Qubit Decoherence in spin baths:
Understanding, Withstanding, and Application

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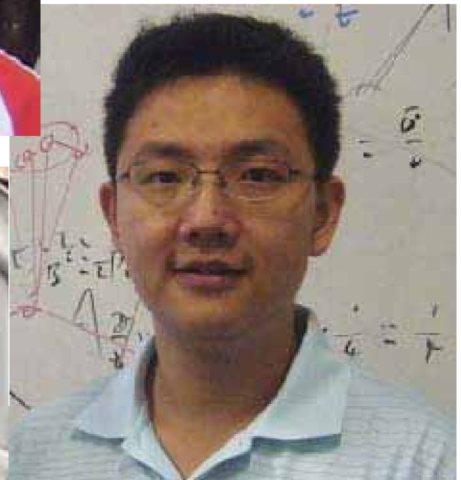


Z. Y. Wang

J. F. Du

Motivation:

Coherence of electron spin for quantum information application

Key issue:

Decoherence (mostly by nuclear spin baths)

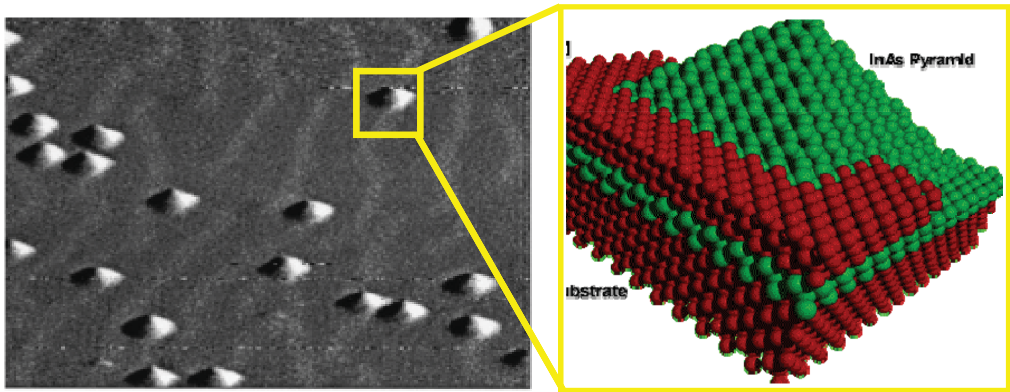
Prerequisites:

Understanding & withstanding the decoherence

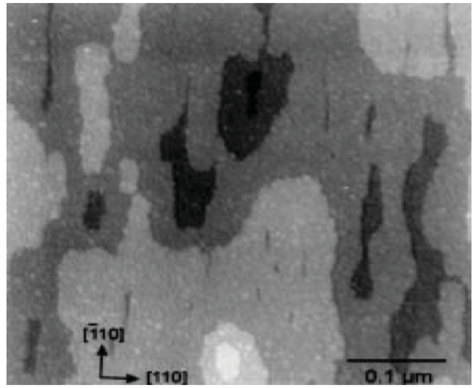
Perspective:

Exploitation of decoherence

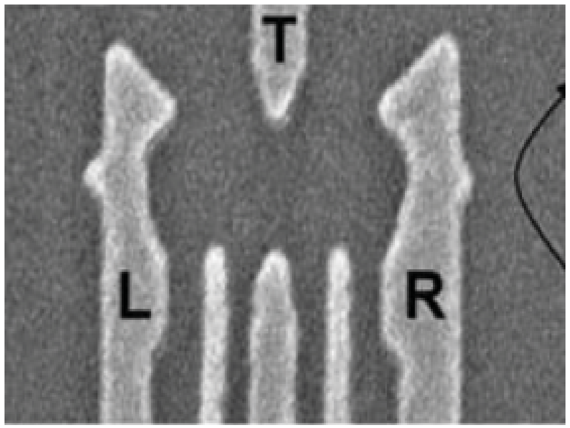
Relevant systems: Electron spin qubit in quantum dots



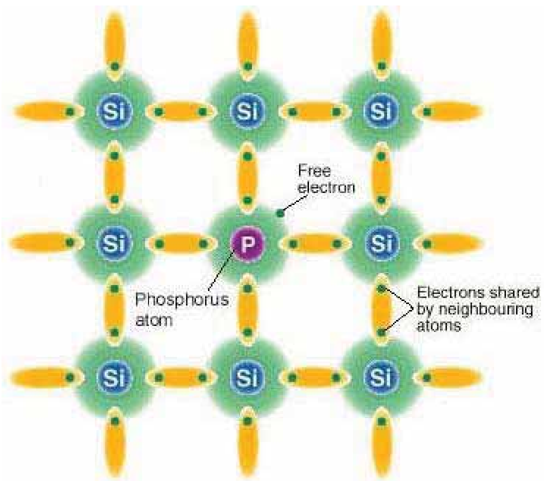
self-assembled dot



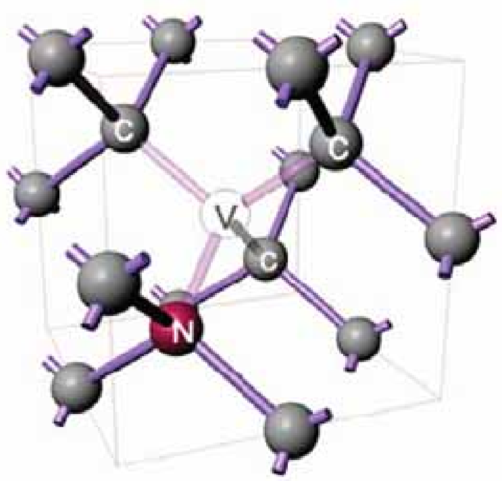
interface fluctuation islands



Gate-defined dot

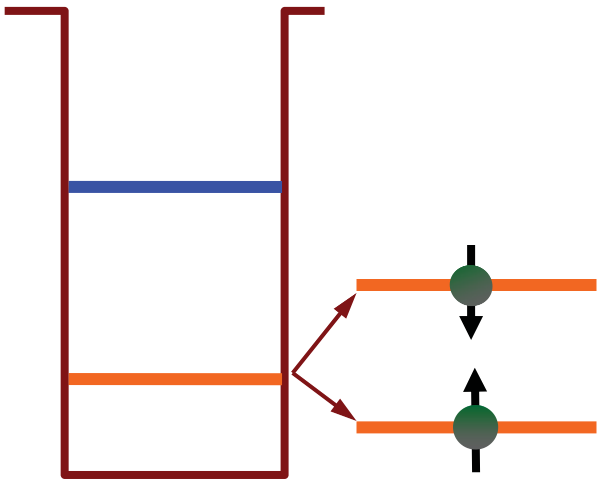


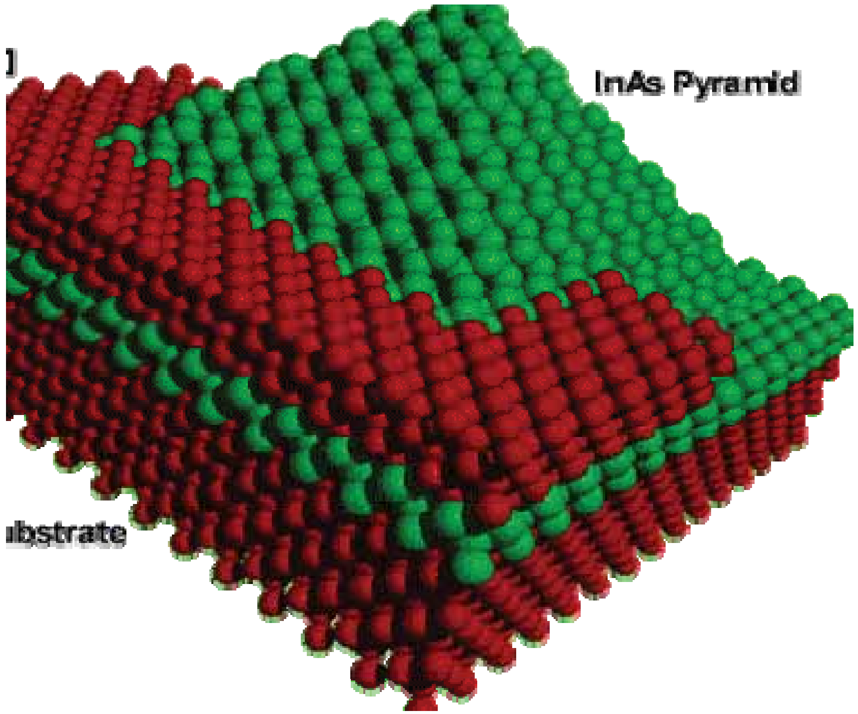
donor impurity P:Si



NV center in diamond

A spin is simple, but simple is difficult.





In a typical quantum dot, a doped electron is spatially overlapped with thousands to millions of atoms. The many-body interaction makes a spin complex.

Energy scales in a QD: From "big bang" to 0 K

"Big bang"

Band gap, visible light	PHz, eV, 10^4 K
LO phonon, confinement splitting	10 THz, 10 meV, 100 K
LA phonon, electron Zeeman splitting	THz, meV, 10 K
Nuclear Zeeman splitting	GHz, μeV, 10 mK
Hyperfine interaction	MHz, neV, 10 μK
Nuclear-nuclear interaction	kHz, peV, 10 nK

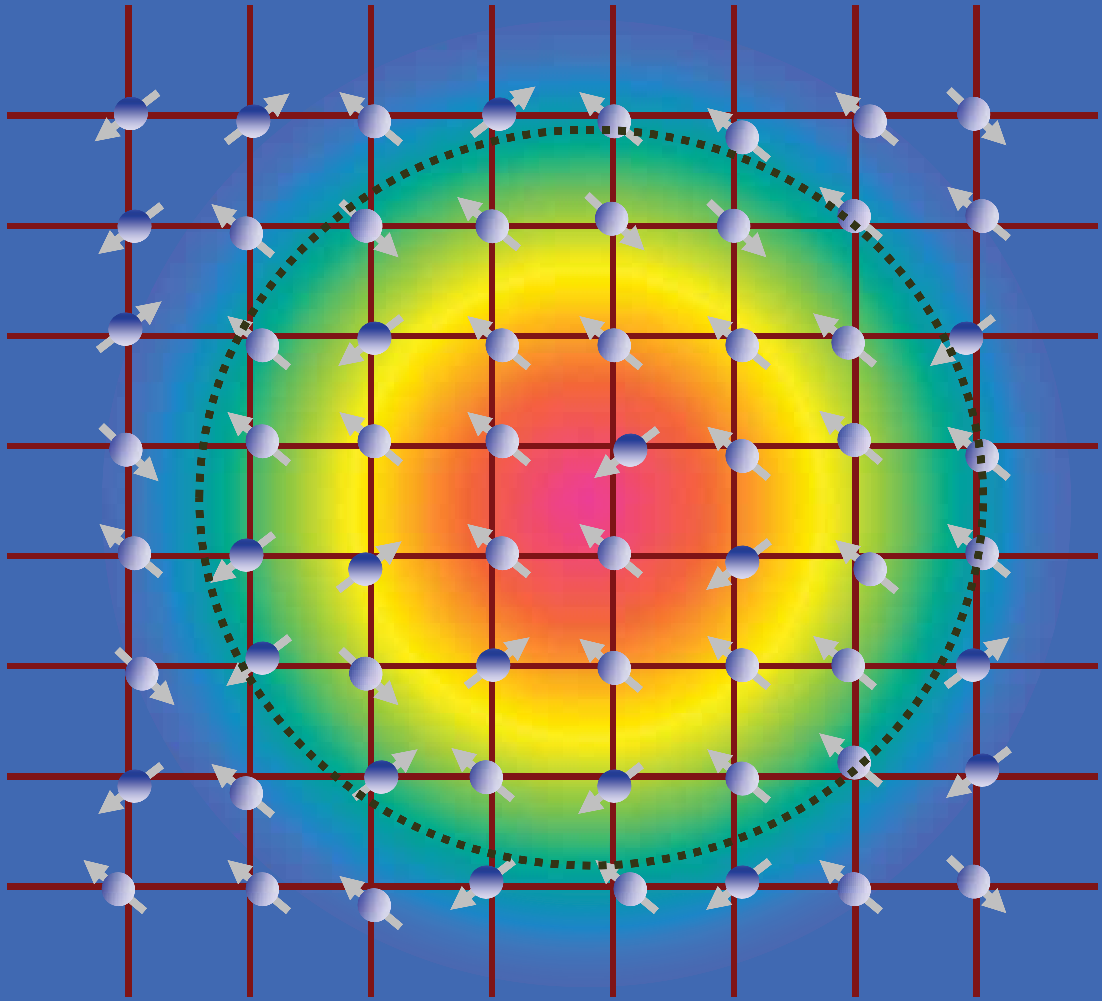
Absolute zero physics
(or "big bang" of a new quantum world)

RBL, W. Yao, and L. J. Sham, Advances in Physics 59, 703-802 (2010)

Electron spin decoherence in quantum dots

			Experiments	Theories
S-O & phonons (T1~ms @ 1K)			Fujisawa et al ‘02 Elzerman et al ‘04 Kroutvar et al ’04	Khaetskii & Nazarov ‘01,’02, Erlingsson & Nazarov ’02, Loss ’04
Nuclear spin baths	hyperfine	T2*~ns	Gurudev et al ’05 Petta et al ’05 Koppens et al ‘05	Merkulov et al ’02 Khaetskii et al ’02, ’03 Coish & Loss ’04
		T1>>ms @ B>100mT	Johnson et al ’ 05, Koppens et al ‘05, Bracker ’05, Braun et al ’05,Imamoglu ’06	Merkulov et al ‘02 Semenov & Kim ’03
	hf & N-N	T2 ~ms (P:Si, NV) ~μs (III-V)	Lyon ’03 (Si:P), Abe et al ‘04 (Si:P), Marcus ’05 (GaAs) Kouwenhoven ’06, ’07 (GaAs) Bayer ‘06 ’07 (InGaAs), Lukin 06 (NV), Du 09 (radicals), …	Das Sarma 03 (semiclassical); Das Sarma 05-07 (CE); Sham 05-07 (PCA & LCE); Loss 05 (2QD w/o n-n); Liu 08 (2QD w/ n-n & CCE)

1 electron spin + N nuclear spins in quantum dot



The nuclear spins in a quantum dot and the qubit electron spin form a relatively isolated system.

Outline

I-1. Semiclassical theory (Kubo, Anderson & Klauder, …)

I-2 Quantum theory of qubit decoherence

II. Control of decoherence and dynamical decoupling

III. Experiments and applications

I-1. Spin decoherence: Semiclassical theory

Reading materials:

R. Kubo, J. Phys. Soc. Jpn. **9**, 935 (1956).

P. W. Anderson, J. Phys. Soc. Jpn. **9**, 316 (1954).

Geometrical representation of spin-1/2

The spin state is a superposition state:

$$|\psi\rangle = \cos\frac{\theta}{2} e^{-i\varphi/2} |\uparrow\rangle + \sin\frac{\theta}{2} e^{+i\varphi/2} |\downarrow\rangle$$

The Bloch Vector or spin polarization:

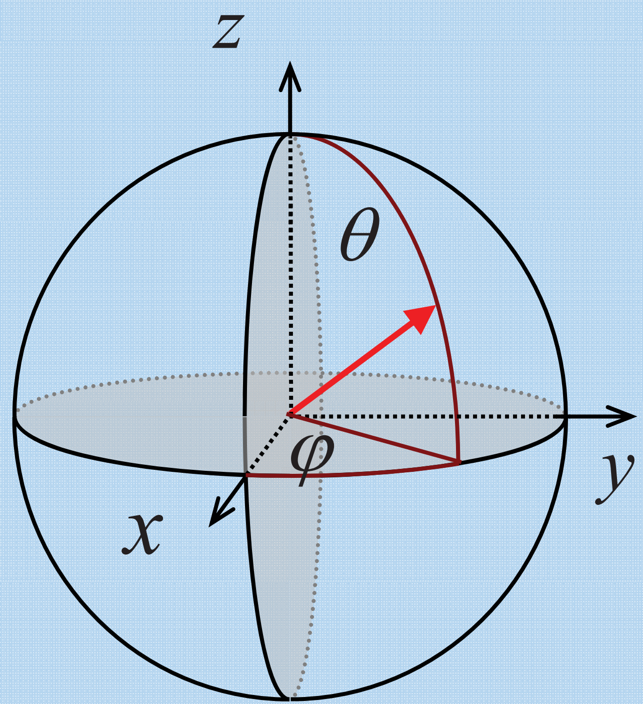
$$\mathbf{S} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$$

$$= \langle\psi|\boldsymbol{\sigma}|\psi\rangle$$

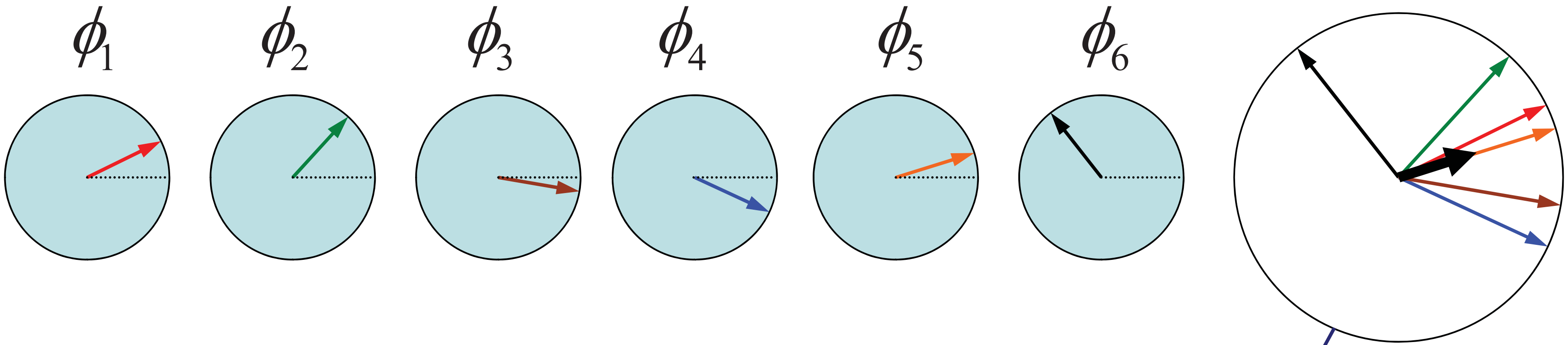
Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \ \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \ \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Bloch sphere



No phase correlation: No coherence



$$\left|\psi_J\right\rangle = \left|\theta, \phi_J\right\rangle$$

Random phase:
Depolarization

$$\mathbf{S} = \mathbf{e}_x \sin\theta\ \Re\left\langle \exp\left(i\phi_J\right)\right\rangle + \mathbf{e}_y \sin\theta\ \Im\left\langle \exp\left(i\phi_J\right)\right\rangle + \mathbf{e}_z \cos\theta$$

Decoherence: Density matrix formalism

Density matrix of a pure state

$$\left|\psi_J\right\rangle = a\left|\uparrow\right\rangle + be^{i\phi_J}\left|\downarrow\right\rangle \quad \Rightarrow \quad \left|\psi_J\right\rangle\left\langle\psi_J\right| = \begin{pmatrix} a^2 & abe^{-i\phi_J} \\ abe^{i\phi_J} & b^2 \end{pmatrix}$$

Average of random phase→ Density matrix of a mixed state

$$\rho = \sum_J P_J \left|\psi(\phi_J)\right\rangle\left\langle\psi(\phi_J)\right| = \begin{pmatrix} a^2 & ab\left\langle e^{-i\phi}\right\rangle \\ ab\left\langle e^{i\phi}\right\rangle & b^2 \end{pmatrix}$$

$$\xrightarrow{\text{random phase}} \begin{pmatrix} a^2 & 0 \\ 0 & b^2 \end{pmatrix}$$

Off-diagonal DM element ⇔ Phase correlation

Decoherence: Density matrix formalism

Bloch vector & density matrix elements

$$\text{With } \sigma_i\sigma_i = 1,\ \sigma_i\sigma_j = i\varepsilon_{ijk}\sigma_k,\ \mathrm{Tr}\left(\sigma_i\right) = 0$$

$$\rho = \begin{pmatrix} a^2 & ab\left\langle e^{-i\phi}\right\rangle \\ ab\left\langle e^{i\phi}\right\rangle & b^2 \end{pmatrix} = \frac{1}{2} + \frac{S_x\sigma_x + S_y\sigma_y + S_z\sigma_z}{2}$$

$$\langle \mathbf{S} \rangle = \sum_\phi P_\phi \langle \psi(\phi)|\boldsymbol{\sigma}|\psi(\phi)\rangle = \mathrm{Tr}\left[\boldsymbol{\sigma}\sum_\phi P_\phi |\psi(\phi)\rangle\langle\psi(\phi)|\right] = \mathrm{Tr}\left[\boldsymbol{\sigma}\rho\right]$$

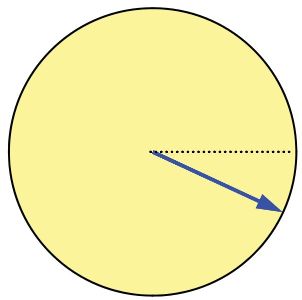
$$S_x = 2\Re\left(\rho_{\downarrow\uparrow}\right),\ S_y = 2\Im\left(\rho_{\downarrow\uparrow}\right),\ S_z = \rho_{\uparrow\uparrow} - \rho_{\downarrow\downarrow}$$

(de)coherence of a single spin

Coherence: Relative phase between down and up states are the same for different spins.

Decoherence: Relative phase between down and up states are randomized for different spins.

What means the coherence and decoherence of a SINGLE spin?



(de)coherence of a single spin

A single-shot measurement gives either 0 or 1, yielding only one bit information.

Many shots required to measure the phase, a real number.

A state cannot be cloned.

$$\left.\begin{array}{l} U|k_1\rangle|0\rangle = |k_1\rangle|k_1\rangle \\ U|k_2\rangle|0\rangle = |k_2\rangle|k_2\rangle \end{array}\right\} \Rightarrow U\left(|k_1\rangle + |k_2\rangle\right)|0\rangle = |k_1\rangle|k_1\rangle + |k_2\rangle|k_2\rangle$$

Next shot the phase will be different!

Single-spin coherence: correlation of many measurements!

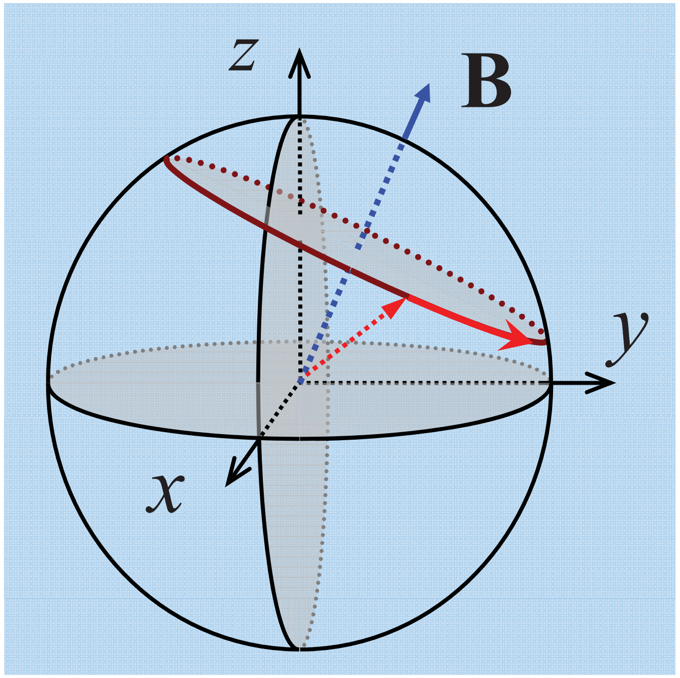
Pictorial Spin Dynamics

Schrödinger equation

$$i\partial_t |\psi\rangle = H|\psi\rangle = -\mathbf{B}\cdot\mathbf{S}|\psi\rangle$$

$$\Updownarrow$$

$$\partial_t \mathbf{S} = \mathbf{B}\times\mathbf{S}$$

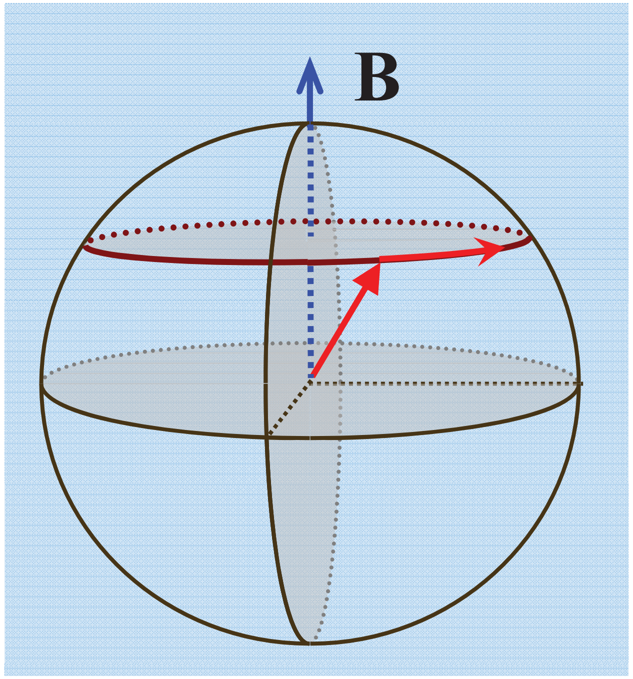


The spin precesses about the magnetic field

Spin Dynamics: Phase angle under a B-field

For B field along the z-axis, the eigen states:

$$H\left|{}^{\uparrow}\!/_{\downarrow}\right\rangle = \pm\frac{B}{2}\left|{}^{\uparrow}\!/_{\downarrow}\right\rangle$$



According to Schrödinger equation

$$\left|\psi(0)\right\rangle = \cos\frac{\theta}{2}e^{-i\varphi/2}\left|\uparrow\right\rangle + \sin\frac{\theta}{2}e^{+i\varphi/2}\left|\downarrow\right\rangle$$

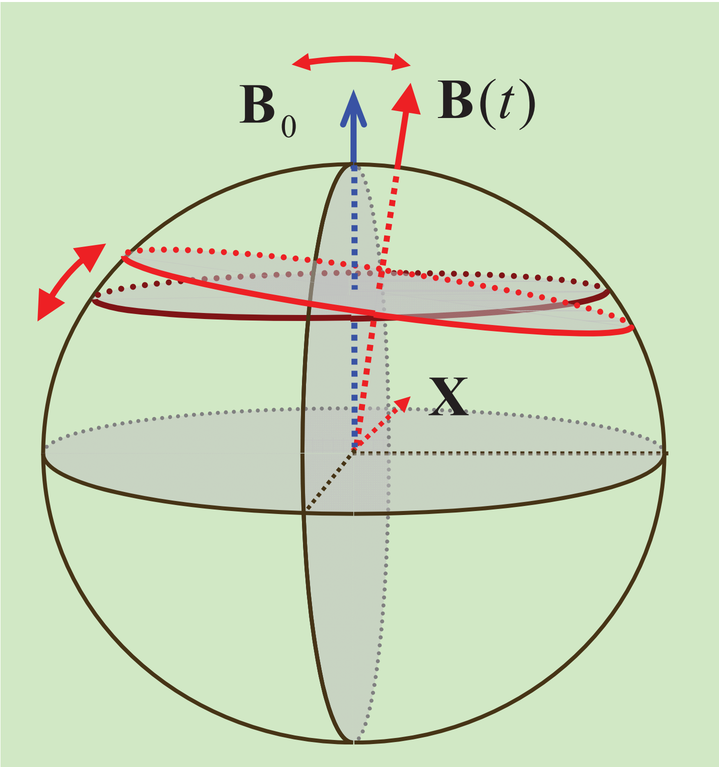
$$\Downarrow$$

$$\left|\psi(t)\right\rangle = \cos\frac{\theta}{2}e^{-i(\varphi+Bt)/2}\left|\uparrow\right\rangle + \sin\frac{\theta}{2}e^{+i(\varphi+Bt)/2}\left|\downarrow\right\rangle = \left|\theta,\varphi+Bt\right\rangle$$

$$\left|\theta,\varphi\right\rangle \Rightarrow \left|\theta,\varphi+Bt\right\rangle$$

Spin decoherence: Random force model

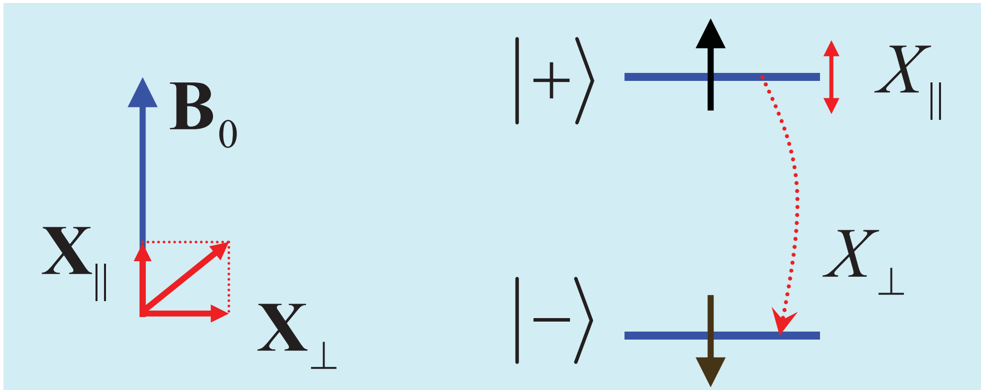
$$\partial_t \mathbf{S} = \mathbf{B}(t) \times \mathbf{S} \quad \text{with } \mathbf{B}(t) = \mathbf{B}_0 + \mathbf{X}(t)$$



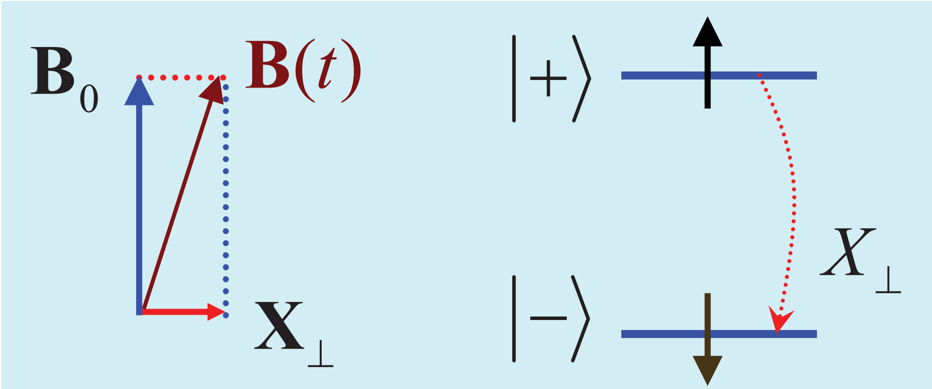
Random field: $\mathbf{X}(t) = \mathbf{X}_{\parallel}(t) + \mathbf{X}_{\perp}(t)$

$\mathbf{X}_{\parallel}(t) \;\rightarrow\;$ energy fluctuation;

$\mathbf{X}_{\perp}(t) \;\rightarrow\;$ spin flip



Spin decoherence: Random force model



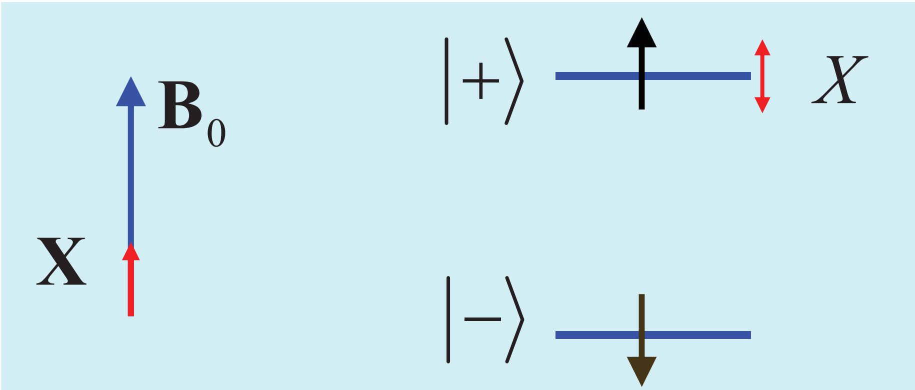
$$\partial_t \mathbf{S} = \mathbf{B}(t) \times \mathbf{S}$$

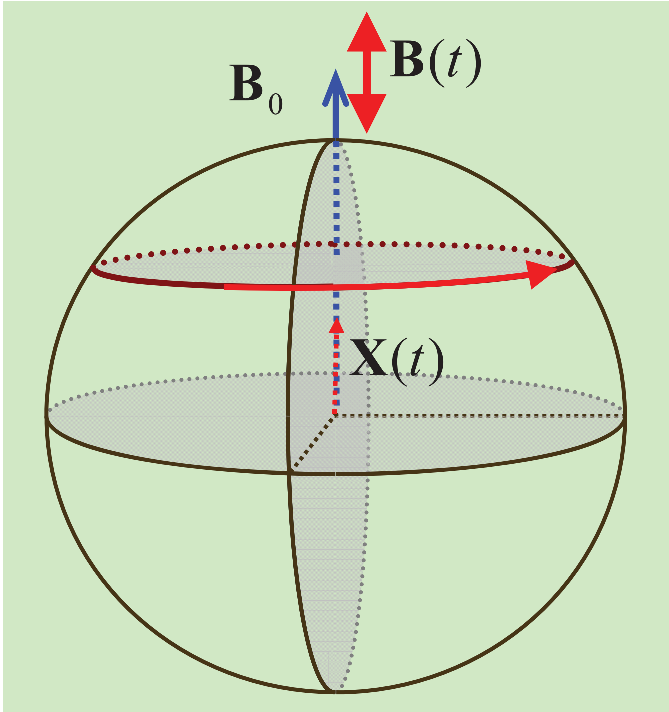
$X_\perp$ causes spin flip or longitudinal relaxation, negligible for $X_\perp << B_0$ (strong field limit), i.e., the spin relaxation time T_1 can be made much longer than spin dephasing time.

When the external field is strong, we can neglect the perpendicular component of the random field.

Random force → random phase

$$\partial_t \mathbf{S} = \mathbf{B}(t)\times\mathbf{S}$$
$$\mathbf{B}(t) = \mathbf{B}_0 + \mathbf{X}(t)$$

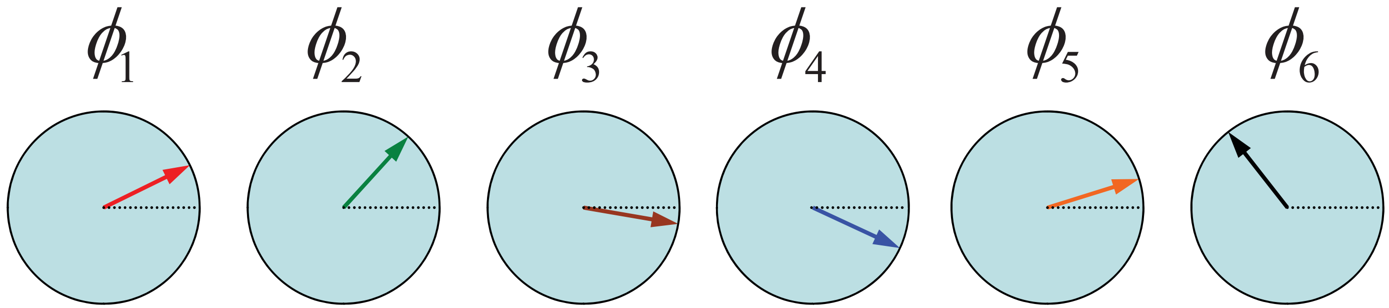




$$\phi_X \equiv \int X(t)dt \quad \Rightarrow \quad |\psi(t)\rangle = |\theta, B_0 t + \phi_X\rangle$$

The uncontrollable environment imposes a random force.
A random phase is accumulated: Decoherence.

Spin decoherence: Random force model



$$\rho = \begin{pmatrix} a^2 & abe^{-iB_0 t}\left\langle e^{-i\phi_X}\right\rangle \\ abe^{+iB_0 t}\left\langle e^{i\phi_X}\right\rangle & b^2 \end{pmatrix}$$

$$\left\langle e^{-i\phi_X}\right\rangle = 1 - i\left\langle \phi_X \right\rangle + \frac{(-i)^2}{2!}\left\langle \phi_X \phi_X \right\rangle + \frac{(-i)^3}{3!}\left\langle \phi_X \phi_X \phi_X \right\rangle + \cdots$$

Spin decoherence: Random force model

Gaussian noise (see Zinn-Justin, QFT & Critical Phenomena, Ch.1):

$$P\left[X(t)\right]=\frac{1}{\sqrt{2\pi\det(A)}}\exp\left(-\frac{1}{2}\sum_{j,k=1}^{N}X\left(t_j\right)A_{jk}X\left(t_k\right)\right)$$

Wick's theorem:

$$\left\langle \phi_X \right\rangle=\left\langle \phi_X\phi_X\phi_X \right\rangle=\left\langle \phi_X\phi_X\phi_X\phi_X\phi_X \right\rangle=\cdots=0$$

$$\left\langle \phi_X\phi_X\phi_X\phi_X \right\rangle=3\cdot 1\cdot\left\langle \phi_X\phi_X \right\rangle\left\langle \phi_X\phi_X \right\rangle$$

$$\left\langle \phi_X\phi_X\phi_X\phi_X\phi_X\phi_X \right\rangle=5\cdot 3\cdot 1\cdot\left\langle \phi_X\phi_X \right\rangle\left\langle \phi_X\phi_X \right\rangle\left\langle \phi_X\phi_X \right\rangle$$

$\cdots$

R. Kubo, in *Stochastic Processes in Chemical Physics* (1969)

Spin decoherence: Random force model

Decoherence determined by the noise correlation

$$\left\langle e^{-i\phi_X} \right\rangle = \sum_{k=0}^{\infty} \frac{(-i)^{2k}}{k!2^k} \left\langle \phi_X \phi_X \right\rangle^k = \exp\left(-\frac{1}{2} \left\langle \phi_X \phi_X \right\rangle \right)$$

$$\text{where } \left\langle \phi_X \phi_X \right\rangle = \int_0^t \int_0^t \left\langle X(t') X(t'') \right\rangle dt'' dt'$$

Spin decoherence: Random force model

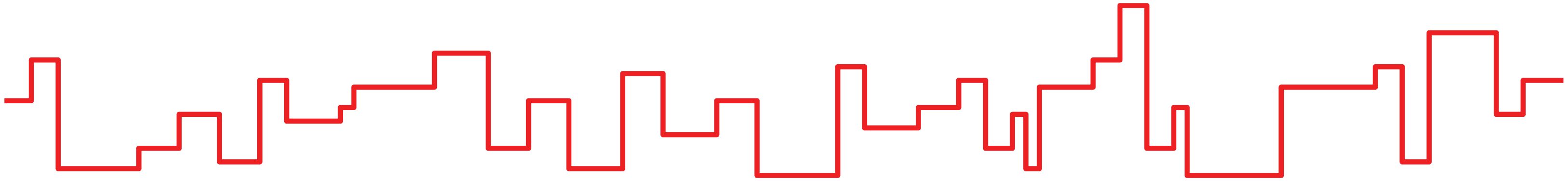
$$\left\langle e^{-i\phi_X}\right\rangle = \exp\left(-\frac{1}{2}\left\langle \phi_X\phi_X\right\rangle\right)$$

In a system with translational symmetry

$$\begin{aligned}
\left\langle \phi_X\phi_X\right\rangle &= 2\int_0^t t'\left\langle X(t')X(0)\right\rangle dt' \\
&\equiv 2\left\langle X(0)X(0)\right\rangle\int_0^t \tau C(t-\tau)\,d\tau \\
&= 2\Gamma^2\int_0^t \tau C(t-\tau)\,d\tau
\end{aligned}$$

$$\boxed{C(\tau)\equiv\frac{\left\langle X(\tau)X(0)\right\rangle}{\left\langle X(0)X(0)\right\rangle}\text{: noise correlation function}}$$

Spin decoherence: Random force model



$$C(\tau) = \exp\left(-|\tau|/\tau_c\right)$$ → Noise correlation time

1. Static fluctuation (inhomogeneous broadening)

$$\tau_c = \infty \;\Rightarrow\; \left\langle \phi_X \phi_X \right\rangle = \Gamma^2 t^2$$

$$\Rightarrow\; \rho_{\uparrow\downarrow} \propto \exp\left(-iB_0 t - \Gamma^2 t^2/2\right)$$

Even if the bath has no dynamics, thermal distribution alone can lead to the static fluctuation and dephasing.

