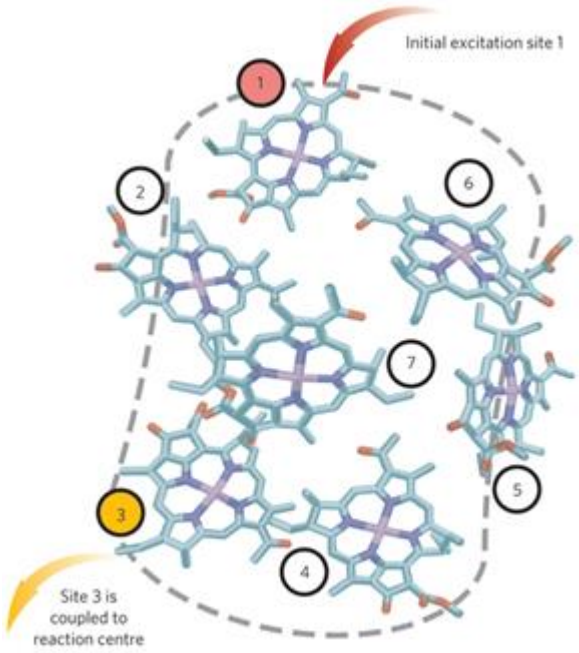
Simulation results: LH2





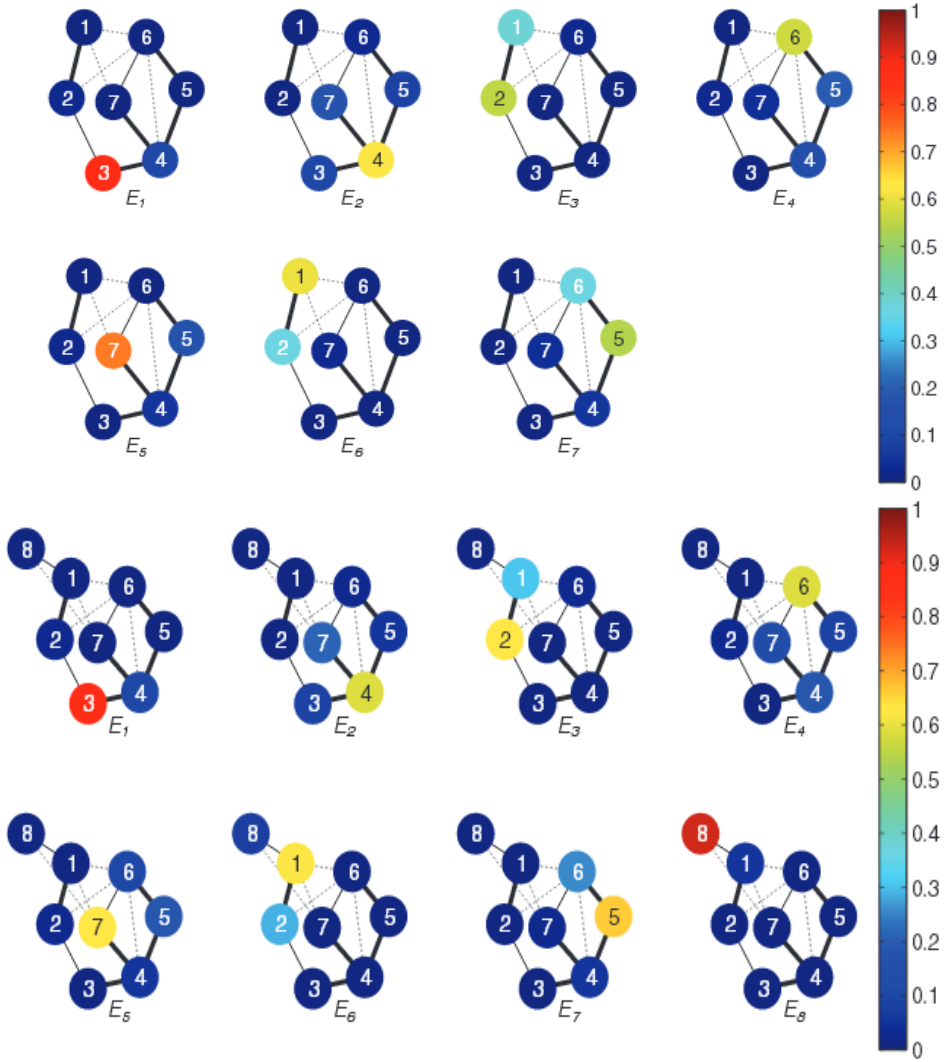
S. Yeh, J. Zhu, S. Kais, ***J. Chem. Phys.*** 137, 084110 (2012);

