# Three Pieces on

# Controlled Quantum Dynamics

**Martin B Plenio**

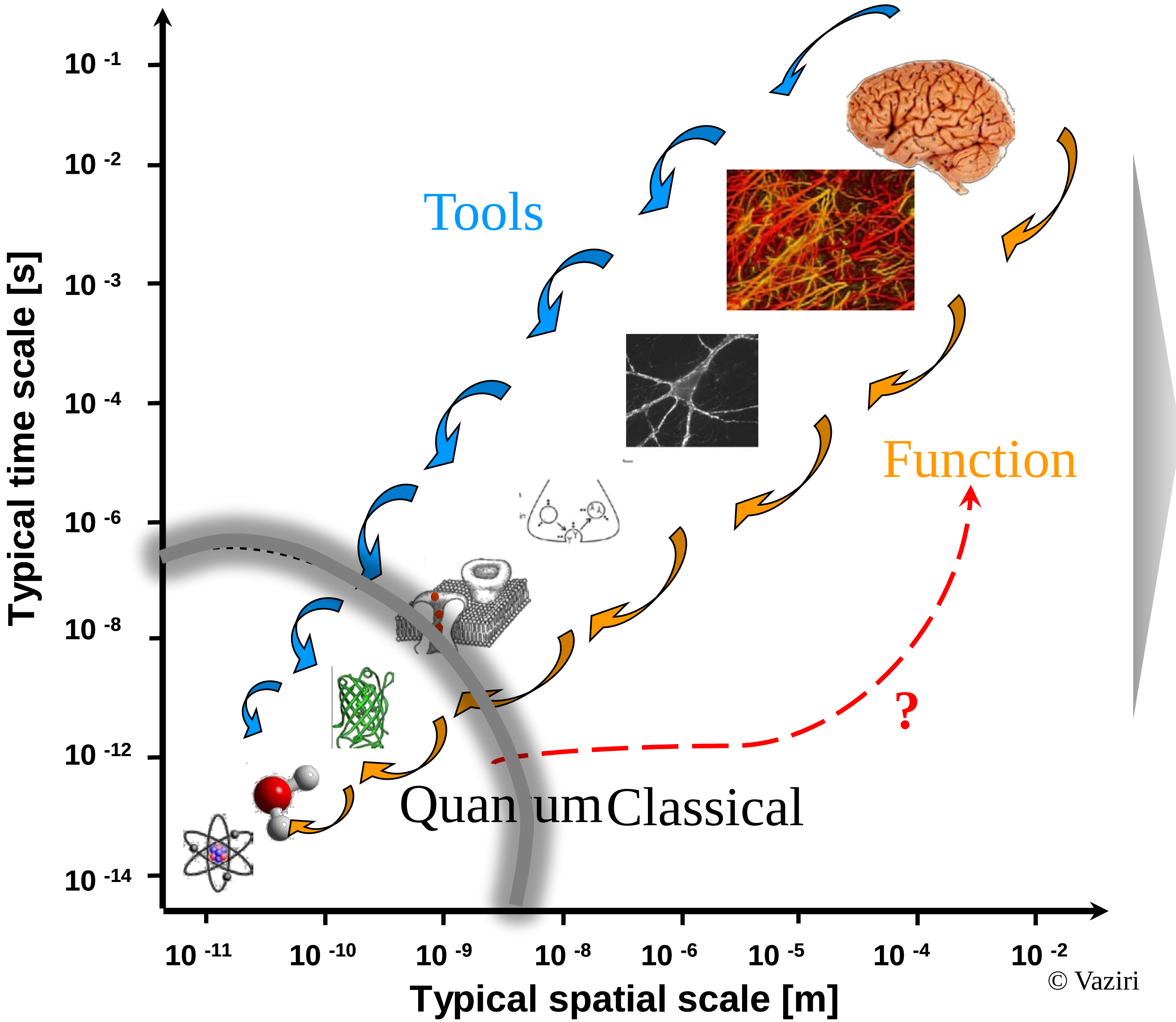
**Institut für Theoretische Physik**
**Universität Ulm**

**&**

**Quantum Optics and Laser Science Group**
**Blackett Laboratory**
**Imperial College London**


Integrated Quantum Science and Technology

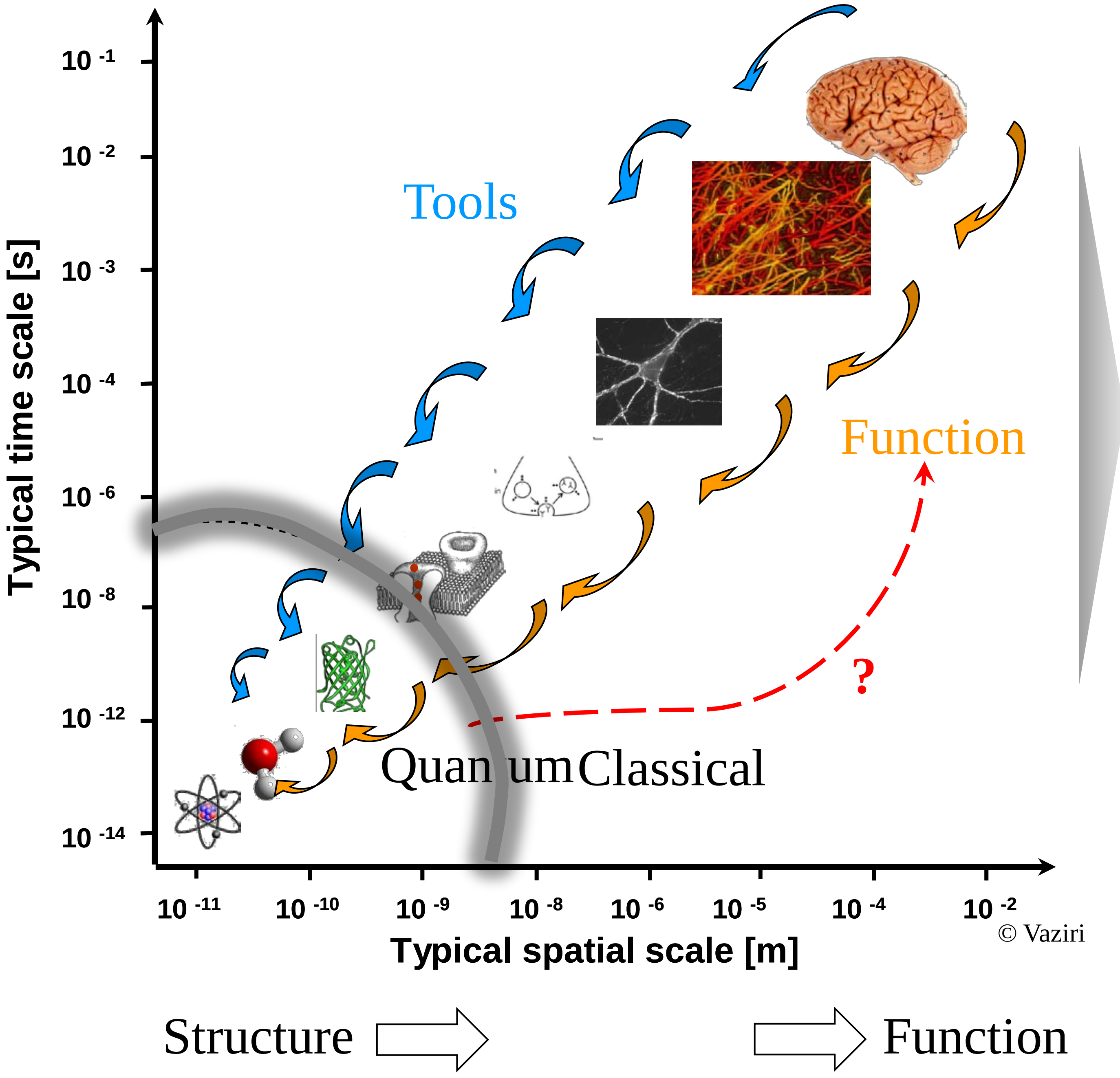
# Part I




**Can quantum coherence be relevant for biological function?**

**Requires tools for studying biological structure and function at unprecedented spatial and temporal resolution**

Huelga & Plenio, Review in preparation for Contemporary Physics 2012

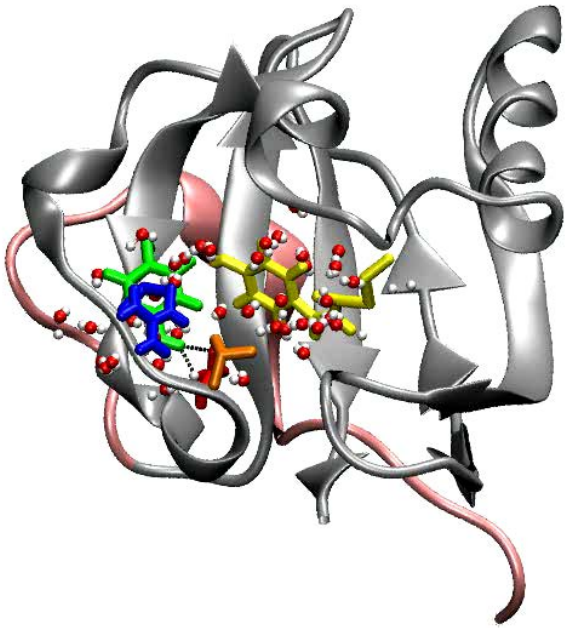



**Can quantum coherence be relevant for biological function?**

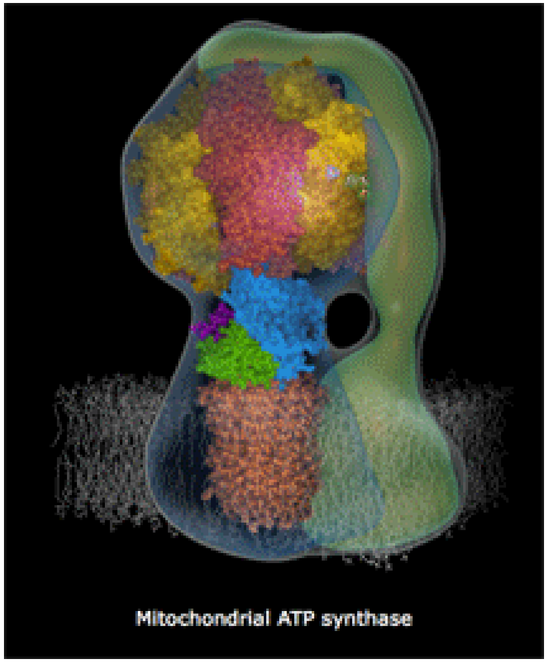
**Requires tools for studying biological structure and function at unprecedented spatial and temporal resolution**

Huelga & Plenio, Review in preparation for Contemporary Physics 2012

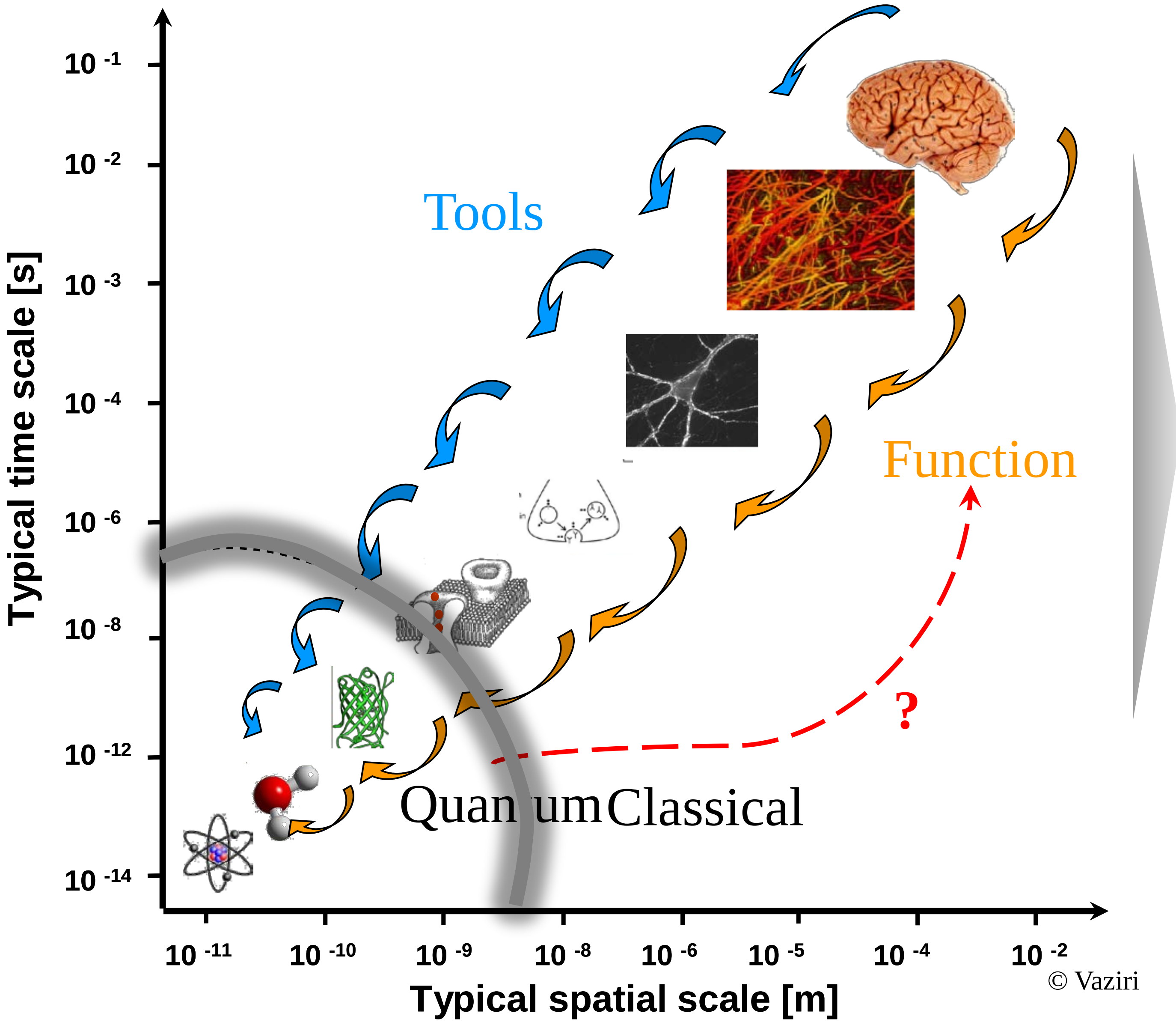
# Biological motion on the nanoscale



Computational Chemistry
Group, Amsterdam




Walker @ Cambridge




**Can quantum coherence be relevant for biological function?**

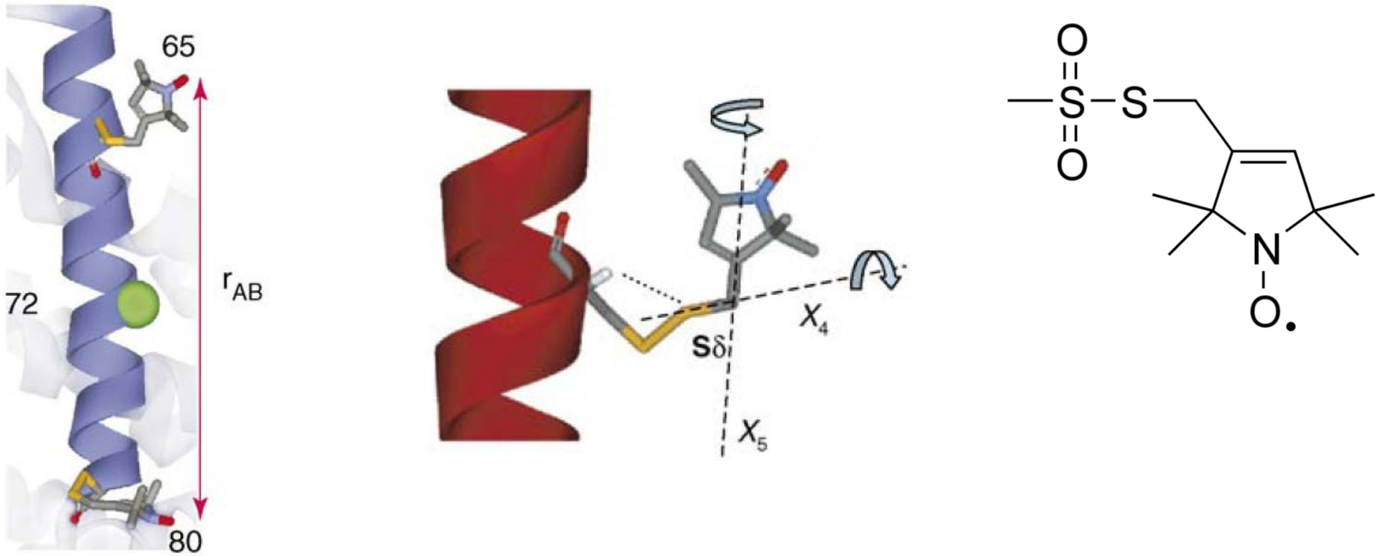
**Requires tools for studying biological structure and function at unprecedented spatial and temporal resolution**

Structure → Dynamics → Function

Huelga & Plenio, Review in preparation for Contemporary Physics 2012

# Biological motion on the nanoscale

- Measure distance between a pair of electron spins: organic spin labels




G. E. Fanucci and D. S. Cafiso, Recent advances and applications of site-directed spin labeling (2006)

- Wide applications of ESR with spin labels:
  - Protein orientation
  - Distance measurements
  - Protein dynamics
  - Structural biology

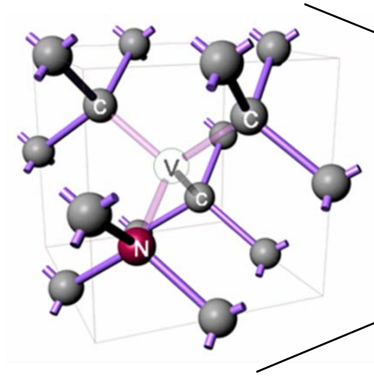
- Determine intra and intermolecular distance via ESR: hard to go beyond 5 nm
  - Inhomogeneous broadening

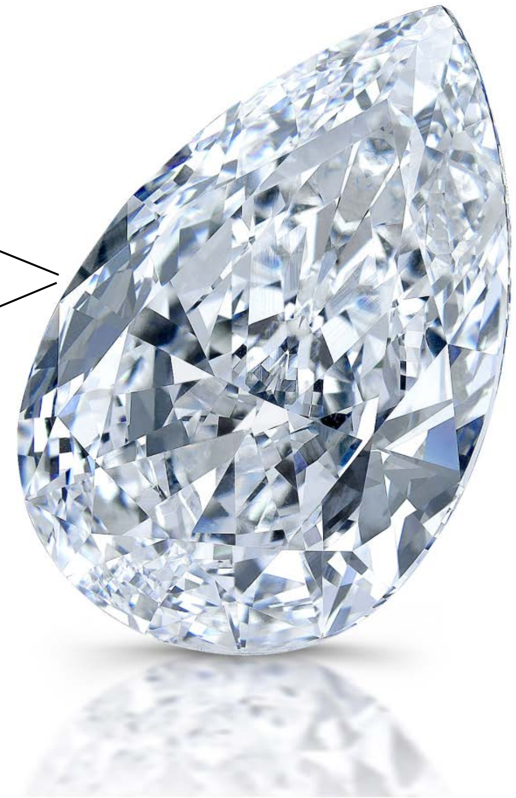
# Nano-diamonds as spin quantum sensors

# Nano-diamonds as spin quantum sensors

Crystals are like people, its only the defects t
hat make them interesting F. Franck

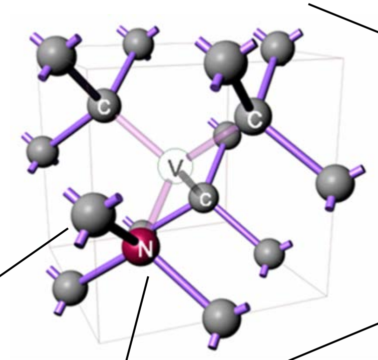
# Nano-diamonds as spin quantum sensors

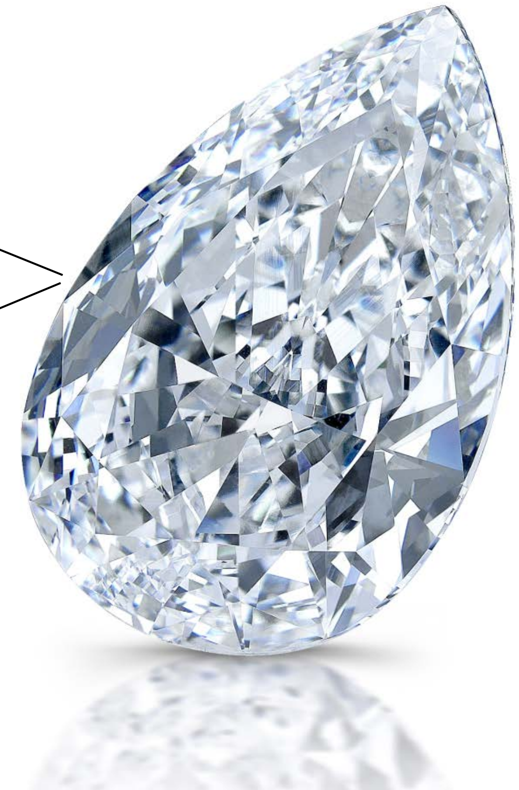


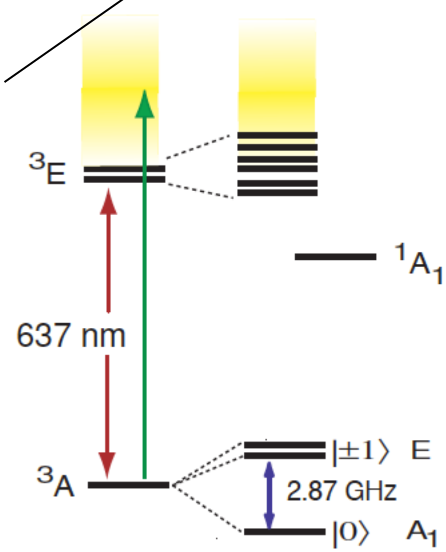



Crystals are like people, its only the defects t
hat make them interesting F. Franck

# Nano-diamonds as spin quantum sensors



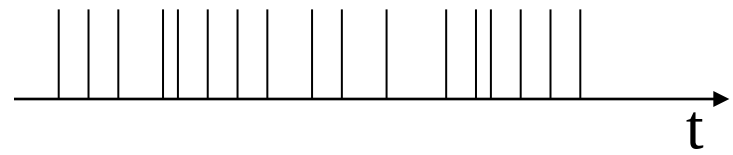


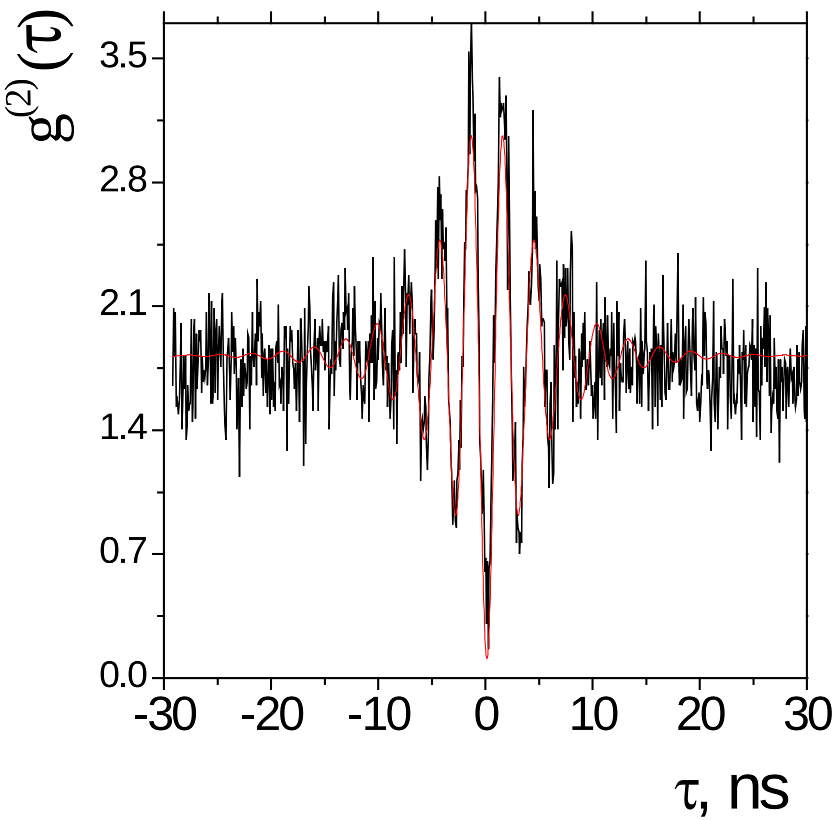

Crystals are like people, its only the defects t
hat make them interesting F. Franck

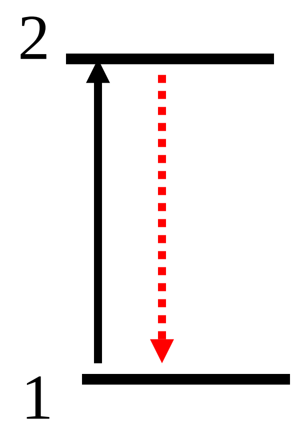
# Single-center signature

$$g^{(2)}(\tau) = \langle I(t) I(t+\tau) \rangle \Big/ \langle I(t) \rangle^2$$

Photon stream



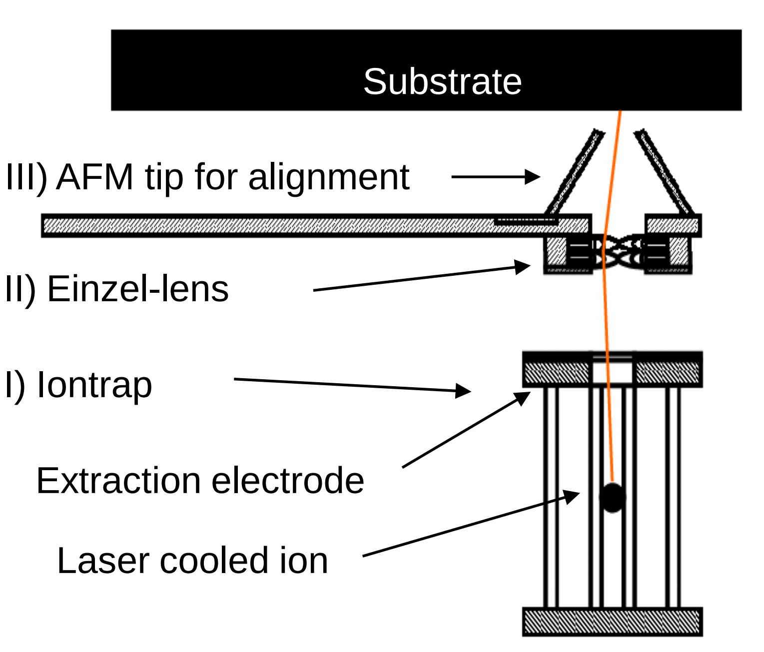




Single photon source:
Kurtsiefer, Weinfurter et al. PRL 85 (2000)

First commercial implementation
QCV, Melbourne, 2008

Transform-limited single photons @4K
Batalov et al., PRL 2008

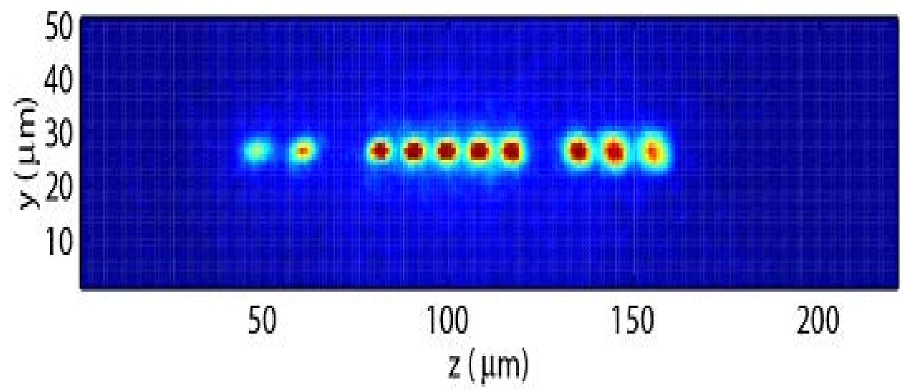
# Deterministic creation of NV-center

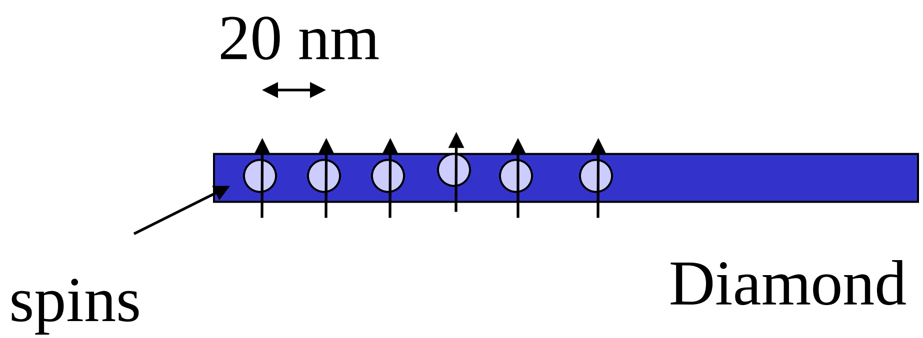



J. Meijer *et al.*, cond-mat/0508756
Applied Physics A 83,   321  (2006)

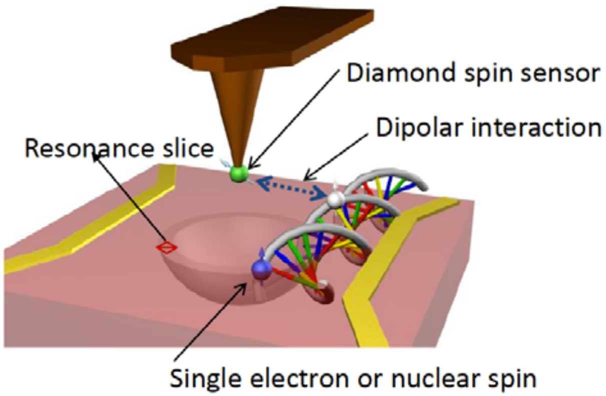
**Sympathetic Cooling of $N^+$ Ions**

H. C.  Nägerl, Innsbruck, unpublished



# Nano-diamonds as spin quantum sensors




J. R. Maze, et al, Nature 2008
G. Balasubramanian, …, Jelezko, Wrachtrup, Nature 2008.

- Chemical and thermal stability
- Optical readout
- Coherent control with microwave
- Long coherence time: spin bath

Challenge: How to detect a single nucleus in real environments?

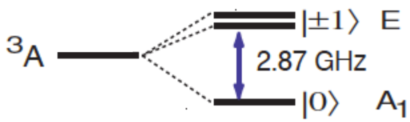
- Small magnetic moment: Long measurement time
- Single out the target nucleus from environment noise
- Detect minute changes in position

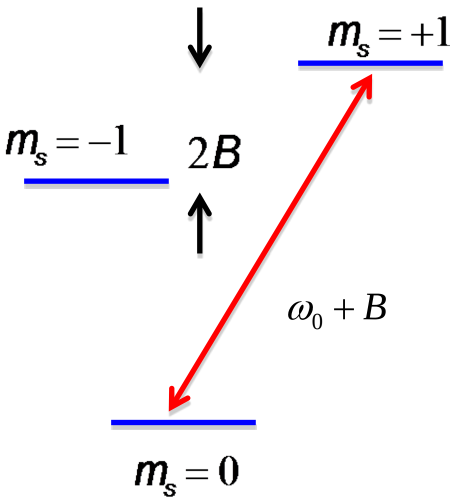
Hardware approach
Reduce noise and imperfections