Spin decoherence: Random force model

2. Motional narrowing regime (rapid fluctuation)

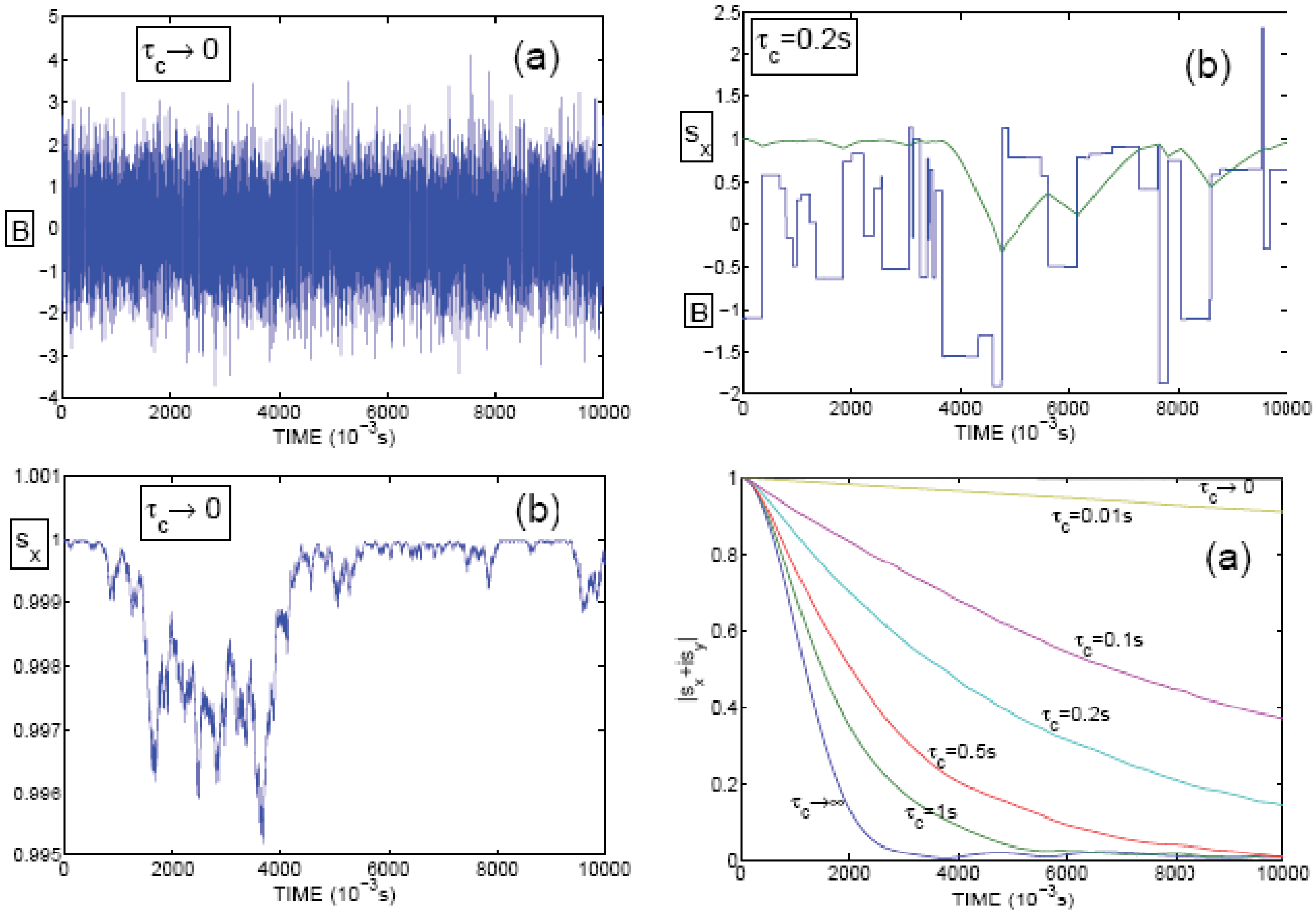
$$\tau_c \to 0 \Rightarrow \left\langle \phi_X \phi_X \right\rangle = 2\Gamma^2 \tau_c t$$

$$\Rightarrow \rho_{\uparrow\downarrow} \propto \exp\left(-iB_0 t - t/T_2\right)$$

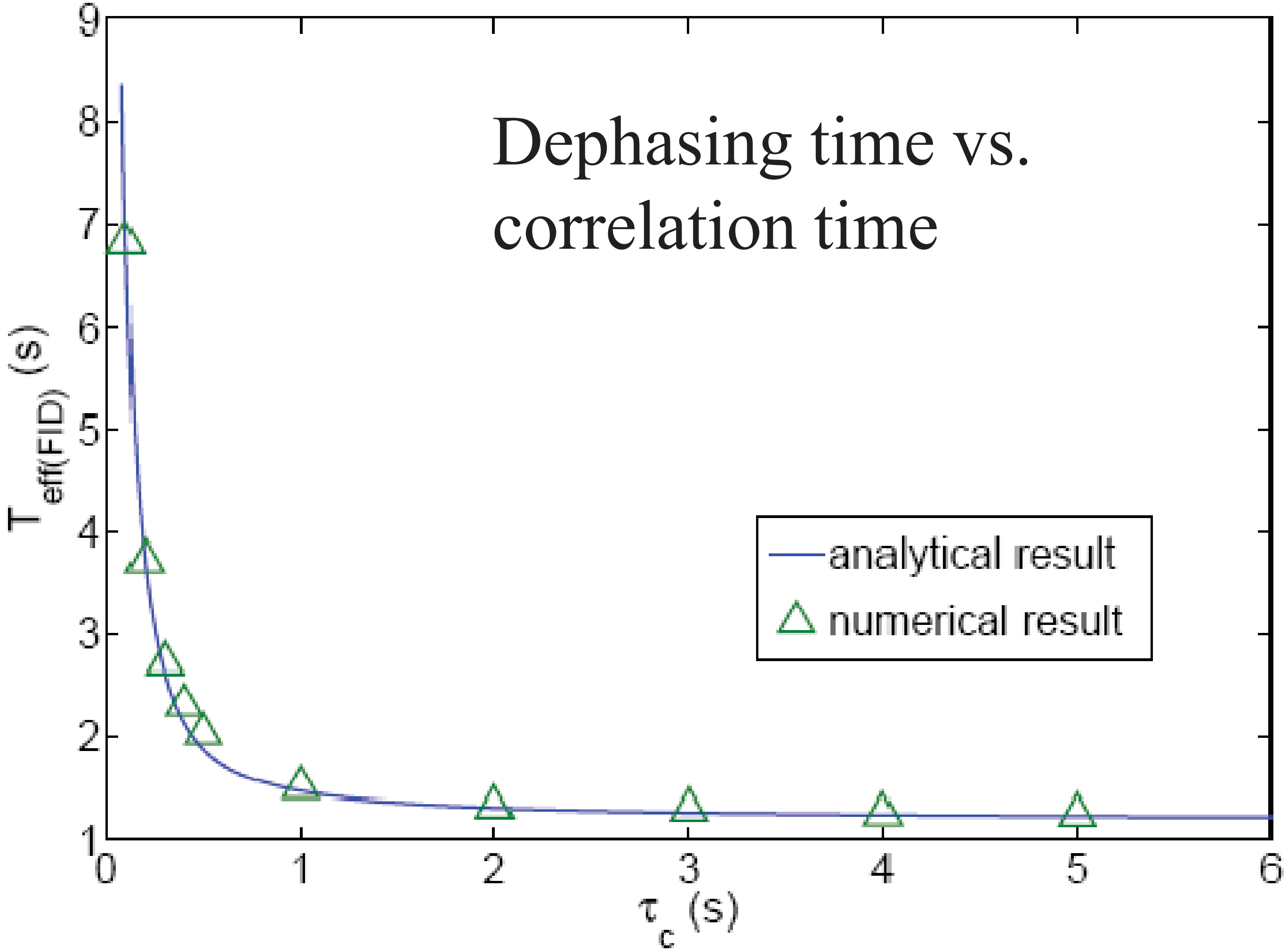
$$\boxed{T_2^{-1} = \Gamma^2 \tau_c}$$

i. It is due to dynamics of the bath
ii. Exponential decay for rapid fluctuation
iii. The faster the fluctuation, the slower the decoherence

Spin decoherence: Random force model



Spin decoherence: Random force model



I-2. Spin decoherence: Quantum Theory

Quantum theory:
Local magnetic field is a Q-number (quantum field)

$$\hat{B}(t)\mathbf{e}_z \times \hat{\mathbf{S}} \qquad \text{or} \quad \exp(-iHt)|S\rangle \otimes |B\rangle$$

Thermal fluctuation: $\rho = \sum P_I |I\rangle\langle I|$ and $\hat{B}_z |I\rangle = B_I |I\rangle$

Classical noise, static inhomogeneous broadening

Quantum fluctuation: $[H, B] \neq 0$

$\hat{B}_z |I\rangle = B_I |I\rangle$ but in general $|I\rangle$ is not eigen state of H

After evolution $e^{-iHt}|I\rangle = \sum C_I(t)|I\rangle$, $\Delta B_z \neq 0$

the local field gets quantum fluctuation fluctuation.

Qubit-bath model for pure dephasing

$$\boxed{H = \Omega S_z + h_z S_z + H_N}$$

Zeeman energy

Overhauser field

Nuclear spin interaction (dipole-dipole, Zeeman energy, etc.)

No qubit spin flip – pure dephasing considered

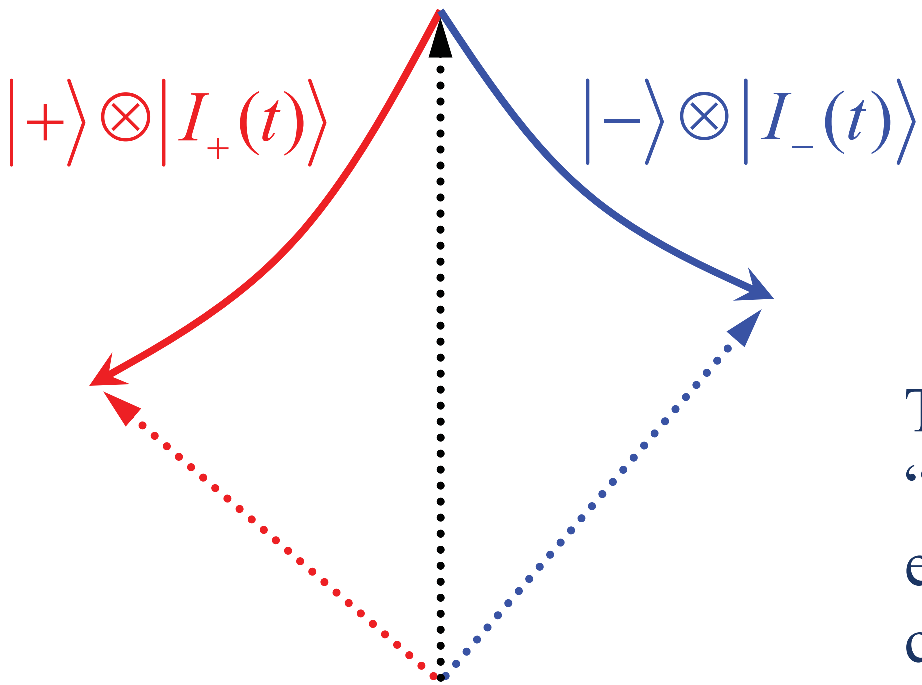
Since $S_Z = \frac{1}{2}\left(|+\rangle\langle+| - |-\rangle\langle-|\right)$

$$\boxed{H = |+\rangle\langle+| \otimes H^{+} + |-\rangle\langle-| \otimes H^{-}}$$

The spin bath Hamiltonian depends on the qubit state

Decoherence by quantum entanglement

$$\left(|+\rangle + |-\rangle\right) \otimes |I\rangle$$



$$|+\rangle \otimes |I_+(t)\rangle + |-\rangle \otimes |I_-(t)\rangle$$

Decoherence: Bifurcated bath evolution → which-way info known → less coherence left

The more the quantum object is "measurement" by the environment, the more it loses its coherence (quantum information).

Decoherence due to nuclear dynamics

The bath state bifurcated depending on the qubit state.

$$\left|I\right\rangle \xrightarrow{H^{\pm}} \left|I^{\pm}(t)\right\rangle \equiv e^{-iH^{\pm}t}\left|I\right\rangle$$

Qubit-bath entanglement established due to the bifurcated evolution

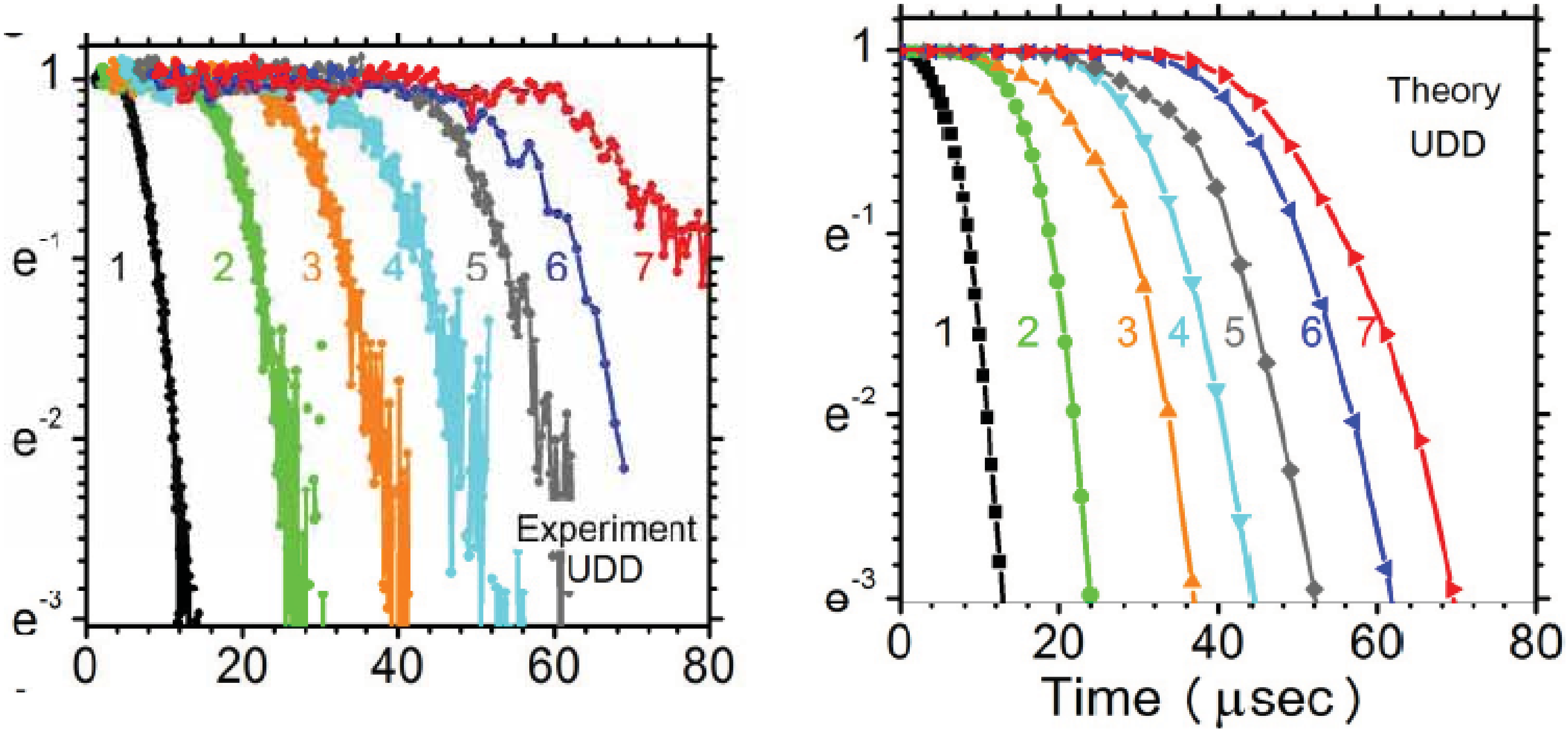
$$\left(C_{-}\left|-\right\rangle + C_{+}\left|+\right\rangle\right)\otimes\left|I\right\rangle \xrightarrow{H} C_{-}\left|-\right\rangle\otimes\left|I^{-}(t)\right\rangle + C_{+}\left|+\right\rangle\otimes\left|I^{+}(t)\right\rangle$$

Coherence depends on the overlap or indistinguishability of the two pathways

$$\rho_{+,-}(t) = C_{+}^{*}C_{-}\left\langle I^{+}(t)\middle|I^{-}(t)\right\rangle$$

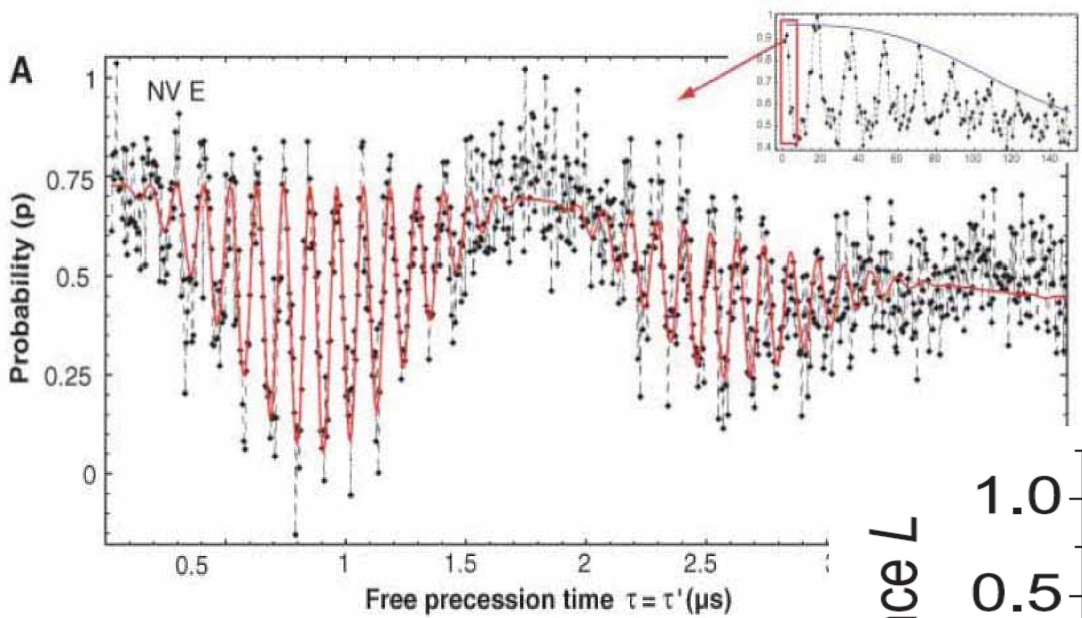
Quantum many-body theory for spin bath dynamics

Experiment vs theory (w/o fitting parameters): Radical spins in irradiated malonbic acid crystals

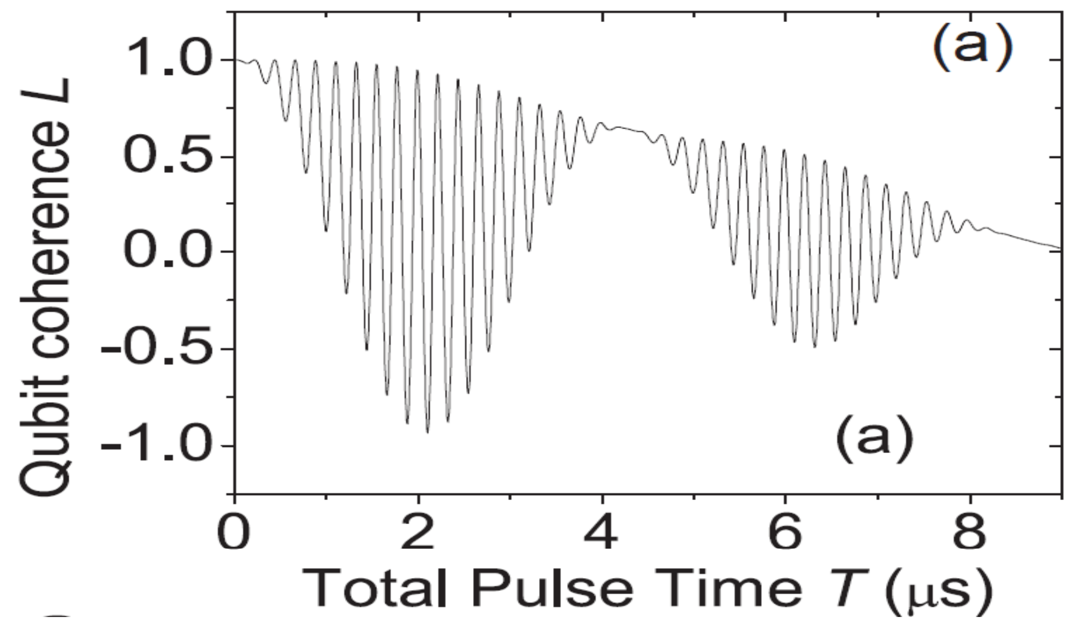


JF Du, X Rong, N Zhao, Y Wang, JH Yang & RBL, Nature **461**, 1265 (2009).

Experiment vs theory (w/o fitting parameters): NV center spin in diamond

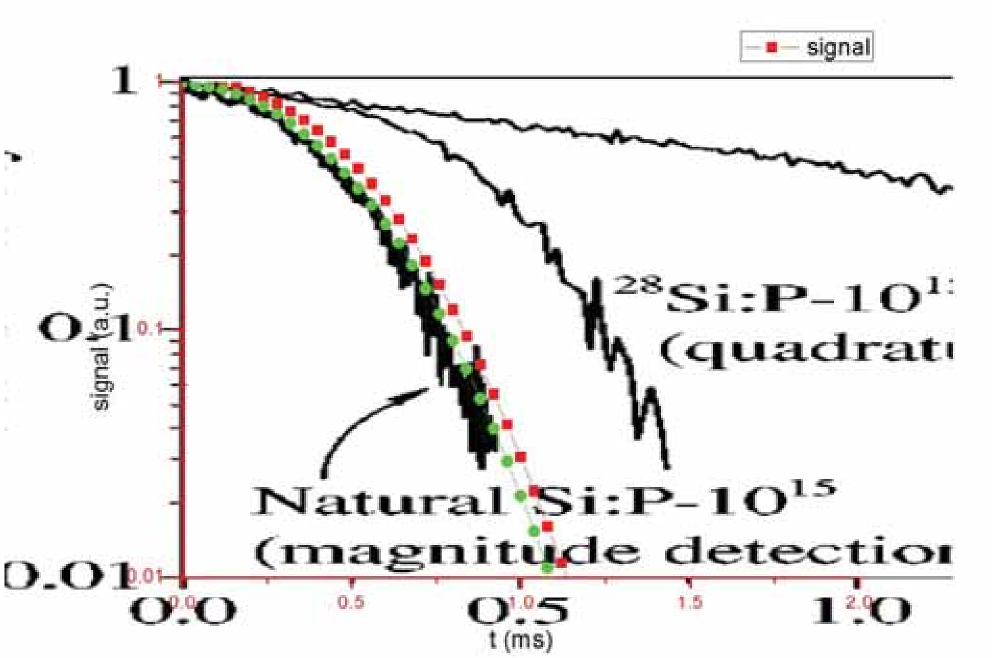


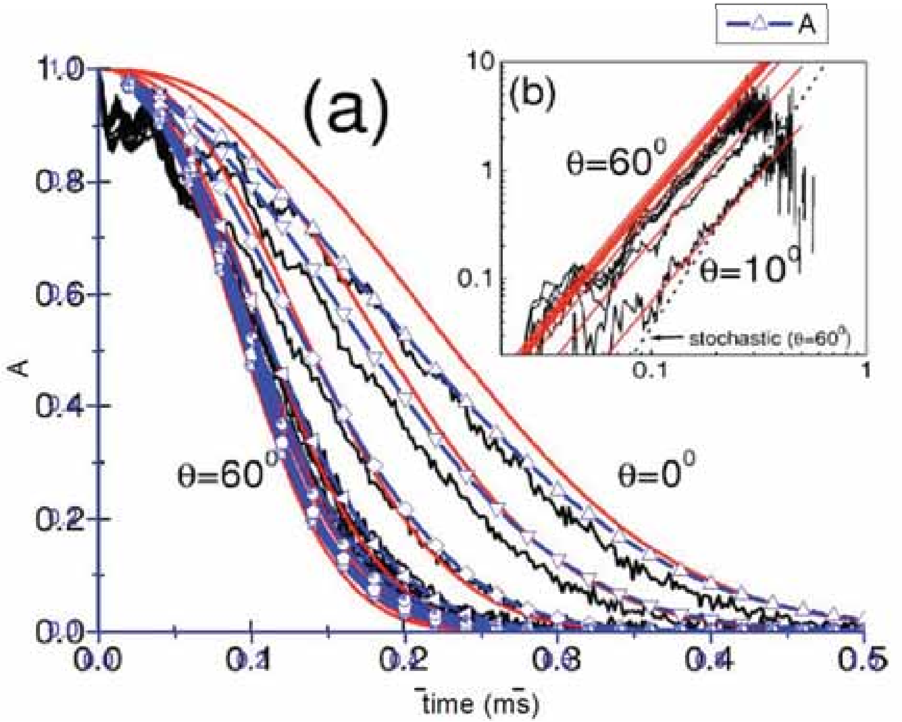
Lukin et al Science 2006



Nan Zhao et al
(unpublished)

Experiment vs theory (w/o fitting parameters): P-donor spins in silicon





Experimental data from S. Lyon et al Phys. Rev. B (2003)
Calculation by Nan Zhao et al (unpublished)

General formalism

Consider the qubit coherence:

$$\rho_{+,-}(t) \propto \langle I | \exp(iH^{+}t) \exp(-iH^{-}t) | I \rangle \equiv U$$

for a general interaction Hamiltonian (w/o two-body interaction only)

$$H^{\pm} = \pm\frac{\Omega}{2} \pm \sum_{n} \omega_n J_n^z + \sum_{m,n} D_{m,n}^{\pm} J_m^z J_n^z + \sum_{m,n} B_{m,n}^{\pm} \left(J_m^+ J_n^- + \text{h.c.} \right)$$

Electron and nuclear spins: Interactions

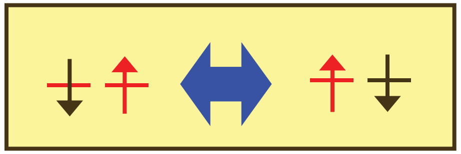
Fermi contact hyperfine interaction (quantum dots, Si:P, e.g.)

$$\hat{H}_{eN} = \sum_n a_n \hat{\mathbf{S}}_e \cdot \hat{\mathbf{J}}_n, \qquad a_n = \frac{\mu_0}{4\pi}\gamma_e \gamma_n \frac{8\pi}{3} |\Psi(\mathbf{R}_n)|^2$$

Dipolar hyperfine interaction (NV centers in diamond, e.g.)

$$\hat{H}_{\mathrm{eN}} = \frac{\mu_0}{4\pi} \sum_n \frac{\gamma_{\mathrm{e}} \gamma_{\mathrm{N}}}{R_n^3} \left(\hat{\mathbf{S}} \cdot \hat{\mathbf{J}}_n - \frac{3 \hat{\mathbf{S}} \cdot \mathbf{R}_n \mathbf{R}_n \cdot \hat{\mathbf{J}}_n}{R_n^2} \right)$$

Nuclear spin dipole-dipole interaction



$$\hat{H}_{NN}^{d} = \sum_{n<m} \frac{\mu_0}{4\pi} \frac{\gamma_n \gamma_m}{R_{n;m}^3} \left(\hat{\mathbf{J}}_n \cdot \hat{\mathbf{J}}_m - \frac{3 \hat{\mathbf{J}}_n \cdot \mathbf{R}_{n;m} \mathbf{R}_{n;m} \cdot \hat{\mathbf{J}}_m}{R_{n;m}^2} \right)$$

W. Yao, RBL & L. J. Sham, PRB 74, 195301 (06)

Electron and nuclear spins: Interactions

Zeeman splitting ($B_0 \sim 10$ T): Electron $H_e = \Omega_e S_e^z$, $\Omega_e \sim 10^{12}\ \mathrm{s}^{-1}$

Nuclear $H_N = \omega_n J_n^z$, $\omega_n \sim 10^9\ \mathrm{s}^{-1}$

Hyperfine interaction: $H_{eN} = a_n \mathbf{S}_e \cdot \mathbf{J}_n$, $a_n \sim 10^6\ \mathrm{s}^{-1}$

Diagonal part $\Rightarrow$ Random local field: $\mathbf{X}(t) = \mathbf{e}_z a_n \left\langle J_n^z \right\rangle$

Off-diagnal $\Rightarrow$ indeirect nuclear interaction: $H_{nm}^{\mathrm{eff}} = \dfrac{a_n a_m}{4\Omega_e} S_e^z J_n^+ J_m^-$

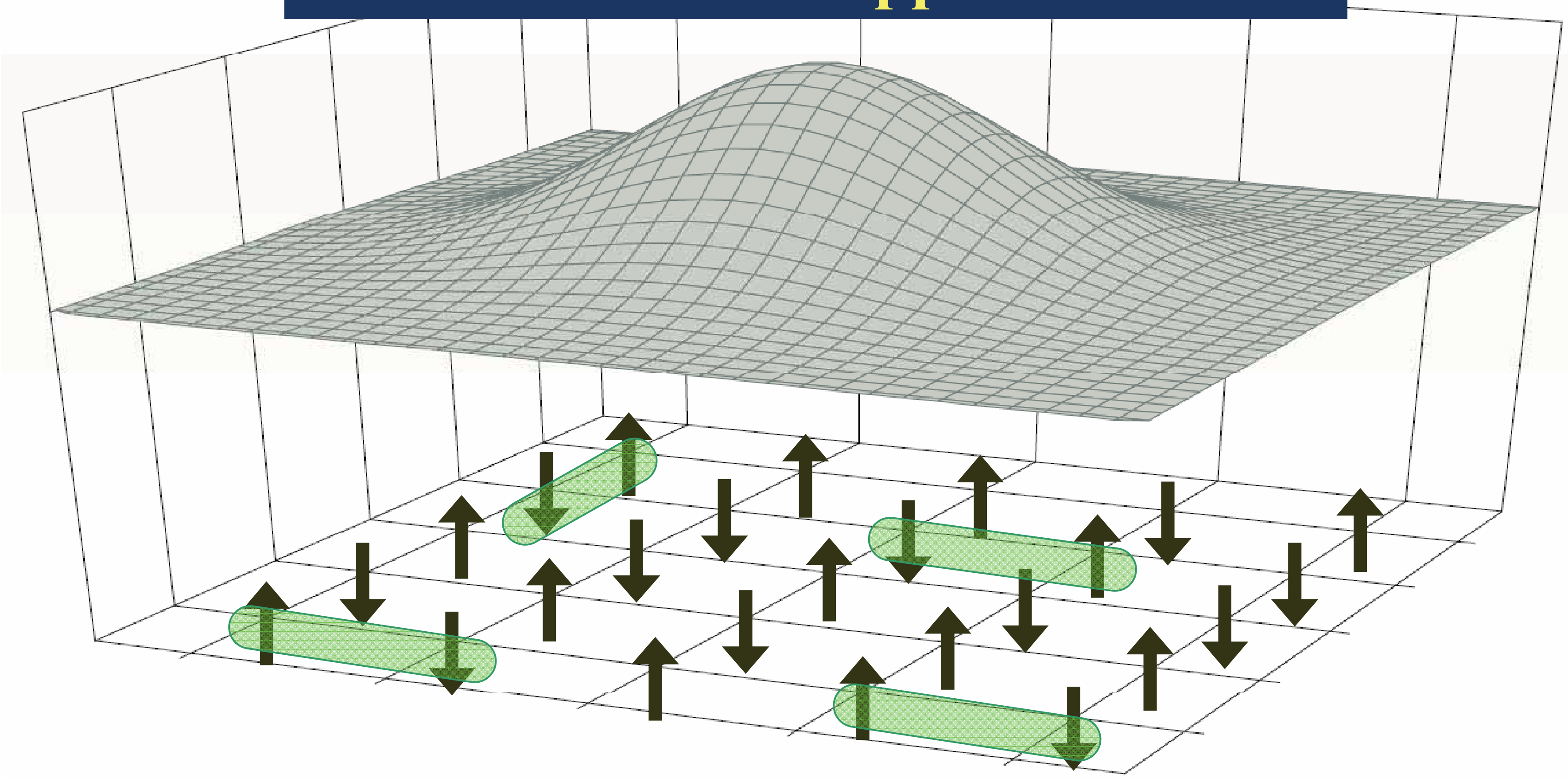
Nuclear spin interaction:

$H_{NN} = D_{nm} J_n^z J_m^z + B_{nm} J_n^+ J_m^-$, $D_{nm} \sim B_{nm} \sim 10^3\ \mathrm{s}^{-1}$

Direct dipolar interaction + Pseudo-dipolar interction,

Pseudo-exchange interaction + Quadrupole interaction + H_{NN}^{eff}

Pair-correlation approximation

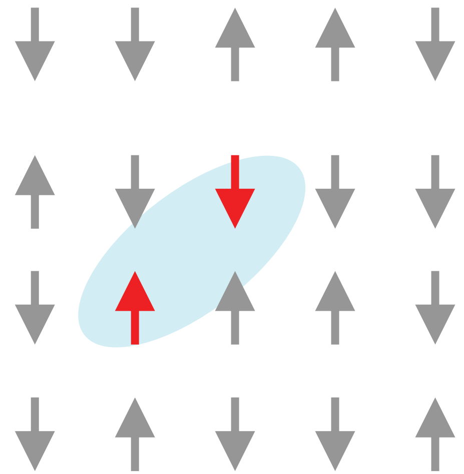


W. Yao, RBL & L. J. Sham, PRB 74, 195301 (06)

1. The dynamics are caused by pairwise flip-flops
2. When the pair-flips are few, there is almost no overlap
3. The pair-flips then can be considered as independent

Contribution by flip-flops of a pair of spins

Consider first the flip-flops of a pair of spins $\{i,j\}$ and neglect the flips of all the others.