Simulation results: FMO



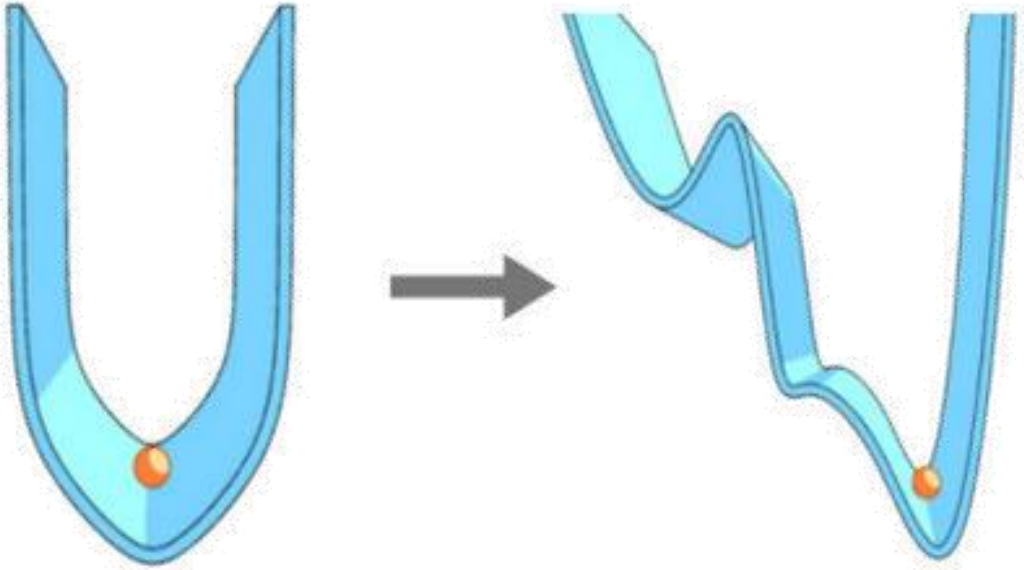
7 sites

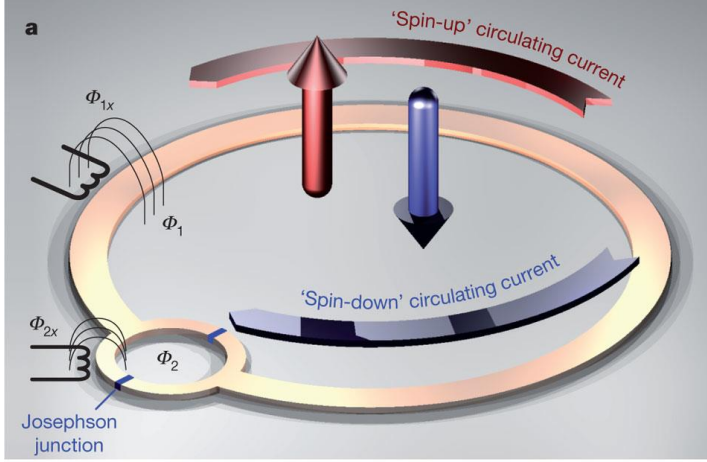
+ additional site

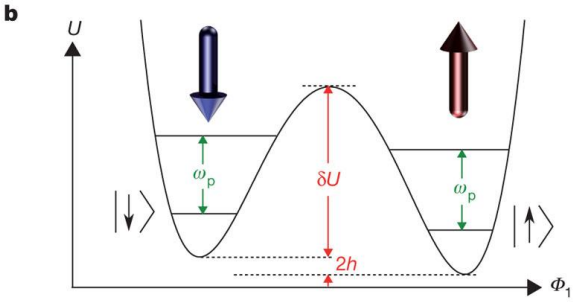


S. Yeh, S. Kais, arXiv:1408.3556v1 (2014)

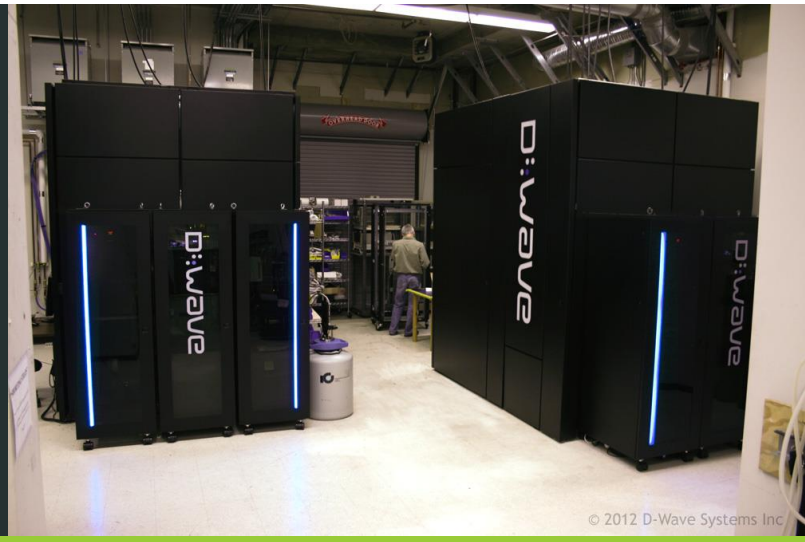
Adiabatic quantum computing







Adiabatic quantum processor chip mounted in cryogenic chip carrier and ready for use.