Software approach
Use radiation to make system immune to noise

→ Single molecule optically detected magnetic resonance spectroscopy

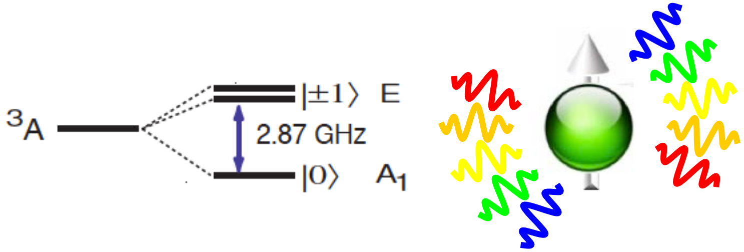
# Protecting against noise



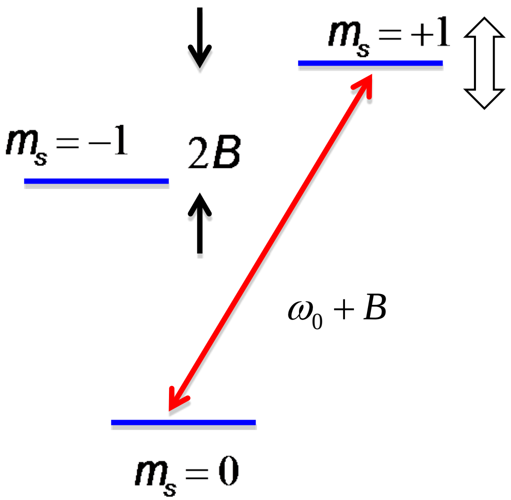

Magnetic field defines two-level system

# Protecting against noise



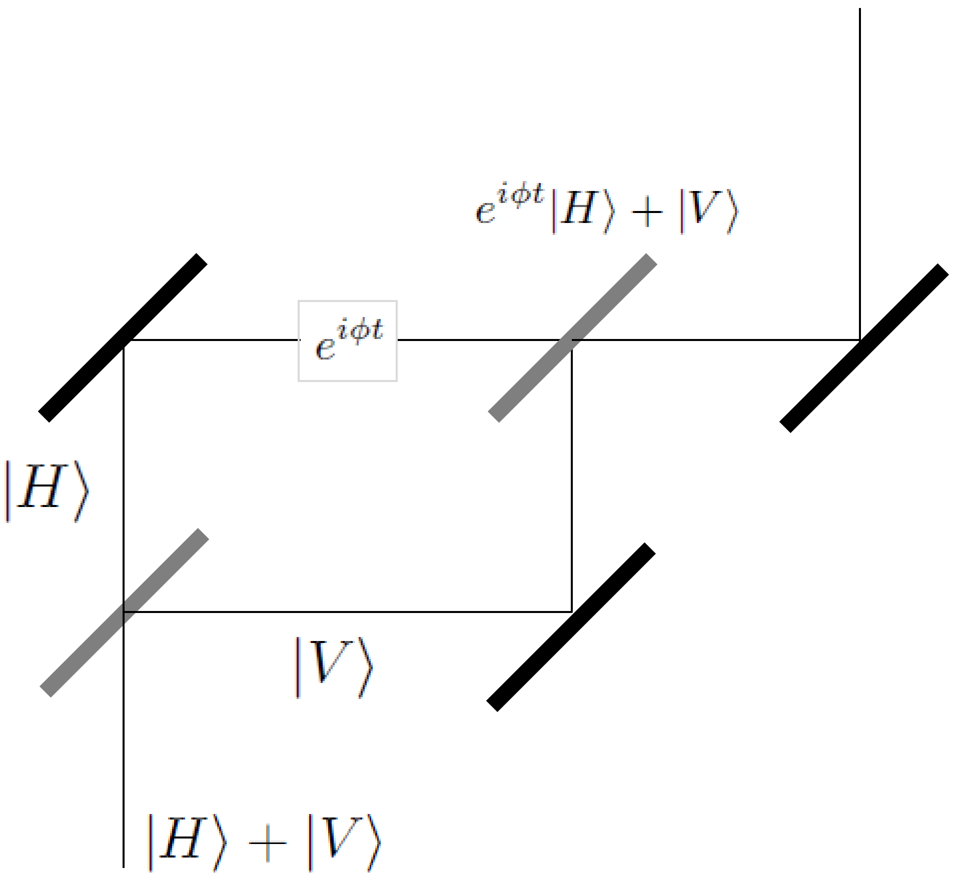

Environmental fluctuations possess finite memory time

⇨ Employ dynamical decoupling techniques

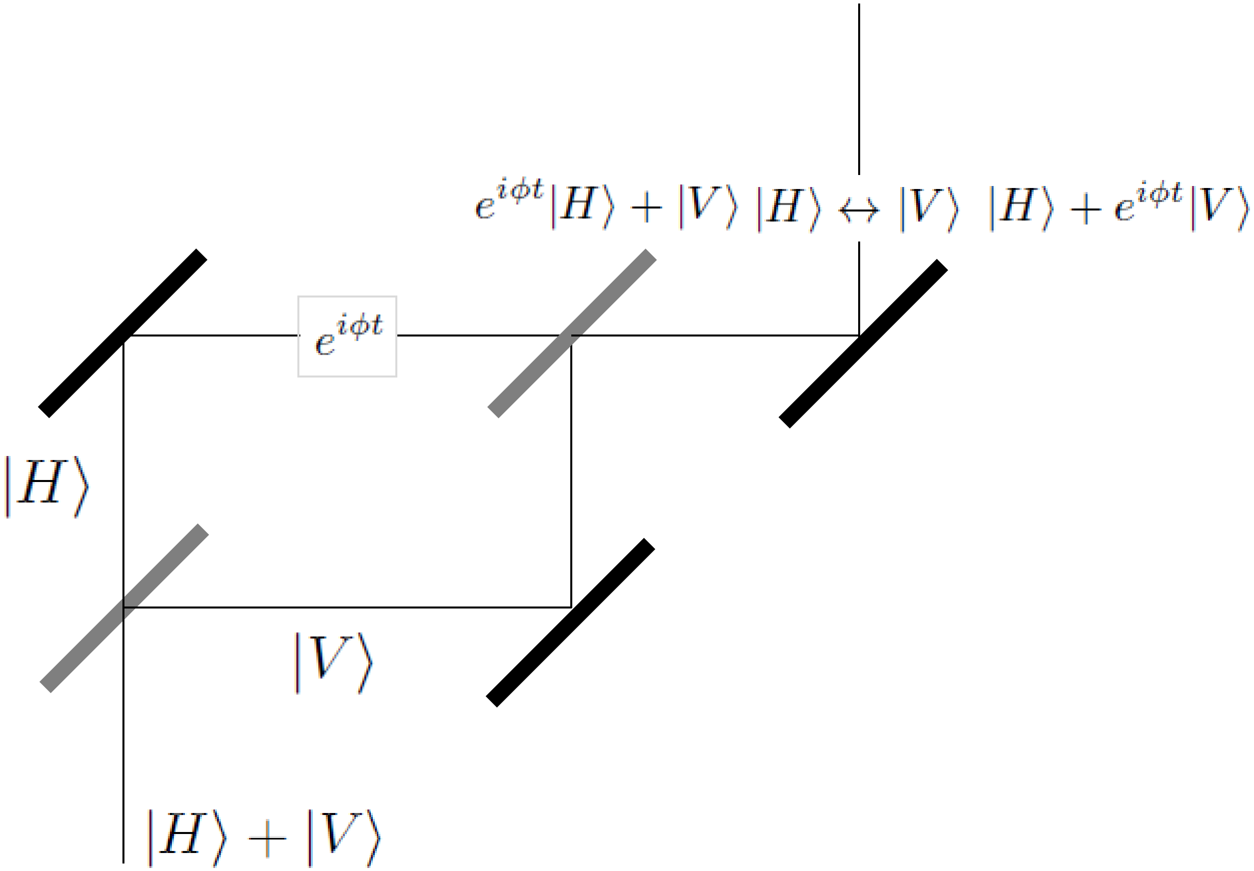



Magnetic field defines two-level system

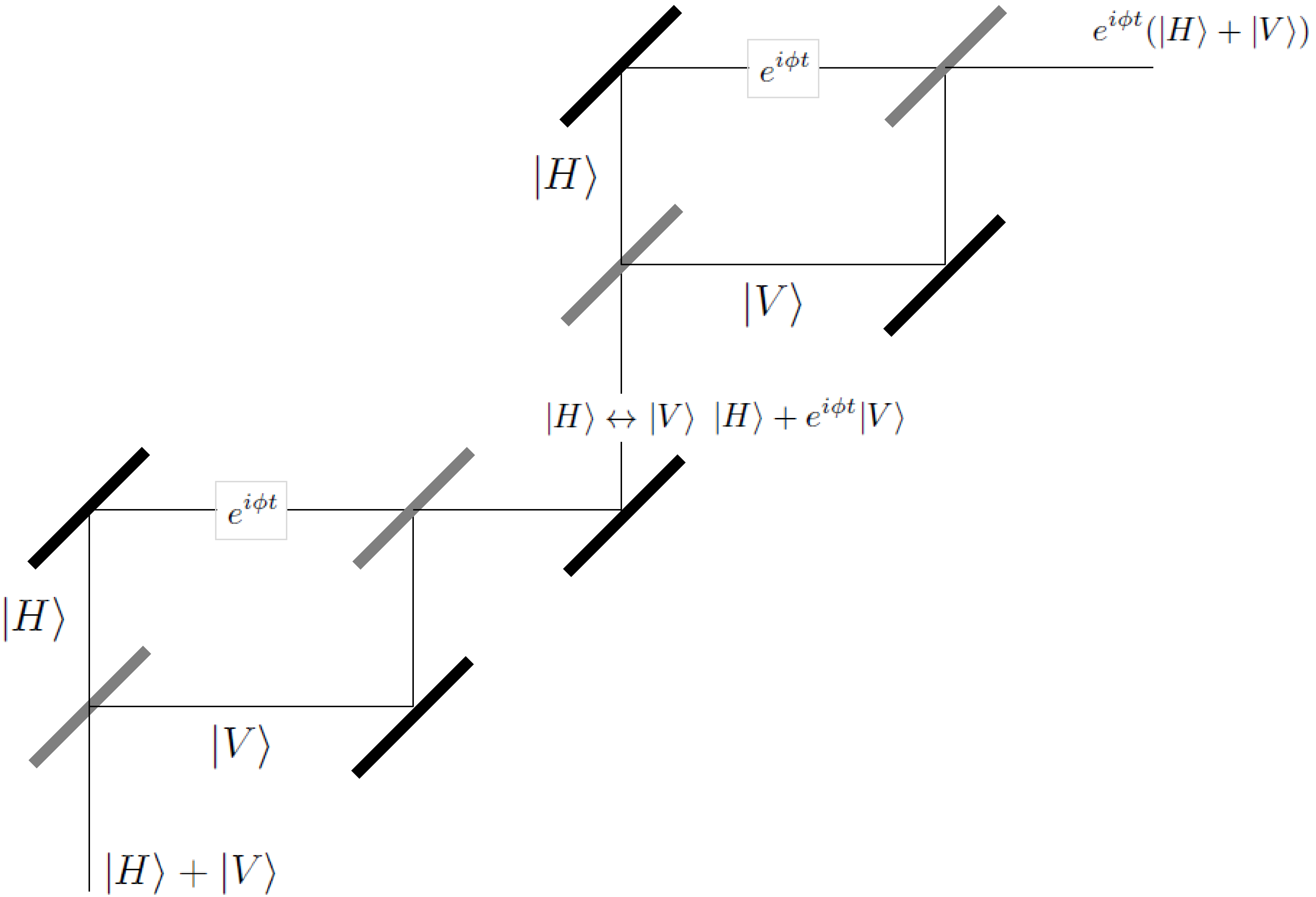
# Protecting against noise



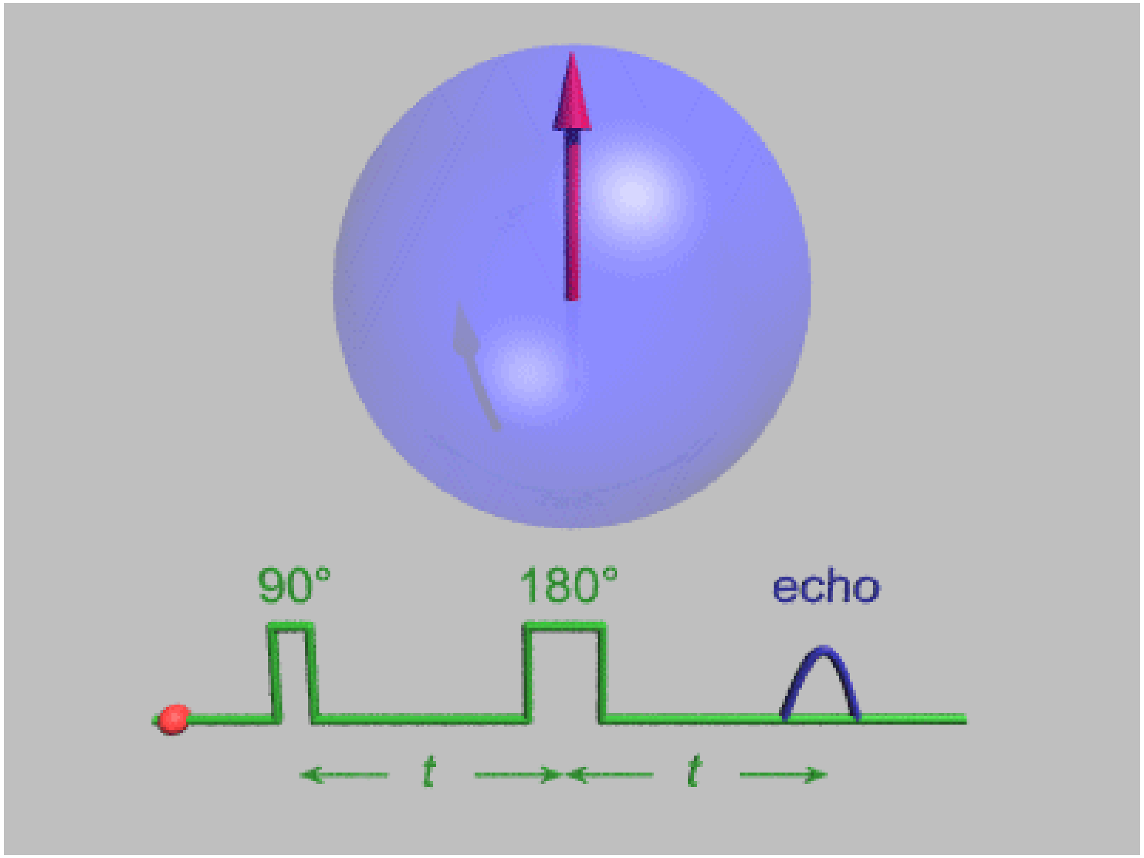
# Protecting against noise



# Protecting against noise

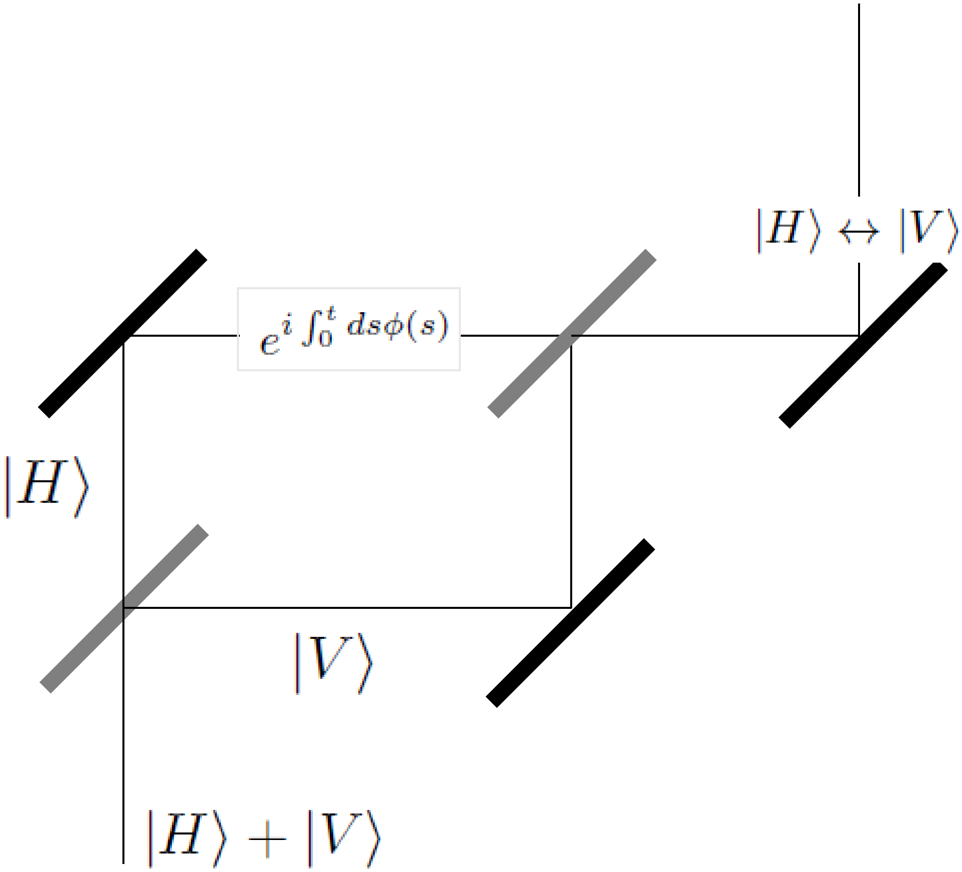


# Hahn echo –

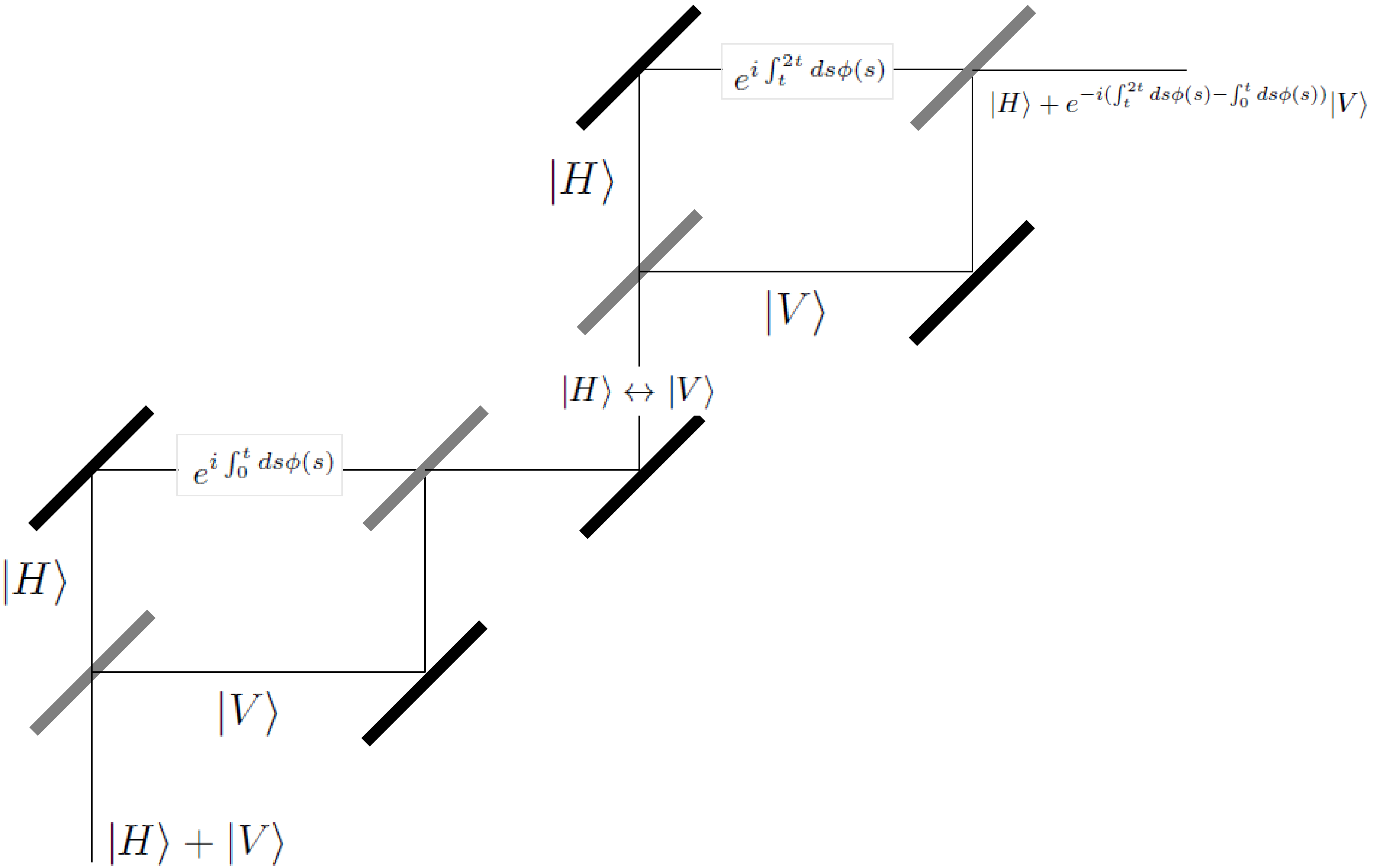



Hahn, Phys. Rev. 1950

# Protecting against noise



# Protecting against noise



# Protecting against noise

## Slow change of frequency

$$e^{i(\int_t^{2t} ds\phi(s) - \int_0^t ds\phi(s))} \cong e^{i(\int_t^{2t} ds(\phi(0)+s\phi'(0)) - \int_0^t ds(\phi(0)+s\phi'(0)))}$$

$$= e^{i(\int_t^{2t} dss\phi'(0) - \int_0^t dss\phi'(0))}$$

$$= e^{it^2\phi'(0)}$$

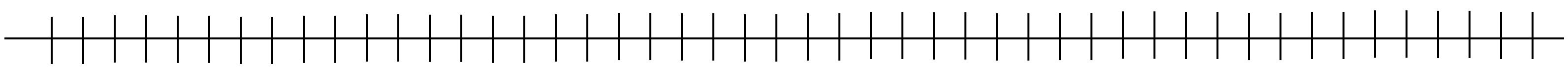
# Protecting against noise

## Slow change of frequency

$$e^{i(\int_t^{2t} ds\phi(s) - \int_0^t ds\phi(s))} \cong e^{i(\int_t^{2t} ds(\phi(0)+s\phi'(0)) - \int_0^t ds(\phi(0)+s\phi'(0)))}$$

$$= e^{i(\int_t^{2t} dss\phi'(0) - \int_0^t dss\phi'(0))}$$

$$= e^{it^2\phi'(0)}$$



t = 0

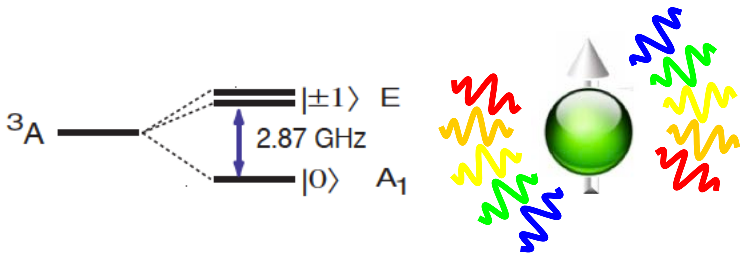
N time intervals
of length T/N

t = T

Total phase: $\left(e^{i(\frac{T}{N})^2\phi'(0)}\right)^N = e^{i\frac{T^2}{N}\phi'(0)} \xrightarrow[N\to\infty]{} 1$

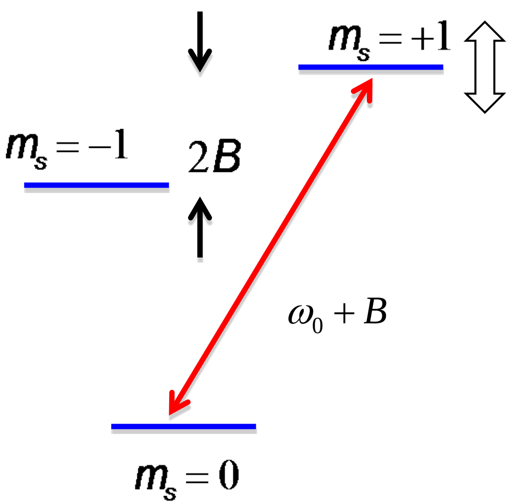
Rapid sequence of π-pulses cancels dephasing noise

# Protecting against noise

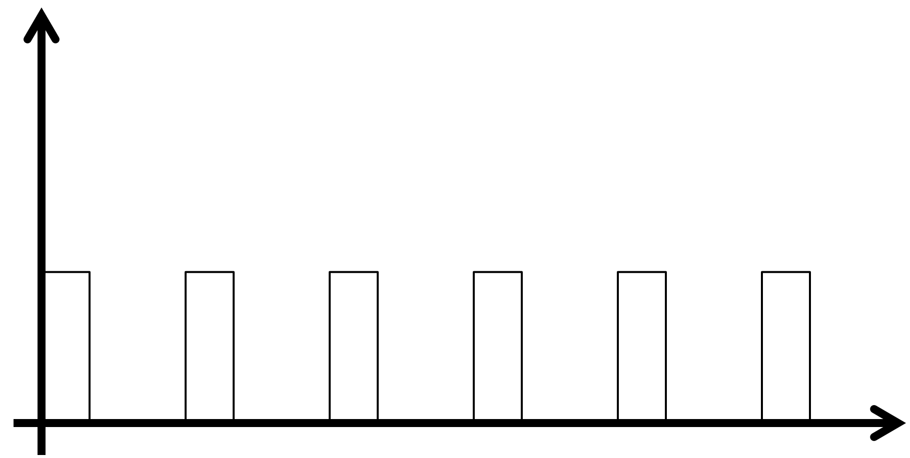



Environmental fluctuations possess finite memory time

⇒ Employ dynamical decoupling techniques



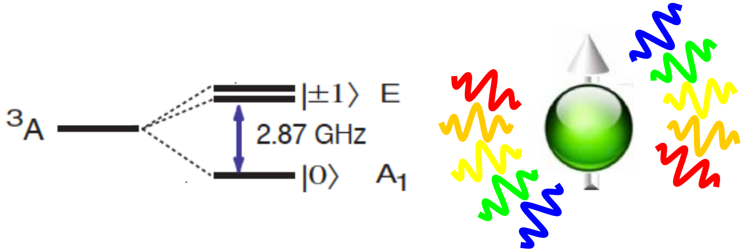

Magnetic field defines two-level system



Pulsed decoupling – Induce short π-pulses to average out interaction with the environment

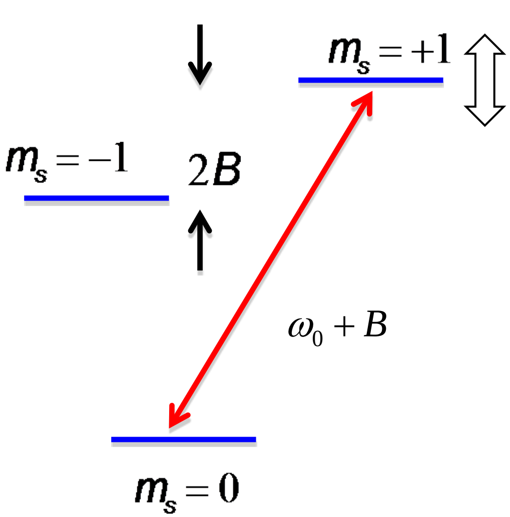
Hahn, Phys. Rev. 1950 ; Carr, Purcell, Phys. Rev. 1954; Meiboom & Gill, Rev.Sci.Inst. 1958, .................

# Protecting against noise

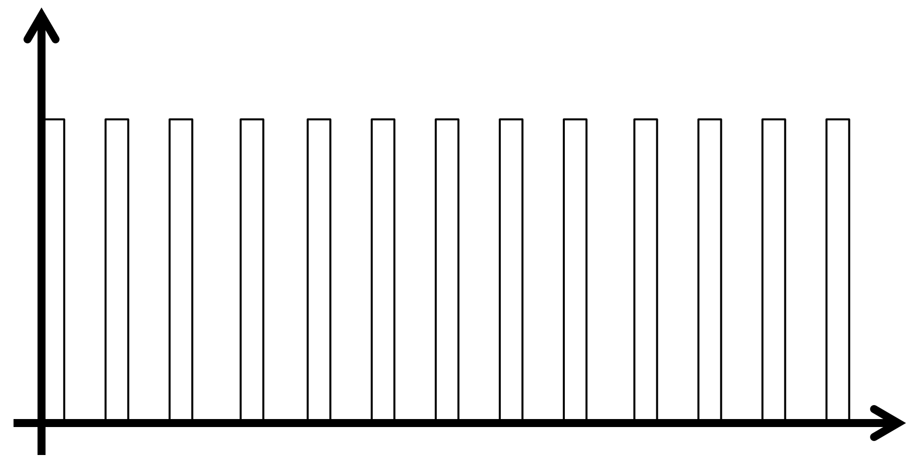



Environmental fluctuations possess finite memory time

⇨ Employ dynamical decoupling techniques




Magnetic field defines two-level system

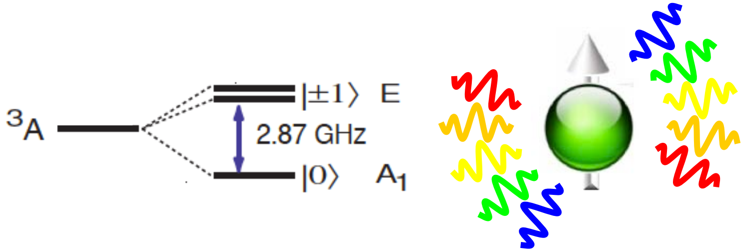


Pulsed decoupling – Induce short π-pulses to average out interaction with the environment

Increase pulse rate to improve decoupling

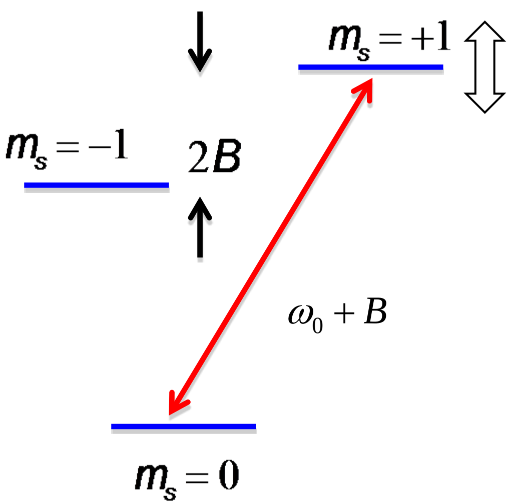
Hahn, Phys. Rev. 1950 ; Carr, Purcell, Phys. Rev. 1954; Meiboom & Gill, Rev.Sci.Inst. 1958, .................

# Protecting against noise

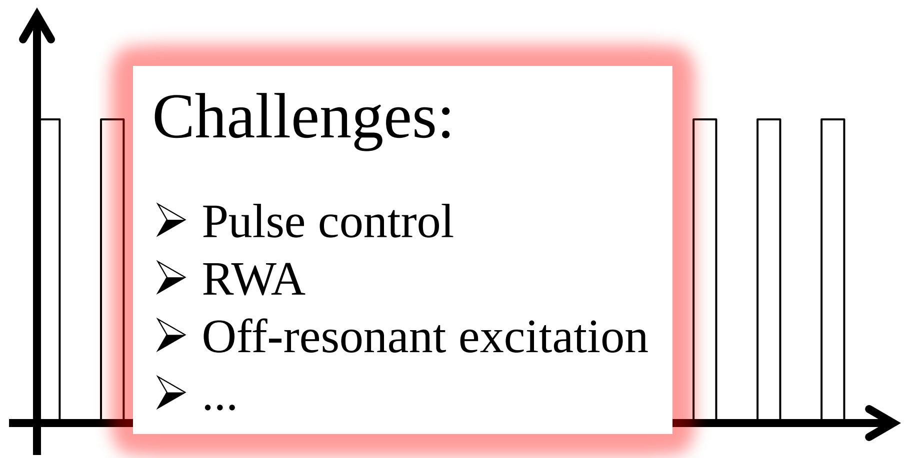



Environmental fluctuations possess finite memory time

⇨ Employ dynamical decoupling techniques




Magnetic field defines two-level system



## Challenges:

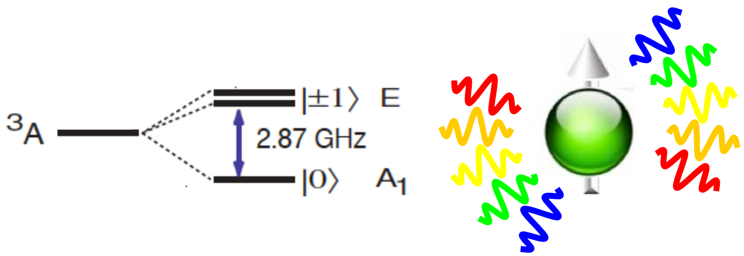
- Pulse control
- RWA
- Off-resonant excitation
- ...

Pulsed decoupling – Induce short π-pulses to average out interaction with the environment

Increase pulse rate to improve decoupling

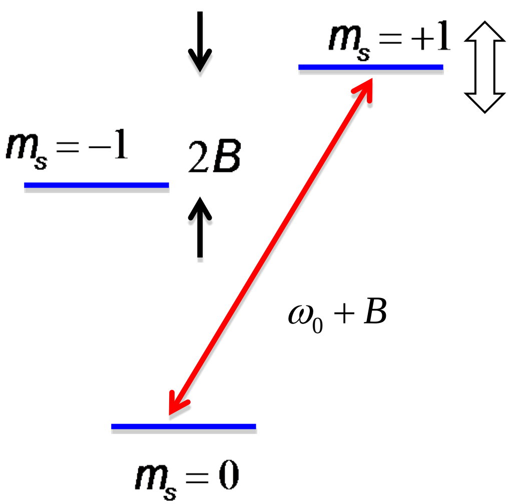
Hahn, Phys. Rev. 1950 ; Carr, Purcell, Phys. Rev. 1954; Meiboom & Gill, Rev.Sci.Inst. 1958, .................

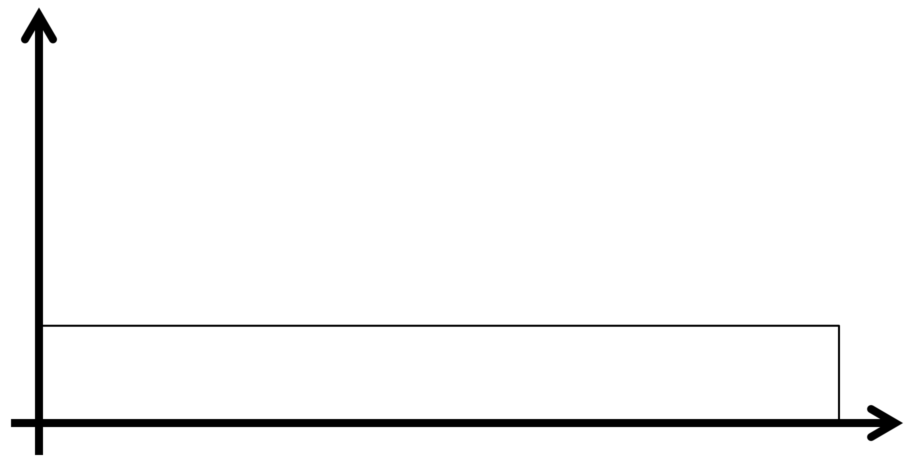
# Protecting against noise




Environmental fluctuations possess finite memory time

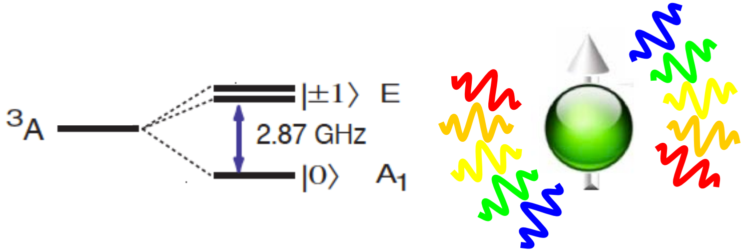
⇨ Employ continuous dynamical decoupling techniques



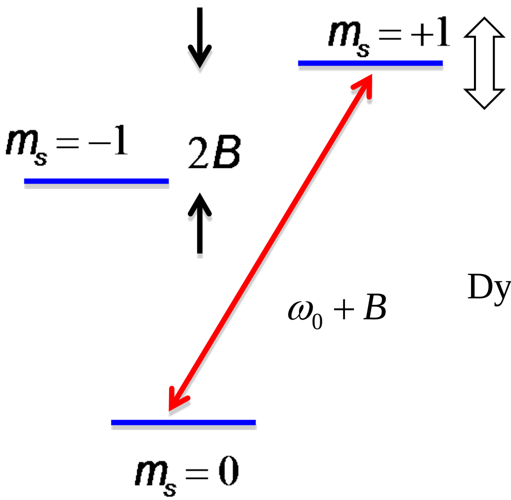
Magnetic field defines two-level system

# Protecting against noise




Environmental fluctuations possess finite memory time

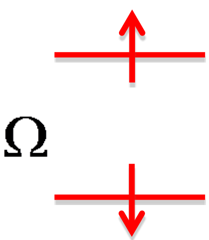
⇒ Employ continuous dynamical decoupling techniques




Continuous ⇒ Dynamical Decoupling

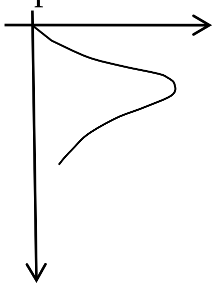
$$H_{NV} = \Omega\sigma_x$$

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




$$|-\rangle = |0\rangle - |+1\rangle$$

Environment spectral density

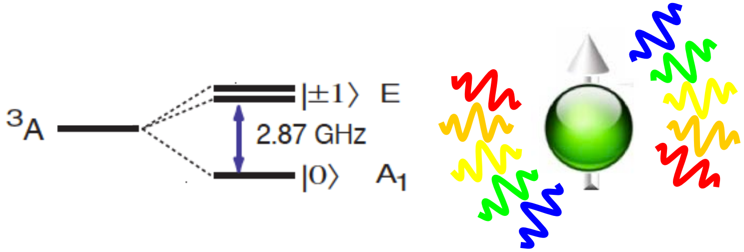


Magnetic field defines two-level system

$$\sigma_z \Leftrightarrow \sigma_x$$

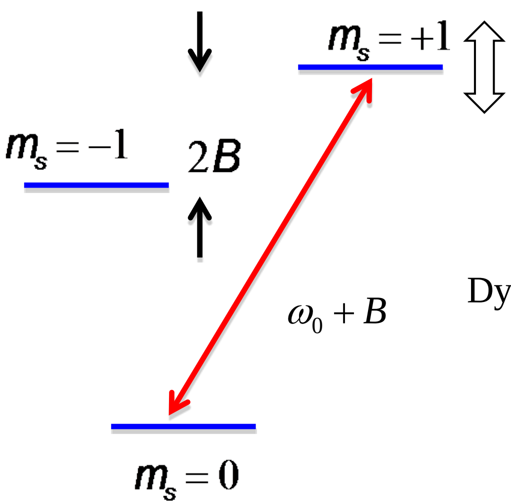
Interaction with environment carries energy penalty

# Protecting against noise

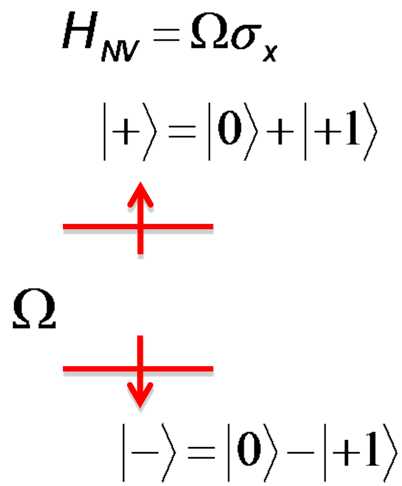


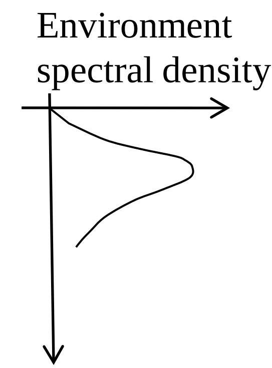

Environmental fluctuations possess finite memory time

⇒ Employ continuous dynamical decoupling techniques




Continuous ⇒ Dynamical Decoupling



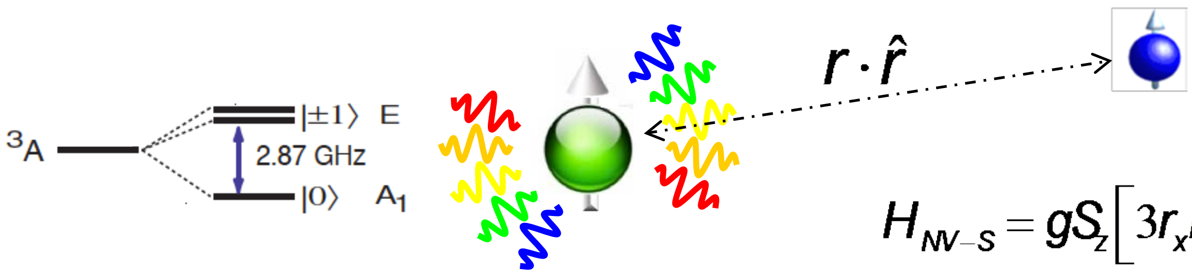

Magnetic field defines two-level system

$\sigma_z \Leftrightarrow \sigma_x$

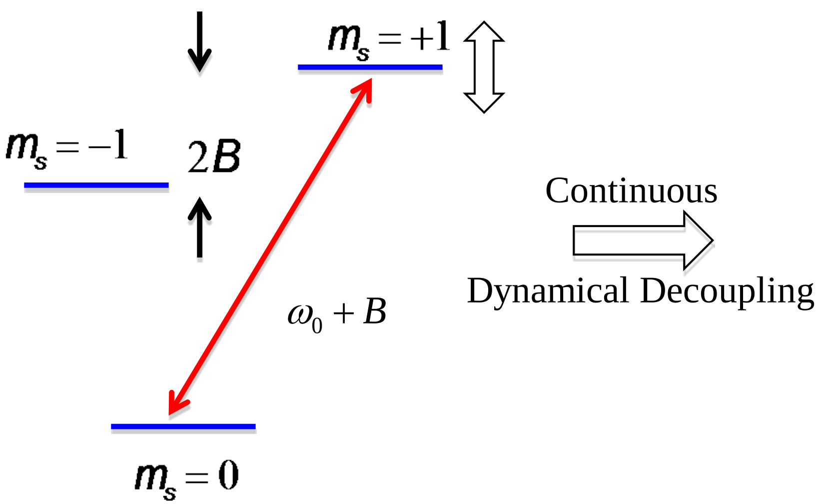
Interaction with environment carries energy penalty

Discovered many times:
F. Bloch 1950's , P. Facchi, D. A. Lidar, and S. Pascazio, Phys. Rev. A 69, 032314 (2004), K.M. Fonesca-Romero, S. Kohler & P. Hänggi, Chem. Phys. 296, 307 (2004); Fortschr. Phys. 54, 804 (2006) , ...

# Protecting against noise

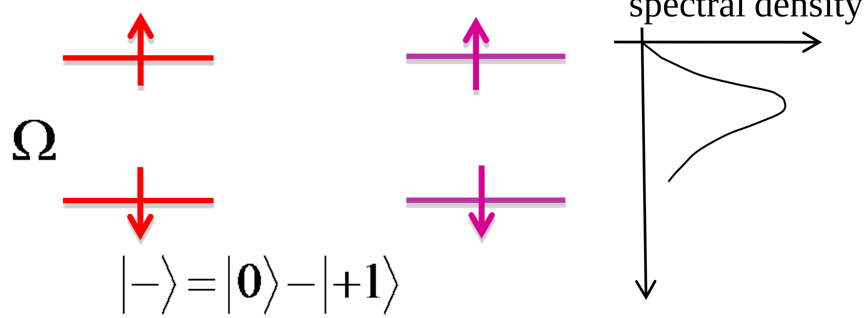



$$H_{NV-S} = gS_z\left[3r_x r_z I_N^x + 3r_y r_z I_N^y + \left(3r_z^2 - 1\right) I_N^z\right]$$




$$H_{NV} = \Omega\sigma_x$$

$$|+\rangle = |0\rangle + |+1\rangle \quad H_S = \gamma_N \vec{B} \cdot \vec{I}_N$$




$$|-\rangle = |0\rangle - |+1\rangle$$

Magnetic field defines two-level system

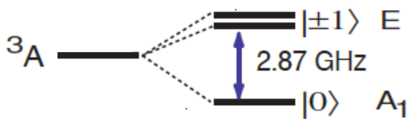
Hartmann-Hahn condition (1962)

