Open Quantum Systems: from qubits to quantum biology

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Resources:
www.qutip.org
Reviews: Lambert *et al.* Nature Physics (2013), Scholes et al., Nature (2017).
J. Preskill, “Quantum Computing 40 years later”, arxiv:2106.10522
Breuer and Petruccione, “The theory of open quantum systems”

Supported by:

- From Manchester (Mancunian) UK, and PhD from the University of Manchester. Supervisor: Tobias Brandes





- 2005: JSPS Fellow @ The University of Tokyo (Prof. Akira Shimizu)

- 2008-2021: @ RIKEN (Dr. Franco Nori), became Senior Research Scientist in 2019.


Overview:

Part 1:

Introduction to qubits and quantum computing

From qubits to quantum biology

Introduction to QuTiP

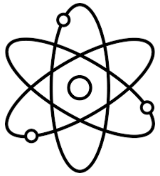
Part 2:

Deriving approximate noise models: Lindblad master equation

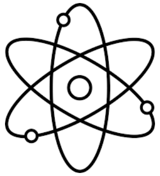
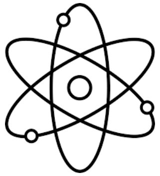
Non-perturbative methods: HEOM and reaction coordinates

What is quantum computing in a nutshell?

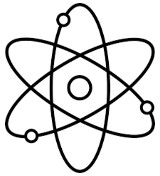
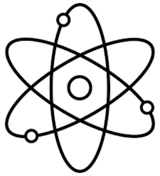
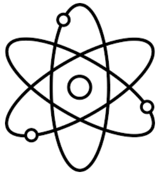
- Quantum systems are difficult to simulate on a classical computer



$$\psi = \alpha|0\rangle + \beta|1\rangle$$

$$\psi = \gamma|00\rangle + \epsilon|01\rangle + \zeta|10\rangle + \eta|11\rangle$$

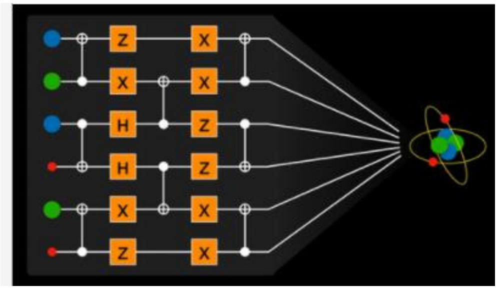
  … 

N atoms require 2^N parameters.

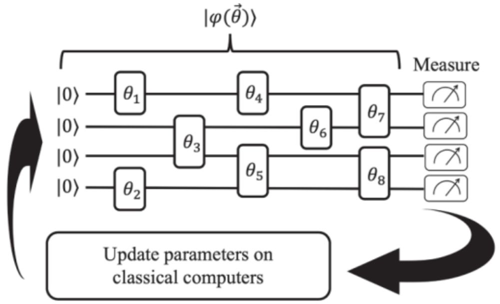
Efficient simulation of a quantum system requires a quantum system

If we build a computer from controllable quantum components (qubits) we can:

- Simulate other quantum systems (digital and analog, practical applications to quantum chemistry?), solve (some) optimization problems (variationally, annealing)



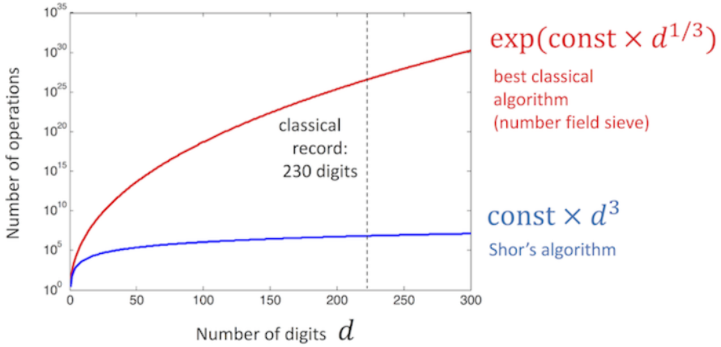
(Aspuru-Guzik)



(S. Endo et al, J. Phys. Soc 2020)

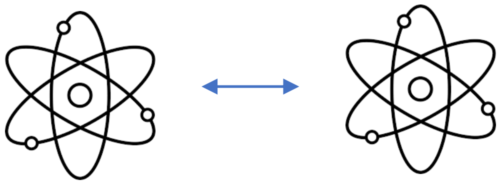
- Run certain algorithms faster than possible on a classical computer, e.g, Shor's algorithm, Grover's algorithm.

Shor's algorithm: Can find the prime factors of an integer exponentially faster than the best known classical algorithm, can then break public-key encryption like RSA.



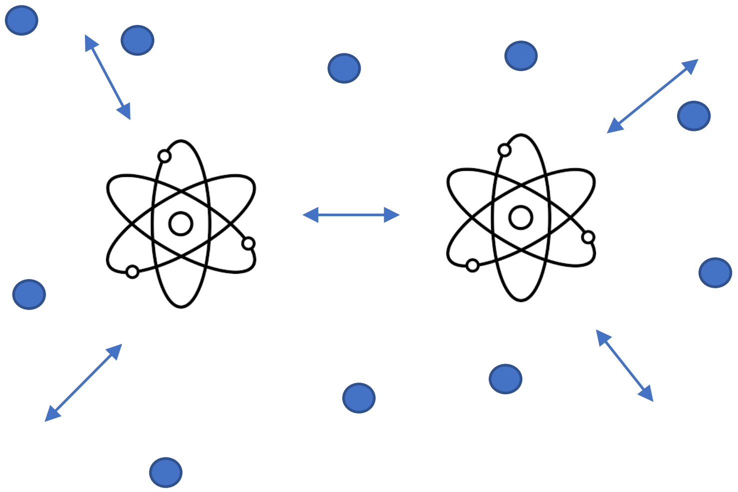
What are the obstacles?

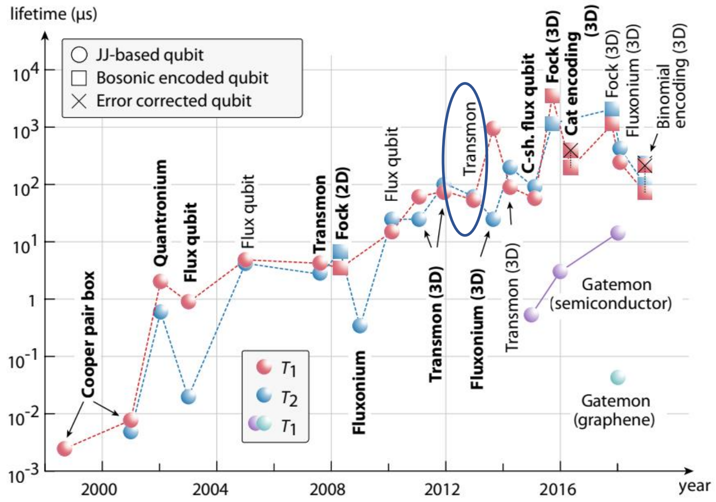
- Quantum systems are difficult to simultaneously control and isolate



$$\psi = \gamma|00\rangle + \epsilon|01\rangle + \zeta|10\rangle + \eta|11\rangle$$

- We need to both make multiple ‘atoms’ interact, while limiting their interaction with the rest of the universe (the dominant source of noise)





Kjaergaard et al, 2019

Amazing progress on many technologies, e.g., superconducting qubits.

Current limits: material imperfections, Cosmic Rays! (even.. Dark matter? axions, Weakly interacting particles)

Timeline of quantum computation

1982 Feynman:
To efficiently simulate a quantum system we need a quantum computer

1984: BB84 (Bennett & Brassard) propose quantum key distribution

1993: Quantum teleportation (Bennett Brassard, Crepeau, Jozsa, Peres and Wooters)

1994: Shor's Algorithm (Peter Shor @ Bell Labs)

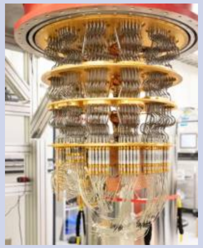
1995: Solovay–Kitaev theorem

1996: Quantum error correction (CSS codes)

2001: Nakamura, Pashkin, Tsai demonstrate coherent superconducting qubit

2011: D-Wave announces annealing device

2014: Google partners with UCSB (John Martiniz)



2016: IBM releases first cloud quantum computer

2018: NISQ era defined (universal quantum computation still distant?)