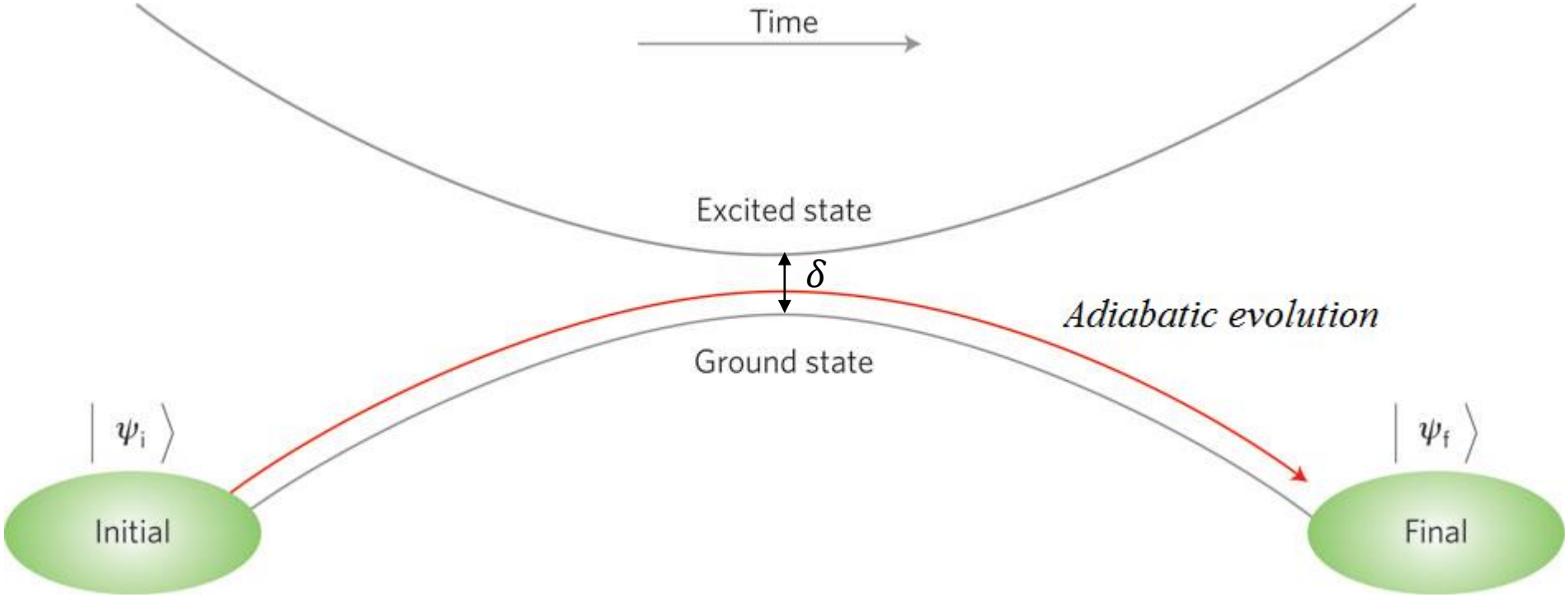


Y. Cao, R. Babbush, J. Biamonte, S. Kais, ***Phys. Rev. A***, 91, 1, 012315, 2015;

Adiabatic quantum computing

$$H(s) = \left(1 - \frac{s}{T}\right) H_1 + \frac{s}{T} H_2$$

$\delta = \frac{1}{\text{poly}(n)}$ for efficient, accurate computation



Transverse Ising Model (TIM)