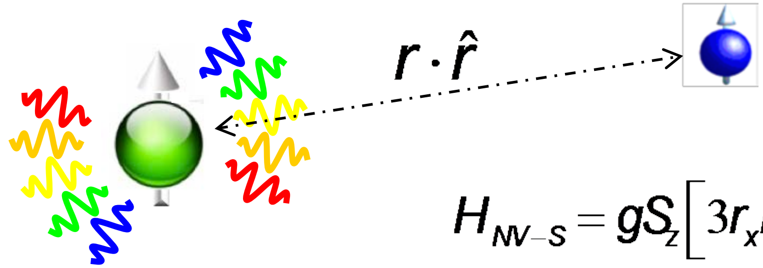
$$\sigma_z \Leftrightarrow \sigma_x$$

Interaction with environment
carries energy penalty

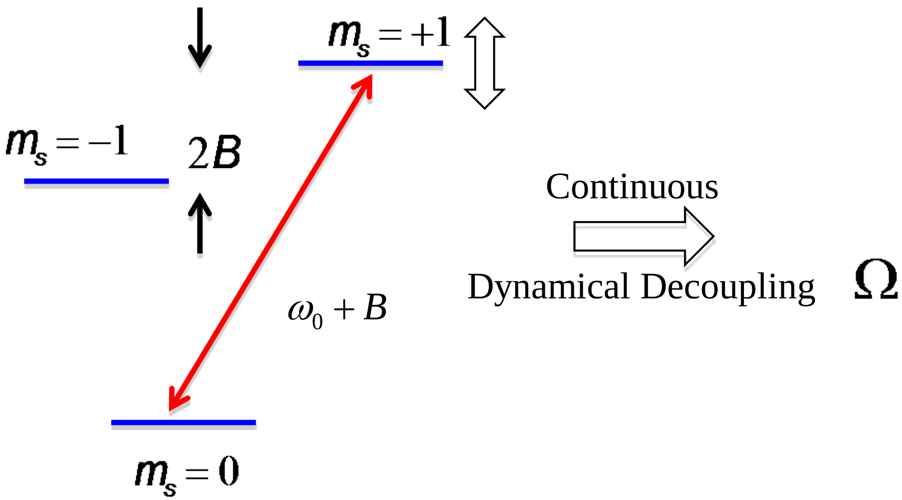
J.-M. Cai et al, arXiv:1112.5502

# Protecting against noise



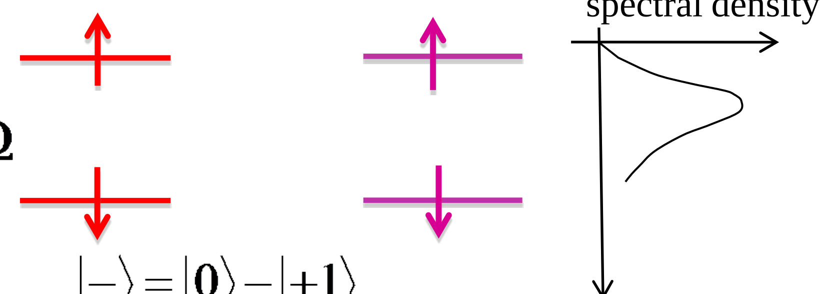




$$H_{NV-S} = g S_z \left[ 3 r_x r_z I_N^x + 3 r_y r_z I_N^y + \left( 3 r_z^2 - 1 \right) I_N^z \right]$$




$$H_{NV} = \Omega \sigma_x$$

$$|+\rangle = |0\rangle + |+1\rangle \quad H_S = \gamma_N \vec{B} \cdot \vec{I}_N$$




$$|-\rangle = |0\rangle - |+1\rangle$$

Magnetic field defines two-level system

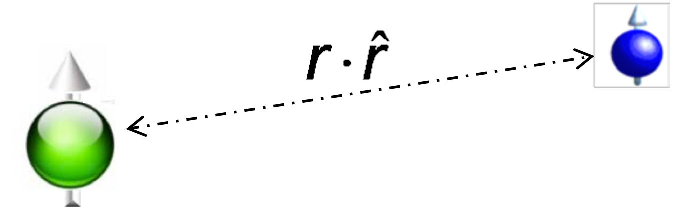
Hartmann-Hahn condition (1962)

$$\sigma_z \Leftrightarrow \sigma_x$$

Interaction with environment
carries energy penalty

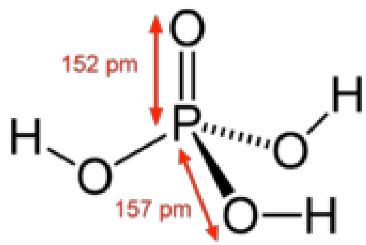
J.-M. Cai et al, arXiv:1112.5502

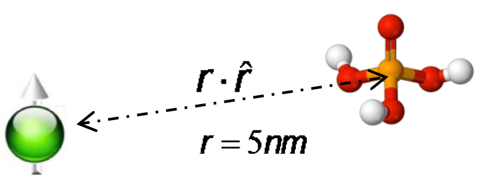
# The sensor in action I



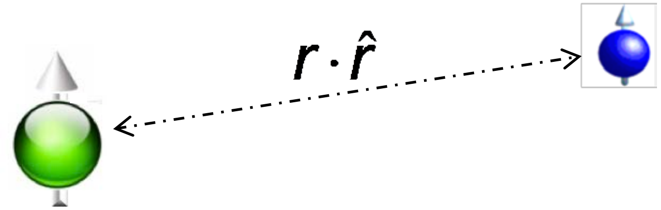

- Measurement on NV spin


Phosphoric acid



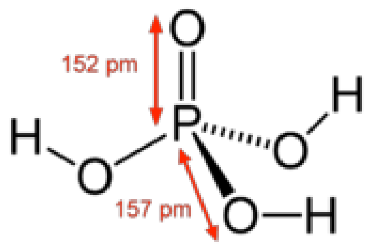



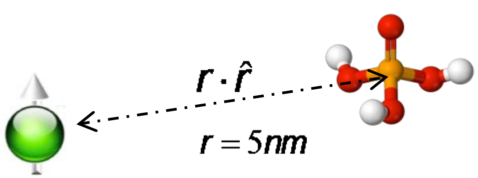
# The sensor in action I

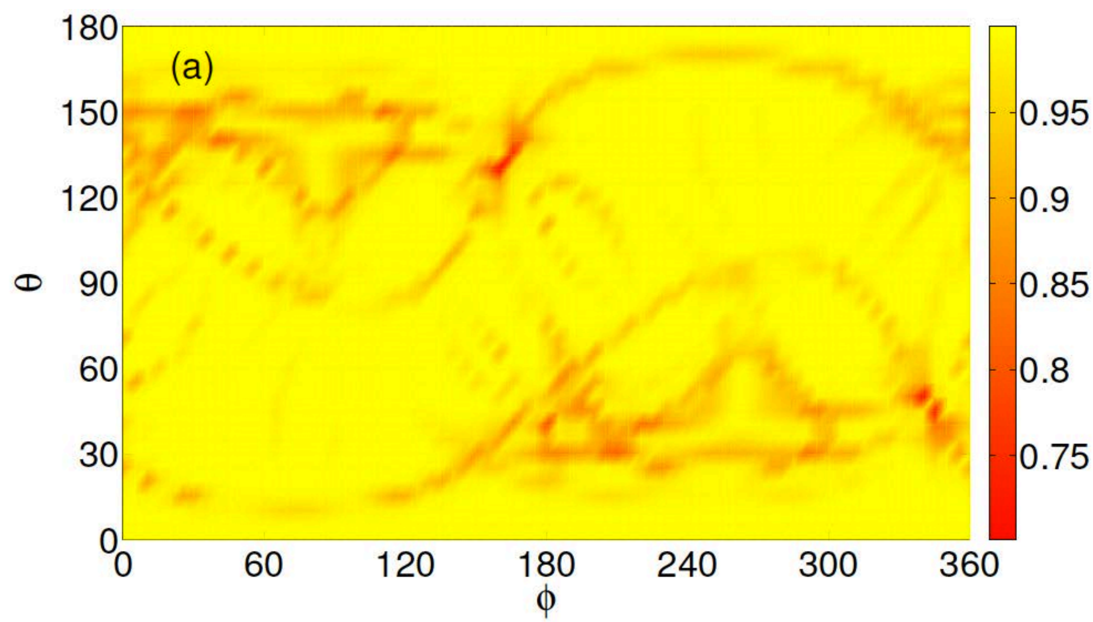



- Measurement on NV spin

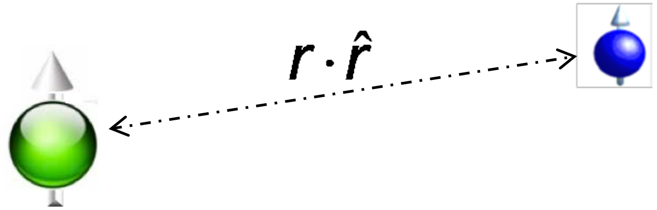

Phosphoric acid



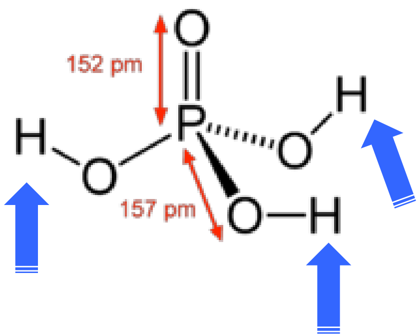



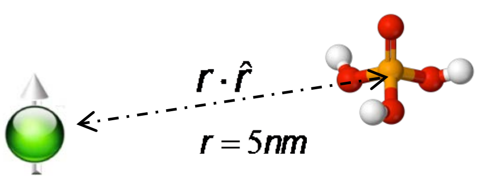
# The sensor in action I

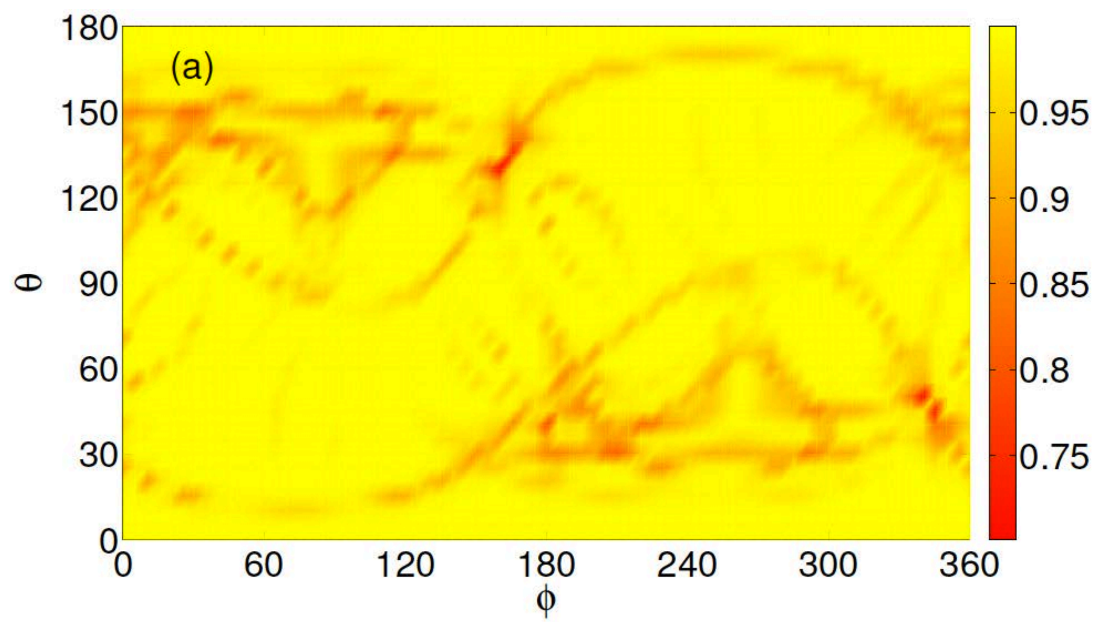



- Measurement on NV spin

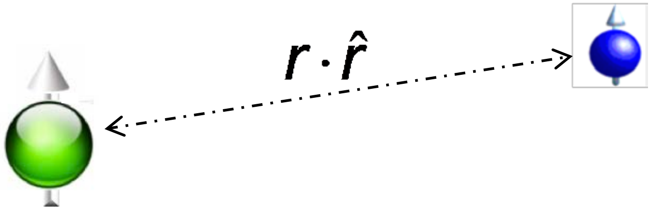

Phosphoric acid



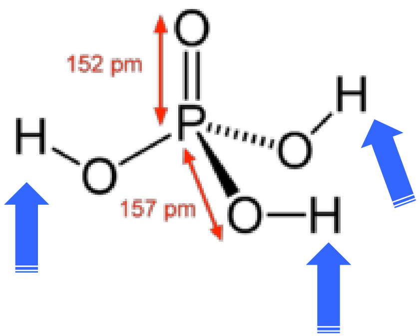



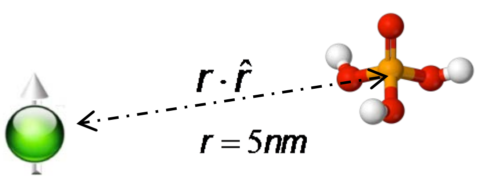
# The sensor in action I

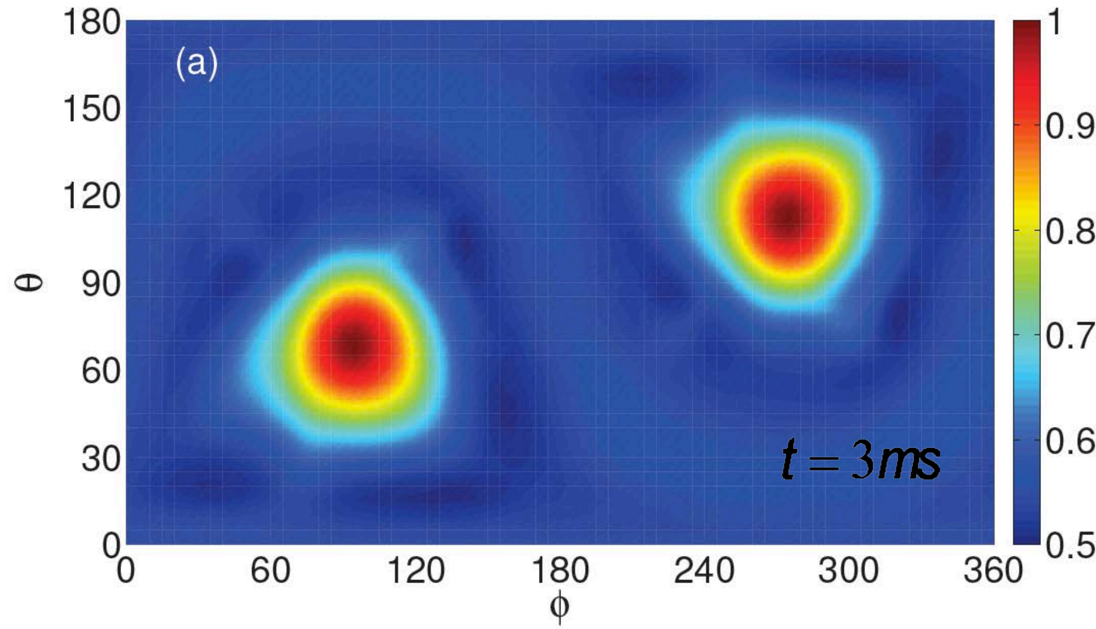



- Measurement on NV spin


Phosphoric acid



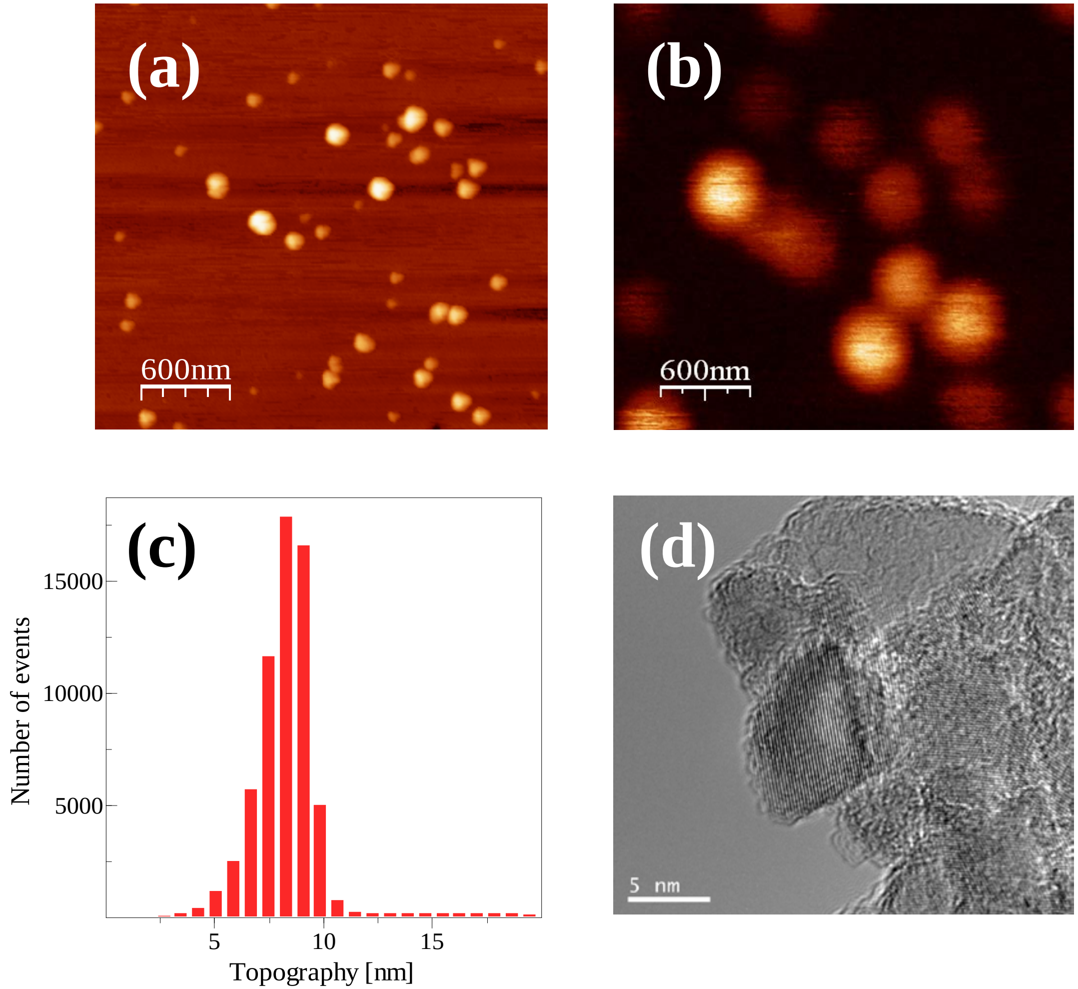




First experimental steps: T.H. Taminiau et al, arXiv:1205.4128 , N. Zhao et al, arXiv:1204.6513 , S. Kolkowitz et al, arXiv:1204.5483

# Part Ia

# Nanodiamonds –



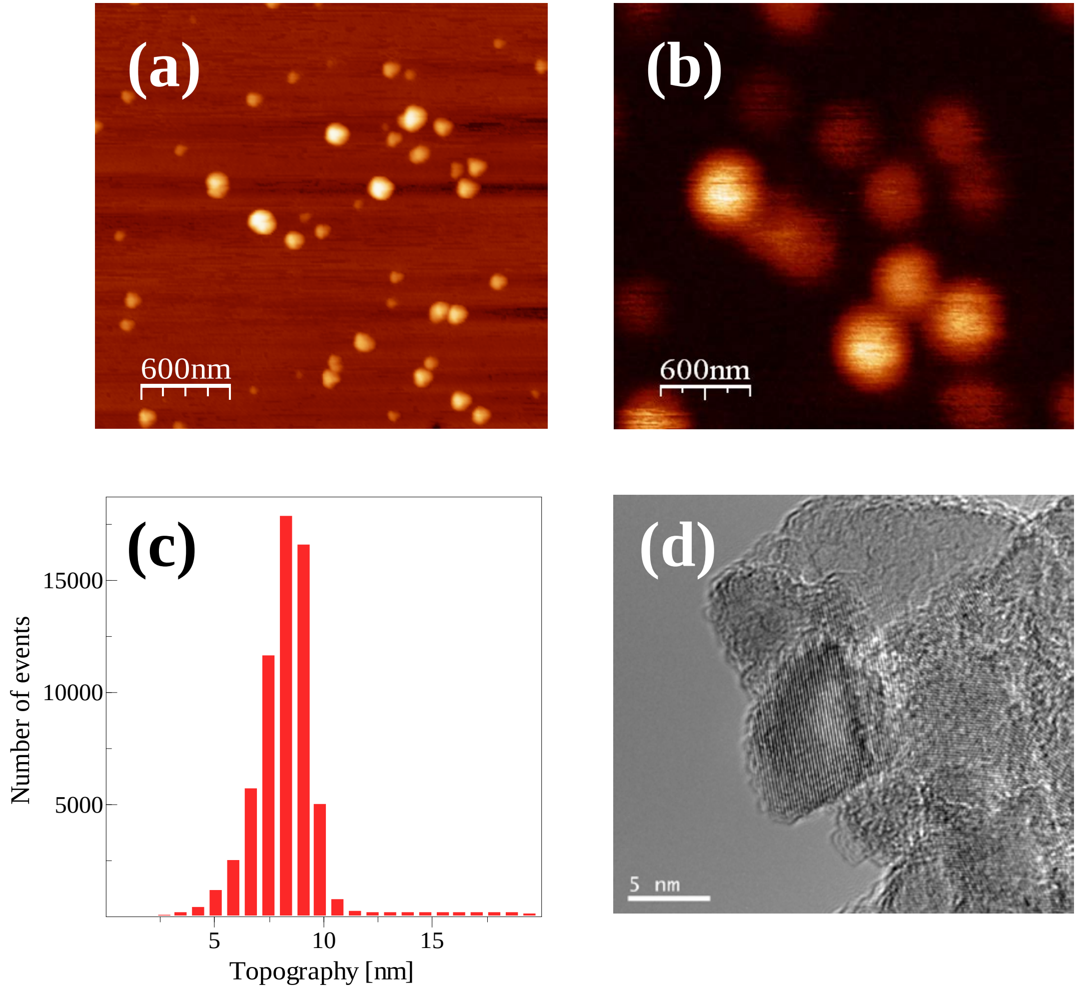

Smalles fluorescent nanodiamonds currently: 5nm

Challenge: Surface is a noisy place and rather close to NV center

Solutions: Clean and terminate the surface with atoms H, OH, F, ...

Problem: These are nuclear spins and thus interact with the NV center → noise

# Nanodiamonds –




Smalles fluorescent nanodiamonds currently: 5nm

Challenge: Surface is a noisy place and rather close to NV center

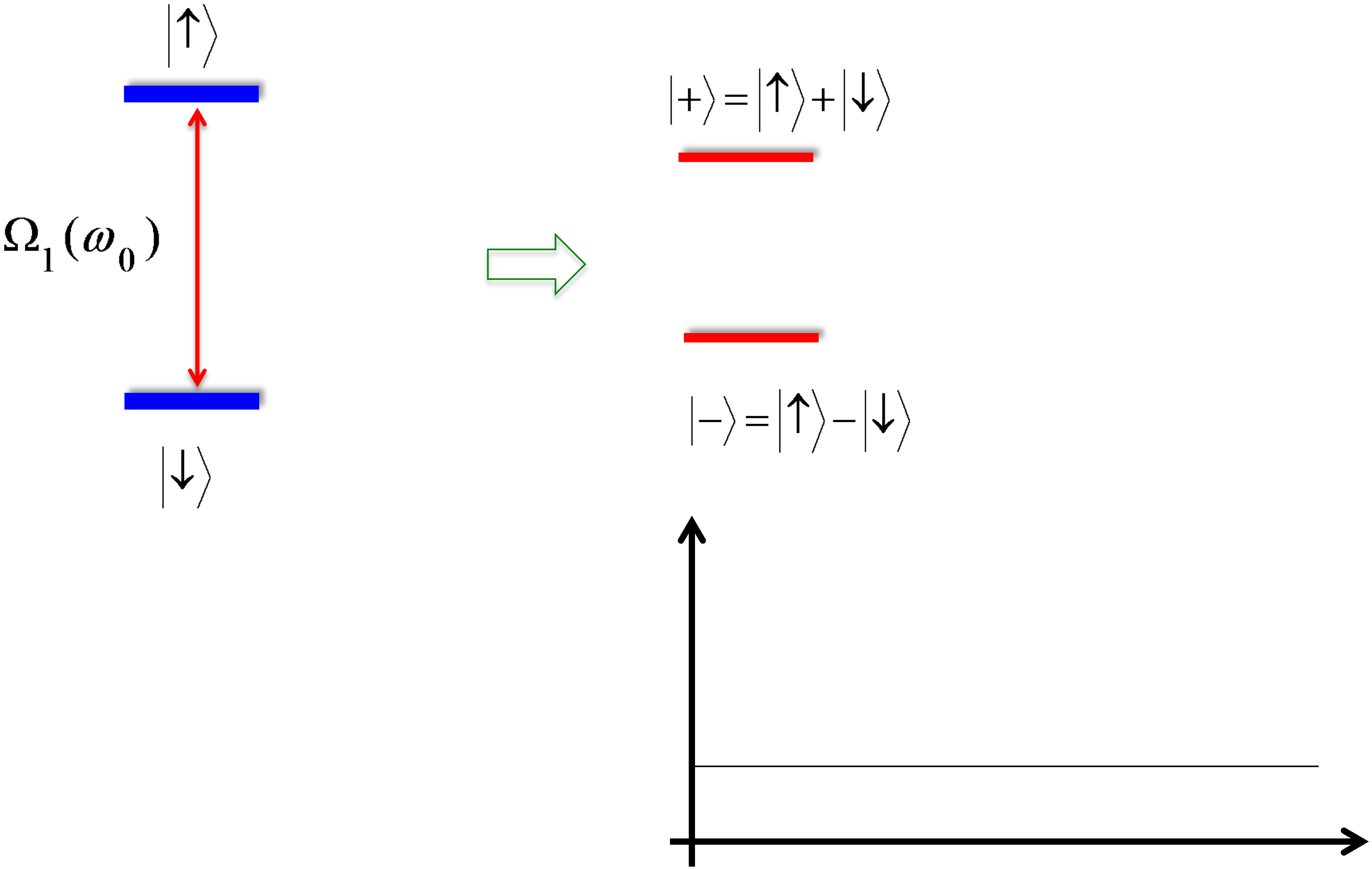
Solutions: Clean and terminate the surface with atoms H, OH, F, ...

Problem: These are nuclear spins and thus interact with the NV center → noise

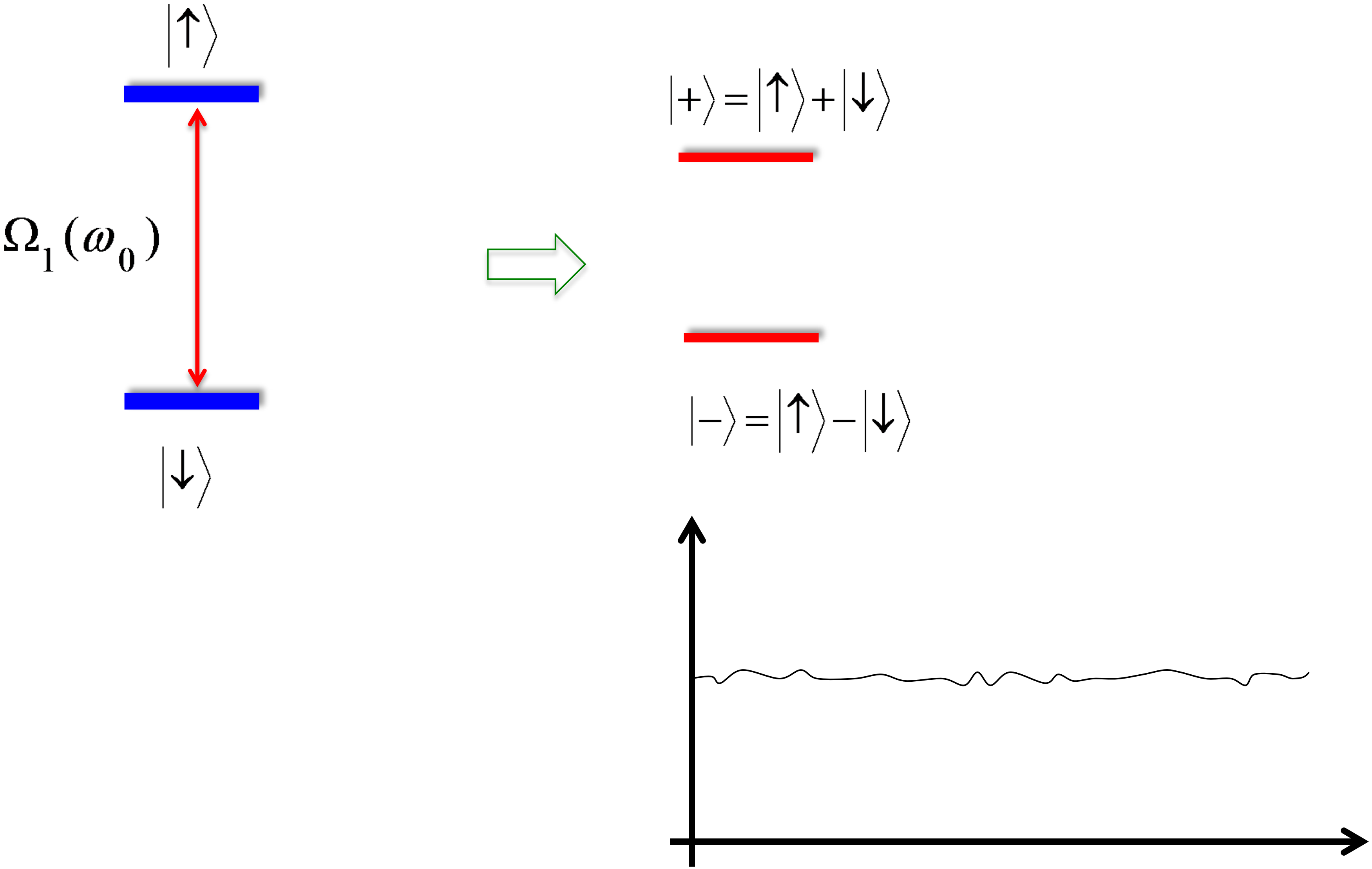
→ Requires quite strong driving to decouple