The propagation amplitude contributed by the pair is

$$U(i,j)=\langle I|\exp\left(ih^{+}_{\{i,j\}}t\right)\exp\left(-ih^{-}_{\{i,j\}}t\right)|I\rangle$$

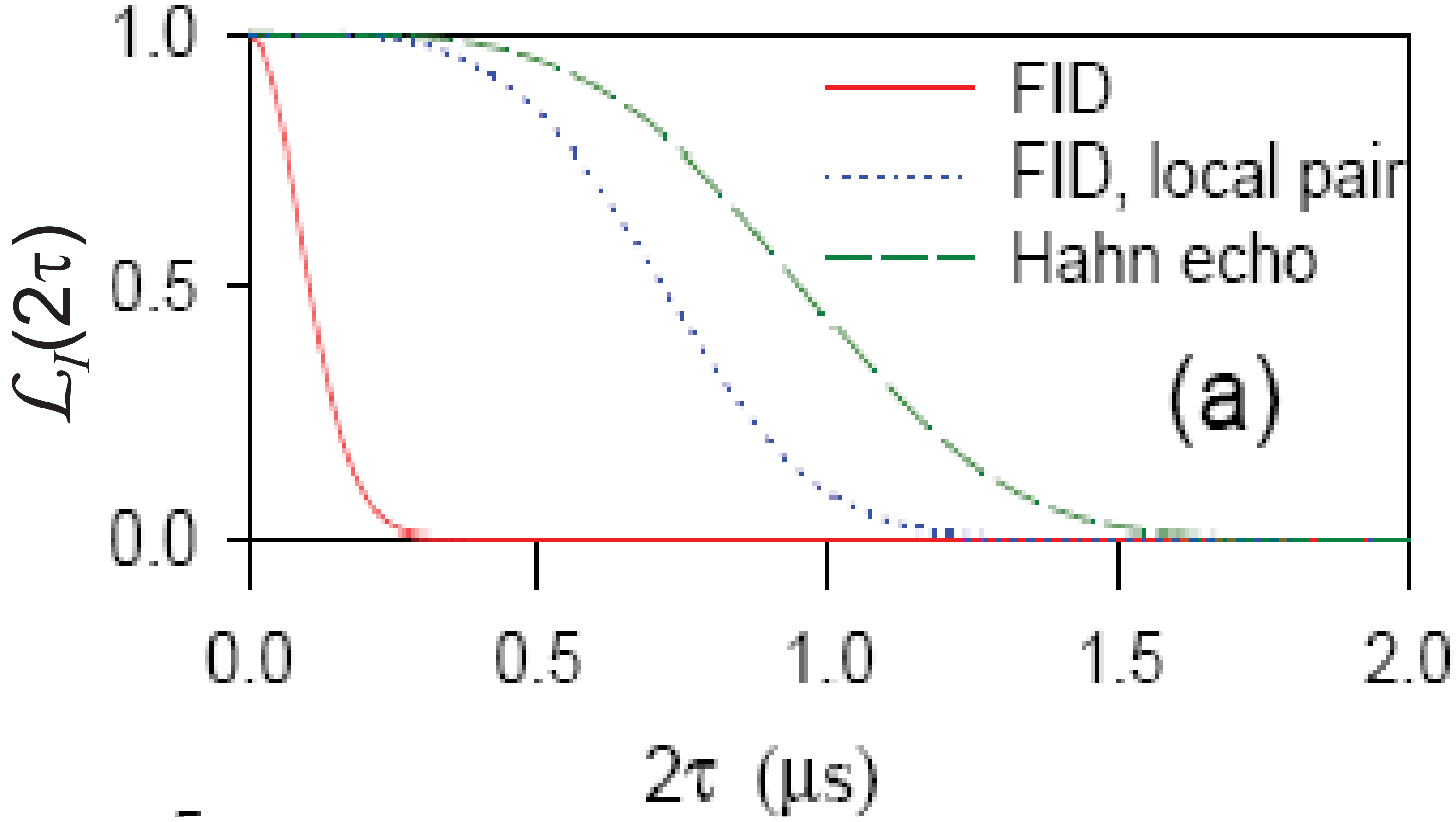
Here the Hamiltonian excludes the flip-flops of other spins

$$h^{\pm}_{\{i,j\}}=\pm\frac{\Omega}{2}\pm\sum_{n}\omega_n J^z_n+\sum_{m,n}D^{\pm}_{m,n}J^z_m J^z_n+B^{\pm}_{i,j}\left(J^{+}_{i}J^{-}_{j}+\text{h.c.}\right)$$

$$U=\langle I|\exp\left(iH^{+}t\right)\exp\left(-iH^{-}t\right)|I\rangle\approx\prod_{\{i,j\}}U(i,j)$$

W. Yao, RBL & L. J. Sham, PRB 74, 195301 (06)

Decoherence due to entanglement with nuclei



W. Yao, R. B. Liu, and L. J. Sham, Phys. Rev. B **74**, 195301 (2006).

Contribution by all the pairs taken independent

The pair correlation approximation is valid when the number of completed pair-flips is much less than the number of bath spins

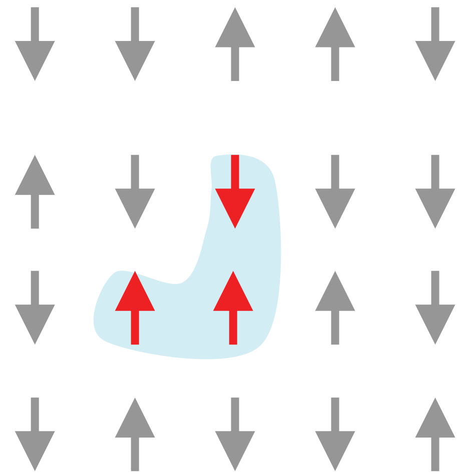
$$N_{\text{flip}} = NB_{m,n}^2 t^2 \ll N$$

$$\Rightarrow \quad t \ll B_{m,n}^{-1}$$

In small baths or for longer time, higher order correlations become relevant.

Contribution by motion of three spins

Consider now flip-flops of 3 spins $\{i,j,k\}$
and neglect the flips of all the others.



The propagation amplitude contributed
by the pair is

$$U(i,j,k)=\langle I|\exp\left(ih^{+}_{\{i,j,k\}}t\right)\exp\left(-ih^{-}_{\{i,j,k\}}t\right)|I\rangle$$

Here the Hamiltonian excludes the flip-flops of other spins

$$h^{\pm}_{\{i,j,k\}}=\pm\frac{\Omega}{2}\pm\sum_{n}\omega_n J_n^z+\sum_{m,n}D^{\pm}_{m,n}J_m^z J_n^z+\sum_{m,n\in\{i,j,k\}}B^{\pm}_{m,n}\left(J_m^+J_n^-+\text{h.c.}\right)$$

which amounts to mean-field treatment of the other spins:

$$h^{\pm}_{\{i,j,k\}}=H^{\pm}\left(\mathbf{J}_i,\mathbf{J}_j,\mathbf{J}_k,\langle\mathbf{J}_{n\neq i,j,k}\rangle\right)$$

Three-spin correlation

To single out the contribution from the authentic collective motion that can not be factorized into pair-correlations:

$$\tilde{U}(i,j,k) = \frac{U(i,j,k)}{U(i,j)U(i,k)U(j,k)}$$

This term is called a 3-spin correlation

Now the propagation amplitude including up to the collective 3-spin correlations can be written as

$$U \approx \prod_{\{i,j\}} U(i,j) \prod_{\{i,j,k\}} \tilde{U}(i,j,k)$$

So on and so forth … …

Cluster correlation expansion

Thus, by definition, the propagation amplitude can be expanded by all the cluster correlations as

$$U = \prod_{C \subset \{1,2,\ldots,N\}} \tilde{U}(C)$$

$$U(C) = \langle I | \exp(i h_C^+ t) \exp(-i h_C^- t) | I \rangle \quad \text{with } h_C^\pm = H^\pm\left(\mathbf{J}_{i \in C}, \langle \mathbf{J}_{n \notin C} \rangle\right)$$

$$\tilde{U}(C) = \frac{U(C)}{\prod_{C' \subset C} \tilde{U}(C')}$$

$\ln\left(\tilde{U}(C)\right)$ is an infinite partial summation of the connected diagrams involving flip-flops of all and only spins in the cluster
(Ref. Linked Cluster Expansion, Many-Particle Physics, Mahan)

*M*th order cluster correlation approximation

Calculating the CCE up to the maximum order amounts to exactly solving the problem which in general is not possible.

In the decoherence problem, we consider a finite-time evolution (or a finite-temperature problem by taking the time to be imaginary), it will often suffice to keep the cluster correlation up to a certain size *M*, which is the *M*th order CCE approximation:

$$U \approx \prod_{|C| \le M} \tilde{U}(C)$$

e.g., pair correlation approximation $\Leftrightarrow M = 2$

Relation to linked cluster expansion (Sham et al)

The propagator can be written as a time-ordered one as

$$U = \langle I | \exp(iH_+ t)\exp(-iH_- t) | I \rangle = \left\langle \mathrm{T}_\tau \exp\left(-i\int_{-t}^{t} H(\tau)\, d\tau\right)\right\rangle$$

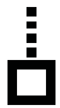
$$\begin{array}{lccccc} H(\tau) = & & H_- & & -H_+ & \\ & & \longrightarrow & & \longrightarrow & \\ \tau = & -t & & 0 & & +t \end{array}$$

By expansion in connected Feynman diagrams (See, e.g., G. D. Mahan, Many-Body Physics):

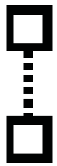
$$U = \exp\left(V_0 + V_1 + V_2 + \cdots\right)$$

$$V_n = (-i)^n \left\langle \mathrm{T}_\tau \int_{-t}^{t}\int_{-t}^{t_1}\cdots\int_{-t}^{t_{n-1}} H(\tau_1) H(\tau_2)\cdots H(\tau_n)\, d\tau_1 d\tau_2 \cdots d\tau_n \right\rangle_{\text{connected}}$$

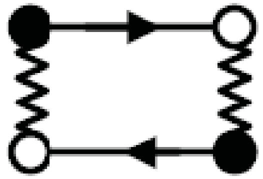
Examples of connected diagrams from Wick's theorem



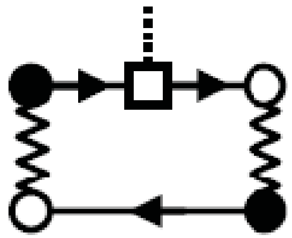
J_i^z



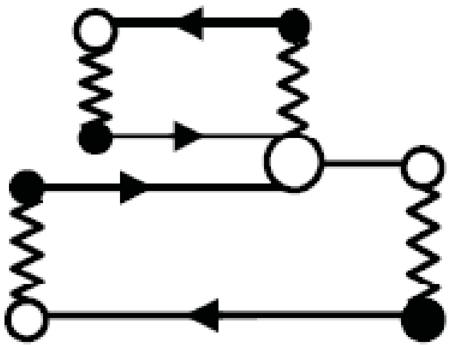
$J_i^z J_j^z$



$J_i^+ J_j^- J_j^+ J_i^-$



$J_i^+ J_j^- J_i^z J_j^+ J_i^-$



$J_i^+ J_j^- J_i^+ J_k^- J_k^+ J_i^- J_j^+ J_i^-$

Rules:

1. Diagonal interaction – dotted lines
2. Off-diagonal interaction – wavy lines
3. Propagation line – solid arrows

Note that unlike fermions or bosons,

$\left[J_i^+, J_j^-\right] = 2J_z$ is not a c-number

$\left[J_i^\pm, J_j^z\right] = \mp J_i^+ \neq 0$

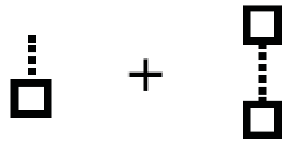
Grouping of connected diagrams according to clusters

The linked cluster expansion can be evaluated order by order.

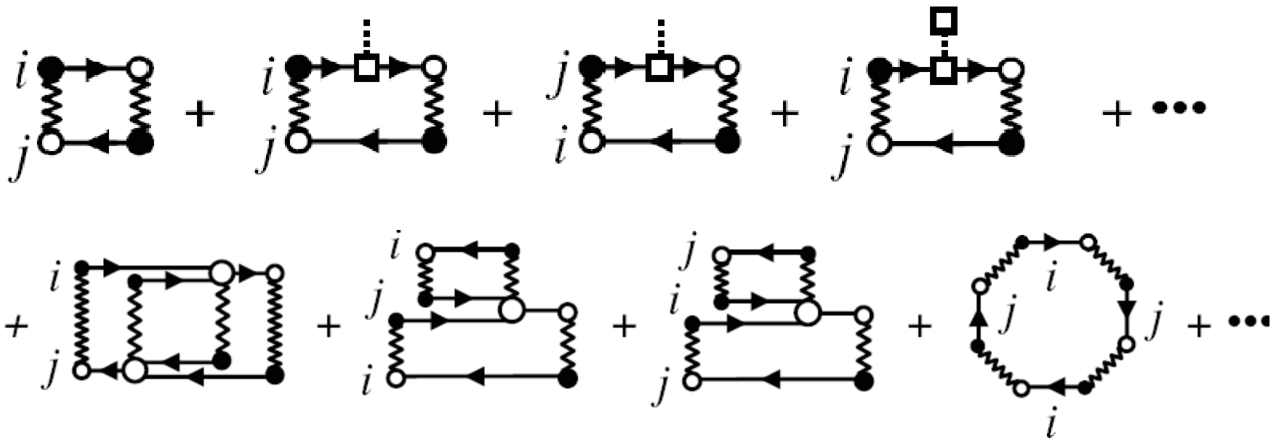
It is very tedious and will soon exhaust all your computing power.

If we sum all the connected diagrams involving the flip-flops of all and only the spins in a certain a set, e.g.

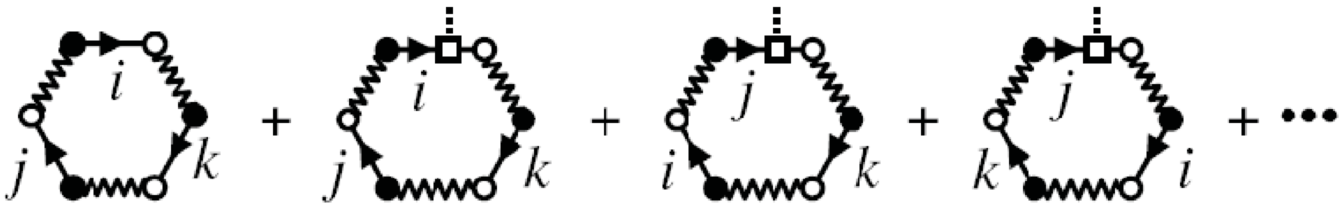
$$\tilde{\pi}(\varnothing) =$$



$$\tilde{\pi}(i,j) =$$



$$\tilde{\pi}(i,j,k) =$$



$$U = \exp\left(\tilde{\pi}(\varnothing) + \sum_{i} \tilde{\pi}(i) + \sum_{i,j} \tilde{\pi}(i,j) + \sum_{i,j,k} \tilde{\pi}(i,j,k) + \cdots \right)$$

$$= \prod_{C \subseteq \{1,2,\ldots,N\}} \exp\left(\tilde{\pi}(C)\right)$$

Comparing to $U = \prod_{C \subset \{1,2,\ldots,N\}} \tilde{U}(C)$

$$\boxed{\therefore \tilde{U}(C) = \exp\left(\tilde{\pi}(C)\right)}$$

CCE versus LCE

A cluster correlation terms is an infinite partial summation of the connected diagrams involving flip-flops of all and only the spins in a cluster.

But the evaluation of the cluster correlation is much simpler – no need of diagrams at all.

Relation to cluster or virial expansion

Following the virial expansion for non-ideal gases in grand canonical ensembles, Das Sarma et al developed a cluster expansion theory:

$$\boxed{W(C)=\left|U(C)\right|=\left|\langle I|\exp\left(ih_C^{+}t\right)\exp\left(-ih_C^{-}t\right)|I\rangle\right|}$$

$$\tilde{W}(i)=W(i)=1 \text{ (for pair-interaction)}$$

$$W(i,j)=\tilde{W}(i,j)+\tilde{W}(i)\tilde{W}(j)$$

$$W(i,j,k)=\tilde{W}(i,j,k)+\tilde{W}(i)\tilde{W}(j)\tilde{W}(k)$$
$$+\tilde{W}(i,j)\tilde{W}(k)+\tilde{W}(i,k)\tilde{W}(j)+\tilde{W}(j,k)\tilde{W}(i)$$

So on and so forth

$$
\begin{aligned}
W(1,2,\ldots,N) = {} & \tilde{W}(1)\tilde{W}(2)\cdots\tilde{W}(N) \\
& +\tilde{W}(1)\tilde{W}(2)\cdots\tilde{W}(N-2)\tilde{W}(N-1,N)+\cdots \\
& +\tilde{W}(1,2)\tilde{W}(3,4)\cdots\tilde{W}(N-1,N)+\cdots \\
& +\cdots \\
& +\tilde{W}(1,2,\ldots,N)
\end{aligned}
$$

A M-th order approximation is to keep the terms containing up to M spins in a cluster, e.g., the 2nd order approximation is

$$
\begin{aligned}
W(1,2,\ldots,N) \approx {} & \tilde{W}(1)\tilde{W}(2)\cdots\tilde{W}(N) \\
& +\tilde{W}(1)\tilde{W}(2)\cdots\tilde{W}(N-2)\tilde{W}(N-1,N)+\cdots \\
& +\tilde{W}(1,2)\tilde{W}(3,4)\cdots\tilde{W}(N-1,N)+\cdots
\end{aligned}
$$

Problem with the cluster expansion

For a non-ideal gas in a grand canonical ensemble with translational symmetry, the summation of the virial expansion can be made compact (See, e.g., T. D. Lee, Statistical Physics - 统计物理):

$$W(1,2,\ldots)=\exp\left(\tilde{W}(1,2)+\tilde{W}(1,3)\cdots+\tilde{W}(1,2,3)+\cdots\right)$$

One obtains the same result as the CCE.

It is easy to calculate $\tilde{W}(1,2),\cdots$ up to the Mth order.

But for a finite system, we don’t have such a compact result, and the summation is tedious, even up to the 2nd order approximation (the pair-correlation approximation).

Consider a 4-spin system up to the 2nd order terms:

With the 1st order terms $\tilde{W}(i)=1,$

$$W(1,2,3,N)\approx 1+\sum_{i,j}\tilde{W}(i,j)$$

$$+\tilde{W}(1,2)\tilde{W}(3,4)+\tilde{W}(1,3)\tilde{W}(2,4)+\tilde{W}(1,4)\tilde{W}(2,3)$$

$$=\prod_{i,j}\left[1+\tilde{W}(i,j)\right]$$

$$-\tilde{W}(1,2)\tilde{W}(2,3)-\tilde{W}(1,3)\tilde{W}(3,4)-\tilde{W}(1,4)\tilde{W}(2,4)\cdots$$

Overlapping terms (which belong to higher-order correlations) are over-counted in the factorized form as in the 1st line.

Validity of the Cluster Expansion

But for a large system in which the decoherence is completed already when all the cluster correlations are still very small:

$$W(1,2,\ldots,N)=\exp\left(\tilde{W}(1,2)+\tilde{W}(2,3)+\cdots+O\left(\tilde{W}^2\right)\right)$$

The CCE and the CE yield the same result.

The textbook CE applies to large systems (grand canonical ensemble). CCE applies to both large and small systems (relevant in modern nanotechnologies).

Systems for numerical check

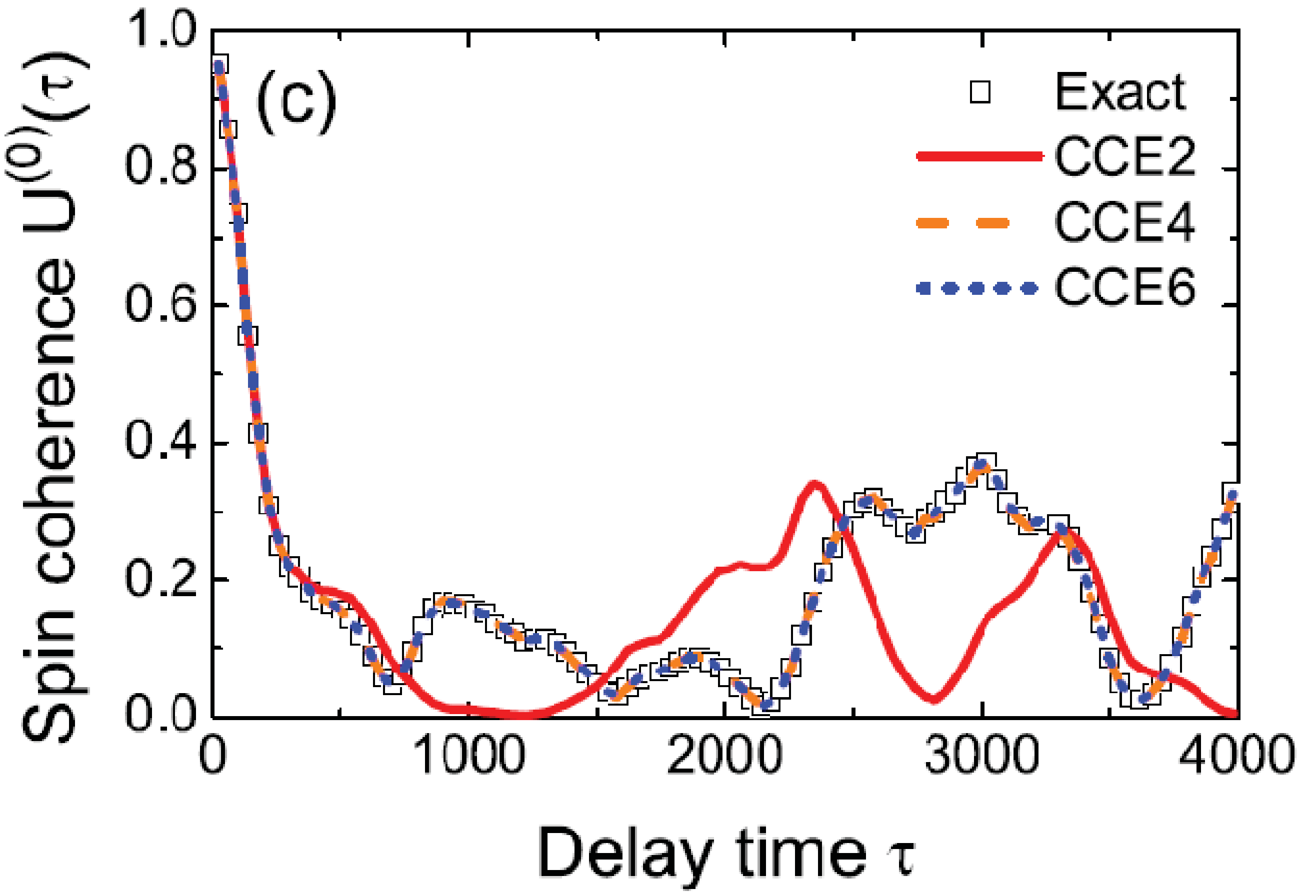
1D XY model which has an exact solution

$$H^{\pm} = \lambda_i^{\pm}\left(X_i X_{i+1} + rY_i Y_{i+1}\right) + \omega_i^{\pm} Z_i$$

$\lambda_i^{\pm}$, $\omega_i^{\pm}$ are sin-functions of i for large bath

and random for small bath

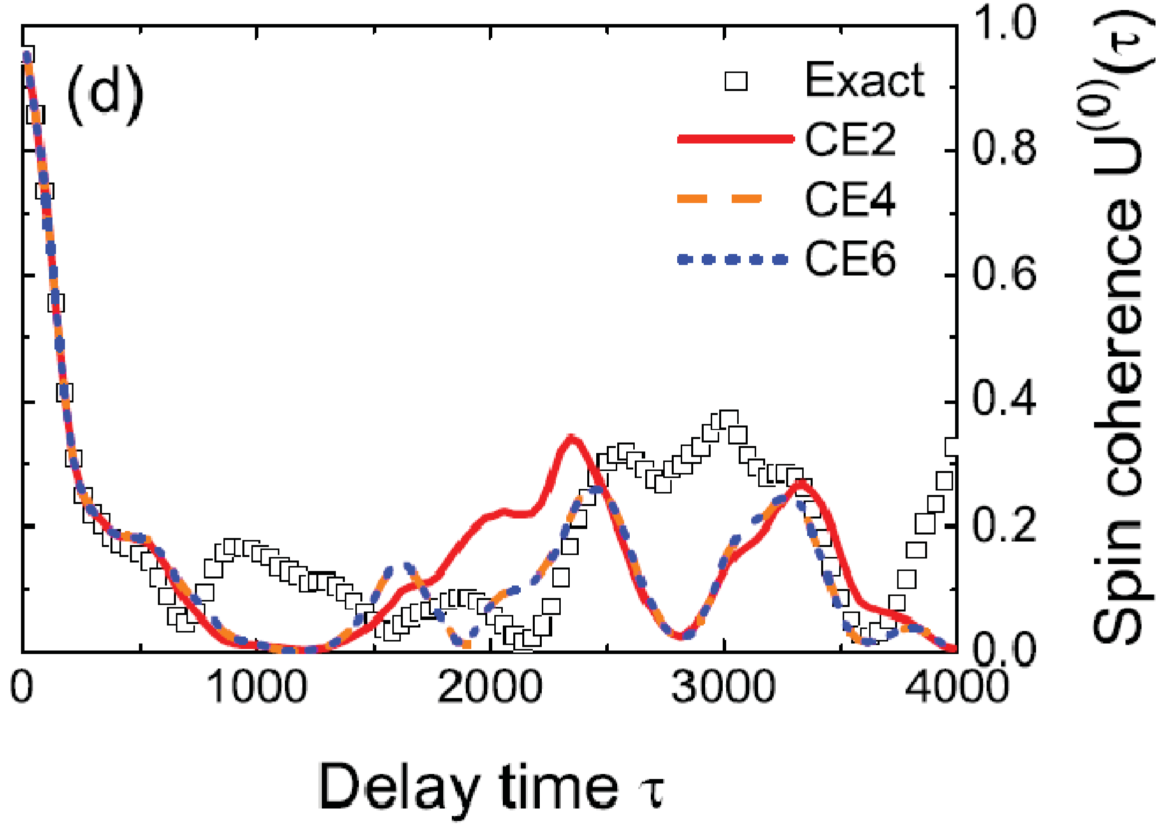
CCE gives correct multi-spin coherence



This small bath (N=100) has 4 spins in near resonance. The 4-spin coherence oscillation is reproduced by CCE-4 or above.

W. Yang & RBL, Phys. Rev. B **78**, 085315 (08).

CE misses the multi-spin coherence



But the CE converges to the wrong results and cannot produces correctly the multi-spin coherence oscillation.

W. Yang & RBL, Phys. Rev. B **78**, 085315 (08).

Summary of the quantum many-body theory for qubit decoherence

1. CCE: A user-friendly quantum many-body theory for spin bath dynamics, capable of reproducing experimental results accurately with relatively small computing resources;
2. The textbook Cluster Expansion (not discussed) applies to large systems (grand canonical ensemble). CCE applies to both large and small systems (relevant in modern nanotechnologies).

Issues to be solved:

Decoherence and relaxation (T1 problem) at low- or zero field. The P-representation theory (L. L. Dobrovitski et al) and the ring-diagram expansion (L. Cywinski et al) are good progresses, but do not apply to the case of spins under dynamical decoupling control.

Homework

1. Generalize CCE to finite interacting fermion/boson systems (e.g., aharmonic phonon dynamics in carbon nanotube)

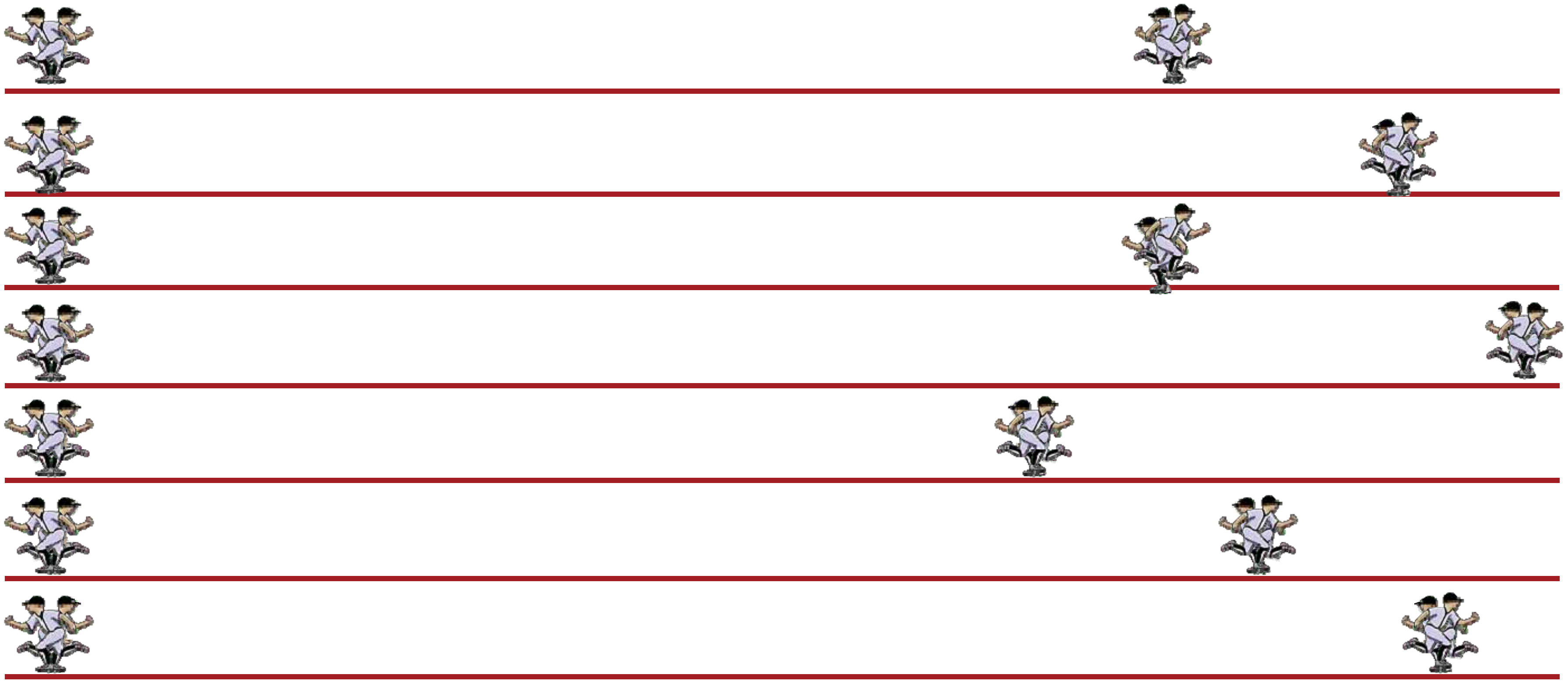
2. Apply CCE to calculating the partition function of a finite system at finite temperature (imaginary time problem)

$$\left\langle \exp\left(+iH^{+}t\right)\exp\left(-iH^{-}t\right)\right\rangle \Rightarrow \left\langle \exp\left(-H\beta\right)\right\rangle$$

II-1. Decoherence control:
Classical picture

<u>**Reading materials:**</u>
J. R. Klauder & P. W. Anderson, Phys. Rev. **125**, 912 (1962).

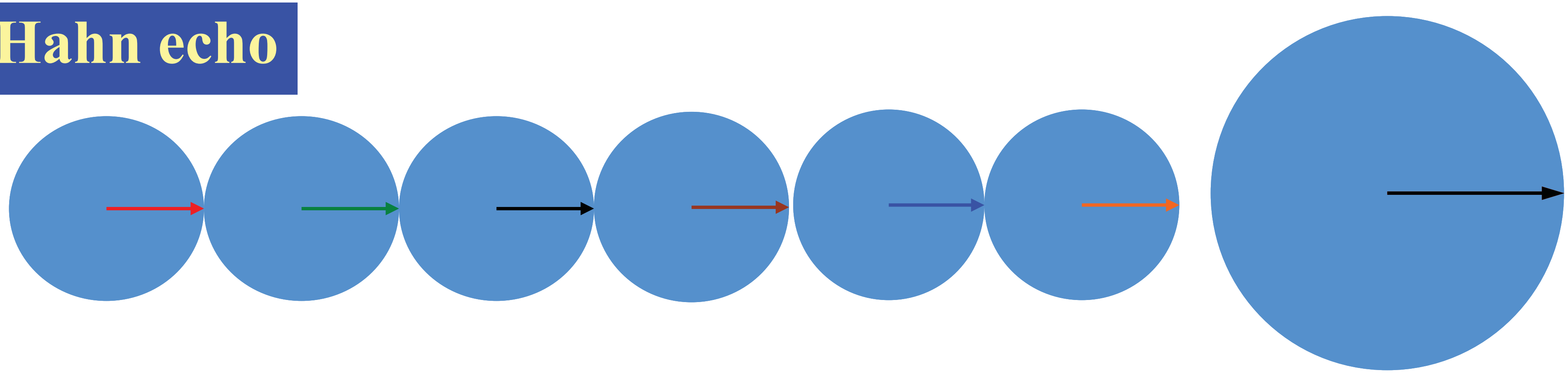
Coherence, lost in translation



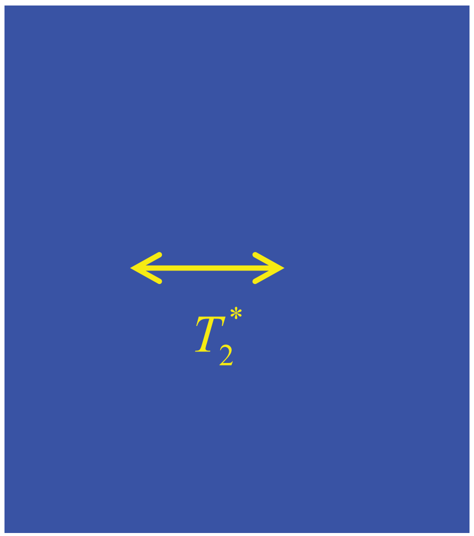
It works when the runners' speeds are kept constant.

$$\boxed{\text{Eq. (1):} \qquad \tau - (t - \tau) = 0}$$

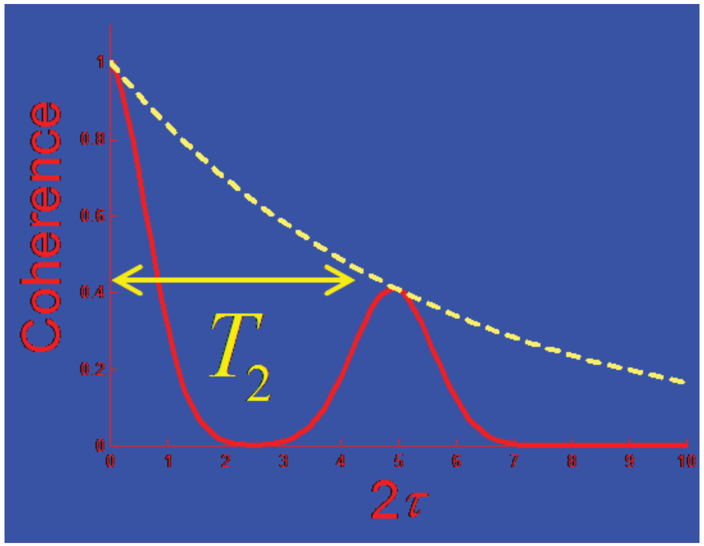
Hahn echo



$$\left(a\left|\downarrow\right\rangle+e^{-iX_J t}b\left|\uparrow\right\rangle\right)\Rightarrow\left(a\left|\uparrow\right\rangle+e^{-iX_J\tau}b\left|\downarrow\right\rangle\right)\Rightarrow\left(a\left|\uparrow\right\rangle e^{-iX_J(t-\tau)}+e^{-iX_J\tau}b\left|\downarrow\right\rangle\right)$$



Works perfectly for static fluctuations.