$$H = \sum_i \Delta_i X_i + \sum_i h_i Z_i + \sum_{i,j} J_{ij} Z_i Z_j$$

Large-scale implementation of TIM

~1000 qubits

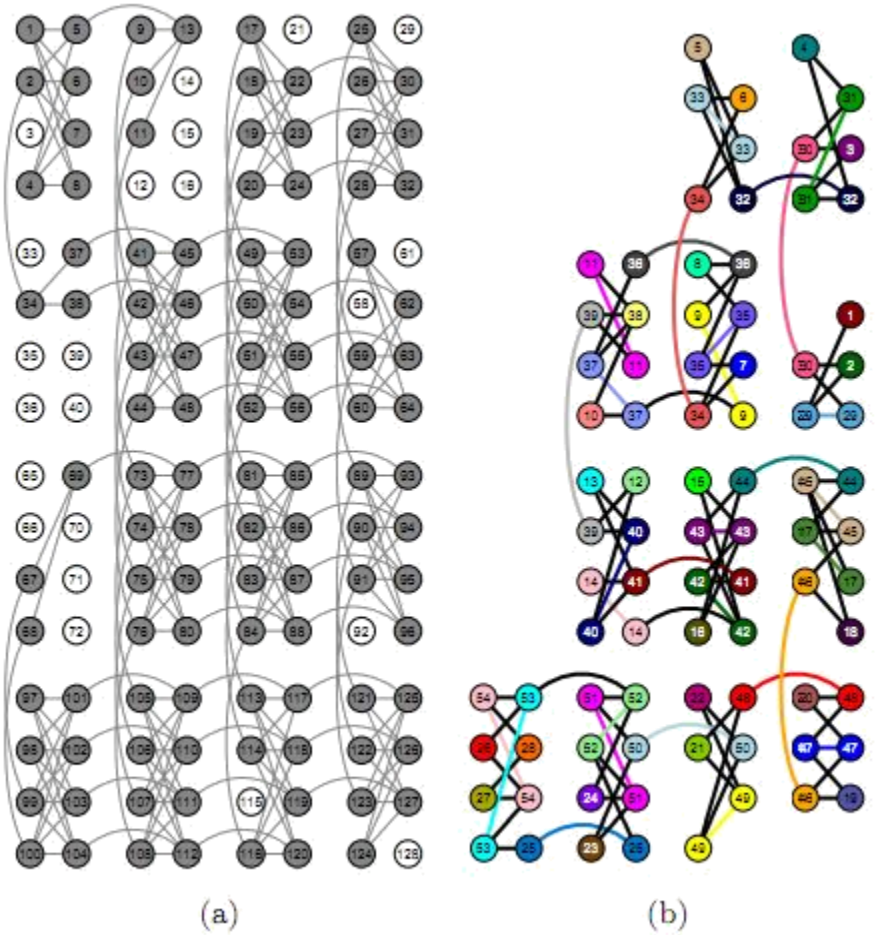
D-Wave
The Quantum Computing Company™

Initial Hamiltonian: single *X* fields

Final Hamiltonian: *ZZ* interactions

$\sum_i h_i Z_i + \sum_{i,j} J_{ij} Z_i Z_j$

Could embed hard optimization problems into the Hamiltonian

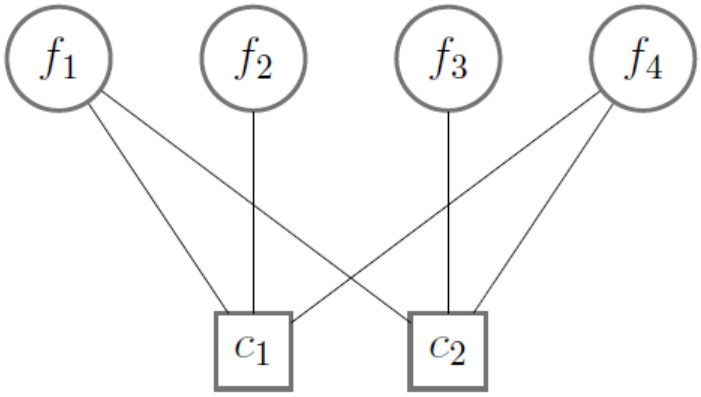


Set Cover with Pairs

Given two sets of nodes *U*, *S* and a graph *G*(*V, E*) where $V = U \cup S$

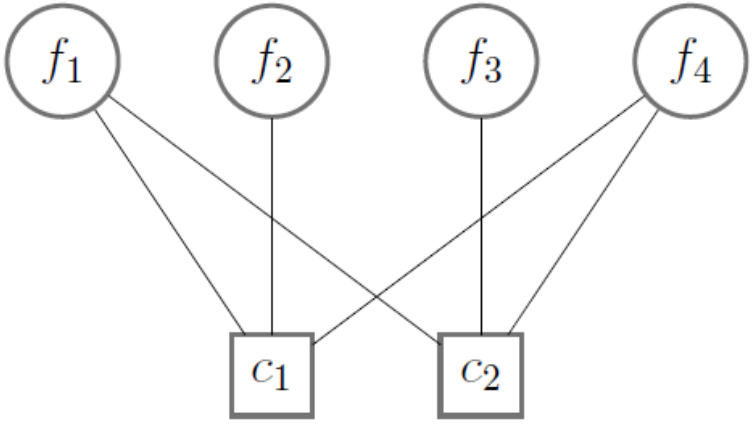