→ Stability of the drive can become a problem

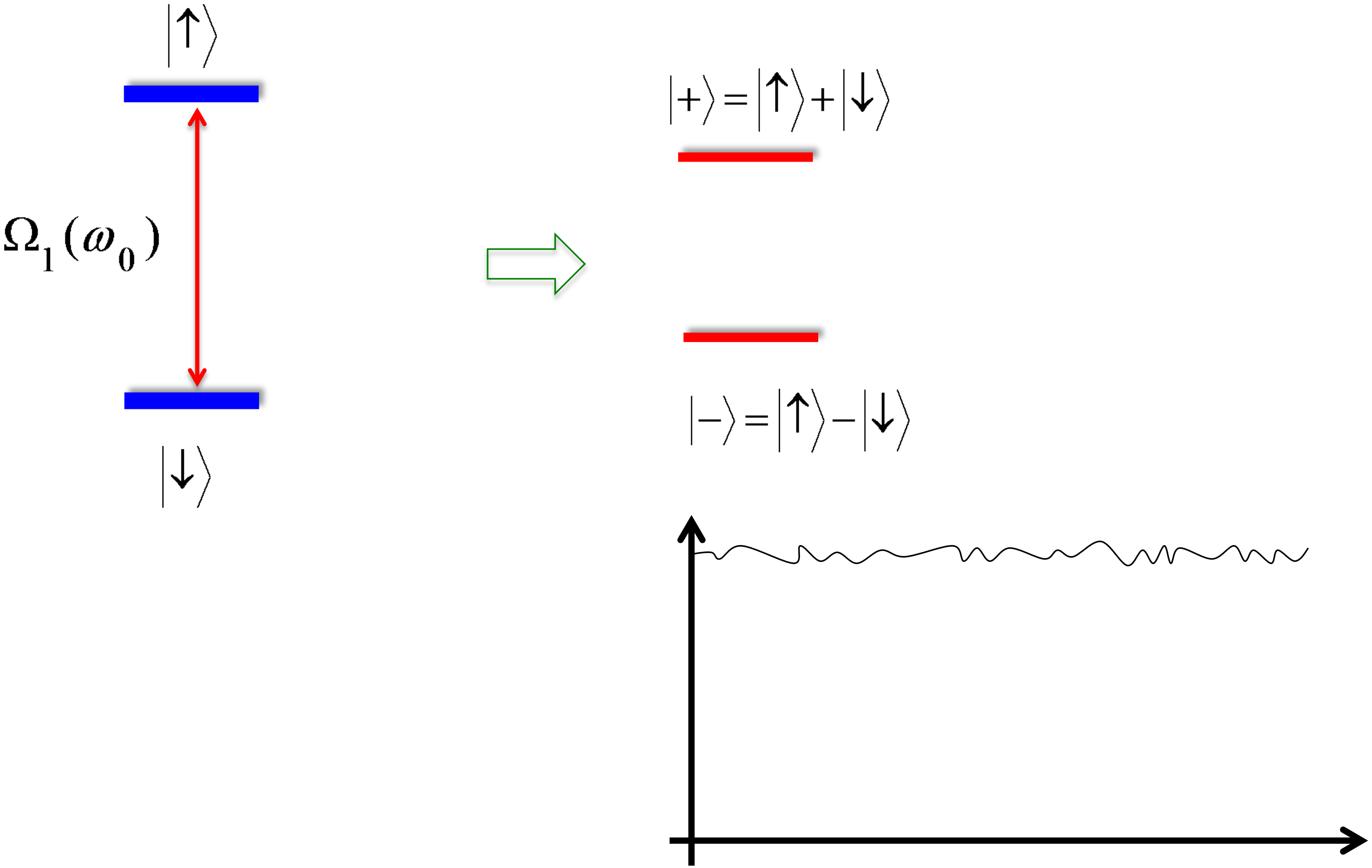
# Concatenated noise protection



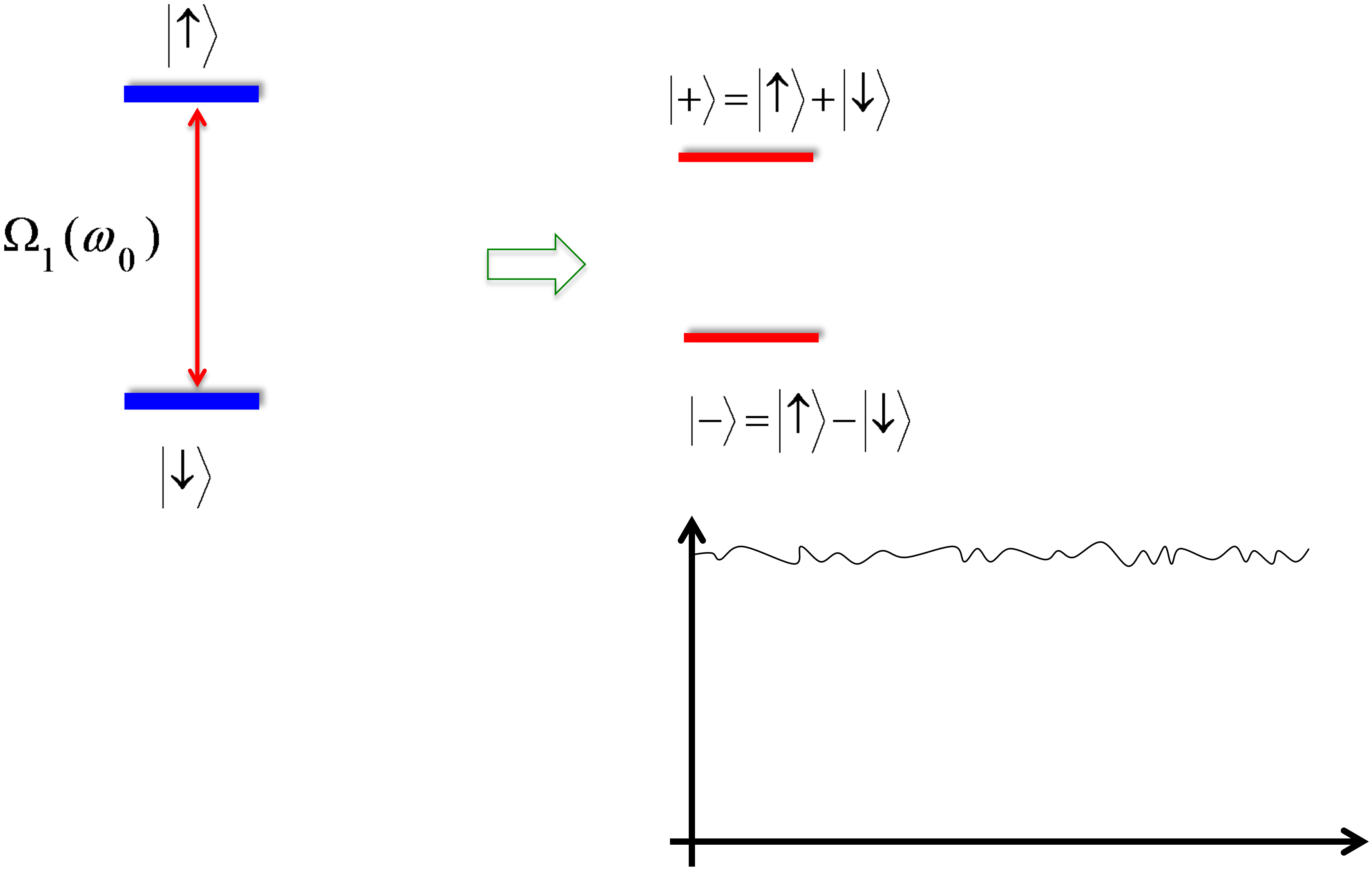
# Concatenated noise protection



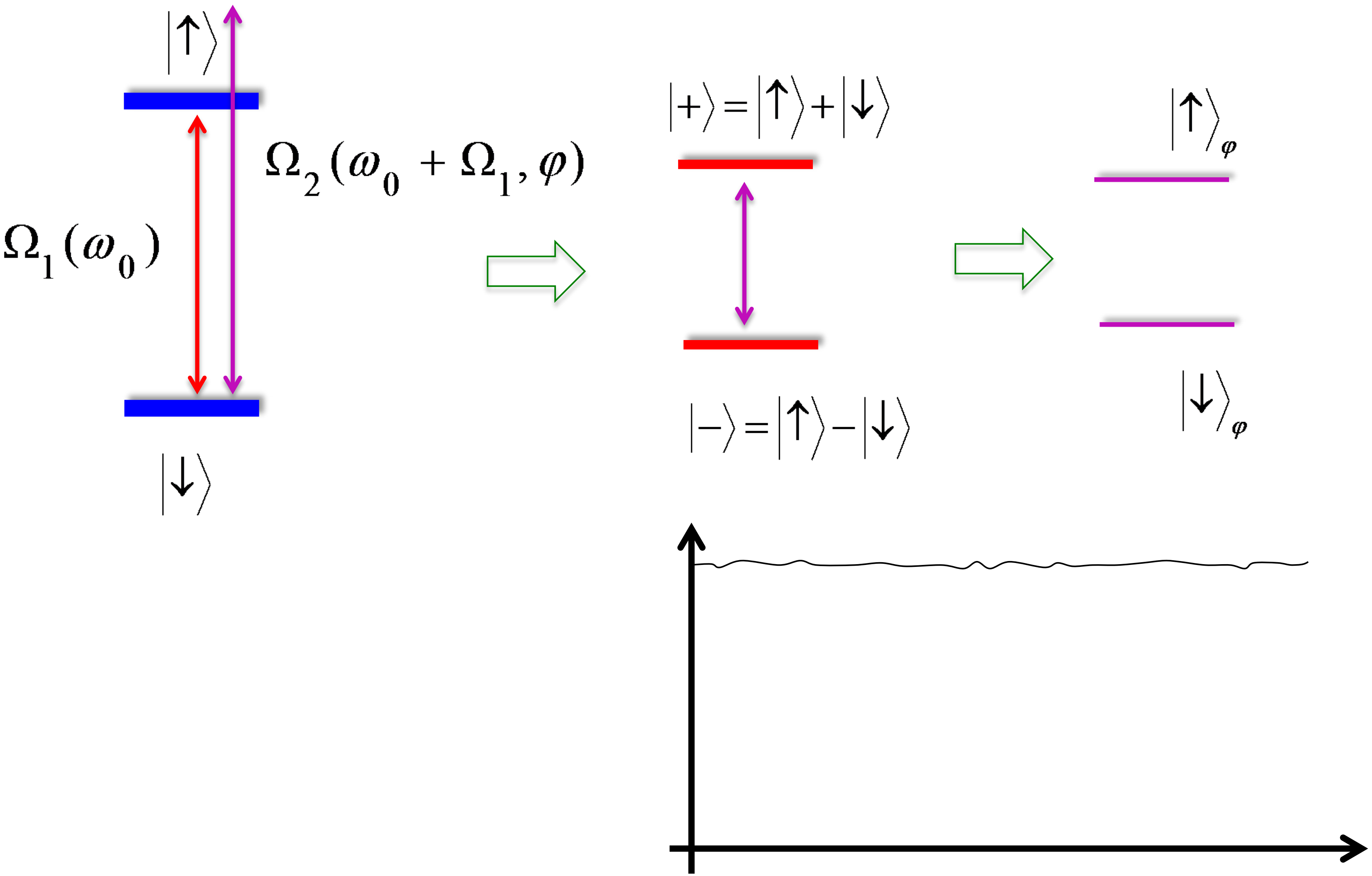
# Concatenated noise protection



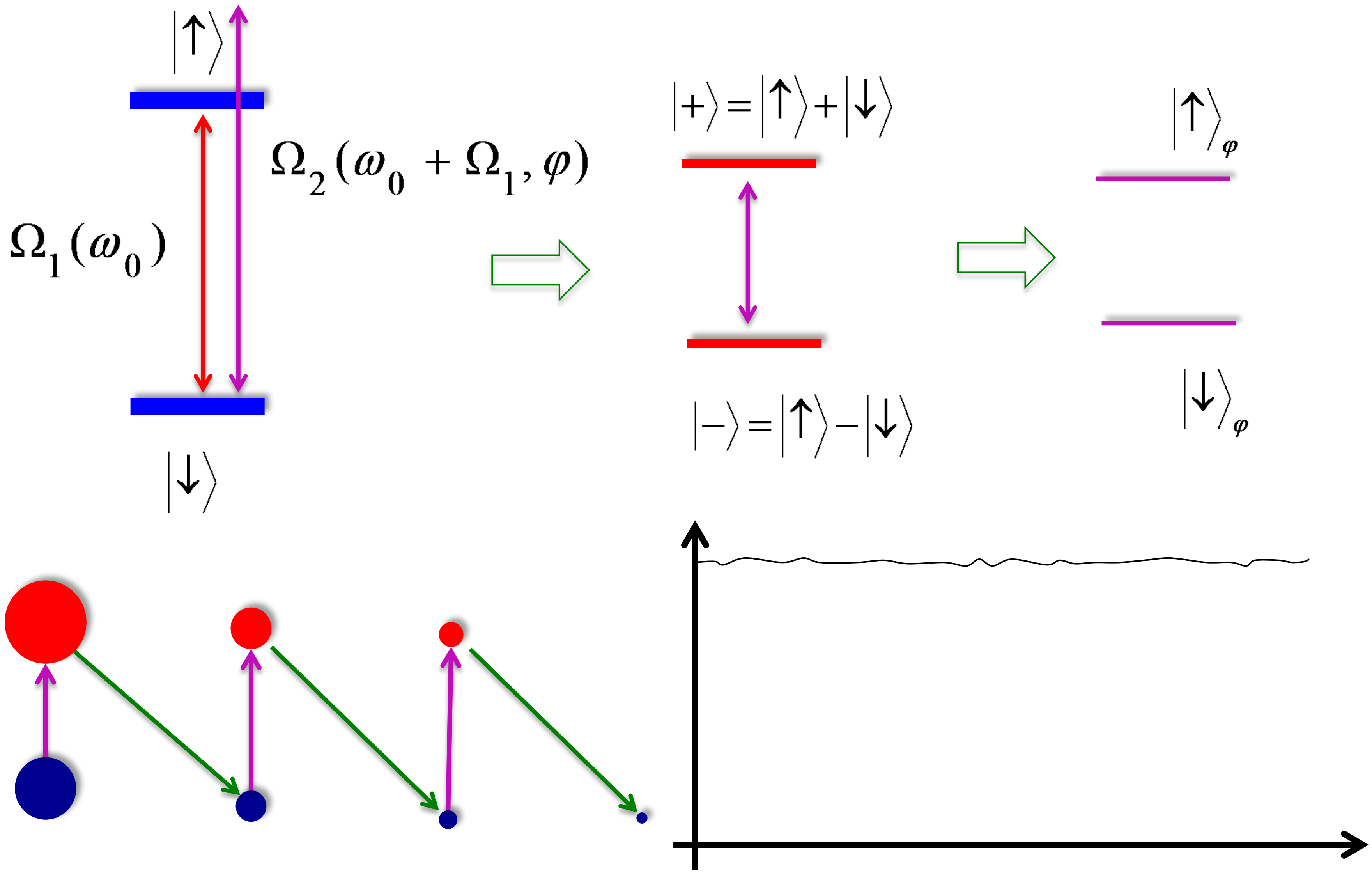
# Concatenated noise protection



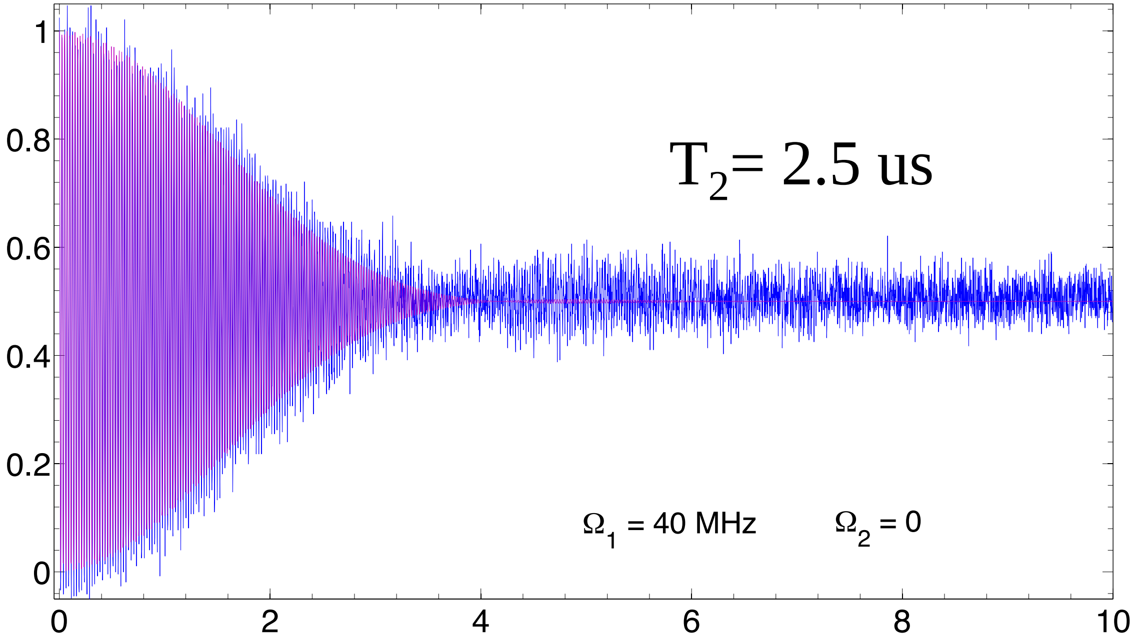
# Concatenated noise protection



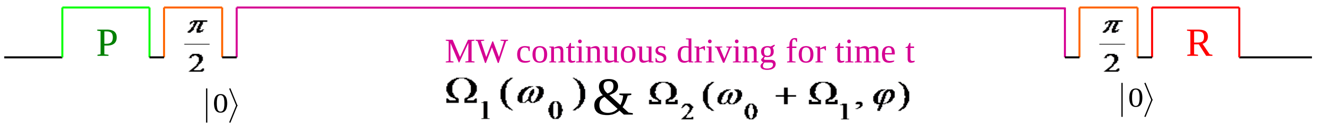
# Concatenated noise protection

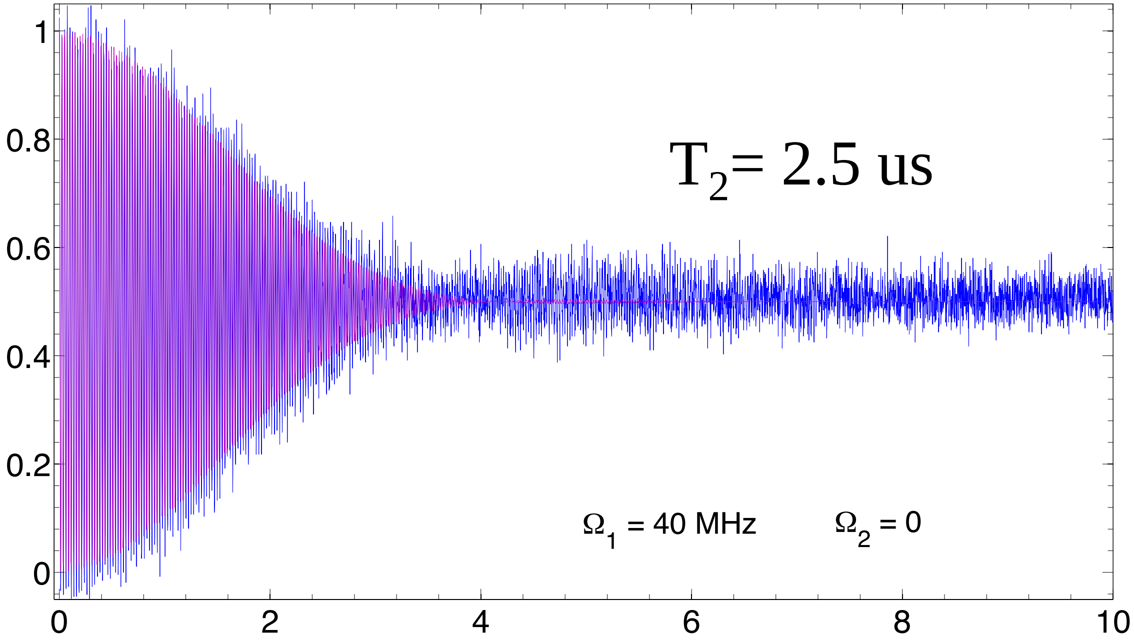


# Experimental results

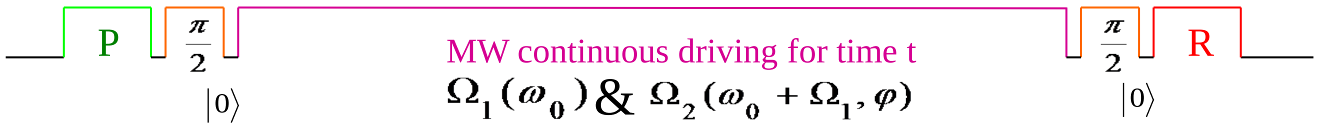



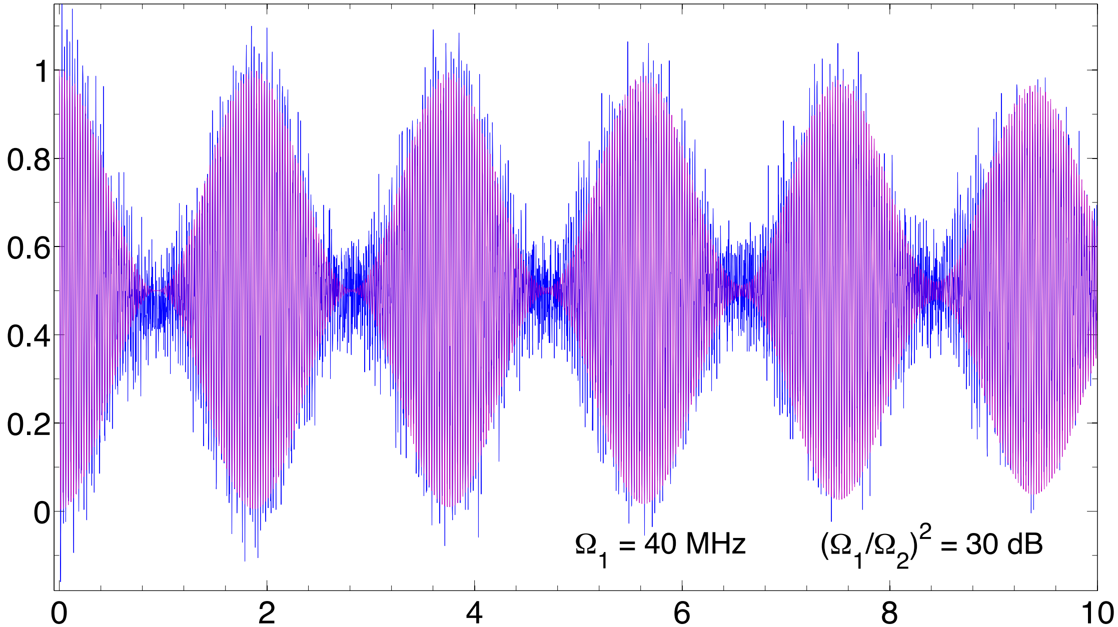
# Experimental results

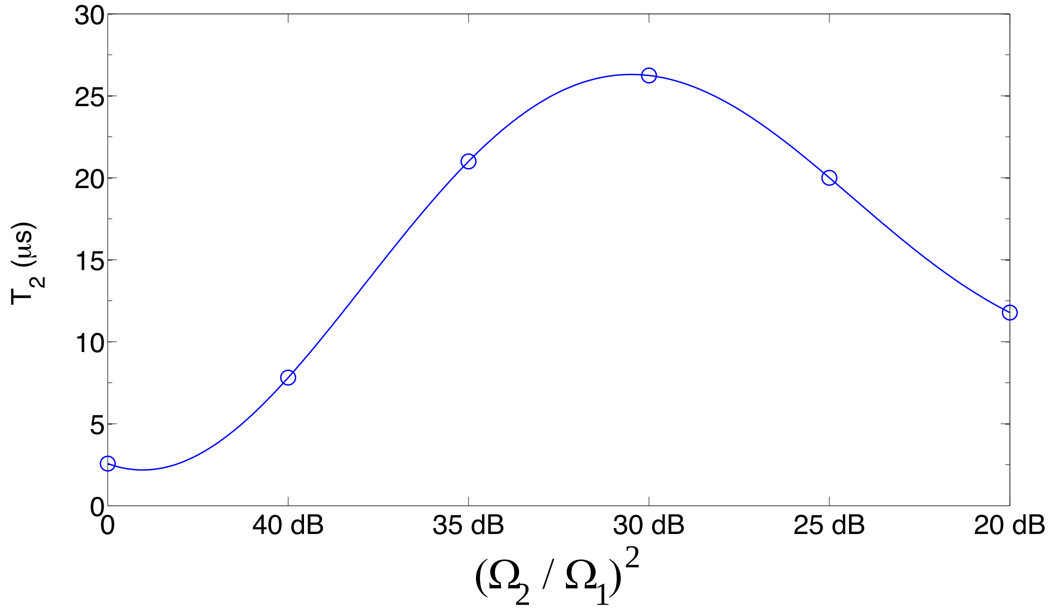


# Experimental results



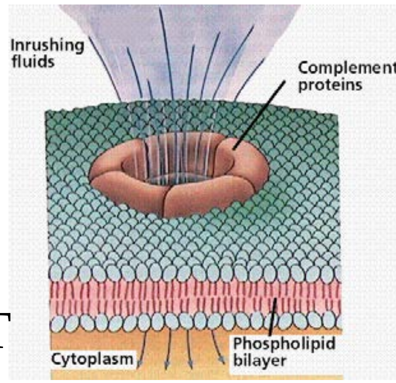



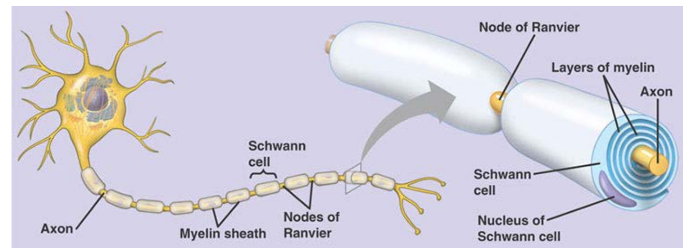



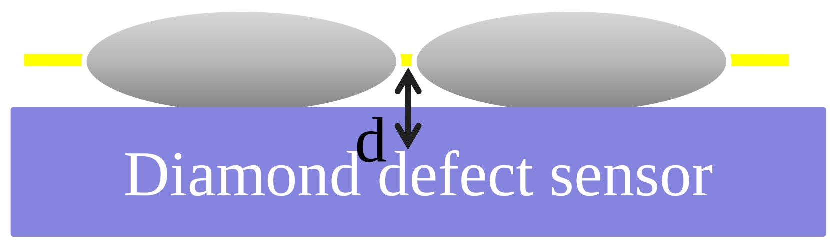

J.-M. Cai, et al arXiv:1111.0930

# Minute magnetic fields are everywhere –

Membrane
pores:
I:10 pA
B field ~ 0.1nT

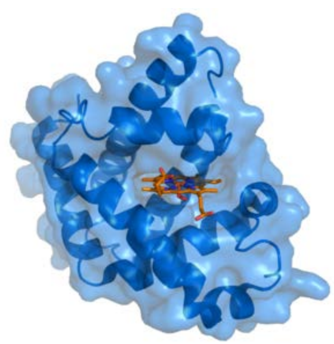



d=100nm; B field ~ 100nT

Catalytic centers
in enzymes:



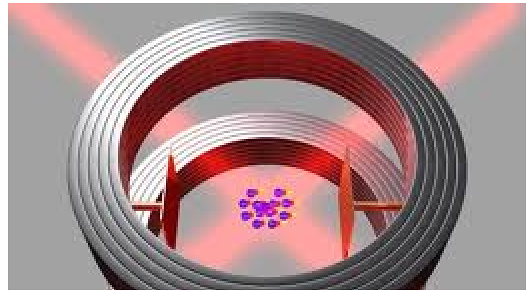
B field ~ 1μT@10nm

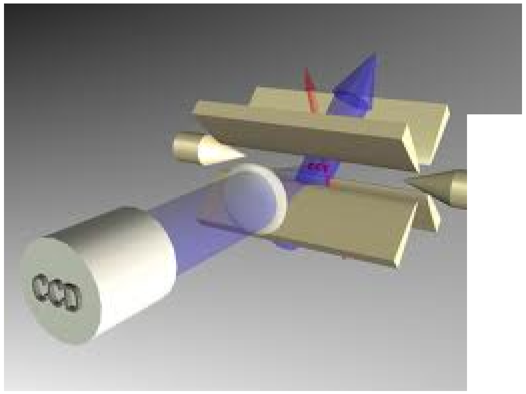
Lloyd Hollenberg et al. PRL 2009

# Comparing sensors

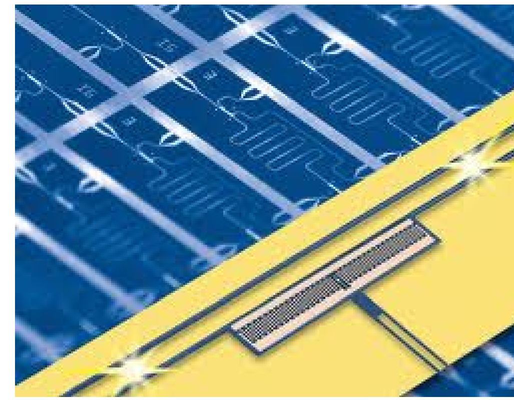
| Attributes | **Atomic Force Microscopy** | **Optical single molecule** | **Nuclear magnetic resonance** | **X Ray diffraction** | **Force detected NMR** | **NV diamond sensor** |
|---|---|---|---|---|---|---|
| Temporal resolution | 10 ms | 1 ms | 1 ns | - | >1s | 1 ms - 1 ns |
| Spatial resolution | 0.5 nm | 10 nm | 0.1 nm | 0.1 nm | 1 nm | 0.1 nm |
| Element specific | no | no | yes | No/yes | yes | yes |
| Ambient conditions | yes | yes | yes | crystals | No | yes |
| Non-invasive? | No | yes | yes | No | No | yes |
| Sensitivity | molecular | molecular | $10^{13}$ molecules | Bulk (crystals) | molecular, atomic (low T) | Single atom |

# Quantum simulators

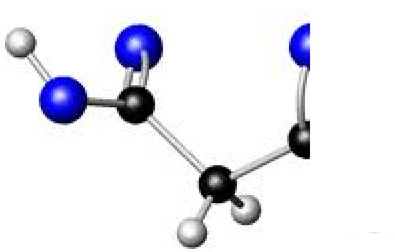


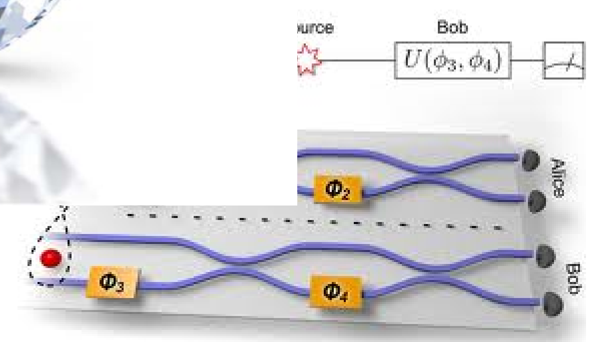



Innsbruck



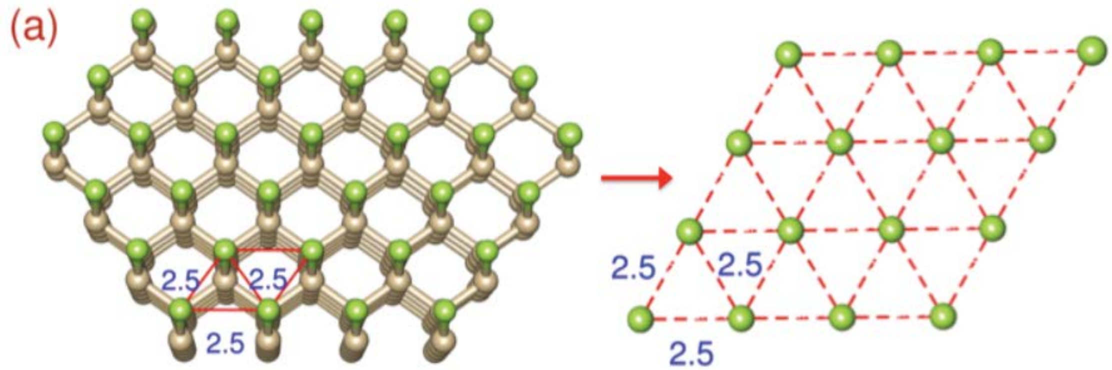
ETH Zürich



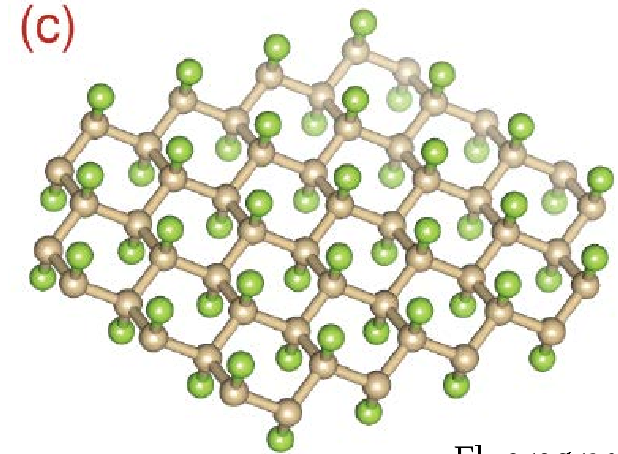



Bristol

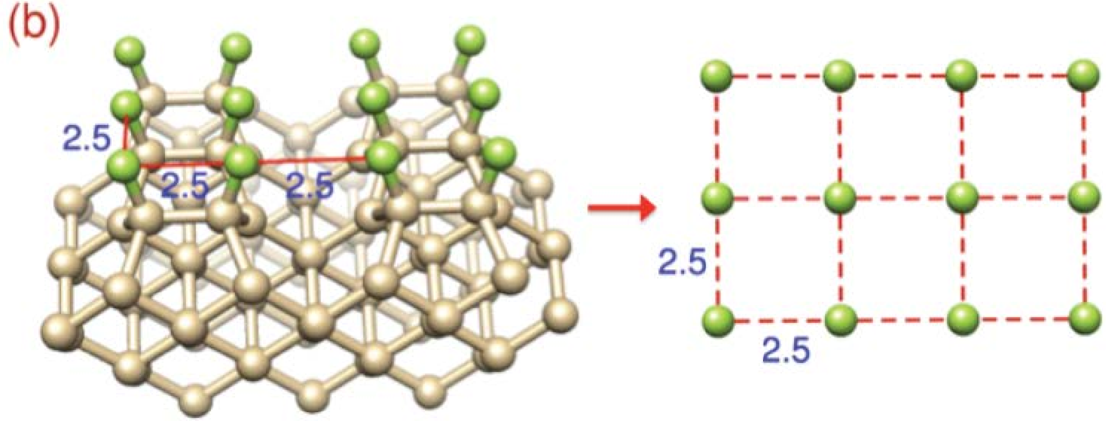
# Surface quantum simulators




Diamond 111-surface

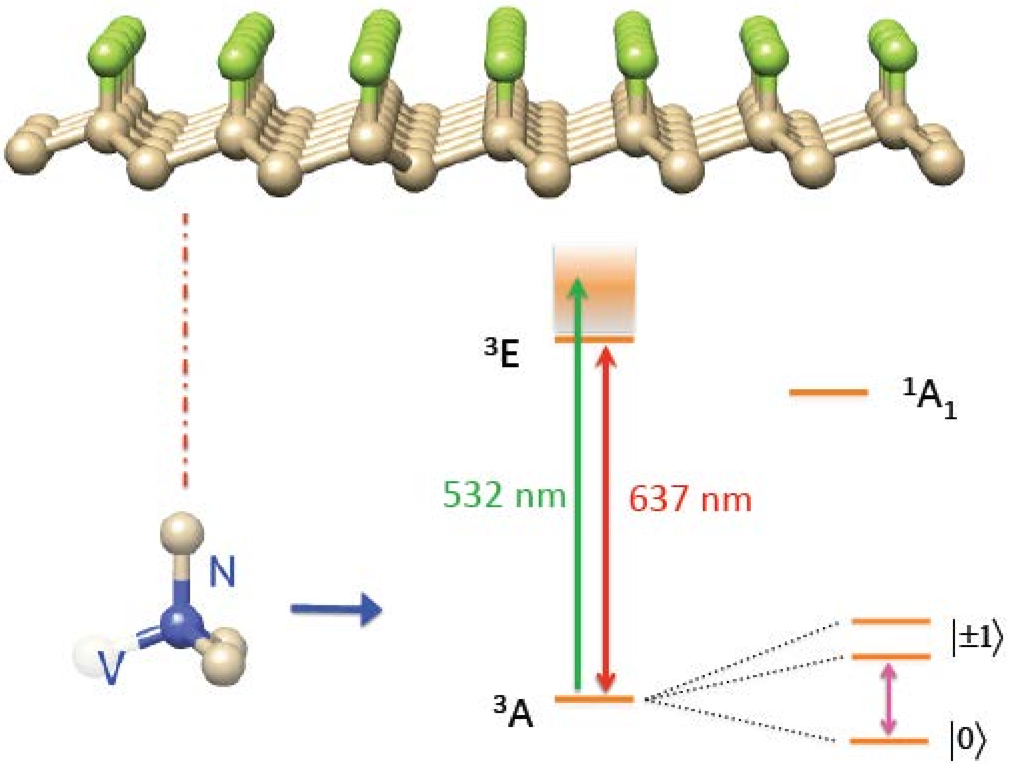



Fluorographene

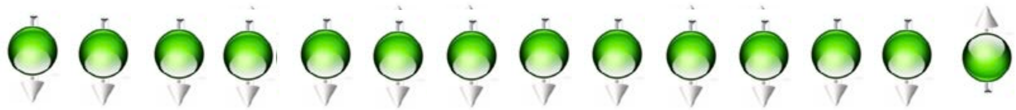



Diamond 100-surface

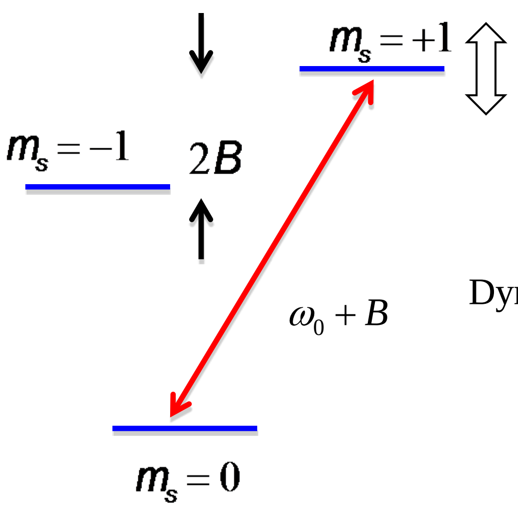
# Surface quantum simulators



# Initializing the simulator



Decouple nuclear spins from each other by radiofrequency driving.




Continuous

Dynamical Decoupling

$$H_{NV} = \Omega\sigma_x$$

$$|+\rangle = |0\rangle + |+1\rangle \quad H_S = \gamma_N \vec{B}\cdot\vec{I}_N$$


$$|-\rangle = |0\rangle - |+1\rangle$$

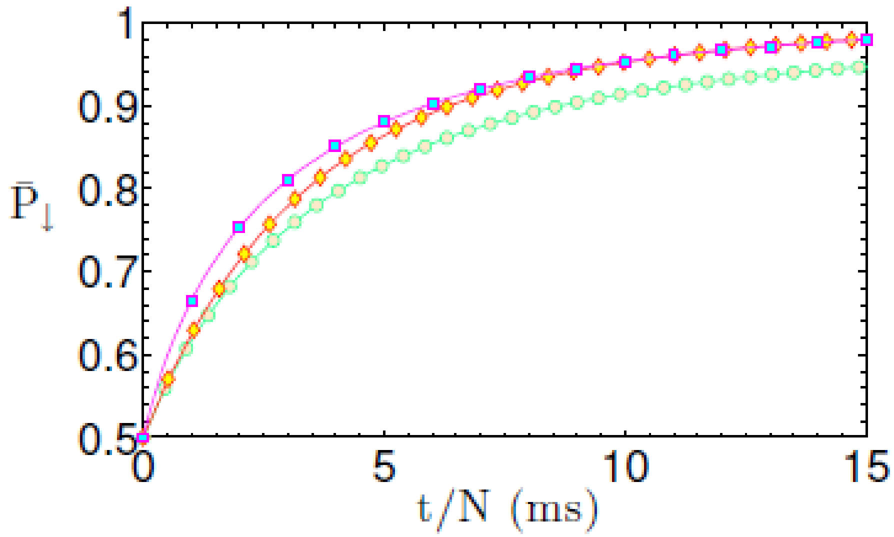
Magnetic field defines two-level system

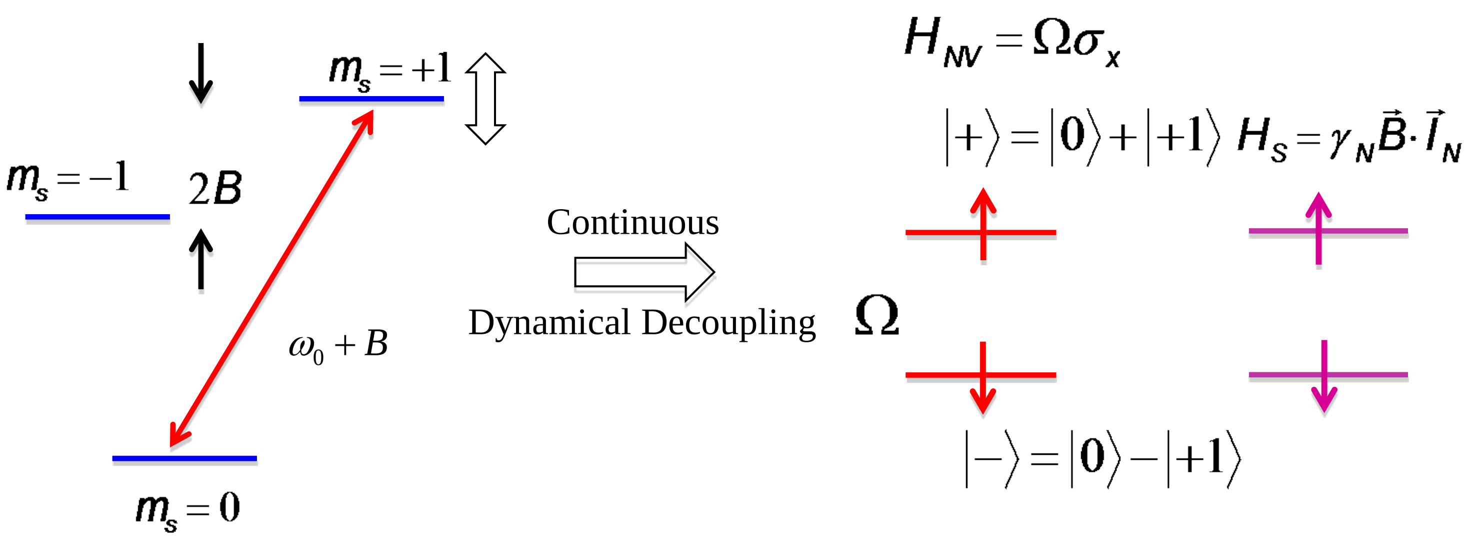
$$\sigma_z \Leftrightarrow \sigma_x$$

Interaction with environment carries energy penalty

Hartmann-Hahn condition (1962)

# Initializing the simulator



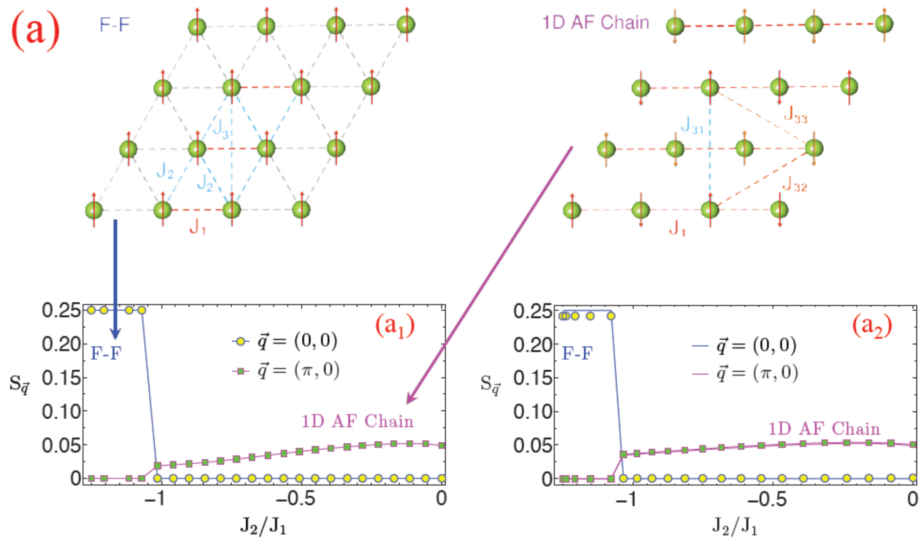

Magnetic field defines two-level system

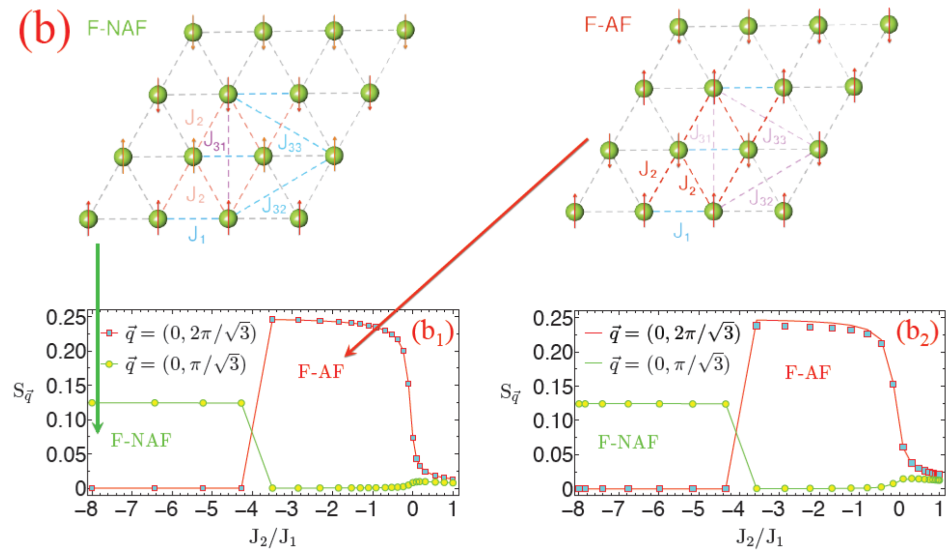
$\sigma_z \Leftrightarrow \sigma_x$

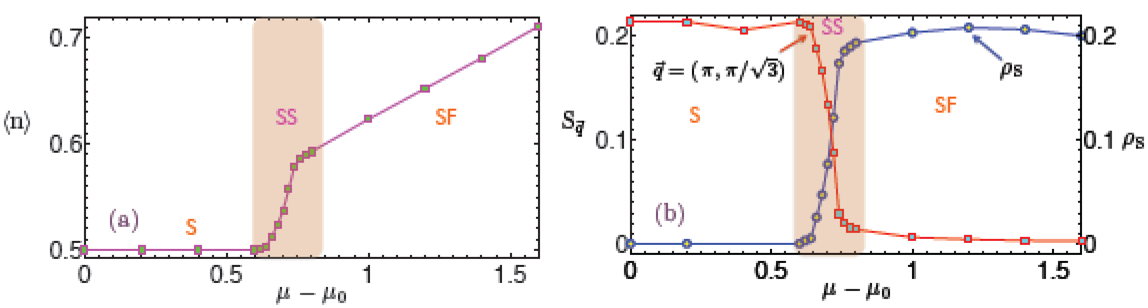
Interaction with environment
carries energy penalty

Hartmann-Hahn condition (1962)

# Surface quantum simulators



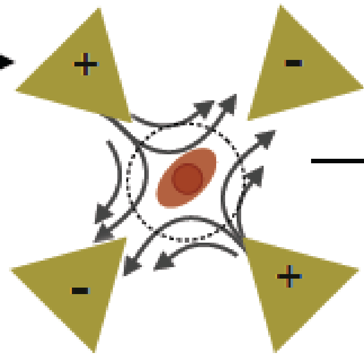



# The Physics of Ion Traps –

- Electromagnetism forbids the creation of a global minimum for the electrostatic field.

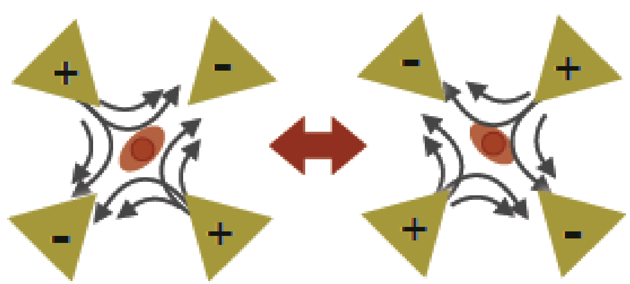
DC electrodes →



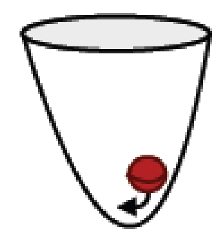

$$\nabla \cdot \mathbf{E} = 0 \quad \text{(Gauss' law)}$$

→ Electric field lines entering a closed region must also exit


- If one alternates the signs of the DC potentials periodically (radio-frequency), the charged particle sees an average confining force corresponding to a **harmonic oscillator**



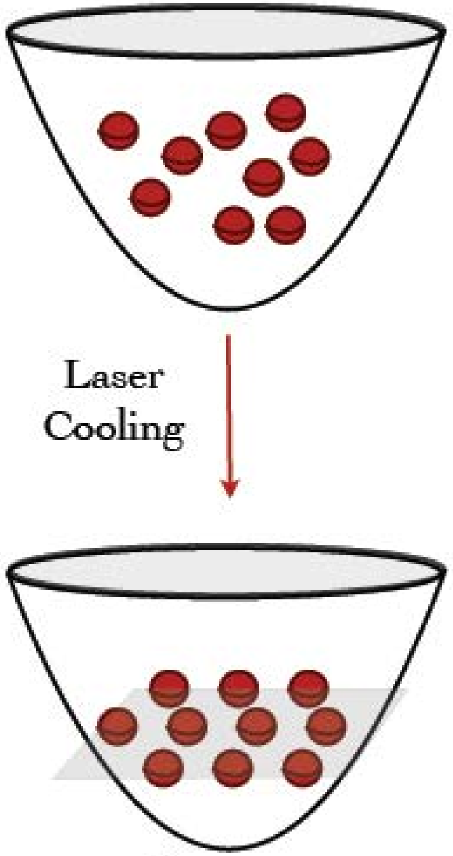

$$\boldsymbol{F} = q\boldsymbol{E} \equiv$$



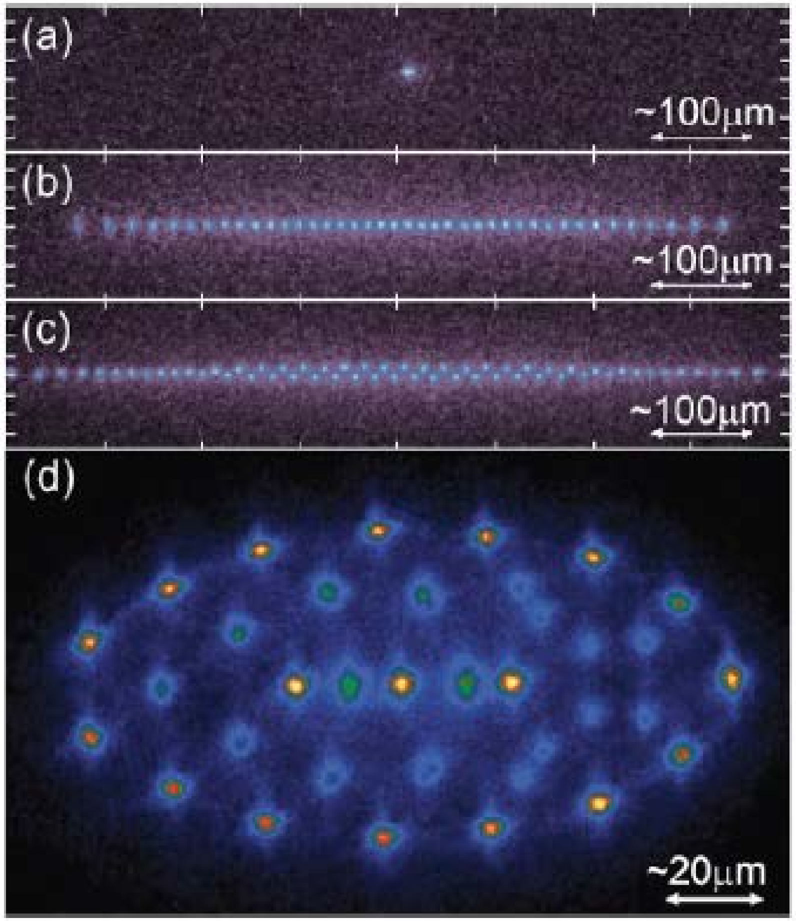
Thanks to Alejandro Bermudez for providing slides

# The Physics of Ion Traps –

- The radio-frequency traps are capable of confining an entire gas of charged particles




Crystalline structure




Experimental Coulomb Crystals (T. Schaetz)

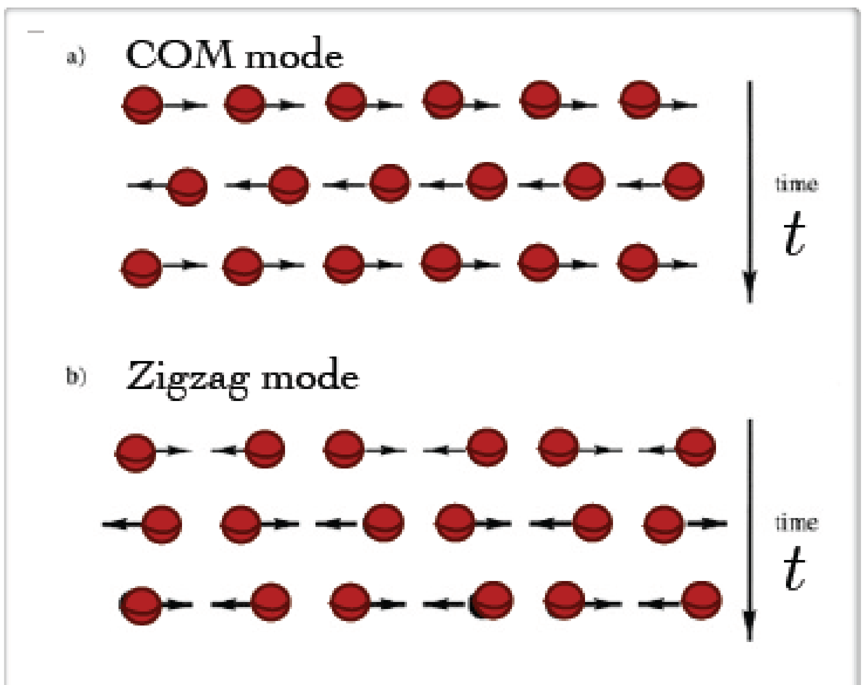
# The Physics of Ion Traps –

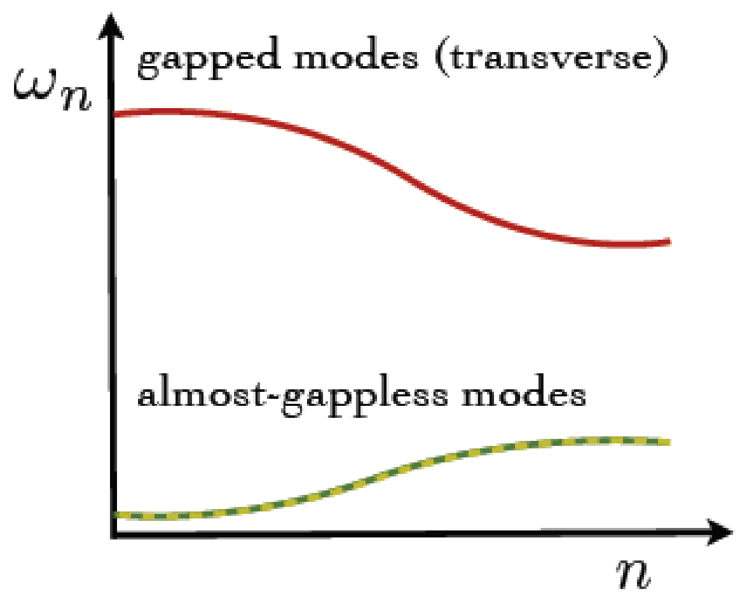
- The small vibrations of these charged particles lead to collective modes

$$H_{\mathrm{v}} = \sum_n \omega_n a_n^\dagger a_n$$

collective vibrational excitations - **phonons**

(e.g. two modes in a linear chain)



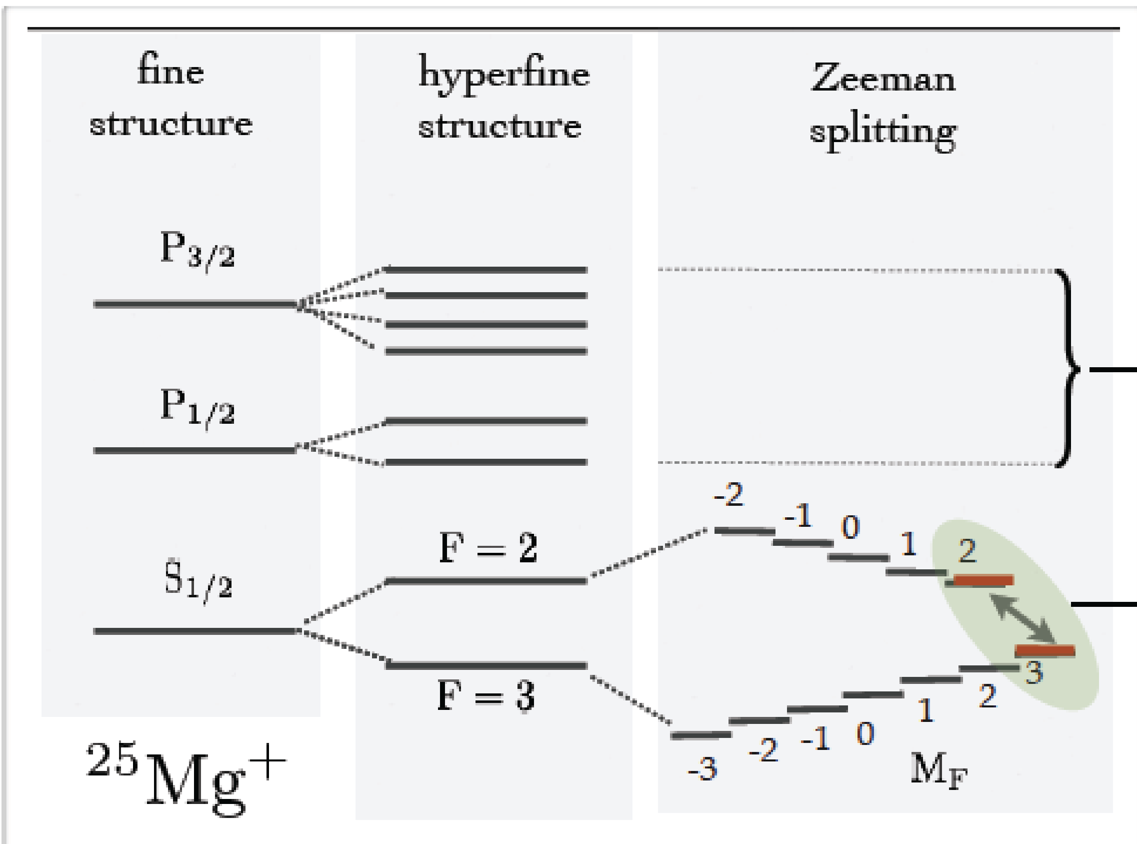
# The Physics of Ion Traps –

- The charged particles of interest will be single-ionized alkaline-earth atoms.

