The Case for *Quantum-Coherent Nuclear Engineering*

Florian Metzler, PhD
2/7/2021

Confidential

Overview

- Quantum 2.0 and Nuclear: Programmatic considerations
- So what is coherence?
- What can coherence do for us? An overview of quantum dynamics
- The future of quantum dynamics simulations
- How can weak couplings have large effects?
- Building intuition on dynamics and transition rate changes
- Quantum-coherent engineering
- Quantum coherence at the nuclear level
- Nuclear reactions and nuclear state transitions
- What's next?
- How to create quantum-coherent nuclear ensembles?
- Reviewing relevant experiments
- Proposed experiments (toward definitive confirmation and applications)
- What does quantum-coherent nuclear engineering look like?

Quantum 2.0 and Nuclear: Programmatic considerations

Two ways to approach research

DEMAND SIDE

What problems need solving?
What do we know that might help address them?

FORTHCOMING ARTICLE:
"Nuclear fusion rate enhancement in solid-state environments"

SUPPLY SIDE

What new tools are emerging?
In what ways can they be applied?

PROPOSED ARTICLE:
"The Case for Quantum-Coherent Nuclear Engineering"

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- Quantum dynamics

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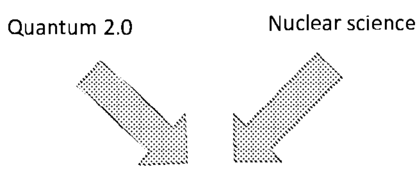
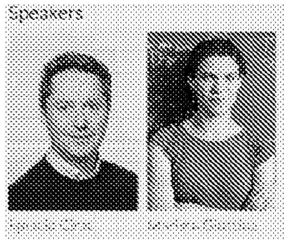


What is Quantum 2.0?

A definition

OSA Quantum 2.0 Conference



*"Quantum 2.0 refers to **the development and use of many-body quantum superposition, entanglement, and measurement** to advance science and technology. Examples are quantum computing and simulation, quantum communications, and quantum sensing.*

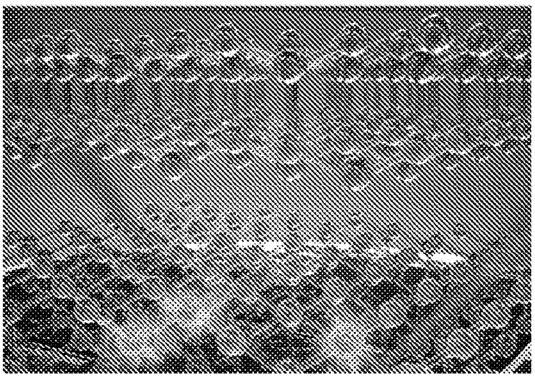
*New resulting technologies will potentially go for beyond the **(quantum 1.0) capabilities offered by systems without the conceptual need for large-scale superposition or entanglement**, examples of which are conventional semiconductor electronics, loser-based communication systems and magnetic-resonance medical imagers."*

https://www.osa.org/en-us/meetings/topical_meetings/quantum/program/

More on Quantum 2.0: Basic Energy Sciences Roundtable

Basic Energy Sciences Roundtable

Opportunities for Basic Research for Next-Generation Quantum Systems



Participants:

- Aashish Clerk, University of Chicago
- Peter Denes, Lawrence Berkeley National Laboratory
- Michael Flatté, University of Iowa
- Danna Freedman, Northwestern University
- Giulia Galli, University of Chicago
- Stephen Jesse, Oak Ridge National Laboratory
- Mark Kasevich, Stanford University
- Chris Monroe, University of Maryland/IonQ
- William Oliver, Massachusetts Institute of Technology
- Chris Palmstrøm, University of California–Santa Barbara
- Nitin Samarth, Pennsylvania State University
- Darrell Schlom, Cornell University
- Irfan Siddiqi, University of California-Berkeley/Lawrence Berkeley National Laboratory
- Jeff Taylor, Los Alamos National Laboratory
- Birgitta Whaley, University of California–Berkeley
- Amir Yacoby, Harvard University
- Jun Ye, JILA, University of Colorado

Awschalom, D., Christen, H., Clerk, A., Denes, P., Flatté, M., Freedman, D., Galli, G., Jesse, S., Kasevich, M., & Monroe, C. (2017). *Basic Energy Sciences Roundtable: Opportunities for Basic Research for Next-Generation Quantum Systems*. USDOE Office of Science (SC) (United States). https://www.osti.gov/servlets/purl/1616258

More on Quantum 2.0: Basic Energy Sciences Roundtable

Emphasizing controlled superposition

"From the transistor to the molecular switch, quantum mechanics is at the heart of nearly all materials properties and chemical processes. Still, the subtleties of quantum behavior are often hidden from view. As a result, ***only a small number of scientific techniques and technological applications take advantage of the unique phenomena of quantum superposition and entanglement****. Harnessing these counterintuitive properties of matter promises to yield revolutionary new approaches to computing, sensing, communication, and metrology. [..]*

Quantum-coherent systems have been discovered that exhibit remarkable properties and ever increasing coherence times. However, ***understanding of how these systems interact (for example, the complexity of entanglement) is currently limited to a small number of systems****. Advances in tahis field require an understanding of the scaling of coherence lengths and times with system size and complexity, and the identification of new signatures of quantum states in artificial quantum-coherent systems."*

More on Quantum 2.0: Basic Energy Sciences Roundtable

Coherent quantum-to-quantum transduction

"[Goals:] ***Discover novel approaches for quantum-to-quantum transduction: The coherent transduction of information [and energy!] from one modality to another, at the single-particle or quantum level****, is at the core of quantum measurement and information processing. The development of quantum science will also contribute to areas outside of computing.* ***Control over quantum-coherent states in artificial systems may lead to enhanced transduction for novel electronics, efficient light harvesting and photovoltaics, new techniques for cosmology and nuclear science****, and sensing capabilities that are orders of magnitude beyond current standards."*

More on Quantum 2.0: Basic Energy Sciences Roundtable

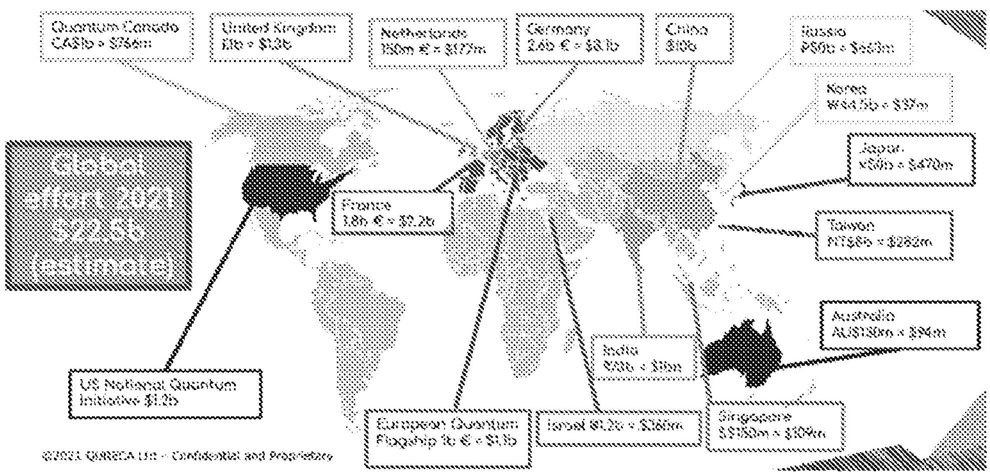
Photosynthesis, strong coupling, tunable lattices

"The light harvesting apparatus of plants and bacteria possesses remarkable capabilities of reaching near unit efficiency for the conversion of an absorbed photon to an electron which goes on to initiate the [..] chemical reactions of photosynthesis. [..] Recent ultrafast spectroscopy and theoretical work have revealed insight into ***the quantum dynamics of the energy transfer and show how the excitonic degrees of freedom interact cooperatively with phonons to ensure the optimality and robustness of the transport in the presence of disorder****. This approach can provide important insights for the design of quantum-to-quantum transducers. [..]*

Theory of quantum state transfer: A key challenge in any quantum transduction scheme is to find a ***quantum system that is flexible enough to couple strongly and coherently to a variety of distinct systems and is thus capable of acting as a "quantum bus."*** *[..] A prime example is the use of vibrational modes of a mechanical resonator as a quantum bus. [..]*

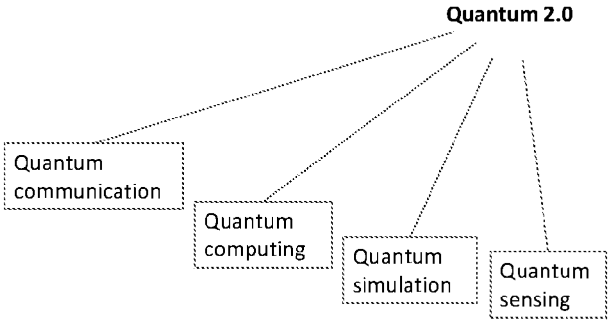
Arrays of dopant atoms, or metal-organic sites, with specified arrangements can be introduced to ***create highly tunable superlattices to enhance particular phonon, plasmon, or optical modes."***

Worldwide efforts



A typical categorization: EU Quantum Flagship

"The Second Quantum Revolution is unfolding now, exploiting the enormous advancements in our ability to detect and manipulate single quantum objects. The Quantum Flagship is driving this revolution in Europe."



Quantum Flagship (2021) Quantum Technology | The future is Quantum. Quantum Technology. https://qt.eu/

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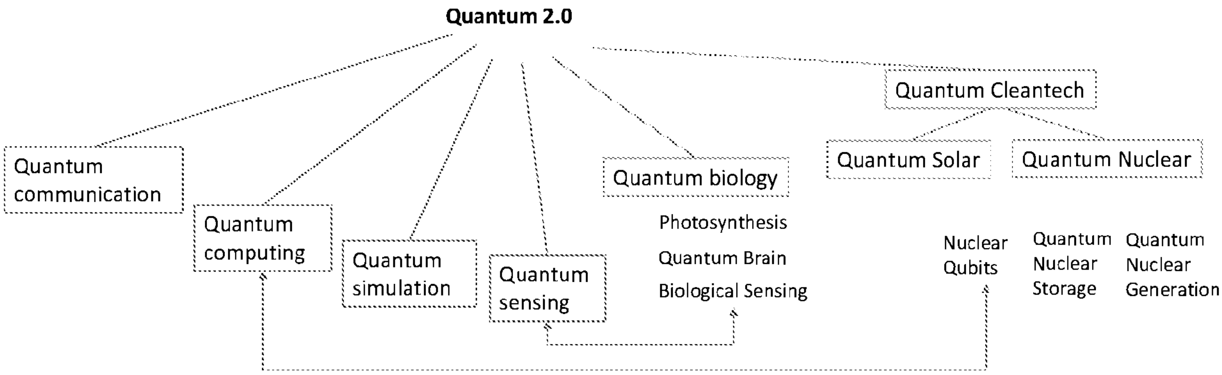

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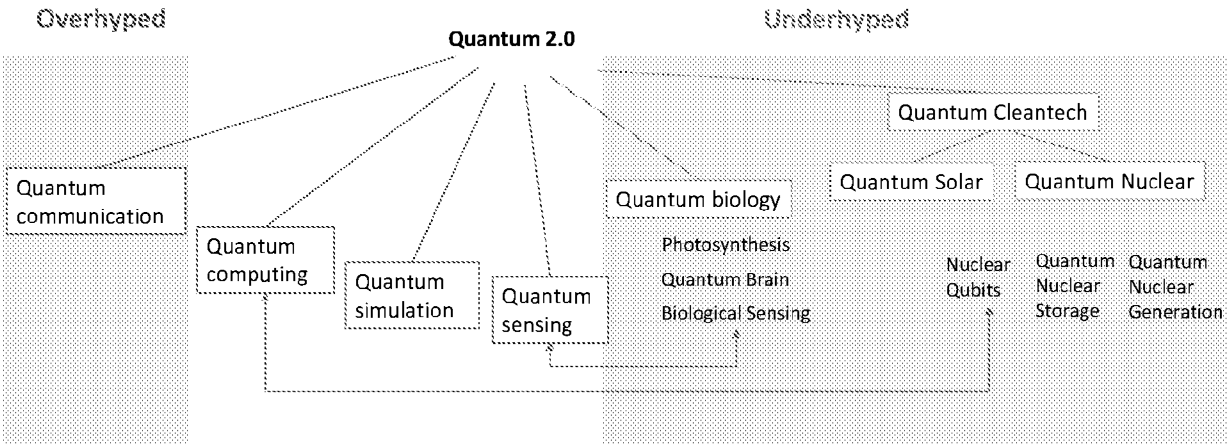


Lack of appreciation of quantum physics in traditional nuclear engineering

Does nuclear engineering involve a lot of quantum physics?