Find a minimum size subset $A \subseteq S$ such that every element of *U* is connected to two elements in *A*.

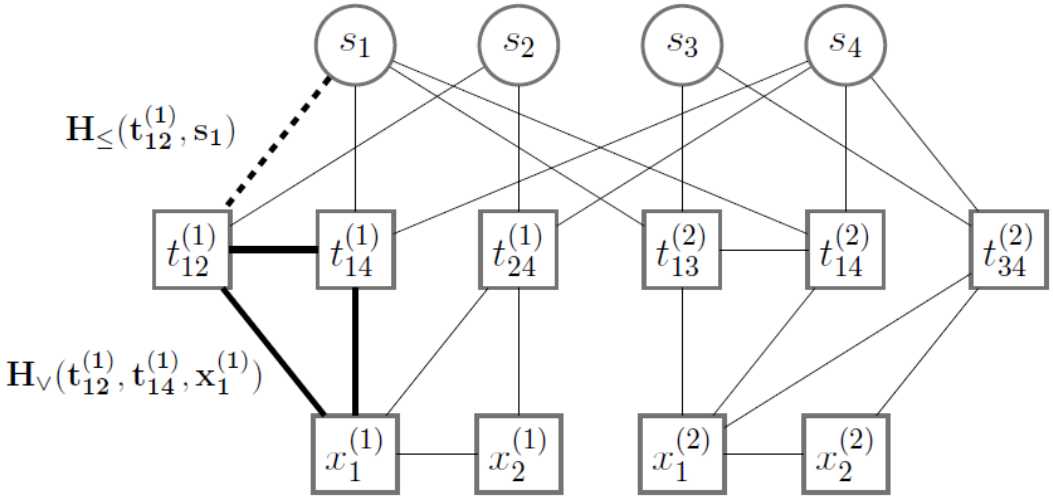
Example. A network of users *U* and facilities *S*. Find the minimum set of facilities such that each user is covered by at least two facilities.



Here $S = \{f_1, f_2, f_3, f_4\}$ and $U = \{c_1, c_2\}$.

Reduction to Ising Model





Set Cover with Pairs (*G*, *U*, *S*) → Integer programming (*G*, *U*, *S*) + auxiliary variables *T* → Ising Hamiltonian $\sum_i h_i Z_i + \sum_{i,j} J_{ij} Z_i Z_j$