$^{9}Be^{+}, ^{25}Mg^{+}, ^{40}Ca^{+}$

↓

they have an atomic level structure



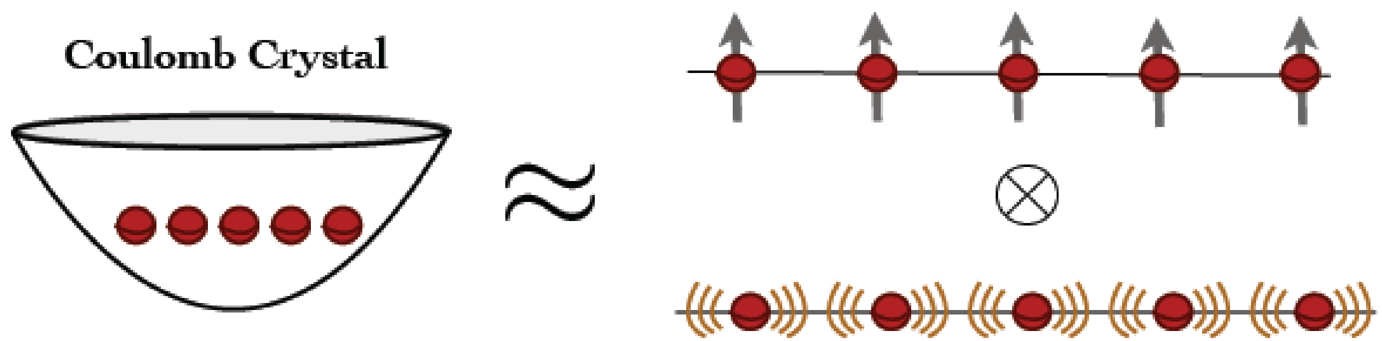

Excited states for cooling, optical pumping, and state-dependent fluorescence-readout

we can drive a particular transition by microwaves or 2-photon processes with optical radiation

**effective spin-1/2 (qubit)**

# The Physics of Ion Traps –

- Therefore, the ion crystal can be described as a **ensemble of harmonic oscillators** and a **lattice of spins**




$$H_{\mathrm{v}} = \sum_n \omega_n a_n^\dagger a_n$$

collective vibrational excitations - **phonons**

$$\omega_n \sim 1\mathrm{MHz}$$

$$H_{\mathrm{s}} = \sum_i \frac{1}{2}\omega_0 \sigma_i^z$$

atomic states - **spins**

$$\omega_0 \sim \mathrm{GHz}$$

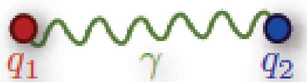
# The Physics of Ion Traps –

- The lattice spins are so far uncoupled. To implement Quantum Information Processing or Quantum Simulations, we need to develop some scheme to couple them.

Physical interactions usually involve 2 particles **linearly** coupled to a carrier

**e.g. Coulomb interaction-** 2 charged particles interchanging a scalar photon

$$H_I = \int \mathrm{d}^3 r J_\mu A^\mu \sim \int \mathrm{d}^3 k a_s(\boldsymbol{k}) \rho^*(\boldsymbol{k}) + \mathrm{H.c.}$$



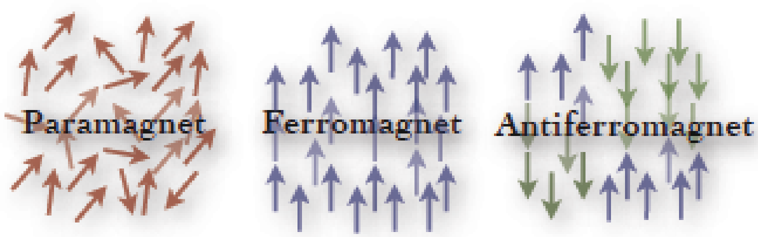

After the adiabatic elimination of the photons, we get the 2-body Coulomb interaction

$$H_{\text{eff}} = \frac{1}{4\pi\epsilon_0} \frac{q_1 q_2}{|\boldsymbol{r}_1 - \boldsymbol{r}_2|}$$

In magnetism, the magnetic dipoles interact via analogous linear exchange processes giving rise to diverse types of **symmetry-breaking order**

$$H = \sum_{\boldsymbol{r},\boldsymbol{r}'} J(|\boldsymbol{r} - \boldsymbol{r}'|) S_{\boldsymbol{r}} \cdot S_{\boldsymbol{r}'}$$

**Eq. Heisenberg model**



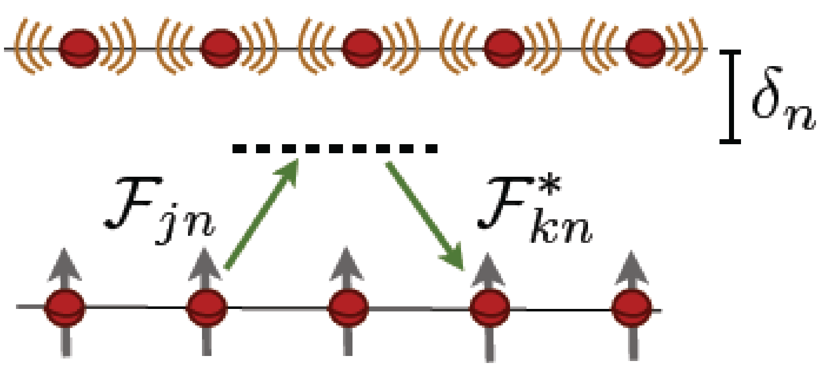
# The Physics of Ion Traps –

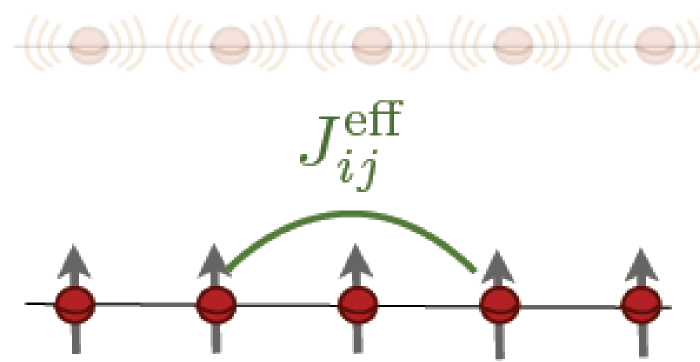
We can get effective magnetism using the **phonons** as interaction **carriers**

The first ingredient we require is a coupling between the spins and the phonons

$$H_{\mathrm{sp}} = \sum_{jn} \mathcal{F}_{jn} \sigma_i^z a_n \mathrm{e}^{\mathrm{i}\omega_{\mathrm{L}} t} + \mathrm{H.c}$$

laser-induced **spin-phonon couplings**



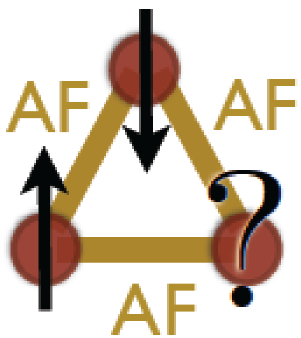

$$|\mathcal{F}_{jn}| \sim 10\mathrm{kHz} \quad \omega_{\mathrm{L}} \sim 100\mathrm{kHz}$$

$$J^{\mathrm{eff}}_{ij} \approx \frac{\mathcal{F}_{jn}\mathcal{F}^*_{kn}}{\delta_n}$$

$$J^{\mathrm{eff}}_{ij} \approx 1\mathrm{kHz}$$

1a It is difficult to understand how the interplay of ***quantum fluctuations*** and ***frustration*** can stabilise new phases of matter (e.g. quantum spin liquids).

L. Balents, Nature **464**, 199 (2010).




magnetic

geometric frustration

$$H_{\text{class}} = \sum_{\langle i,j \rangle} |J_{ij}| \sigma_i^z \sigma_j^z$$

Exponential degeneracy of the groundstate manifold

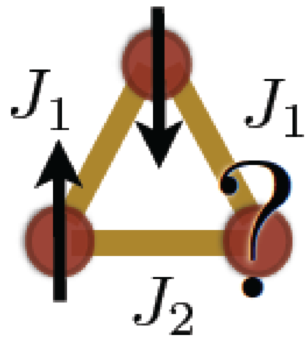
$$H_{\text{quant}} = \sum_{\langle i,j \rangle} |J_{ij}| \sigma_i^z \sigma_j^z - \sum_i h \sigma_i^x$$

? How is this degeneracy lifted by quantum fluctuations?

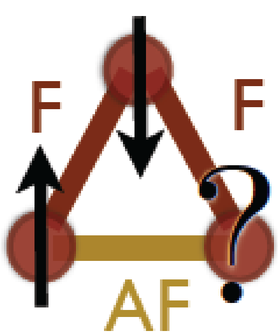
Does a new phase emerge out of this degenerate manifold?

(reminiscent of the FQHE)

1b It is difficult to find materials that realise ***low-dimensional quantum Ising models***




$$J_1/J_2 \in (-\infty, +\infty)$$




"… a real-life constraint is that most spins are vectors

and not scalar Ising spins as frequently used in models…"

A. P. Ramirez, Annu. Rev. Mat. Sci. **24,** 453 (1994).

and even more difficult that those materials display a ***variable range of frustration***

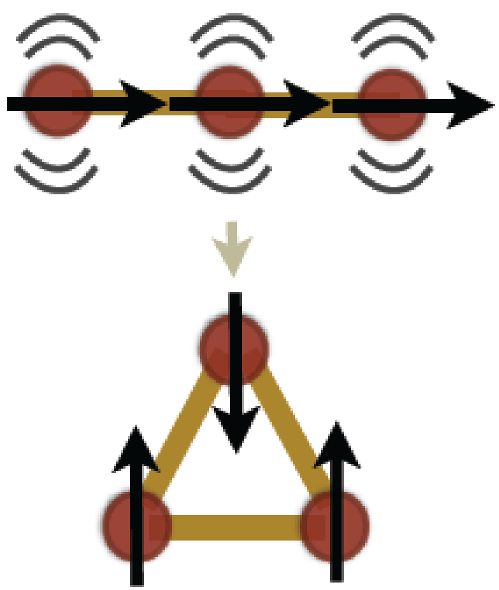
"… most real compounds differ significantly from idealized models. One example of departure… the inability to precisely control the interaction strength, range, and anisotropy…"

A. P. Ramirez, Annu. Rev. Mat. Sci. **24,** 453 (1994).

? Is it possible to design the range of Ising frustration in different lattices and control the quantum fluctuations?

1b It is very difficult to understand completely the physics of ***spin-phonon coupled quantum magnets***

$$H = \sum \omega_n a_n^\dagger a_n + \sum_{\langle i,j \rangle} |J_{ij}| \left( 1 + \sum_n \xi_n (a_n^\dagger + a_n) \right) \sigma_i^z \sigma_j^z - h \sum_i \sigma_i^x$$



magnetic structural phase transition

The condensation of a particular phonon mode (i.e. structural phase transition) may lead to an order-disorder magnetic phase transition (and viceversa)

spin-version of **Peielrs instability** 1D metals

R. E. Peierls, Quantum Theory of Solids (1955),

? What happens with non-adiabatic effects (no separation of scales for spin and phonons)?

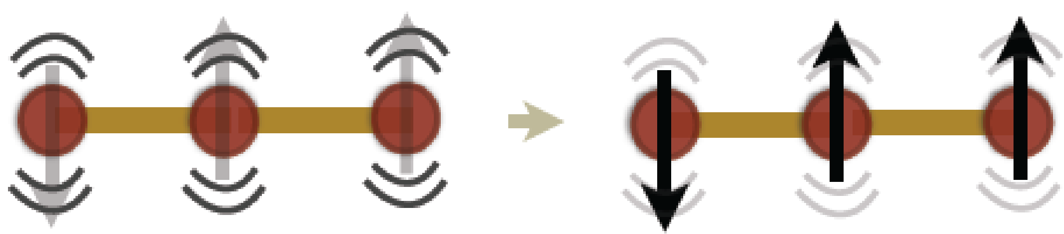
2b It is very difficult to find materials that realize spin-phonon coupled quantum Ising models.

Heisenberg Peierls samples

| | | |
|---|---|---|
| Heisenberg Peierls samples | TTF-$CuS_4C_4(CF_3)_4$ | J.W.Bray et al., Phys. Rev. Lett. **35,** 744 (1975). |
| | TTF-$AuS_4C_4(CF_3)_4$ | I.S. Jacobs et al., Phys. Rev. B. **14,** 3036 (1976). |
| | $CuGeO_3$ | M. Hase, et al., Phys. Rev. Lett. **70,** 3651 (1993). |
| | TiOCl | A. Seidel et al., Phys. Rev. B. **67,** 020405 (2003). |

$$|J_{ij}|/\omega_n \in [0, \infty)$$

and even more difficult that those materials display a ***variable range of adiabaticity***



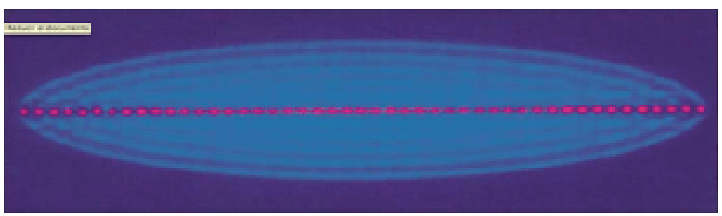
faster phonon excitations    faster spin excitations

? Is it possible to design the range of phonon/ spin adiabaticity?

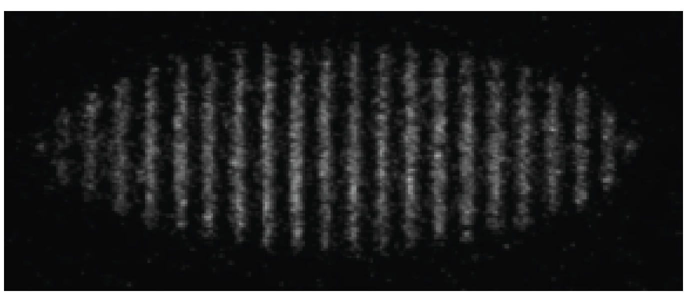
**Coulomb Crystals** are self-assembled structures of trapped ions

$$H = \sum_{j=1}^{N} \sum_{\alpha=x,y,z} \left( \frac{1}{2m} p_{j\alpha}^2 + \frac{1}{2} m \omega_\alpha^2 r_{j\alpha}^2 \right) + \frac{e^2}{2} \sum_{j \neq k} \frac{1}{|\mathbf{r}_j - \mathbf{r}_k|}$$

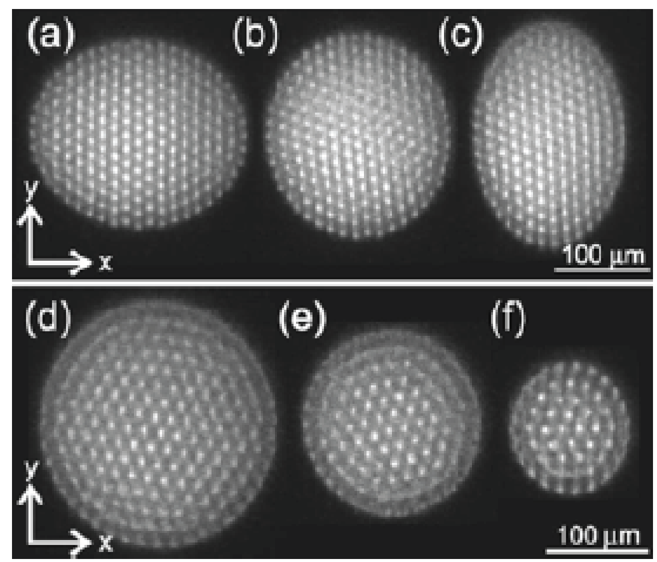
equilibrium positions



L. Hornekaer, et al. PRL **86**, 1994 (2001).



N. Kjaergaard et al., PRL **91**, 095002 (2003).




A. Mortensen, et al., PRL. **96**, 103001 (2006).

By controlling the trapping frequencies in a Paul trap, we can create **ladders of bond-sharing triangles** with any **desired number of legs.**

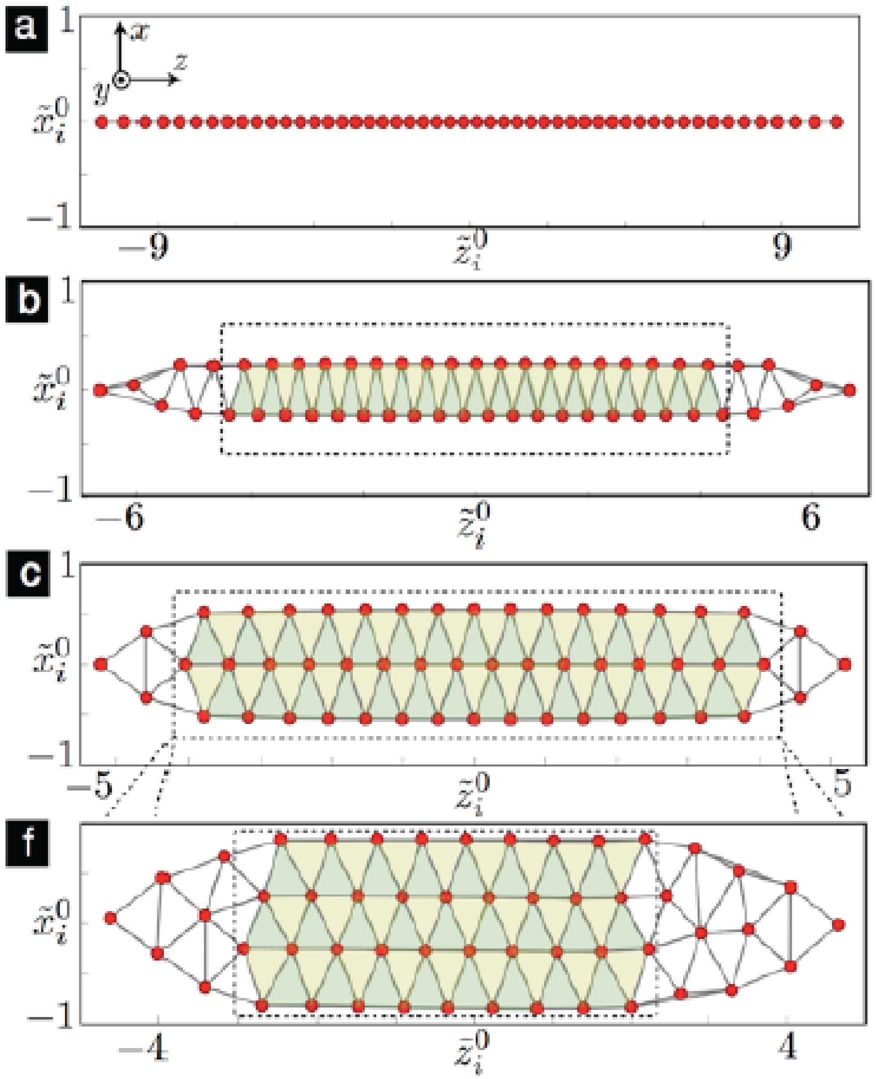
$$\kappa_x = \left(\frac{\omega_z}{\omega_x}\right)^2$$

$n_l = 1$

$n_l = 2$

$n_l = 3$

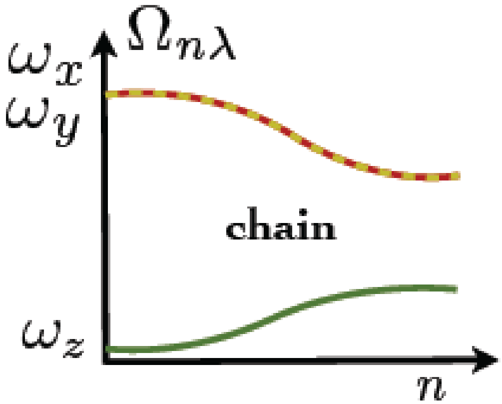
$n_l = 4$



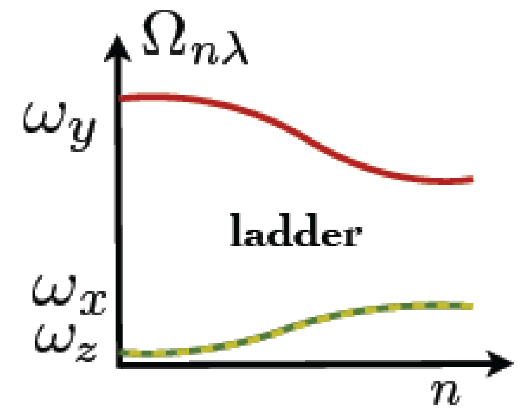

**dimensional crossover**

$0^+$ → $\kappa_{c,2}$ → $\kappa_{c,3}$ → $\kappa_{c,4}$ → $1$

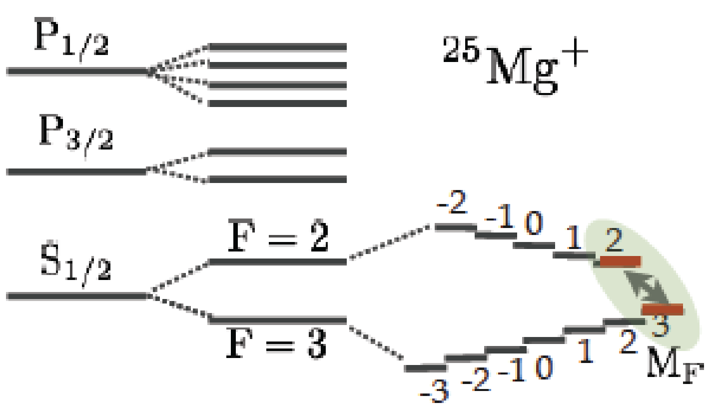
**Harmonic approximation.-** The small vibrations around the equilibrium positions are coupled by the Coulomb interaction ➔ **Collective phonon modes**




$$H_{\rm p} = \sum_{n\lambda} \Omega_{n\lambda} a^\dagger_{n\lambda} a_{n\lambda}$$




**Two-level approximation.-** The atomic energy structure presents several levels, two of which can be addressed by lasers ➔ **Pseudo-spins s=1/2**

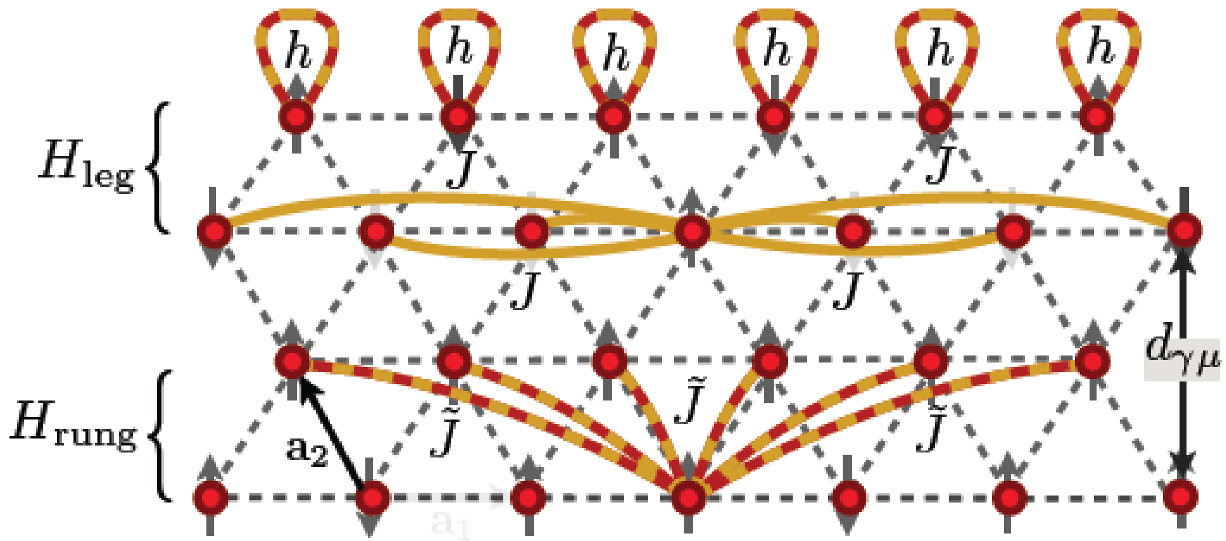



$$H_{\rm s} = \sum_i \frac{1}{2}\omega_0 \sigma_i^z - h \sum_i \sigma_i^x$$

We obtain a quantum simulator for frustrated **quantum Ising Ladders** 1a

$$H_{\text{leg}} = \sum_{\gamma} \sum_{i_s \neq j_s} J^{\gamma}_{i_s,j_s} \sigma^z_{i_s}(\gamma)\sigma^z_{j_s}(\gamma) - h \sum_{\gamma} \sum_{i_s} \sigma^x_{i_s}(\gamma)$$

$$H_{\text{rung}} = \sum_{\gamma \neq \mu} \sum_{i_s \neq j_s} \tilde{J}^{\gamma,\mu}_{i_s,j_s} \sigma^z_{i_s}(\gamma)\sigma^z_{j_s}(\mu).$$

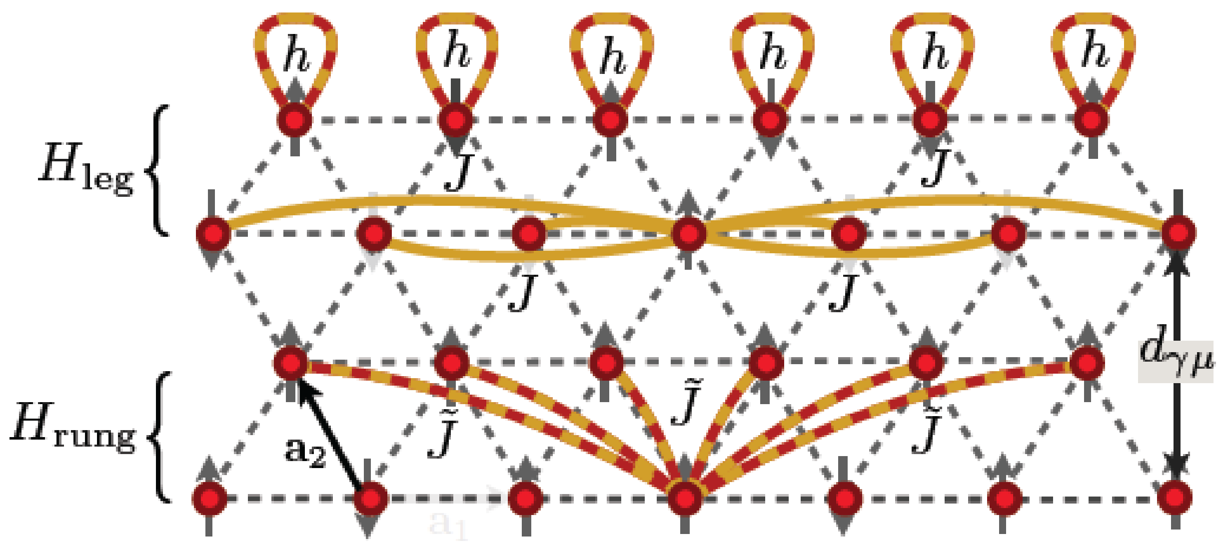



1b It is even more difficult to find materials with a variable range of Ising frustration

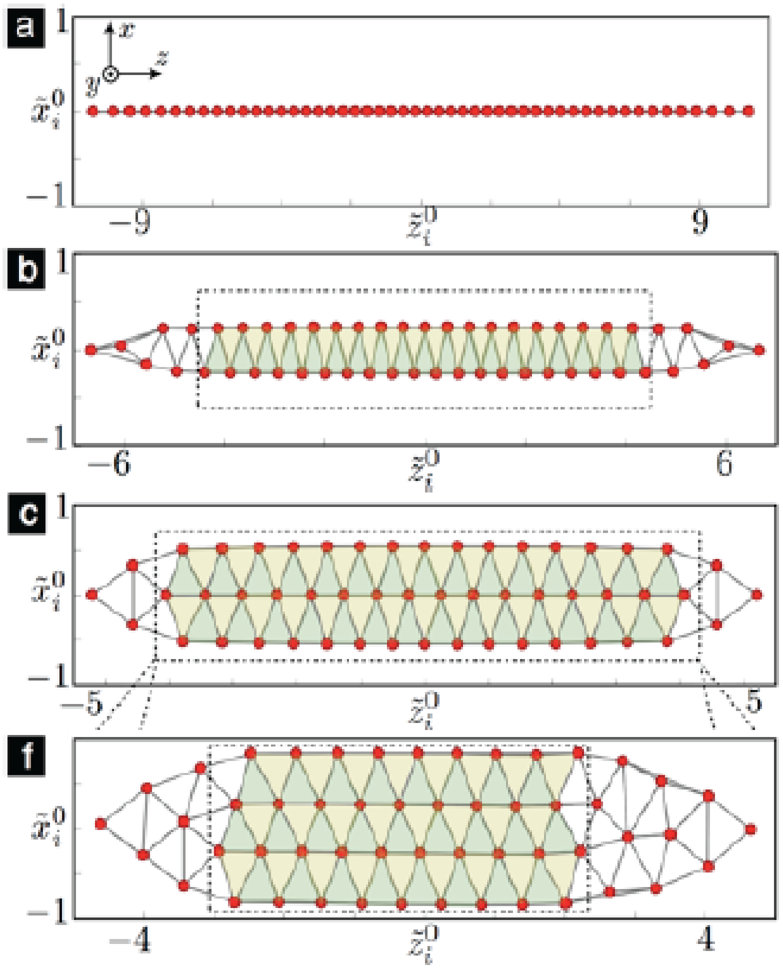
We obtain a quantum simulator for frustrated **quantum Ising Ladders** 1a

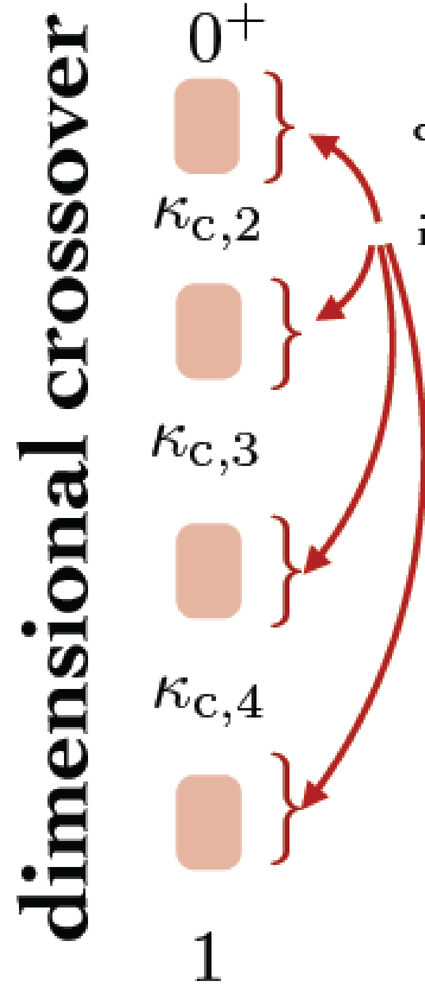
$$H_{\mathrm{leg}} = \sum_{\gamma} \sum_{i_s \neq j_s} J^{\gamma}_{i_s, j_s} \sigma^z_{i_s}(\gamma) \sigma^z_{j_s}(\gamma) - h \sum_{\gamma} \sum_{i_s} \sigma^x_{i_s}(\gamma)$$

$$H_{\mathrm{rung}} = \sum_{\gamma \neq \mu} \sum_{i_s \neq j_s} \tilde{J}^{\gamma, \mu}_{i_s, j_s} \sigma^z_{i_s}(\gamma) \sigma^z_{j_s}(\mu).$$

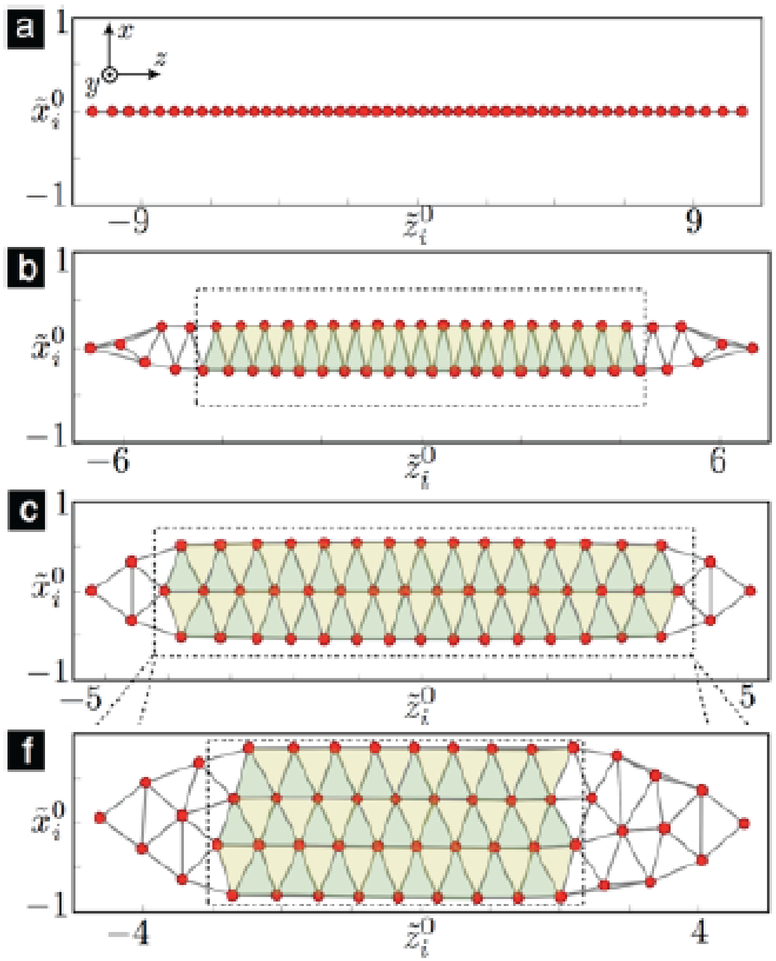


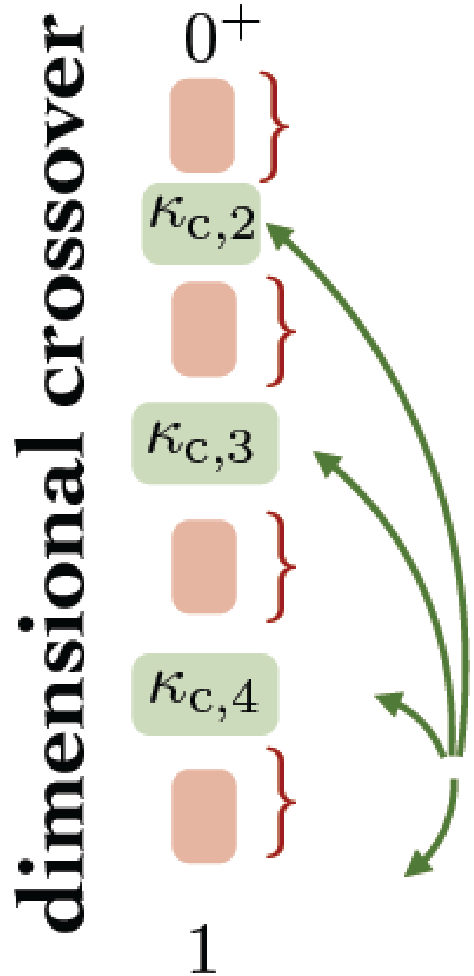

1b It is ~~even more difficult to find~~ materials with a variable range of Ising frustration
possible to synthesize




So far, we have focused only on the stable regions in between the structural phase transitions



