Problems of Modern Physics

Lecture 5

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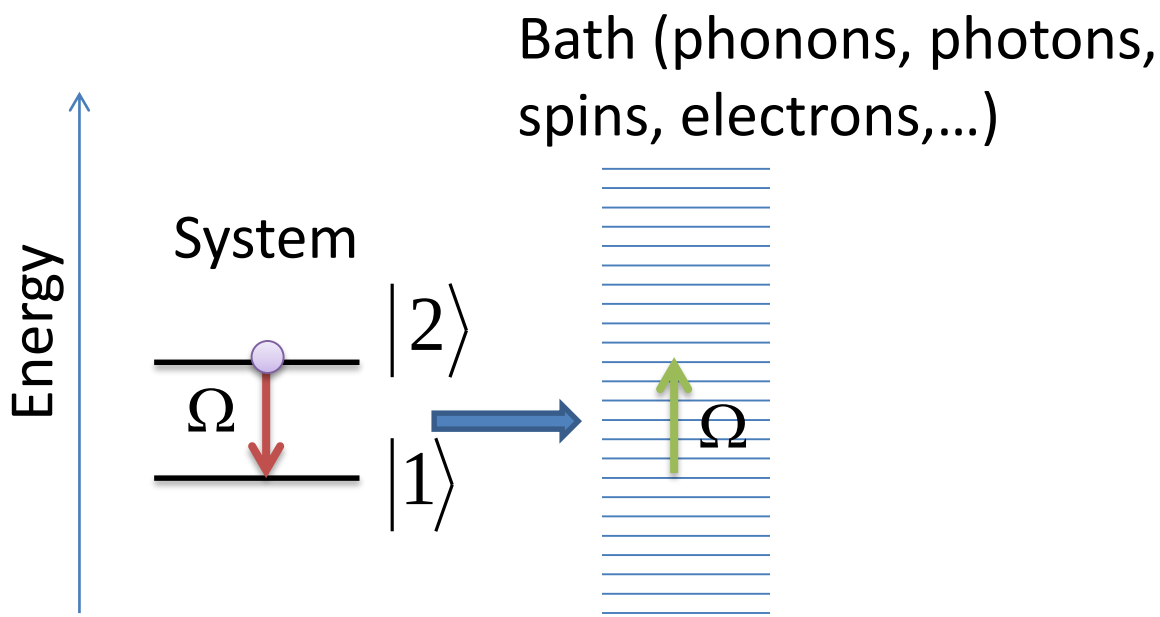
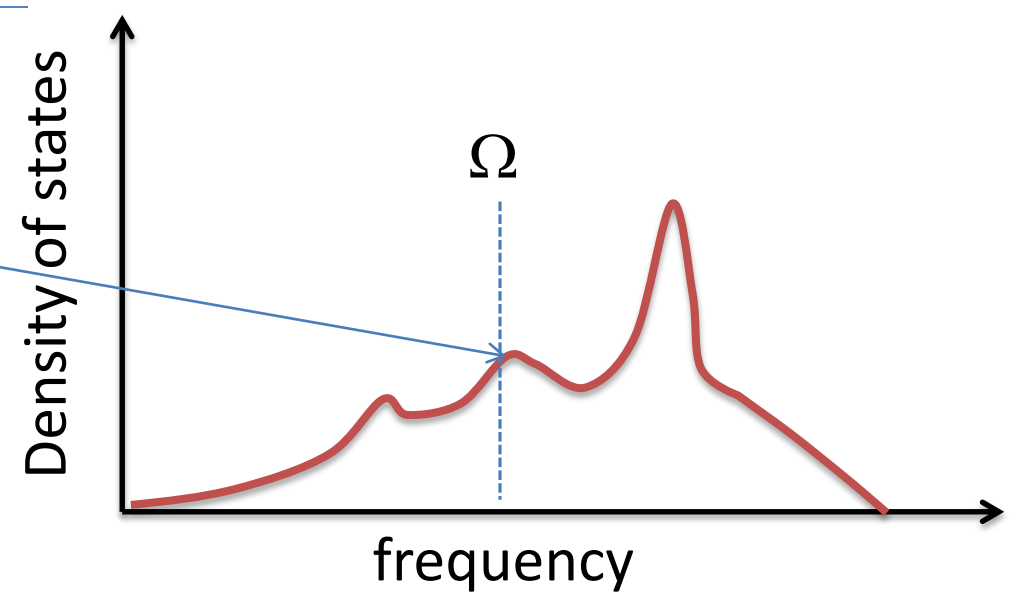
Decoherence