Solution ⟵ **Ground state** $|\psi\rangle$

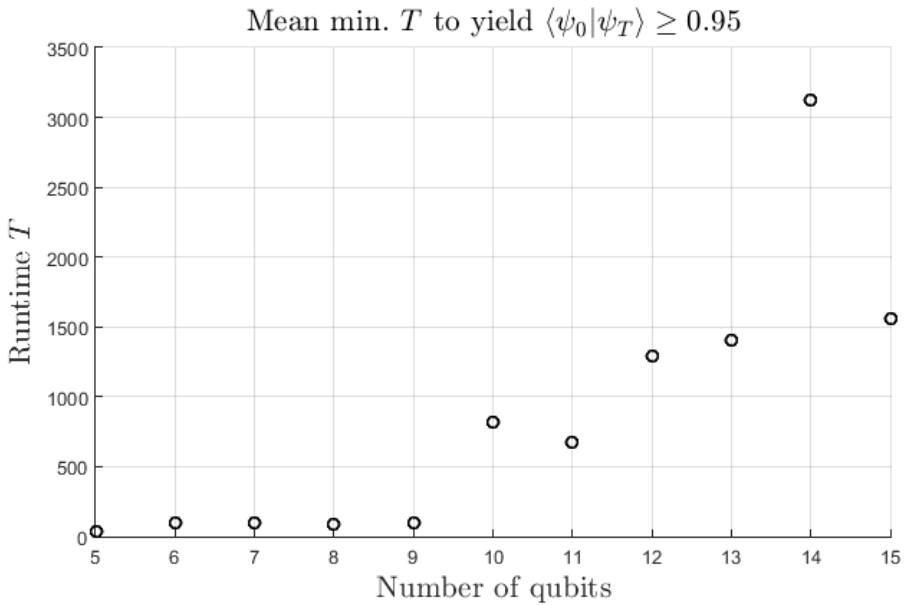
Runtime analysis

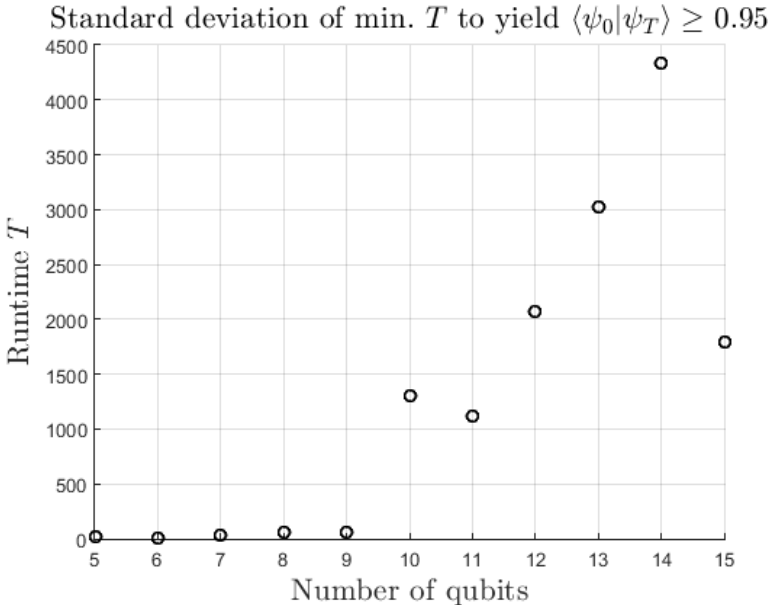
Consider SCPP instances with different input sets *U*, *S* and random *G*;

For each SCPP instance, construct an Ising Hamiltonian *H'*;

Start from $\sum_i \Delta_i X_i$ and evolve it adiabatically to *H'*;

Find the minimum time *T* needed to yield a final state encoding the solution with probability 0.95.