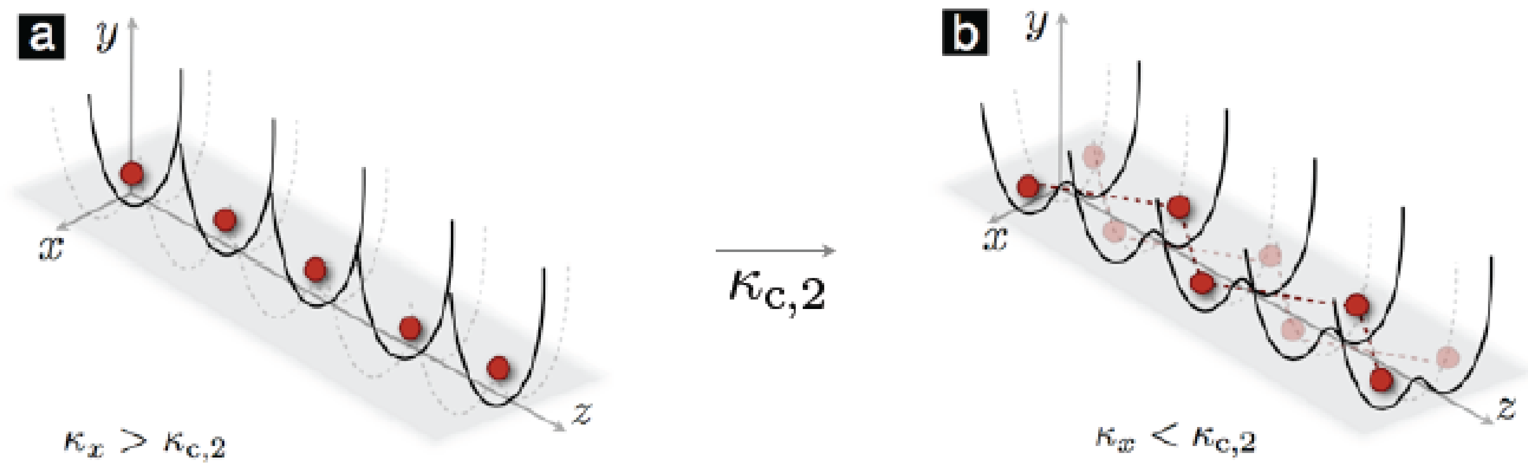




Now, we would like to study what happens close to criticality

**Inhomogeneous $\phi^4$model.-** Close to the first structural phase transition $\kappa_{c,2}$ , there is a soft phonon mode (zigzag distortion) that condenses

$$q_{ix} = (-1)^i \delta q_i^{zz} \quad \langle \delta q_i^{zz} \rangle \neq 0$$

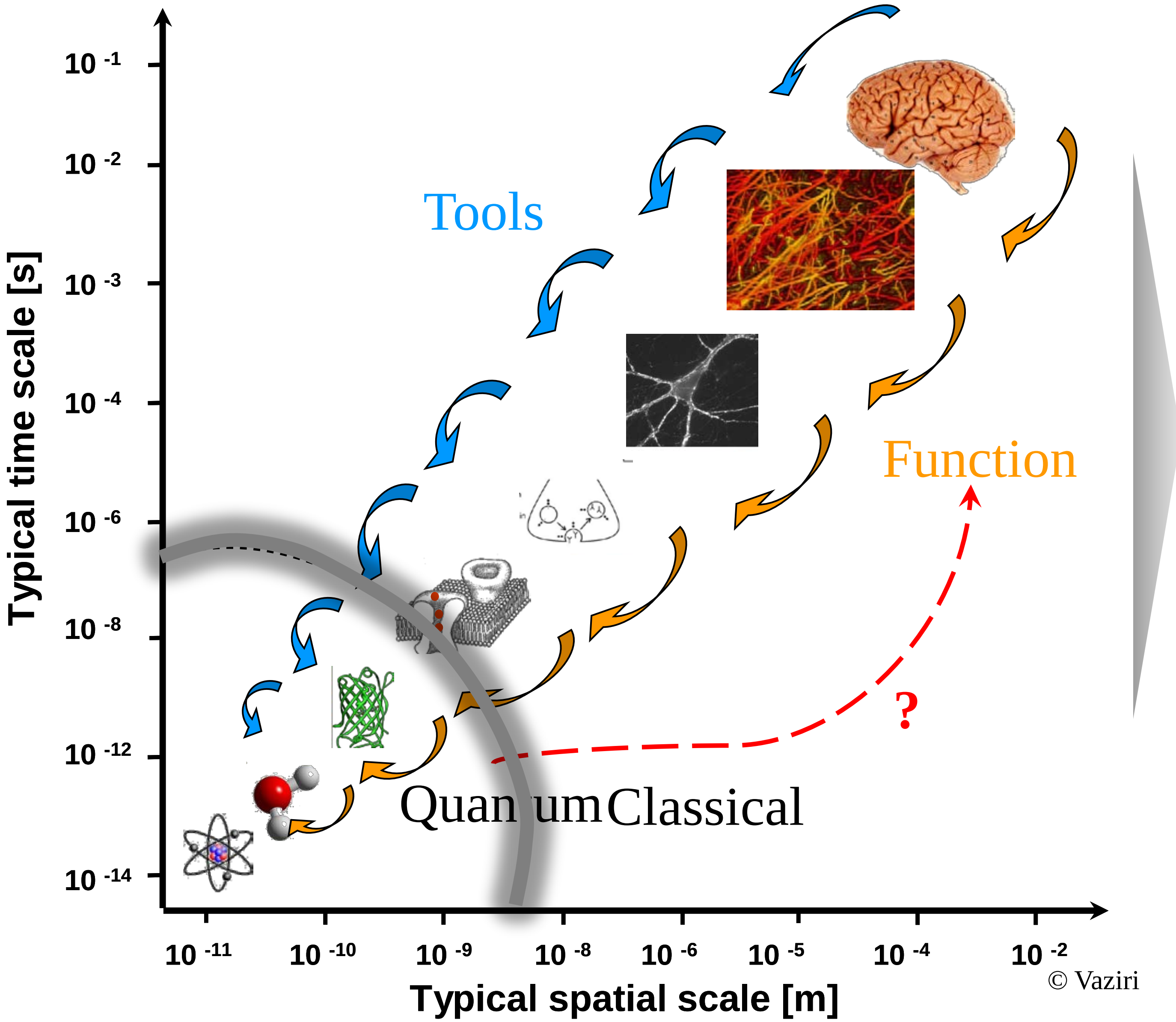
Bermudez & Plenio, PRL 2012




$$H_x = \sum_i \left( \frac{m l_z^2}{2} (\partial_t \delta q_i^{zz})^2 + \frac{r_i^x}{2} (\delta q_i^{zz})^2 + \frac{u_i^x}{4} (\delta q_i^{zz})^4 \right) + \sum_{i \neq j} \frac{K_{ij}^x}{2} (\partial_j \delta q_i^{zz})^2$$

$$r_i^x > 0 \xrightarrow[\kappa_{c,2}]{} r_i^x < 0$$

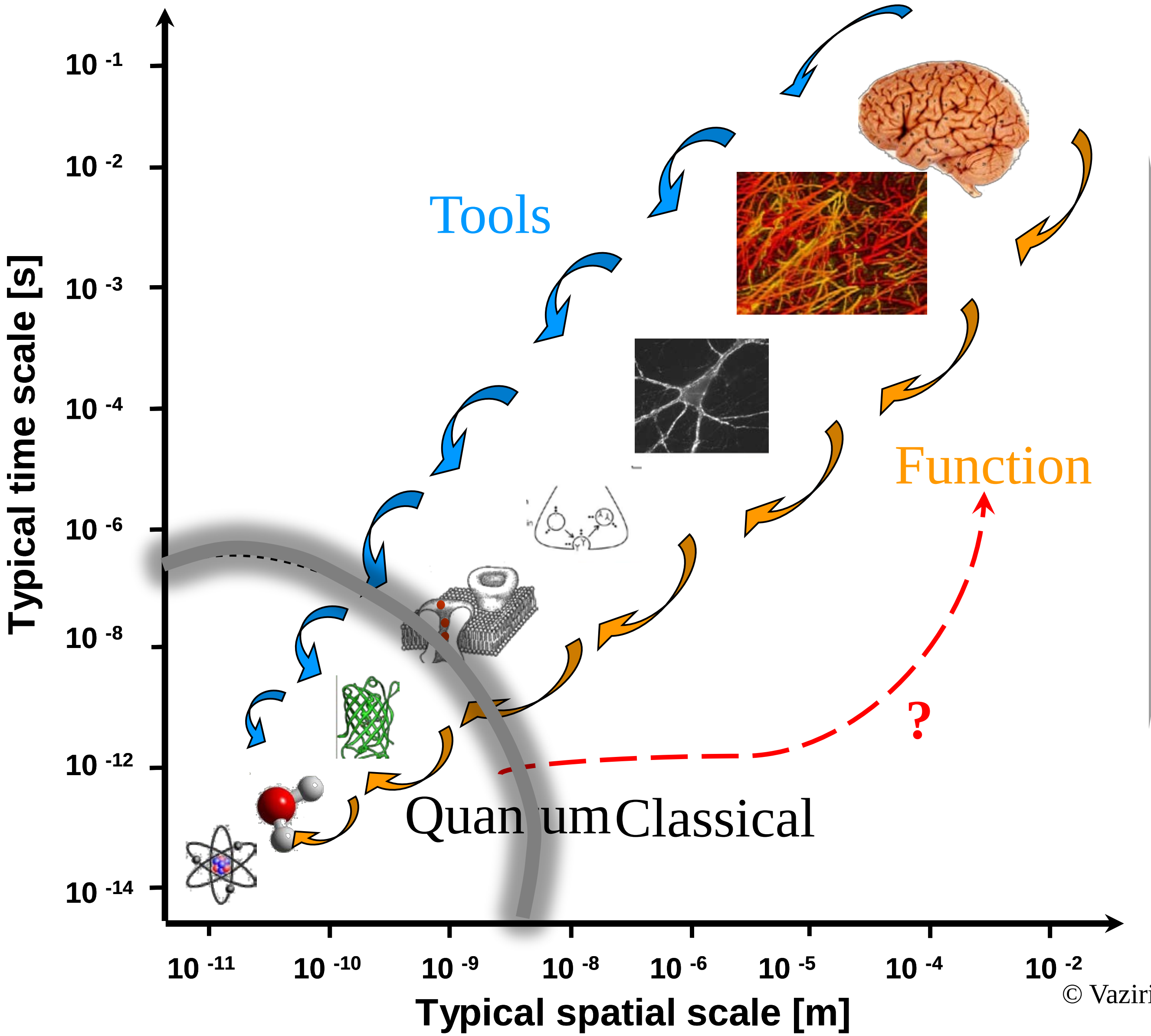
# Part II




**Can quantum coherence be relevant for biological function?**

**Requires tools for studying biological structure and function at unprecedented spatial and temporal resolution**

Huelga & Plenio, Review in preparation for Contemporary Physics 2012



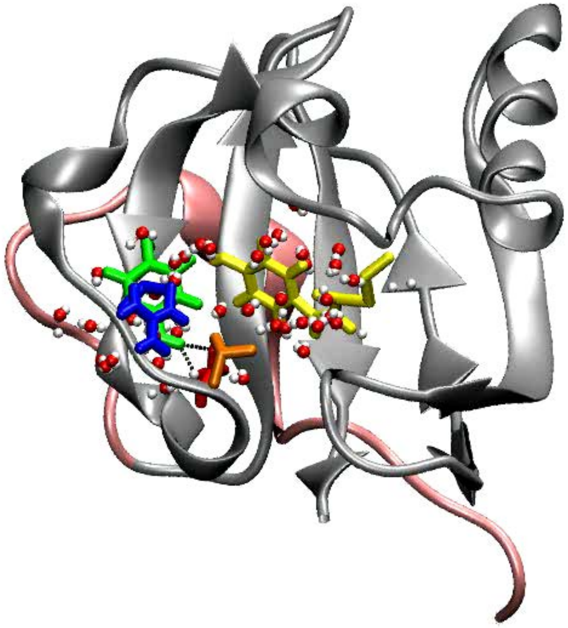

**Can quantum coherence be relevant for biological function?**

**Requires tools for studying biological structure and function at unprecedented spatial and temporal resolution**

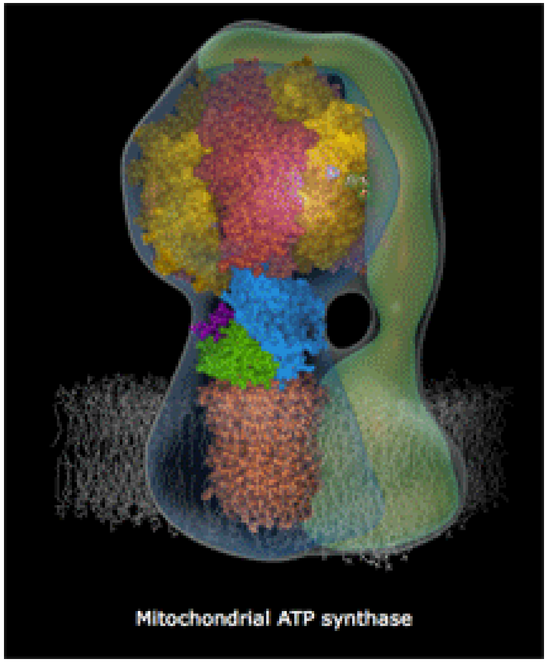
Structure ⇨ ⇨ Function

Huelga & Plenio, Review in preparation for Contemporary Physics 2012

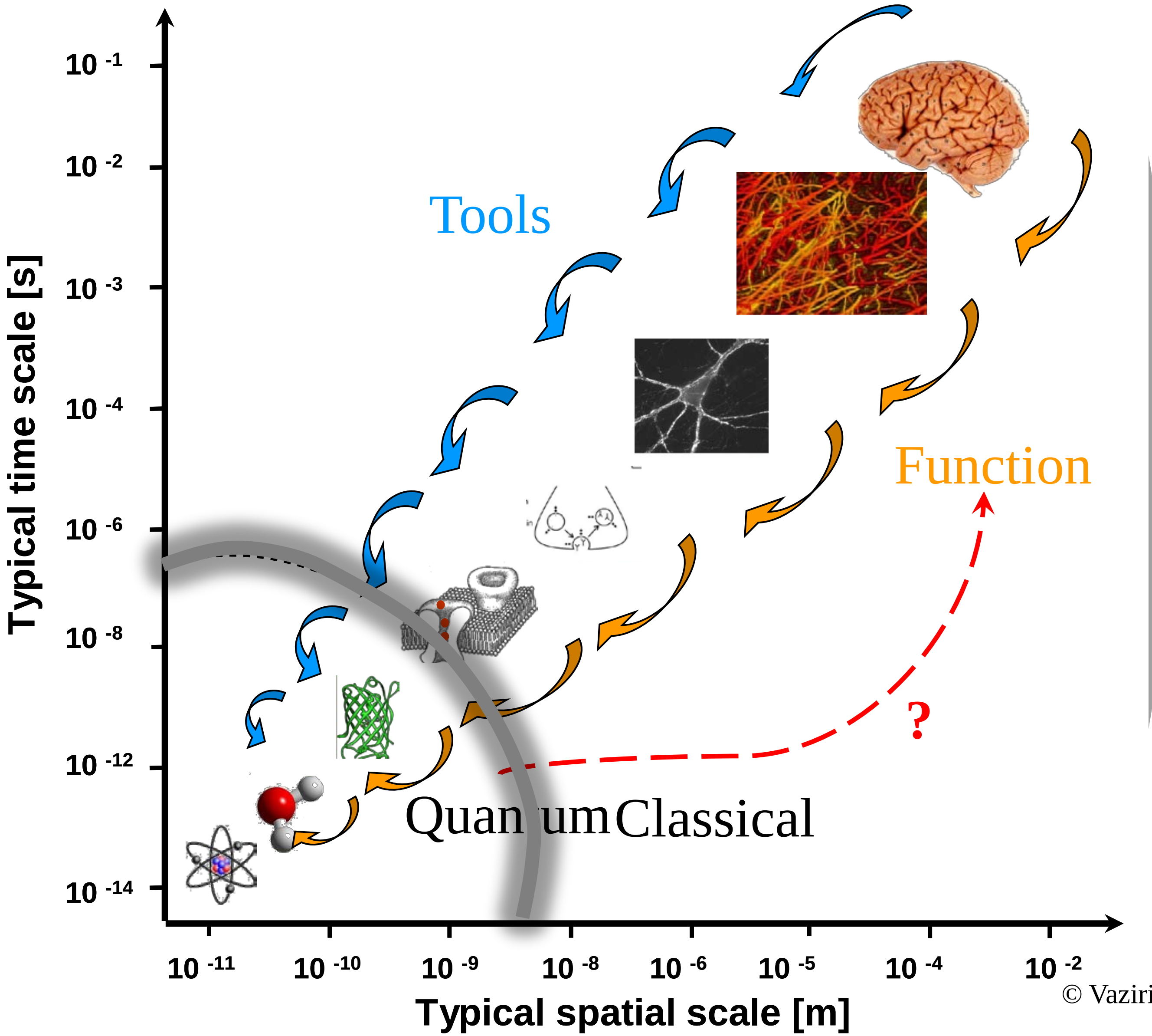
# Biological motion on the nanoscale



Computational Chemistry
Group, Amsterdam




Walker @ Cambridge




**Can quantum coherence be relevant for biological function?**

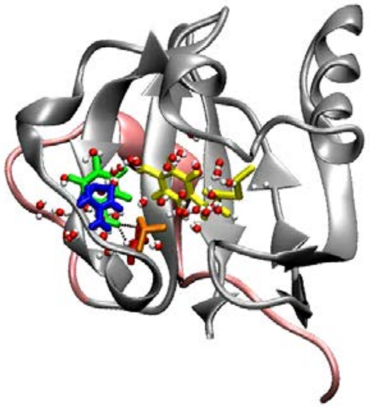
**Requires tools for studying biological structure and function at unprecedented spatial and temporal resolution**

Structure ⇨ Dynamics ⇨ Function

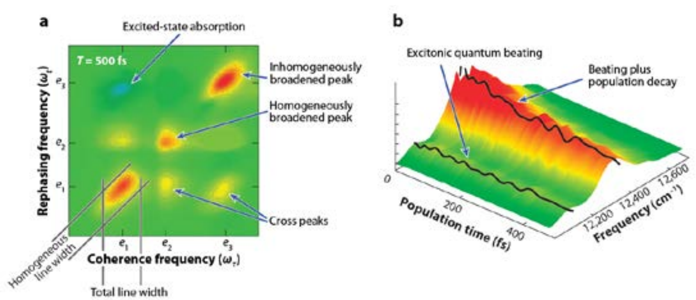
Huelga & Plenio, Review in preparation for Contemporary Physics 2012

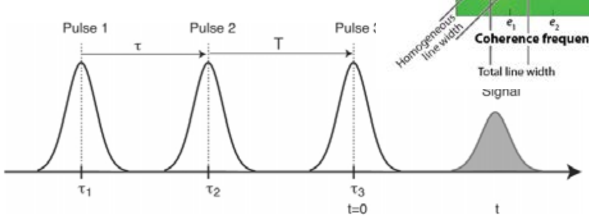
# What are we looking for ?

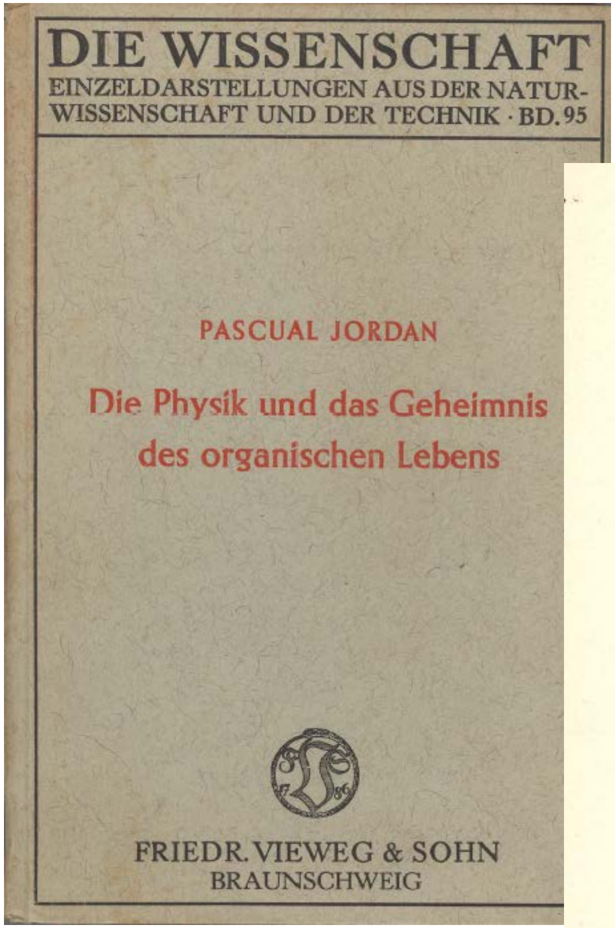
- In dynamical processes
  - Coherence length and time scales
  - Role of coherence & environmental noise
  - Design principles
  - Experimental verification



Convergence of optics and biophysics techniques have led to the ability to explore these questions experimentally.





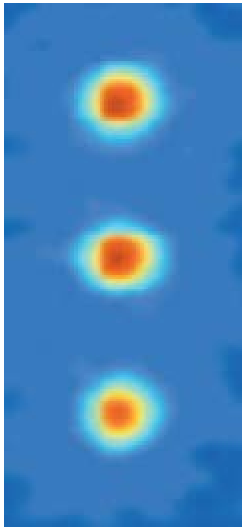

## Quanten-Biologie

Der rasche Fortgang der wissenschaftlichen Forschungsarbeit läßt immer neue Spezialgebiete entstehen, und verschärft durch die unausweichlichen Notwendigkeiten der Arbeitsteilung die — so oft beklagte — hochgradige Spezialisierung des Wissenschaftlers. Aber gleichzeitig ergibt sich aus den Ergebnissen einer immer eindringlicheren Forschung ganz von selbst auch eine gegenläufige Tendenz: eine Tendenz zur Vereinheitlichung von Gebieten, die vorher getrennt und beziehungslos dazustehen schienen. So haben die gr[illegible] Erfolge der modernen Physik auf dem Gebiete der A[illegible] letzte[illegible] beseit[illegible] Hand [illegible] in de[illegible] ihrer [illegible] Arbei[illegible] auch ihre unbequemen Seiten. Der Physiker, der die allgemeinen Erkenntnisse seiner Wissenschaft für konkrete Einzelfragen fruchtbar machen will, ist oft genötigt, sich über spezielle chemische Gebiete zu unterrichten, die ihm früher ein unbekanntes Land gewesen sind; und mancher Chemiker andererseits stöhnt insgeheim über die Zumutung, daß er nun auch noch die „Wellenmechanik" und ähnliche gewissenmaßen zum unzugänglichsten Gletschergebiet der theoretischen Physik gehörige Dinge lernen soll. Aber solche Schwierigkeiten des Weges der heutigen Forschung können doch nicht die stolze Gewißheit verdunkeln, daß wir die inneren Zusammenhänge der Naturerscheinungen in einer Tiefe und mit einer Eindringlichkeit erfaßt haben, die es uns erlaubt, fast unübersehbar große Gebiete mannigfaltigster



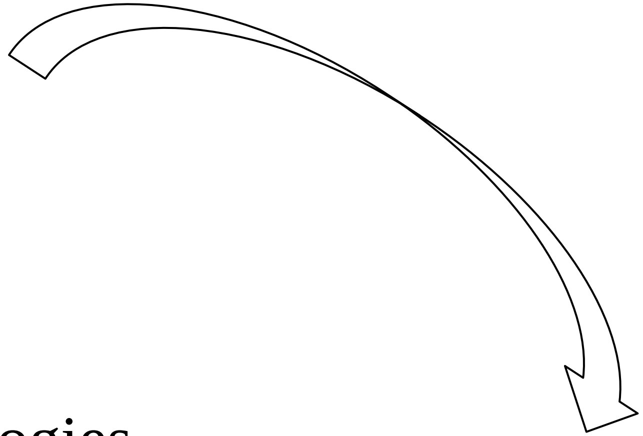
lichkeiten erschöpfend zu untersuchen strebt. Dabei aber erhebt sich eine Frage: Sind die Gesetze der Atomphysik und Quantenphysik für die Lebensvorgänge von wesentlicher Bedeutung? Machen wir uns, um die Tragweite dieser Frage zu ersehen, bewußt,

# Coherence & Environments



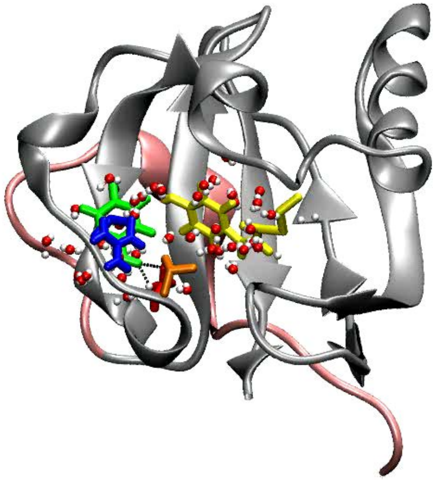
Quantum technologies

Isolate system to observe & exploit quantum behaviour



Biology

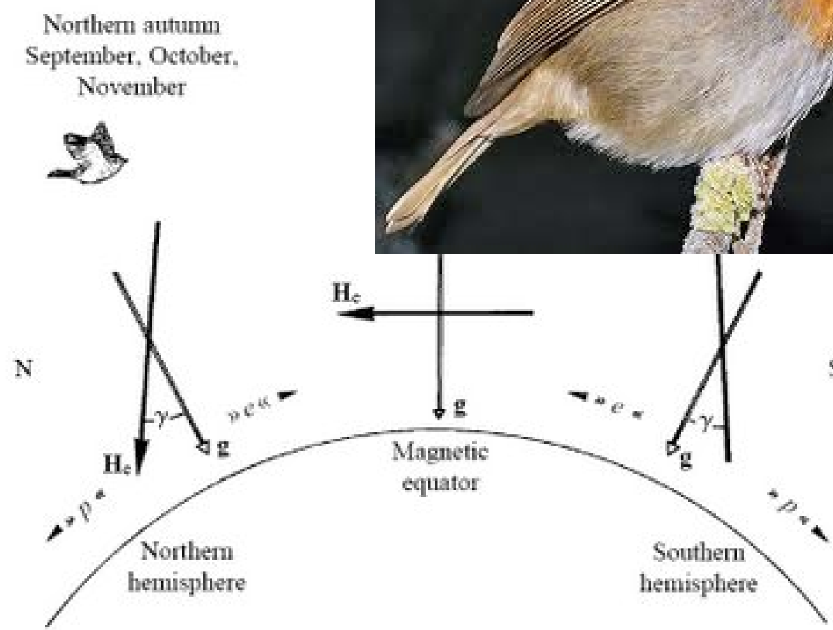
Systems in strong contact with surrounding world

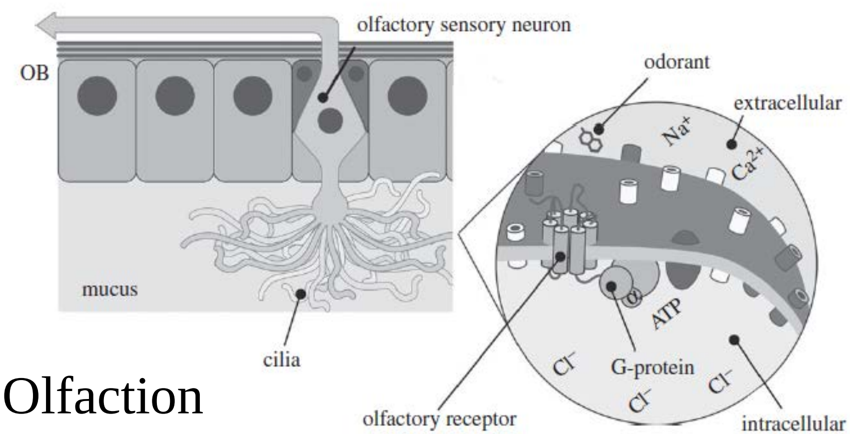


# Coherence and environments

Photosynthesis

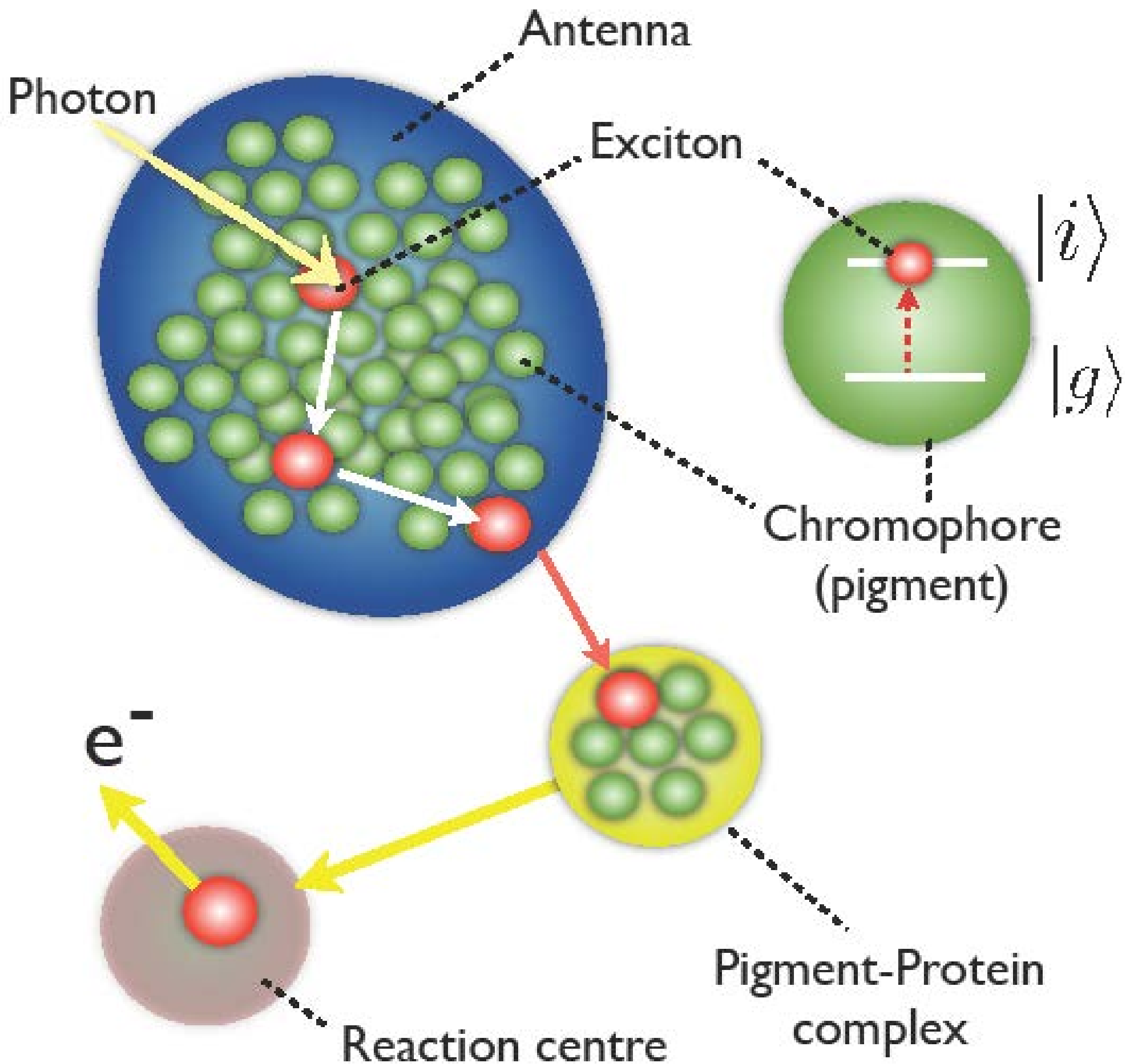
Magnetic Sensing

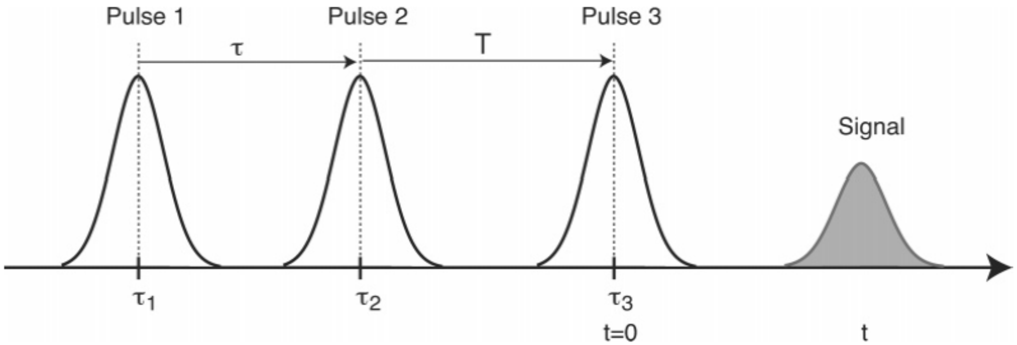


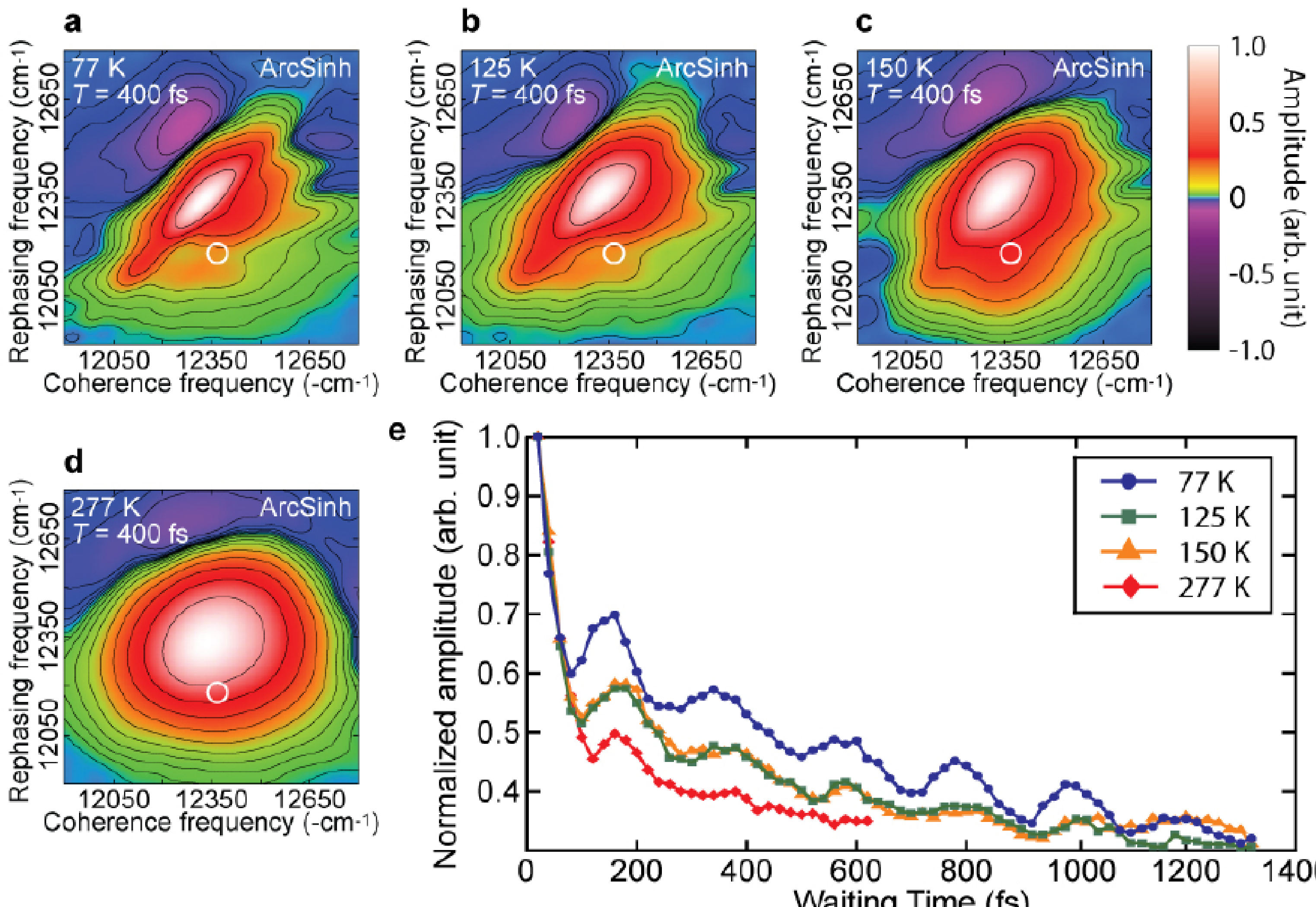




Olfaction

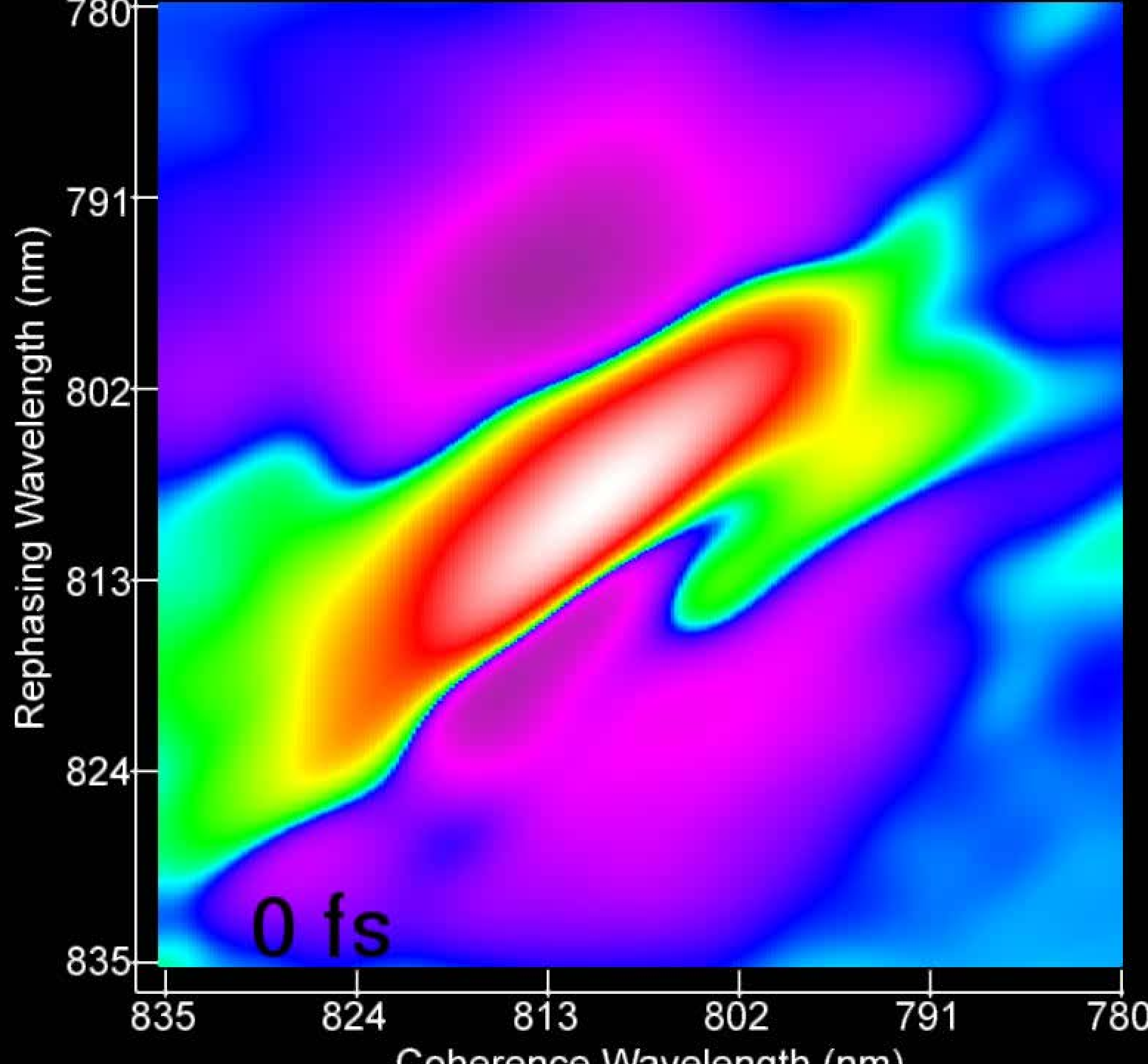
# Excitation energy transport






Engel et al, Science 2007
Panitchayangkoon et al, PNAS 2010



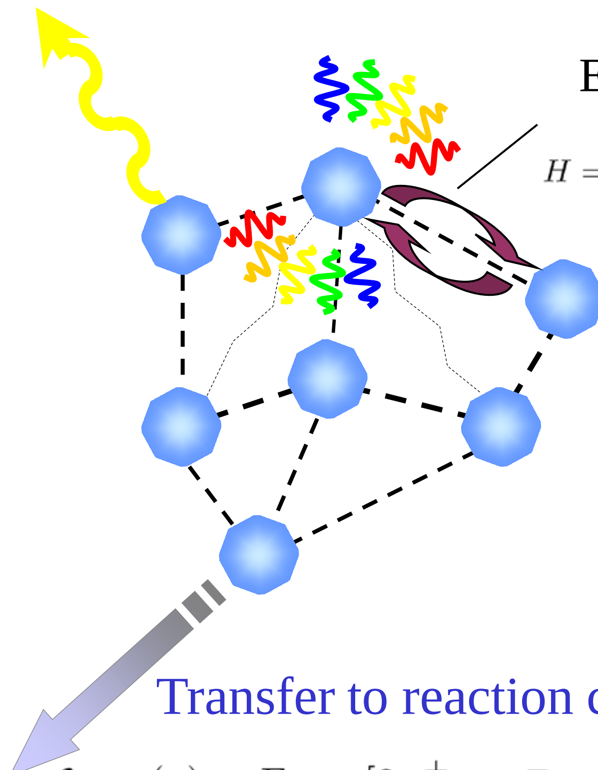
780
791
802
813
824
835
Rephasing Wavelength (nm)
0 fs
835
824
813
802
791
780
Coherence Wavelength (nm)