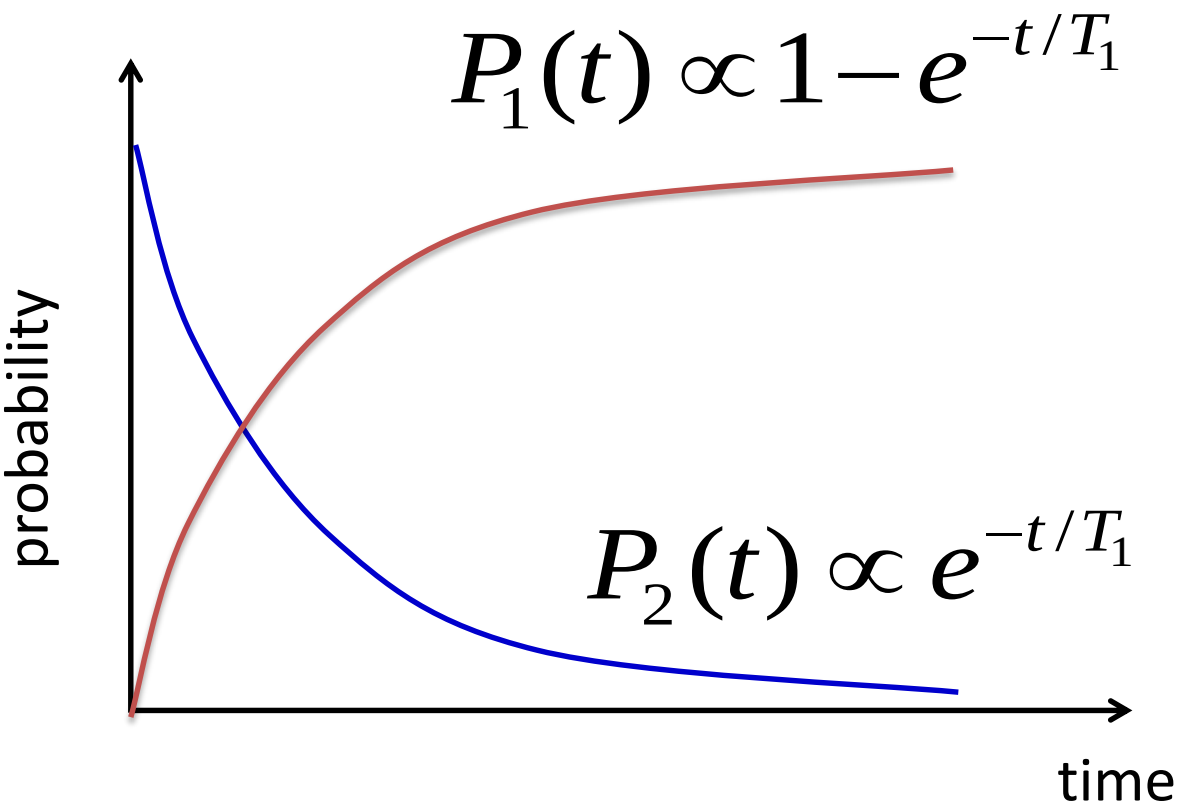
Relaxation



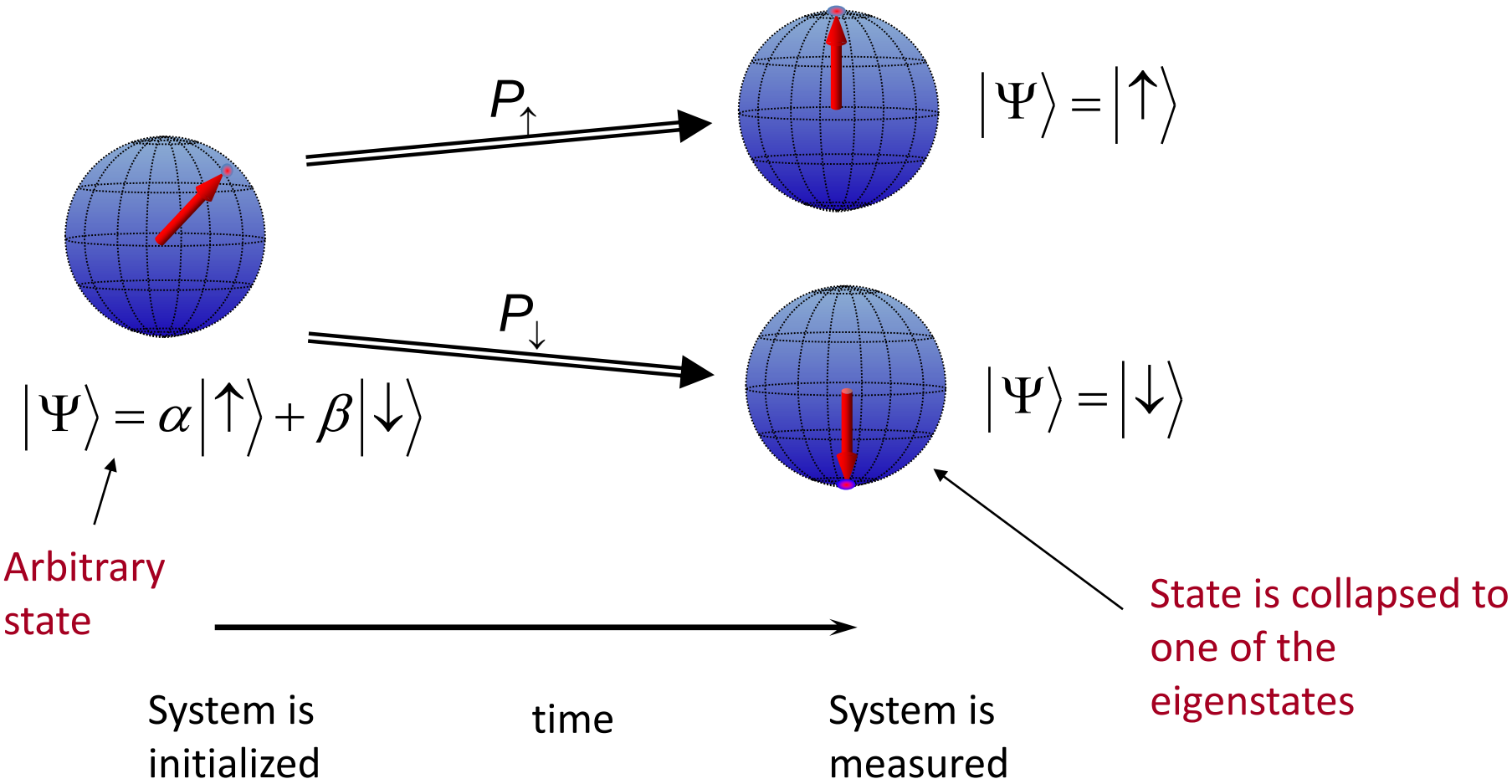
These modes determine energy relaxation



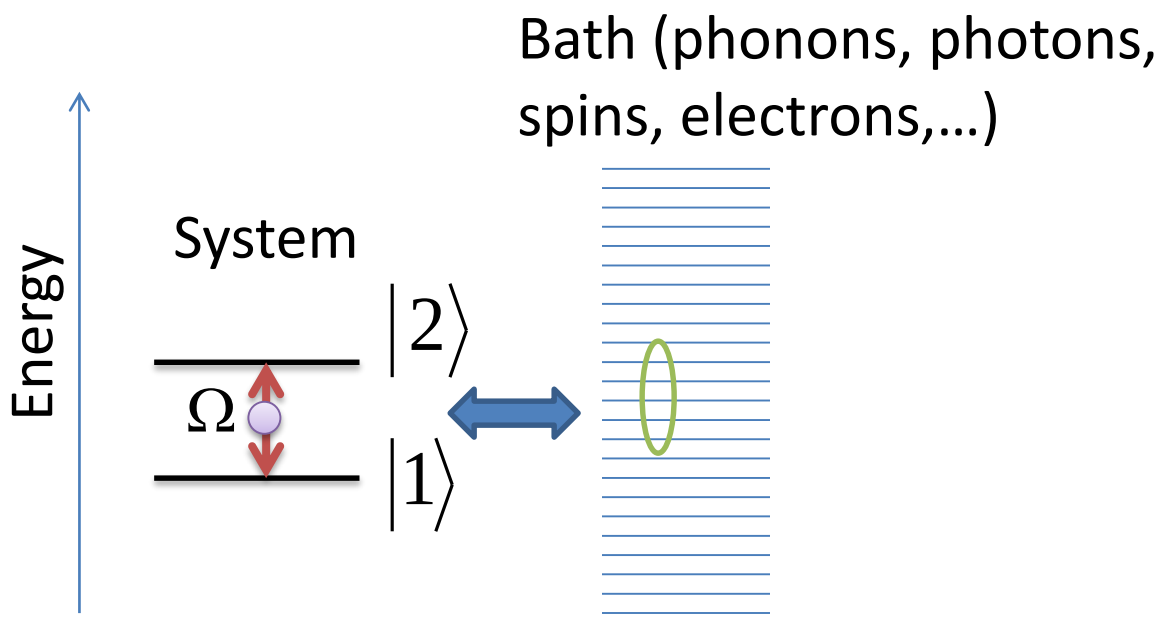
Relaxation



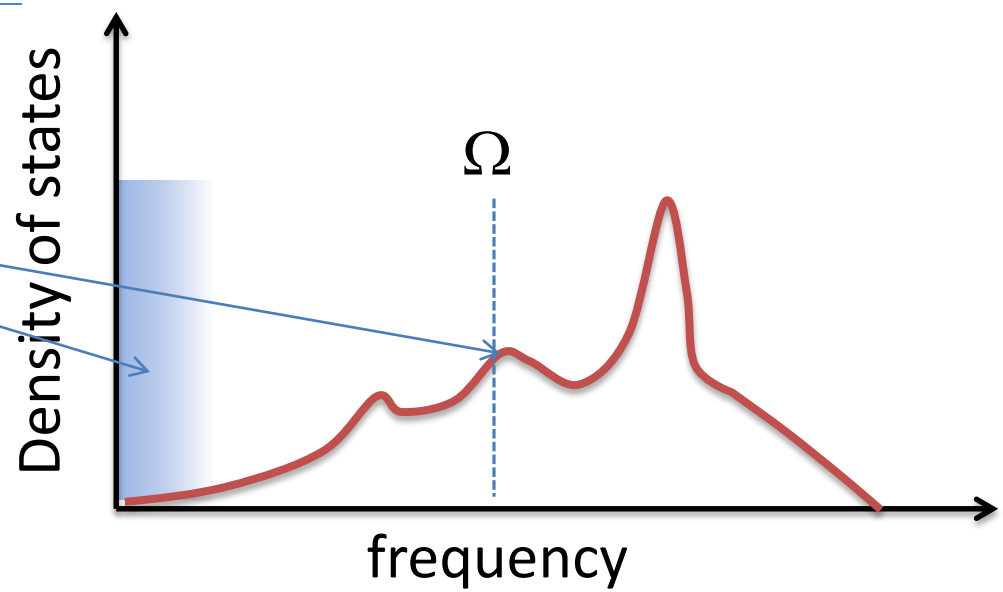
Decoherence: simple picture



Decoherence



These modes determine decoherence



System and bath: example – no relaxation

$$H = H_{\text{sys}} + H_{\text{int}} + H_{\text{bath}}$$

$$H_{\text{sys}} = \sum_i \Omega_i |i\rangle\langle i|$$ Electronic states

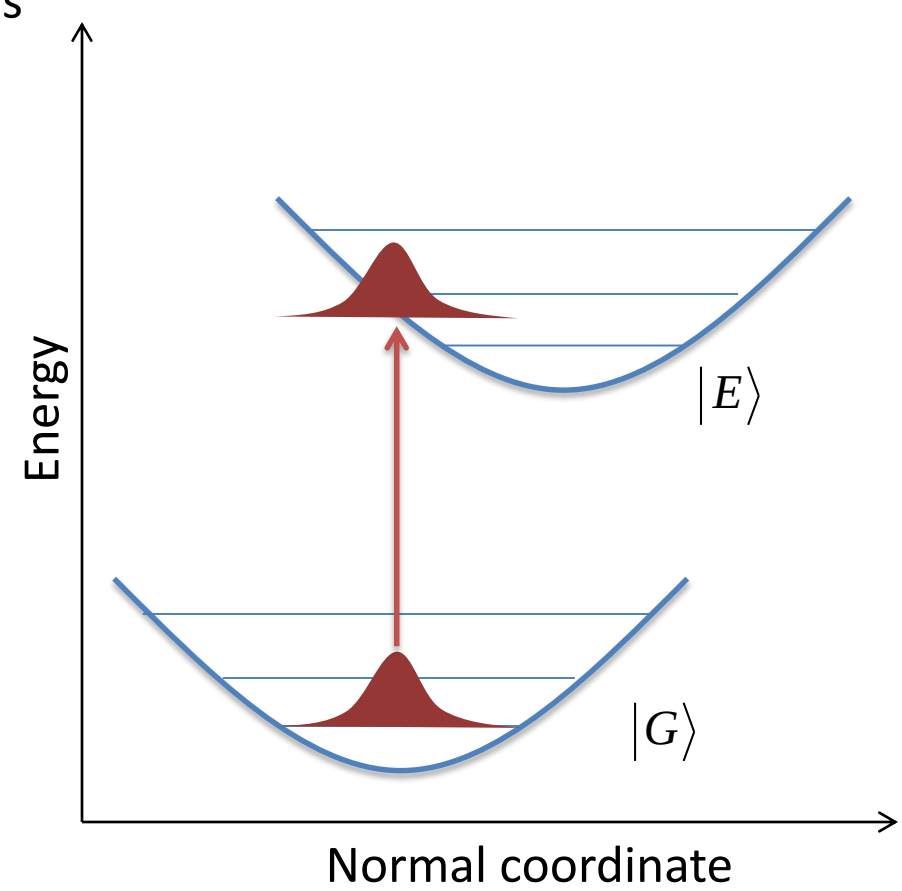
$$H_{\text{bath}} = \sum_k \omega_k b_k^+ b_k$$ Bosonic bath

$$H_{\text{int}} = \sum_{i,k} \kappa_{ik} |i\rangle\langle i| \left(b_k^+ + b_k\right)$$

Diagonal system-bath coupling

No relaxation! Bath induces fluctuations only.

Electronic states in a molecule: displaced harmonic oscillators

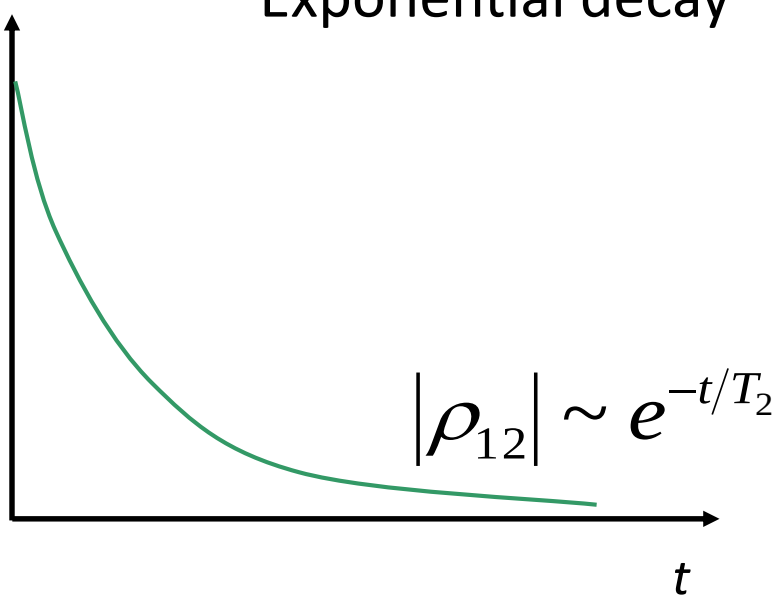


Non-exponential decay

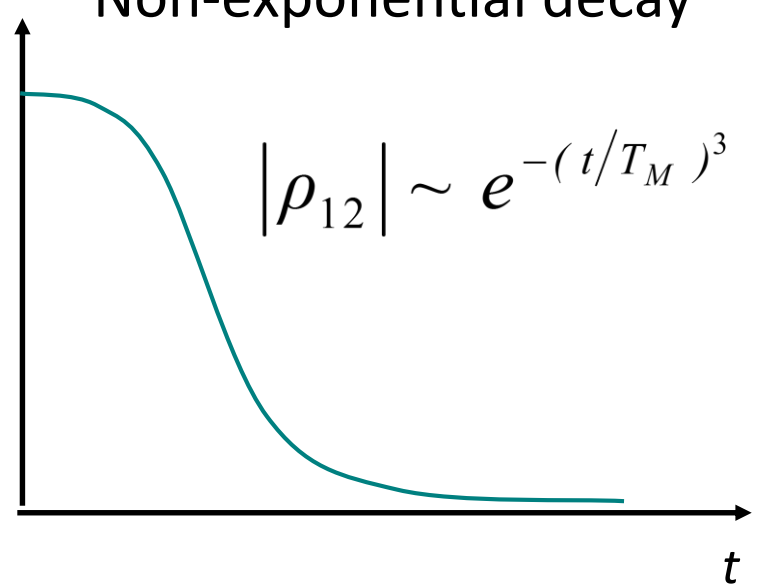
System's density matrix:

$$\rho(t) = \begin{pmatrix} \rho_{11}(t) & \rho_{12}(t) \\ \rho_{21}(t) & \rho_{22}(t) \end{pmatrix}$$

Exponential decay



Non-exponential decay



System and bath

No-relaxation model

System is entangled with the bath

$$|\Psi(0)\rangle = \left(\alpha|\uparrow\rangle + \beta|\downarrow\rangle\right)|J\rangle \Rightarrow |\Psi(t)\rangle = \alpha(t)|\uparrow\rangle|J_\uparrow\rangle + \beta(t)|\downarrow\rangle|J_\downarrow\rangle$$

system bath

$$\rho = \begin{pmatrix} |\alpha(t)|^2 \langle J_\uparrow|J_\uparrow\rangle & \alpha(t)\beta^*(t)\langle J_\downarrow|J_\uparrow\rangle \\ \beta(t)\alpha^*(t)\langle J_\uparrow|J_\downarrow\rangle & |\beta(t)|^2\langle J_\downarrow|J_\downarrow\rangle \end{pmatrix}$$

Quantum model of decoherence

$$\rho = \begin{pmatrix} |\alpha(t)|^2 \langle J_\uparrow | J_\uparrow \rangle & \alpha(t)\beta^*(t)\langle J_\downarrow | J_\uparrow \rangle \\ \beta(t)\alpha^*(t)\langle J_\uparrow | J_\downarrow \rangle & |\beta(t)|^2 \langle J_\downarrow | J_\downarrow \rangle \end{pmatrix}$$

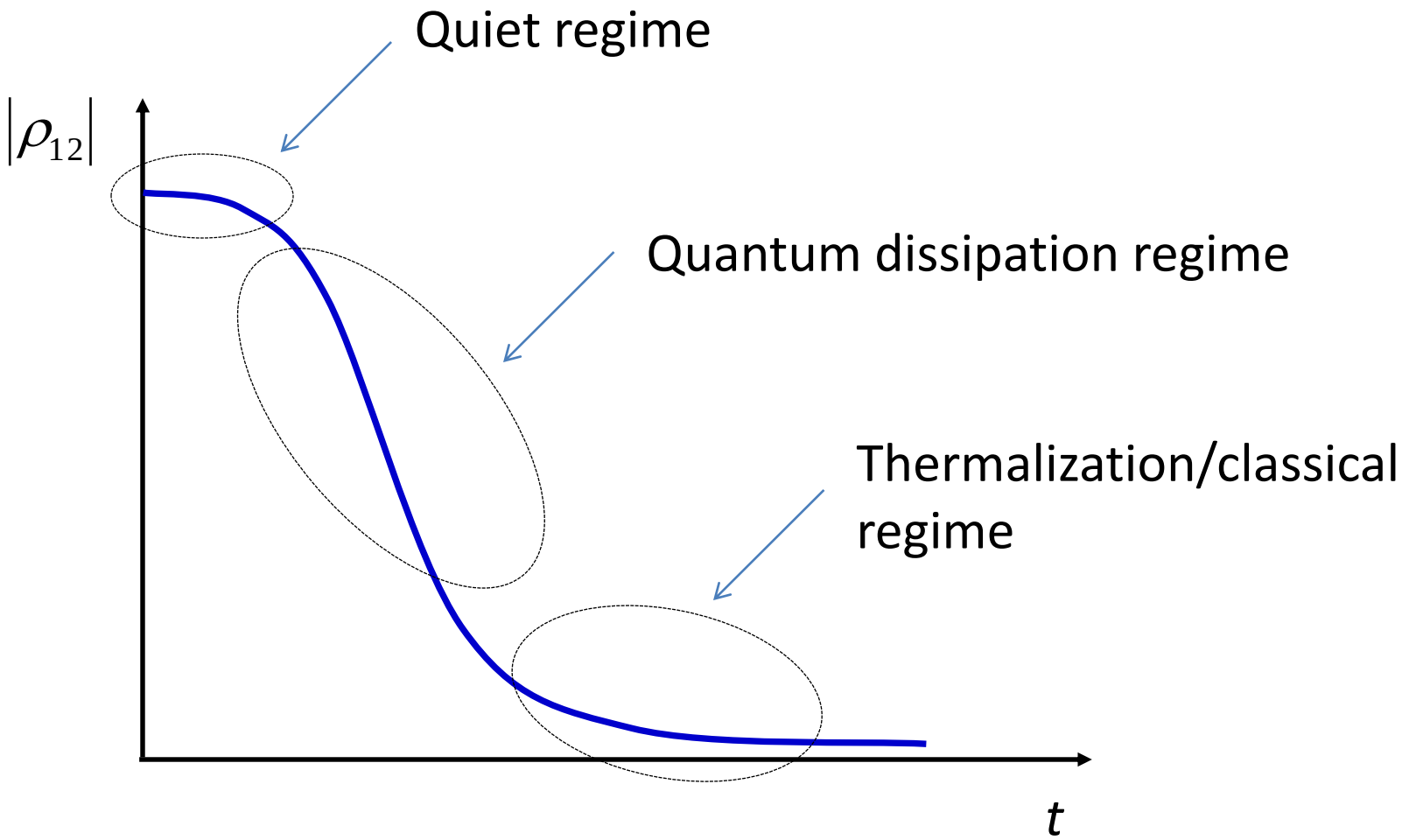
$\langle J_\uparrow(t) | J_\downarrow(t) \rangle$ determines decoherence

It decays monotonically/non-monotonically to 0

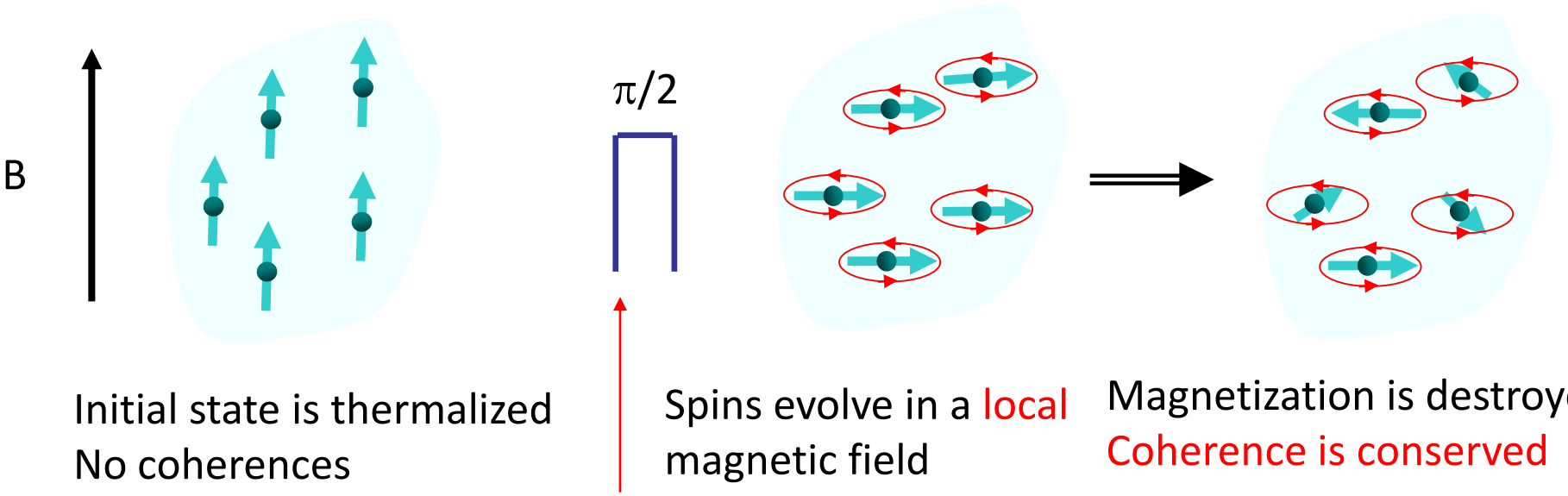
Finally, we get a mixed density matrix:

$$\rho = \begin{pmatrix} |\alpha(t)|^2 & 0 \\ 0 & |\beta(t)|^2 \end{pmatrix} = |\alpha(t)|^2 \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + |\beta(t)|^2 \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