Dynamical Fluctuations

Spin Echo: Random force model

Spin flip

State before flip: $a|\uparrow\rangle + b|\downarrow\rangle$ State after flip: $a|\downarrow\rangle + b|\uparrow\rangle$

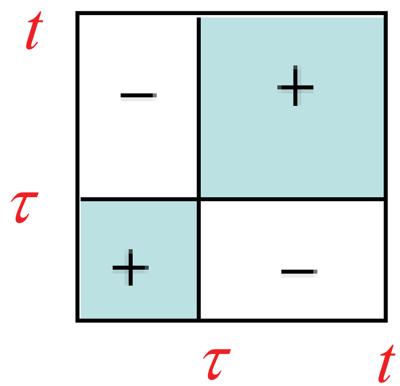
τ t

$$\langle \phi_X \phi_X \rangle = \left(\int_0^\tau \int_0^\tau dt'' dt' - 2\int_\tau^t \int_0^\tau dt'' dt' + \int_\tau^t \int_\tau^t dt'' dt' \right) \langle X(t') X(t'') \rangle$$

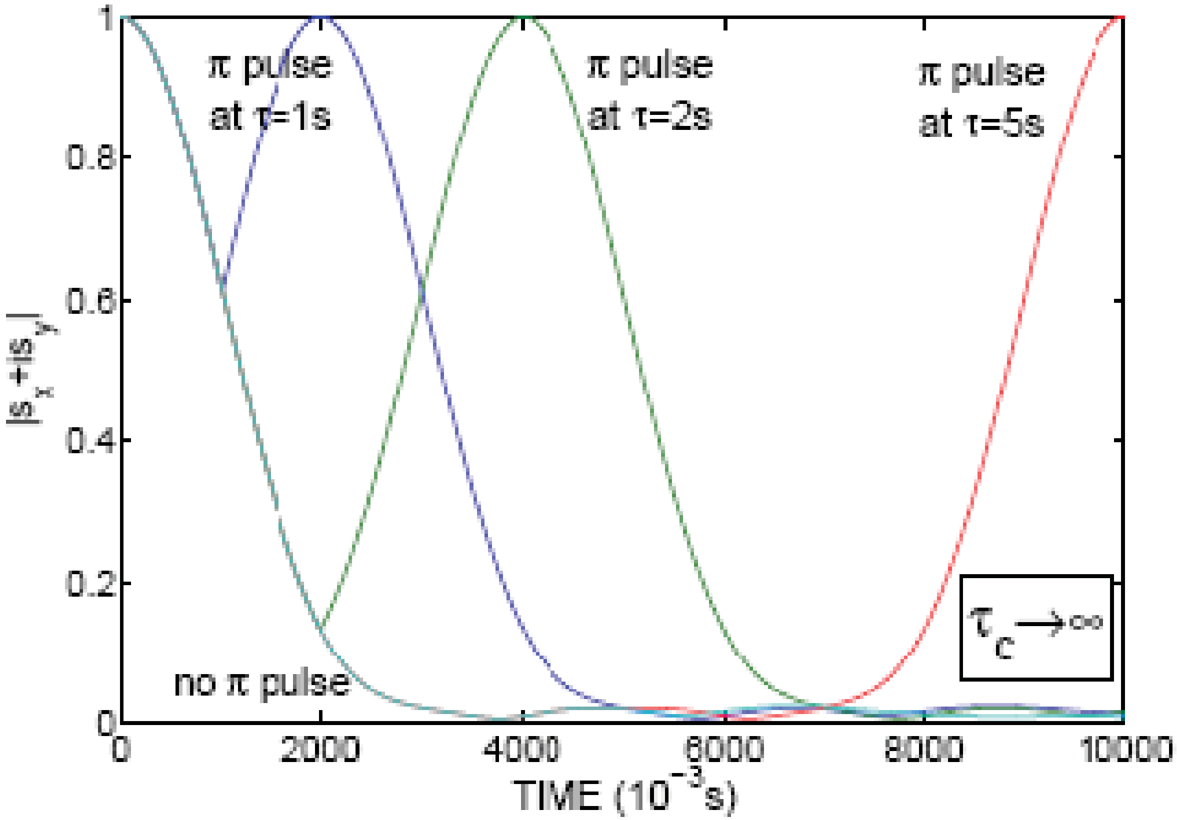
$$= \Gamma^2 \left(\int_0^\tau \int_0^\tau dt'' dt' - 2\int_\tau^t \int_0^\tau dt'' dt' + \int_\tau^t \int_\tau^t dt'' dt' \right) C(t' - t'')$$

$$= \begin{cases} \Gamma^2 (t - 2\tau)^2, & (\tau_c \to \infty) \\ 2\Gamma^2 \tau_c t, & (\tau_c \to 0) \end{cases}$$

for $C(t' - t'') = \exp\left(-|t' - t''|/\tau_c\right)$

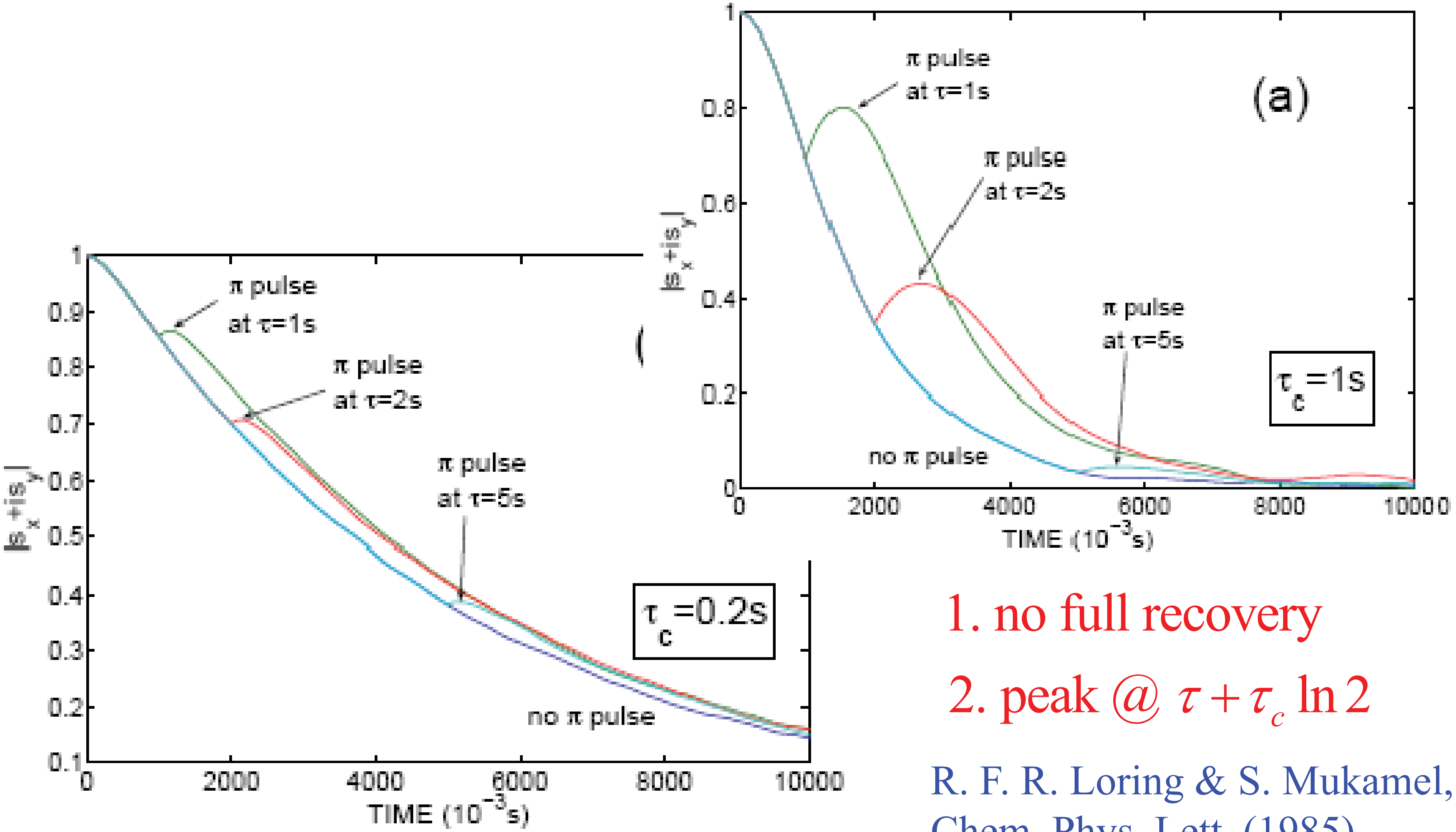


Spin Echo: Static random force



Dephasing due to inhomogeneous broadening can be fully eliminated by spin echo,

Spin Echo: Dynamical Random force

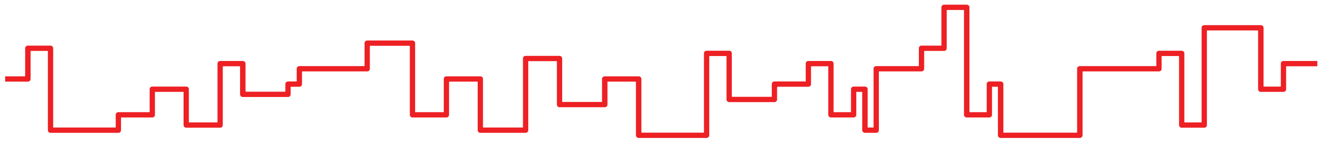


1. no full recovery

2. peak @ $\tau + \tau_c \ln 2$

R. F. R. Loring & S. Mukamel, Chem. Phys. Lett. (1985)

Summary of the semiclassical picture



$$B(t)\mathbf{e}_z \times \hat{\mathbf{S}} \xrightarrow{\text{Average}} \left\langle \hat{S}_\perp \right\rangle \propto \exp\left(-\frac{1}{2} \int \left\langle B(t_1) B(t_2) \right\rangle dt_1 dt_2 \right)$$

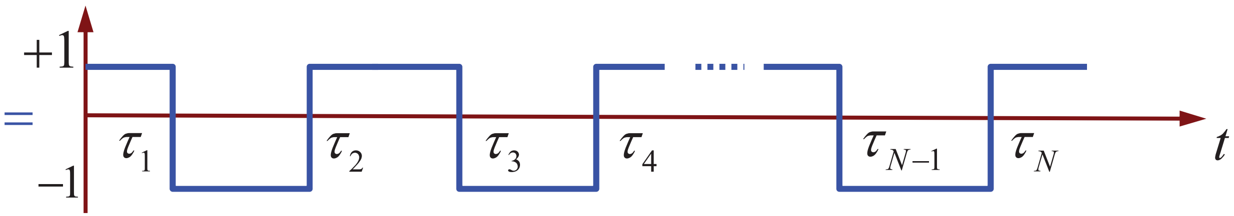
Decoherence control by spin-flips (rooted in spin echo)

$$F(t) B(t)\mathbf{e}_z \times \hat{\mathbf{S}} \xrightarrow{\text{Average}} \left\langle \hat{S}_\perp \right\rangle \propto \exp\left(-\frac{1}{2} \int \left\langle B(t_1) B(t_2) \right\rangle F(t_1) F(t_2) dt_1 dt_2 \right)$$

$$= \exp\left(-\int_0^\infty \frac{S(\omega)}{\omega^2} \left| F(\omega, t) \right|^2 \frac{d\omega}{\pi} \right)$$

e.g., periodic Carr-Purcell-Meiboom-Gill (CPMG) sequence:

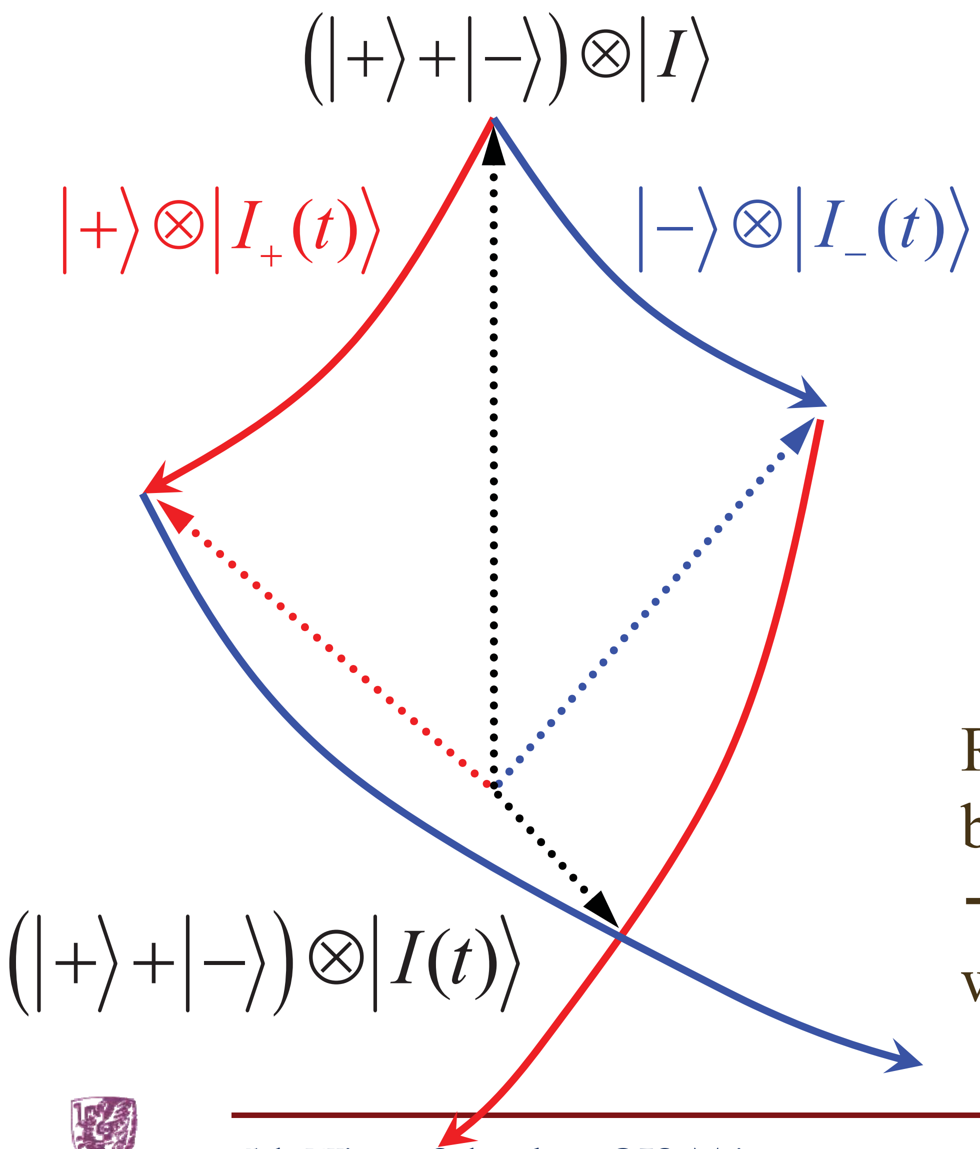
$F(t) =$



with $\tau_n = T \frac{2n-1}{2N}$

II-2. Quantum picture: How to control decoherence?

Recoherence by disentanglement (quantum erasure)

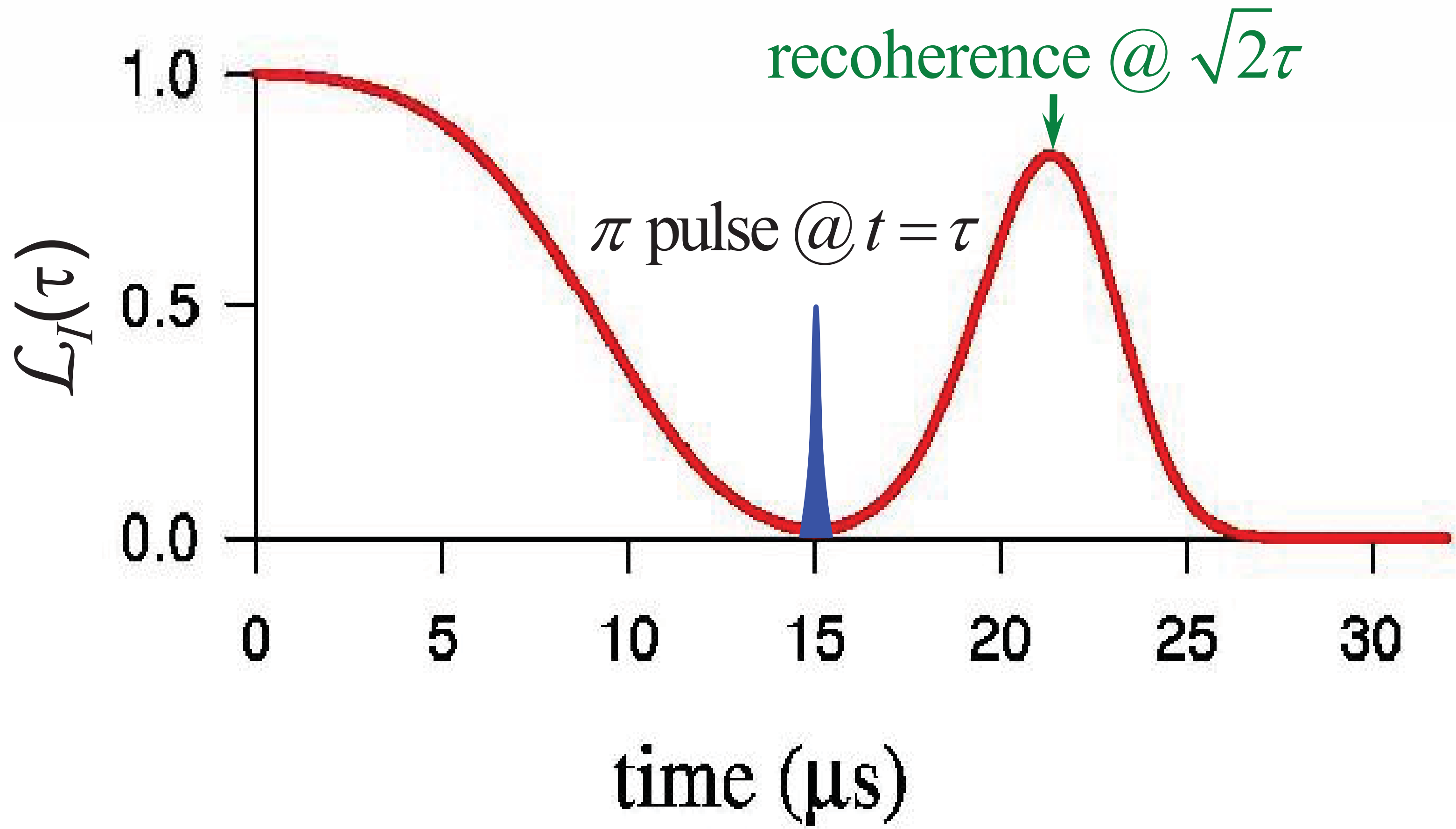


Decoherence: Bifurcated bath evolution → which-way info known → less coherence left

Mesoscopic systems: The bath and the spin is a closed system. The which-way info goes nowhere but stored in the bath

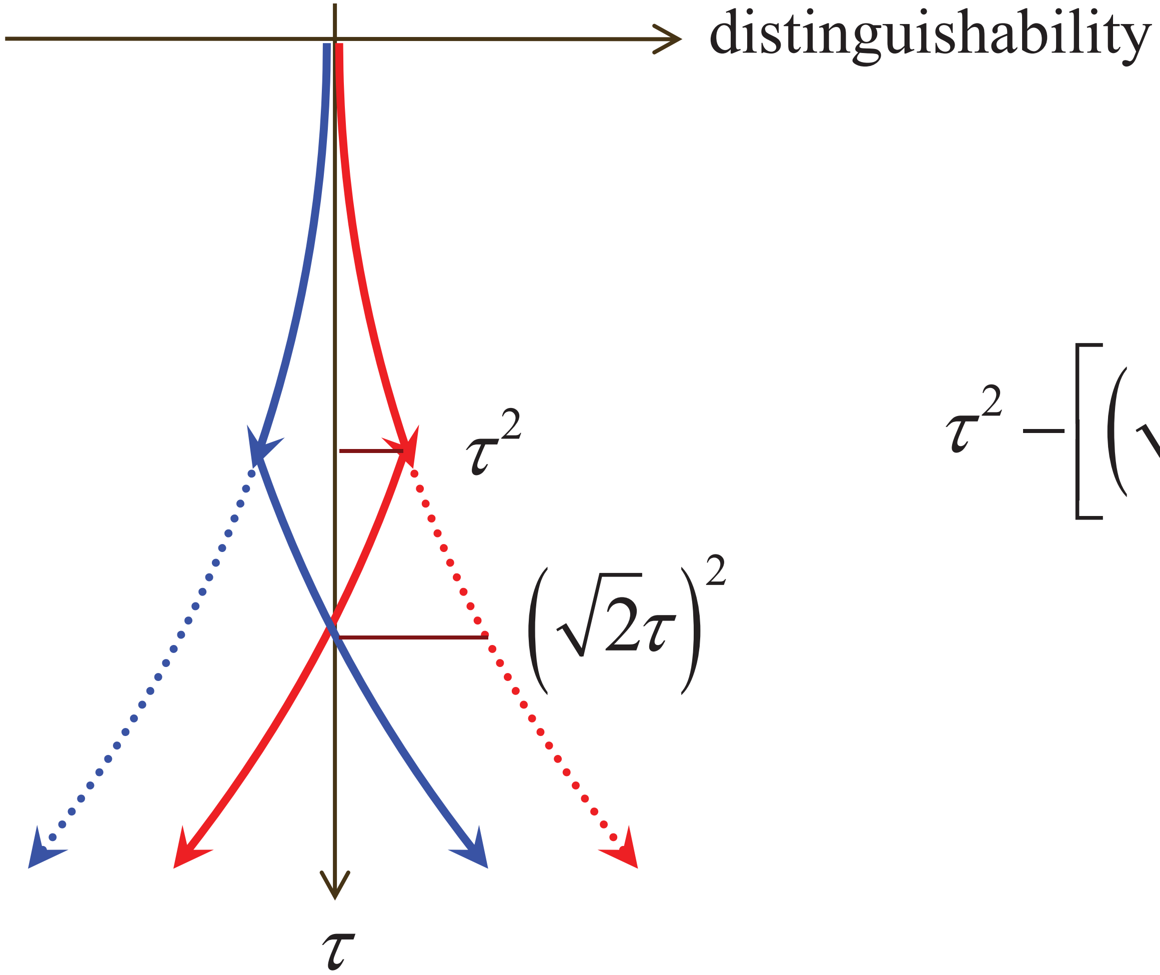
Recoherence: e-spin flipped → bath pathways exchange directions → pathway intercross → which-way info erased → recoherence

Resurrecting from ashes: When disentangled



W. Yao, RBL, and L. J. Sham, Phys. Rev. Lett. **98**, 077602 (07).

Understanding the magic sqrt(2) recovery



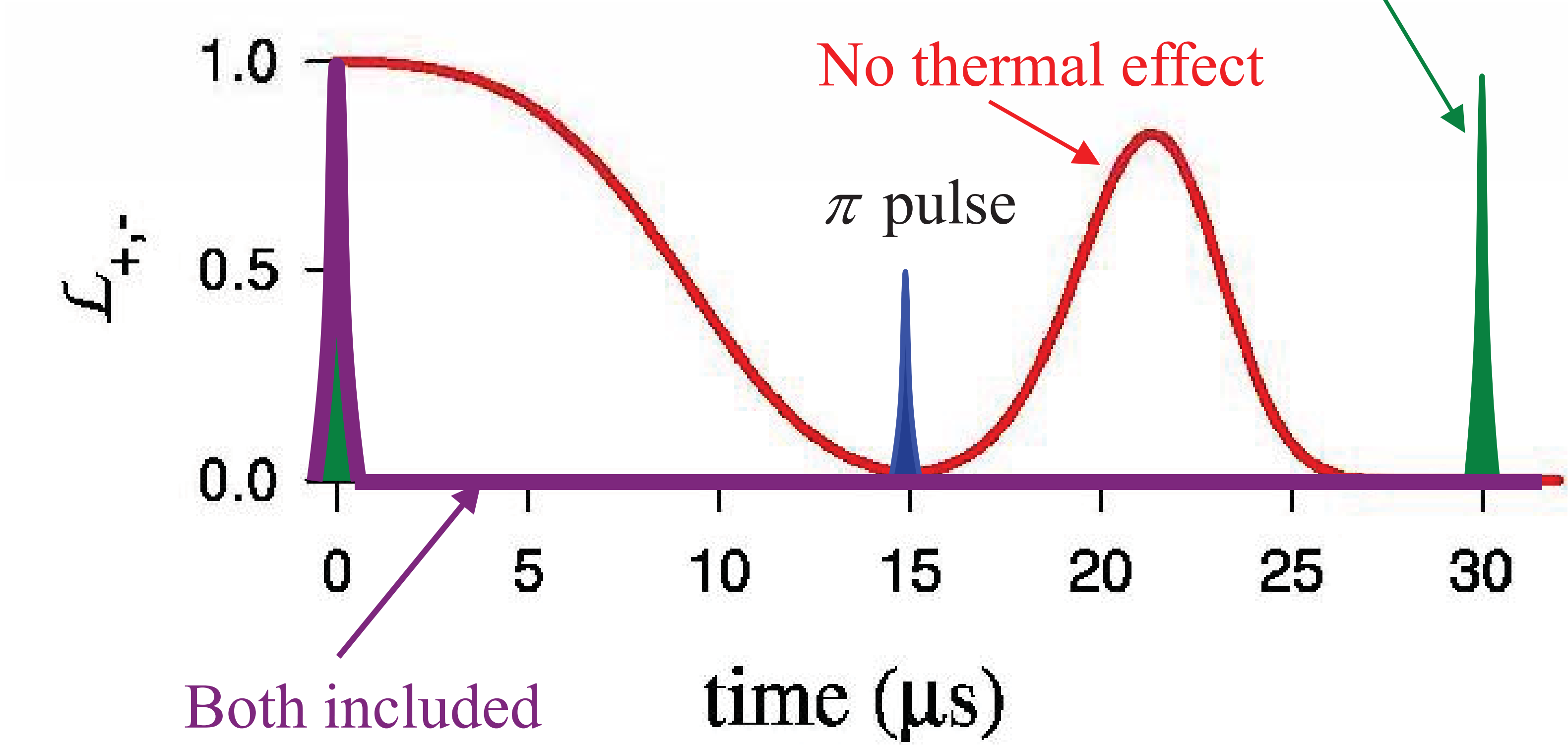
$$\tau^2 - \left[\left(\sqrt{2}\tau\right)^2 - \tau^2\right] = 0$$

Why the magic recovery not observed?

The thermal distribution of the initial nuclear spin configurations leads to inhomogeneous broadening dephasing.

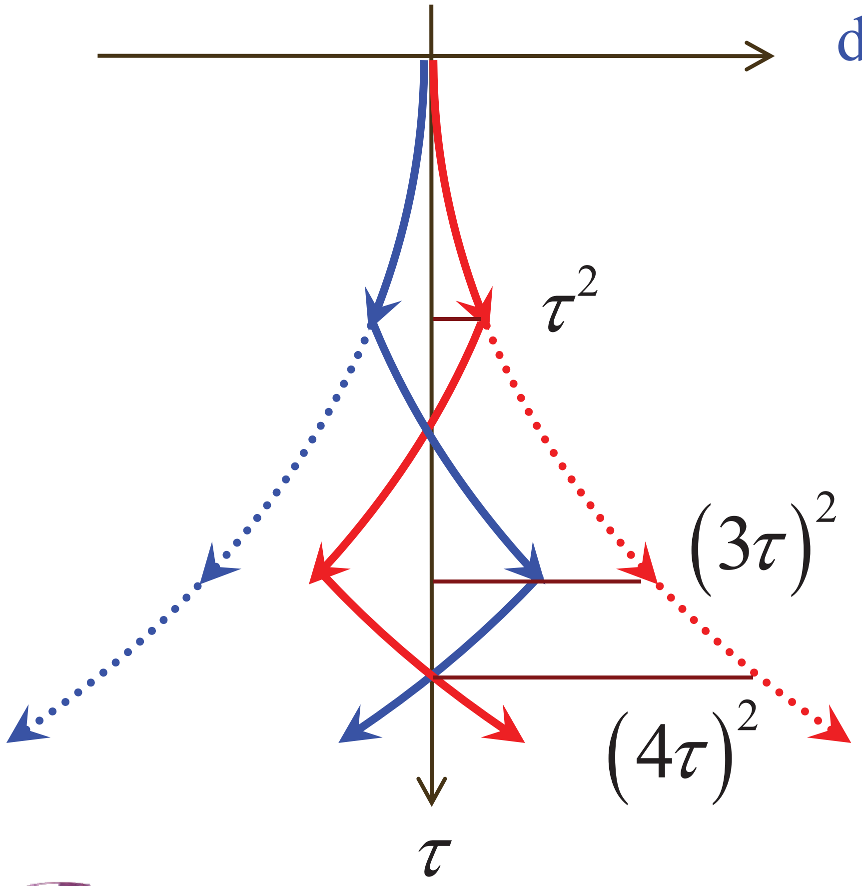
$$\rho^N = \sum P_J |J\rangle\langle J| = \exp\left(-\mu B_0 \hat{J}_z / k_B T\right)$$

$$L \sim \exp\left(-(t-2\tau)^2 / T_2^{*2}\right)$$



To see the hidden disentanglement

1. Filter out the inhomogeneous broadening, e.g., by mode-locking (Greilich et al, Science, 2006), narrowing nuclear spin distribution (Xu et al, Nature 2009), or
2. One more pulse control

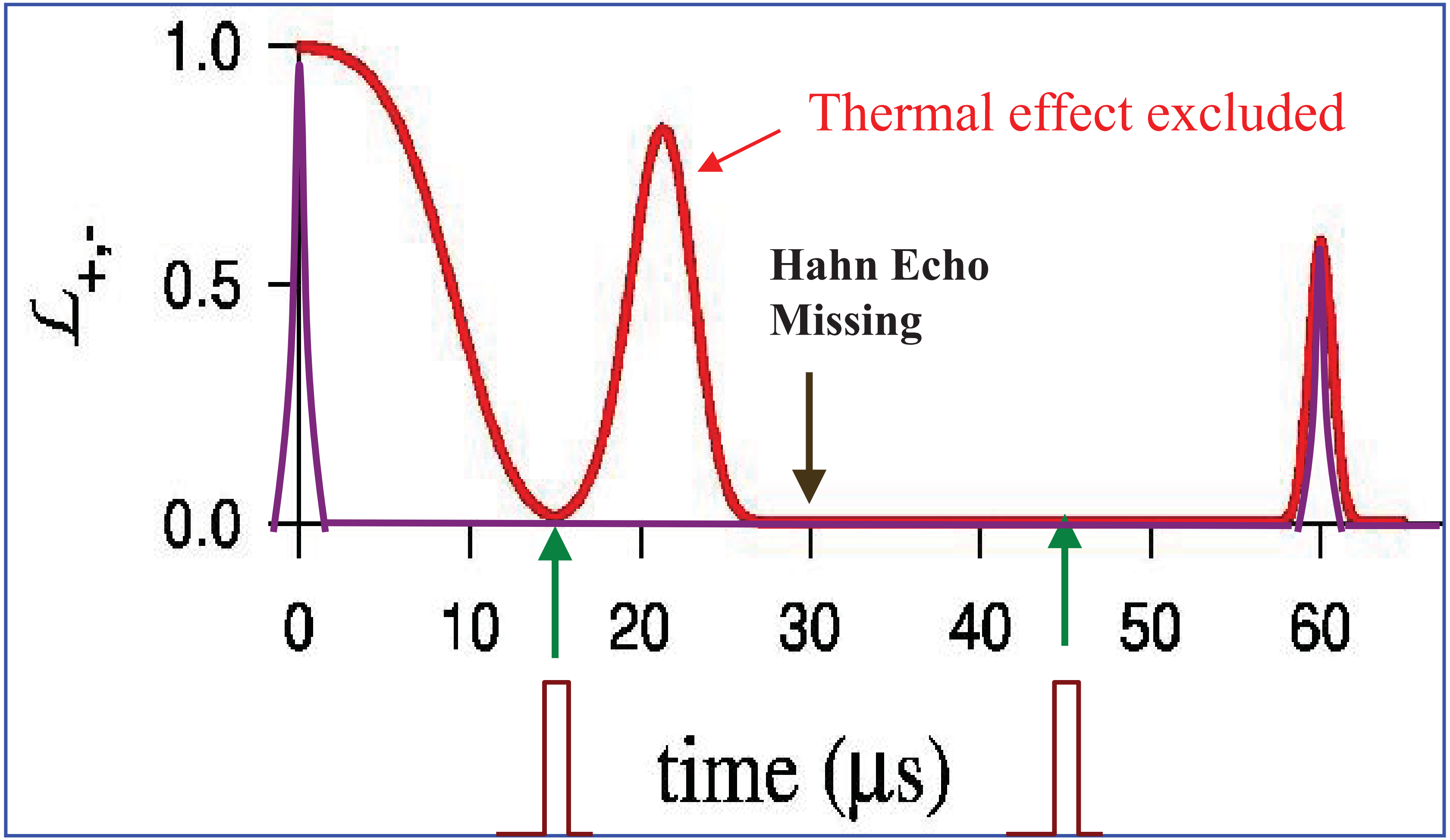


$$\boxed{\begin{gathered}\tau-(3\tau-\tau)+(4\tau-3\tau)=0\\ \tau^2-\left[(3\tau)^2-\tau^2\right]+\left[(4\tau)^2-(3\tau)^2\right]=0\end{gathered}}$$

Both thermal fluctuation and quantum entanglement are eliminated (in the leading order)

It is just the Carr-Purcell

Two-pulse control: Disentanglement at echo time



W. Yao, RBL, and L. J. Sham, Phys. Rev. Lett. **98**, 077602 (07).

Concatenated disentanglement

Iteration to higher-order control

FID $U_0^{\pm} \equiv e^{-i(C_0 \pm D_0)\tau}$

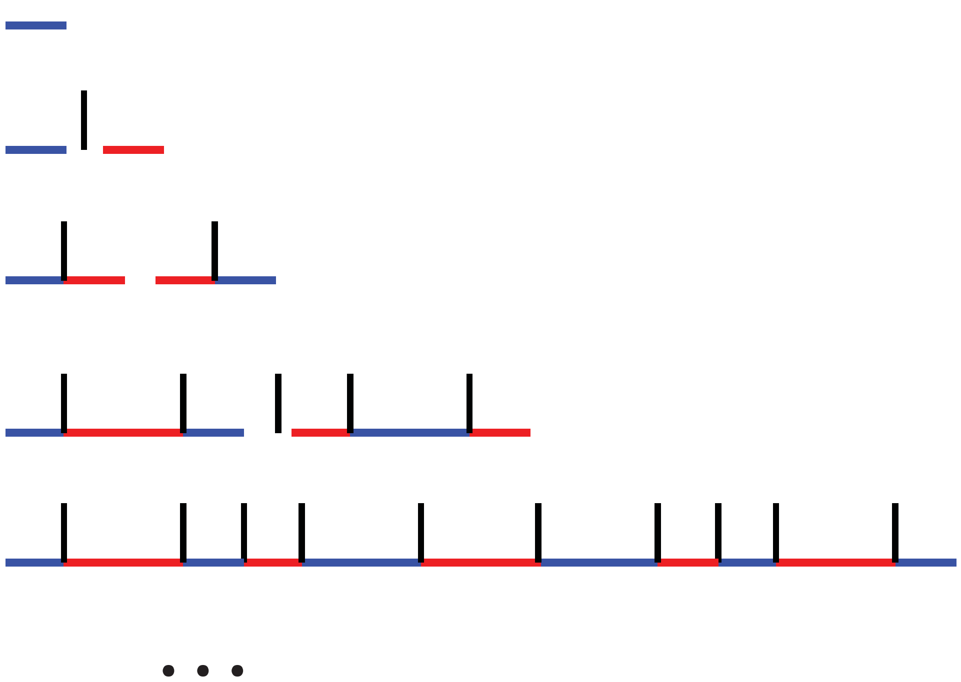
Hahn echo $U_1^{\pm} \equiv U_0^{\mp} U_0^{\pm}$

Carr-Purcell $U_2^{\pm} \equiv U_1^{\mp} U_1^{\pm}$

$U_3^{\pm} \equiv U_2^{\mp} U_2^{\pm}$

$U_4^{\pm} \equiv U_3^{\mp} U_3^{\pm}$

$\cdots$



1. K. Khodjasteh and D. A. Lidar, Phys. Rev. Lett. **95**, 180501 (2005).
2. W. Yao, RBL, and L. J. Sham, Phys. Rev. Lett. **98**, 077602 (2007).

Recap of the quantum model

$$H_I = \hat{B}\sigma_z/2 \text{ and } H = H_I + H_b$$

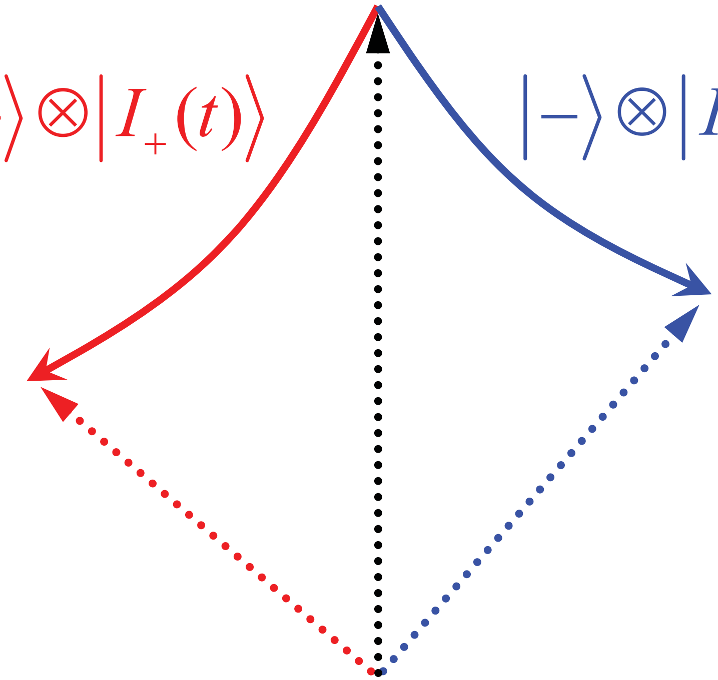
$$H = |+\rangle\langle+| \otimes (C_0 + D_0) + |-\rangle\langle-| \otimes (C_0 - D_0)$$

with $C_0 \equiv H_b$ and $D_0 \equiv \hat{B}/2$

Decoherence by quantum entanglement

$$\left(|+\rangle + |-\rangle\right) \otimes |I\rangle$$

$$|+\rangle \otimes |I_+(t)\rangle \qquad |-\rangle \otimes |I_-(t)\rangle$$



$$|+\rangle \otimes |I_+(t)\rangle + |-\rangle \otimes |I_-(t)\rangle$$

Bifurcated bath evolution → which-way info known → decoherence

$$\boxed{e^{-i\left(C_0 \pm D_0\right)t} |I\rangle = |I_\pm(t)\rangle}$$

$$S = \langle I_+(t) | I_-(t) \rangle = \langle I | U_+^\dagger U_- | I \rangle$$

$$U_\pm = \exp\left(-i\left(C_0 \pm D_0\right)t\right)$$

$$S \sim 1 - t^2 \langle D_0^2 \rangle / 2 = 1 + O\left(t^2\right)$$

Quantum: Decoherence by under one flip control

$$\boxed{e^{-i(C_0 \mp D_0)\tau_1} e^{-i(C_0 \pm D_0)\tau} \left| I \right\rangle = \left| I_\pm(t) \right\rangle}$$

$$S = \left\langle I_+(t) \middle| I_-(t) \right\rangle = \left\langle I \middle| U_{1,+}^\dagger U_{1,-} \middle| I \right\rangle$$

$$U_{1,\pm} = U_\mp(\tau_1) U_\pm(\tau) = \exp\left(-i\left(C_0 \mp D_0\right)\tau_1\right)\exp\left(-i\left(C_0 \pm D_0\right)\tau\right)$$

Let us check Hahn echo to the 1st order of time

$$U_{1,\pm} = \exp\left(-i\left(C_1 \pm D_1\right)\right) \quad \begin{cases} C_1 = 2C_0\tau + O\left(\tau^2\right) \\ D_1 = i\left[C_0, D_0\right]\tau^2 + O\left(\tau^3\right) \end{cases}$$

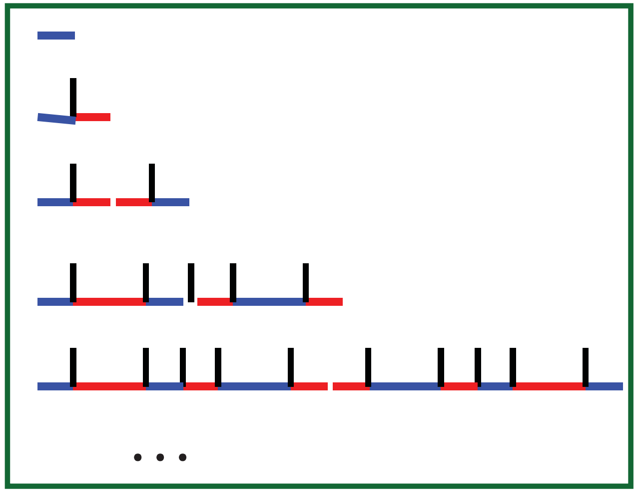
$$S \sim 1 - \left\langle D_1^2 \right\rangle / 2 = 1 - O\left(\tau^4\right)$$

The field is renormalized.