James Miller

My nuclear engineering course involved zero quantum physics.

Even when dealing with theoretical parts like neutron absorption cross-sections and stuff like that, the treatment was entirely classical: neutrons and atoms thought of as ball-bearings with momentum crashing into each other, rather than as wavefunctions interacting at quantized energy levels in bra-ket notation.

If you want a quantum-heavy course, nuclear engineering is about as appropriate for you as majoring in gender studies.

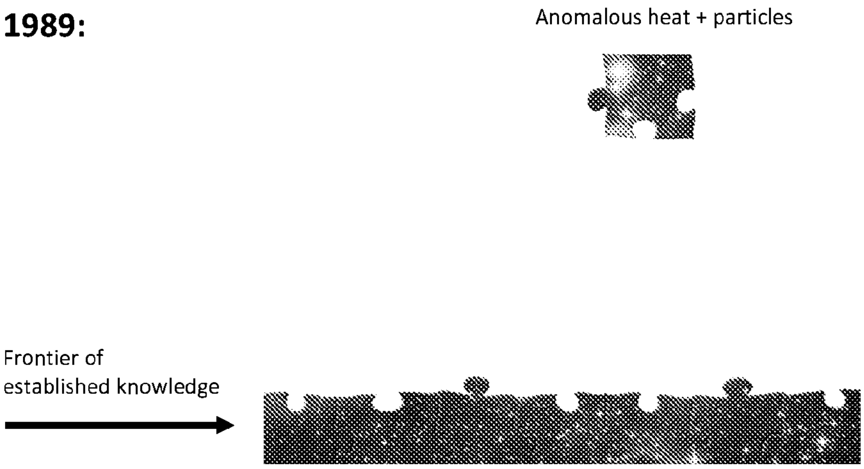
Michael Flagg, Nuclear Engineer

I'd say no, nuclear engineering does not involve a lot of quantum physics. You must be conversant in the theory and I regard it as useful to return to when trouble-shooting problems involving nuclear core management. That said, the vast majority of your work can be handled using classical physics, though when dealing with materials challenges, quantum mechanics can also play a role in investigating the root cause of some issues

https://www.quora.com/Does-nuclear-engineering-involve-a-lot-of-quantum-physics

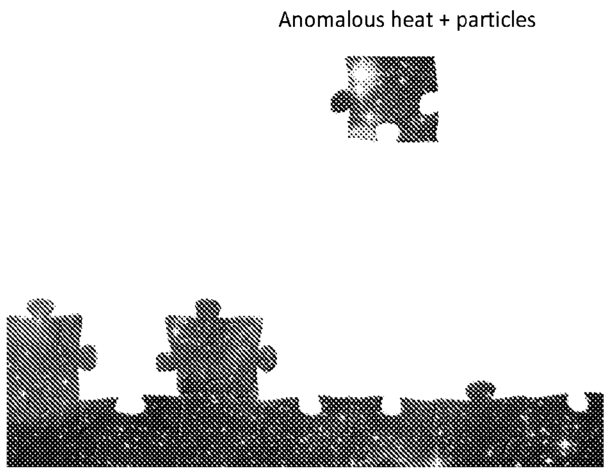
Situating solid-state nuclear anomalies

1989:



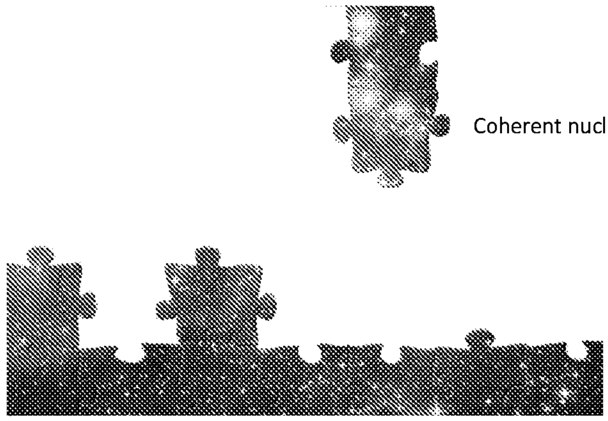
Situating solid-state nuclear anomalies

1999:



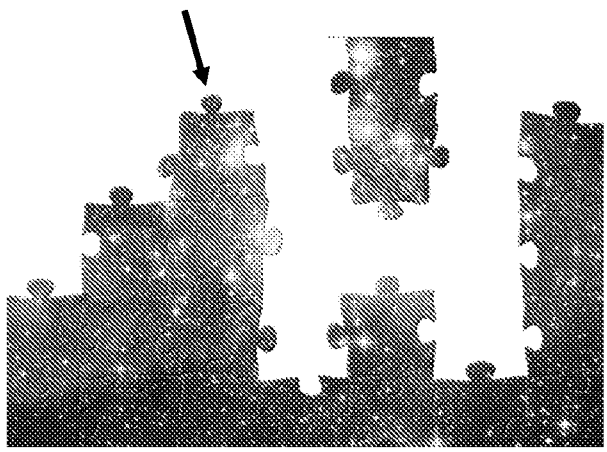
Situating solid-state nuclear anomalies

2000:



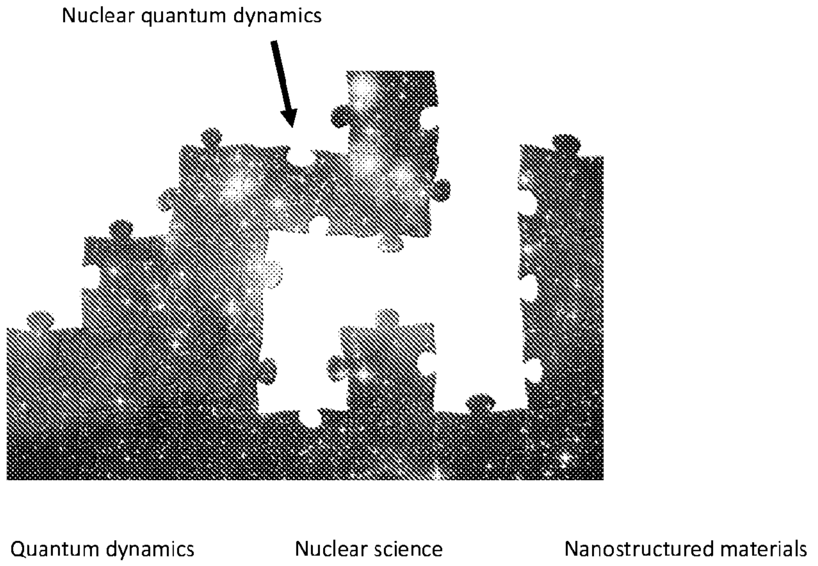
Situating solid-state nuclear anomalies

2020:



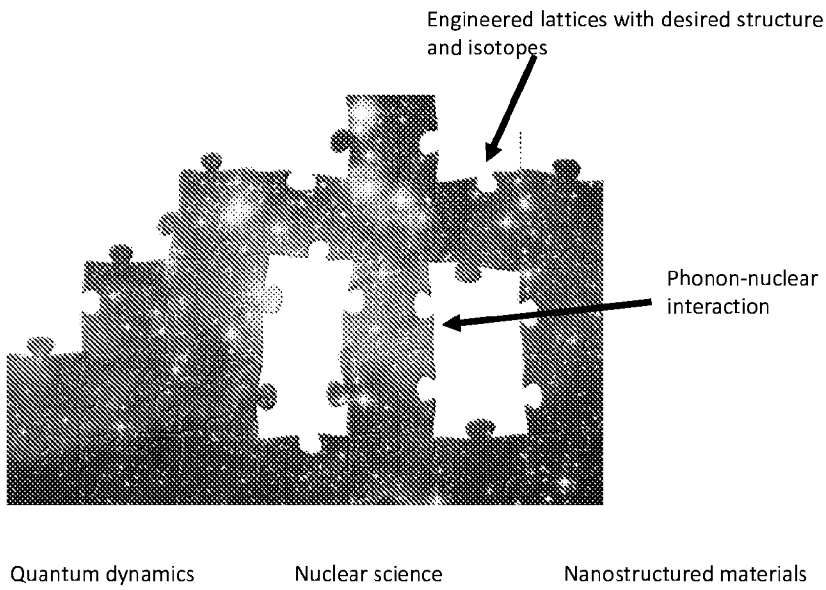
Situating solid-state nuclear anomalies

2021-2025:



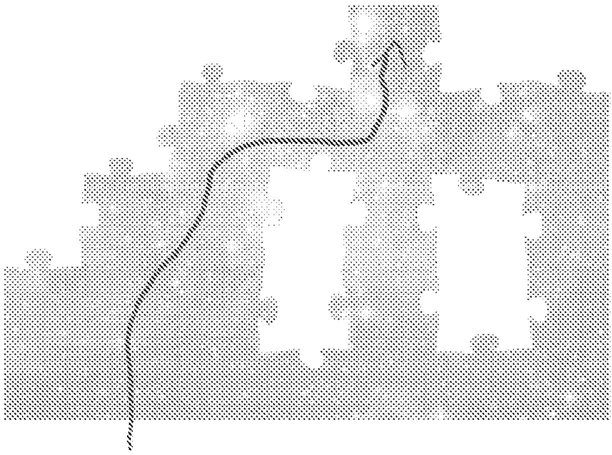
Situating solid-state nuclear anomalies

2025-2030:



Situating solid-state nuclear anomalies

This presentation:



Quantum dynamics Nuclear science Nanostructured materials

A timely frontier

Outlook

I will show the gradual transition from quantum computing to quantum-coherent nuclear engineering.

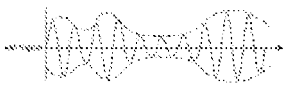
Spoiler:
Quantum-coherent nuclear engineering is essentially quantum computing with high-energy qubits!