Non-exponential decay



Free induction decay



Measured macroscopic transverse magnetization ⟹ Ensemble dephasing, T_2^*

Spin echo

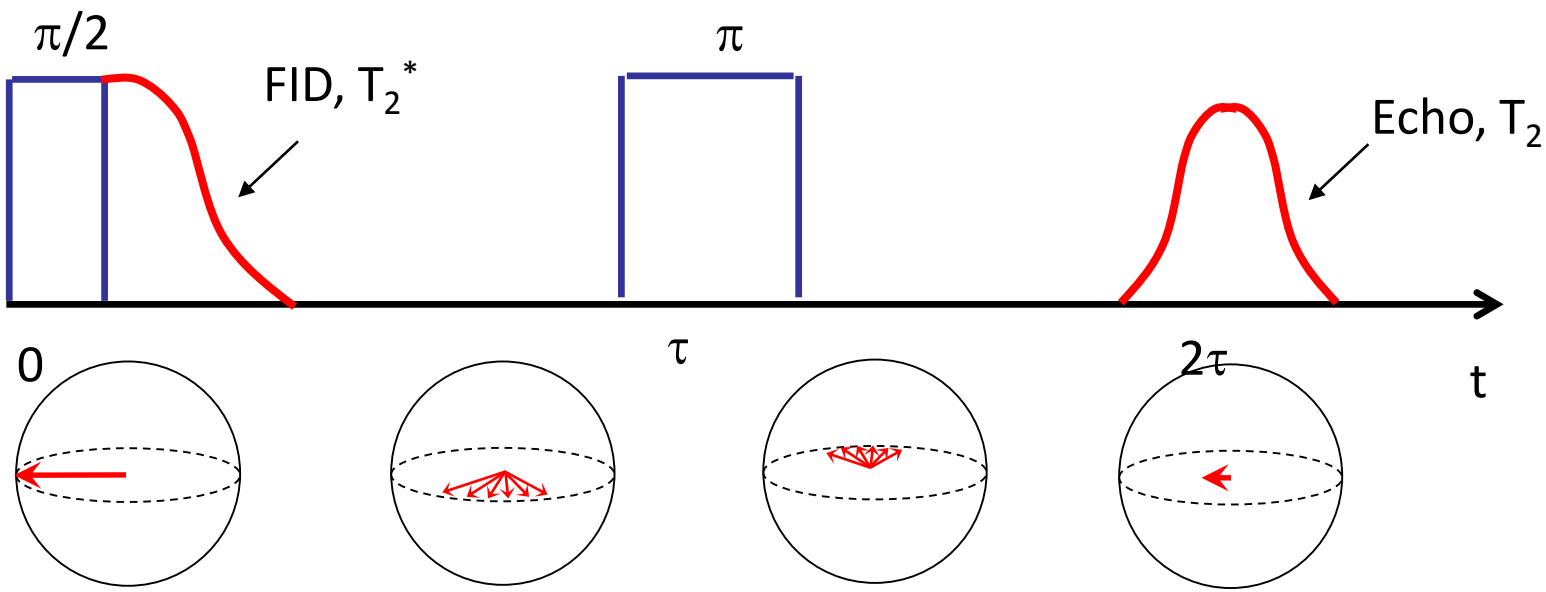
PHYSICAL REVIEW VOLUME 80, NUMBER 4 NOVEMBER 15, 1950

Spin Echoes*†

E. L. HAHN‡
Physics Department, University of Illinois, Urbana, Illinois

(Received May 22, 1950)

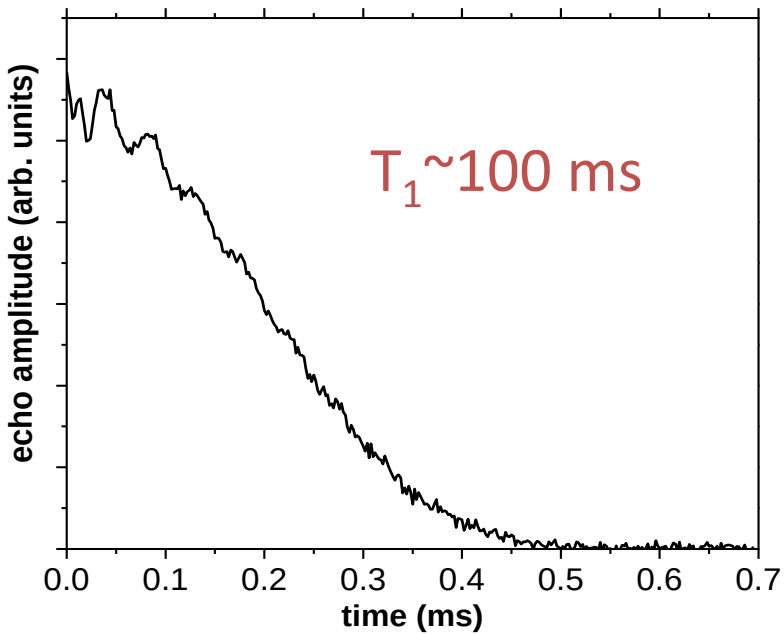
Intense radiofrequency power in the form of pulses is applied to an ensemble of spins in a liquid placed in a large static magnetic field H_0. The frequency of the pulsed r-f power satisfies the condition for nuclear magnetic resonance, and the pulses last for times which are short compared with the time in which the



Measured macroscopic transverse magnetization → "Ensemble decoherence", T_2

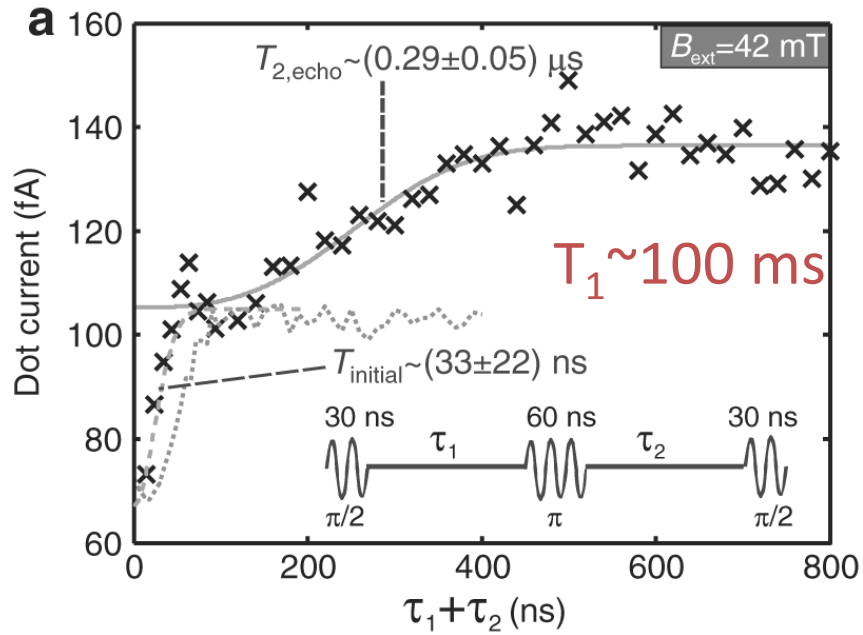
Spin echo decay

Electron spin echo in a Si:P system



A. M. Tyryshkin et al., J. Phys.: Condens. Matter **18**, S783 (2006)

Electron spin echo in a gated QD



F. H. L. Koppens, et al., PRL **100**, 236802 (2008)

Spectral diffusion model

PHYSICAL REVIEW VOLUME 125, NUMBER 3 FEBRUARY 1, 1962

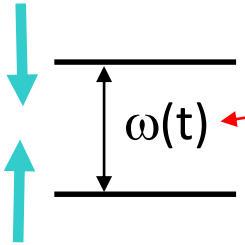
Spectral Diffusion Decay in Spin Resonance Experiments

J. R. KLAUDER AND P. W. ANDERSON
Bell Telephone Laboratories, Murray Hill, New Jersey

(Received September 1, 1961)

In spin resonance experiments random flipping by T_1 or T_2 processes of nearby, nonresonant spins introduces fluctuations into the precessional frequency of the observed spins. These fluctuations may be described by means of a stochastic model, and for wide classes of both Markoffian and non-Markoffian

in detail for samples in which T_1 processes control the source of local frequency fluctuations and for samples in which T_2 processes dominate. Recent two- and three-pulse spin-echo experiments of Mims *et al.* dramatically confirm the predictions of Lorentzian diffusion for electron paramagnetic resonances in samples with



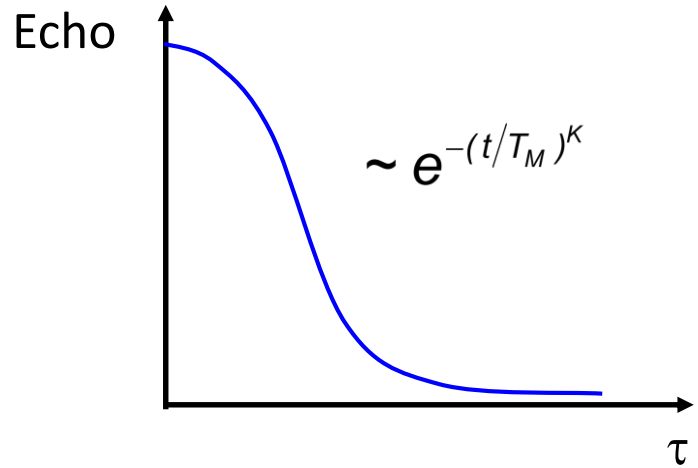
Frequency fluctuates due to interaction with the environment

Since we are only interested in the real part of equations such as (1.5), we can equally well, from a mathematical point of view, negate the frequency $\omega(t')$ after τ rather than negate the phase acquired before τ. Thus the sum of the individual moments can be expressed in the general form

$$M(t)=\left\langle \exp\left[i\int_0^t s(t'')\omega(t'')dt''\right]\right\rangle, \qquad (1.6)$$

where, for the two-pulse spin-echo experiment just described,

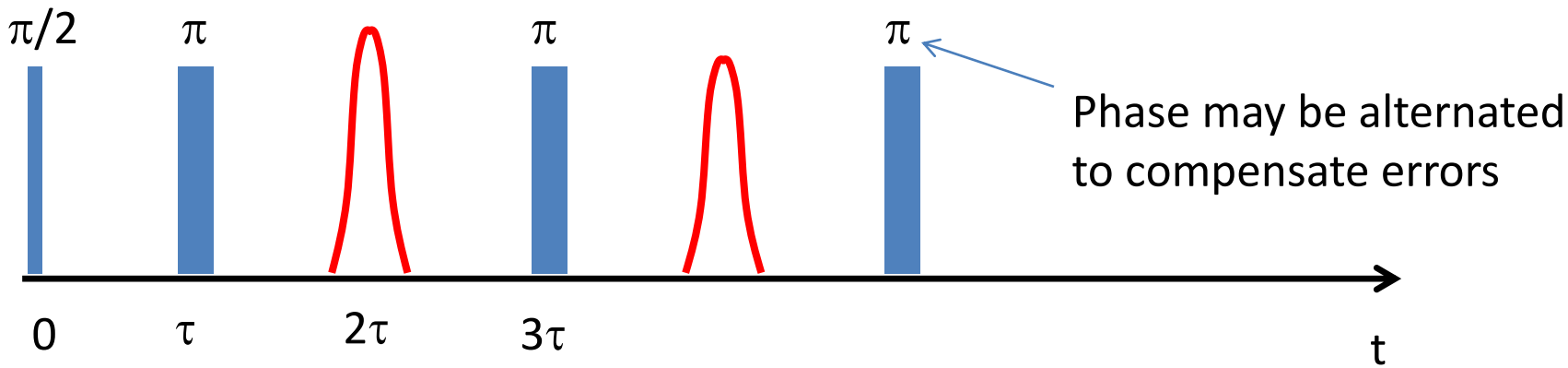
$$\begin{aligned} s(t')&=1, \quad 0<t<\tau; \\ s(t')&=-1, \quad \tau<t. \end{aligned} \qquad (1.7)$$