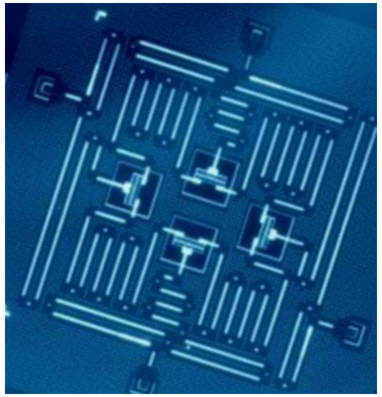
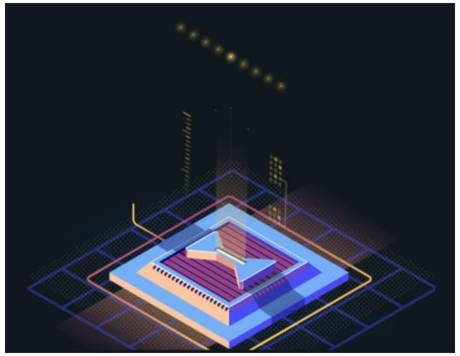
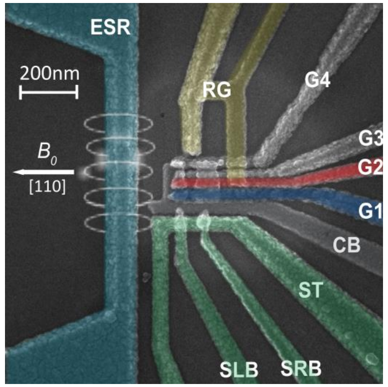
2019: Google's quantum supremacy

Universal quantum computation vs. NISQ

Requirement:	NISQ	Univ. QC (error corrected)
# of qubits	50 - 1000?	> 1,000,000 ?
Error correction	None, or error mitigation	Yes: Surface code, etc
Acceptable gate error rate	Unclear (error mitigation can compensate to some degree)	$<10^{-2}$?
Applications	Exploring quantum physics, limited analog quantum simulations of quantum systems, hybrid/variational approaches, annealing	Shor's algorithm, Grover's algorithm, digital quantum simulation of quantum systems
Scalability issues	May become a problem O(100) qubits	Fabrication, wiring complexity, sheer size

These are not Independent

Current technologies

	Superconducting qubits (Google, IBM)	Ion traps (IonQ)	Semiconductor spin (Intel?)
			
# of qubits:	50+ qubits	30+ qubits	2-5 qubits
Errors:	$\sim 10^{-3}$ two qubit gate error rate (best case)	$\sim 10^{-3}$ two qubit gate error rate (best case)	$\sim 10^{-3}$ two qubit gate error rate (best case)
Scalability:	+ parallel gates - large circuits, wiring, big variations in fab	+ identical ions, long-range interactions, - How to connect traps?	+ small circuits, well established fab - tuning/variability

Others:
- NV centers in diamond
- Topological (Microsoft)
- Photons (Psi Quantum)
- GKP code

NISQ applications

Exploring quantum physics

Theorists can do experiments!

- 500 papers published using IBM-Q
- E.g., H-Y. Ku et al., NPJ-QI 2020

In NISQ-era, one can study:

- many-body entanglement,
- quantum chaos,
- phase transitions,
- analog simulation of quantum dynamics,

and many other features of quantum systems that are inaccessible on classical computers

Hybrid quantum-classical variational approaches

QAOA (Quantum Approximate Optimization Algorithm), Farhi et al, 2014

- Encode optimization problem (e.g., max-cut) into Hamiltonian (e.g, Ising model), classically vary parameters in two unitaries to find solution

$$|\psi(\boldsymbol{\beta},\boldsymbol{\gamma})\rangle = \underbrace{U(\boldsymbol{\beta})U(\boldsymbol{\gamma})\cdots U(\boldsymbol{\beta})U(\boldsymbol{\gamma})}_{p \text{ times}}|\psi_0\rangle$$

To minimize:

$$\langle\psi(\boldsymbol{\beta}_{opt},\boldsymbol{\gamma}_{opt})|H_P|\psi(\boldsymbol{\beta}_{opt},\boldsymbol{\gamma}_{opt})\rangle$$

Others:

VQE: Like QAOA for general problems (quantum chemistry)

Annealing (D-wave)

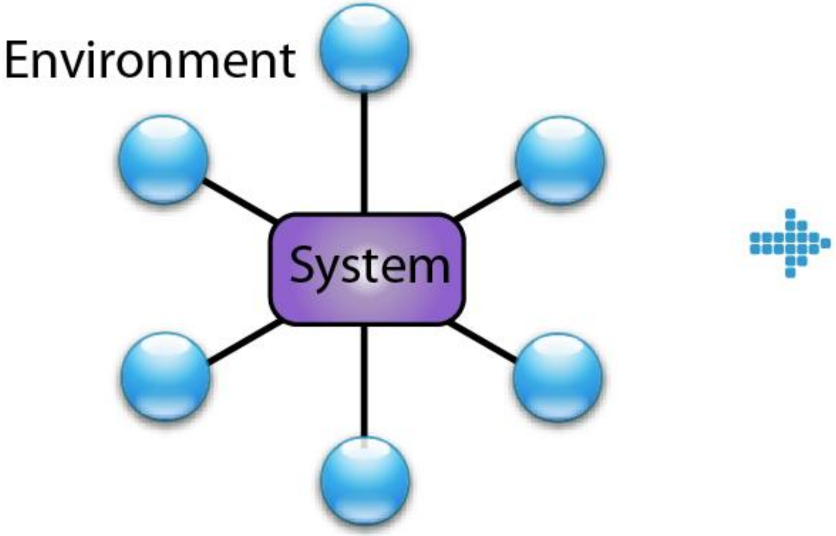
Coherent Ising Machine (NTT)

....

What is noise in the context of quantum computing?

Despite having access to NISQ devices, it is still important to perform classical modelling on a classical computer, to confirm results and understand errors.

In particular, we must model these devices as open systems, and understand how they interact with their environments, and how errors in control and measurements arise or can be mitigated.



The environment is typically composed of infinite degrees of freedom. However, if it is only weakly coupled to the system, one can adopt several perturbative approaches.

Spin-boson model

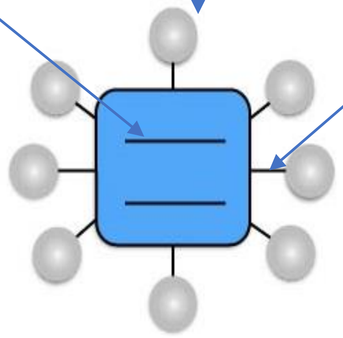
- We can usually capture the main influence of environment degrees of freedom with as a continuum of bosonic modes:

$$H_{\mathrm{SB}} = \frac{\epsilon}{2}\sigma_z + \frac{\Delta}{2}\sigma_x + \sum_k \omega_k a_k^\dagger a_k + \sigma_z \sum_k \frac{g_k}{\sqrt{2\omega_k}}(a_k + a_k^\dagger)$$

System energy

Bath mode frequencies

Coupling strengths



Remarkably this model can reproduce classical friction, and explain decoherence (the emergence of the classical world)

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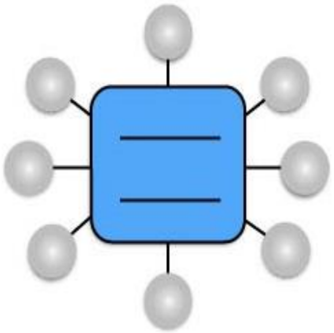


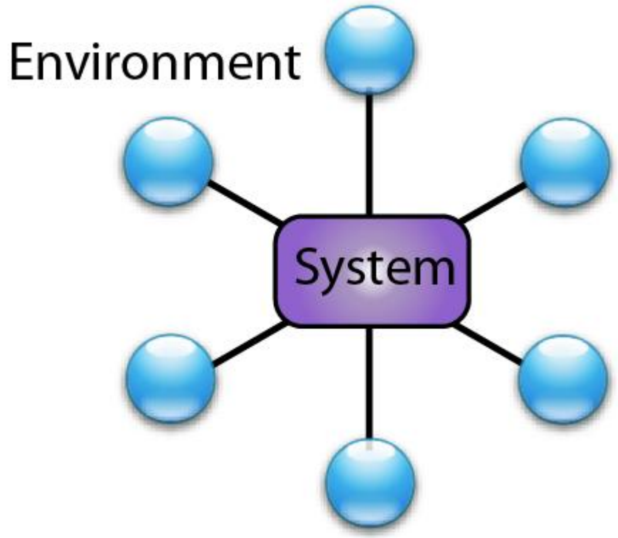
Environment characterized by spectral density and correlation functions

$$J(\omega) = \pi \sum_k \frac{g_k^2}{2\omega_k}\delta(\omega - \omega_k)$$

$$C(t) = \frac{1}{\pi}\int_0^\infty d\omega J(\omega)\left[\coth\left(\frac{\beta\omega}{2}\right)\cos(\omega t) - i\sin(\omega t)\right].$$

While complex, we can impose perturbative approximations and arrive at a range of different simple methods that model most noise sources accurately.