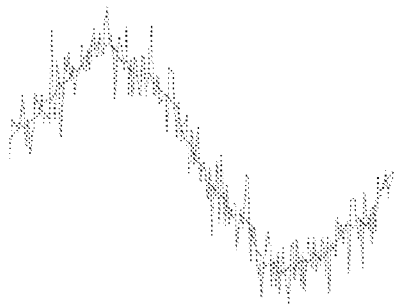
A timely frontier

The fidelity/energy tradeoff

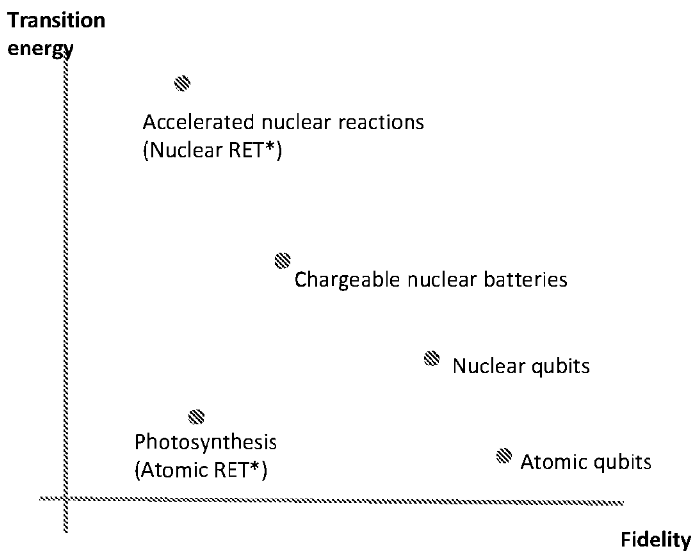
Compare with classical electromagnetics:

- A low-energy electromagnetic wave constitutes a signal
- A high-energy electromagnetic wave constitutes energy transfer



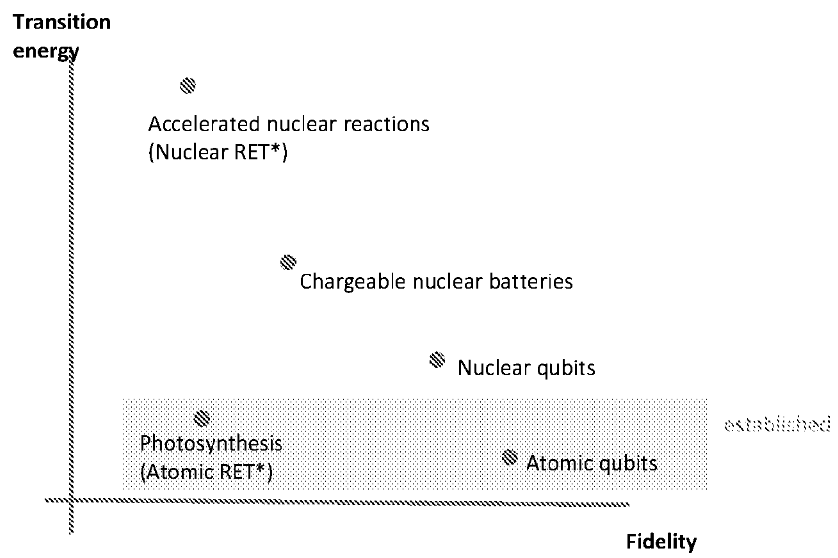


A timely frontier



* RET = Resonance Energy Transfer

A timely frontier



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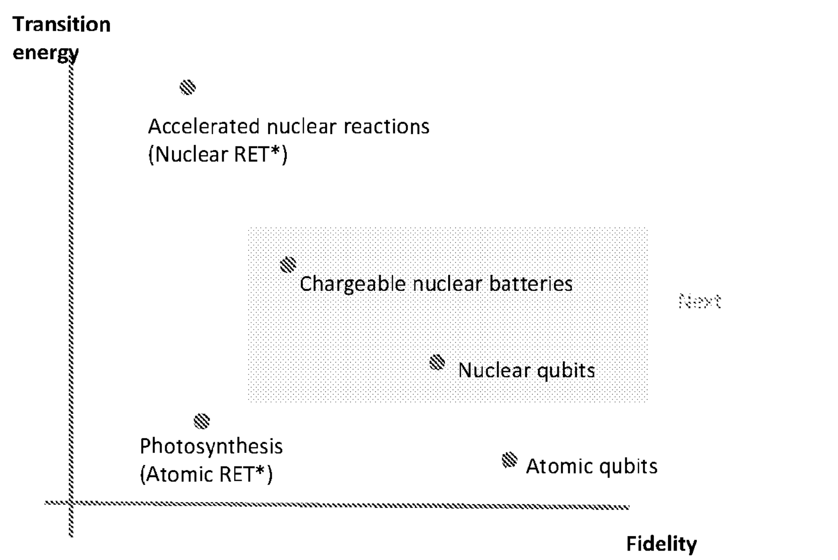
A timely frontier



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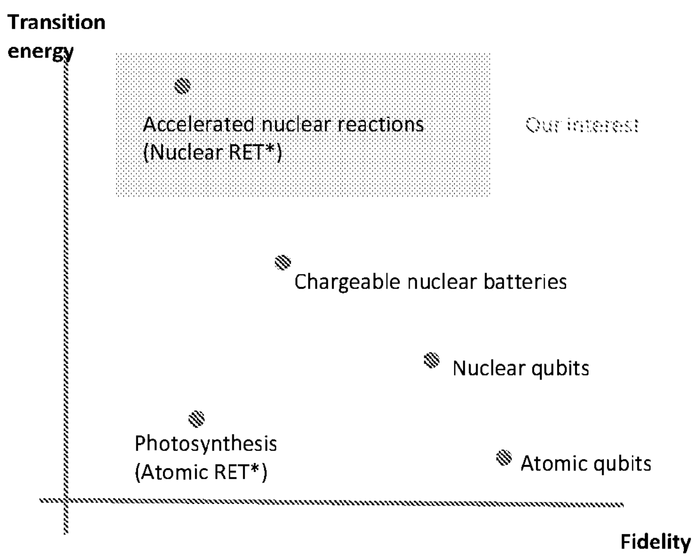


* RET – Resonant Energy Transfer

So what is coherence?

Introduction to coherence

A definition:

A quantum system sufficiently stable so that it can maintain discrete energy/information states, including superposition with coupled subsystems (i.e. energy/information is held collectively by multiple subsystems).

→ allows for precise control of individual quantum states

The opposite is decoherence:

Irreversible dissipation of energy/information into the environment, akin to heat losses in thermodynamics.

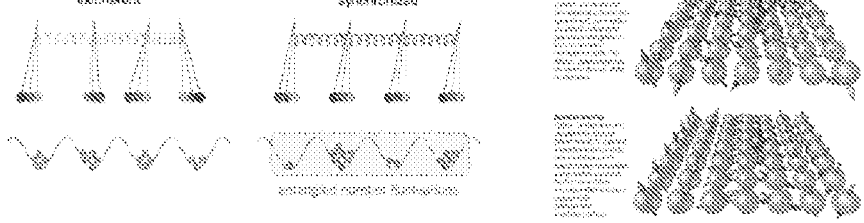
→ allows only to work with statistical aggregates (Quantum 1.0)

Introduction to coherence

More concretely:

To achieve this stability, need:

- Strong coupling internally (between discrete states)
- Weak coupling to the environment (to infinite states/continuum)
- Phase synchronization (often follows from strong coupling)

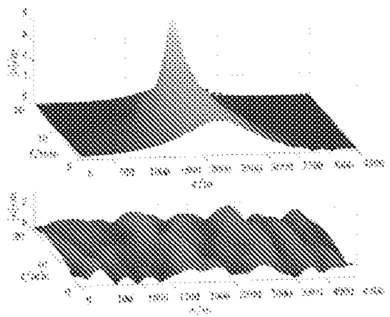


Introduction to coherence

Another way of putting it:

There is a degree of order in the system that allows for the occupation of a few high-energy states vs. many lower-energy states.

Compare with classically coherent wave mechanics:

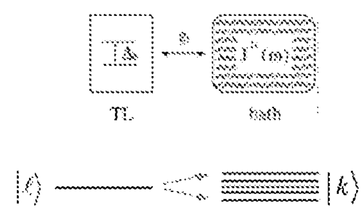


Dematteis, G., Grafke, T., & Vanden-Eijnden, E. (2018). Rogue waves and large deviations in deep sea. Proceedings of the National Academy of Sciences, 115(5), 855-860. https://doi.org/10.1073/pnas.1710670115

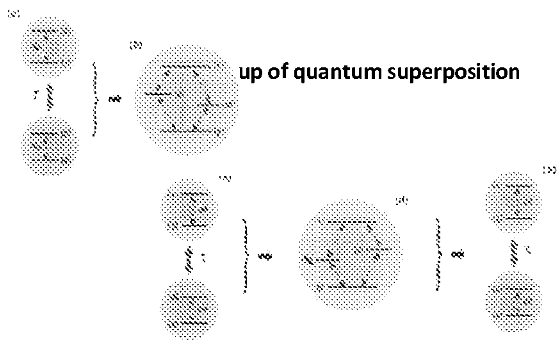
Introduction to coherence

Distinguishing between two (related) types of decoherence:

Dissipation of energy from a discrete quantum state to the environment



up of quantum superposition



Cohering Decohering

Huang, R., & Zhang, H. (2010). Effects of bath temperature on the quantum decoherence. Chemical Physics Letters, [illegible]

Introduction to coherence

We can think about the degree of coherence on a spectrum

	Energy is completely distributed across environment	**Energy is stably held in a single quantum system**	**Energy is held collectively through a superposition of quantum systems**
Characteristics:	strong coupling to outside	weak coupling to outside	weak coupling to outside strong coupling within
Examples:	Quantum 1.0	Nuclear decay Qubits	BEC, photosynthesis
		Incoherent nuclear engineering →	Coherent nuclear engineering

Introduction to coherence

From an exotic state towards a common tool

Previous belief:

Coherence is an exotic and extremely rare state, only possible under exceptional circumstances (close to 0K, very short lived).

Increasingly common realization:

Coherence shows up in all kinds of places, especially in nature. It often can be stabilized by boundary conditions and can be surprisingly long-lived.

Introduction to coherence

Example: growth of coherence lifetimes in qubits

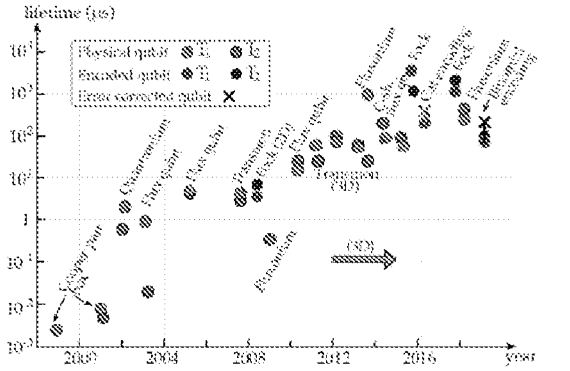
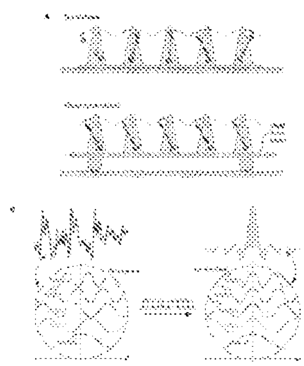


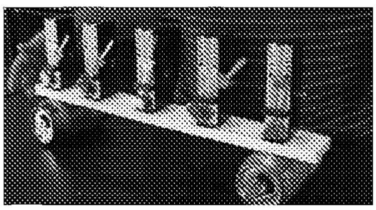
Figure 3.6: Evolution of lifetimes and coherence times in superconducting qubits.