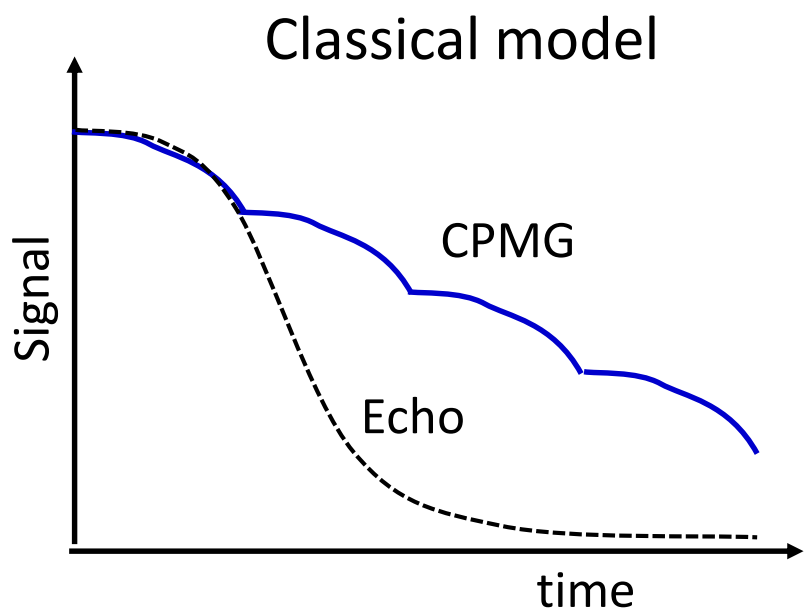


Stochastic model – no dynamics

Dynamical decoupling: classical model

CPMG – Carr Purcell Meiboom Gill pulse sequence





Application to QIP:

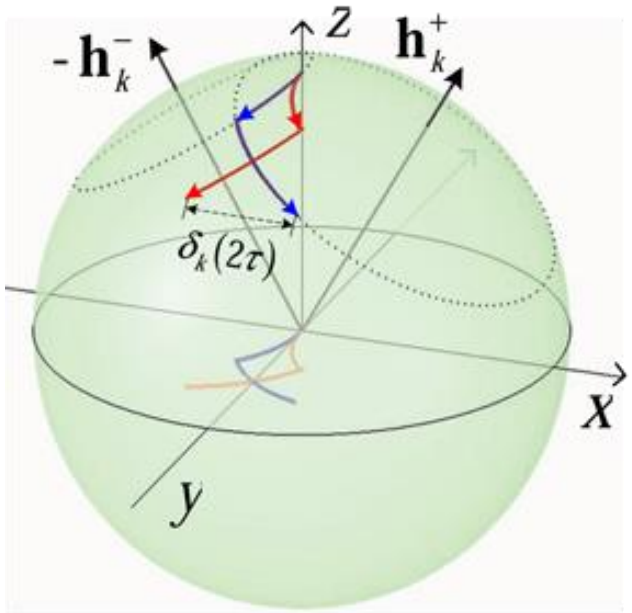
L Viola, S. Lloid, PRA **58**, 2733 (1998)

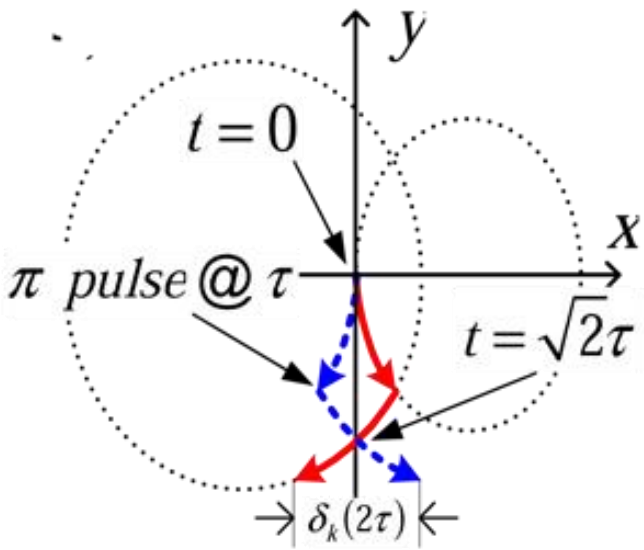
Dynamical decoupling: quantum model

Pseudospin model

$$\left|\Psi(t)\right\rangle = \alpha(t)\left|\uparrow\right\rangle\left|J_{\uparrow}\right\rangle + \beta(t)\left|\downarrow\right\rangle\left|J_{\downarrow}\right\rangle \qquad \left|J_{\uparrow\downarrow}(t)\right\rangle = e^{-\sum_k \mathbf{h}_k^{\pm}\boldsymbol{\sigma} t}\left|J_{\uparrow\downarrow}(0)\right\rangle$$

External pulses change the direction of effective fields





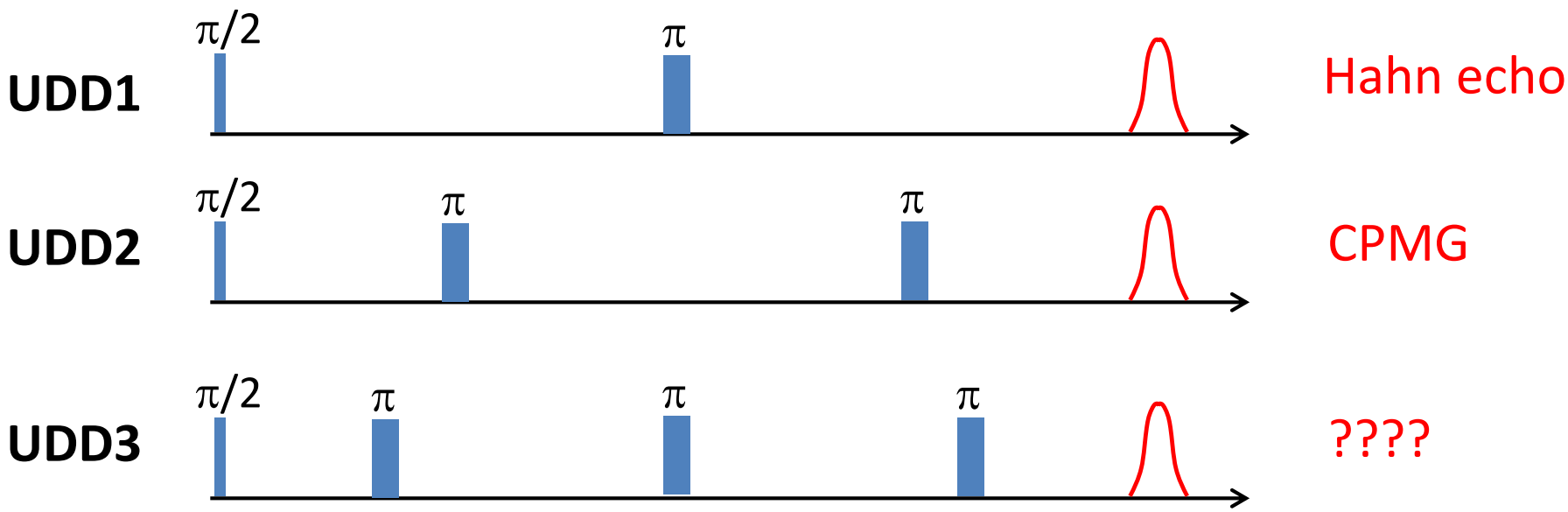
Wang Yao, Ren-Bao Liu and L. J. Sham, Phys. Rev. Lett. **98**, 077602 (2007)

Uhrig's dynamical decoupling

Pulse timing:

$$\tau_j = \tau \sin^2 \frac{j\pi}{2(N+1)} \qquad j = 1,2,\ldots,N$$

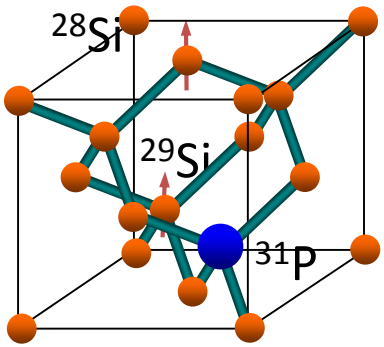
eliminates terms $O(t^{N+1})$



G. S. Uhrig, PRL 98, 100504 (2007)

Electron spin in a nuclear spin bath

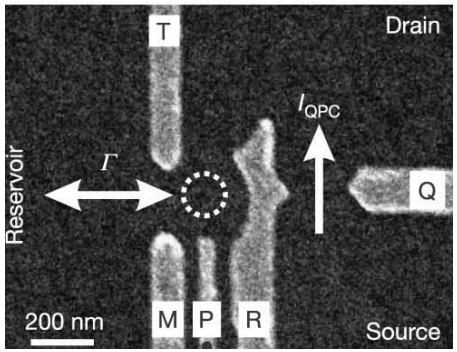
Electron spin of ^{31}P donor in Si



Natural Silicon:

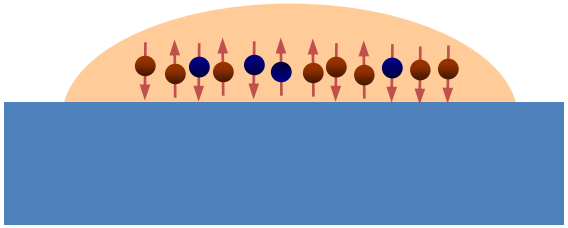
^{29}Si – 4.7% I=1/2

Electron spin in gated GaAs QD



Elzerman et al.
Nature **430**, 431(2004)