By iteration: Concatenated dynamical decoupling

$$U_{l,\pm} = \exp\left(-i\left(C_l \pm D_l\right)\right)$$

$$U_{l+1,\pm} = U_{l,\mp} U_{l,\pm}$$

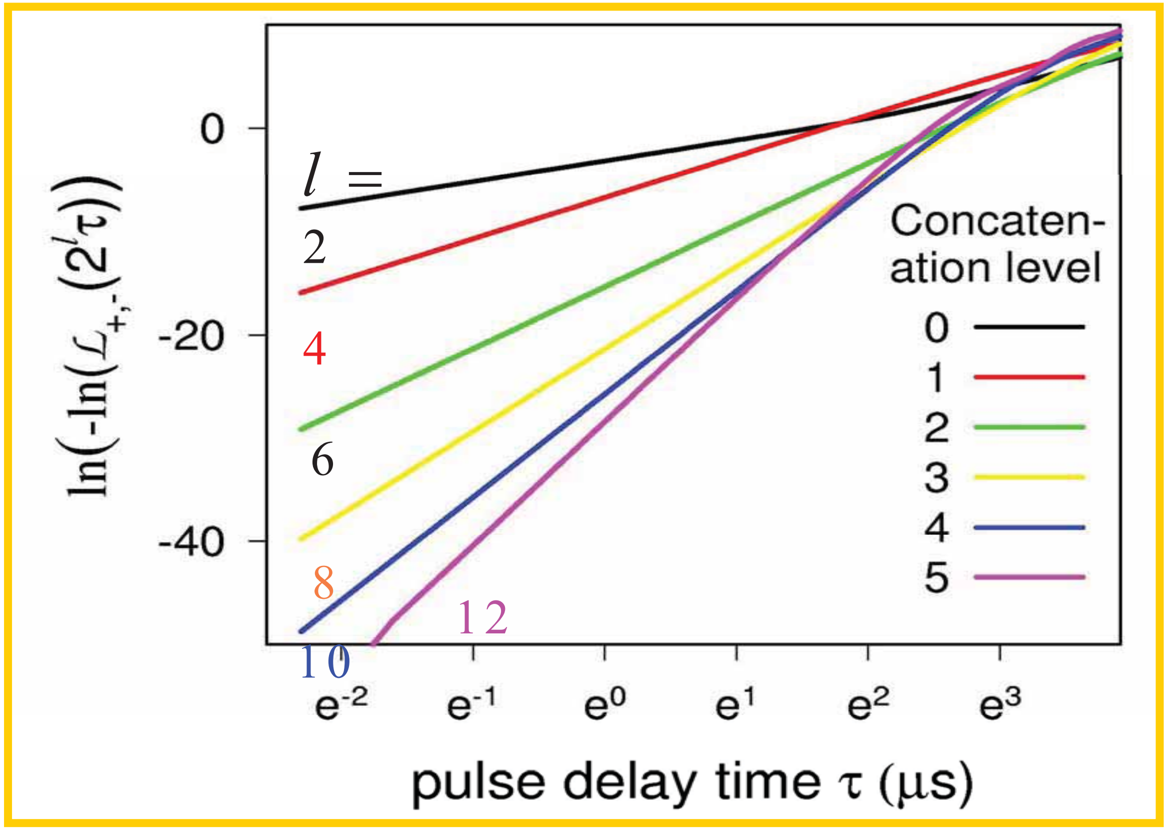


$$\begin{cases} C_{l+1} = 2C_l + \text{higher order} \\ D_{l+1} = i\left[C_l, D_l\right] + \text{higher order} \end{cases}$$

$$\boxed{S \sim 1 - \left\langle D_l^2 \right\rangle / 2 = 1 - O\left(\tau^{2l+2}\right)}$$

Decoherence control by concatenated DD

$$\exp\left(-\frac{t^{2l+1}}{T_{c,l}^{2l+2}}\right)$$

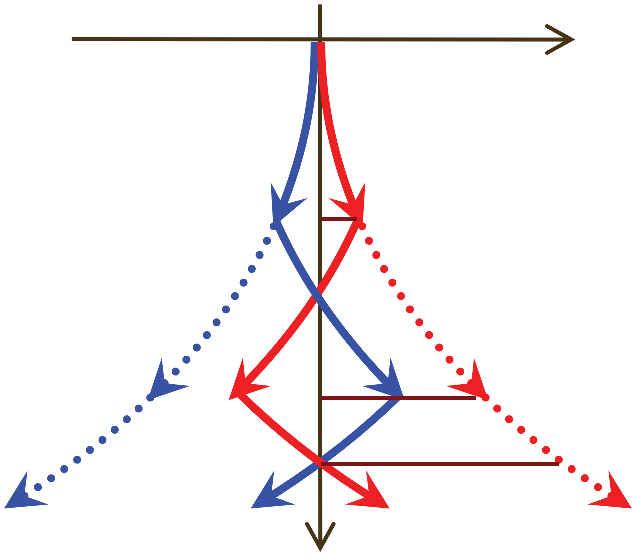


W. Yao, RBL, and L. J. Sham, Phys. Rev. Lett. **98**, 077602 (2007).

# of pulses, however, scales exponentially with order of DD

Optimal pulse sequences

What is the minimal number of pulses needed (optimal solution)?



If the distance: $D_k(t) = a_k t + b_k t^2 + c_k t^3 + \cdots$

$$\tau_1 - (\tau_2 - \tau_1) + (\tau_3 - \tau_2) - \cdots + (-1)^n (T - \tau_n) = 0$$

$$\tau_1^2 - (\tau_2^2 - \tau_1^2) + (\tau_3^2 - \tau_2^2) - \cdots + (-1)^n (T^2 - \tau_n^2) = 0$$

$$\tau_1^3 - (\tau_2^3 - \tau_1^3) + (\tau_3^3 - \tau_2^3) - \cdots + (-1)^n (T^3 - \tau_n^3) = 0$$

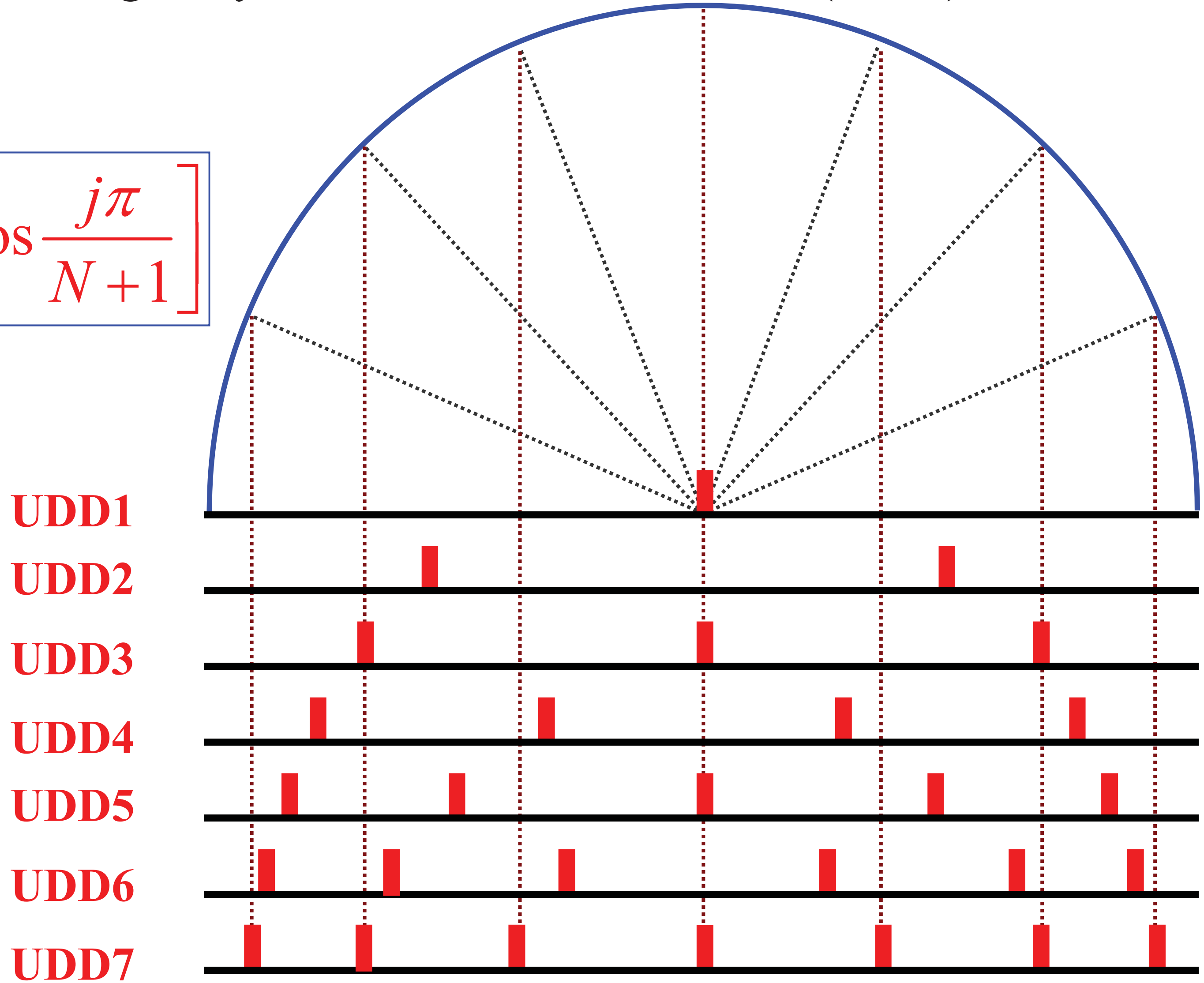
$$\cdots\cdots\cdots$$

$$\tau_1^n - (\tau_2^n - \tau_1^n) + (\tau_3^n - \tau_2^n) - \cdots + (-1)^n (T^n - \tau_n^n) = 0$$

UDD: Uhrig dynamical decoupling

G. Uhrig, Phys. Rev. Lett. **98**, 100504 (2007).

$$\tau_j = \frac{t}{2}\left[1 - \cos\frac{j\pi}{N+1}\right]$$



UDD means Uhrig dynamical decoupling

G. Uhrig, Phys. Rev. Lett. **98**, 100504 (2007).

A little more quantum: Spin boson pure dephasing model

$$H_I = B_z \sigma_z / 2 \quad \text{where } B_z = \sum_q \lambda_q \left(a_{-q}^\dagger e^{i\omega_q t} + a_q e^{-i\omega_q t} \right)$$

The bath has no interaction. It has exact solution.
The thermal state has Gaussian noise:

$$\left\langle B(t+\tau) B(t) \right\rangle = \int J(\omega) e^{-i\omega t} d\omega$$

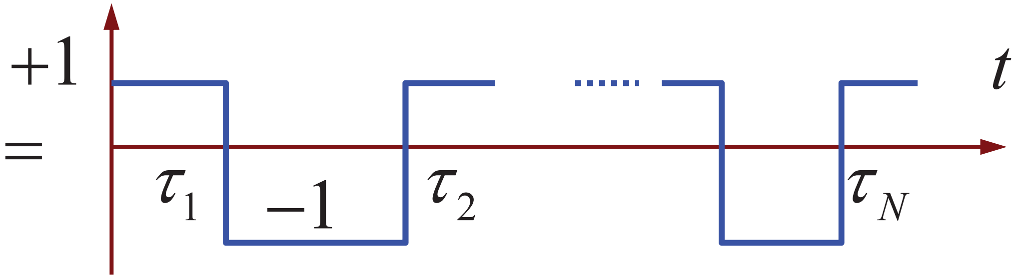
Noise spectrum, i.e., DOS: $J(\omega) = \sum_q \delta(\omega - \omega_q) \left|\lambda_q\right|^2$

The solution for classical Gaussian noise cancel the pure dehasing in free boson bath up to (2N+2)th order of short time.

How about a general interacting quantum bath?

$$H = |+\rangle\langle+| \otimes (C + D) + |-\rangle\langle-| \otimes (C - D)$$

Under control of N flips:

$F(t) =$ 

$$H(t) = |+\rangle\langle+| \otimes \left[C + F(t) D\right] + |-\rangle\langle-| \otimes \left[C - F(t) D\right]$$

$$U_\pm(t) = T \exp\left(-i \int_0^t \left[C \pm F(t) D\right] dt\right)$$

$$S = \langle I | U_+^\dagger U_- | I \rangle$$

Expansion by order (time-dependent perturbation)

$$U_+(t) = T\exp\left(-i\int_0^t \left[C + F(t)D\right]dt\right)$$

$$= \exp(-iCt)\,T\exp\left(-i\int_0^t F(t)\tilde{D}(t)dt\right) \equiv \exp(-iCt)\,\tilde{U}_+(t)$$

$$\tilde{D}(t) = D + [iC, D]t + \frac{1}{2!}\left[iC,[iC,D]\right]t^2 + \cdots \equiv \sum_k D_k t^k$$

What counts is the interaction part:

$$\tilde{U}_+(t) = 1 - i\int_0^t F(t)Ddt$$

$$-i\int_0^t F(t_1)t_1 D_1 dt_1 - i\int_0^t\int_0^{t_1} F(t_1)F(t_2)DDdt_2dt_1$$

$$+O(t^3)$$

Tedious!

$$\tilde{U}_{+}(t)=1-i\int_0^t F(t)D\,dt\;-i\int_0^t F(t_1)t_1D_1dt_1-i\int_0^t\int_0^{t_1}F(t_1)F(t_2)DDdt_2dt_1$$

$$-i\int_0^t F(t_1)t_1^2D_2dt_1-i\int_0^t\int_0^{t_1}F(t_1)F(t_2)t_2D_1Ddt_2dt_1-i\int_0^t\int_0^{t_1}F(t_1)F(t_2)t_1DD_1dt_2dt_1$$

$$-i\int_0^t\int_0^{t_1}\int_0^{t_2}F(t_1)F(t_2)F(t_3)DDDdt_3dt_2dt_1$$

$$-i\int_0^t\int_0^{t_1}\int_0^{t_2}\int_0^{t_3}F(t_1)F(t_2)F(t_3)F(t_4)DDDDdt_4dt_3dt_2dt_1$$

$$-i\int_0^t\int_0^{t_1}\int_0^{t_2}F(t_1)F(t_2)F(t_3)t_3D_1DDdt_3dt_2dt_1$$

$$-i\int_0^t\int_0^{t_1}\int_0^{t_2}F(t_1)F(t_2)F(t_3)t_2DD_1Ddt_3dt_2dt_1$$

$$-i\int_0^t\int_0^{t_1}\int_0^{t_2}F(t_1)F(t_2)F(t_3)t_1DDD_1dt_3dt_2dt_1$$

$$-i\int_0^t\int_0^{t_1}F(t_1)F(t_2)t_2t_1D_1D_1dt_2dt_1-i\int_0^t\int_0^{t_1}F(t_1)F(t_2)t_2^2D_2Ddt_2dt_1$$

$$-i\int_0^t\int_0^{t_1}F(t_1)F(t_2)t_1^2DD_2dt_2dt_1-i\int_0^t F(t_1)t_1^3D_3dt_1$$

$$+O(t^5)$$

Indeed, # of terms scales exponentially, all independent for general bath

RMB100 Award Problem

A RMB100 award (value appreciating) is provided to the first student (professors excluded) in this lecture hall who expands it and finds out the solution of the modulation function so that all the integrals vanish to the 5th order of time before Jan 17th, 2011.

Try Uhrig DD: Clues

1. UDD first discovered for the spin boson model
2. B. Lee, W. M. Witzel, and S. Das Sarma [Phys. Rev. Lett. 100, 160505 (2008)] checked with computer up to the 9th order
3. G. Uhrig [New J. Phys. 10, 083024 (2008)] checked with computer up to the 14th order..

Now we prove it.

Proof: Step 1 (Only odd terms counts)

Let us work in the interaction picture

$$\tilde{U}_{\pm} = T\exp\left(-i\int_0^t \pm F(t)\tilde{D}(t)dt\right)$$

$$= 1 - i\int_0^t \pm F(t)\tilde{D}(t)dt - \int_0^t\int_0^{t_1} F(t_1)F(t_2)\tilde{D}(t_1)\tilde{D}(t_2)dt_2dt_1$$

$$+(-i)^3\int_0^t\int_0^{t_1}\int_0^{t_2}(\pm)F(t_1)F(t_2)F(t_3)\tilde{D}(t_1)\tilde{D}(t_2)\tilde{D}(t_2)dt_3dt_2dt_1$$

$$+\cdots$$

Qubit coherence: $\left\langle \tilde{U}_+^{\dagger}\tilde{U}_- \right\rangle = 1 - \left\langle \tilde{U}_+ - \tilde{U}_- \right\rangle + \text{higher order}$

So we just need to make the terms with odd # of integrals vanish.

Step 2: All terms up to (N+1)th order

Recall: $\tilde{D}(t) = D + [iC, D]t + \frac{1}{2!}[iC,[iC,D]]t^2 + \cdots \equiv \sum_k D_k t^k$

We just need to make

$$0 = \int_0^t \int_0^{t_1} \cdots \int_0^{t_{k-1}} F(t_1) t_1^{m_1} F(t_2) t_2^{m_2} \cdots F(t_k) t_k^{m_k} dt_k \cdots dt_2 dt_1 \propto t^{m_1+m_2+\cdots+m_k+k}$$

if

(i) k is odd, and

(ii) $m_1 + m_2 + \cdots + m_k + k < N + 1$

There are still exponentially many terms.

Step 3: Transform time into angle

UDD, spin flips at $t_j = \frac{t}{2}\left(1-\cos\theta_j\right)$

$F(t) \to f(\theta)$ is a periodic function jumping between $+1$ and -1

Now we just need to make

$$0 = \int_0^{\pi}\int_0^{\theta_1}\cdots\int_0^{\theta_{k-1}}\prod_{j=1}^{k} f\left(\theta_j\right)\sin\left(q_j\theta_j\right)d\theta_k\cdots d\theta_2 d\theta_1$$

if (i) k is odd, and (ii) $q_1+q_2+\cdots+q_k < N+1$

Step 4: Fourier transformation of modulation function

$$f(\theta) = \sum_{s=1,3,5,\ldots} \frac{k\pi}{4} \sin\left(s(N+1)\theta\right)$$

It contains only odd harmonics of $(N+1)$ th order sine wave

By using repeatedly product-to-sum trigonometric formula, the multiple integral will be reduced to contain only terms like:

$$\int_0^{\pi} \cos\left(Q\theta + R\theta\right) d\theta$$

with $Q =$ odd numbers of odd multiples of $(N+1)$ and

$$R = \pm q_1 \pm q_2 \cdots \pm q_k \in [-N, N]$$

So, all the terms satisfying the prescribed conditions vanish.

The proof is done.

Generalization I: Non-ideal is better

From the proof, we found that

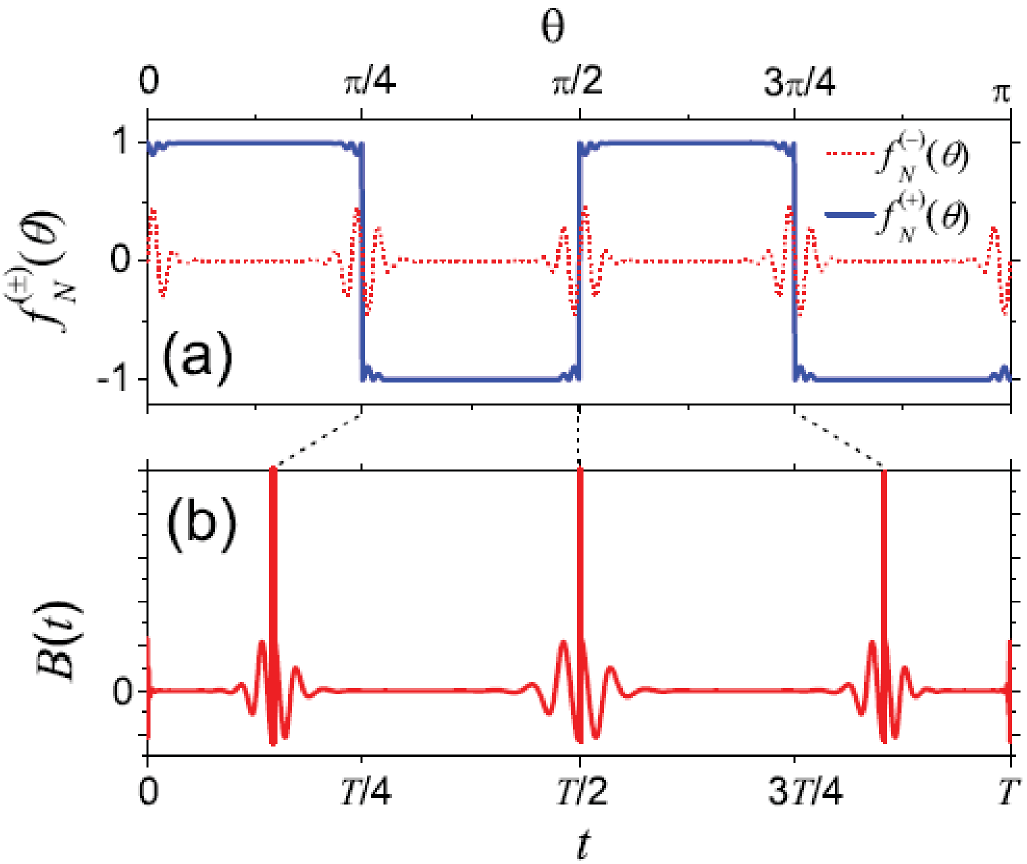
Suffices it

$$f(\theta) = \sum_{s=1,3,5,\ldots} A_k \sin\left(s\left(N+1\right)\theta\right)$$ for arbitrary expansion coefficients A_k

So we can generalize to sequences containing finite-duration pulses superimposed on the ideal UDD.

Useful for quantum control during coherence protection.

Universal optimal control



Extra finite-duration pulses can be tolerated if it satisfies:

$$\theta_j = j\pi/(N+1)$$

$$B'(\theta_j+\phi) = -B'(\theta_j-\phi)$$

$$B'\left(\theta_{j+\frac{1}{2}}+\phi\right) = B'\left(\theta_{j+\frac{1}{2}}-\phi\right)$$

$$B'(\theta_{j+1}) = B'(\theta_j)$$

Generalization II: Combating spin-flip relaxation & beyond

Homework 1: Prove for a general qubit-bath Hamiltonian

$H = C + D_x\sigma_x + D_y\sigma_y + D_z\sigma_z$,

that, a generalized *N*th order UDD sequence $\mathbf{B}(t)$ applied along, say, z-axis, keep the spin coherence along z-axis $\langle\sigma_z\rangle$ without decay up to $O\left(t^{N+1}\right)$

Homework 2: Prove for a general Hamiltonian H, and an arbitrary *Hermitian* operator Σ which satisfies $\Sigma^2 = 1$, a generalized *N*th order UDD sequence $e^{-iH(t_1-t_0)}\Sigma e^{-iH(t_2-t_1)}\Sigma e^{-iH(t_3-t_2)}\cdots\Sigma e^{-iH(t_N-t_{N-1})}$ preserves the physical quantity $\langle\Sigma\rangle$ up to $O\left(t^{N+1}\right)$.

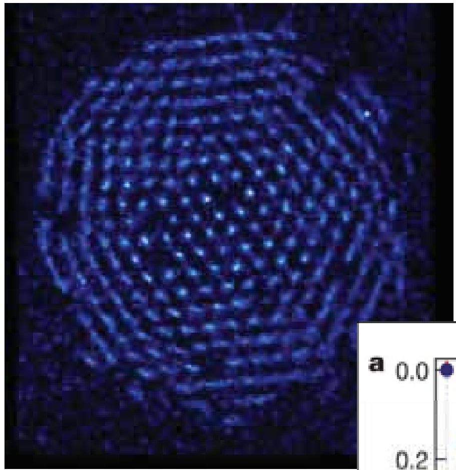
Further developments

1. Nearly optimal for arbitrary coupling – by two hierarchies of UDD [West, Fong & Lidar, PRL 104, 130501 (2010)]
2. Sequences made of pulses with finite amplitudes [Uhrig & Pasini, New J. Phys. 12, 045001 (2010)]
3. To arbitrary coupled multi-qubits [Zhen-Yu Wang & RBL, arXiv:1006.1601, Phys. Rev. A, in press]

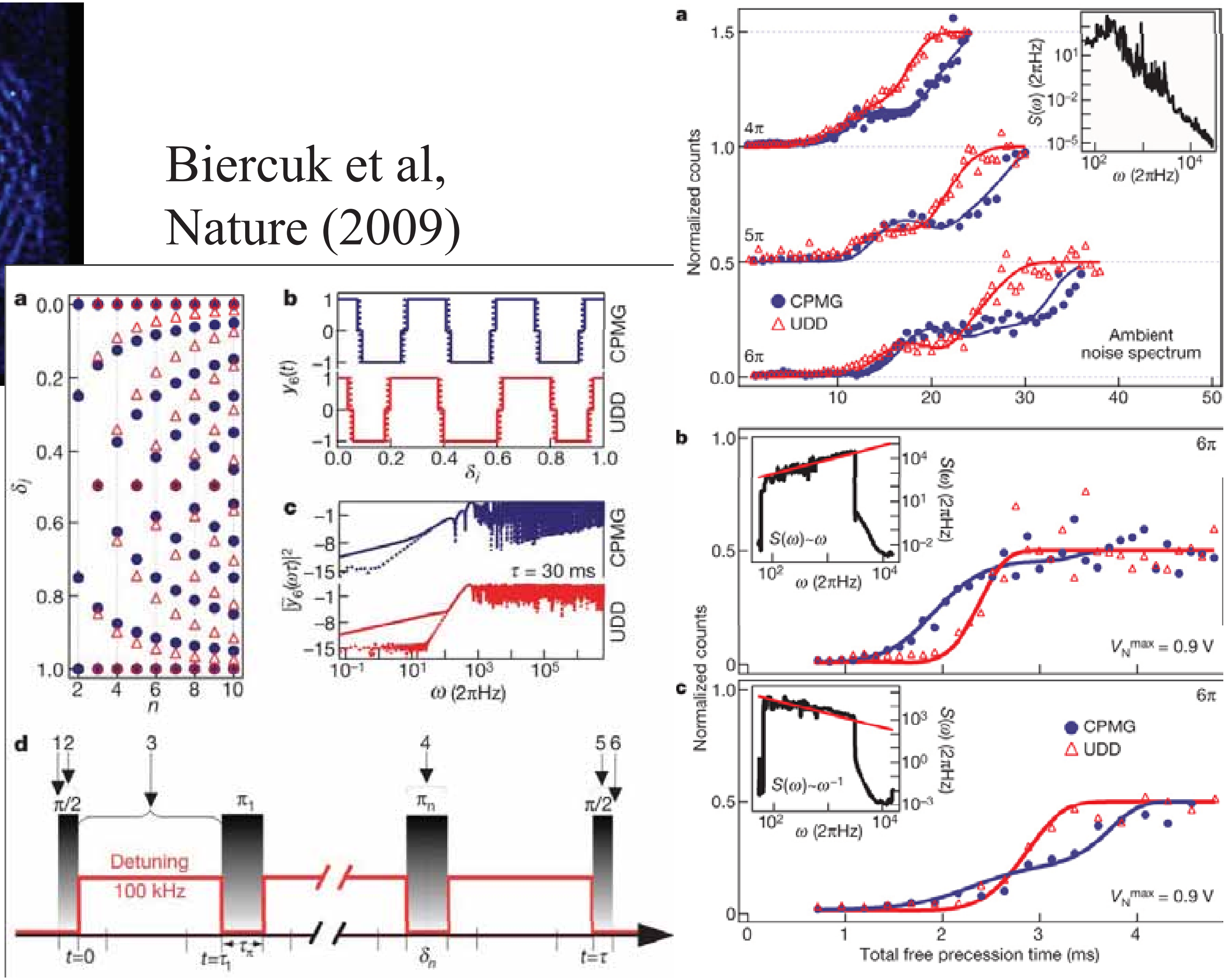
For a review, see W. Yang, Z. Y. Wang, & RBL, Frontiers of Physics 6, 2 (2011); arXiv:1007.0623.

III. Experiments and applications

Protection of coherence of trapped ions

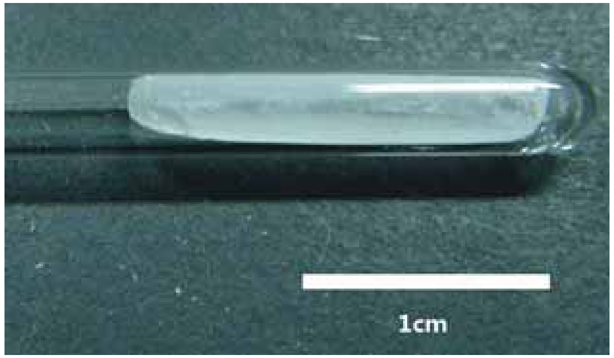


Biercuk et al, Nature (2009)

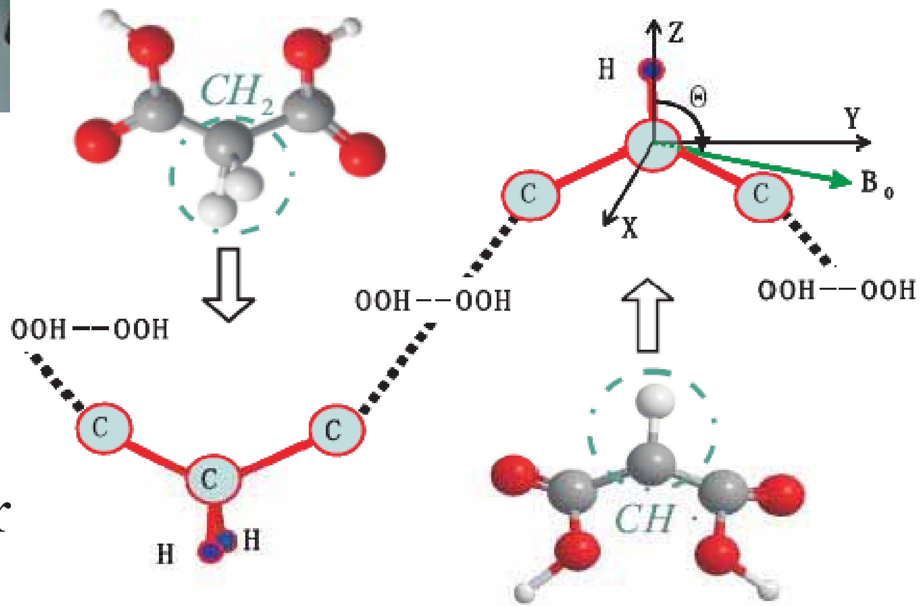


Preserving solid-state qubit coherence

Brucker ESR spectrometer
(X-Band, about US$1.0M)



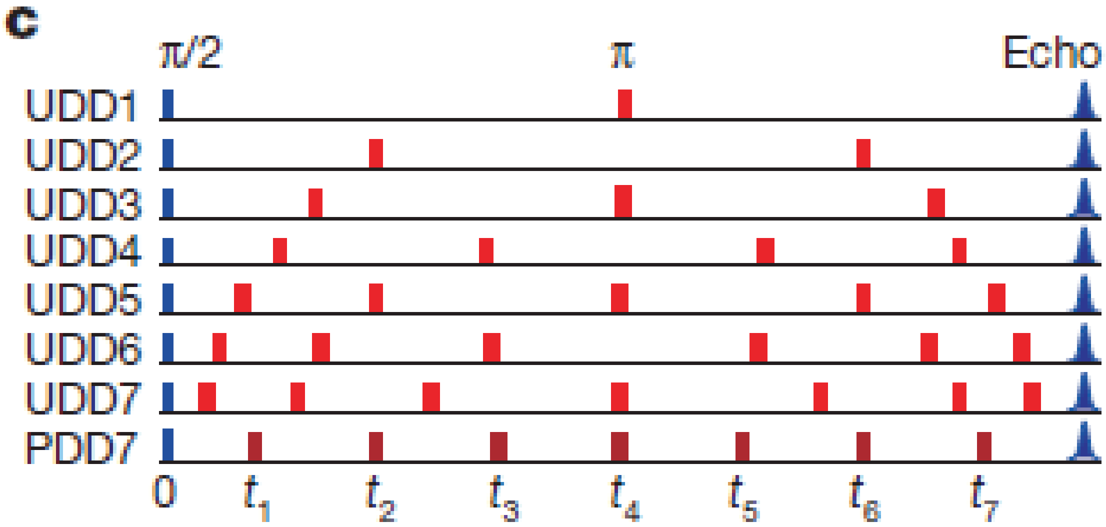
Irradiated malonic acid single crystals

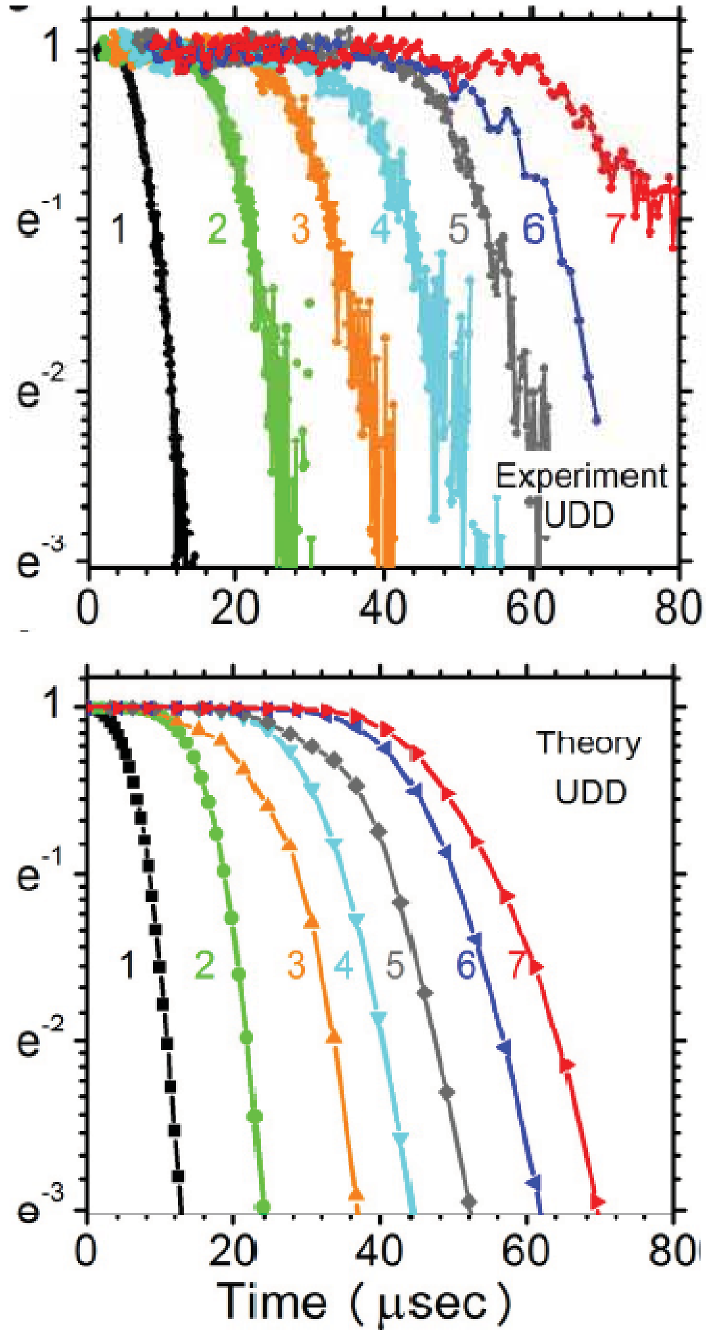


Electron spin of a radical interacting with H nuclear spins

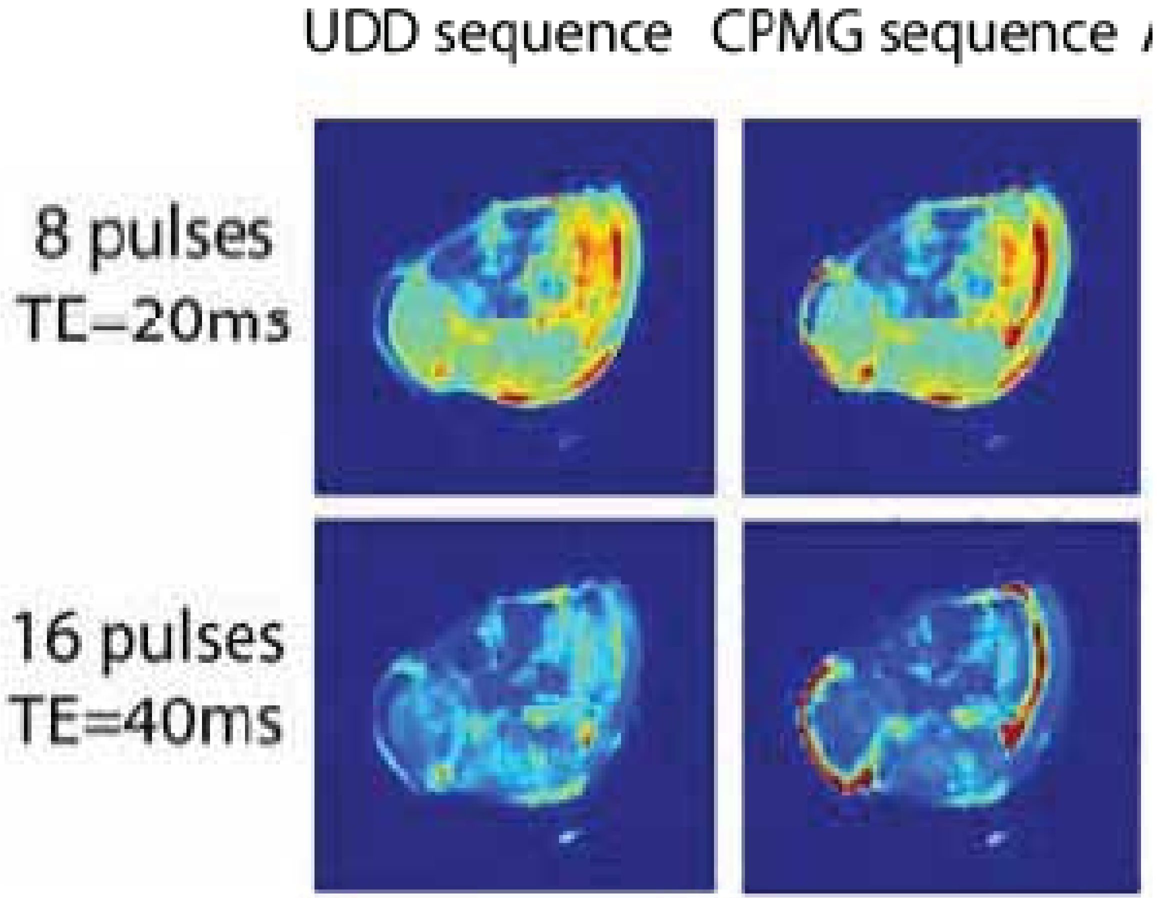
Spin coherence preservation by UDD

JF Du, X Rong, N Zhao, Y Wang, JH Yang & RBL, Nature **461**, 1265 (2009).