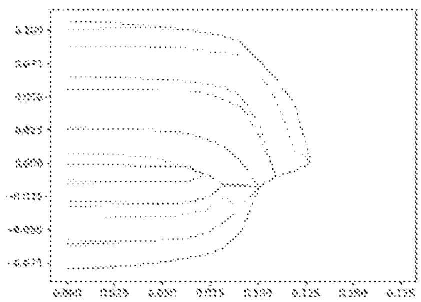
[illegible] (2020). Superconducting qubits: Current state of play. Annual Review of Condensed Matter Physics, 11, [illegible]

Inducing coherence through couplings

Formation of coherence as synchronization





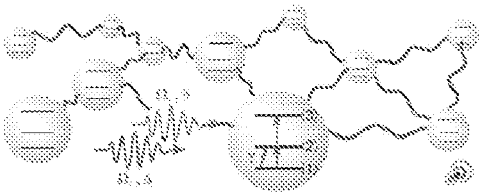


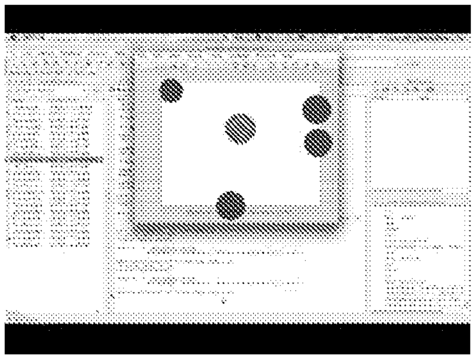
Fig}9 The Kuramoto model for 75 Poincare oscillators showing the frequencies as a function of the coupling coefficient}

[illegible] (2018). Quantum coherence-driven self-organized criticality [illegible]. Science advances, [illegible]
[illegible]
[illegible] The Physics of [illegible] (with Python Programs) [illegible]

Inducing coherence through couplings

Formation of coherence as synchronization (2)

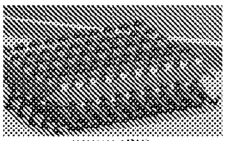


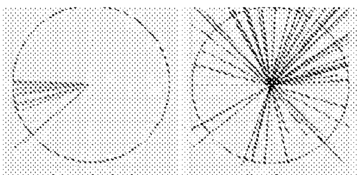


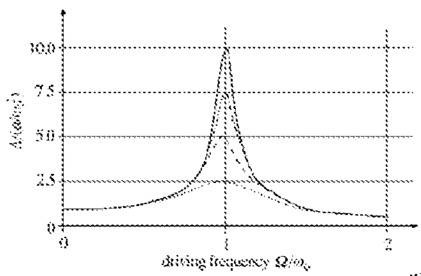
(2011, October 4). Coupled Oscillator Simulation.

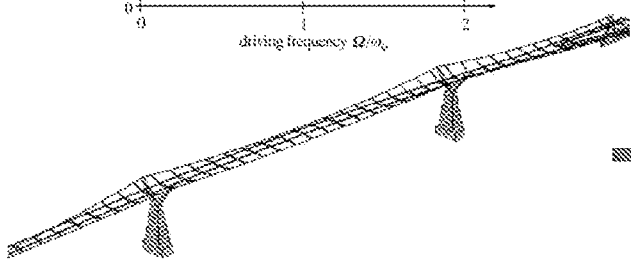
Collective effects from coherence

Building intuition for coherence-based collective effects





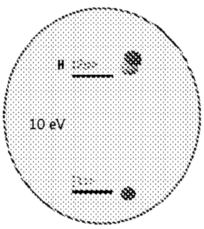


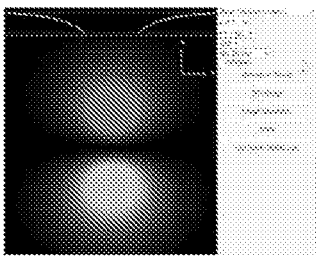


What can coherence do for us?
An overview of quantum dynamics

Quantum dynamics overview

Excited states in the absence of an environment are stable oscillators





$\hat{H}_M =$ [illegible]

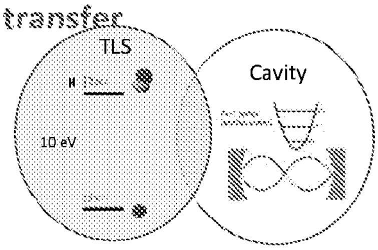
$$i\hbar \frac{\partial}{\partial t}\psi = \hat{H}\psi$$

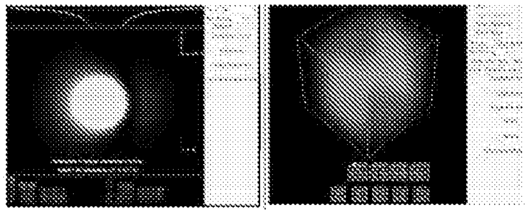
$$\psi(\mathbf{r}, t) = e^{-iE_n t/\hbar}\,\psi(\mathbf{r})$$

$$P(\mathbf{r}, t) = |\psi(\mathbf{r}, t)|^2 = |\psi(\mathbf{r})|^2$$

Quantum dynamics overview

A coupling can lead to discrete energy transfer

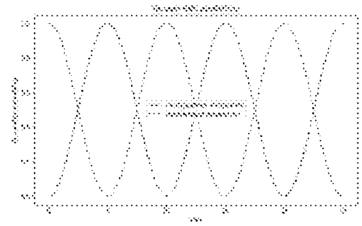




$a_m^\dagger|0\rangle\langle 1|$ Atom decays from $|1\rangle \to |0\rangle$ and emits a photon (in the m^{th} mode).
$a_m|1\rangle\langle 0|$ Atom is excited from $|0\rangle \to |1\rangle$ and absorbs a photon (from the m^{th} mode).
$a_m^\dagger|1\rangle\langle 0|$ Atom is excited from $|0\rangle \to |1\rangle$ and emits a photon (in the m^{th} mode).
$a_m|0\rangle\langle 1|$ Atom decays from $|1\rangle \to |0\rangle$ and absorbs a photon (from the m^{th} mode).

$$\mathcal{H} = \mathcal{H}_0 + V = \frac{\hbar}{2}\omega_0\sigma_z + \sum_m \hbar\omega_m\left(a_m^\dagger a_m + \frac{1}{2}\right) + V$$

TLS | Electromagnetic field | Coupling strength



Cappellaro, P. (2020). Open Quantum Systems. Lecture notes, MIT NSE 2020

Quantum dynamics overview

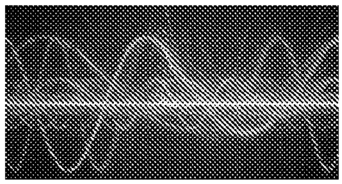
The option for many discrete energy transfer pathways leads to exp. decay

$$\hat{H} = \hat{H}_M + \hat{H}_R + \hat{H}_I$$

Radiation field as an infinite set of oscillators:

$$\hat{H}_R = \sum_{\mathbf{k},\sigma} \hbar\omega_{\mathbf{k}}\left[\hat{a}^\dagger_{\mathbf{k},\sigma}\hat{a}_{\mathbf{k},\sigma} + \frac{1}{2}\right]$$

With coupling: $\hat{H}_I = -\hat{\mathbf{d}}\cdot\hat{\mathbf{E}}(\mathbf{r})$



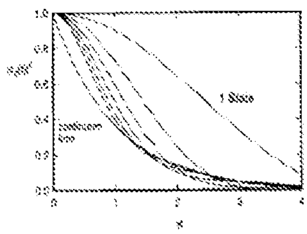


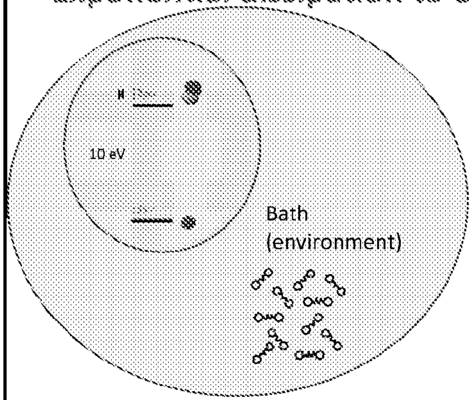
Fig. 24.2 Occupation probability as a function of normalized time for finite-basis models

Hagelstein, P. L., Senturia, S. D., & Orlando, T. P. (2004). Introductory applied quantum and statistical mechanics. John Wiley & Sons.

Quantum dynamics overview

Radiative decay:

Exponential dissipation to environment



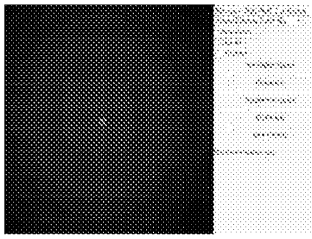
$$i\hbar\frac{\partial}{\partial t}\Psi(t) = \left[\hat{H}_0 + \hat{V}\right]\Psi(t)$$

$$\Psi(t) = \sum_j c_j u_j e^{-iE_jt/\hbar}$$

$$P(t) = \sum_j |c_j(t)|^2$$

$$P_i \sim e^{-\gamma t}$$

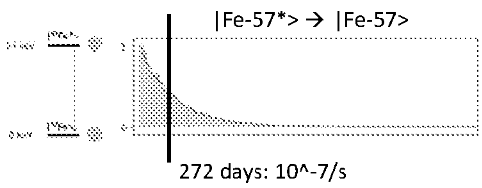
$$\gamma = \frac{2\pi}{\hbar}|\langle\Phi_f|\hat{V}|\Phi_i\rangle|^2\rho(E_f)$$

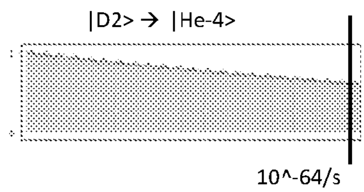


Quantum dynamics overview

A brief intermezzo: nuclear decay and nuclear reactions

- According to convention, nuclear reactions are always treated like spontaneous emission (i.e. as occurring incoherently)
- In other words: The assumption is that there is not one preferred pathway for released nuclear energy. E.g. it can go into many different modes at different angles in space.

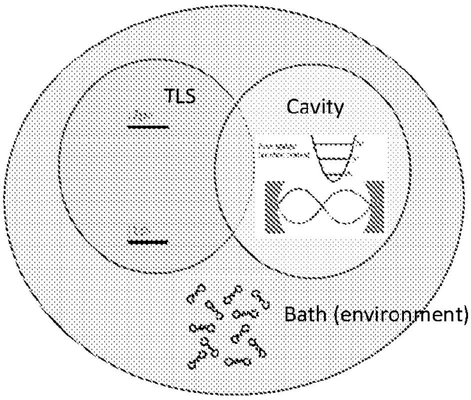


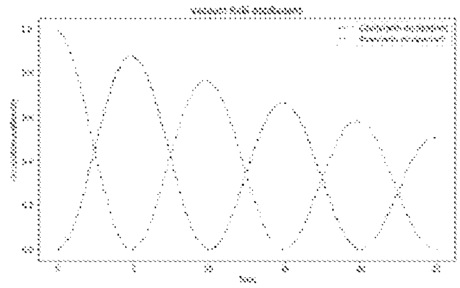


Quantum dynamics overview

Coupling to field with dissipation

$$H_{Rabi} = \omega_r(a^\dagger a + \tfrac{1}{2}) + \tfrac{\omega_a}{2}\sigma_z + g(a^\dagger + a)(\sigma_+ + \sigma_-) + \sqrt{\gamma}a$$