# Transport dynamics

$$\mathcal{L}_{diss}(\rho) = \sum_{j=1}^{N} \Gamma_j[-\{\sigma_j^+\sigma_j^-, \rho\} + 2\sigma_j^-\rho\sigma_j^+]$$

Loss of excitation

$$\frac{d\rho}{dt} = -\frac{i}{\hbar}[H, \rho] + \mathcal{L}$$



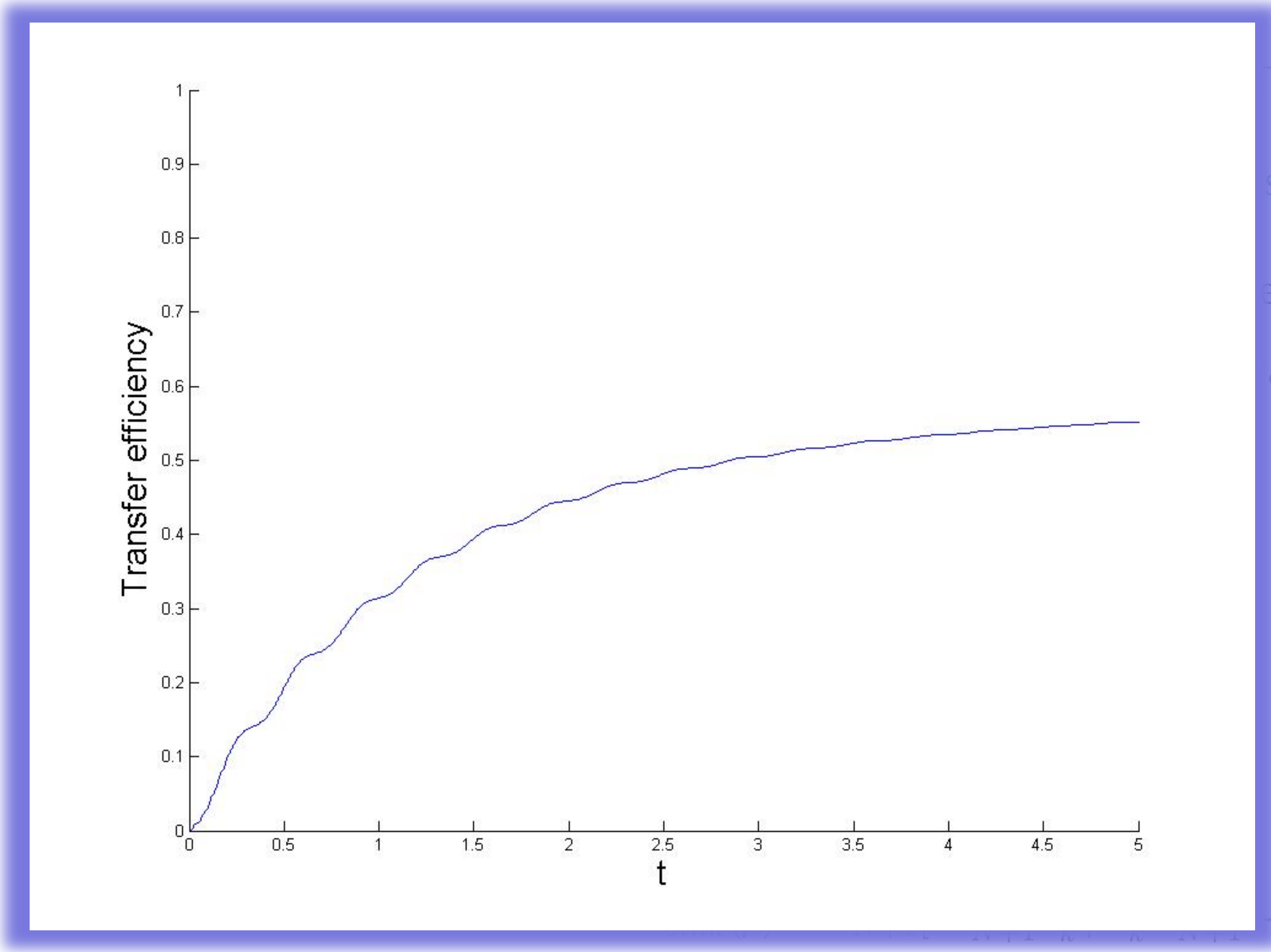
Exchange of excitation

$$H = \sum_{j=1}^{N} \hbar\omega_j \sigma_j^+\sigma_j^- + \sum_{j\neq l} \hbar v_{j,l}(\sigma_j^-\sigma_l^+ + \sigma_j^+\sigma_l^-)$$

Transfer to reaction centre

$$\mathcal{L}_{sink}(\rho) = \Gamma_{N+1}[2\sigma_{N+1}^+\sigma_k^-\rho\sigma_k^+\sigma_{N+1}^- - \{\sigma_k^+\sigma_{N+1}^-\sigma_{N+1}^+\sigma_k^-, \rho\}]$$

# Transport dynamics




$, \rho\} + 2\sigma_j^+\sigma_j^-\rho\sigma_j^+\sigma_j^-]$

sing

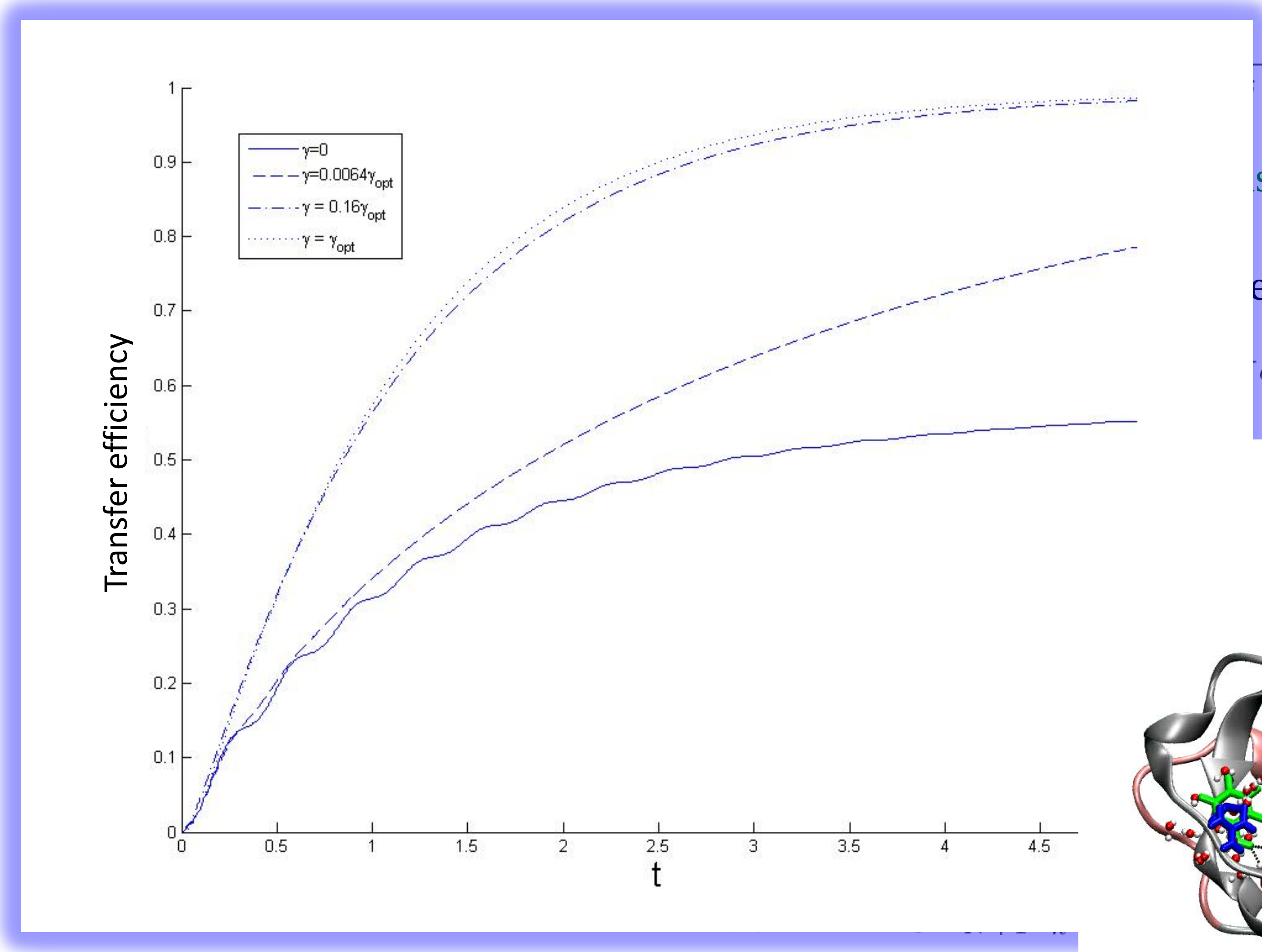
of excitation

$\sigma_j^- + \sum_{j\neq l} \hbar v_{j,l}(\sigma_j^-\sigma_l^+ + \sigma_j^+\sigma_l^-)$

$\{\sigma_k^+\sigma_{N+1}^-\sigma_{N+1}^+\sigma_k^-, \rho\}]$

Plenio & Huelga, New J. Phys. 2008

# Transport dynamics with noise

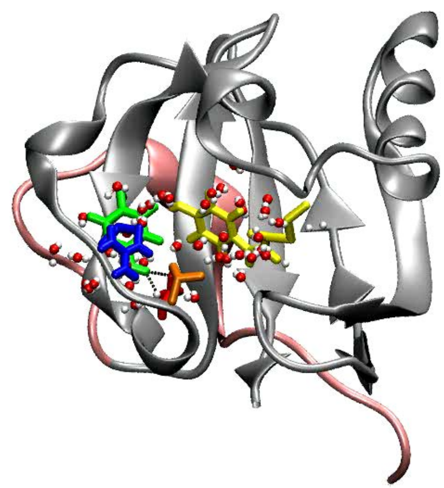



$, \rho\} + 2\sigma_j^+ \sigma_j^- \rho \sigma_j^+ \sigma_j^- ]$

sing

e of excitation

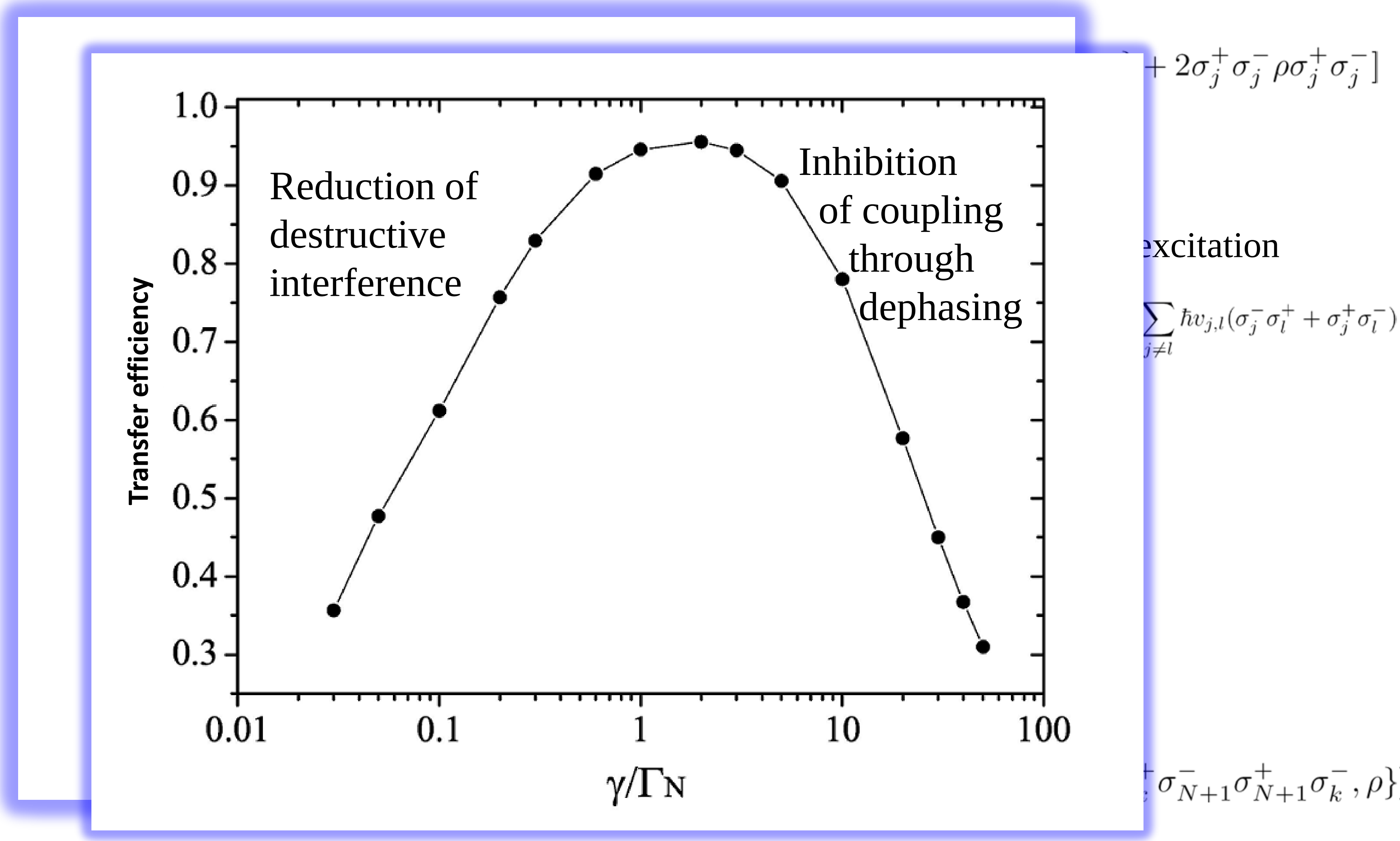
$\sigma_j^- + \sum_{j \neq l} \hbar v_{j,l} (\sigma_j^- \sigma_l^+ + \sigma_j^+ \sigma_l^-)$



$\}]$

Plenio & Huelga, New J. Phys. 2008

# Transport dynamics with noise




Plenio & Huelga, New J. Phys. 2008

# Transport dynamics

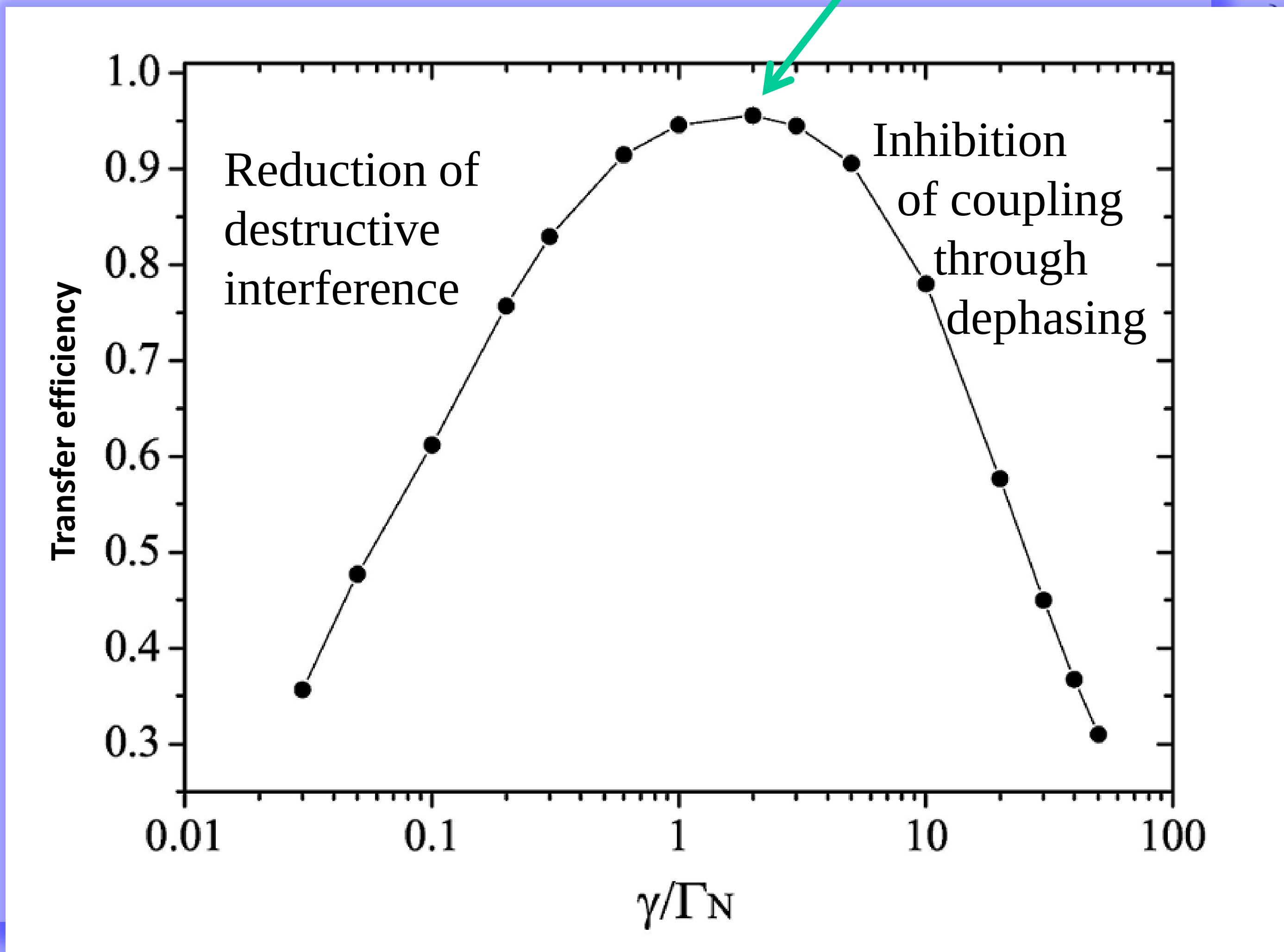
Optimal operating regime is on boundary between coherent and incoherent system

Caruso, Chin, Datta, Huelga, Plenio, J Chem Phys 2009

$+ 2\sigma_j^+ \sigma_j^- \rho \sigma_j^+ \sigma_j^- ]$

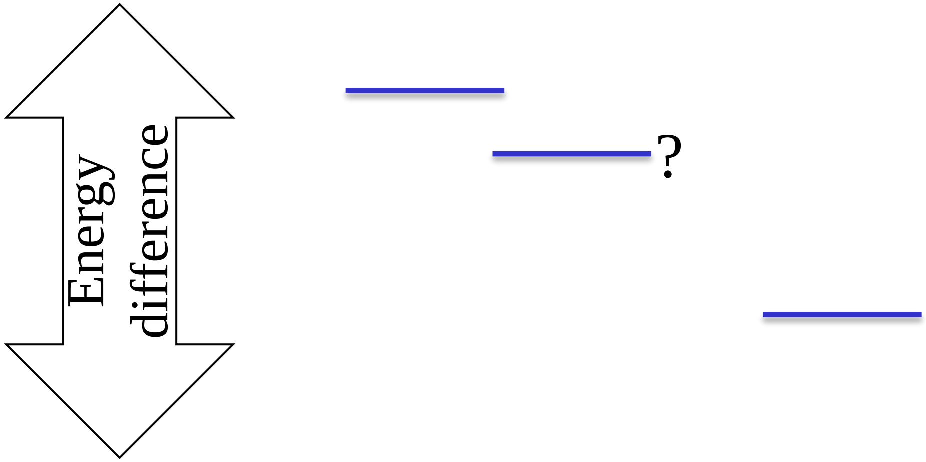
excitation

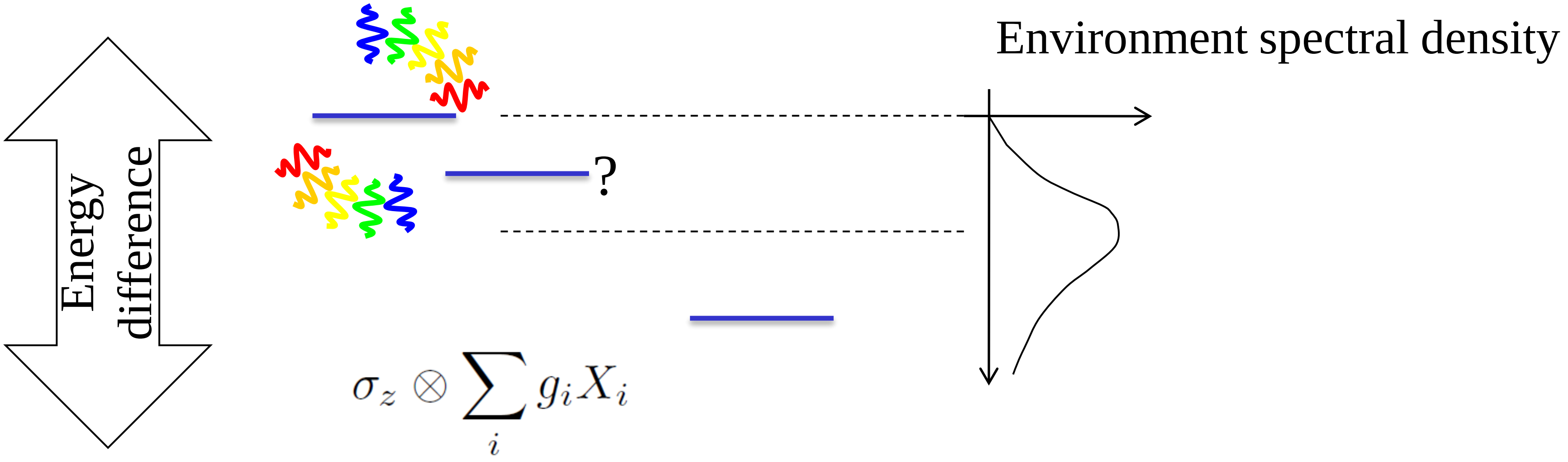
$\sum_{j \neq l} \hbar v_{j,l} (\sigma_j^- \sigma_l^+ + \sigma_j^+ \sigma_l^-)$

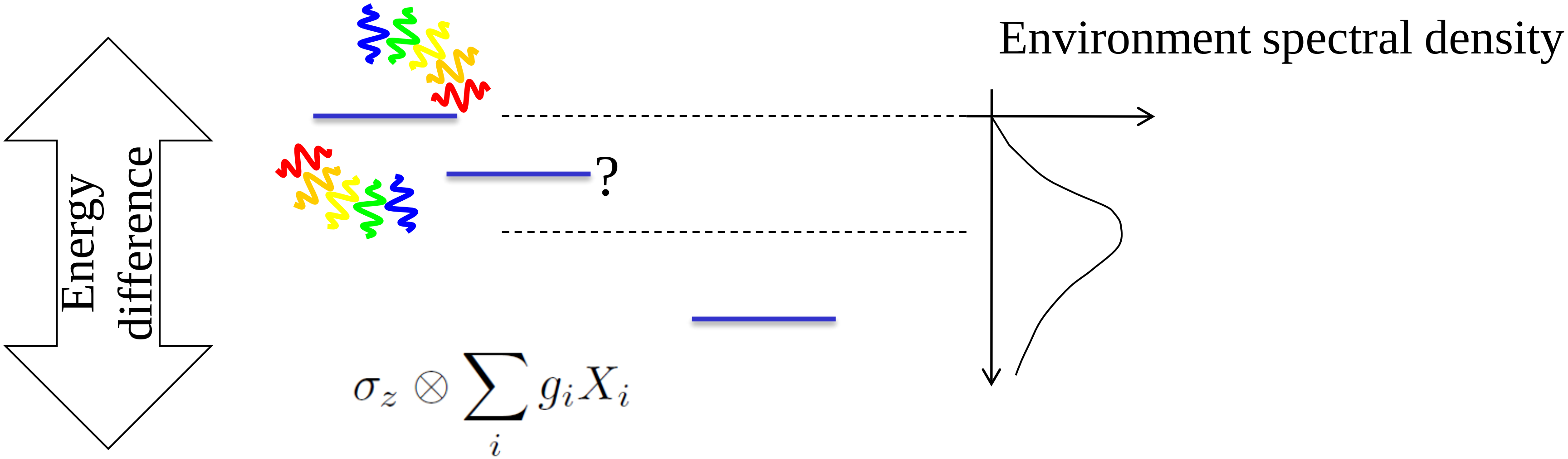


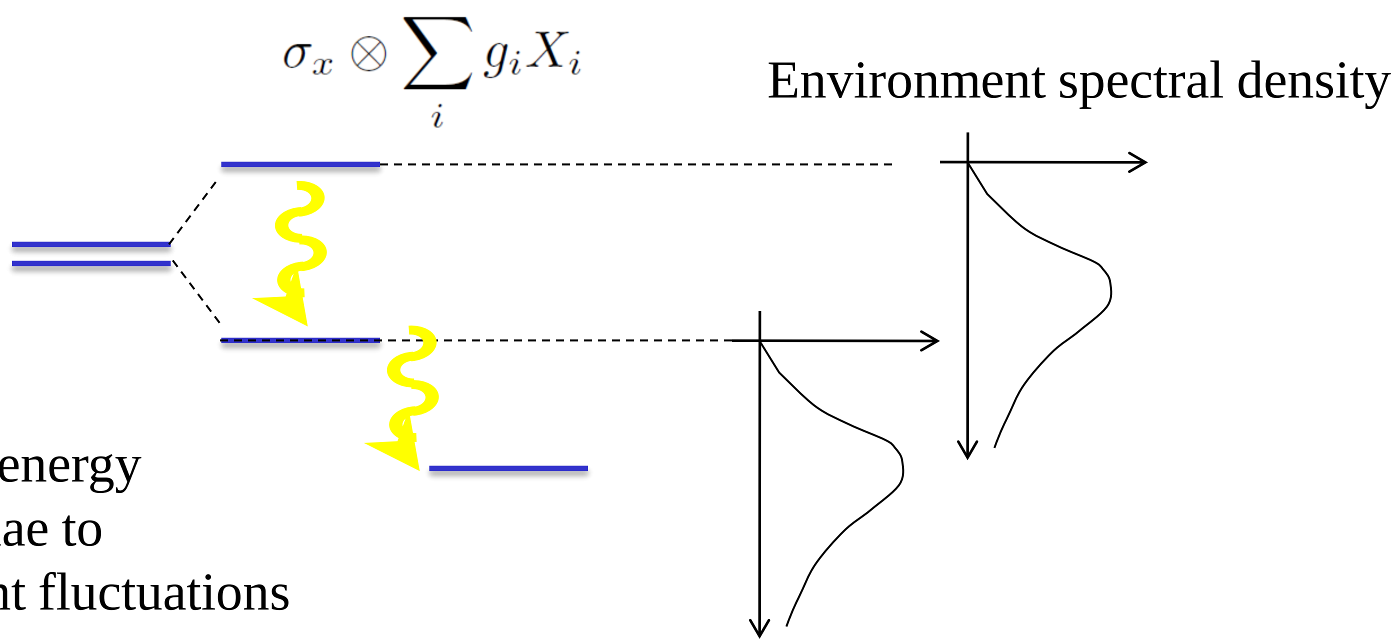

$\sigma_{N+1}^- \sigma_{N+1}^+ \sigma_k^-, \rho\}]$

Require new methods for the accurate description of dynamics in intermediate regime


Energy difference
?


Environment spectral density
Energy difference
?
$\sigma_z \otimes \sum_i g_i X_i$




Coherently shifted energy levels act as antennae to harvest environment fluctuations

Chin, Huelga, Plenio, Phil. Trans. Act. Roy. Soc. A 2012

# Long-lived coherences

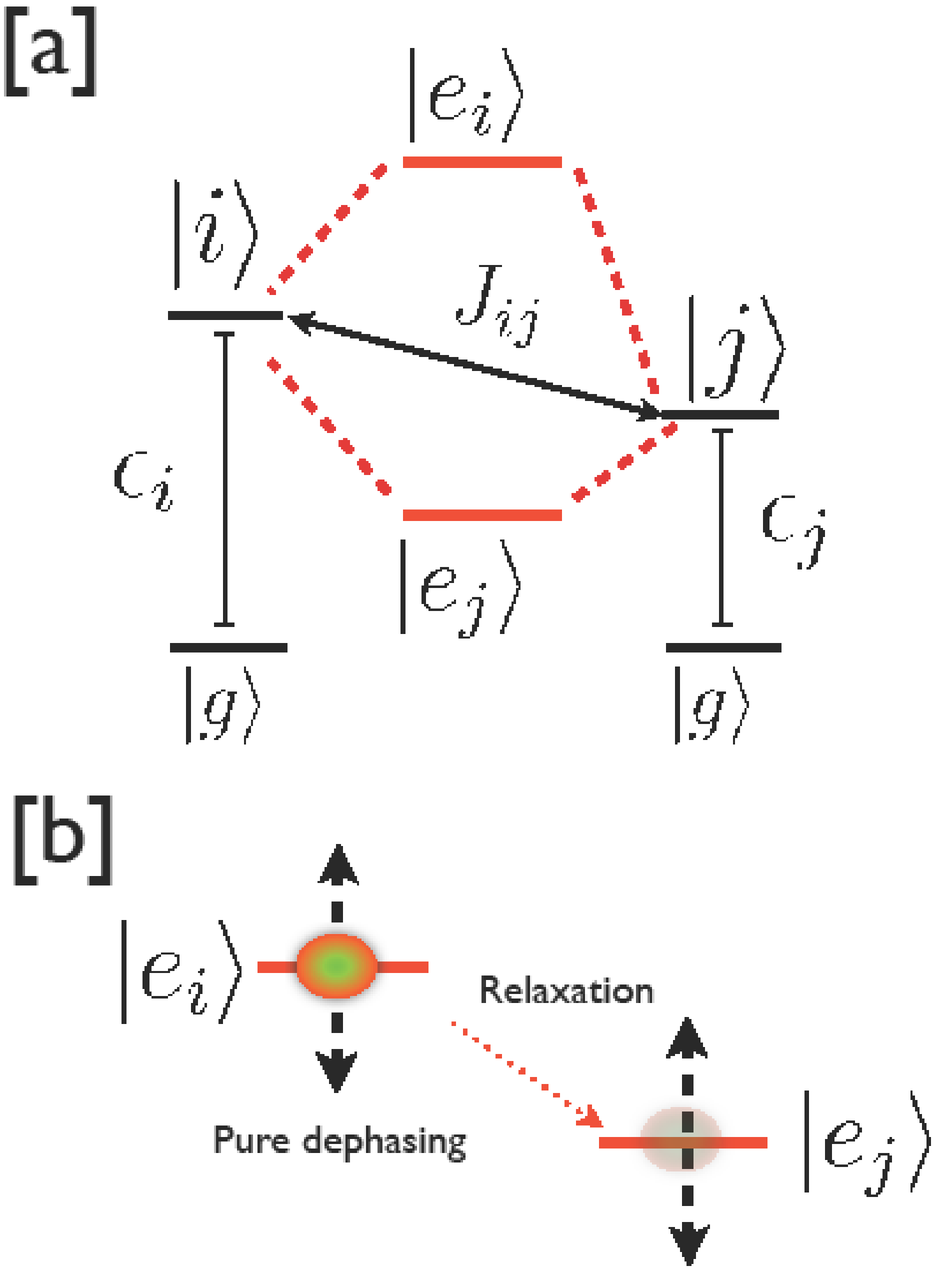
Need to explain:

(i)
Ground-excited state coherence is short lived

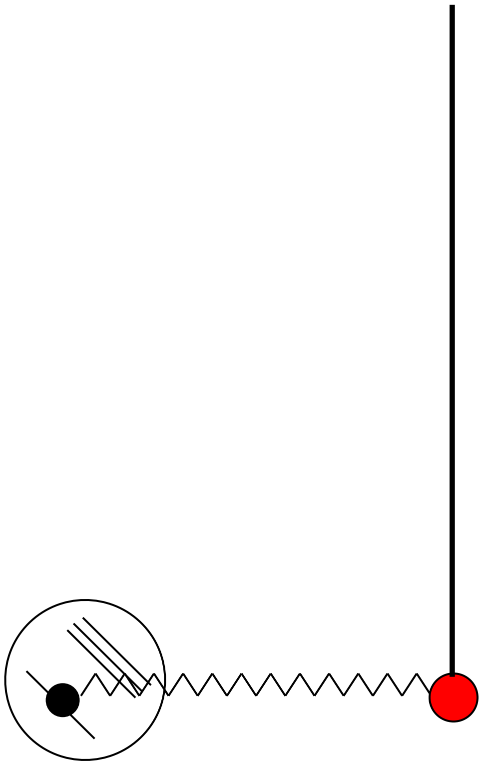
compared to

exciton-exciton coherences

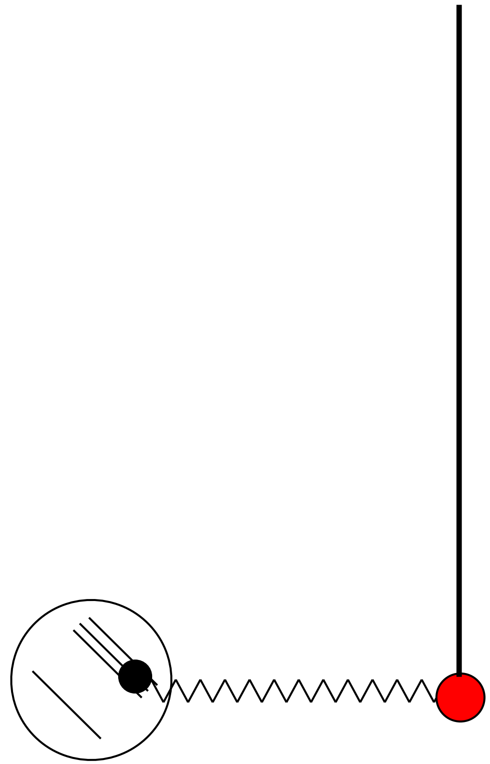
(ii)
and for the same model yielding correct energy transfer rates, spectra etc



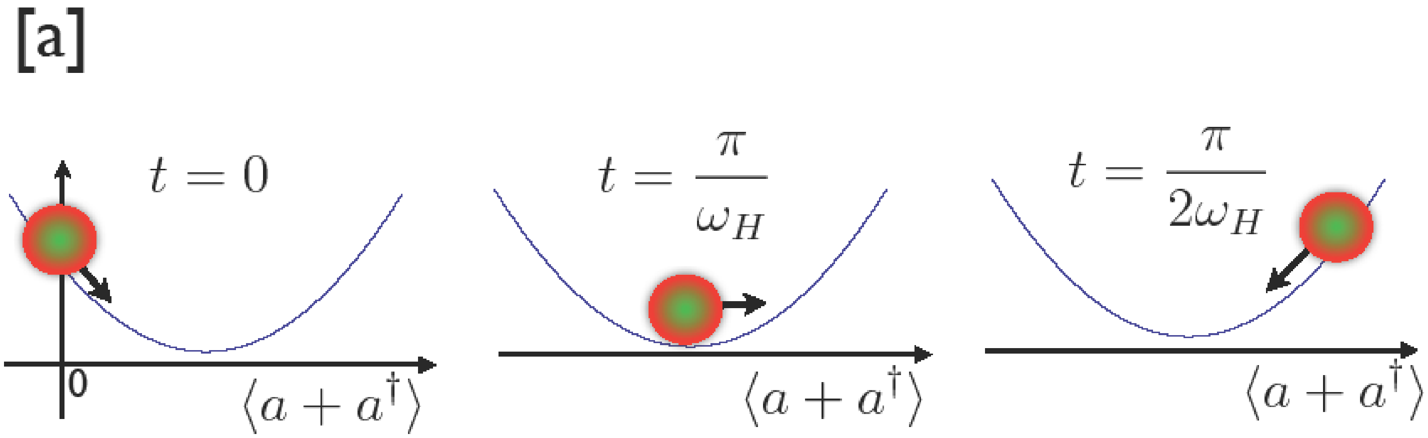
# Vibration induced electronic coherence

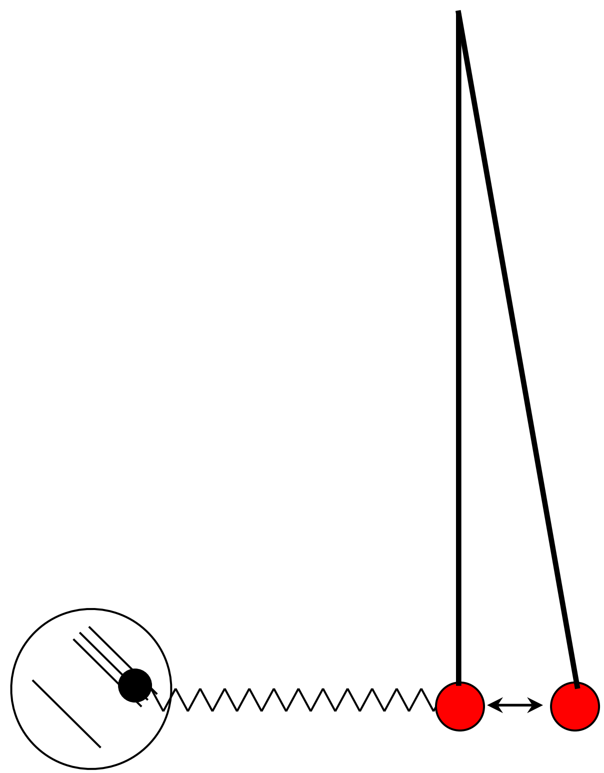


# Vibration induced electronic coherence



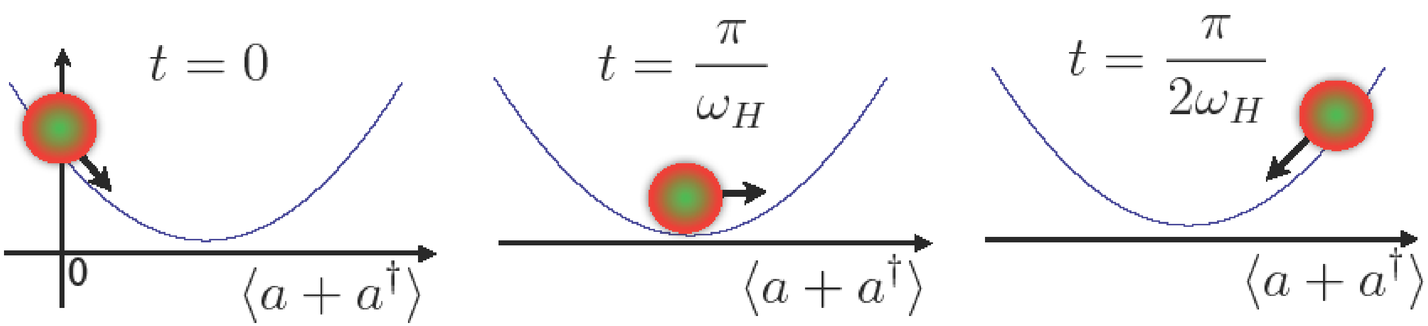
# Vibration induced electronic coherence