Perturbative methods



Perturbative approaches:

- Lindblad master equations
- Polaron methods
- Bloch-Redfield/non-Secular master equations
- Higher order expansions

To model noise in quantum circuits on a classical computer, we can either:

- Take a `discrete trajectory’ approach, and model bit flips and phase noise as discrete random events (like quantum Monte-Carlo) while frequency and strength depend on environment properties

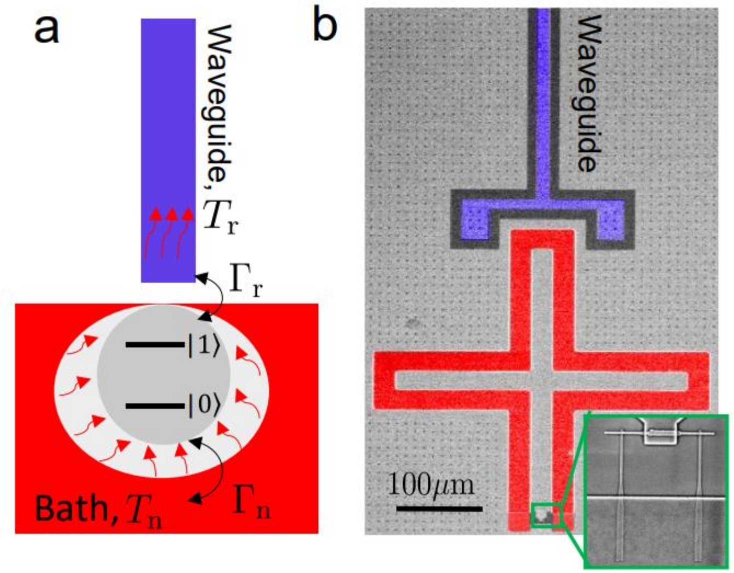
- Model the average behavior with a `density matrix’ and Liouvillian equation of motion

Many powerful software packages make this easier than ever!

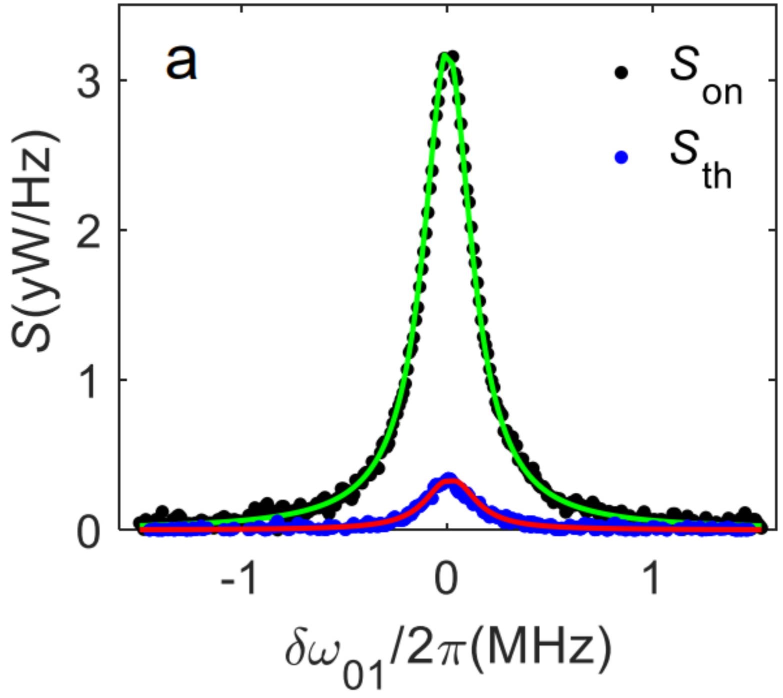
Example: Nonequilibrium heat transport and work with a single artificial atom coupled to a waveguide: emission without external driving

Yong Lu, Neill Lambert, Anton Frisk Kockum, Ken Funo, Andreas Bengtsson, Simone Gasparinetti, Franco Nori, and Per Delsing

By very weakly coupling a qubit to a waveguide we can monitor other noise sources



If we monitor the output of the waveguide,
without driving, what do we expect to see?



Superconducting qubits are strongly affected by quasiparticles (breakdown of superconductivity) and two-level systems in their environment

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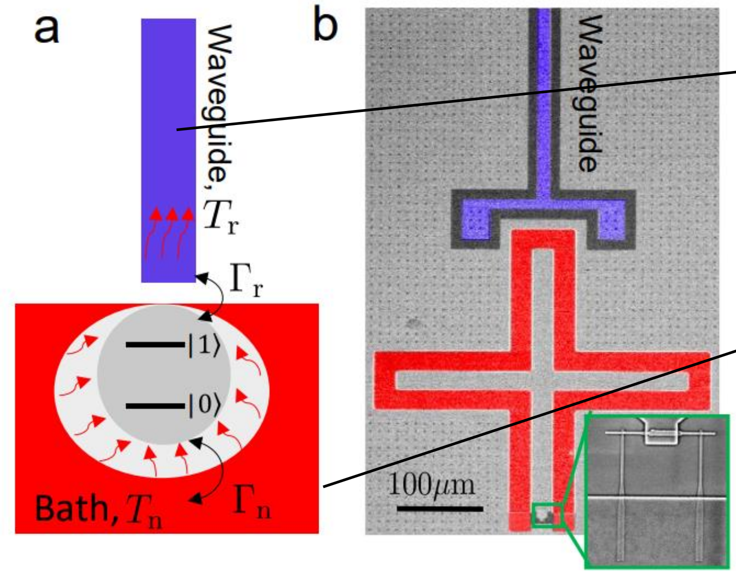
$$\frac{H_{\mathrm{q}}}{\hbar} = -\frac{\Delta}{2}\sigma_z + \frac{\Omega}{2}\sigma_x,$$

$$\frac{\partial}{\partial t}\rho_S(t) = -\frac{i}{\hbar}[H_{\mathrm{q}}, \rho(t)] + \mathcal{L}[\rho(t)],$$



$$\begin{aligned}\mathcal{L}[\rho(t)] = & \boxed{\frac{\Gamma_{\mathrm{r}}}{2}(n_{\mathrm{r}}+1)\,\mathcal{D}[\sigma_-]\rho + \frac{\Gamma_{\mathrm{r}}}{2}n_{\mathrm{r}}\mathcal{D}[\sigma_+]\rho} \\ & + \boxed{\frac{\Gamma_{\mathrm{n}}}{2}(n_{\mathrm{n}}+1)\,\mathcal{D}[\sigma_-]\rho + \frac{\Gamma_{\mathrm{n}}}{2}n_{\mathrm{n}}\mathcal{D}[\sigma_+]\rho} \\ & + \frac{\Gamma_\phi}{4}\mathcal{D}[\sigma_z]\rho,\end{aligned}$$

$$S(\omega) = \frac{\hbar\omega_{01}}{2\pi}\int_{-\infty}^{\infty} dt e^{-i\omega t}\langle b_{\mathrm{out}}^\dagger(t) b_{\mathrm{out}}(t')\rangle_{(t'\to\infty)}$$

$$\begin{aligned}\langle b_{\mathrm{out}}^\dagger(t) b_{\mathrm{out}}(t')\rangle = & \,\Gamma_{\mathrm{r}}(n_{\mathrm{r}}+1)\langle\sigma_+(t)\sigma_-(t')\rangle \\ & - \Gamma_{\mathrm{r}} n_{\mathrm{r}}\langle\sigma_-(t')\sigma_+(t)\rangle + \langle f_{\mathrm{in}}^\dagger(t) f_{\mathrm{in}}(t')\rangle \\ & - \frac{i\Omega^*}{2}\langle\sigma_-(t')\rangle + \frac{i\Omega}{2}\langle\sigma_+(t)\rangle + \frac{|\Omega|^2}{4\Gamma_{\mathrm{r}}}.\end{aligned}$$