Enhanced MRI of tumors in mice by UDD



(W. S. Warren, 09)

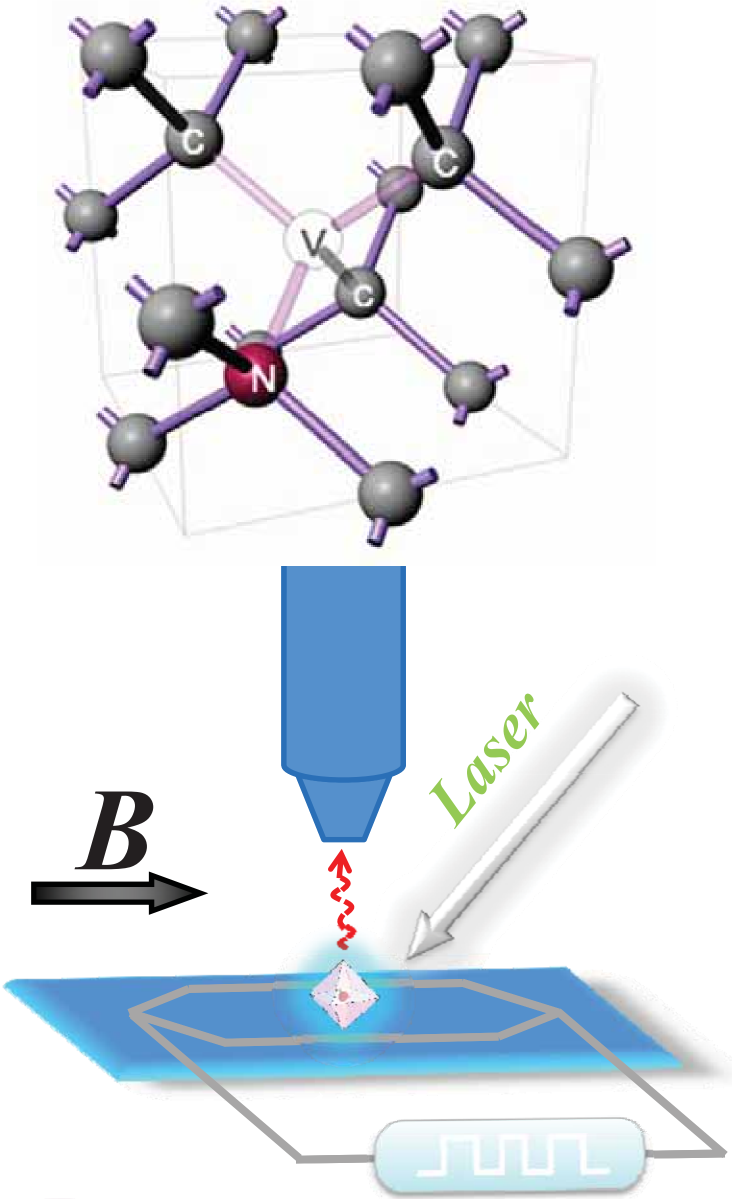
NV center spins in diamond

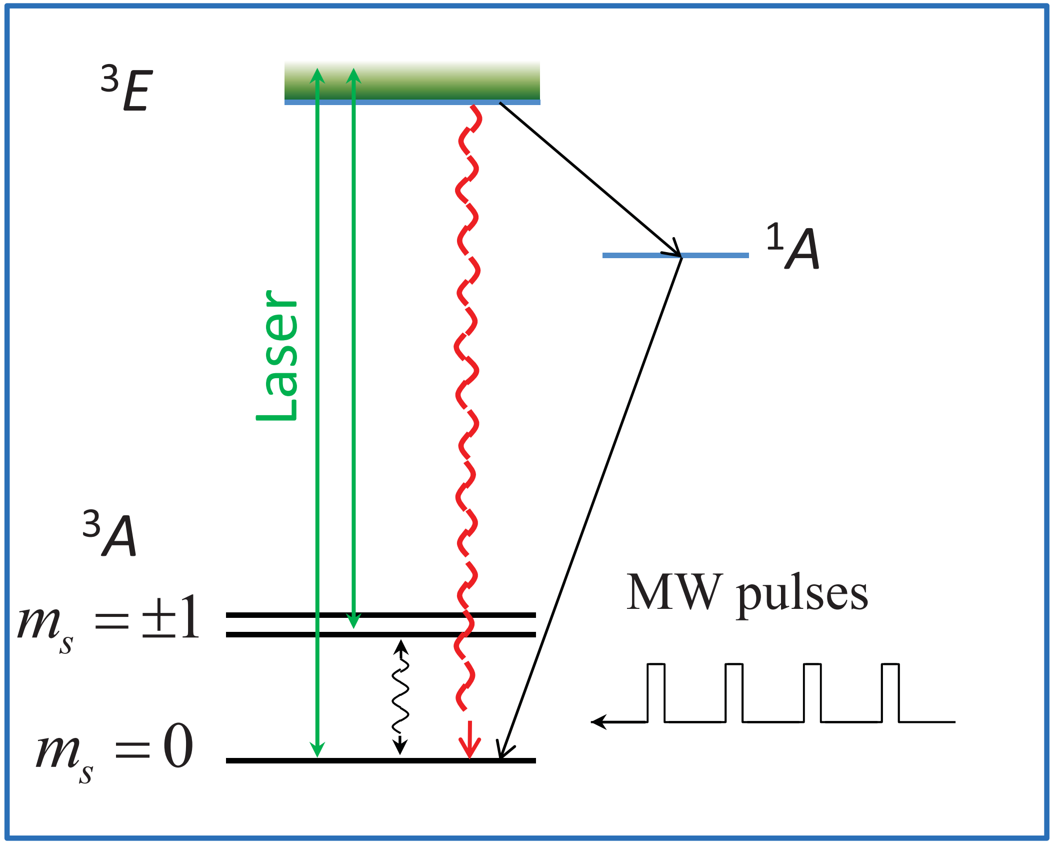
Awschalom, Epstein & Hanson,
The Diamond Age of Spintronics,
Scientific American **297**, 84 (2007).

- Chemical stability
- Weak Spin-orbit interaction (light C atoms, coherence @ RT)
- Low ^{13}C abundance
- Transparent (optical access)
- Non-toxic (medicine)

Long spin coherence time (T2~ ms) @ RT for solid-state quantum computing & magnetometry, optically accessible

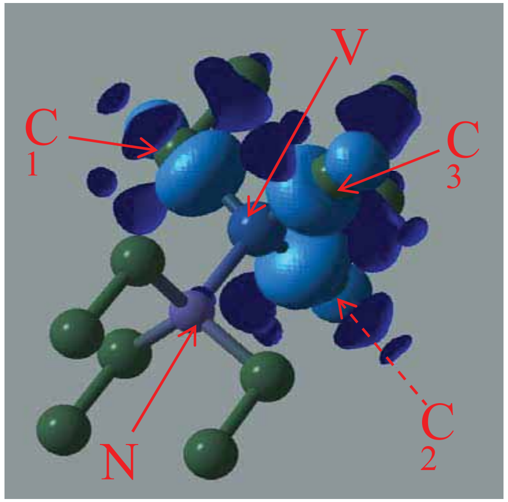
NV Center in diamond: Structure, levels & setup

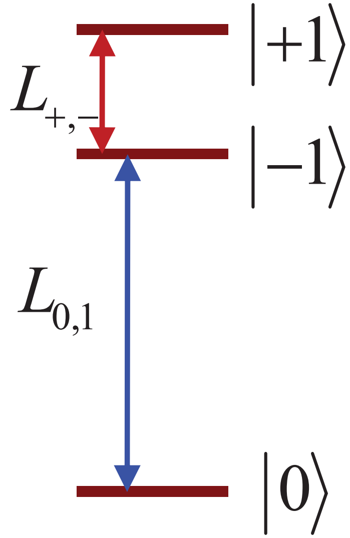




- Type I samples: N-rich, decoherence caused by N electron spins
- Type IIa (hi-purity) samples: Decoherence caused by ^{13}C spins

Spin coherence of NV centre in diamond

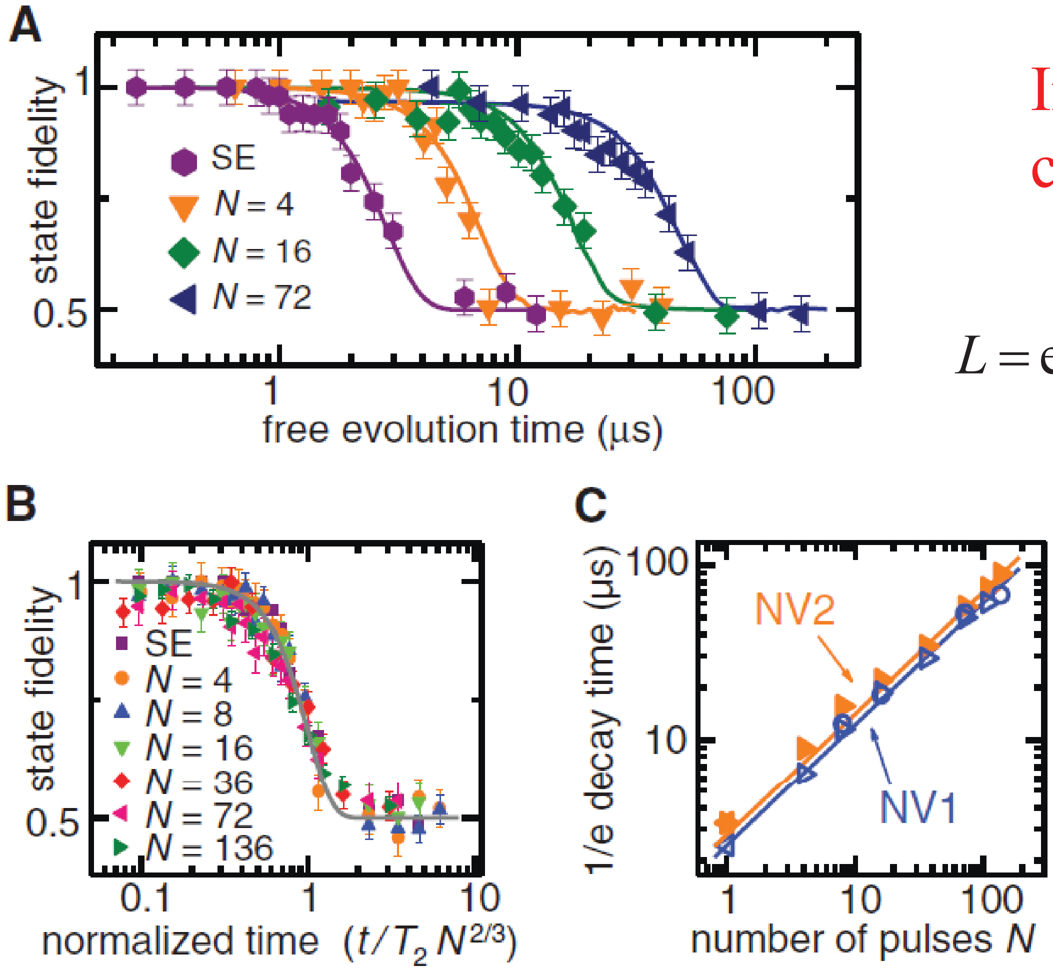




- We consider high-purity diamond (w/ low N density), with ^{13}C bath as the main decoherence channel
- First-principles calculation of structure and interactions
- Quantum many-body theory of centre spin coherence evolution

DD protection of NV center spin coherence in diamond. I

Hanson et al (TU Delft), Science (2010)



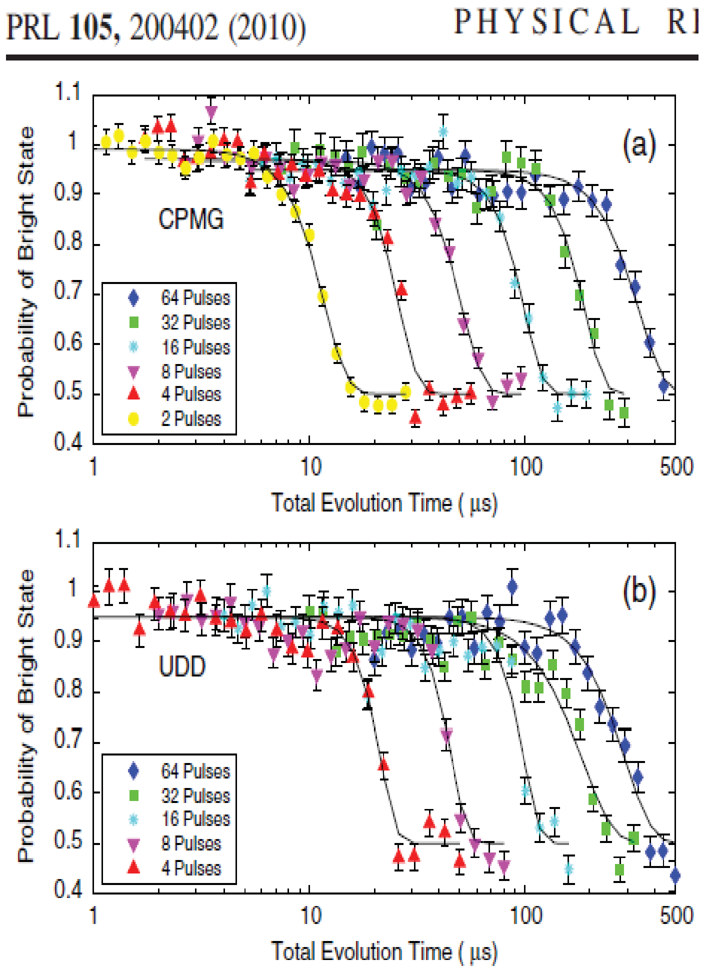
In good agreement with classical noise theory

$$L = \exp\left(-\frac{1}{2}\int\left\langle B(t_1)B(t_2)\right\rangle F(t_1)F(t_2)\right)$$

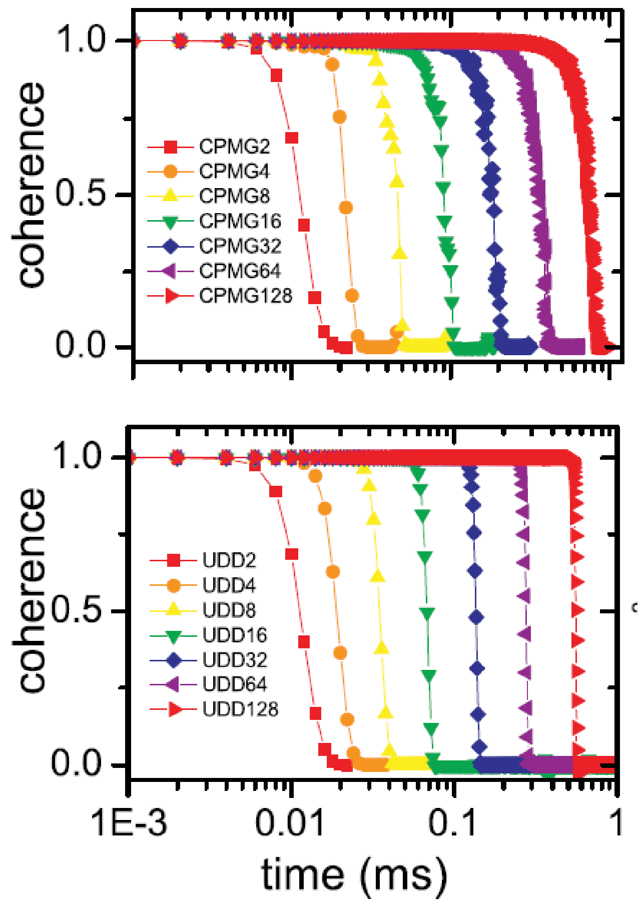
$$\left\langle B(t_1)B(t_2)\right\rangle = \sigma^2 \exp\left(-\frac{\left|t_1 - t_2\right|}{\tau_c}\right)$$

DD protection of NV center spin coherence in diamond. II

D. Cory et al. High-purity sample (^{13}C nuclear spin bath)



N. Zhao, quantum theory calculation w/o adjustable parameters



Quantum or classical, that is a question

N. Zhao, X. Kong, P. Huang, F. Shi, P. Wang, X. Rong, Z. Y. Wang, J. Du & RBL, preprint available upon request by email

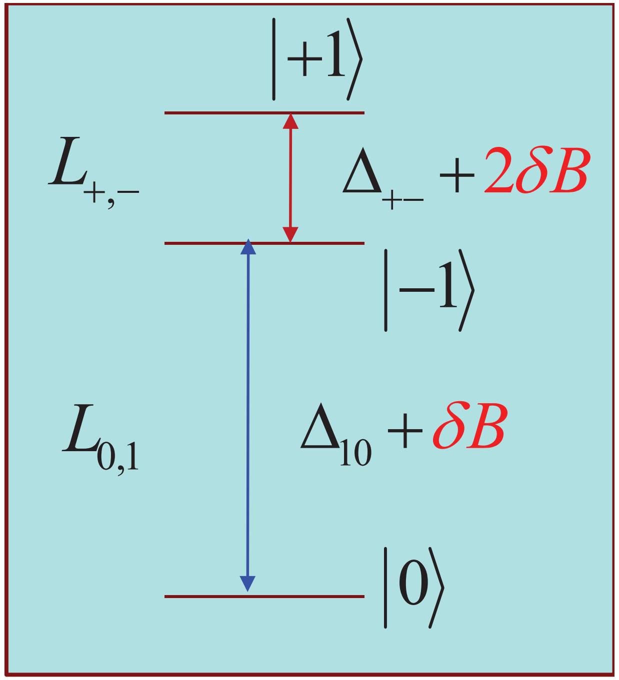
Classical random force:

$$F(t)B(t)\mathbf{e}_z \times \hat{\mathbf{S}} \xrightarrow{\text{Average}}$$

$$L_{0,1} = \exp\left(-\frac{1}{2}\int \langle B(t_1)B(t_2)\rangle F(t_1)F(t_2)\,dt_1 dt_2\right)$$

$$L_{+,-} = \exp\left(-2\int \langle B(t_1)B(t_2)\rangle F(t_1)F(t_2)\,dt_1 dt_2\right)$$

$$\left|L_{+,-} = L_{0,1}^4\right|$$



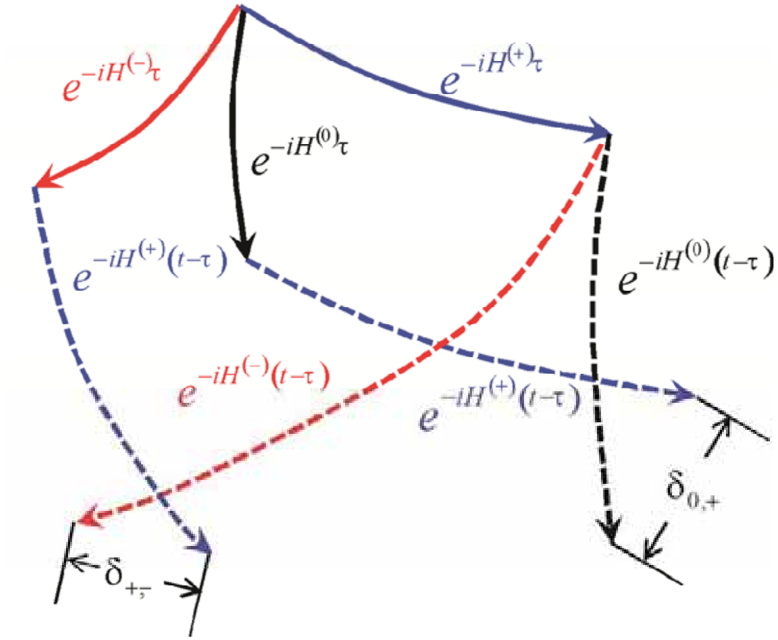
Quantum bath:

$$\left(|-1\rangle + |0\rangle + |+1\rangle\right) \otimes |B\rangle \xrightarrow{|\alpha\rangle\langle\alpha|\otimes H^{(\alpha)}}$$

$$\sum_\alpha |\alpha\rangle \otimes |B_\alpha(t)\rangle$$

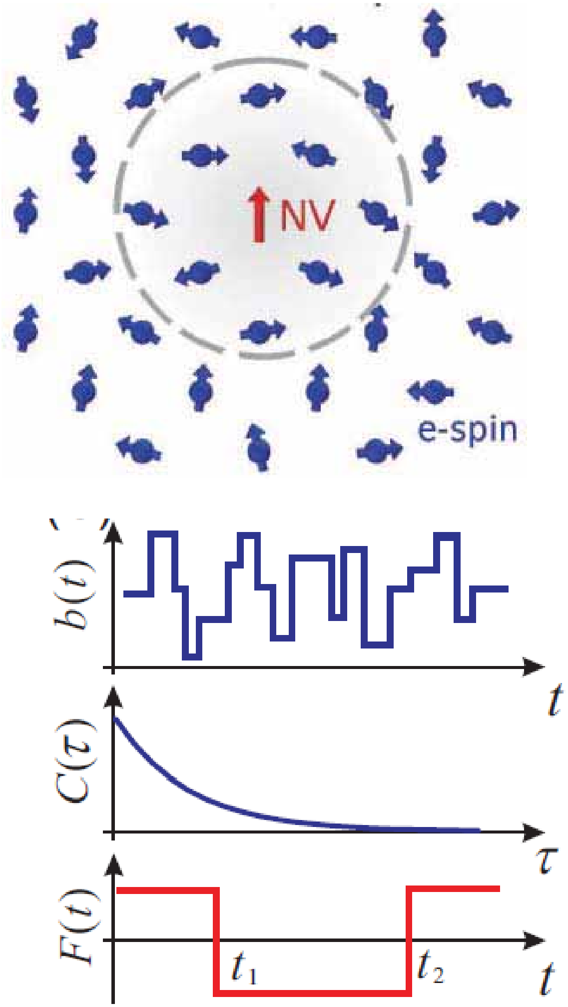
$L_{0,1} \propto \langle B_0(t)|B_{+1}(t)\rangle$, but $L_{+,-} = \langle B_{-1}(t)|B_{+1}(t)\rangle$

Quantum evolution under control

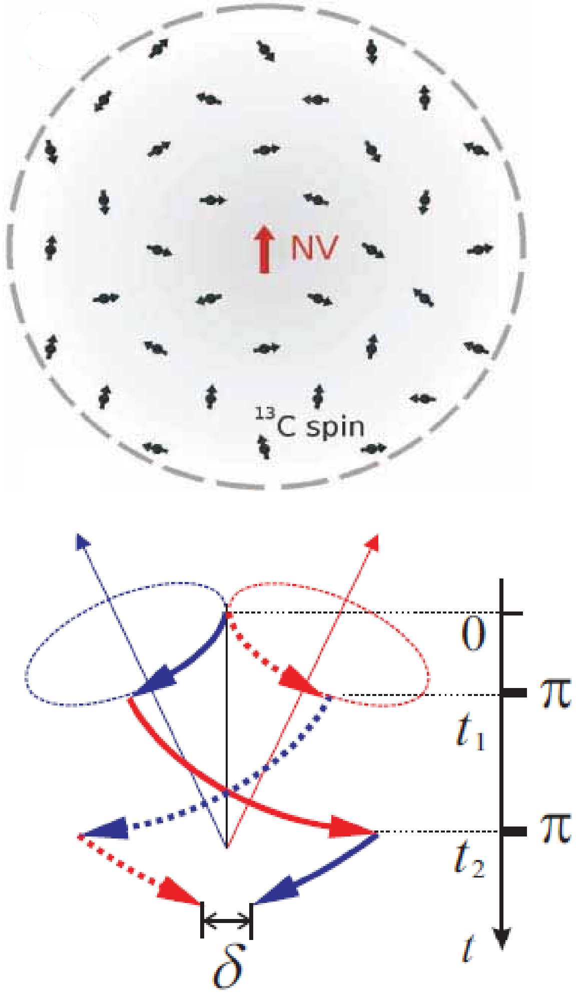


Quantum versus Classical

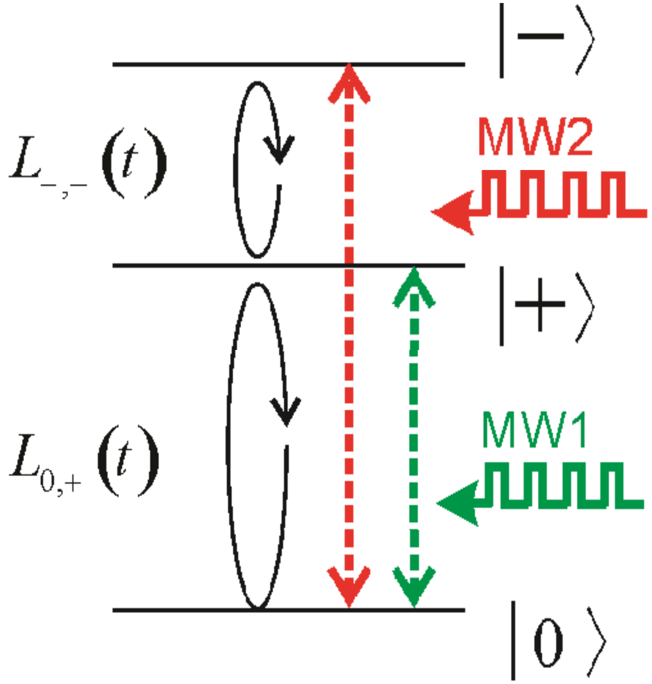
N-spin bath, fast diffusion ➔ classical

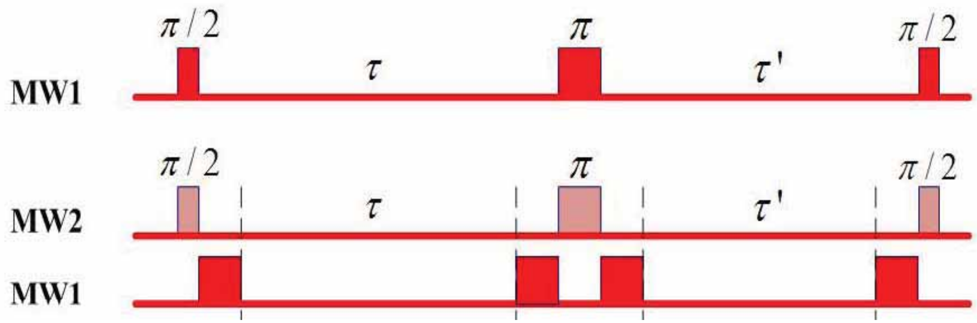


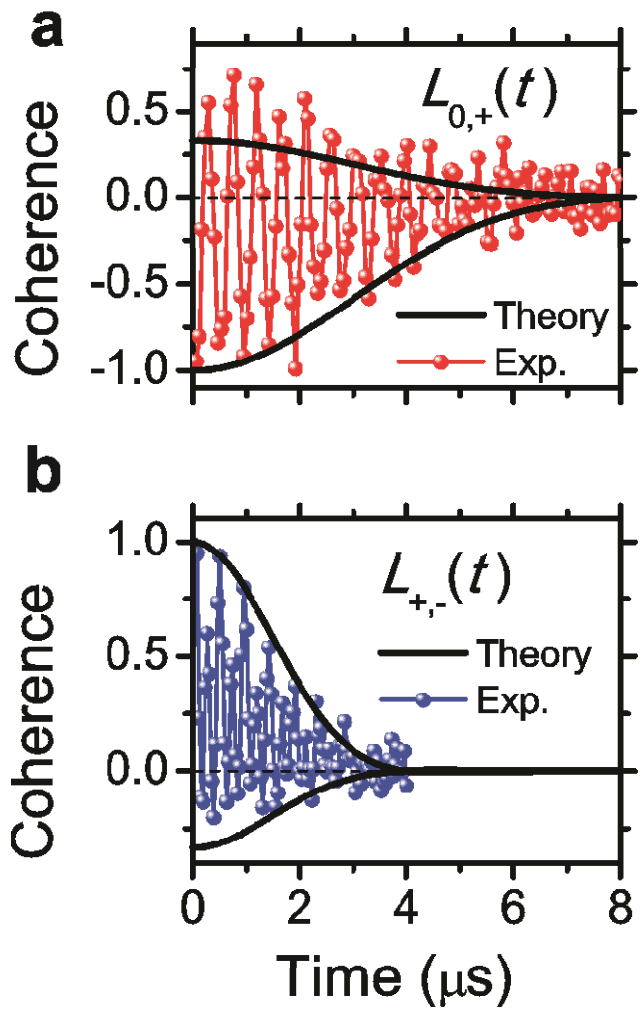
^{13}C-spin bath, slow diffusion ➔ NV which-way info. stored in bath



FID due to thermal (classical) noises from ^{13}C spins







$$\left|L_{+,-} = L_{0,1}^{4}\right|$$

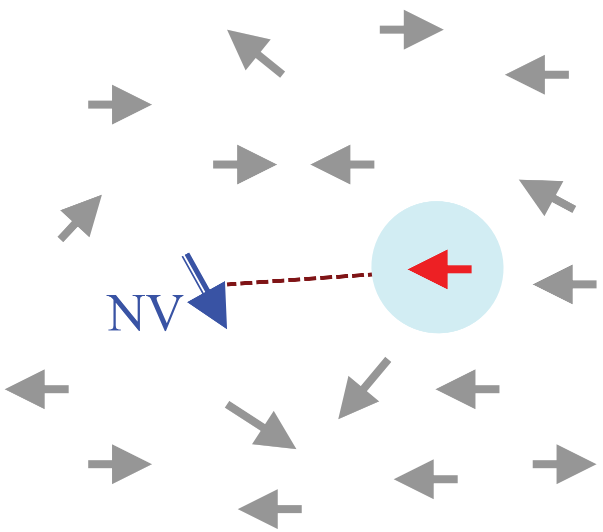
Quantum fluctuations I: Single nuclear spin precession

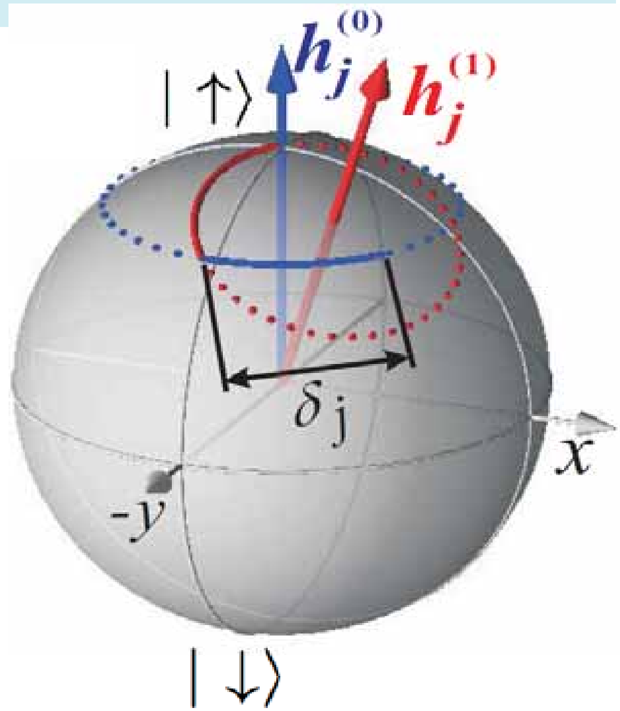
When the thermal noise cancelled by spin echo,
quantum fluctuations become important

$$H=\sum_{\alpha=0,\pm1}\mathbf{I}_j\cdot\mathbf{h}_j^{(\alpha)}\otimes|\alpha\rangle\langle\alpha|$$

Effetive fields $\mathbf{h}_j^{(\alpha)}=\mathbf{B}+\alpha A_j$, conditioned on $|\alpha\rangle$

$\mathbf{h}_j^{(0)}=\mathbf{B}$ $\left(\text{no hf at }|0\rangle\right)$



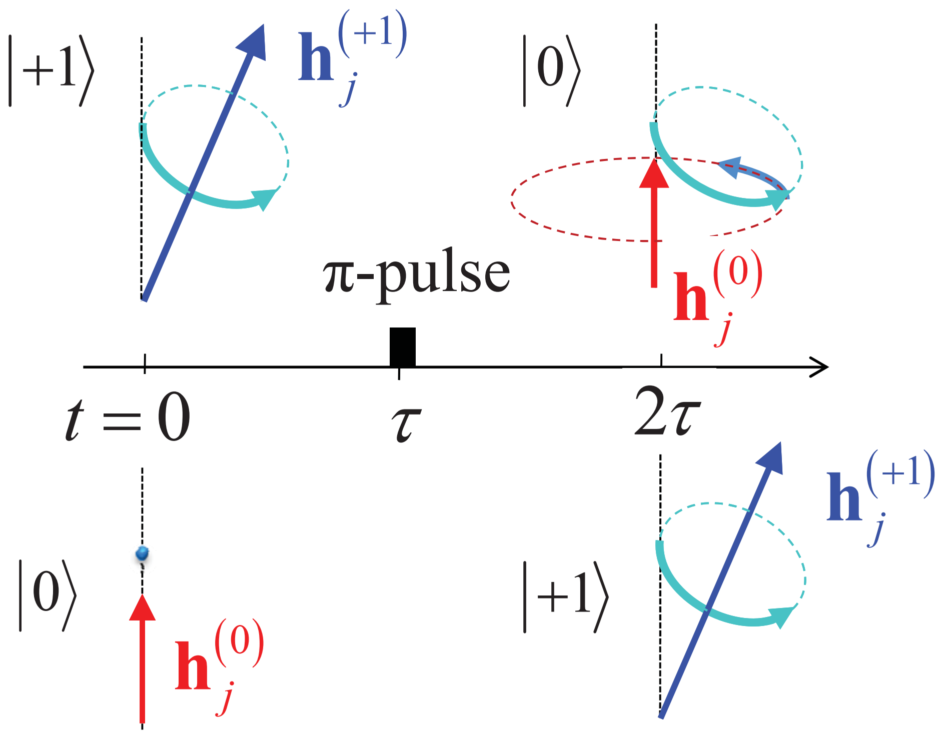


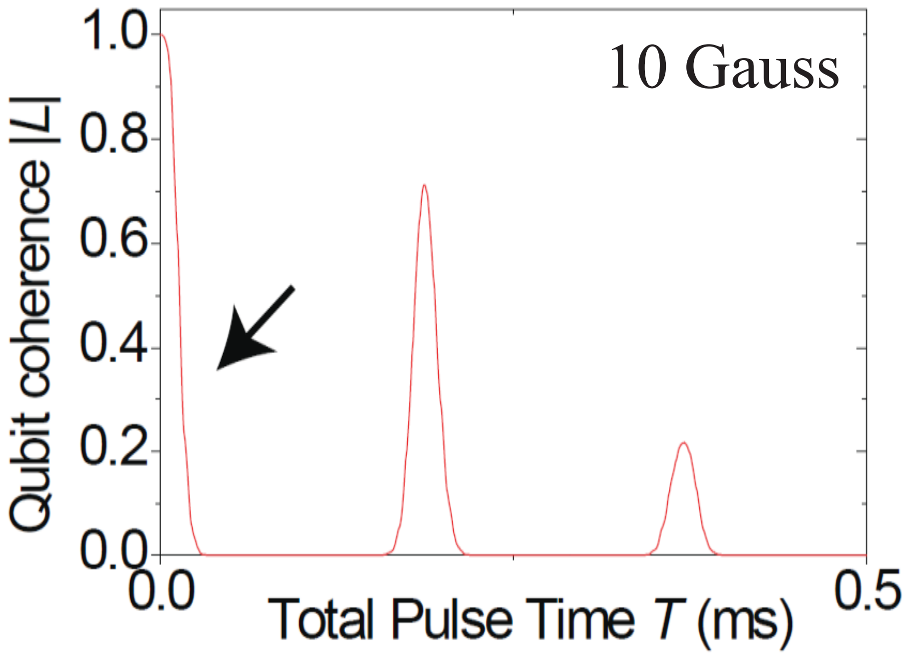
bifurcated evolution of a bath spin

$$\left(|0\rangle+|1\rangle\right)\otimes|\uparrow\rangle\Rightarrow|0\rangle\otimes\left|I^{(0)}(t)\right\rangle+|1\rangle\otimes\left|I^{(1)}(t)\right\rangle$$

$$L_{0,1}(t)=\left\langle I^{(0)}(t)\middle|I^{(1)}(t)\right\rangle$$

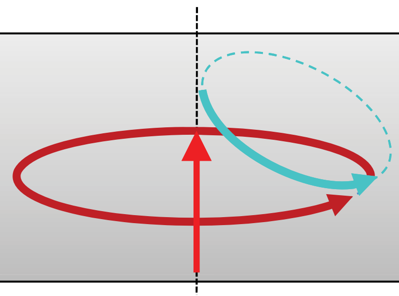
Single nuclear spin dynamics in Hahn echo



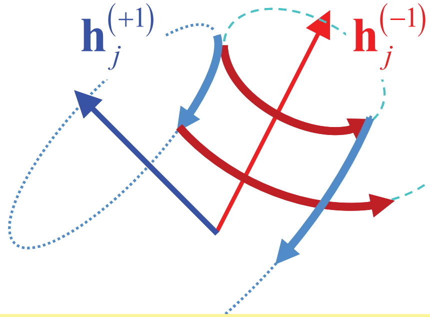


Recovery at

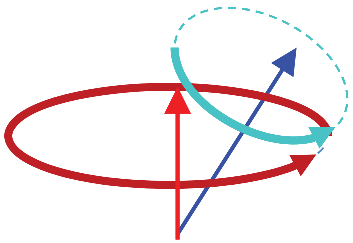
$\gamma_e B \tau = 2\pi$



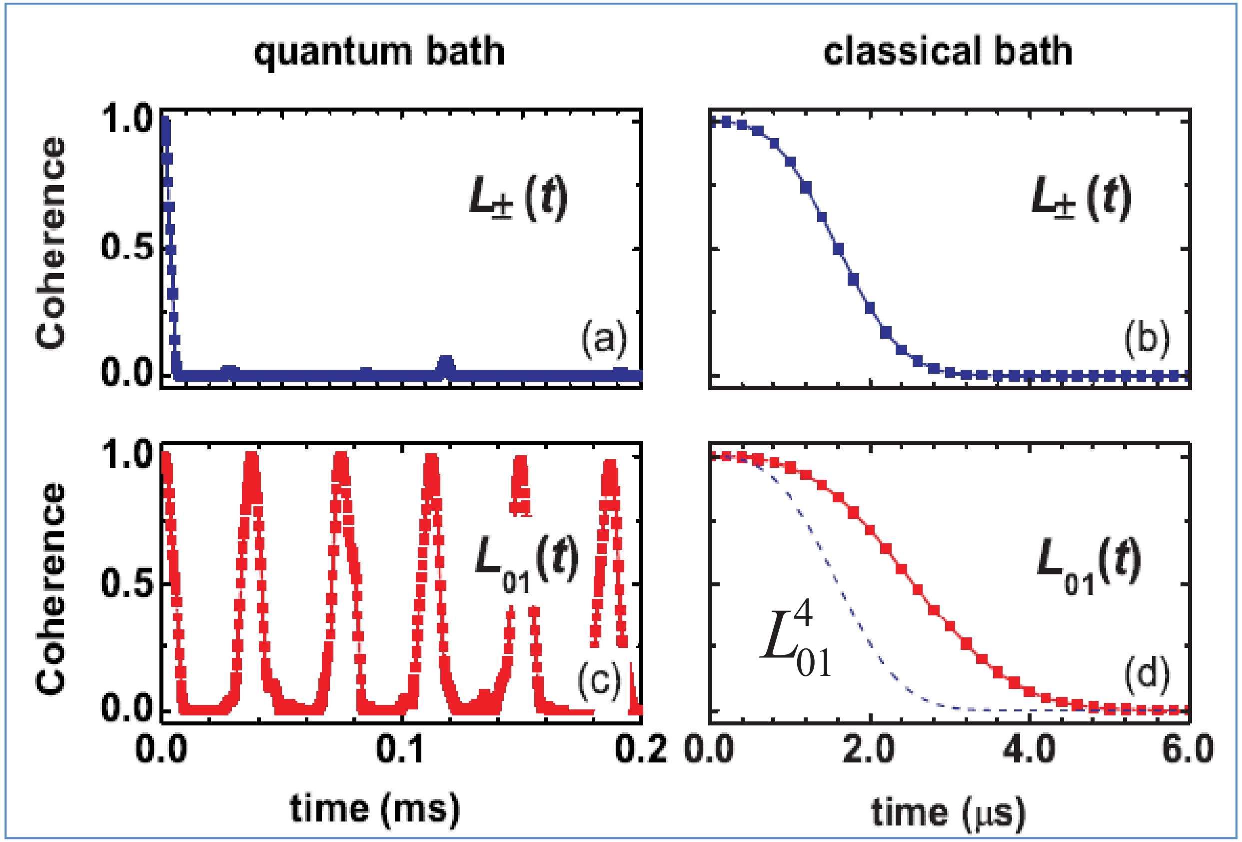
Detecting quantumness of a spin bath I: Weak field