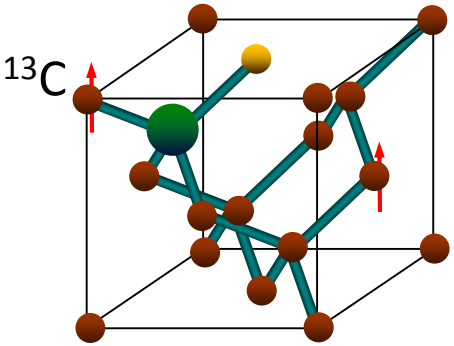
Electron spin in self-assembled GaAs/InAs QD



Natural isotope concentrations:

^{28}Ga – 100% I=3/2
^{29}In – 100% I=3/2
^{30}As – 100% I=3/2

NV-centers in diamond



Natural Diamond:

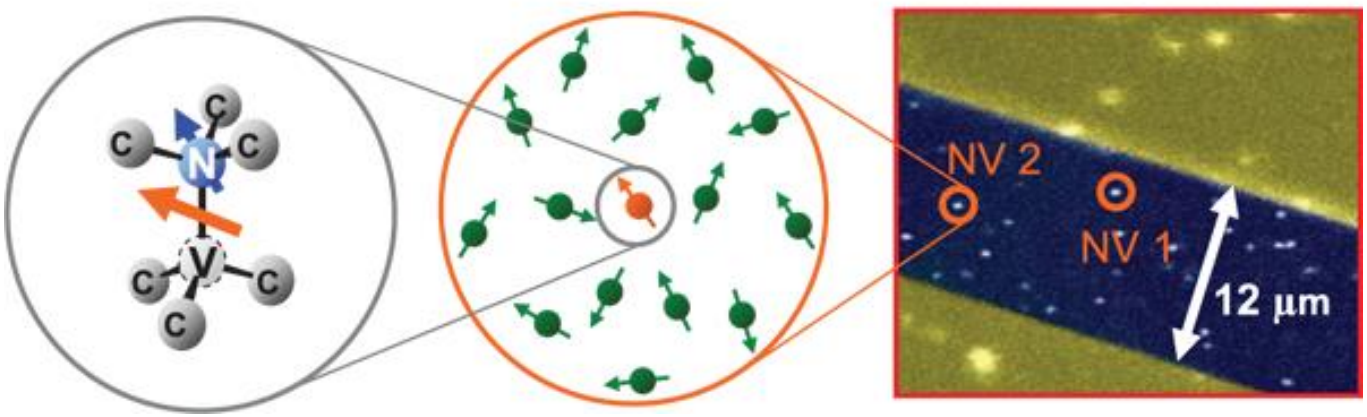
^{13}C – 1.1% I=1/2

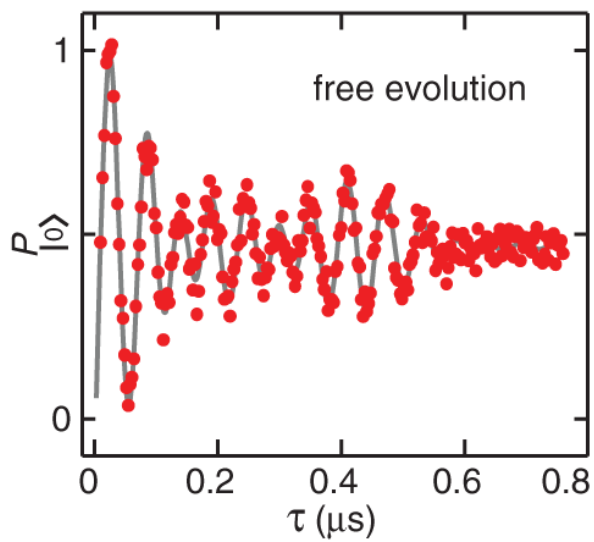
- Single-spin dynamics is important

X Difficult to control with temperature

V Long memory

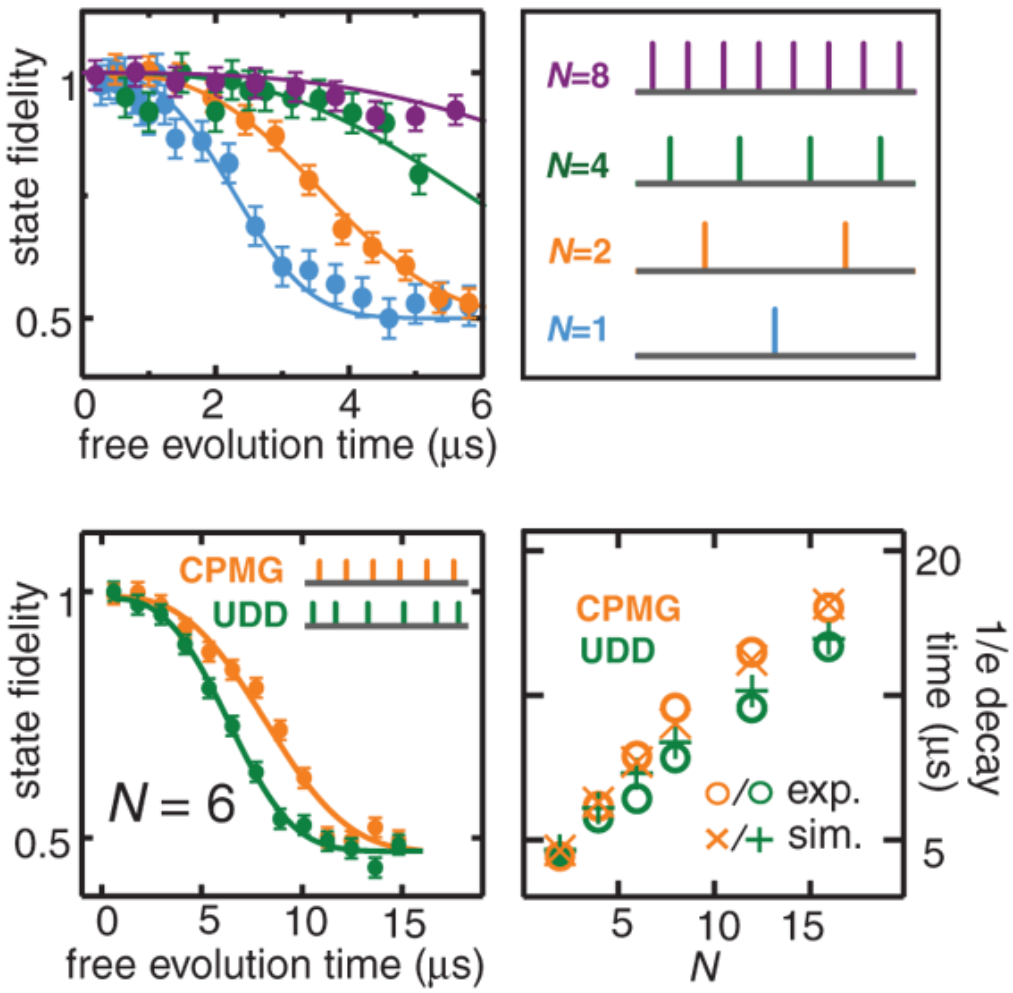
Dynamical decoupling





G. de Lange *et al. Science 330, 60 (2010)*

Dynamical decoupling



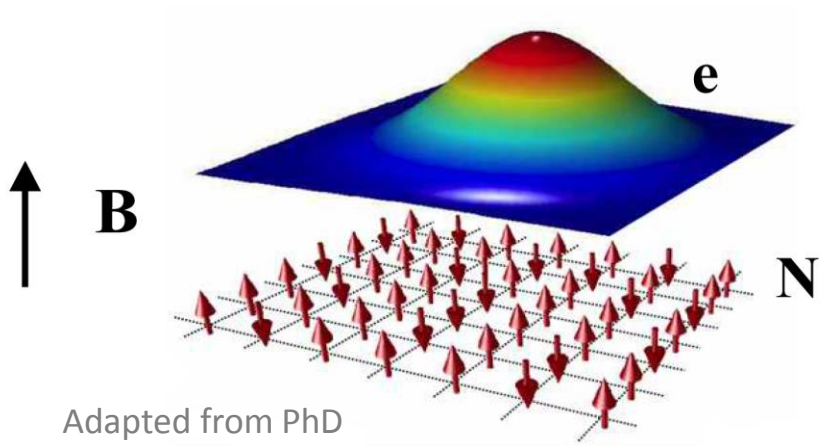
G. de Lange *et al. Science 330, 60 (2010)*

Additional material

How to calculate decoherence

Electron spin in a nuclear spin bath

1+N problem



Adapted from PhD thesis of W. Yao

$$H_{\text{Spin}} = \underbrace{H_{\text{Z}}^{e} + \sum_{i} H_{\text{Z}}^{\text{nucl}}(i)}_{\text{Coupling to external fields}} + \underbrace{\sum_{i} H_{\text{Hf}}(i)}_{\text{Hyperfine interaction}} + \underbrace{\sum_{i \neq j} H_{\text{Dip}}(i, j)}_{\text{Nuclear spin-spin interaction}}$$

Simple, *O*(*N*)

Complicated, O(2^N)

Hyperfine coupling

$$H_{\mathrm{Hf}} = \begin{pmatrix} S_x & S_y & S_z \end{pmatrix} \begin{pmatrix} A_{xx} & A_{xy} & A_{xz} \\ A_{yx} & A_{yy} & A_{yz} \\ A_{zx} & A_{zy} & A_{zz} \end{pmatrix} \begin{pmatrix} I_x \\ I_y \\ I_z \end{pmatrix}$$

Contact terms only:

$$\mathbf{A} = \begin{pmatrix} A_{xx} & 0 & 0 \\ 0 & A_{yy} & 0 \\ 0 & 0 & A_{zz} \end{pmatrix}$$

High field:

$$\mathbf{A} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ A_{zx} & A_{zy} & A_{zz} \end{pmatrix}$$

ESEEM removed

$$\mathbf{A} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & A_{zz} \end{pmatrix}$$