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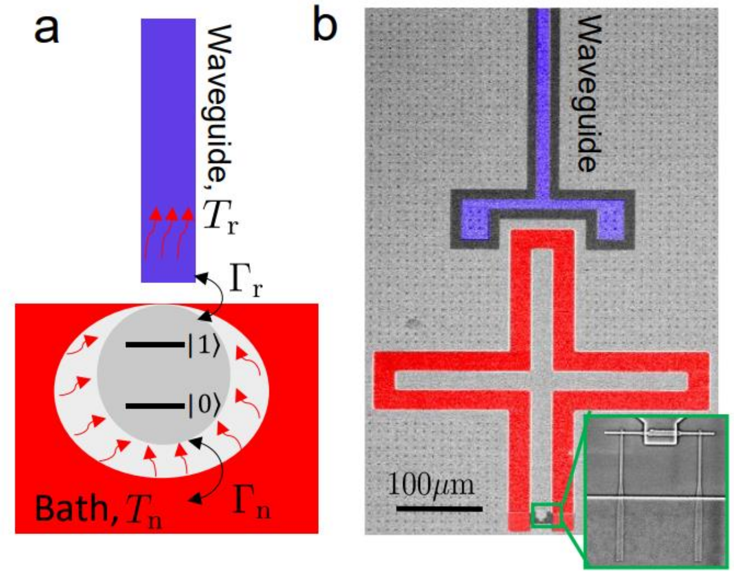
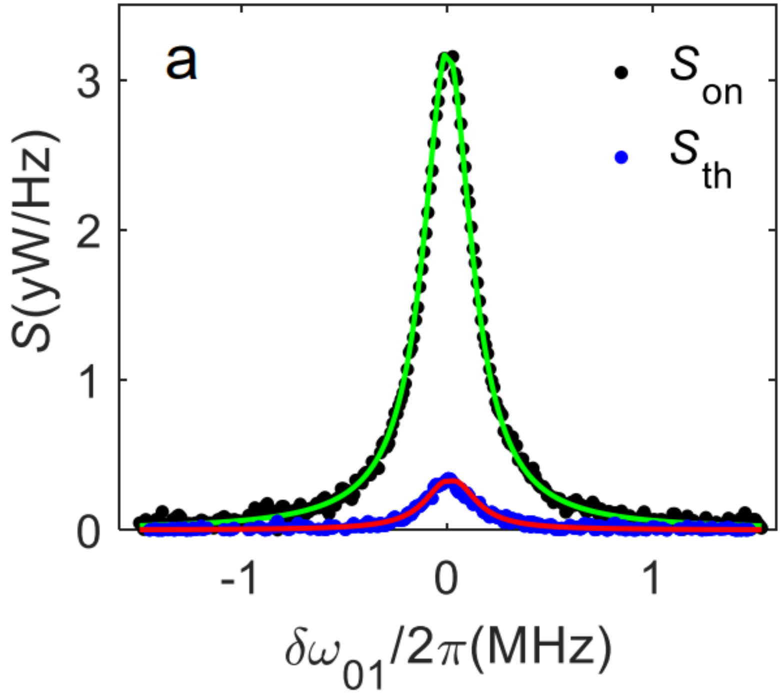


If we monitor the output of the waveguide,
without driving, what do we expect to see?

$$S_{\rm th}(\omega) = \hbar\omega_{01}\frac{\Gamma_{\rm r}}{2\pi}\frac{2\Gamma_2\Gamma_{\rm n}\Delta n/\Gamma_1}{\delta\omega_{01}^2+\Gamma_2^2},$$

$$\Delta n = n_{\rm n} - n_{\rm r}$$



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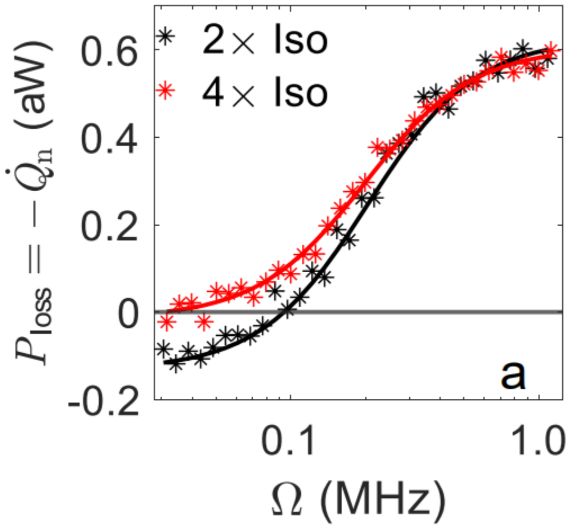
Simple noise models are very robust: If we add coherent drive, we can also characterize the power loss, work and heat

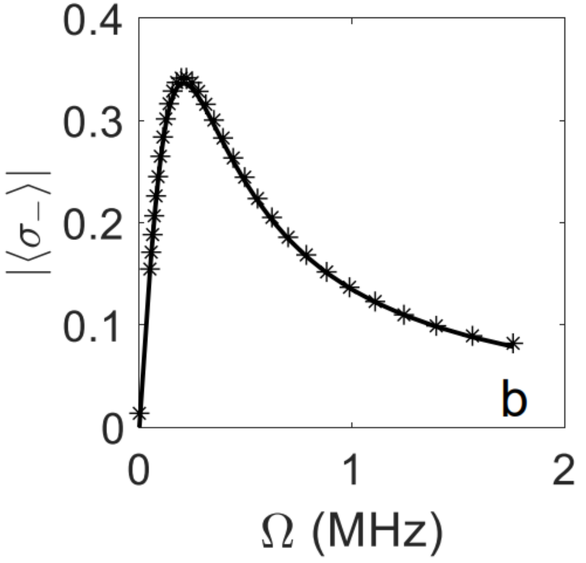


Power loss = Input – output power

Zero drive: gain from thermalization of qubit from secondary bath

Strong drive: saturation of qubit

Adding isolators reduces temperature of secondary bath



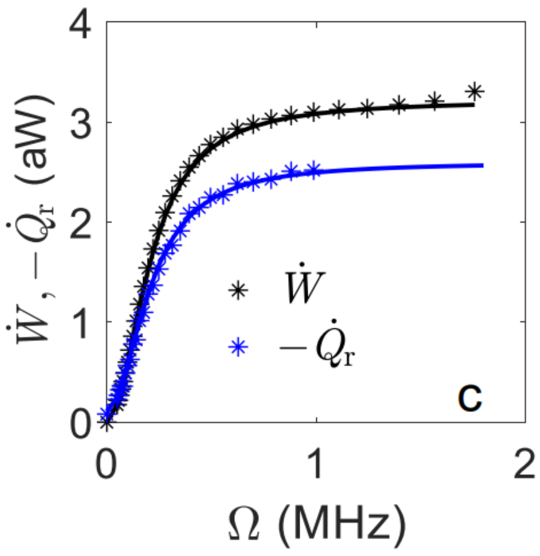
We can extract the qubit coherence from the single-tone spectroscopy

$$\langle \sigma_- \rangle = i(\langle b_{\text{out}} \rangle - \langle b_{\text{in}} \rangle)/\sqrt{\Gamma_{\text{r}}}$$

And use it to calculate the work done by the coherent drive

$$\dot{W} = \text{Tr}\left\{-i[H_0, H_1]\rho\right\} = \frac{\hbar\Omega}{2}\langle \sigma_y \rangle = \hbar\Omega\Re[i\langle \sigma_- \rangle]$$

$$\dot{Q}_{\text{i}} = \hbar\omega_{01}(\Gamma_{\text{i}} n_{\text{i}} \langle \sigma_- \sigma_+ \rangle - \Gamma_{\text{i}}(n_{\text{i}} + 1)\langle \sigma_+ \sigma_- \rangle)$$



Essentially, we show that the power loss is given by the heat flow to the secondary bath, and that work and the two heat flows of course obey the first law

$$\dot{Q}_{\text{r}} + \dot{Q}_{\text{n}} + \dot{W} = \dot{U}$$

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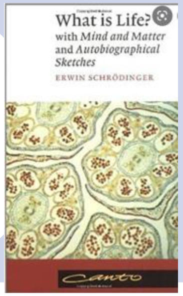
Timeline of quantum effects in biology (focus on photosynthesis and magnetoreception)

2007-??: Large range of explanations for the role of coherence and noise in optimal efficiency (Plenio, Aspuru-Guzik, Manczel, etc)

1944 Schrodinger:

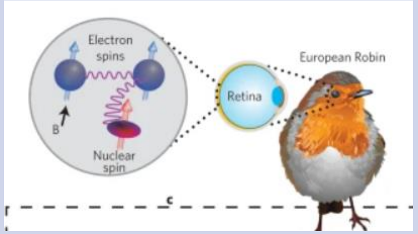
Quantum effects important in some biological processes?