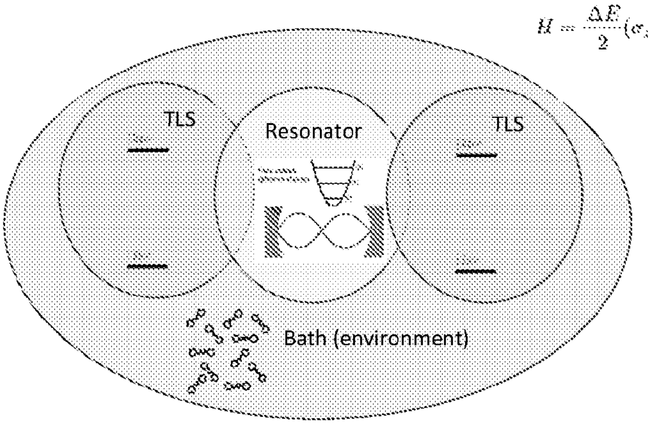


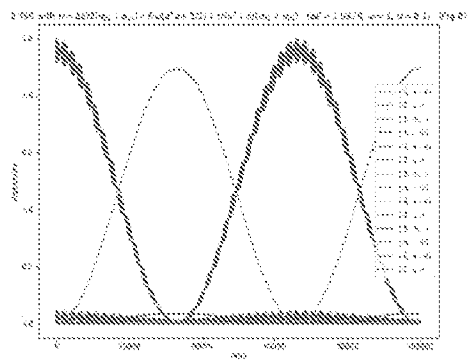


Quantum dynamics overview

Weak coupling via field between two resonant systems

$$H = \frac{\Delta E}{2}(\sigma_{z1} + \sigma_{z2}) + \hbar\omega\left(a^\dagger a + \frac{1}{2}\right) + U\left(a^\dagger + a\right)(\sigma_{x1} + \sigma_{x2}) + \sqrt{\gamma}a$$



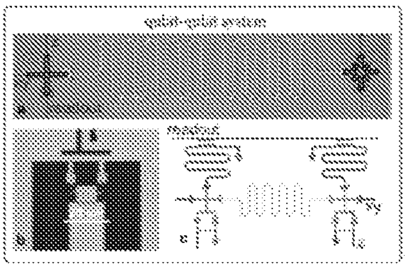


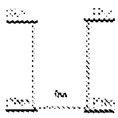
Quantum dynamics overview

Two qubits in superposition

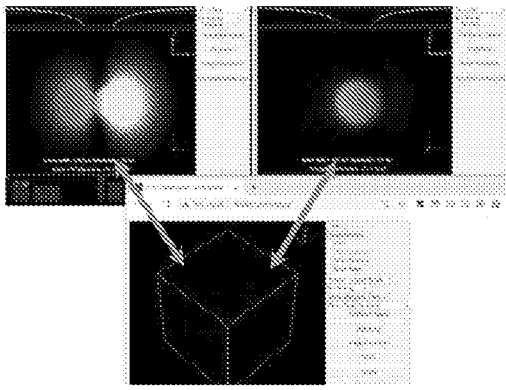
Superposition lasts as long as no other decay channels are open/faster.

$$|0\rangle_A \otimes |1\rangle_B = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \otimes \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}$$



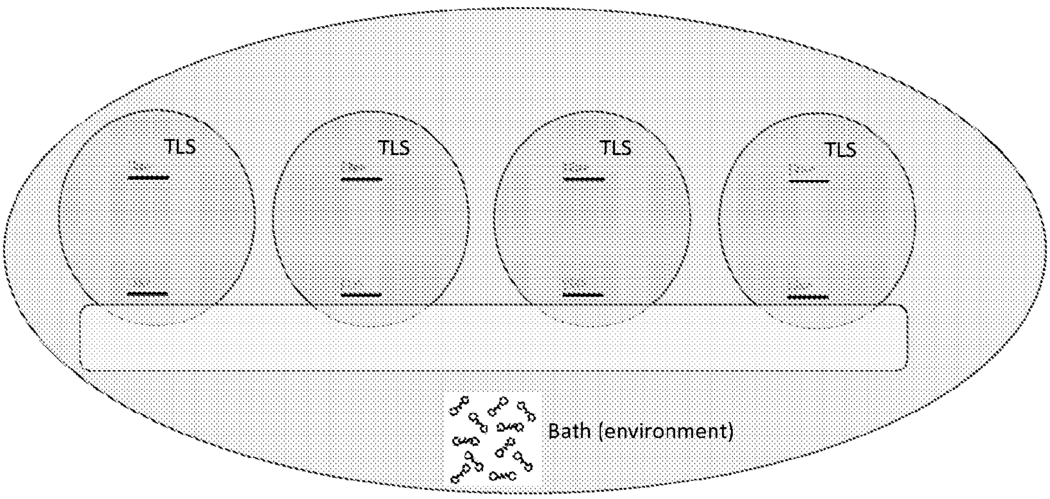


Nonradiative transfer:



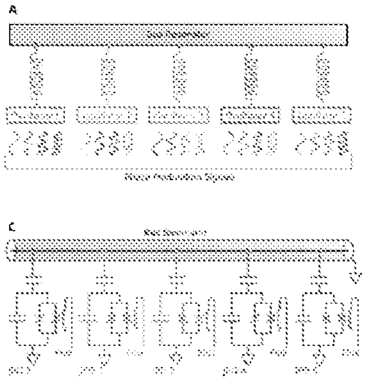
Quantum dynamics overview

Multiple qubits coupled to the same field/oscillator



Quantum dynamics overview

Multiple qubits coupled via a quantum bus



$$H = H_0 + V, \quad V = \frac{U}{2}\sum_{i=1}^{N} d_i^\dagger d_i (d_i^\dagger d_i - 1).$$

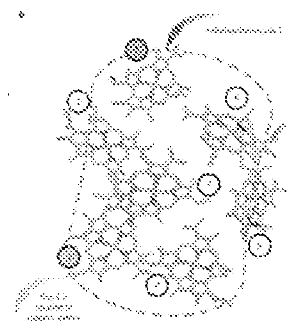
If you have multiple qubit gates, can have superposition of many systems (less relevant for quantum computing but for other techniques such as quantum annealing).

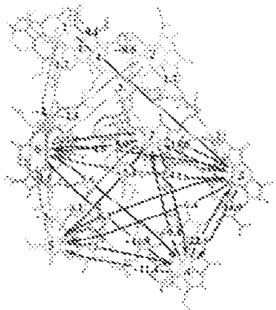
Fang, Y.-L. L., Zheng, H., & Baranger, H. U. (2014). One-dimensional waveguide coupled to multiple qubits: Photon-photon correlations. EPJ Quantum Technology, 1(1), 1-13. https://doi.org/10.1140/epjqt3
Onodera, T., Ng, E., & McMahon, P. L. (2020). A quantum annealer with fully programmable all-to-all coupling via Floquet engineering. npj Quantum Information, 6(1), 48. https://doi.org/10.1038/s41534-020-0279-z

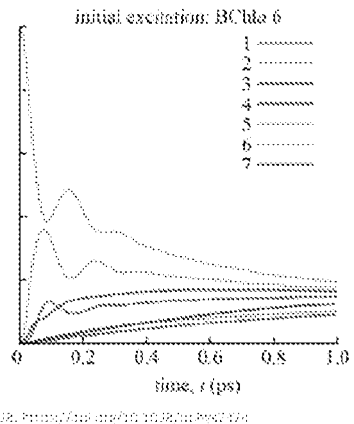
Quantum dynamics overview

Formation of an ensemble: superposition of multiple subsystems

$$\rho_{ensemble}(t) = \frac{1}{N}\sum_{n=1}^{N} |\psi^{(n)}(t)\rangle\langle\psi^{(n)}(t)|.$$







Lambert, N., Chen, Y.-N., Cheng, Y.-C., Li, C.-M., Chen, G.-Y., & Nori, F. (2013). Quantum biology. Nature Physics, 9(1), 10-18. https://doi.org/10.1038/nphys2474
Rebentrost, P., Mohseni, M., & Aspuru-Guzik, A. (2009). Role of quantum coherence and environmental fluctuations in chromophoric energy transport. The Journal of Physical Chemistry B, 113(29), 9942-9947.
Dawlaty, J. M., Ishizaki, A., De, A. K., & Fleming, G. R. (2012). Microscopic quantum coherence in a photosynthetic-light-harvesting antenna. Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences, 370(1972), 3672-3691.

Quantum dynamics overview

Photosynthesis

$$\hat{H}_{tot} = \hat{H}_{sys} + \hat{H}_{env} + \hat{H}_{int}.$$

$$\hat{H}_{sys} = \frac{\hbar\omega_0}{2}\hat{\sigma}_z + \hbar\hat{\sigma}_x$$

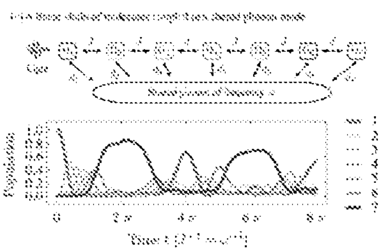
$$\hat{H}_{env} = \sum_{\mathbf{k}} \hbar\omega_{\mathbf{k}} \hat{a}^{\dagger}_{\mathbf{k}} \hat{a}_{\mathbf{k}}.$$

$$\hat{H}_{int} = \sum_{\mathbf{k}} \hat{\sigma}_z \otimes \left(\hbar g_{\mathbf{k}} \hat{a}^{\dagger}_{\mathbf{k}} + \hbar g^{*}_{\mathbf{k}} \hat{a}_{\mathbf{k}}\right).$$

[illegible]

Quantum dynamics overview

Phonon-mediated exciton transfer



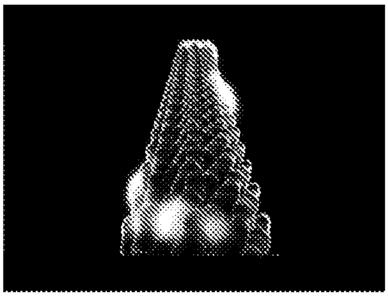
$$\hat{H} = \hat{H}_e + \hat{H}_{ph} + \hat{H}_{e-ph}$$

$$\hat{H}_e = \sum_{j=1}^{N} \hbar\left(\Omega_j + f_j \omega^{-1}\right) |j\rangle\langle j| + \sum_{j \neq k} \hbar J_{jk} |j\rangle\langle k|$$

$$\hat{H}_{ph} = \hbar\omega\left(\hat{b}^{\dagger}\hat{b} + \frac{1}{2}\right)$$

$$\hat{H}_{e-ph} = -\sum_{j=1}^{N} \hbar f_j |j\rangle\langle j| \otimes \left(\hat{b}^{\dagger} + \hat{b}\right)$$

VIDEO: accelerated state transitions due to genetically engineered spacing of excitons:
https://www.youtube.com/watch?v=91vhoxR1Lts



[illegible]

[illegible]

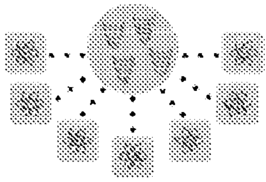
Quantum dynamics overview

Multiple qubits interacting via multiple field modes: Spin-boson model

More specifically we consider a system of N qubits interacting with K bosonic modes (Fig. 1(a)) by means of a spin-boson Hamiltonian Massimo Palma et al. (1996); Wu et al (2013) of the form:

$$H = \sum_{i=1}^{N} \frac{\Omega_i}{2}\sigma_z^i + \sum_{k=1}^{K} \omega_k b_k^\dagger b_k + \sum_{i,k} \lambda_{i,k}\sigma_z^i (b_k^\dagger + b_k). \quad (1)$$

(a)



[illegible] (2018). Processing quantum coherence using the spin-boson model

Modelling the full picture

Sneak preview

This is the model for quantum-coherent nuclear engineering:

$$\hat{H} = \sum_j \mathbf{M}_j c^2 + \sum_{\mathbf{k},\sigma} \hbar\omega_{\mathbf{k},\sigma} \hat{a}_{\mathbf{k},\sigma}^\dagger \hat{a}_{\mathbf{k},\sigma} + \sum_j \sum_{\mathbf{k},\sigma} V_{j,\mathbf{k},\sigma}$$