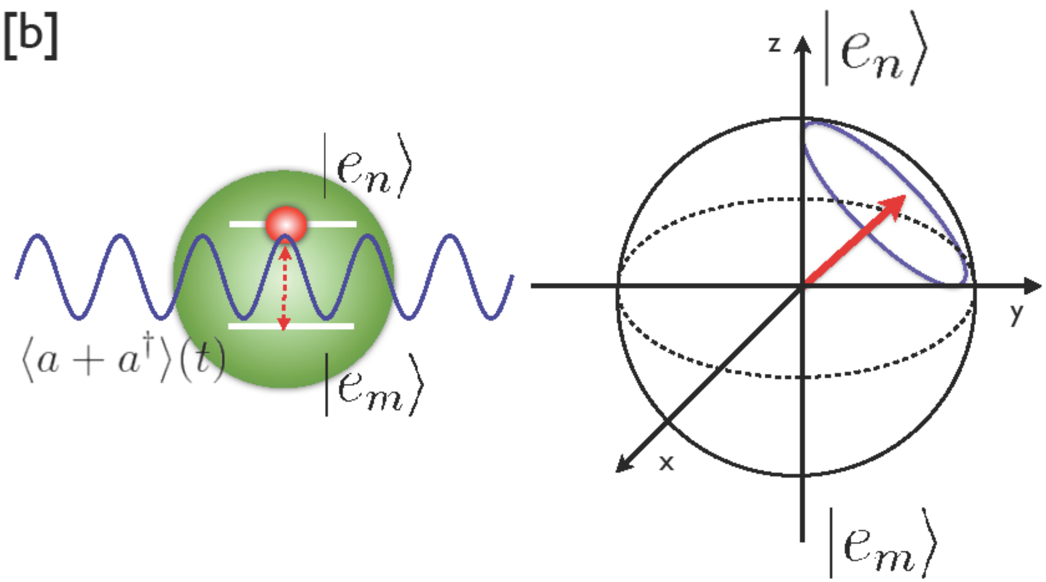



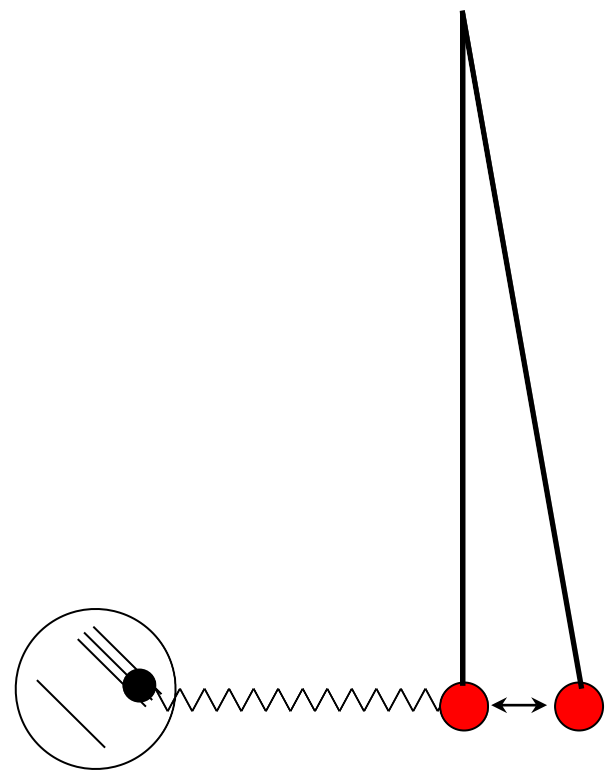
# Vibration induced electronic coherence

[a]

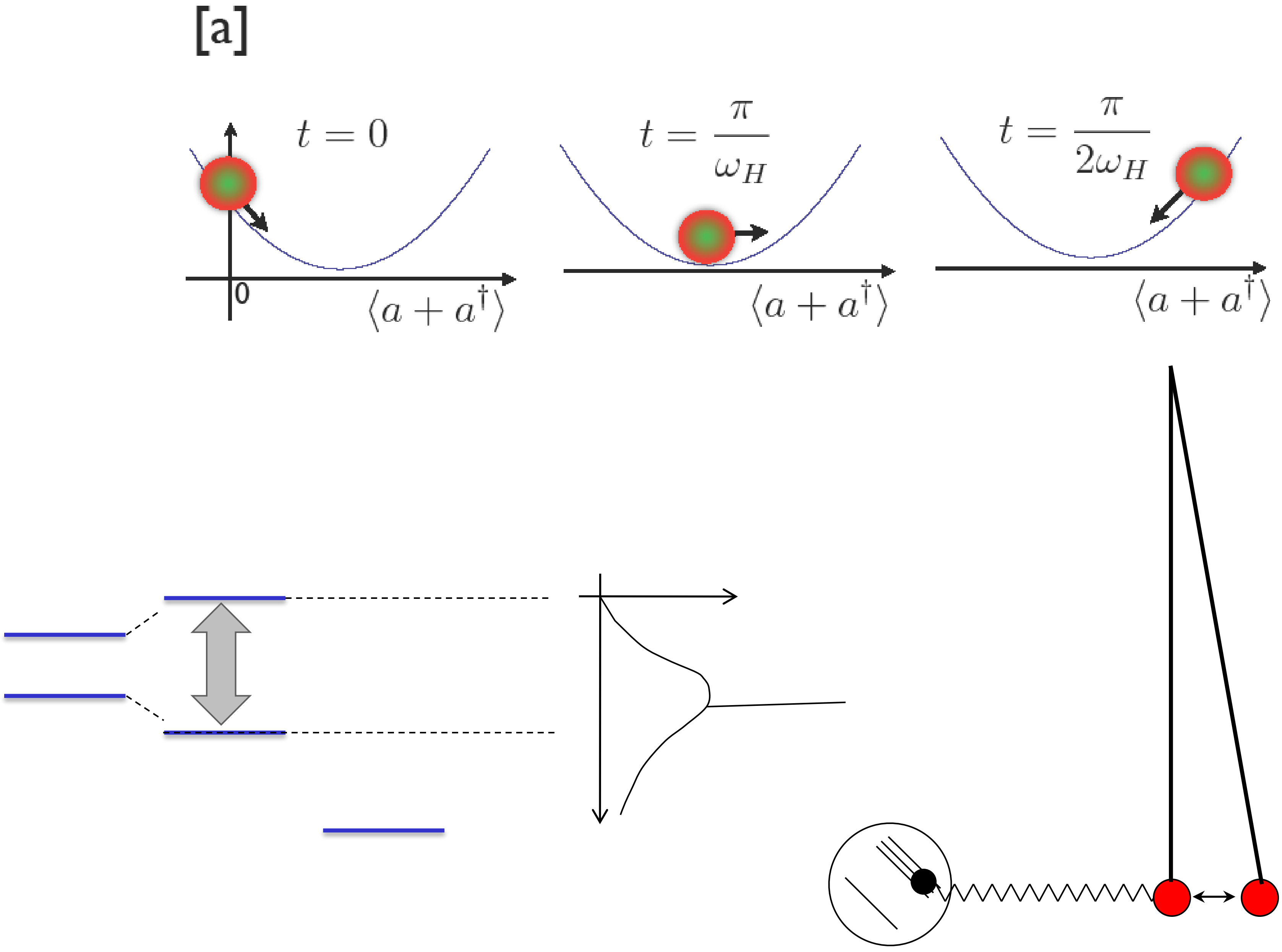



[b]

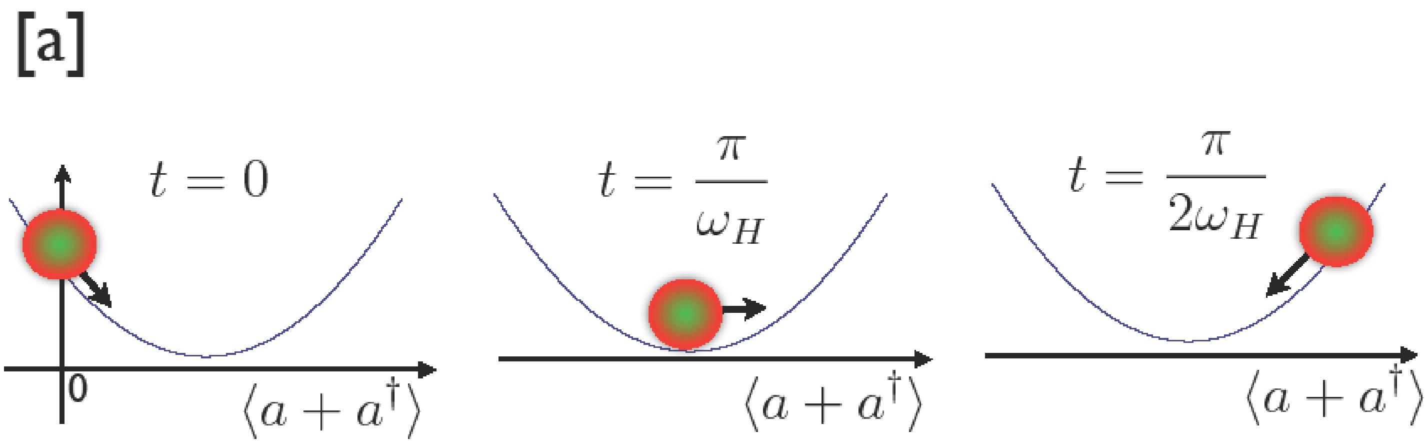


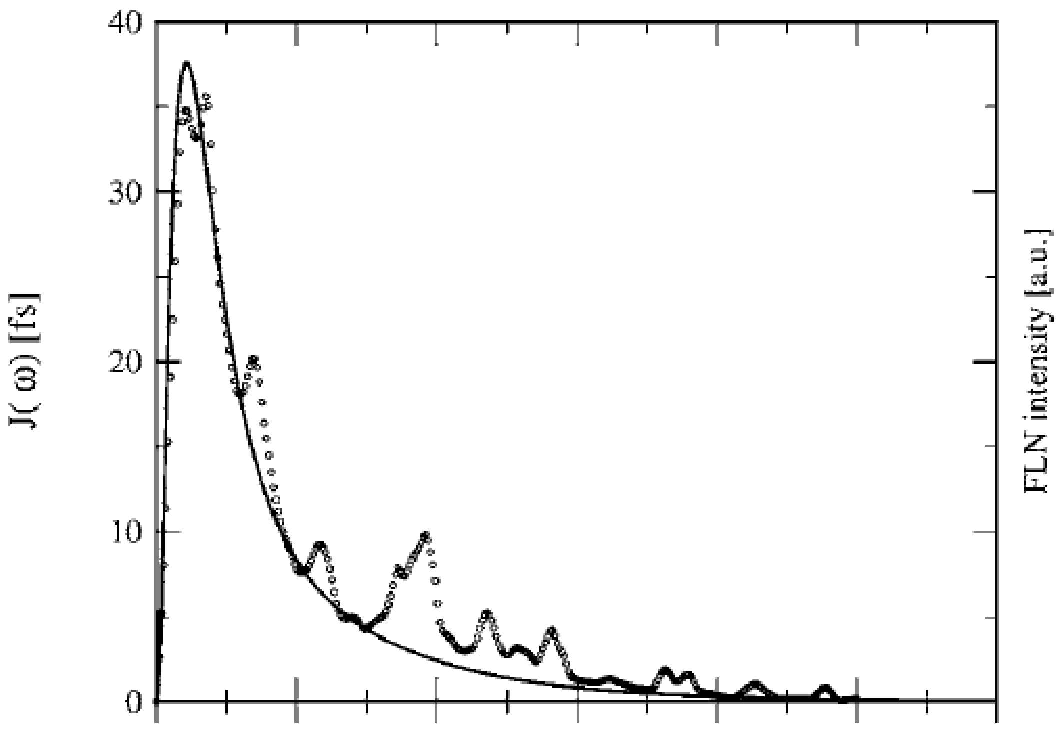



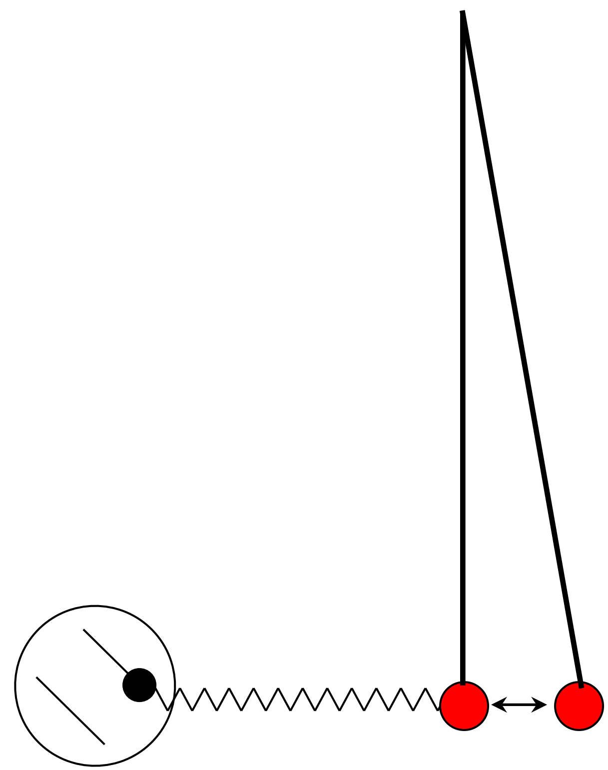
# Vibration induced electronic coherence



# Vibration induced electronic coherence

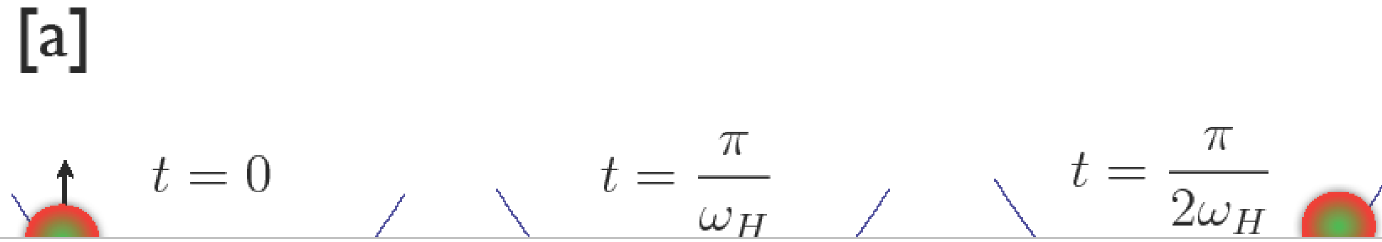


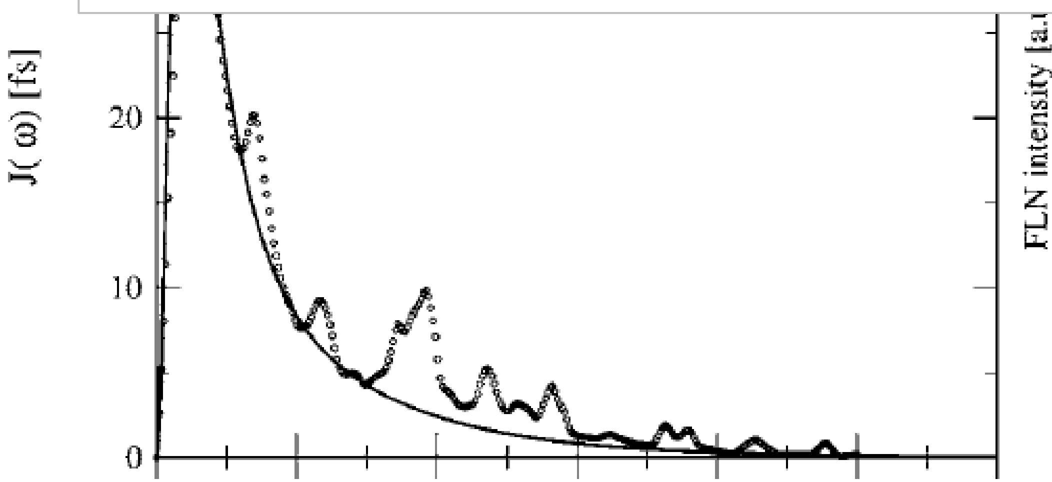
Taken from Wendling et al, J Phys Chem B 2000

# Vibration induced electronic coherence

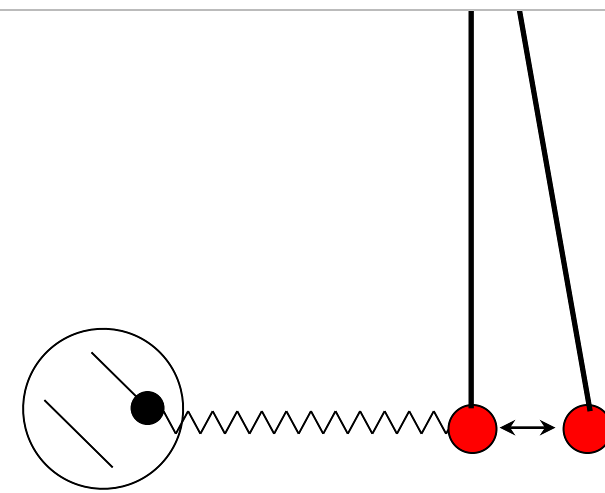



## Two ways forward
## (both taken and compared)

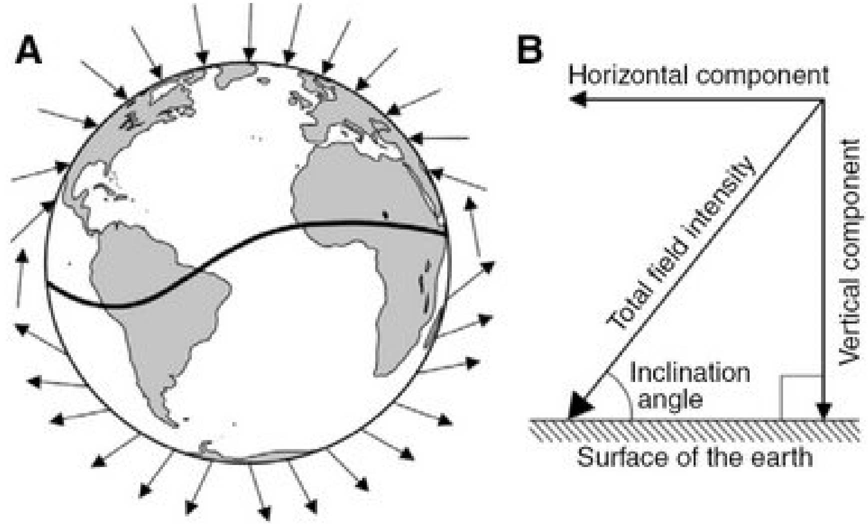
- Semi-classical approximation of environment modes
  In preparation J. Prior, A.W. Chin, R. Rosenbach, S.F. Huelga and M.B. Plenio
- Non-perturbative modeling of the system environment dynamics
  Prior, Chin, Huelga, Plenio, PRL 2010

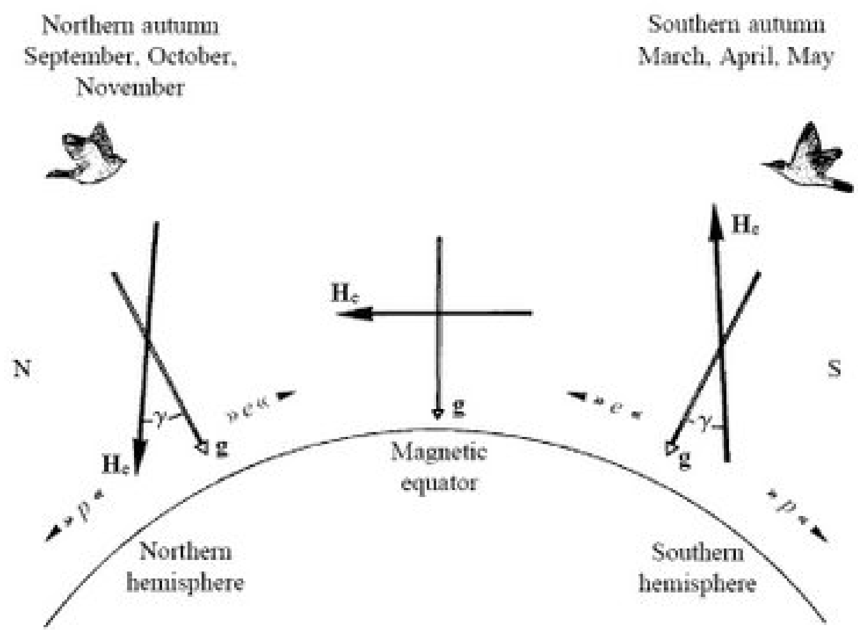



Taken from Wendling et al, J Phys Chem B 2000



# Magnetic sense of birds: Coherence and noise



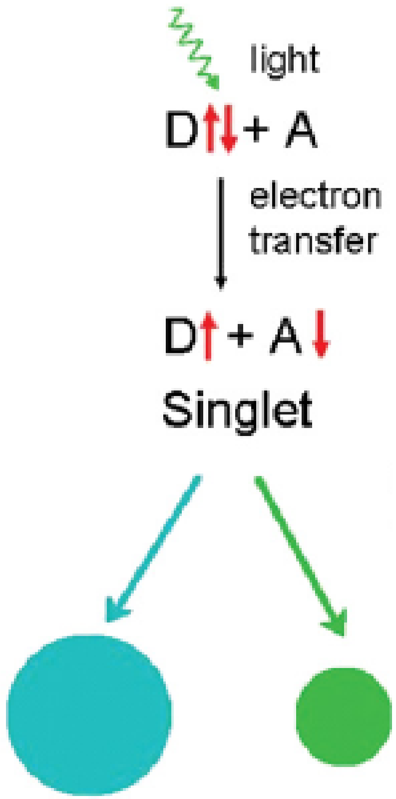

Birds and other animals sense the magnetic field.

How do they do this ?

- Magnetic particles
- Chemical compass

Wiltschko & Wiltschko since the 1960‘s

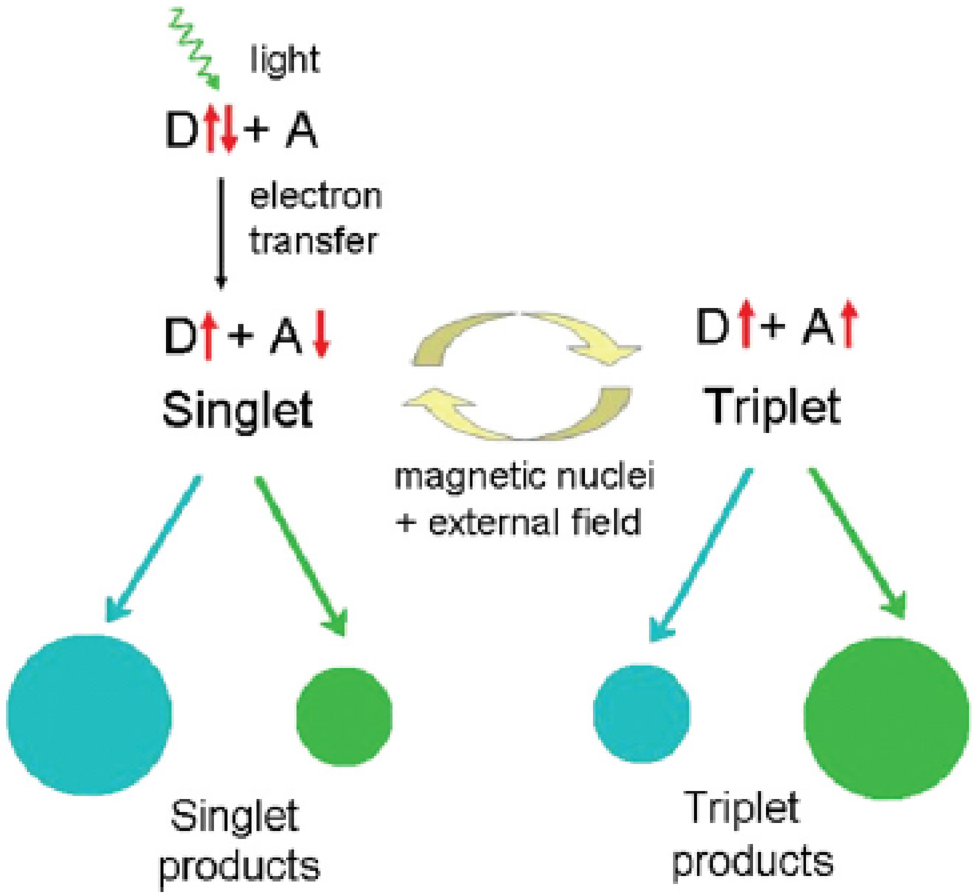
# Magnetic sense of birds: Coherence and noise




Photon absorption creates radical pair in singlet state

Ritz, Adem, and Schulten., Biophys. J. (2000)

# Magnetic sense of birds: Coherence and noise



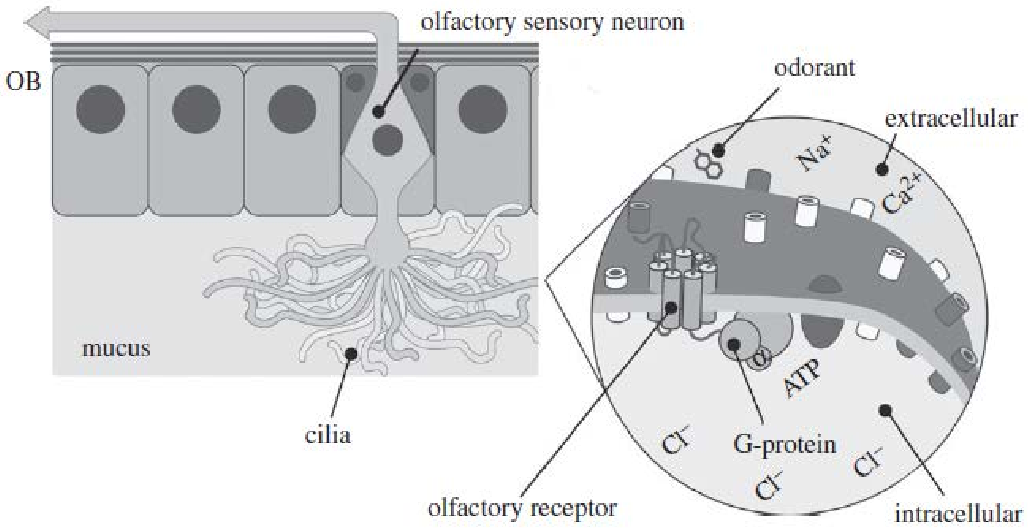

Photon absorption creates radical pair in singlet state

Interaction with nuclear spin environment lead to singlet-triplet interconversion

Conversion rates depend on external magnetic field

Ritz, Adem, and Schulten., Biophys. J. (2000)

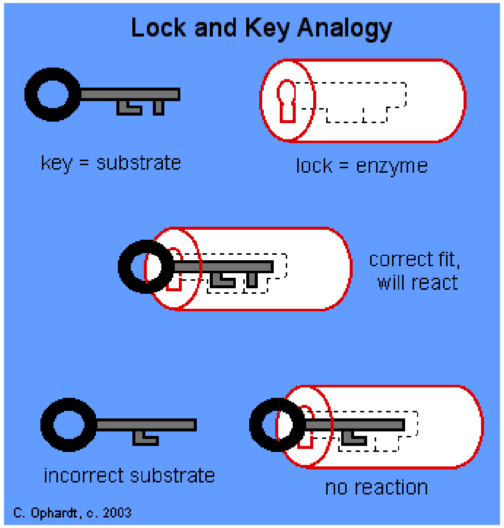
# Olfaction



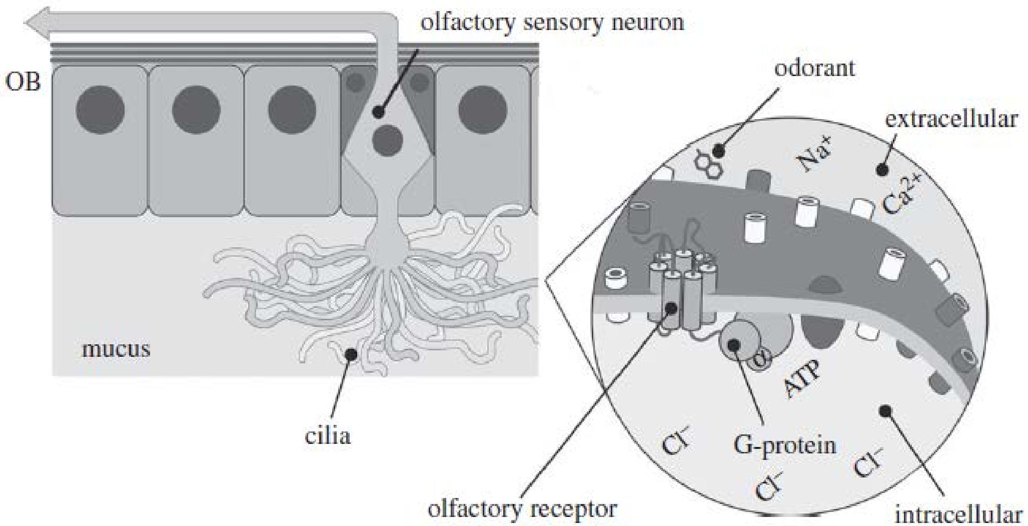

Standard theory:

Different receptors are sensitive to different scents

Origin is shape sensitivity, lock and key principle

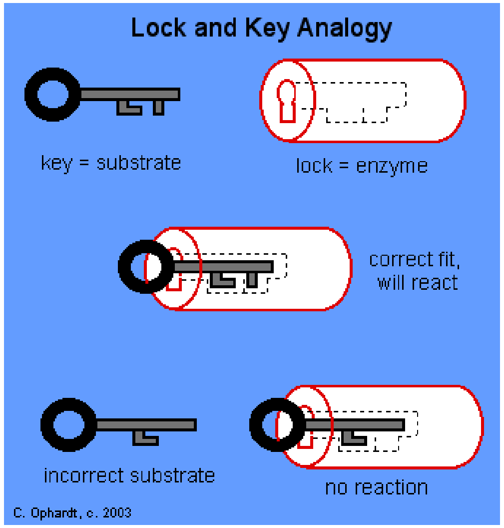


# Olfaction




Standard theory:
Different receptors are sensitive to different scents

Origin is shape sensitivity, lock and key principle




Weakness: Odorants are small molecules, and very similar shaped molecules may smell rather differently.

Replace hydrogen by deuterium, Drosphila flies can smell the difference

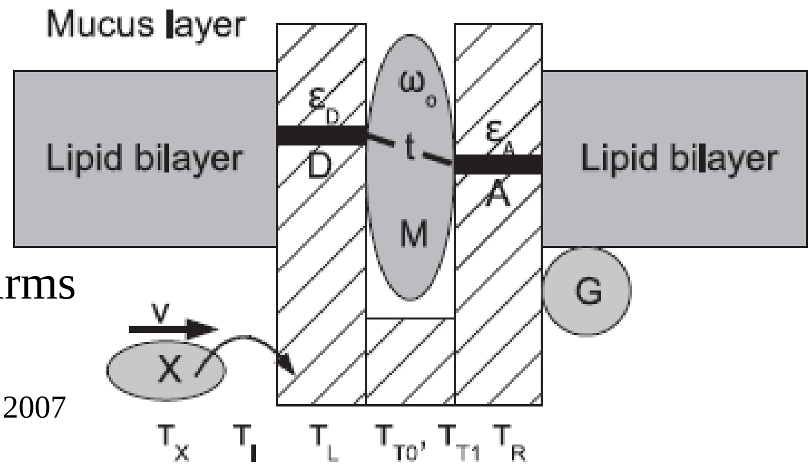
Franco, Turin, Mershin, Skoulakis, PNAS 9 3797 (2011)

# Olfaction and phonon assisted electron tunneling

Dyson (1938) / Wright(1977): What we smell are molecular vibrations

Turin (1996): Sense molecular vibrations through phonon assisted tunneling

Turin, Chem. Senses 21, 773 (1996)




Quantum theoretical treatment of phonon-assisted electron tunneling for reasonable parameters confirms that the idea is at least theoretically plausible.

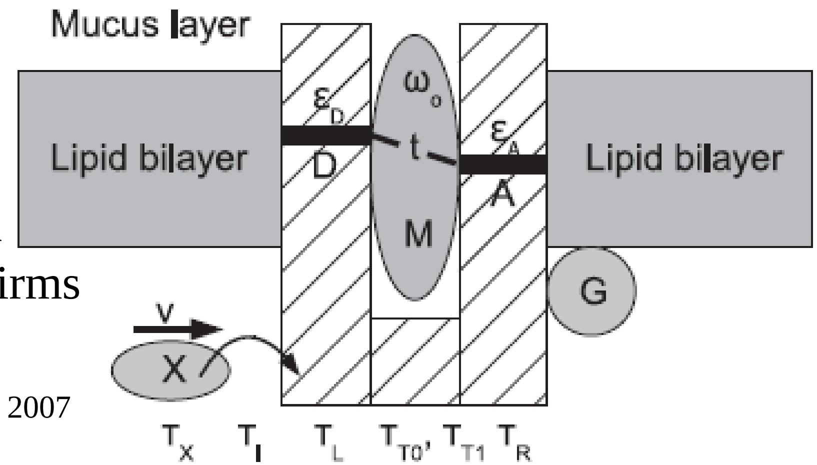
Brookes, Hartoutsiou, Horsfield and Stoneham, Phys. Rev. Lett. 2007

# Olfaction and phonon assisted electron tunneling

Dyson (1938) / Wright(1977): What we smell are molecular vibrations

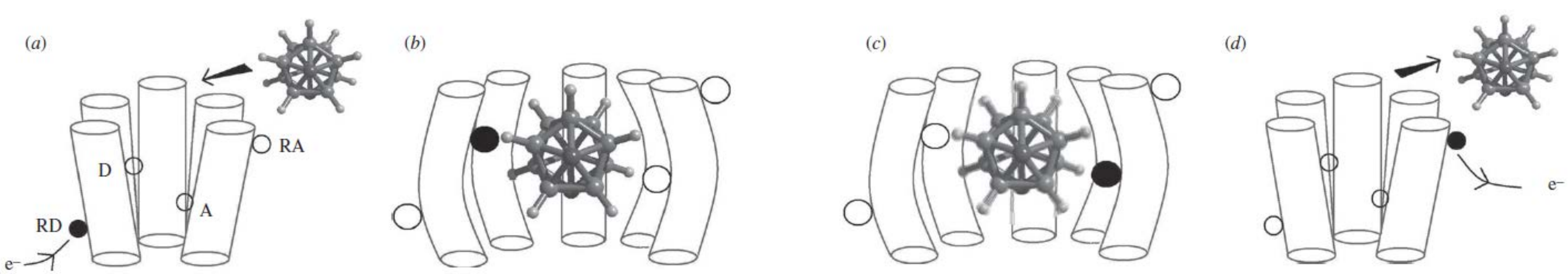
Turin (1996): Sense molecular vibrations through phonon assisted tunneling

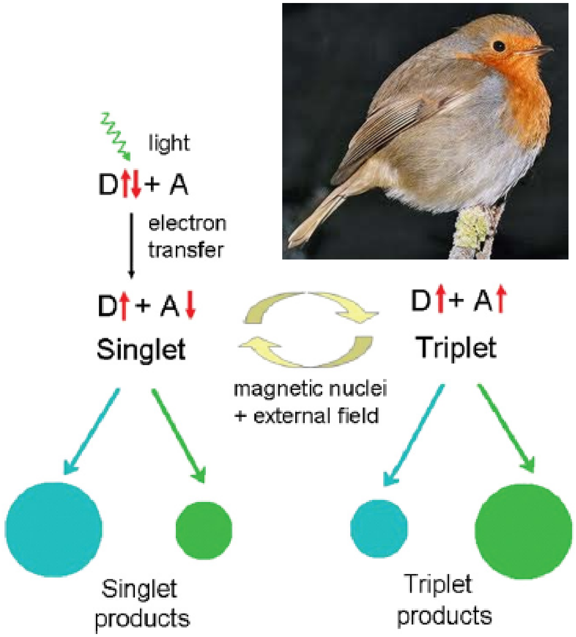
Turin, Chem. Senses 21, 773 (1996)

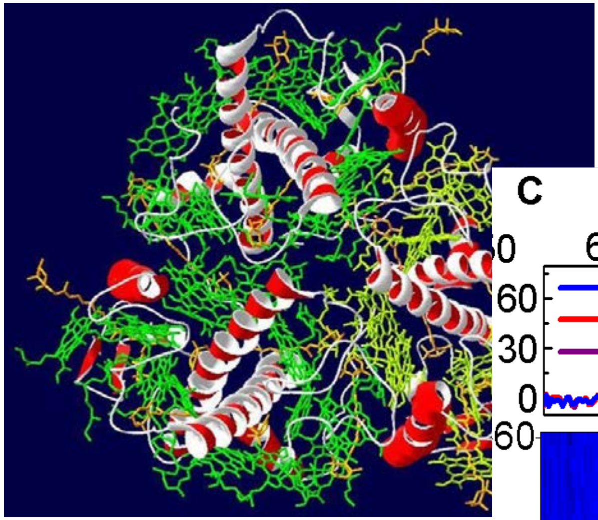


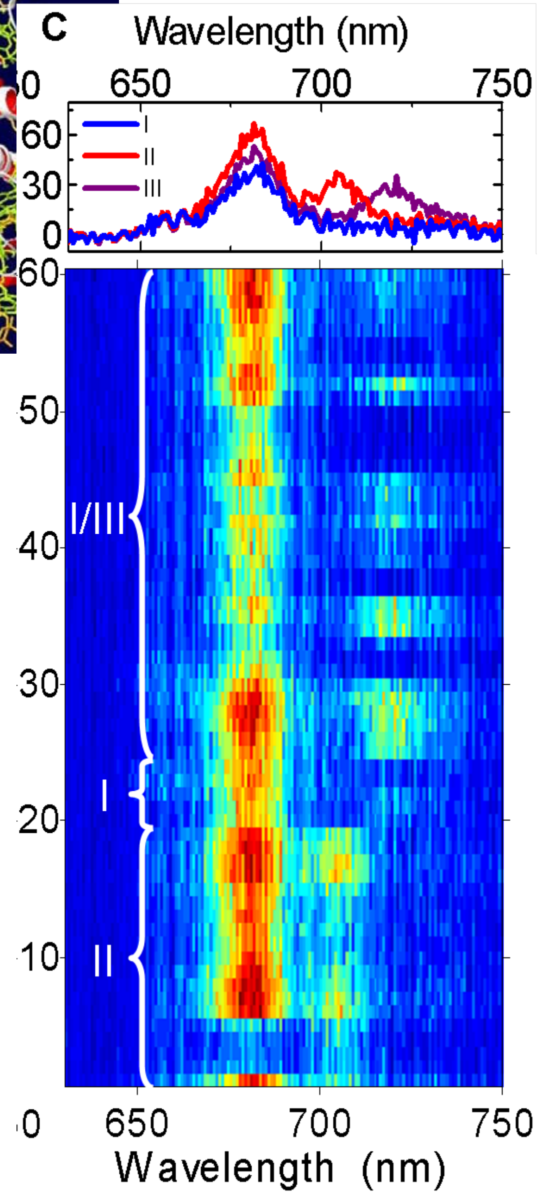

Quantum theoretical treatment of phonon-assisted electron tunneling for reasonable parameters confirms that the idea is at least theoretically plausible.

Brookes, Hartoutsiou, Horsfield and Stoneham, Phys. Rev. Lett. 2007



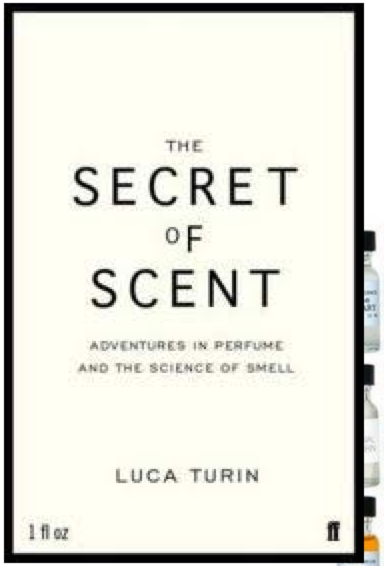


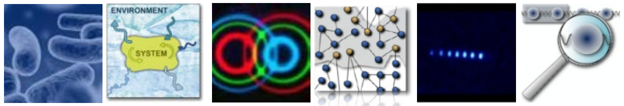



Interaction between coherent dynamics and noise, between electrons &vibrations are key to understand fundamental biological effects at the quantum – classical boundary.

Quantum technology can provide novel sensors to study these phenomena




# Institut für Theoretische Physik




**Profs**
Martin Plenio
Susana Huelga

**Postdocs**
Javier Almeida
Abolfazl Bayat
Alejandro Bermudez
Jianming Cai
Felipe Caycedo
Marcus Cramer
Shai Machnes
Gor Nikoghosyan
Alex Retzker

**PhD students**
Andreas Albrecht
Tillmann Baumgratz
Javier Cerrillo-Moreno
Clara Javaherian
Ramil Nigmatullin
Robert Rosenbach
Mischa Woods

**Academic Visitors**
Koenraad Audenaert
Filippo Caruso
Mauro Paternostro
Javier Prior
Illai Schwartz

IQ^ST Integrated Quantum Science and Technology
Marie Curie Actions
QESSENCE
HIP
PICC
Gefördert vom Bundesministerium für Bildung und Forschung
DFG Deutsche Forschungsgemeinschaft
Alexander von Humboldt Stiftung / Foundation