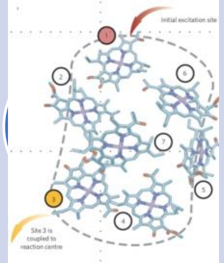
1972: Wiltschko: Bird’s have an inclination compass:

1978:

Radical-pair magneto-reception proposal (Schulten et al.)

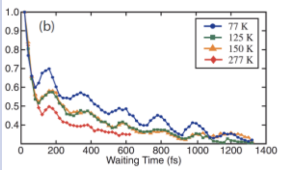


2007: Engel et al. demonstrate beating in FMO complex @ 77K

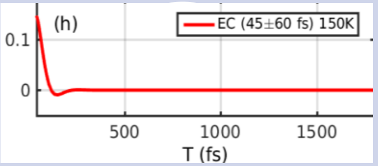


2006/2010: Wiltschko: Bird’s ability to navigate dependent on ambient light, affected by external oscillating Magnetic fields.
Hore/Schulten: Cryptochromes.
Maeda: Demonstration in solution

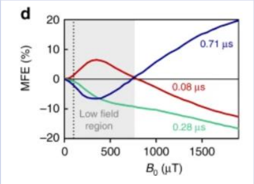
2010: FMO complex experiment repeated at room temperature (PNAS)



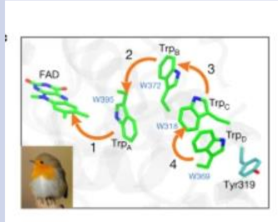
2017/2021: Repeated FMO experiments show limited coherence (Thorwart, Miller). Focus on the influence of noise?



2019: Kerpal et al, Nat. Comms, Demonstration of sensitivity of radical pair to 50 micro-tesla

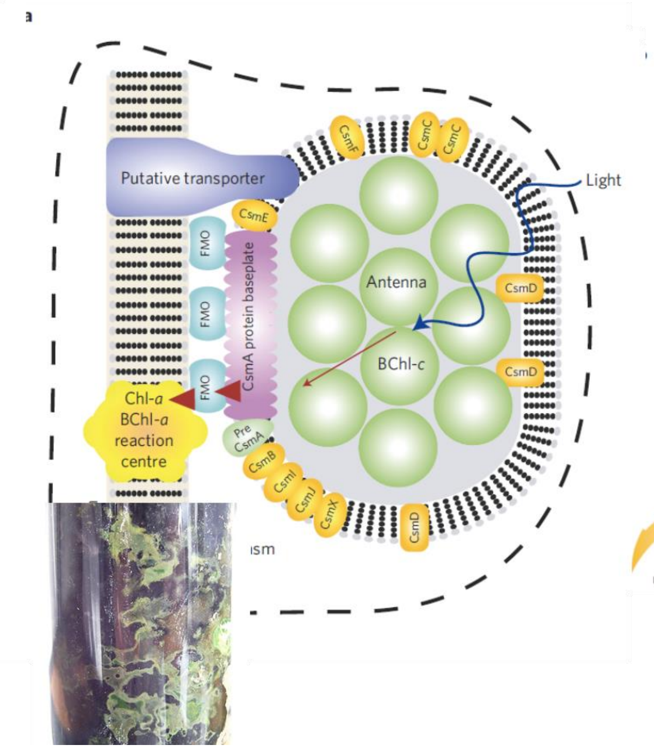


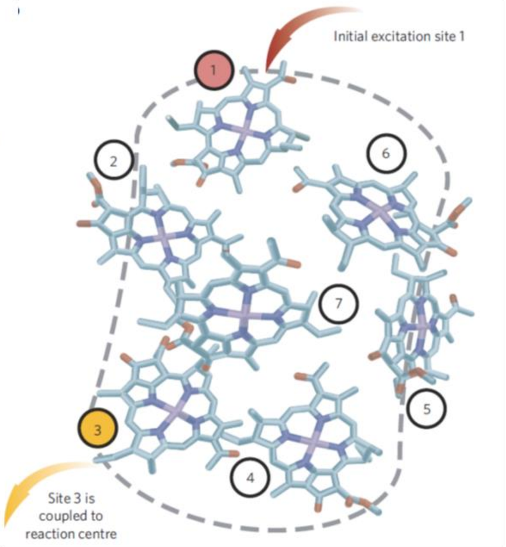
2021: Demonstration of magnetic sensitivity in cryptochrome from migratory songbird (Xu, Hore, Nature)

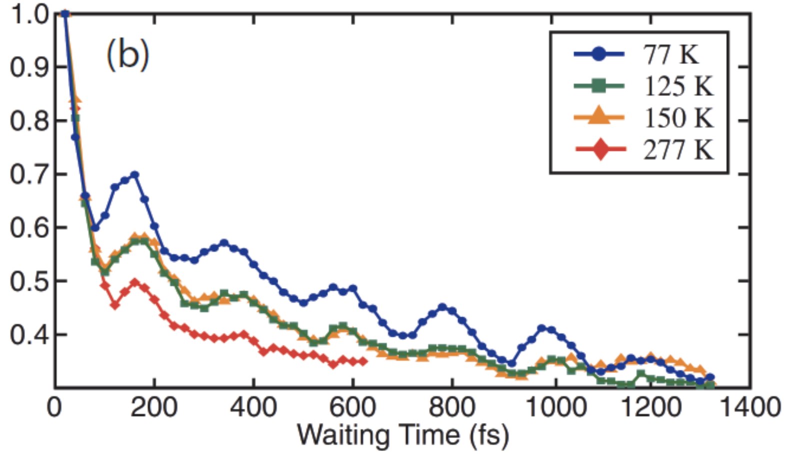


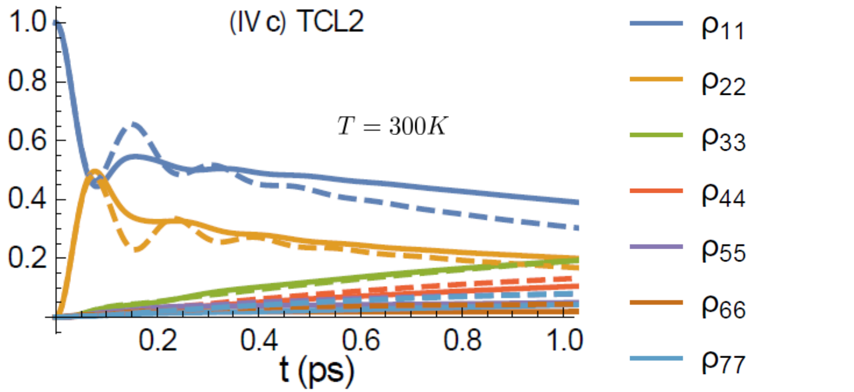
Photosynthesis: A simple physics picture

Light-harvesting in the Fenna-Matthews-Olsen complex: does quantum coherence persist on time scales relevant for energy transfer?