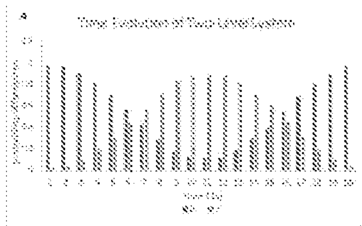
$$V_{j,\mathbf{k},\sigma} = \mathbf{a}_j \cdot \left(\frac{\partial \mathbf{P}_j}{\partial a_{\mathbf{k},\sigma}^\dagger} \hat{a}_{\mathbf{k},\sigma} + \frac{\partial \mathbf{P}_j}{\partial a_{\mathbf{k},\sigma}^\dagger} \hat{a}_{\mathbf{k},\sigma}^\dagger \right)$$

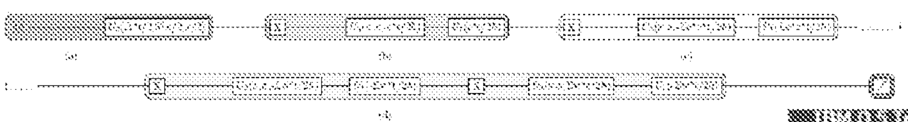
The future of quantum dynamics simulations

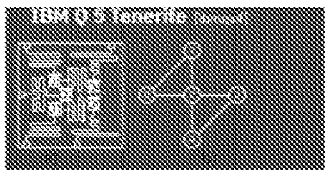
Using quantum computing to evolve Hamiltonians

Spin-Boson Model to Demonstrate Quantum Tunneling in Biomolecules using IBM Quantum Computer

$$\mathcal{H} = -\frac{\hbar\Delta\sigma_x}{2} + \frac{\epsilon\sigma_z}{2} + \frac{q\sigma_z\Sigma c_\alpha x_\alpha}{2\hbar} + \Sigma\hbar\omega_\alpha b_\alpha^\dagger b_\alpha$$







Mohanta, Y., Abhishek, ... S., ..., K., Kumar, V., Behera, B. K., & Panigrahi, P. K. (2018). Spin-boson model to demonstrate quantum tunneling in biomolecules using IBM quantum computer. ArXiv Preprint ...

Using quantum simulation to evolve Hamiltonians

ARTICLE

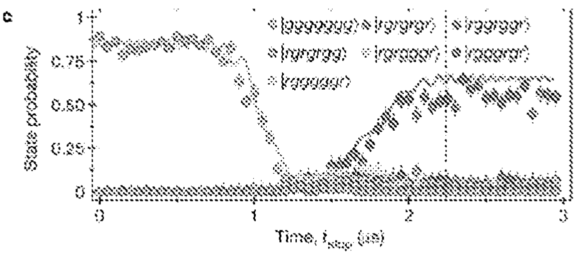
Probing many-body dynamics on a 51-atom quantum simulator

$$\frac{\mathcal{H}}{\hbar} = \sum_i \frac{\Omega_i}{2}\sigma_x^i - \sum_i \Delta_i n_i + \sum_{i<j} V_{ij} n_i n_j$$

$$\sigma_x^i = |g_i\rangle\langle r_i| + |r_i\rangle\langle g_i|$$

a

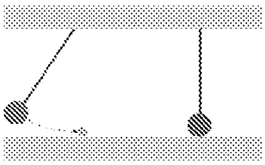
c

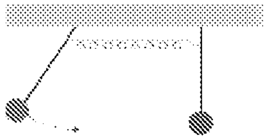


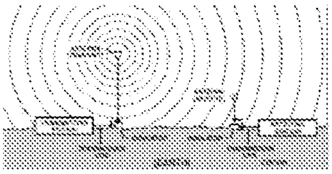
Bernien, H., Schwartz, S., Keesling, A., Levine, H., Omran, A., Pichler, H., Choi, S., Zibrov, A. S., Endres, M., Greiner, M., Vuletić, V., & Lukin, M. D. (2017). Probing many-body dynamics on a 51-atom quantum simulator. Nature, 551(7682), 579–584. https://doi.org/10.1038/nature24622

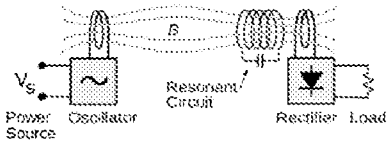
How can weak couplings have large effects?

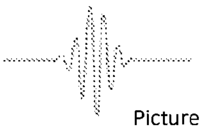
Radiative vs nonradiative



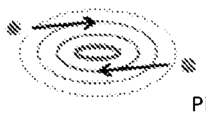








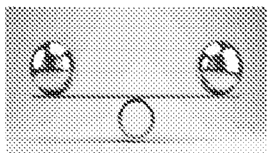
Picture as wave package



Picture as disturbance of E-field

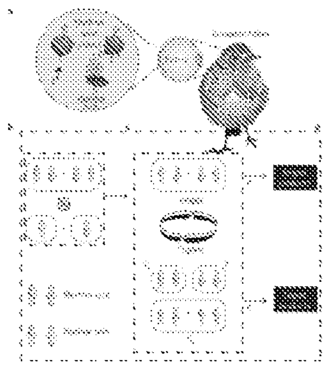
Judo analogy

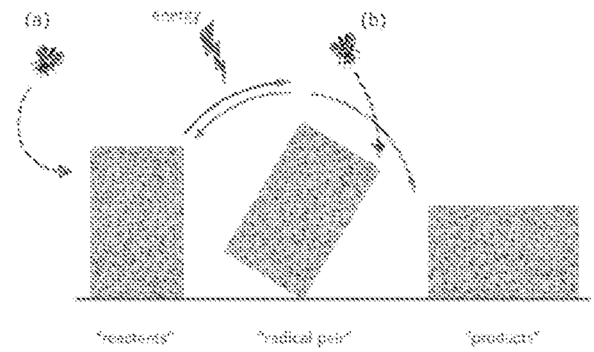
Only a very small tipping force is needed if a system is well-balanced



Compare with quantum sensing in quantum biology

Extremely weak magnetic field triggers chemical reactions



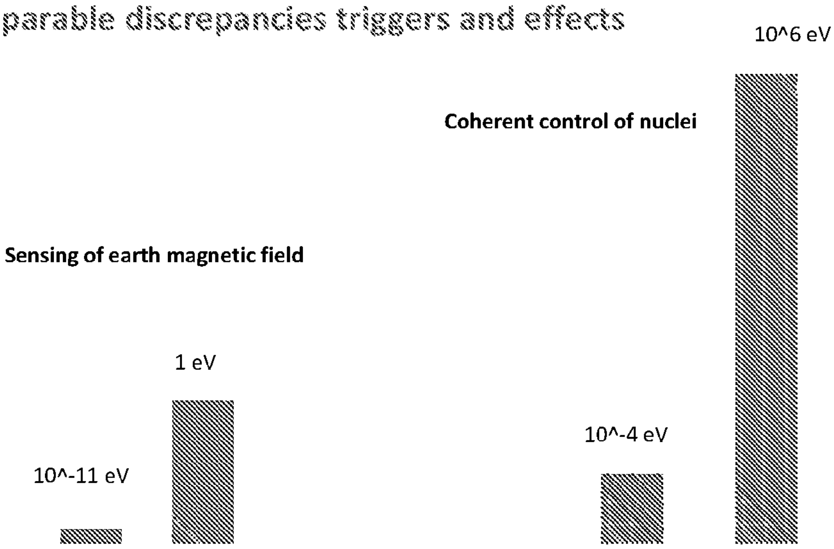


Lambert, N., Chen, Y.-N., Cheng, Y.-C., Li, C.-M., Chen, G.-Y., & Nori, F. (2013). Quantum biology. Nature Physics, 9(1), 10–18. https://doi.org/10.1038/nphys2474

Hore, P. J., & Mouritsen, H. (2016). The Radical-Pair Mechanism of Magnetoreception. Annual Review of Biophysics, 45, 299–344. https://doi.org/10.1146/annurev-biophys-032116-094545

Compare with quantum sensing in quantum biology

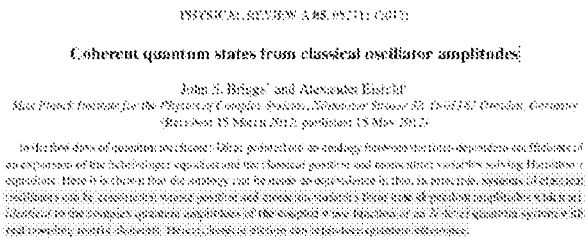
Comparable discrepancies triggers and effects



Building intuition on dynamics and transition rate changes

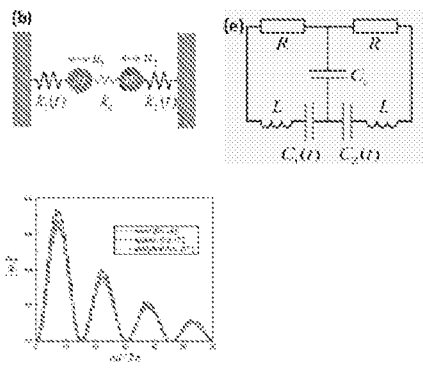
Dynamics and transition rate changes

Classical dynamics can reproduce quantum dynamics precisely


PHYSICAL REVIEW A 85, 052111 (2012)

Coherent quantum states from classical oscillator amplitudes

John S. Briggs and Alexander Eisfeld
(Received 15 March 2012; published 15 May 2012)

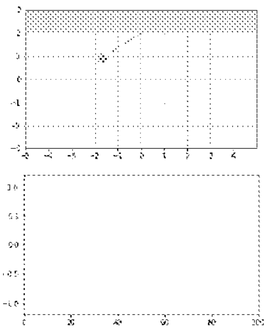


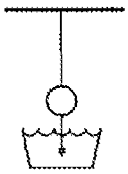
Briggs, J. S., & Eisfeld, A. (2012). Coherent quantum states from classical oscillator amplitudes. Physical Review A, 85(5), 052111.

Ivakhnenko, O. V., Shevchenko, S. N., & Nori, F. (2018). Simulating quantum dynamical phenomena using classical oscillators: Landau-Zener-Stückelberg-Majorana interferometry, latching modulation, and motional averaging. Scientific Reports, 8, 12218.

Dynamics and transition rate changes

Dissipative exponential decay





$$\frac{dx}{dt} = \frac{p(t)}{m}, \quad \frac{dp}{dt} = -m\omega^2 x \quad \rightarrow \quad \frac{d\alpha}{dt} = -i\omega\alpha(t)$$

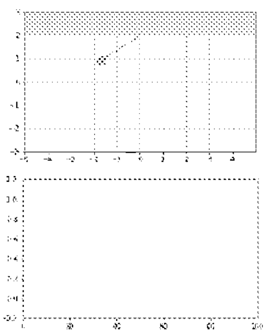
$$\langle X\rangle = \frac{1}{\sqrt{2}}(\alpha_0 e^{-i\omega t} + \alpha_0^* e^{i\omega t})$$
$$\langle P\rangle = \frac{-i}{\sqrt{2}}(\alpha_0 e^{-i\omega t} - \alpha_0^* e^{i\omega t})$$

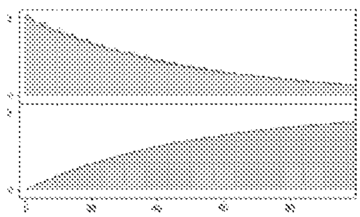
$$X = (a + a^\dagger)/\sqrt{2}, \quad P = -i(a - a^\dagger)/\sqrt{2}, \quad \mathcal{H} = \omega(a^\dagger a + \frac{1}{2}).$$

Hemmer, P. R., & Prentiss, M. G. (1988). Coupled-pendulum model of the stimulated resonance Raman effect. JOSA B, 5(8), 1619-1625.