No full revival for multi-transition

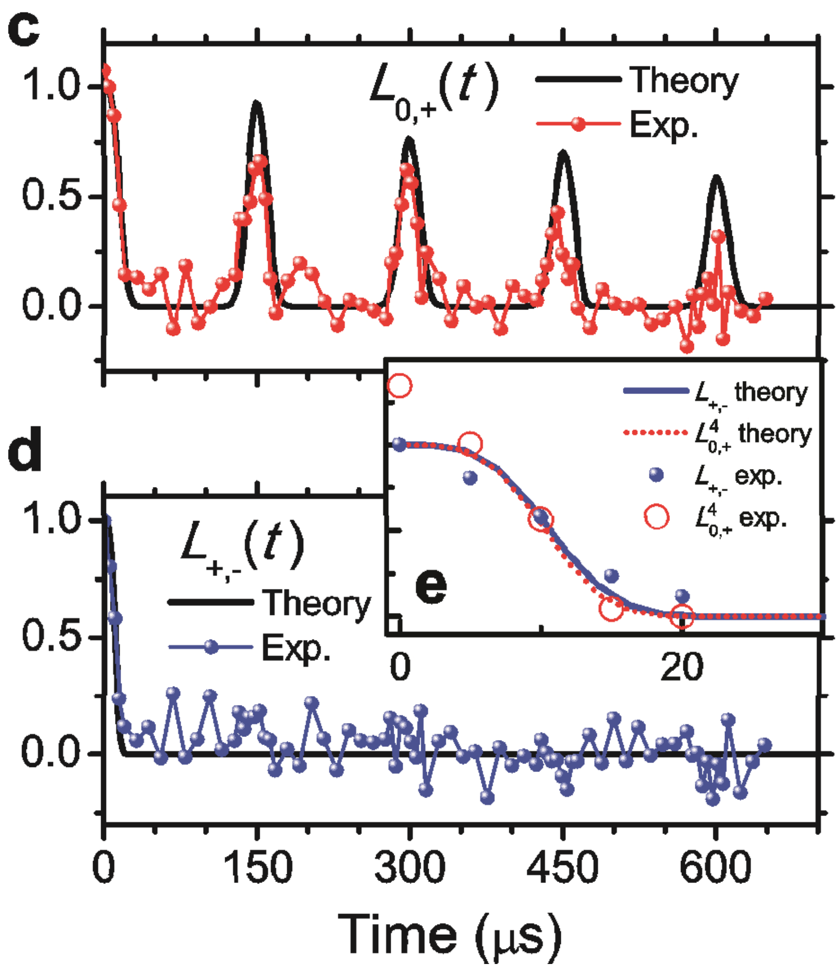


Revival @ $4\pi/(\gamma_N B)$



$B = 50$ Gauss

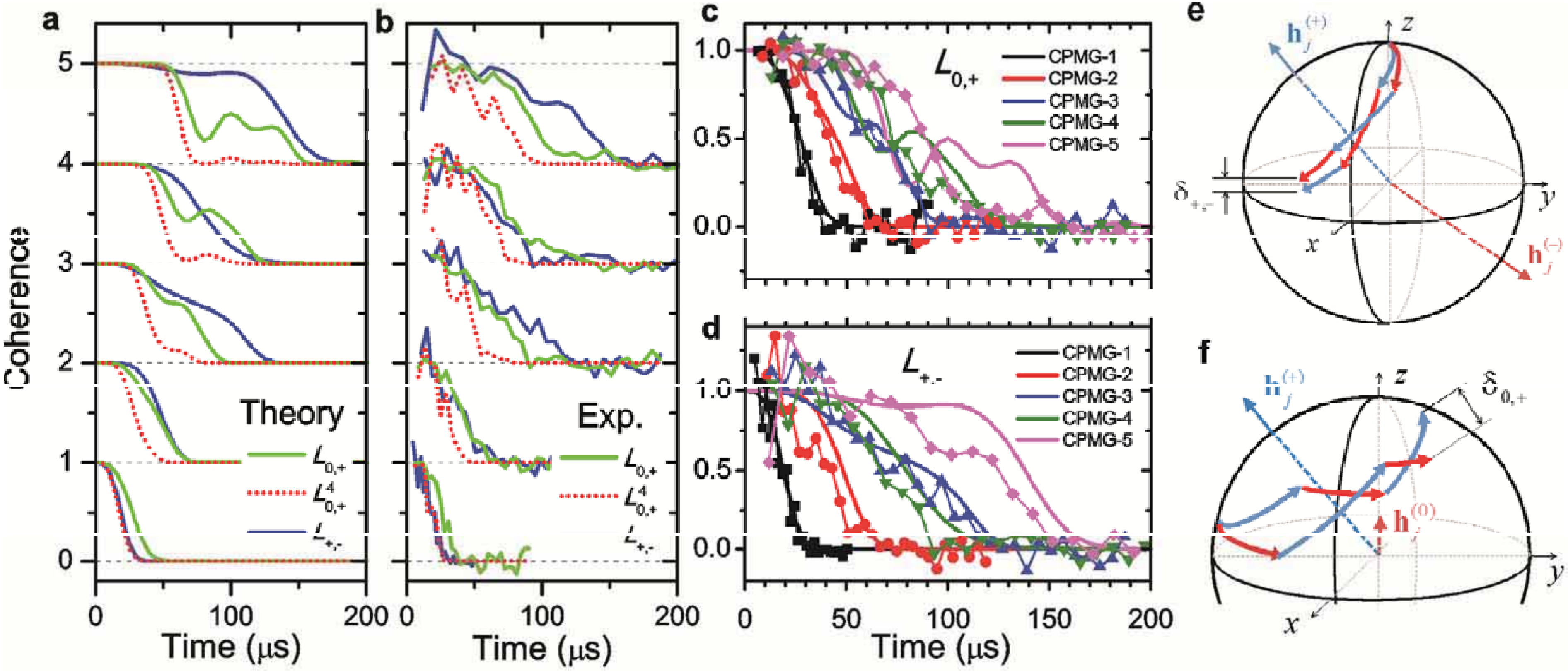
Experimental study II: spin echo



- ➢ Single-transition has recovery.
- ➢ Multi-transition has no.
- ➢ In good agreement with quantum theory with no fitting parameters.

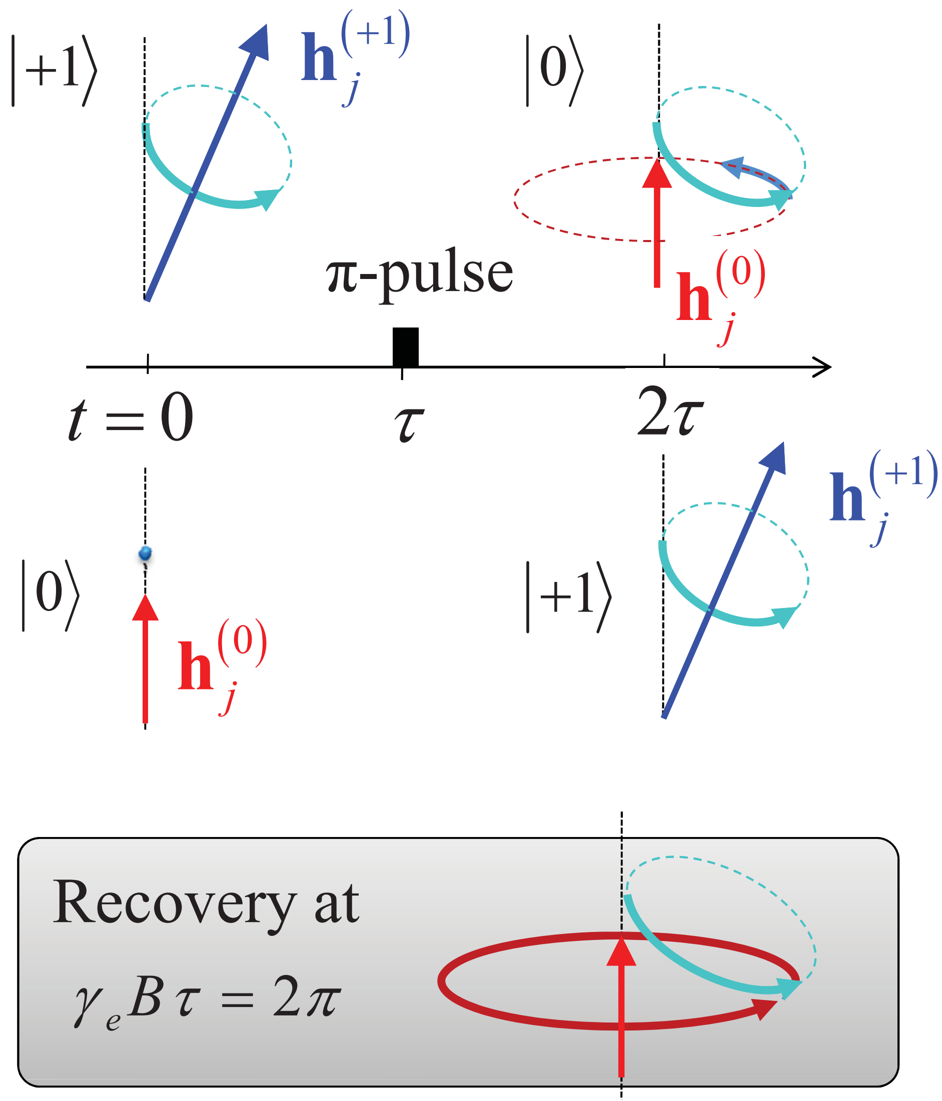
Single- & multi-coherence under DD

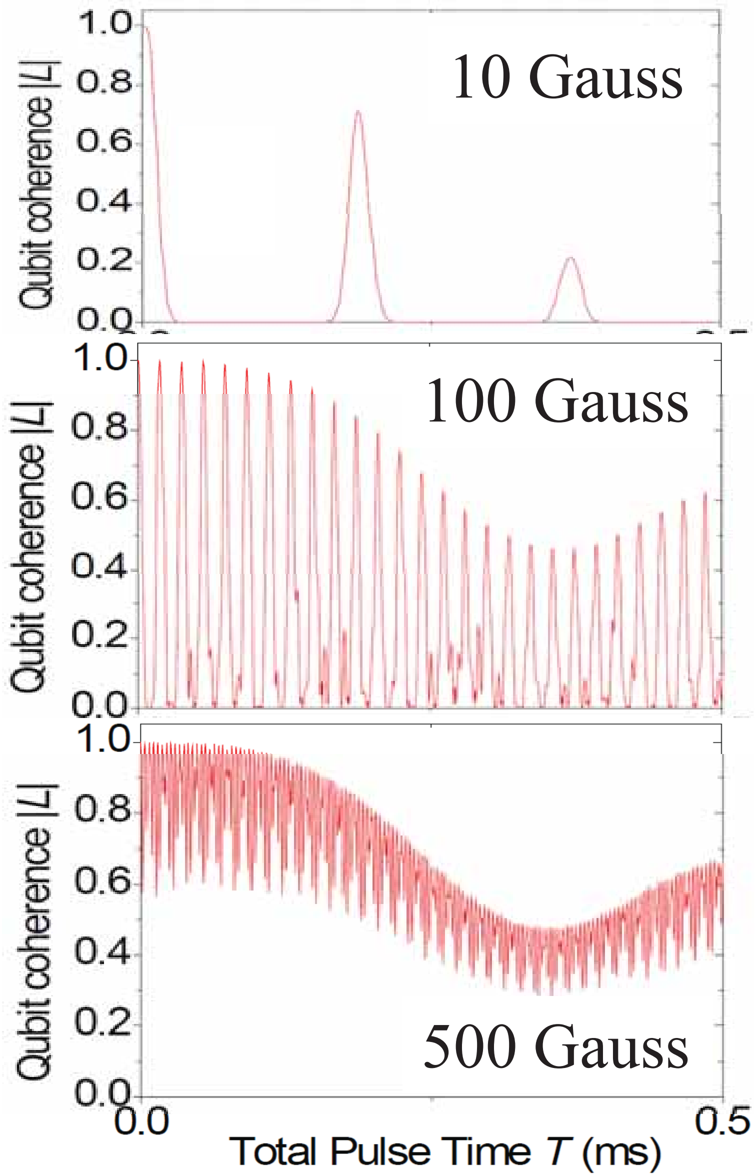
N. Zhao et al, unpublished



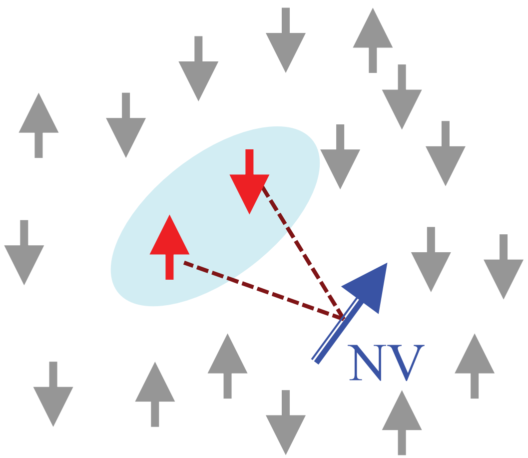
Multi-transition suffers twice stronger noises than single-transitions, but has longer coherence time!

Single nuclear spin dynamics suppressed by strong field





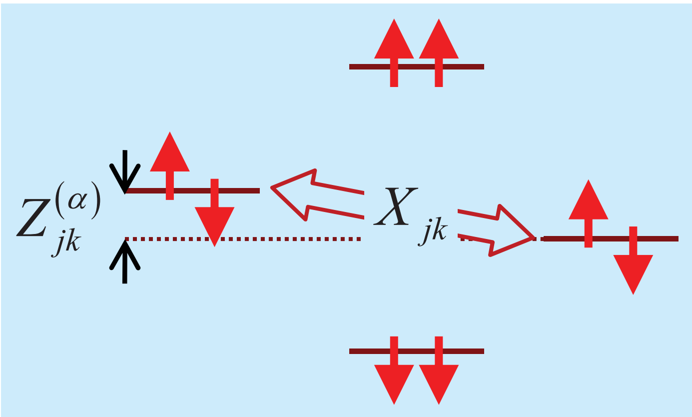
Quantum Fluctuations II: Pairwise nucelar spin flip-flop

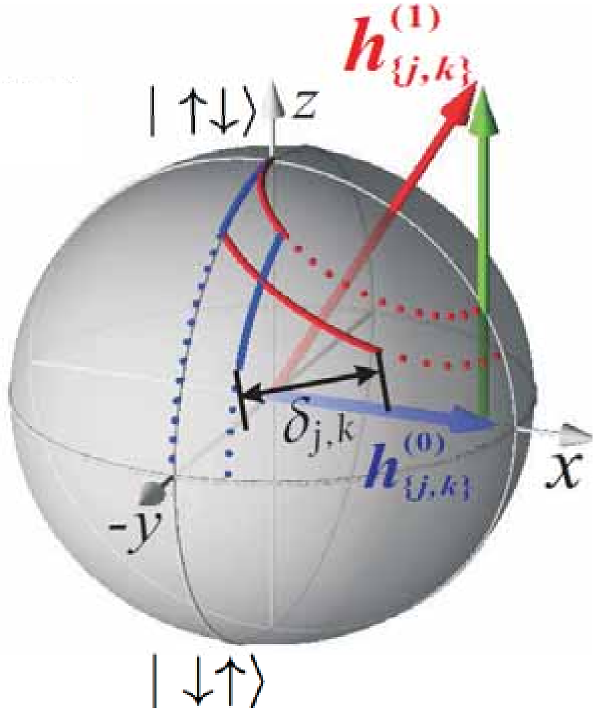


Mapped to a pseudo-spin under pseudo-fields conditioned on $|\alpha\rangle$

$\mathbf{h}_{jk}^{(0)} = \left(X_{jk}, 0, 0\right)$ no hf energy cost

$\mathbf{h}_{jk}^{(\pm)} = \left(X_{jk}, 0, \pm Z_{jk}^{(1)}\right)$





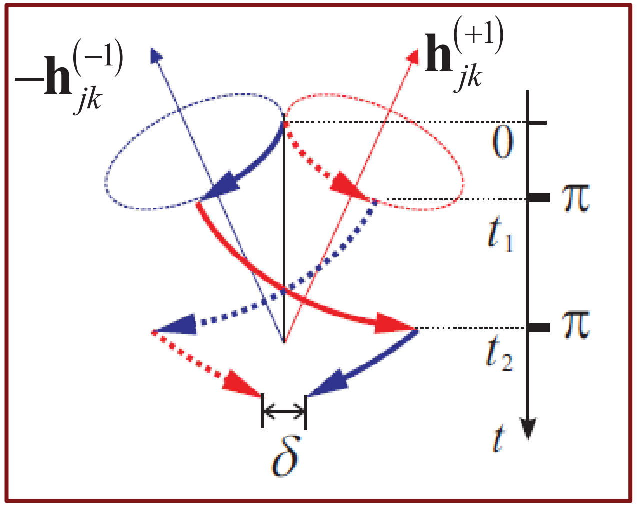
$Z_{jk}^{(\alpha)}$ hf energy cost

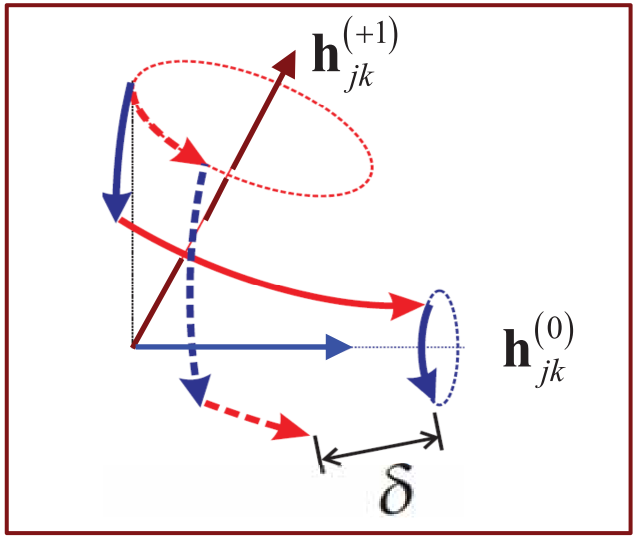
X_{jk} dipolar flip-flop rate

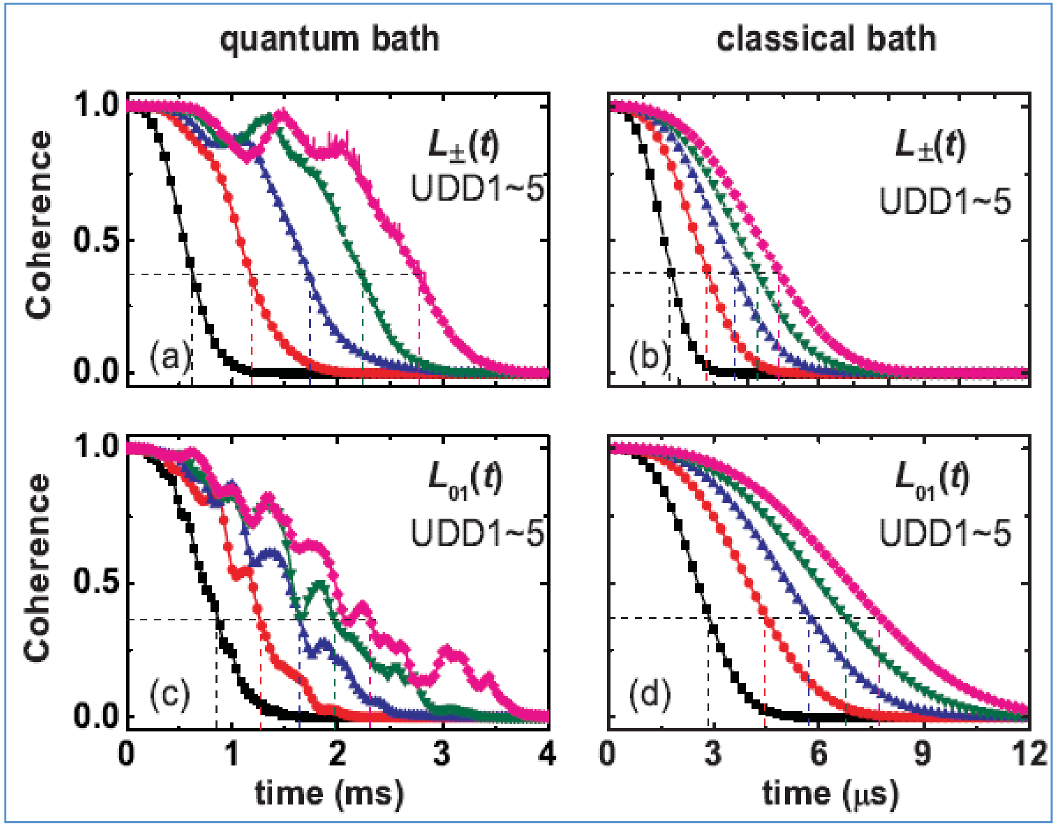
Detecting quantumness of a spin bath II: Strong field

Symmetric bath evolutions for ±1 NV states lead to better coherence recovery.

B=.15 T, decoherence by pair flip-flops

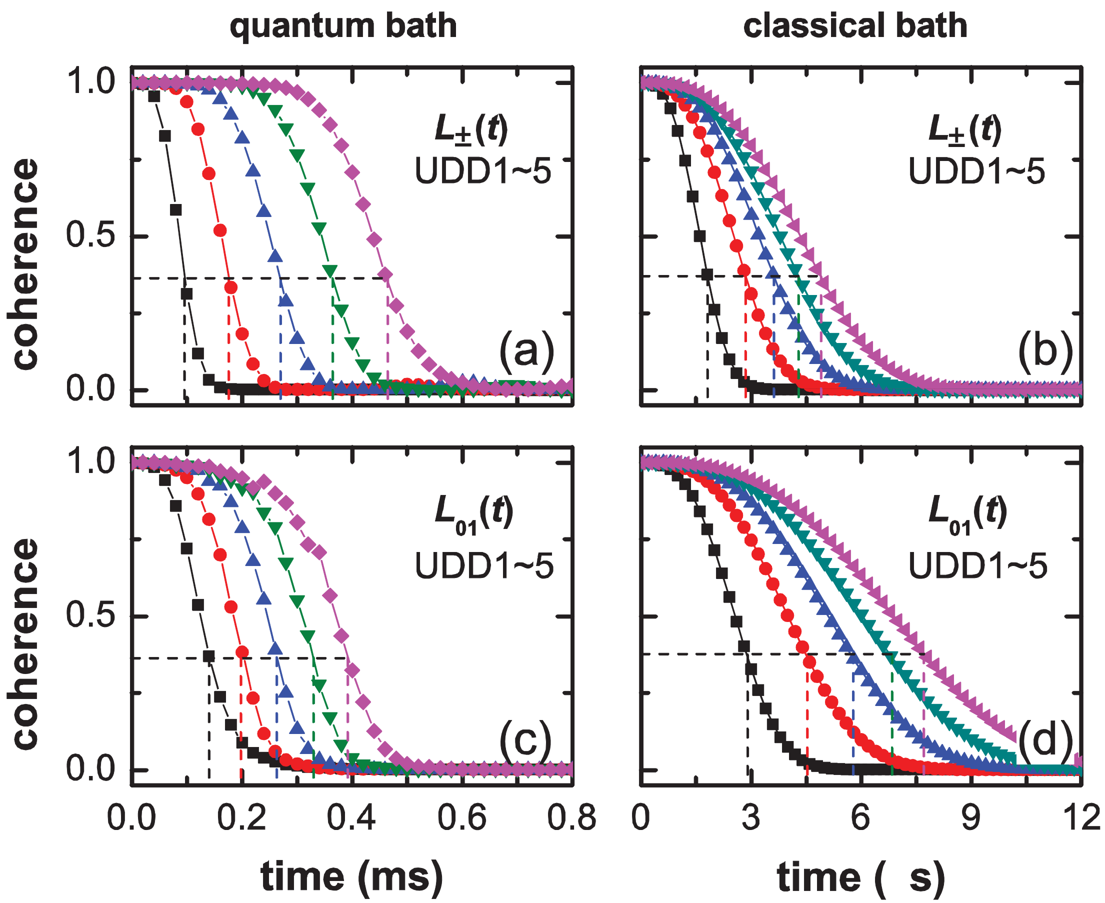






Multiple-transition has LONGER coherence time than single-transition, even though the former suffers stronger fluctuations

Detecting quantumness of a spin bath III: Zero field

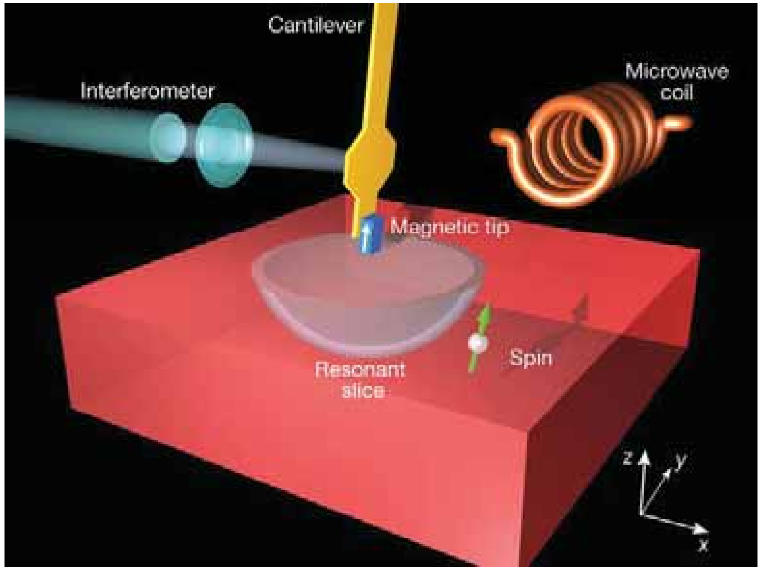


Multiple-transition has LONGER coherence time than single-transition

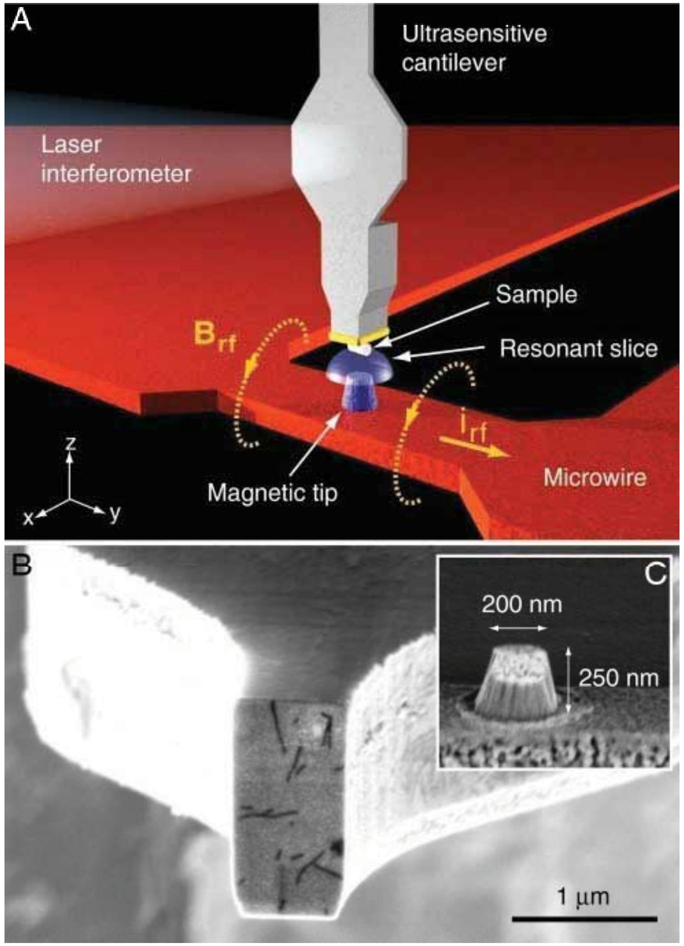
Application I: Atomic scale magnetometry using pair coherence

N. Zhao, J. L. Hu, S. W. Ho, J. T. K. Wan & RBL, arXiv:1003.4320, updated preprint available upon request by email

Toward single-spin detection: MRFM



Detection of single electron spins [Rugar et al (IBM), Nature, 2004]

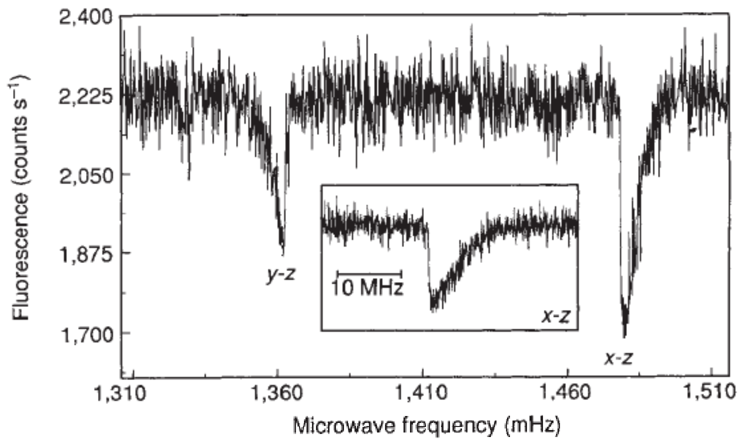


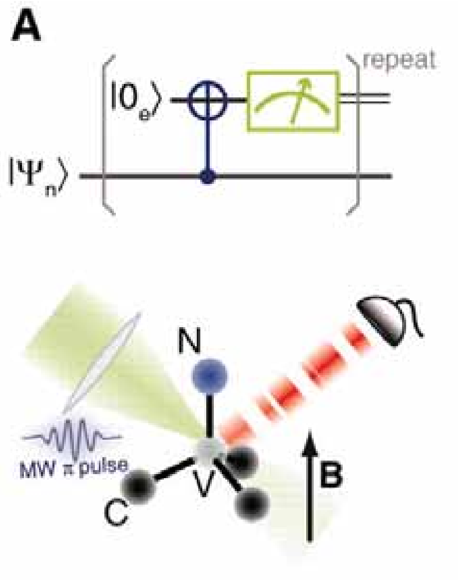
MRI w/ 10 nm res. By sensitivity of ~ 10^4 H nuclear spins [Rugar et al (IBM), PNAS, 2009]

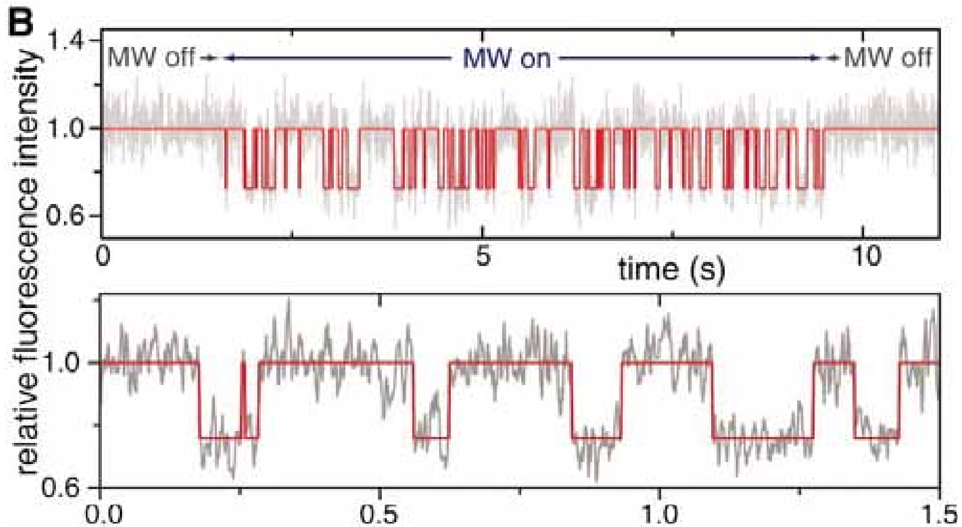
Long way to go to reach single-nucleus sensitivity

Toward single-spin detection: ODMR

ODMR of single molecule
[Wrachtrup et al, Nature, 1993]







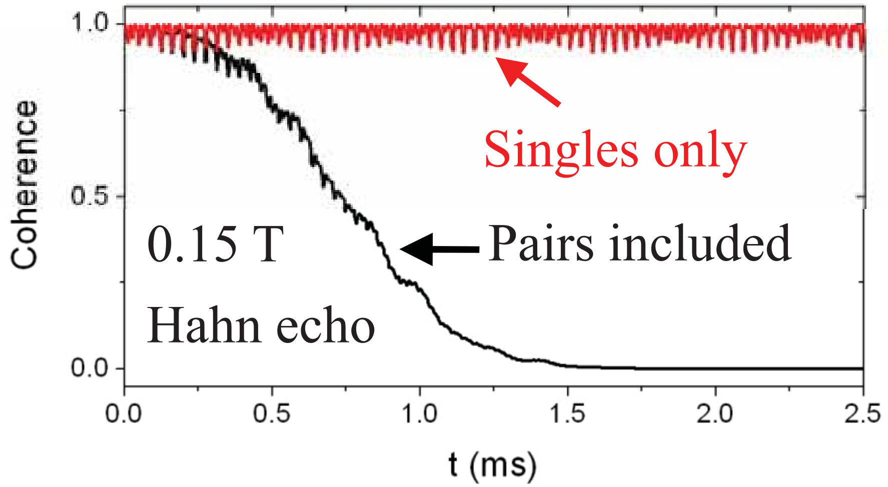
Single nuclear spin readout (Wrachtrup et al, Science, 2010)

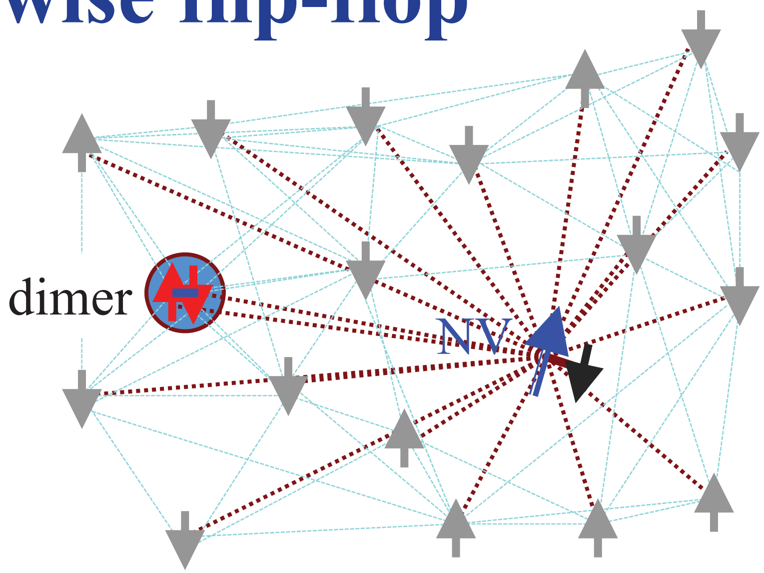
But limited to nuclei located closely to an electron spin

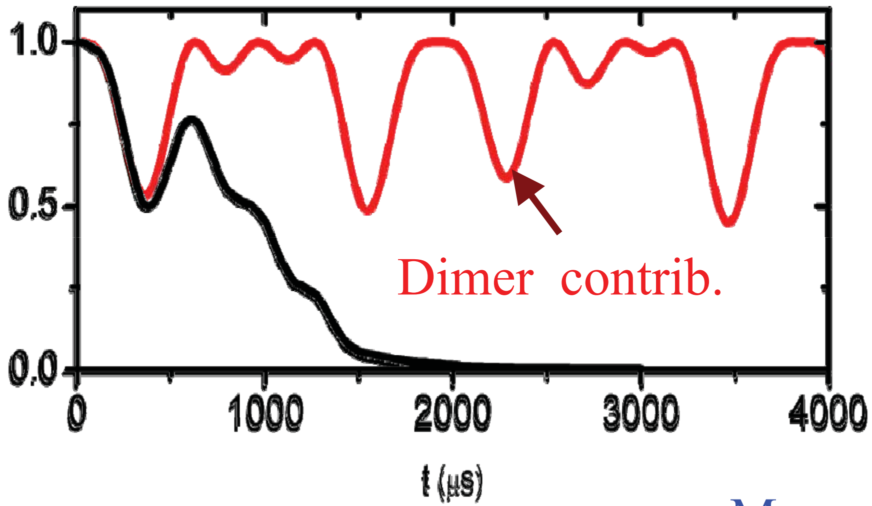
Toward single-spin detection

- Sensing single nuclear spins at distance from an e-spin, by ODMR?
- Long coherence time of center electron spin is the key
- Under DD, the center electron spin is sensitive to nuclear spin noises