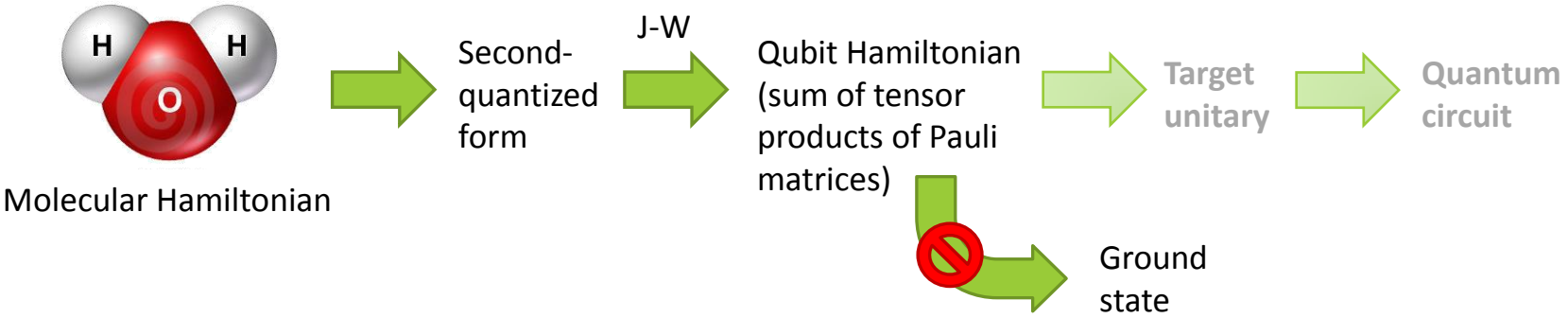


Adiabatic quantum simulation

Goal: simulate properties of quantum systems

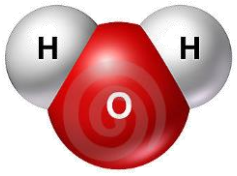
1) Dynamic properties: time evolution e^{-iHt} for a given Hamiltonian *H*

2) Static properties: for example the ground state of a given *H*



The qubit Hamiltonian is usually many-body

Adiabatic quantum simulation



Molecular Hamiltonian

Second-quantized form

J-W

Qubit Hamiltonian (sum of tensor products of Pauli matrices)

Target unitary

Quantum circuit

Ground state

The qubit Hamiltonian is usually many-body, which is unphysical to realize

Example: H_2 in minimal STO-3G basis

$$\begin{aligned}\hat{H}_{JW} = & -0.81261\ \mathbf{1} + 0.171201\ \sigma_0^z + 0.171201\ \sigma_1^z - 0.2227965\ \sigma_2^z - 0.2227965\ \sigma_3^z \\ & +0.16862325\ \sigma_1^z\sigma_0^z + 0.12054625\ \sigma_2^z\sigma_0^z + 0.165868\ \sigma_2^z\sigma_1^z + 0.165868\ \sigma_3^z\sigma_0^z \\ & +0.12054625\ \sigma_3^z\sigma_1^z + 0.17434925\ \sigma_3^z\sigma_2^z - 0.04532175\ \sigma_3^x\sigma_2^x\sigma_1^y\sigma_0^y \\ & +0.04532175\ \sigma_3^x\sigma_2^y\sigma_1^y\sigma_0^x + 0.04532175\ \sigma_3^y\sigma_2^x\sigma_1^x\sigma_0^y - 0.04532175\ \sigma_3^y\sigma_2^y\sigma_1^x\sigma_0^x.\end{aligned}$$

Need to reduce the Hamiltonian to 2-body

Reduction by perturbation theory

Basic idea:

Given a *k*-local target Hamiltonian H_{targ} on *n* qubits;

Find a 2-local Hamiltonian $\widetilde{H}$ on *n* + poly(*n*) qubits such that

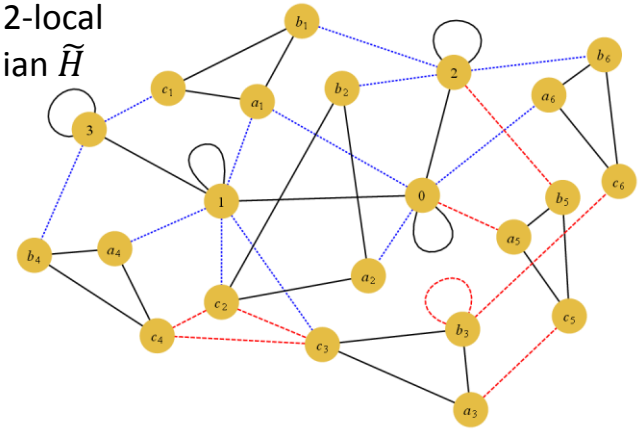
$$\left|\lambda\left(H_{\text{targ}}\right) - \lambda(\widetilde{H})\right| \leq \varepsilon$$

Lowest 2^n energy levels

Qubit Hamiltonian H_{targ}
(sum of tensor products of Pauli matrices)