Dynamics and transition rate changes

Dissipative exponential decay





$$i\hbar\frac{\partial}{\partial t}\Psi(t) = \left[\hat{H}_0 + \hat{V}\right]\Psi(t)$$

$$\Psi(t) = \sum_j c_j u_j e^{-iE_j t/\hbar}$$

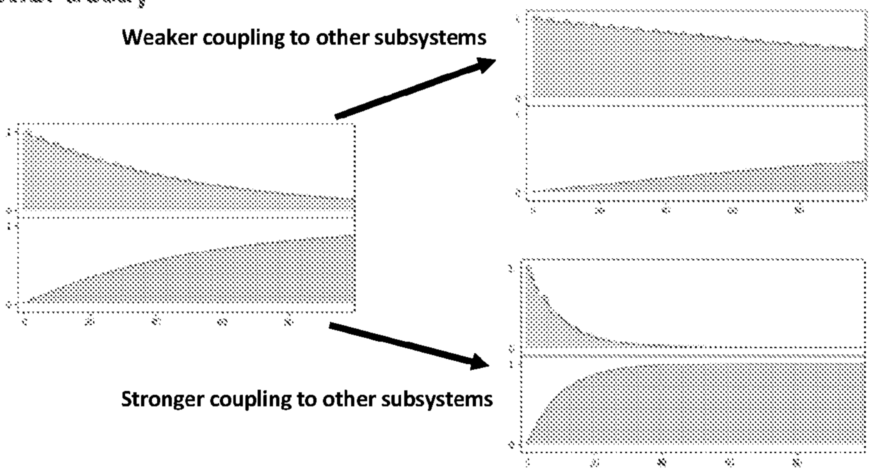
$$P(t) = \sum_j |c_j(t)|^2$$

$$P_i \sim e^{-\gamma t}$$

$$\gamma = \frac{2\pi}{\hbar} |\langle\Phi_f|\hat{V}|\Phi_i\rangle|^2 \rho(E_f)$$

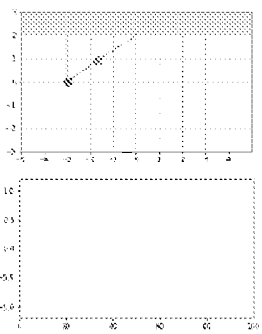
Dynamics and transition rate changes

Dissipative exponential decay



Dynamics and transition rate changes

Strong coupling to single resonant subsystem

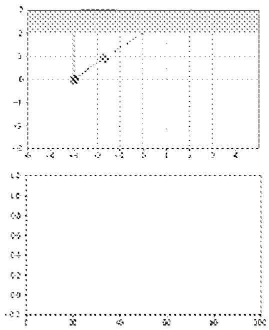


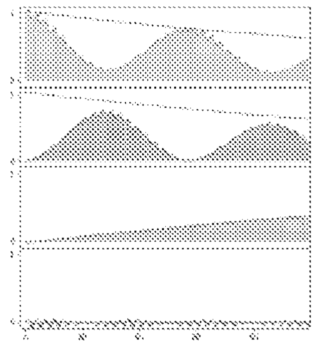
$$H = \frac{|\mathbf{p}_1|^2}{2m} + \frac{1}{2} m\omega_0^2 |\mathbf{r}_1|^2 + \frac{|\mathbf{p}_2|^2}{2m} + \frac{1}{2} m\omega_0^2 |\mathbf{r}_2|^2 + \frac{e^2}{4\pi\varepsilon_0 R^3}\left[\mathbf{r}_2 \cdot \mathbf{r}_1 - 3(\mathbf{r}_2 \cdot \mathbf{i}_{21})(\mathbf{r}_1 \cdot \mathbf{i}_{21})\right]$$

$$H = \frac{\Delta E}{2}(\sigma_{21} + \sigma_{22}) + \hbar\omega\left(a^\dagger a + \frac{1}{2}\right) + U\left(a^\dagger + a\right)(\sigma_{21} + \sigma_{12})$$

Dynamics and transition rate changes

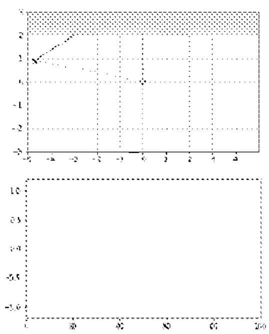
Strong coupling to single resonant subsystem





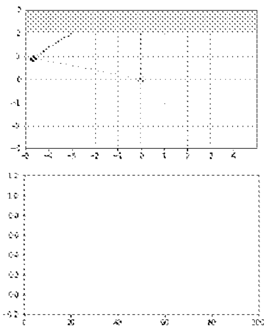
Dynamics and transition rate changes

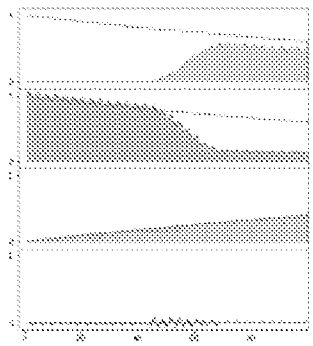
Qubit flip through induced coupling



Dynamics and transition rate changes

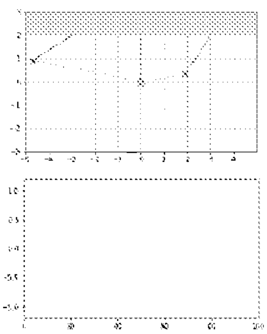
Qubit flip through induced coupling





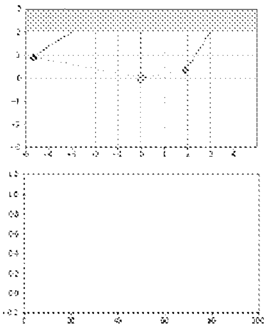
Dynamics and transition rate changes

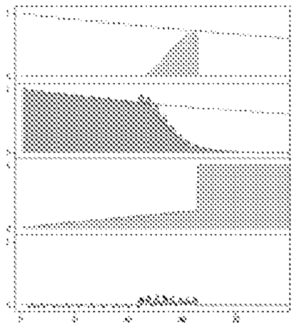
Cooperative upconversion (quantum pooling) due to induced coupling



Dynamics and transition rate changes

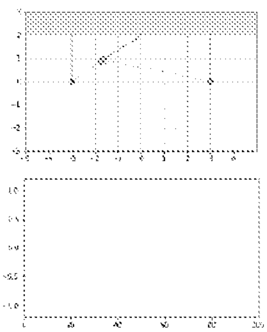
Cooperative upconversion (quantum pooling) due to induced coupling





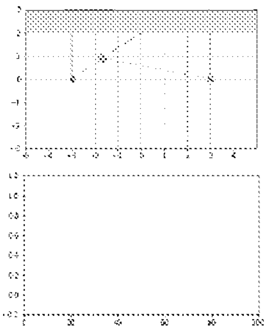
Dynamics and transition rate changes

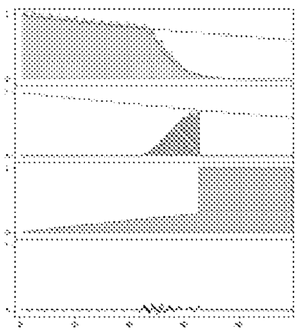
Cooperative downconversion (quantum cutting) due to induced coupling

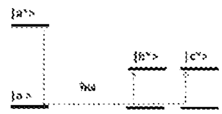


Dynamics and transition rate changes

Cooperative downconversion (quantum cutting) due to induced coupling



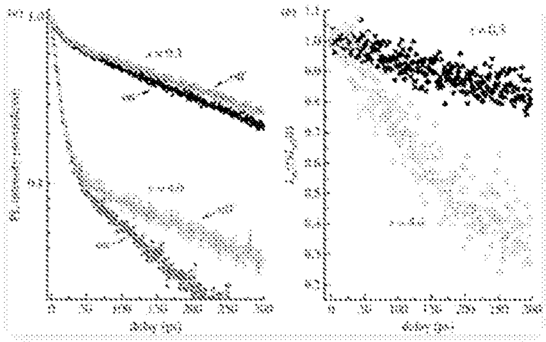




Quantum-coherent engineering

Quantum-coherent engineering

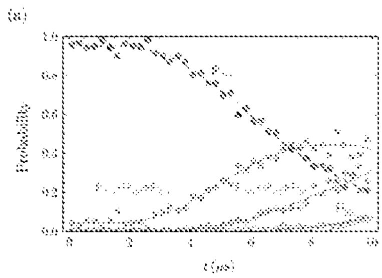
Engineering transition rates



Schmidt, S. A., ... (2012). ... Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences, ...

Quantum-coherent engineering

Engineering state transitions, including downconversion



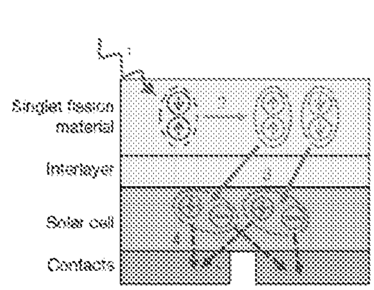


Figure S1. (a) Recapture probabilities ... (solid circles), ...
circles) for three atoms in a line as a function of the release trapping ...
extract ... Solid lines are the prediction of our loss model with the ...
of ... for ... is due to losses induced by background gas collision...

... (2015). Coherent Excitation Transfer in a Spin Chain of Three Rydberg Atoms. Physical Review Letters, 114(11), 113002. https://doi.org/10.1103/PhysRevLett.114.113002

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Quantum-coherent engineering

Engineering state transitions, including upconversion

$$H = H_0 + V,$$

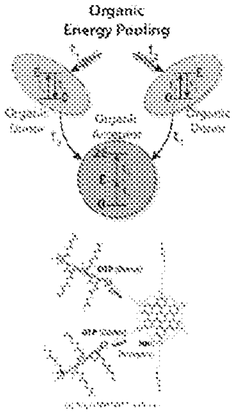
with

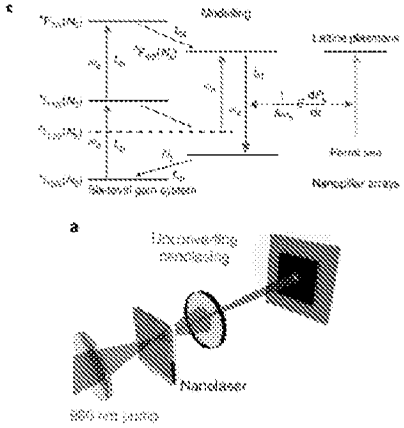
$$H_0 = H_{rad} + \sum_{\xi=A,B,C} H^{\xi}_{mol},$$

$$V = \sum_{\xi=A,B,C} H^{\xi}_{int},$$

and

$$H_{mol} = H_{rad} + \sum_{\xi=A,B,C} (H^{\xi}_{mol} + H^{\xi}_{int})$$





LaCount, M. D., Weingarten, D., Hu, N., Shaheen, S. E., van de Lagemaat, J., Rumbles, G., Walba, D. M., & Lusk, M. T. (2015). Energy Pooling Upconversion in Organic Molecular Systems. The Journal of Physical Chemistry A, 119(17), 4009–4016. https://doi.org/10.1021/acs.jpca.5b00509

Fernandez-Bravo, A., Wang, D., Barnard, E. S., Teitelboim, A., Tajon, C., Guan, J., Schatz, G. C., Cohen, B. E., Chan, E. M., & Schuck, P. J. (2019). Ultralow-threshold, continuous-wave upconverting lasing from subwavelength plasmons. Nature Materials, 18(11), 1172–1176.