Hyperfine-mediated nuclear spin-spin interaction:

- Electron spin dephasing only

$$H_{\mathrm{hf}}(i,j) = S_z \cdot \frac{A_i A_j}{2\Omega_e}\left(I_i^+ I_j^- + I_i^- I_j^+\right)$$

Evolution of an open system

$$\rho_{\text{sys}}(t) = \text{Tr}\left\{e^{-iHt}\rho(0)e^{iHt}\right\}$$

$$H = H_0 + V$$

Simple single-spin part

Complicated interaction part

Factorizable initial state:

$$\rho(0) = \underbrace{\left(a_{s's}\,|s\rangle\langle s'|\right)}_{\rho_s(0)} \otimes \underbrace{\left(\sum_j p_j\,|j\rangle\langle j|\right)}_{\rho_{bath}(0)}$$

spin

bath state

Simple part

$$H_0 = \Omega_e S^z + \omega_I \sum_i I_i^z + S^z \sum_i A_i^{zz} I_i^z$$

Complicated part

$$V_{dd} = \sum_{i \neq j} D_{ij}^{dd} I_i^z I_j^z + B_{ij}^{dd} I_i^+ I_j^-$$ dipole-dipole term

$$V_{hf} = 2S^z \sum_{i \neq j} B_{ij}^{hf} I_i^+ I_j^-$$ Hyperfine-modulated term

Quantum models of spectral diffusion

N. Prokof'ev and P.C.E. Stamp, Rep. Prog. Phys. 63, 669 (2000)

I.A.Merkulov, Al.L.Efros, M.Rosen, PRB 65, 205309 (2002)

A. V. Khaetskii, D. Loss, and L. Glazman, PRL 88, 186802 (2002)

S.Saikin, D.Mozyrsky, V.Privman, Nano Letters 2, 651 (2002)

R. de Sousa, S.Das Sarma, PRB 68, 115322 (2003)

S.Saikin, L. Fedichkin, PRB 67, 161302(R) (2003)

W. M. Witzel, R. de Sousa, S. Das Sarma, PRB 72, 161306(R) (2005)

W. Yao, R.-B. Liu, L. J. Sham, PRB 74, 195301 (2006)

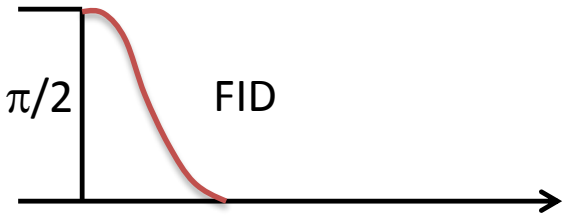
…

LCE approach in two steps

Step I: Write the complicated system dynamics in an exponential form

Step II: Calculate only those terms that correspond to "linked" spin diagrams

Step 1: single-spin FED



$$\rho_{\uparrow\downarrow}(t) = \rho_{\uparrow\downarrow}(0)\sum_j p_j \left\langle j \middle| e^{i(H_0^- + V_-)t} e^{-i(H_0^+ + V_+)t} \middle| j \right\rangle$$

$$e^{-i(H_0^+ + V_+)t} = T\left\{ e^{-i\int_0^t V_+(t'-t)dt'} \right\} e^{-iH_0^+ t}$$

$$\boxed{\rho_{\uparrow\downarrow}(t) = \rho_{\uparrow\downarrow}(0) e^{-i\Omega_e t} \sum_j p_j e^{-i\omega_n t} \left\langle j \middle| T\left\{ e^{i\int_0^t V_-(t')dt'} \right\} T\left\{ e^{-i\int_0^t V_+(t'-t)dt'} \right\} \middle| j \right\rangle}$$

Statistical factor determined by initial spin state

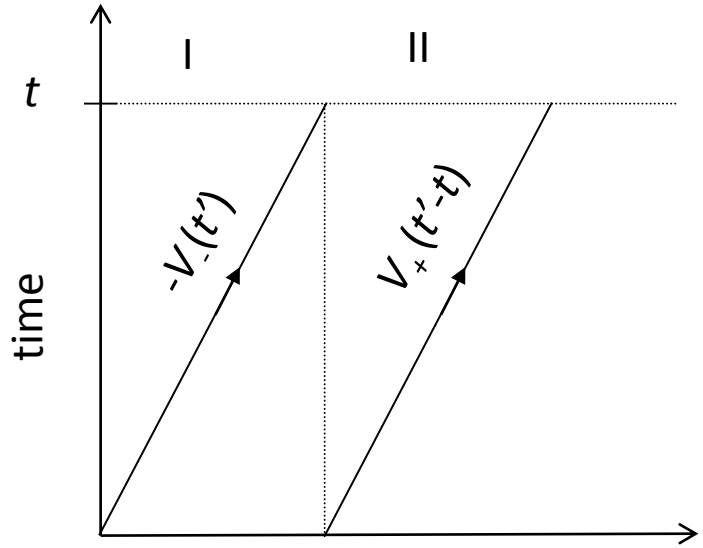
Phase due to the Overhauser field

e-n spin entangement

Inhomogeneous boradening

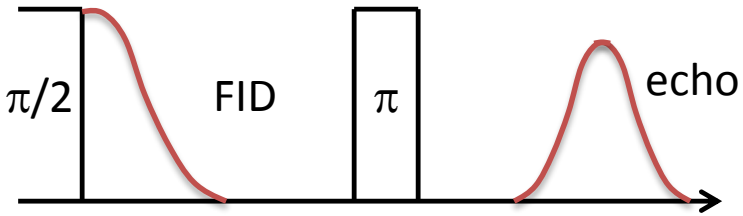
Decoherence

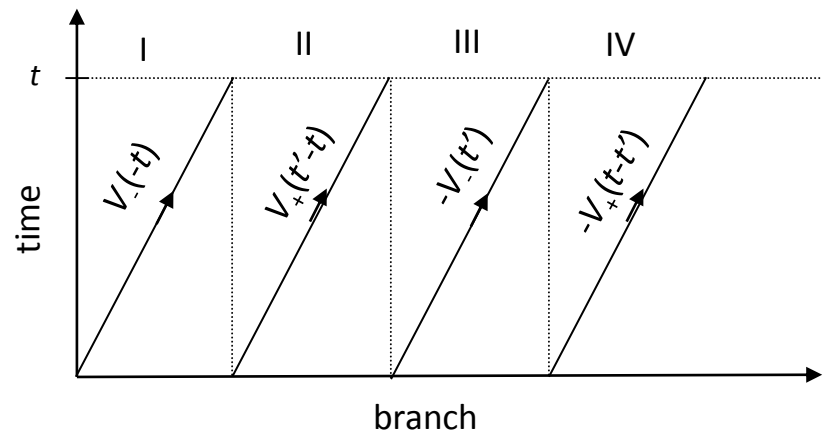
FID: two-branch propagation



$$\overbrace{\langle j | T\left\{ e^{i\int_0^t V_-(t')dt'} \right\}}^{\text{Branch I}} \overbrace{T\left\{ e^{-i\int_0^t V_+(t'-t)dt'} \right\} | j \rangle}^{\text{Branch II}}$$

Step 1: Hahn echo





$$\rho_{\uparrow\downarrow}(2t) = -\rho_{\uparrow\downarrow}(0)\left\langle j\right| T\left\{e^{i\int_0^t V_+(t-t')dt'}\right\} T\left\{e^{i\int_0^t V_-(t')dt'}\right\} T\left\{e^{-i\int_0^t V_+(t'-t)dt'}\right\} T\left\{e^{-i\int_0^t V_-(-t')dt'}\right\}\left|j\right\rangle$$

- Inhomogeneous broadening: The phase factor due to Overhauser field is removed
- Suppression of spectral diffusion: Electron-nuclear spin entanglement term is modified
- Can be straightforwardly extended to more pulses

Linked cluster expansion

$$\left\langle j \middle| T\left\{ e^{-i\int_0^t V(t')dt'} \right\} \middle| j \right\rangle = e^{\langle V_1(t)\rangle + \frac{1}{2}\langle V_2(t)\rangle + \frac{1}{3}\langle V_3(t)\rangle + \ldots}$$

- LCE describes dynamics in a convenient exponential form.
- Summation of terms in LCE differs from the Dyson type.
- LCE provides a partial sum of infinite series of terms

for example: $$e^{\frac{1}{2}\langle V_2(t)\rangle} = 1 + \frac{1}{2}\langle V_2(t)\rangle + \frac{1}{2!}\left(\frac{1}{2}\langle V_2(t)\rangle\right)^2 + \ldots$$

X-ray singularity, G. D. Mahan (1975) (fermions)

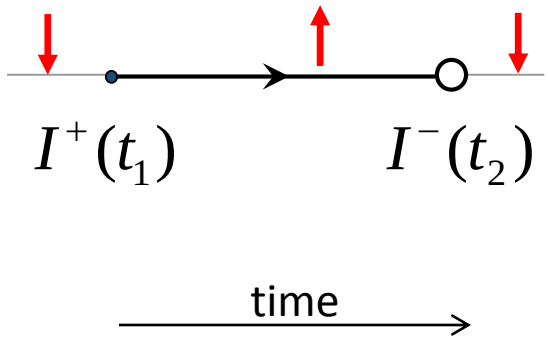
Polaron problem, D. Dunn (1975) (bosons)

Qubit dephasing, Y Makhlin, A. Shnirman (2004) (bosons)

Charge dephasing in QD, E. A. Muljarov, R. Zimmermann (2004)(bosons)

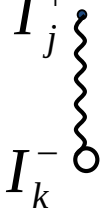
Nuclear spin diagrams

Spin propagation:



Spin-spin interactions:

$A_{jk} I_j^+ I_k^- =$



$A_{jk} I_j^z I_k^z =$

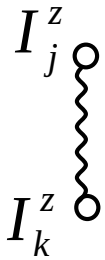
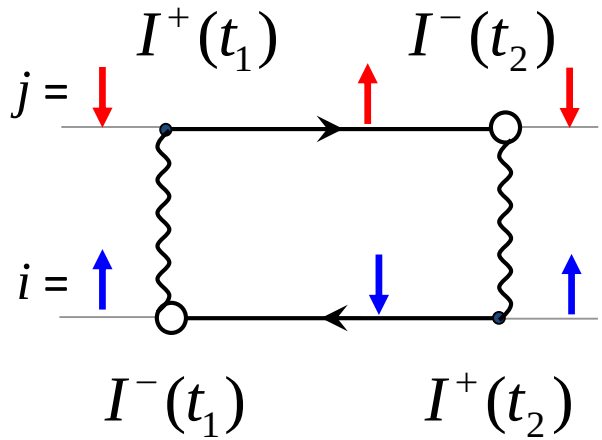
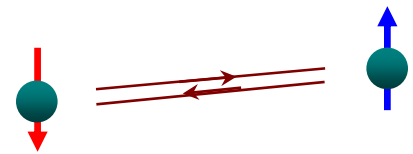