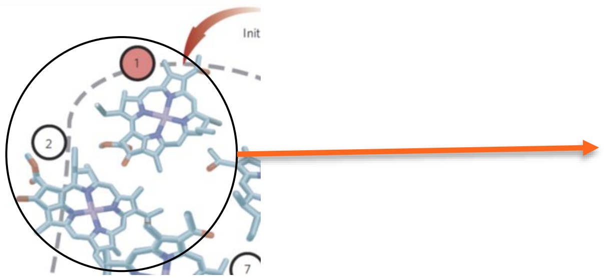
Fruchtman, Lambert, Gauger, Sci. Rep. 2016

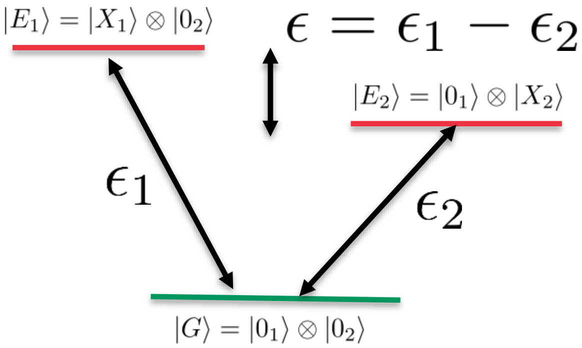
Modelling the energy transfer might be tricky:

- Electrical excitations strongly couple to nuclear motion
- Thermal energy is on the same order as reorganization energy, electronic coupling, etc

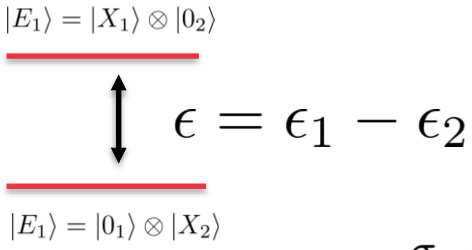
Photosynthesis: A simple physics picture

- A minimal model of a single excitation being transported through the complex: lets focus on just two sites





- If we focus on a single excitation subspace, we can just describe the two molecules as an effective spin:

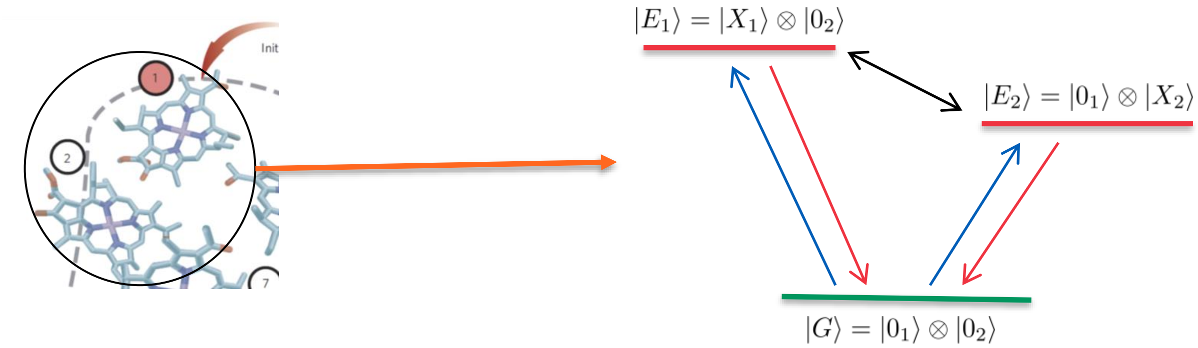


$$H_E = \frac{\epsilon}{2}\sigma_z$$

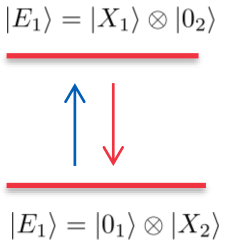
$$\sigma_z = |X_1, 0_2\rangle\langle X_1, 0_2| - |0_1, X_2\rangle\langle 0_1, X_2|$$

Photosynthesis: A simple physics picture

- Energy transfer between sites is given by dipole coupling:



- Energy transfer between sites does not involve an actual movement of charge. We can also capture the contribution to the total energy (Hamiltonian) with two-site model

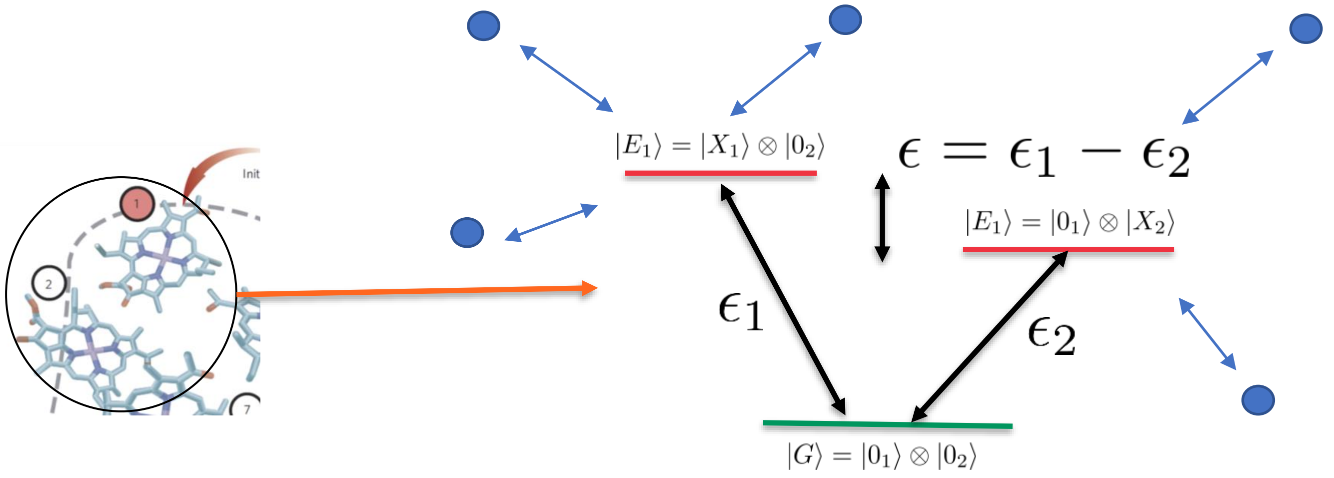


$$H_D = \frac{\Delta}{2}\sigma_x$$

$$\sigma_x = |X_1, 0_2\rangle\langle 0_1, X_2| + |0_1, X_2\rangle\langle X_1, 0_2|$$

Spin-boson model

- The nuclear motion+molecular vibrations and protein scaffold, modulate the eletronic excitation energy. We describe these with a bath of harmonic oscillators



a_k Is the annihilation operator for mode k In the environment (destroys a vibrotational Excitation at frequency ω_k)

$[a_k, a_k^\dagger] = 1$

$$H_{\mathrm{SB}} = \frac{\epsilon}{2}\sigma_z + \frac{\Delta}{2}\sigma_x + \sum_k \omega_k a_k^\dagger a_k + \sigma_z \sum_k \frac{g_k}{\sqrt{2\omega_k}}(a_k + a_k^\dagger)$$

$$\sigma_x = |X_1, 0_2\rangle\langle 0_1, X_2| + |0_1, X_2\rangle\langle X_1, 0_2| \qquad \sigma_z = |X_1, 0_2\rangle\langle X_1, 0_2| - |0_1, X_2\rangle\langle 0_1, X_2|$$

- Note that in general, each chromophore couples to an independent bath (though correlated baths have been studied).

Spin-boson model

- The nuclear motion+molecular vibrations and protein scaffold, modulate the eletronic excitation energy. We describe these with a bath of harmonic oscillators

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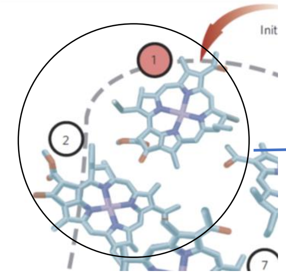
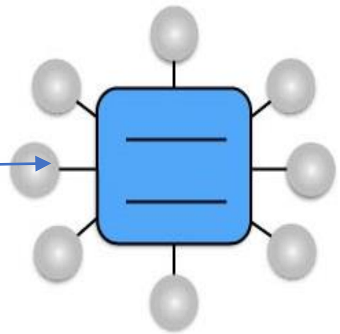




Environment characterized by spectral density and correlation functions

$$J(\omega) = \pi \sum_k \frac{g_k^2}{2\omega_k}\delta(\omega - \omega_k)$$

$$C(t) = \frac{1}{\pi}\int_0^\infty d\omega J(\omega)\left[\coth\left(\frac{\beta\omega}{2}\right)\cos(\omega t) - i\sin(\omega t)\right].$$

We can use a lot of the tools we use for quantum information to model this noise, but what happens when we cannot impose those perturbative approximations?

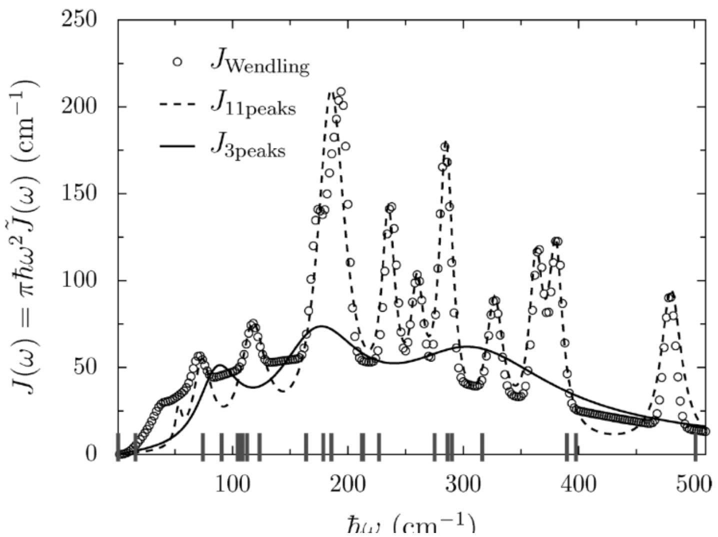
What are the properties of this ‘bath”?