Decoherence by pairwise flip-flop



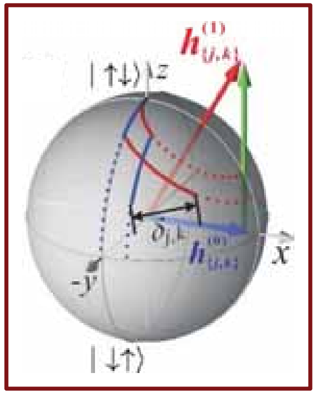




$\mathbf{h}_{jk}^{(\alpha)} = \left(X_{jk}, 0, Z_{jk}^{(\alpha)} \right)$

$X_{jk} \ll Z_{jk}^{(1)}$, incoherent pairs

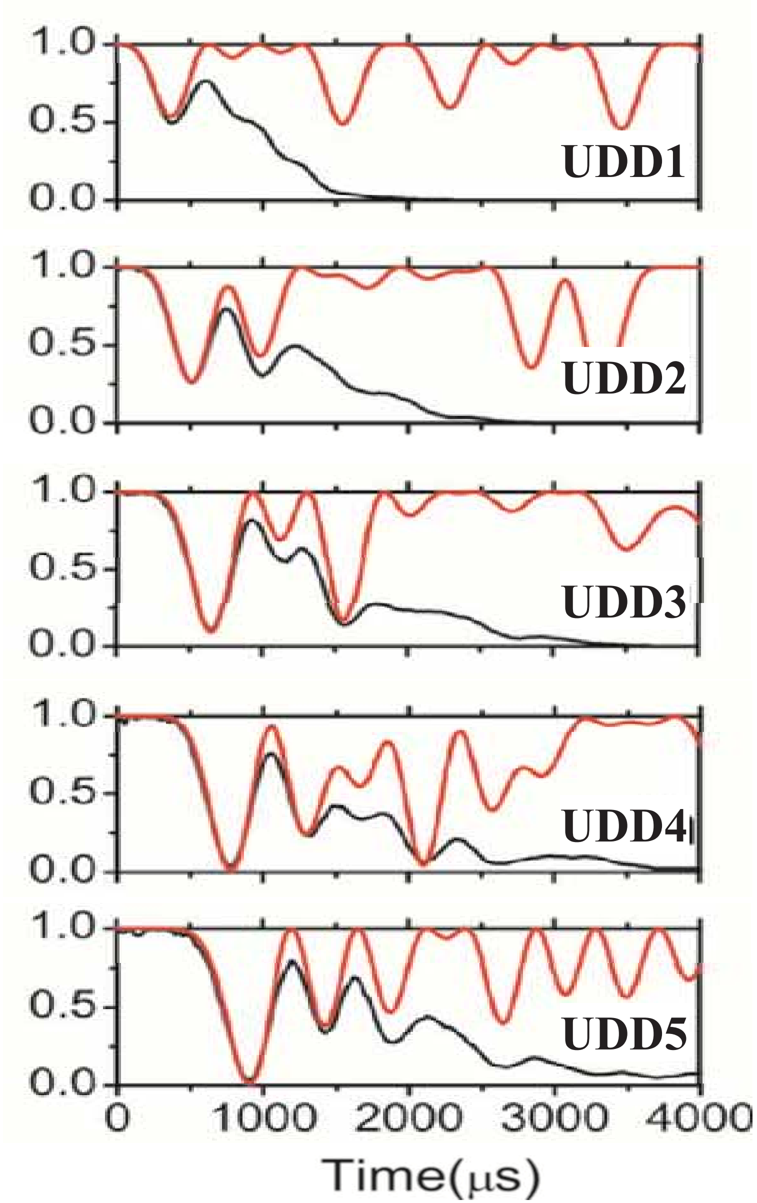
$X_{jk} \sim Z_{jk}^{(1)} \sim$ kHz, coherent pairs



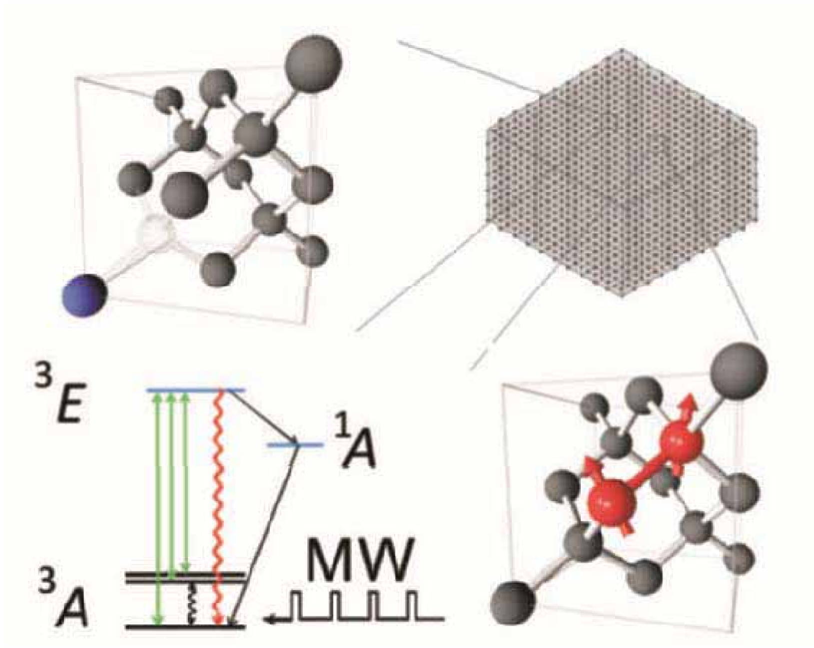
Many incoherent pairs ➔ smooth decoherence

Rare coherent pairs ➔ coherent oscillations

A dancing couple out of random walkers



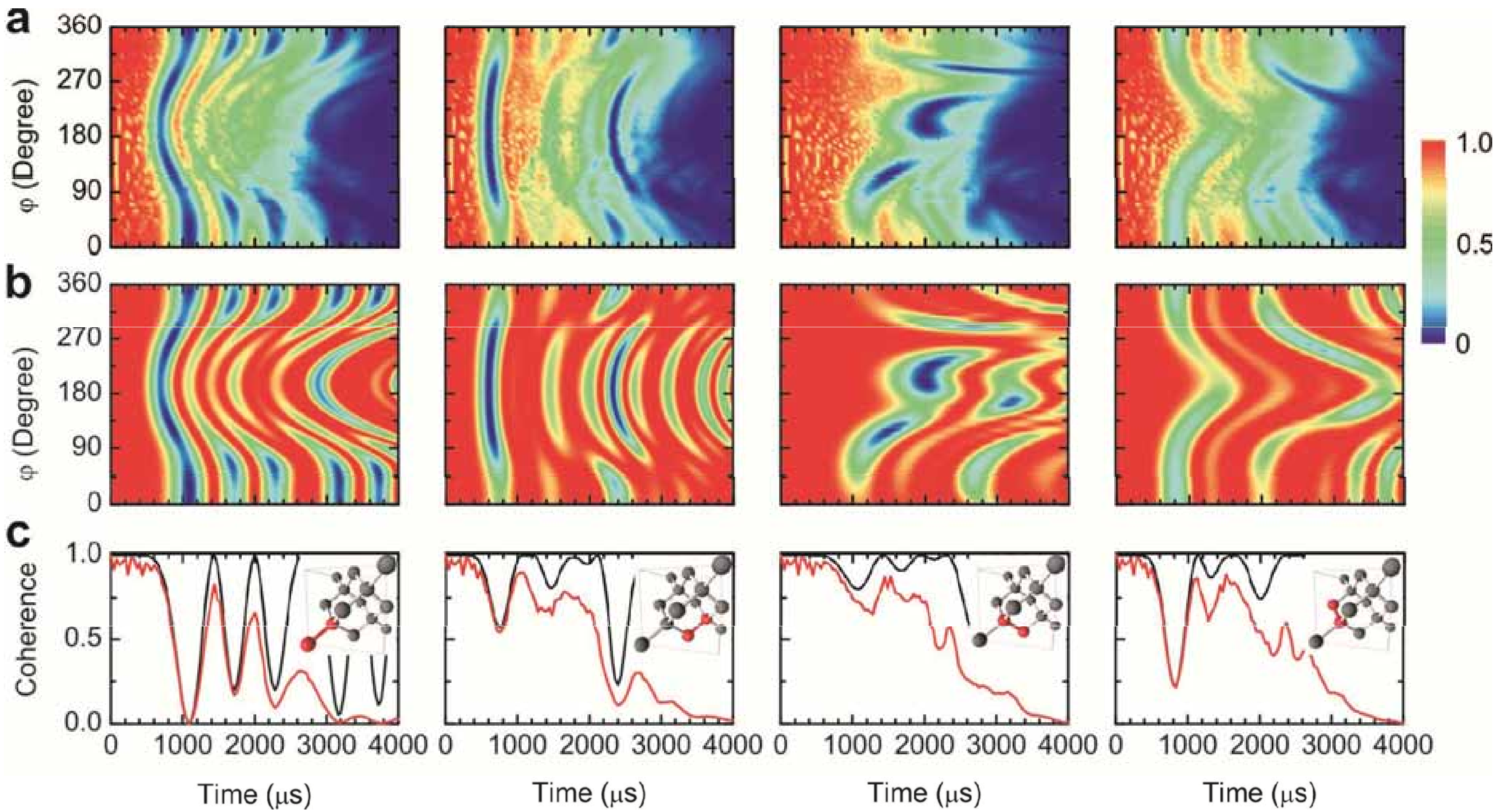
a dimer @ 1.2nm; B=.15 T



Uhrig DD: $t_j = T\sin^2\left(\dfrac{j\pi}{2N+2}\right)$

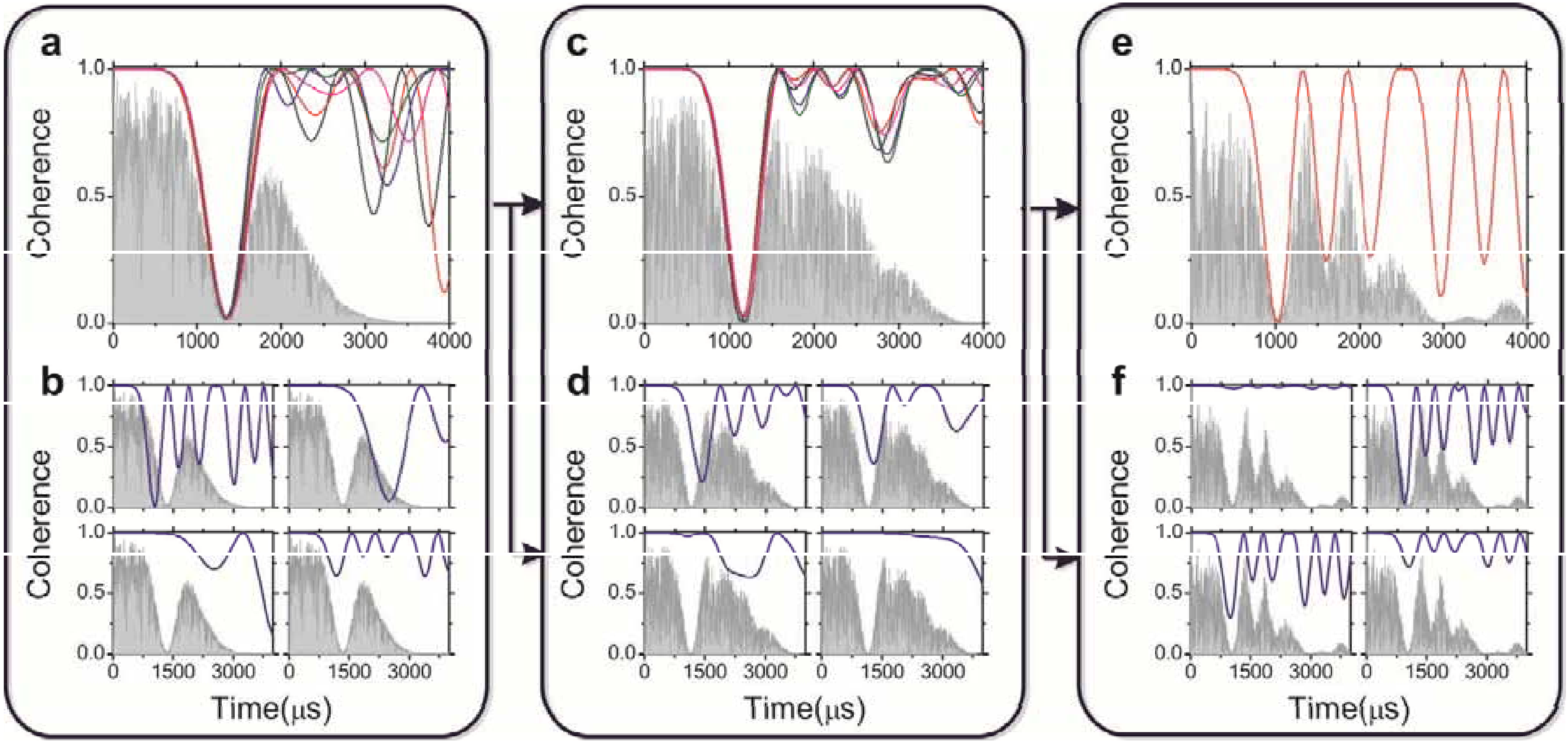
Coherence time prolonged by DD, oscillation feature of the dimer is more pronounced.

Atomic-sensitivity magnetometry of a dimer



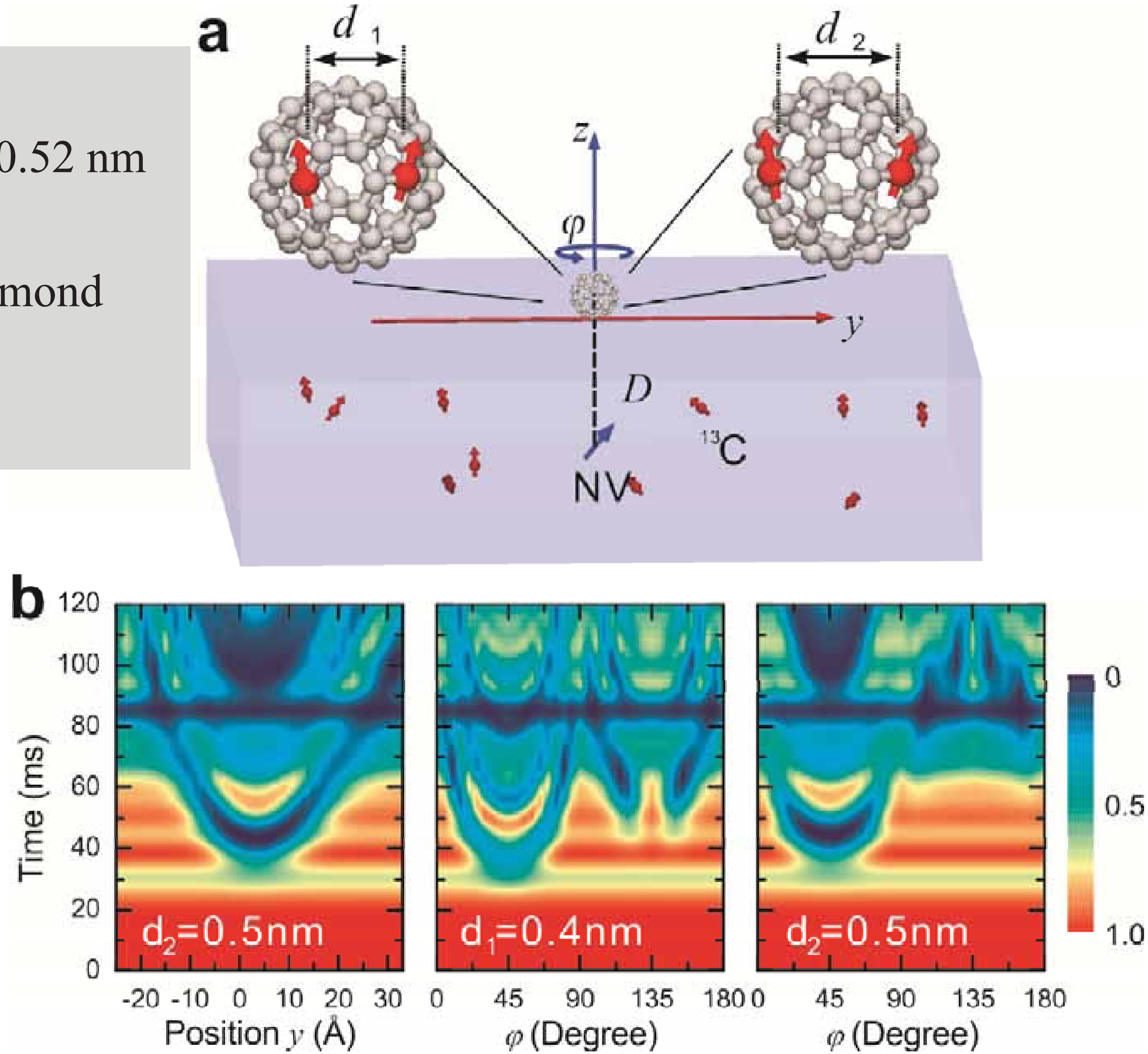
A dimer @ ~1.2nm from NV; *B*=.15 T, tilted from [111] by 10° (to break symmetry about the [111] axis w/o affecting optical initialization & detection)

Fingerprint screening



Single-molecule detection at diamond surface

- C_{60} with two ^{13}C
- d_1=0.41 nm; d_2=0.52 nm
- NV at D=4nm
- 0.03% ^{13}C in diamond
- UDD7 control
- **B**=0.2 T [111]

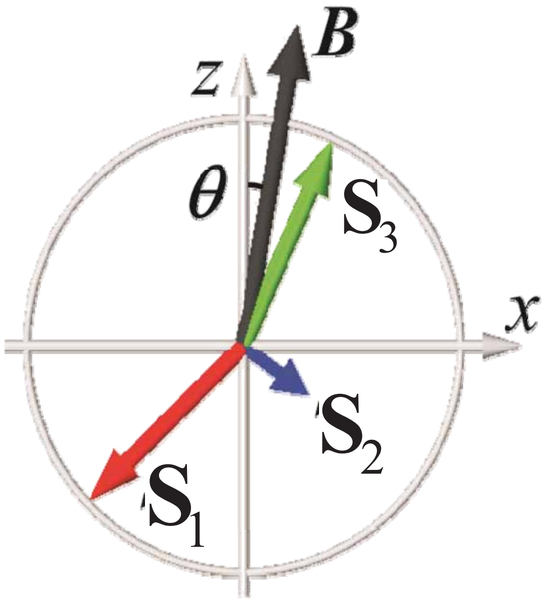


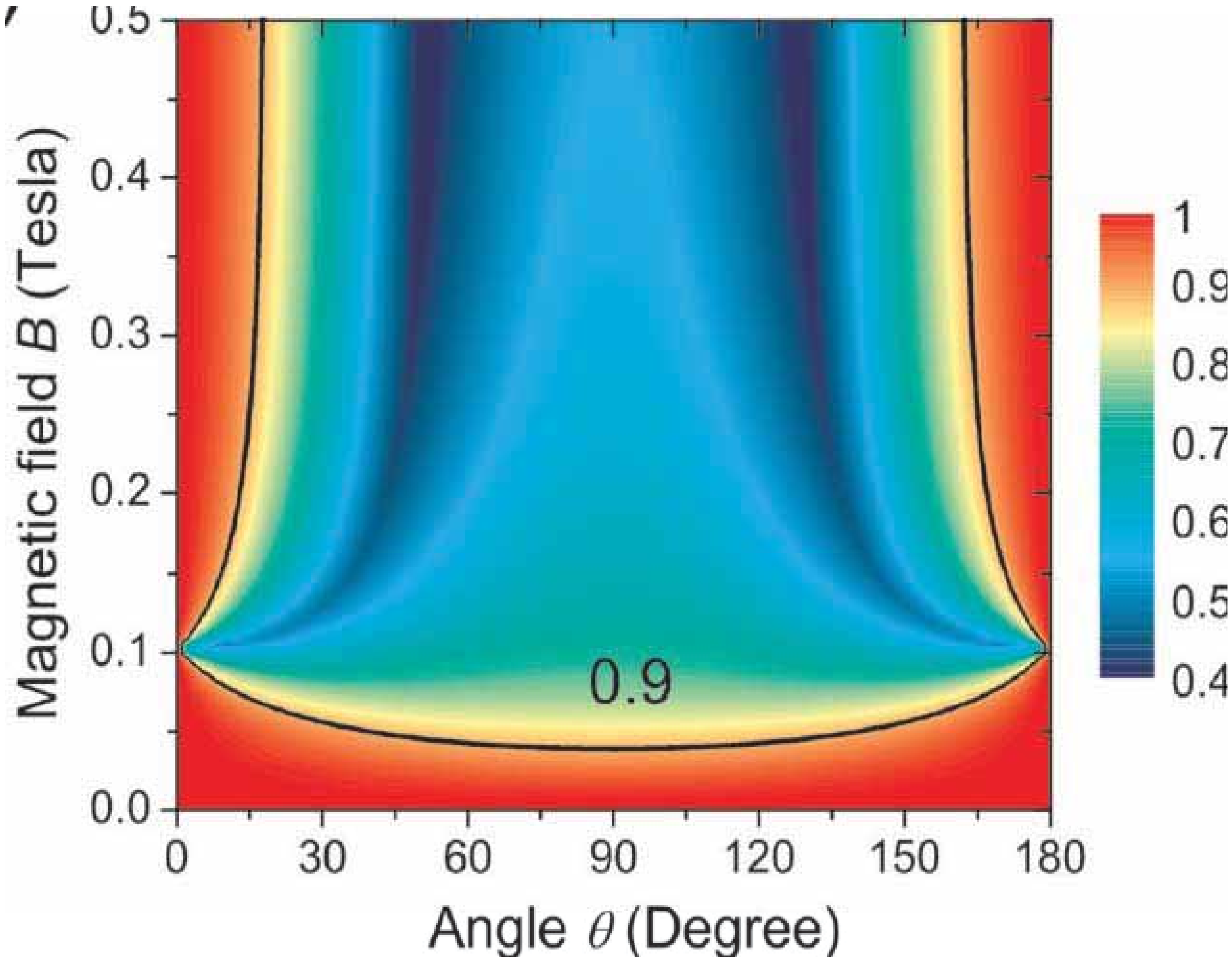
A few practical issues

- when decoherence by nuclear spins is suppressed – low-temperature
- Fidelity of pulse control (loss of overall signal strength)
- Tilt field (optical initialization and readout efficiency)

Issue of tilted field (for optical initialization and readout)

$$\max_{\alpha}\left(\left|\langle m=0|\alpha\rangle\right|^{2}\right)$$





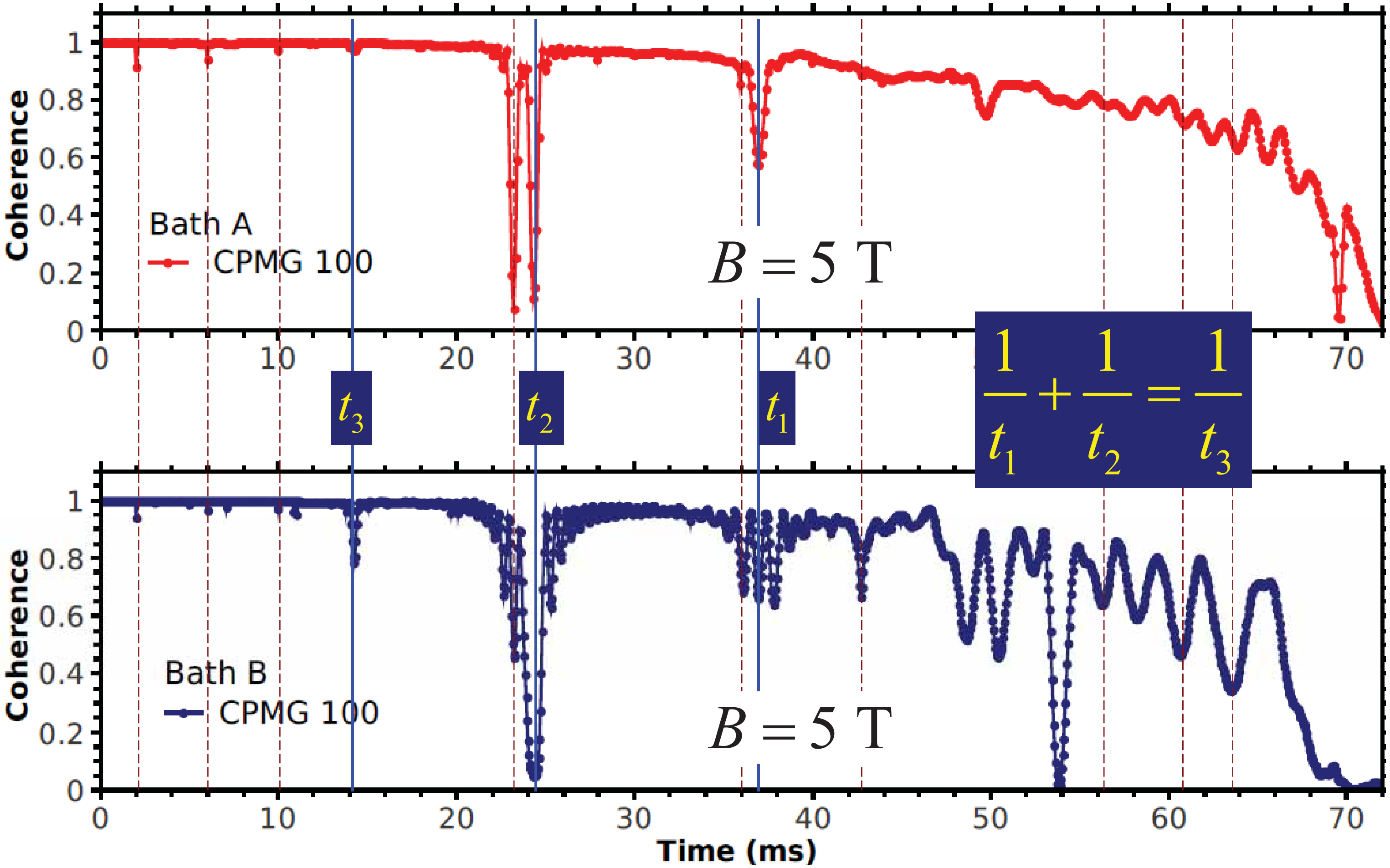
One-sentence take-home message:

Sensing one individual spin is difficult, but sensing one pair/cluster is feasible.

Application II: Many-pulse DD and single molecule NMR

N. Zhao, J. L. Hu, S. W. Ho, J. T. K. Wan & RBL, arXiv:1003.4320, updated preprint available upon request by email

Many-pulse control for many-body physics



Under many-pulse DD control, universal dip structures emerge (with universal timing and intrinsic correlations)

Universal classes of sudden collapses

Noise spectrum caused by elementary excitations in the many-body system

$$S(\omega)=\sum_k \left|g_k^2\right|\delta(\omega-\omega_k)$$

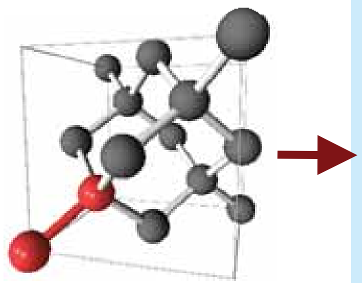
Pulse sequences give filtering function

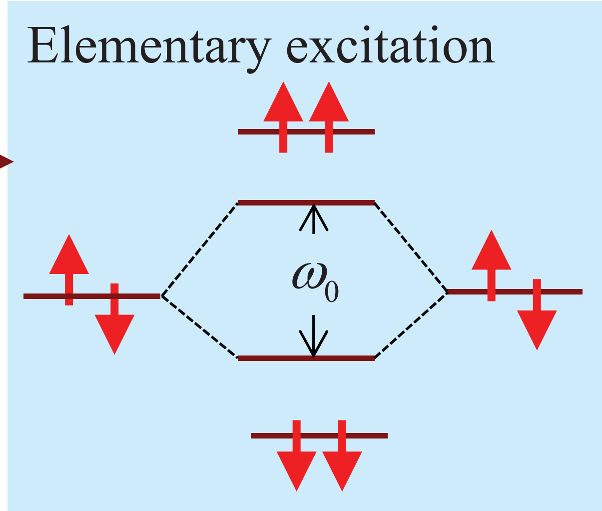
$$F(\omega,t)=\sum_{n=0}^{N}(-1)^n\left(e^{i\omega t_{n+1}}-e^{i\omega t_n}\right)$$

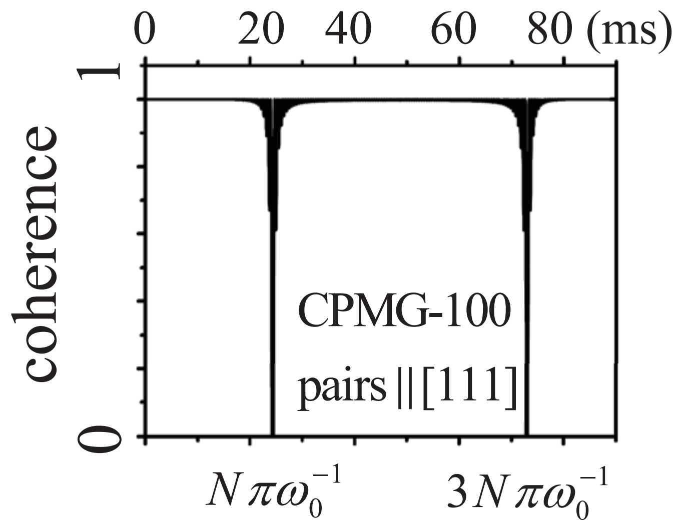
Decoherence under control:

$$L(t)=\exp\left(-\int_0^\infty \frac{S(\omega)}{\omega^2}\left|F(\omega,t)\right|^2\frac{d\omega}{\pi}\right)$$

For many-pulse control, the filtering function has a large value ($\sim N^2$) at $\omega_k t=(2j+1)N\pi$, but almost vanishes elsewhere. Clusters of the same structures have the same excitation spectra. Thus universal features result.

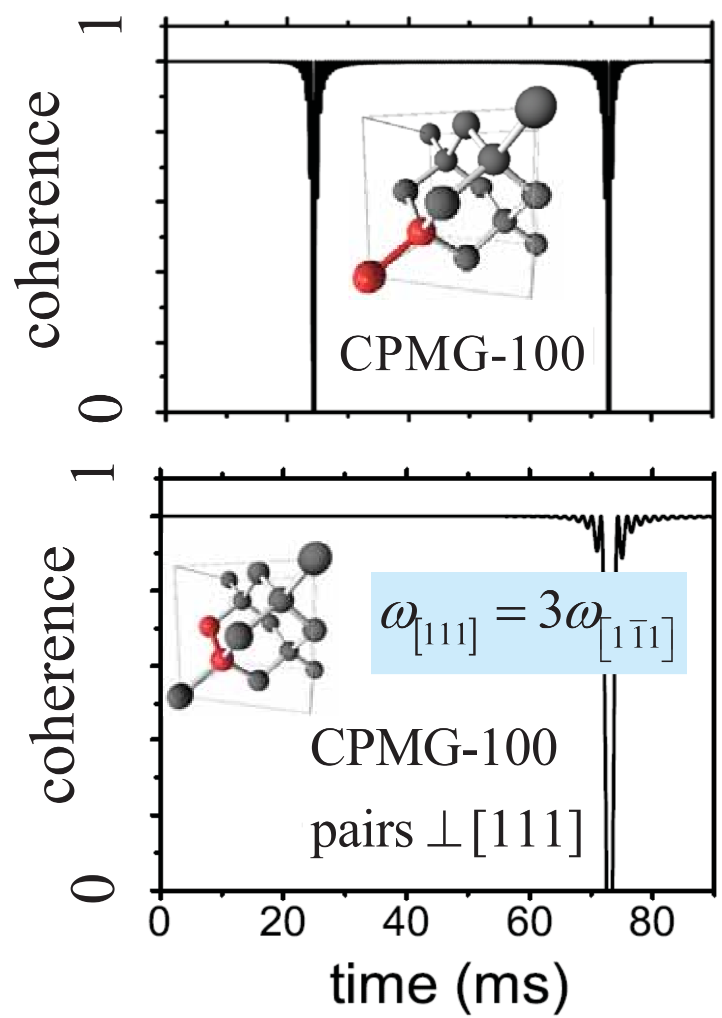




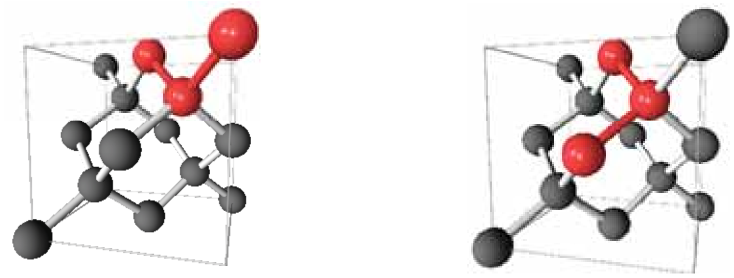


Decoherence by a dimer 3 nm away

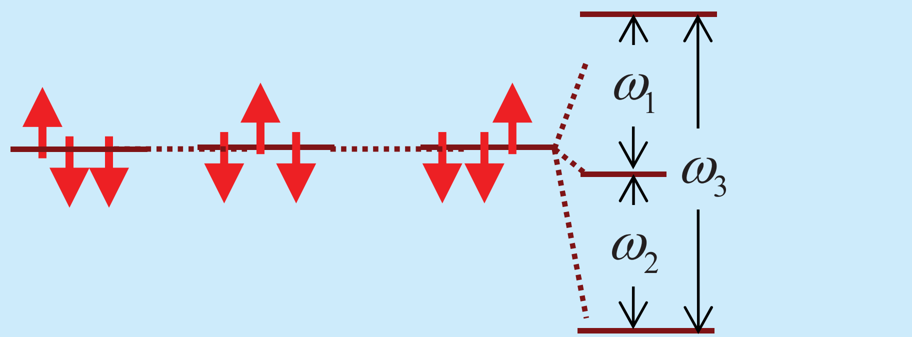
Correlation between transitions revealed by high order DD



Two inequivalent connected 3-spin clusters



Elementary excitations in a 3-spin cluster

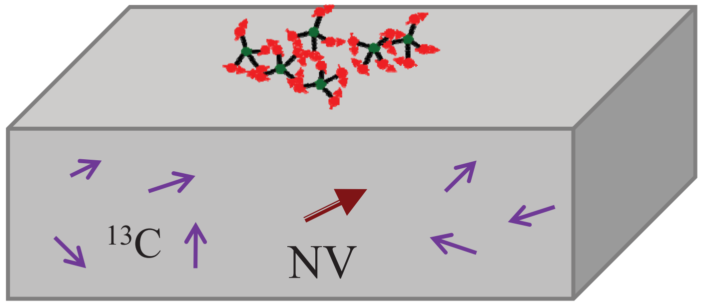


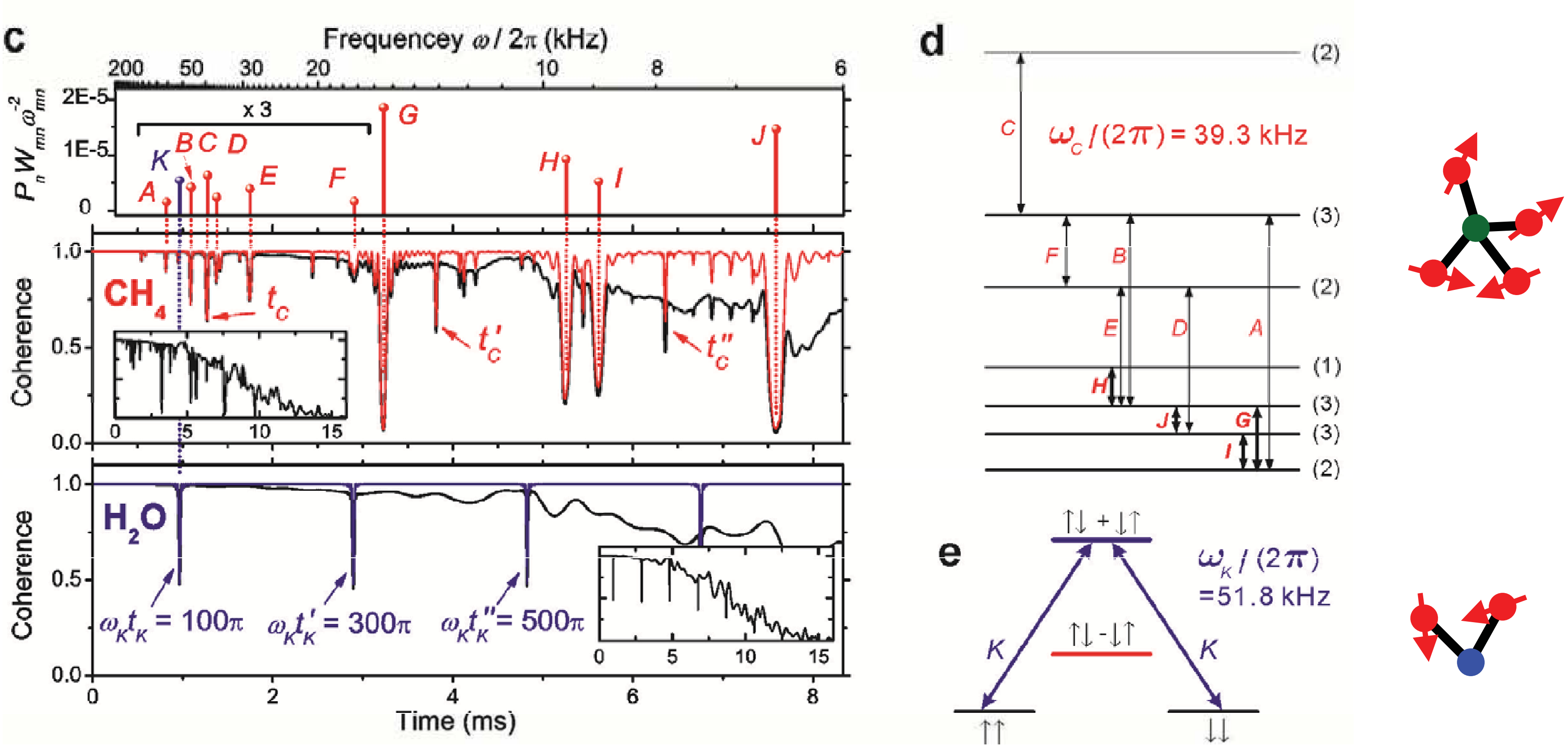
$$\Rightarrow t_3^{-1} = t_2^{-1} + t_1^{-1}$$

Correlation between transitions detected
(c.f. multi-dimensional NMR)

Toward few-nucleus "NMR": Single molecule detection

Spin coherence of an NV center 10 nm below **5(五, five)** $^{1}H_2{}^{16}O$ or $^{12}C^{1}H_4$ molecules, under **100**-pulse CPMG dynamical decoupling, at 0 B field





One-sentence take-home message:

Weak signal of single molecules can be greatly enhanced by many-pulse dynamical decoupling.

Reading materials

Review of quantum computing with electron spins:

1. RBL, W. Yao & L. J. Sham, Advances in Physics **59**, 703-802 (2010).

Quantum theories of decoherence & coherence recovery:

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Summary

1. Quantum picture and many-body theory of qubit decoherence in spin bath
2. Coherence recovery and dynamical decoupling
3. Quantumness & Controllability of nuclear spin baths
4. Atomic scale magnetometry application

Openings are available for postdoc and students.

Thank you