Diagram technique : Yu. A. Izyumov and F. A. Kassan-Ogly, Fiz. Met. Metalloved. 26, 385 (1968); 30, 225 (1970)

Nuclear spin diagrams: flip-flop terms

$$V_2^{ij} =$$





Coherent precession of nuclear spin pairs

Spin echo in the pair approximation:

$$\rho_{\uparrow\downarrow}(t) = \rho_{\uparrow\downarrow}(0) e^{\sum_{i,j=\uparrow\downarrow} V_2^{ij}}$$

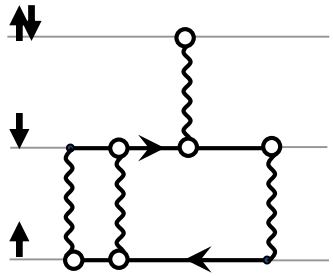
We can have analytical expressions for V_2 terms:

$$\mathrm{Re}(V_2) = \frac{32 \sin^4 \frac{\omega_{ij} t}{2}}{\omega_{ij}^2} \qquad \mathrm{Im}(V_2) = \frac{8 \sin \omega_{ij} t}{\omega_{ij}^2} \left(1 - \cos \omega_{ij} t\right)$$

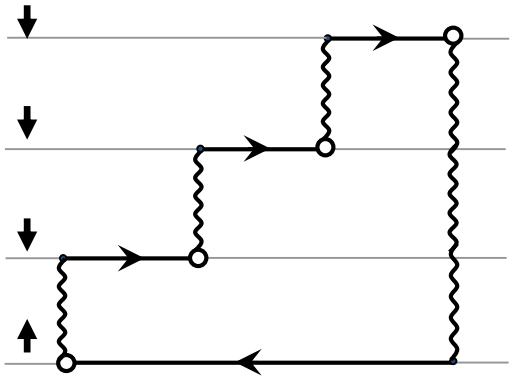
Nuclear spin diagrams: more to the zoo

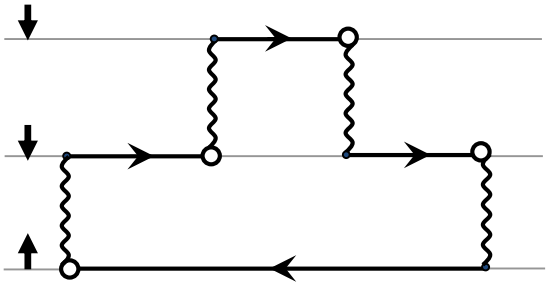
Group I

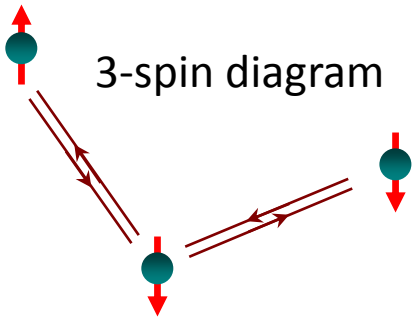
Lower order diagrams renormalized by DI^zI^z



Group II
4-spin ring diagram

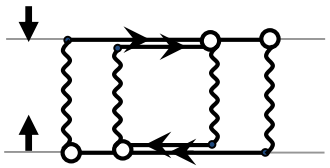


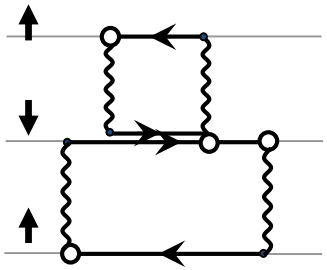




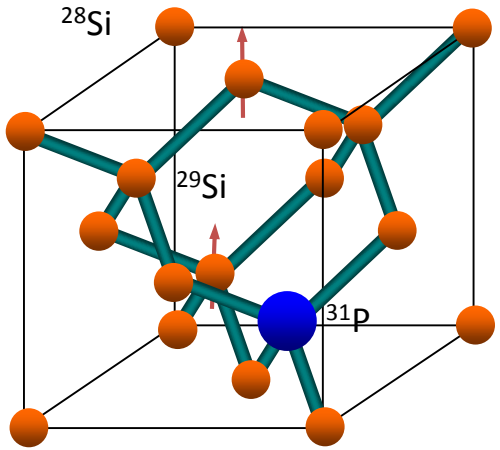
3-spin diagram

Group III
Spin-locked diagrams compensate overlapping of excitations



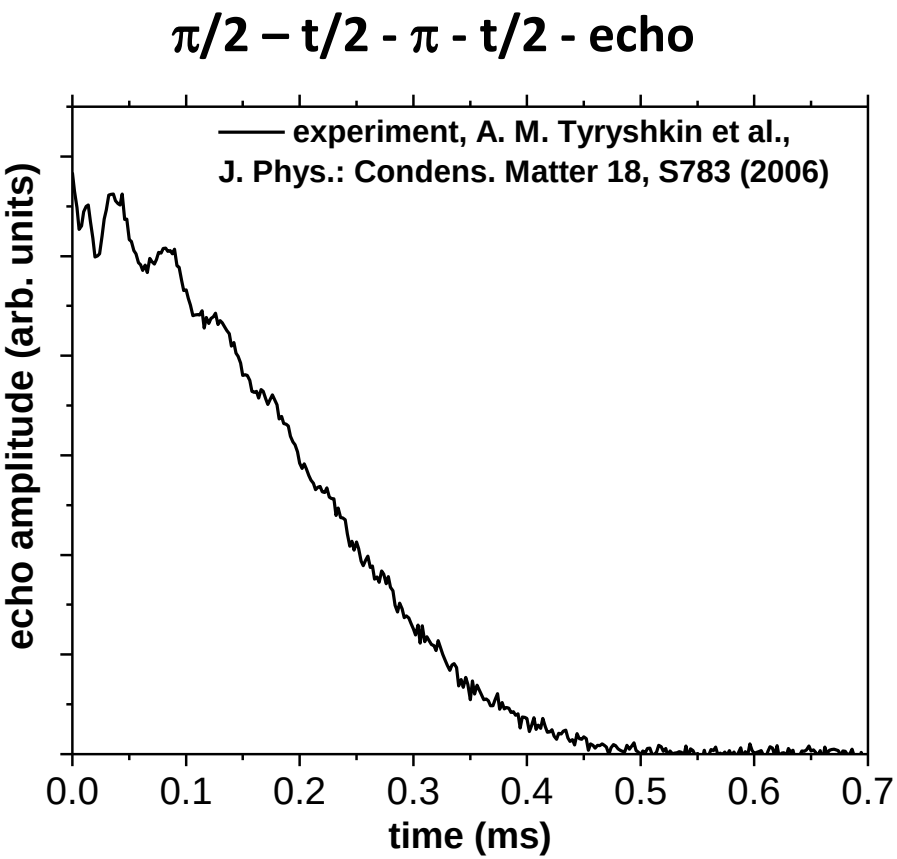
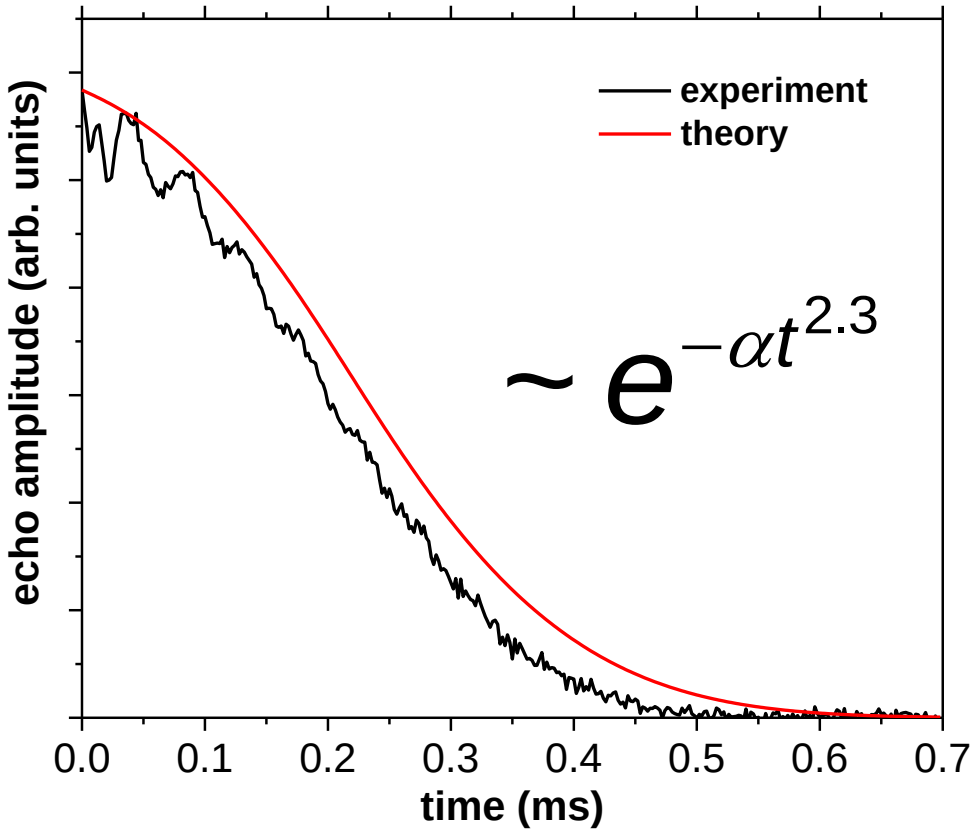


Example: electron spin in Si:P



Natural Silicon:
^{28}Si – 92%
^{29}Si – 4.7% I=1/2
^{30}Si – 3.1%

Natural Phosphorus:
^{31}P – 100% I=1/2



Spin echo: theory vs. experiment