- Modelling of the dynamics of a real photosynthetic complex is hard because of the complex environment. Are simple perturbative methods sufficient?

- Can we capture this influence in a transparent way with new methods?

- Can we understand better how the electronic and vibronic degrees of freedom are correlated, and how that affects coherence, transport, etc?

- Can these features be measured in an experiment?



Kreisbeck and Kramer,
J. Phys. Chem. Lett. 2012

Existing methods:

Matrix-product-state based approaches:
A. Chin *et al. Nat. Phys.* 2013

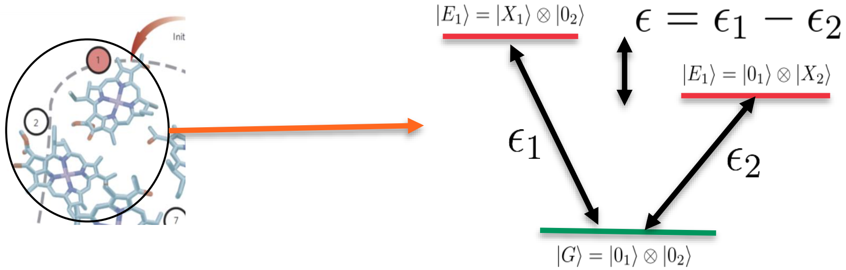
The hierarchy equations of motion:
Tanimura and Kubo, J. Phys. Soc. Jpn. 1989,
Ishizaki and Fleming, PNAS 2009.

An an example of the utility of modelling non-perturbative noise:

Example: role of environment structure using RC method

Illes-Smith, Lambert, Nazir, Phys. Rev. A (2014), and J. Chem. Phys. (2016) , Ishizaki and Fleming, J. Chem. Phys. (2009)

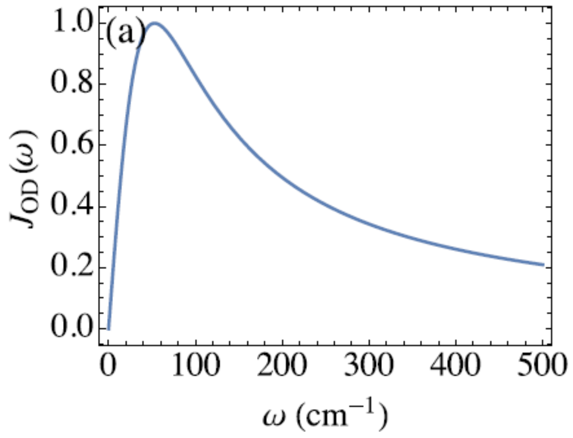
We parameterize the speed of energy transfer by fitting an effective ‘rate’ to the movement of an excitation from one site to another:



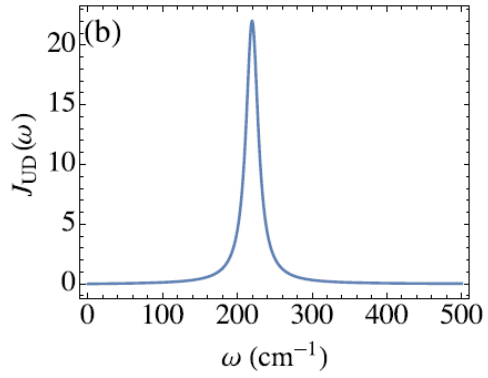
$$\frac{dP_1(t)}{dt} = -k_{1\to2}P_1 + k_{2\to1}P_2,$$
$$\frac{dP_2(t)}{dt} = k_{1\to2}P_1 - k_{2\to1}P_2.$$

Using non-perturbative method, we can study resonant vs. broad environments:

$$J_{\mathrm{SB}}^{\mathrm{OD}}(\omega) = \alpha_{\mathrm{OD}}\omega_c \frac{\omega}{\omega^2 + \omega_c^2}.$$

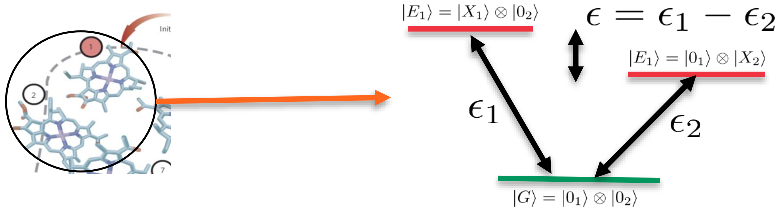


$$J_{\mathrm{SB}}^{\mathrm{UD}}(\omega) = \frac{\alpha_{\mathrm{UD}}\Gamma\omega_0^2\omega}{(\omega_0^2 - \omega^2)^2 + \Gamma^2\omega^2}$$



$\epsilon = 100$ cm^{-1}, $\Delta = 40$ cm^{-1}, $\omega_c = 53$ cm^{-1}, and $T = 300$ K.

An an example of the utility of modelling non-perturbative noise:



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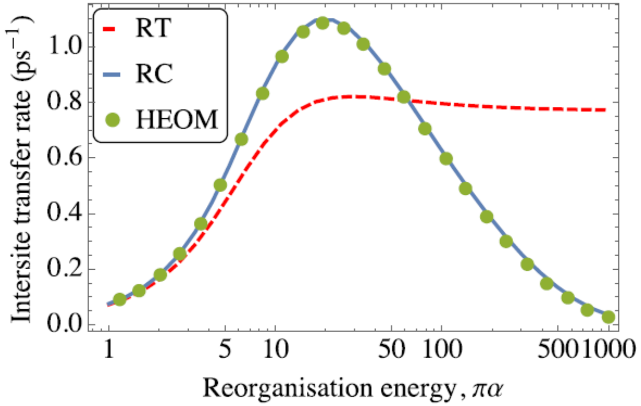

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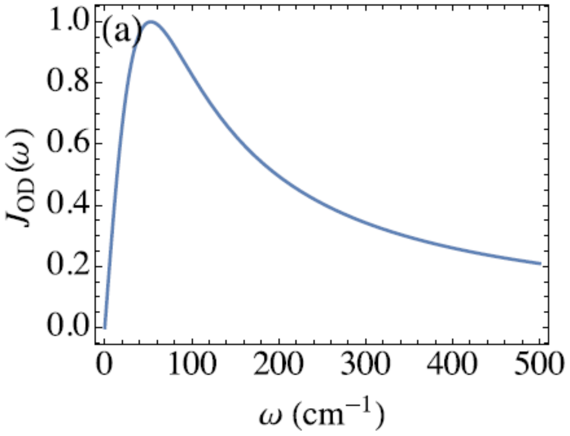

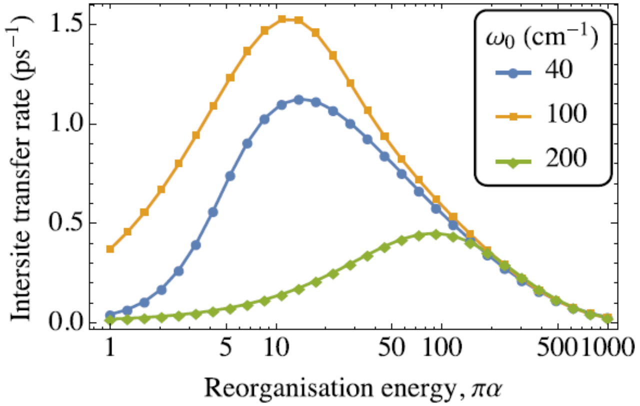

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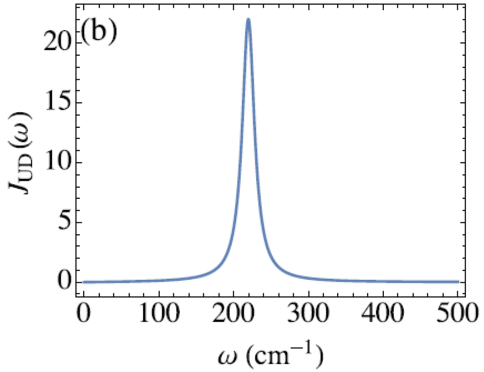