Quantum-coherent engineering

Predicting dynamic outcomes from system parameters

TABLE I. Table of transitions between lanthanide dopant ions in crystal field environs: i-energy pooling, ii-two photon APTE, iii-sensitization, iv-quantum cutting.

A (Transition)	B (Transition)	C (Transition)	Type	References
$Yb^{3+}(^2F_{5/2}\rightarrow{}^2F_{7/2})$	$Yb^{3+}(^2F_{5/2}\rightarrow{}^2F_{7/2})$	$Tb^{3+}(^7F_6\rightarrow{}^5D_4)$	i	18, 23, 28
$Yb^{3+}(^2F_{5/2}\rightarrow{}^2F_{7/2})$	$Yb^{3+}(^2F_{5/2}\rightarrow{}^2F_{7/2})$	$Tm^{3+}(^3H_6\rightarrow{}^1G_4)$	i, ii	21, 22
$Yb^{3+}(^2F_{5/2}\rightarrow{}^2F_{7/2})$	$Yb^{3+}(^2F_{5/2}\rightarrow{}^2F_{7/2})$	$Eu^{3+}(^7F_0\rightarrow{}^5D_2)$	i	25
$Pr^{3+}(^1D_2\rightarrow{}^3H_4)$	$Pr^{3+}(^1D_2\rightarrow{}^3H_4)$	$Pr^{3+}(^1D_2\rightarrow{}^1S_0)$	i	29, 30
$Yb^{3+}(^2F_{5/2}\rightarrow{}^2F_{7/2})$	$Yb^{3+}(^2F_{5/2}\rightarrow{}^2F_{7/2})$	$Ho^{3+}(^5I_8\rightarrow{}^5S_2,{}^5F_4)$	ii	13, 21
$Yb^{3+}(^2F_{5/2}\rightarrow{}^2F_{7/2})$	$Yb^{3+}(^2F_{5/2}\rightarrow{}^2F_{7/2})$	$Er^{3+}(^4I_{15/2}\rightarrow{}^4F_{7/2})$	ii	18, 19, 21, 24, 26
$Pr^{3+}(^3P_0\rightarrow{}^1G_4)$	$Yb^{3+}(^2F_{7/2}\rightarrow{}^2F_{5/2})$	$Pr^{3+}(^3H_4\rightarrow{}^1G_4)$	iii	36
$Er^{3+}(^4I_{13/2}\rightarrow{}^4I_{15/2})$	$Tm^{3+}(^3H_6\rightarrow{}^3H_4)$	$Er^{3+}(^4I_{15/2}\rightarrow{}^4F_{9/2})$	iii	33
$Ho^{3+}(^5F_5\rightarrow{}^5I_8)$	$Yb^{3+}(^2F_{7/2}\rightarrow{}^2F_{5/2})$	$Ho^{3+}(^5I_6\rightarrow{}^5S_2,{}^5F_4)$	iii	35
$Tm^{3+}(^3F_4\rightarrow{}^3H_6)$	$Yb^{3+}(^2F_{7/2}\rightarrow{}^2F_{5/2})$	$Tm^{3+}(^3H_5\rightarrow{}^3H_4)$	iii	37, 38
$Nd^{3+}(^4F_{3/2}\rightarrow{}^4I_{11/2})$	$Yb^{3+}(^2F_{7/2}\rightarrow{}^2F_{5/2})$	$Tb^{3+}(^5D_4\rightarrow{}^5D_1)$	iii	39
$Eu^{3+}(^7F_1\rightarrow{}^5D_0)$	$Eu^{3+}(^7F_1\rightarrow{}^5H_3)$	$Gd^{3+}(^6G_J\rightarrow{}^6S_{7/2})$	iv	41
$Tb^{3+}(^5D_3\rightarrow{}^7F_3)$	$Er^{3+}(^4S_{3/2}\rightarrow{}^4I_{13/2})$	$Er^{3+}(4f^{10}5d\rightarrow{}^4S_{3/2})$	iv	42
$Pr^{3+}(^3H_4\rightarrow{}^3P_2)$	$Pr^{3+}(^3H_4\rightarrow{}^3P_2)$	$Pr^{3+}(^1S_0\rightarrow{}^3H_4)$	iv	43

Andrews, D. L., & Jenkins, R. D. (2001). A quantum electrodynamical theory of three-center energy transfer for upconversion and downconversion in rare earth doped materials. The Journal of Chemical Physics, 114(2), 1089–1100.

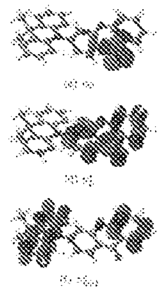
Quantum-coherent engineering

Predicting dynamic outcomes from system parameters

Table 1. Vertical Absorption ΔE_{abs} and Emission ΔE_{em} Energies (eV) as well as Adiabatic Excitation Energies ΔE_{adia} (eV) of ACRXTN[a]

[illegible]		[illegible]	ΔE_{abs} DFT/MRCI-R	ΔE_{abs} RI-CC2	ΔE_{abs} TDDFT B3LYP	[illegible] DFT/MRCI-R	[illegible] DFT/MRCI-R	[illegible] DFT/MRCI-R	[illegible]
[illegible]		(0.93) CS	0.00	0.00	0.00			3.58	
[illegible]	CT	(0.85) [illegible]	3.09	3.41	3.50	2.56	3.27	22.03	4 × 10[illegible]
[illegible]	[illegible]	(0.76) [illegible]	3.61	3.92	3.60[b]	3.20	2.90	3.55	[illegible]
[illegible]	[illegible]	(0.70) [illegible]	3.65	4.21	3.82[c]	3.60	3.35	3.60	0.13442
[illegible]	CT	(0.79) [illegible]	3.93	3.94	2.86	2.58	2.71	21.74	
[illegible]	[illegible]	(0.83) [illegible] (0.30) [illegible]	3.25	3.77	3.43	3.04	2.87	3.25	
[illegible]	[illegible]	(0.45) [illegible] (0.26) [illegible]	3.38	3.73	3.48			3.59	
[illegible]	[illegible]	(0.67) [illegible]	3.42	3.65	3.37	3.04	2.61	3.56	

[a]The electric dipole moments μ (Debye) and oscillator strengths f(r) were computed at the ground-state minimum. [b]S_2 state: S_1 (3.56 eV) is a CT state in TDDFT(B3LYP) calculation, found as S_4 at 4.05 eV (DFT/MRCI-R) and at 4.20 eV in RI-CC2. [c]S_4 state; S_3 (2.82 eV) is a CT state in TDDFT(B3LYP) calculation, not found among the lowest six excited singlet states in DFT/MRCI-R and RI-CC2.



orbitals in the optimized ground state

[illegible] (2016). Mechanism of [illegible] The Journal of Physical Chemistry C, [illegible]

Quantum-coherent engineering

Engineering structures with optimized parameters for desired dynamics and outcomes ("energy transfer editing")

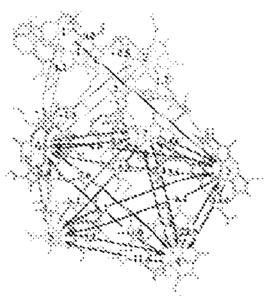
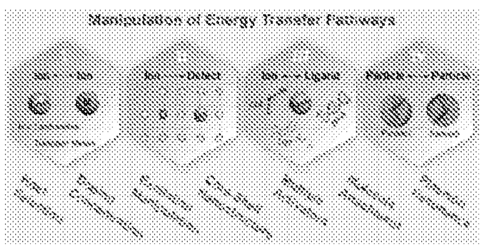


Figure 2



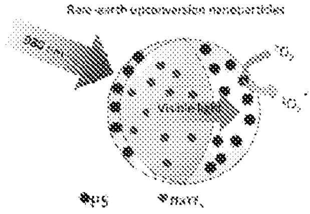


Figure 2. Schematic illustration showing four major energy transfer pathways dominated in upconverting nanosystems. A list of chemical and physical approaches to energy transfer manipulation is included in the scheme.

Qin, X., Xu, J., Wu, Y., & Liu, X. (2019). Energy-transfer editing in lanthanide-activated upconversion nanocrystals: A toolbox for emerging applications. ACS Central Science, 5(1), 29-42.
Keshef, [illegible] (2017). Advances in antimicrobial photodynamic inactivation at the nanoscale. Nanophotonics, 6. https://doi.org/10.1515/nanoph-2016-0189

Quantum-coherent engineering

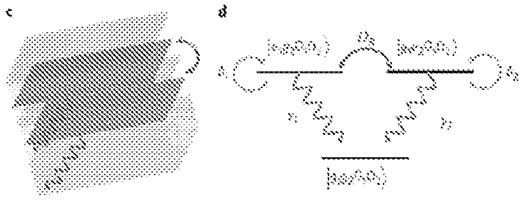
Summary

- So it's all about deliberately moving energy/information around in coupled systems.

Quantum coherence at the nuclear level

Quantum dynamics

Accelerating state transitions via couplings: nuclei



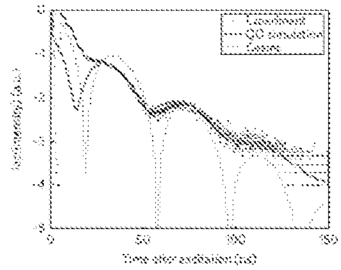


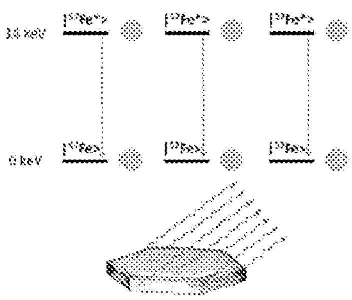
Fig. 3 | Measurement of Rabi oscillations. Temporal response of the sample, showing clearly visible Rabi oscillations. The theoretical curves are a Fourier transform of the energy-resolved reflectivity, derived from the quantum optical (QO) model, and an exponentially damped cosine whose period is the Rabi frequency, respectively. Note that these temporal oscillations are evenly spaced, in contrast to propagation quantum beats (also known as dynamical beats), the period of which increases with increasing time after excitation.

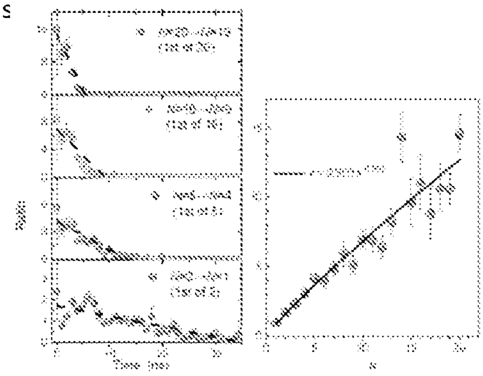
Haber, J., Kong, X., Strohm, C., Willing, S., Gollwitzer, J., Bocklage, L., Rüffer, R., Pálffy, A., & Röhlsberger, R. (2017). Rabi oscillations of X-ray radiation between two nuclear ensembles. Nature Photonics, 11(11), 720–725. https://doi.org/10.1038/s41566-017-0013-3

Quantum dynamics

Accelerating state transitions via couplings: nuclei

- The more systems participate, the stronger the coupling.
- The stronger the coupling, the faster the state transitions





Chumakov, A. I., et al (2018). Superradiance of an ensemble of nuclei excited by a free electron laser. Nature Physics, 14