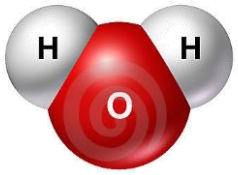
$$H_{\mathrm{H}_2} = f_0\mathbb{1} + f_1 Z_0 + f_2 Z_1 + f_3 Z_2 + f_1 Z_0 Z_1 + f_4 Z_0 Z_2 + f_5 Z_1 Z_3$$
$$+ f_6 X_0 Z_1 X_2 + f_6 Y_0 Z_1 Y_2 + f_7 Z_0 Z_1 Z_2 + f_4 Z_0 Z_2 Z_3 + f_3 Z_1 Z_2 Z_3$$
$$+ f_6 X_0 Z_1 X_2 Z_3 + f_6 Y_0 Z_1 Y_2 Z_3 + f_7 Z_0 Z_1 Z_2 Z_3$$

Reduced 2-local Hamiltonian $\widetilde{H}$



Summary

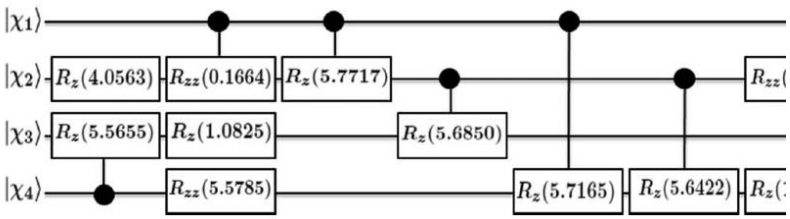
Quantum algorithms. In particular for quantum chemistry



Target unitary evolution

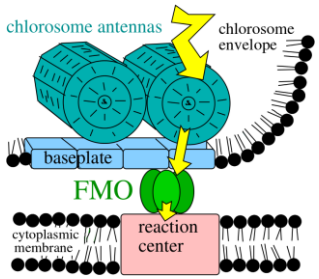
Gate decomposition

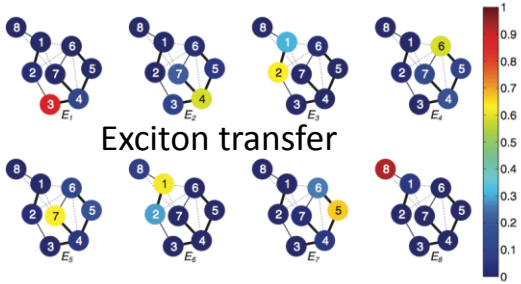
$$\min_{U'} \left| 1 - \left[\alpha \cdot \frac{1}{N} \mathbf{Tr}\left(U' U^{\dagger}\right) + \frac{\beta}{\text{Cost}} \right] \right|$$



Quantum circuit

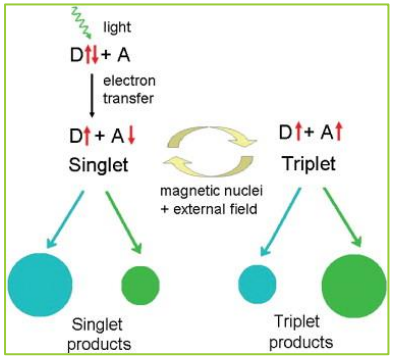
Entanglement for complex chemical and biological systems



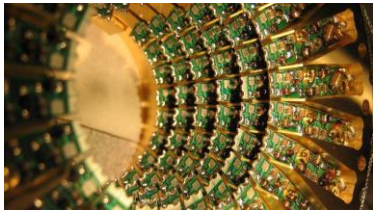


Exciton transfer

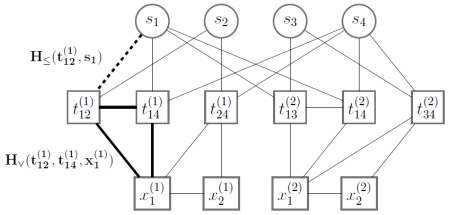
Radical pair mechanism



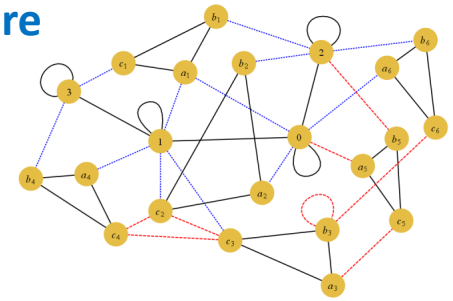
Adiabatic quantum algorithms for quantum simulation and more



Adiabatic quantum device (quantum annealer)



Set cover with pairs



Electronic structure calculation

Thanks for your attention!