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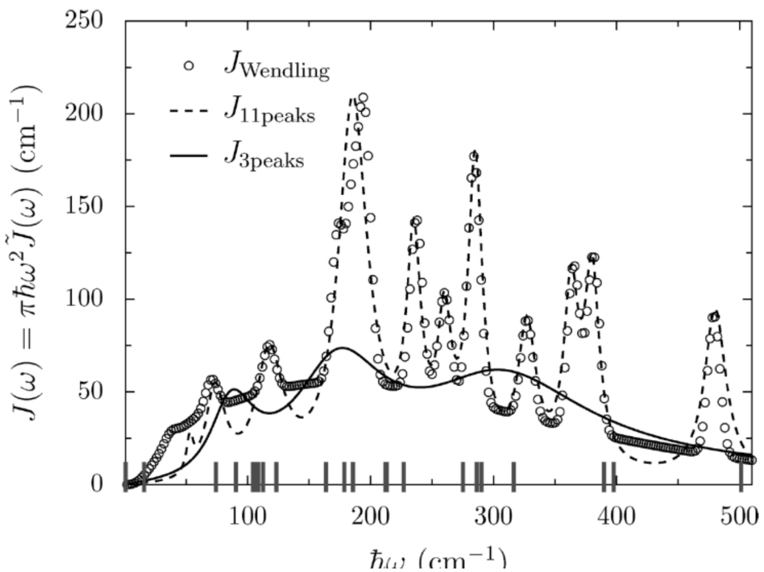
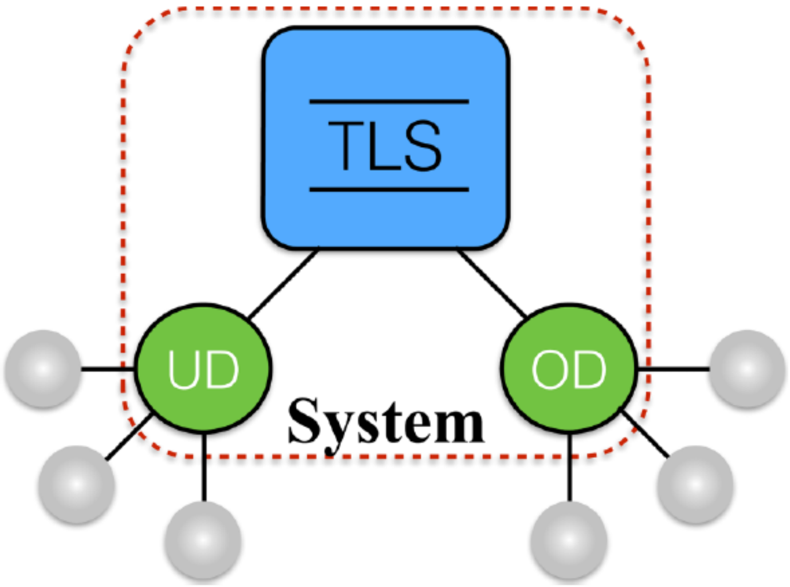
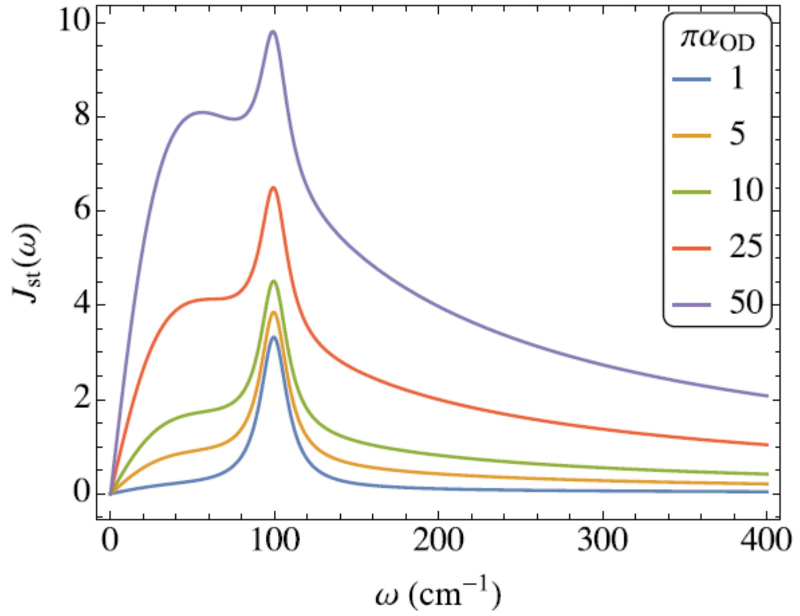
What about when both broad and resonant baths co-exist?







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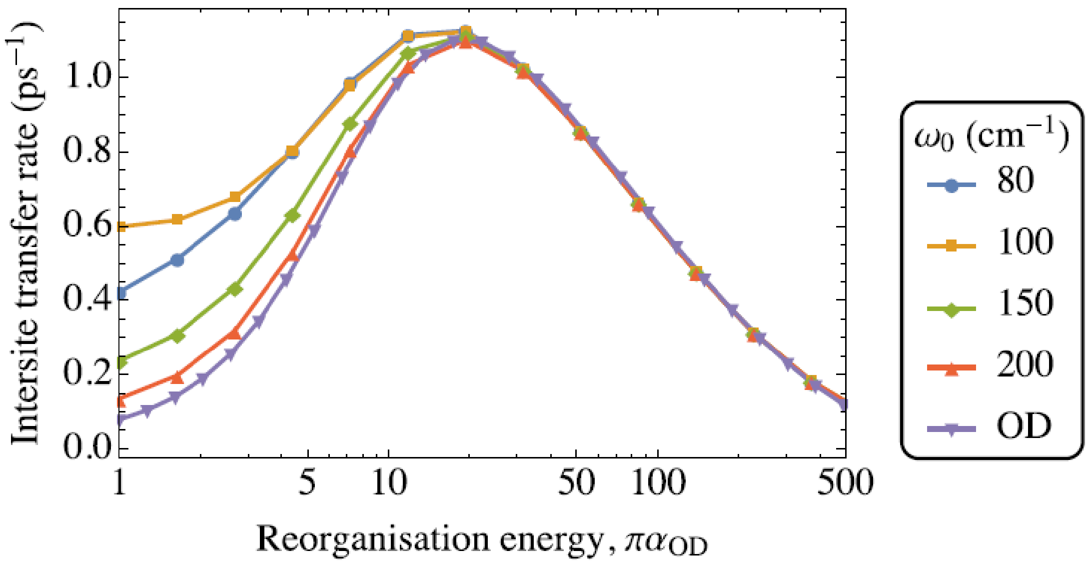

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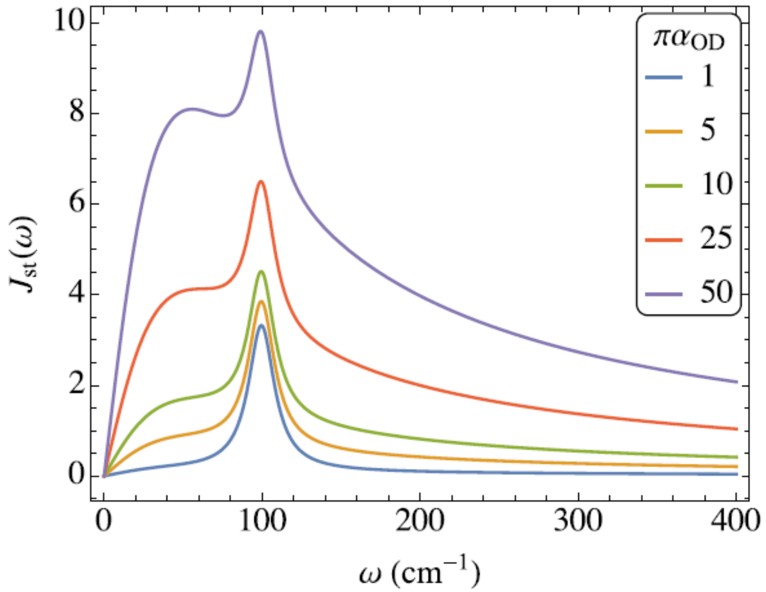

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Resonant structured baths enhance energy transfer, but their influence is diminished if the broad background is sufficiently strong

Overview:

Part 1:

Introduction to qubits and quantum computing

From qubits to quantum biology

Introduction to QuTiP

Part 2:

Deriving approximate noise models: Lindblad master equation

Non-perturbative methods: HEOM and reaction coordinates