QUANTUM MECHANICS on the LARGE SCALE

Banff-BIRS conference, 12-17 April 2003

This conference to be followed by a workshop (see next slide)

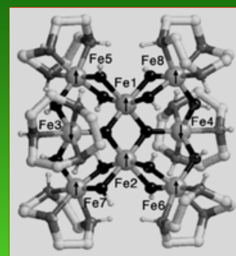
QUANTUM MECHANICS on the LARGE SCALE

Peter Wall Institute for Advanced Studies (UBC, Vancouver)

(April 17-27, 2003)

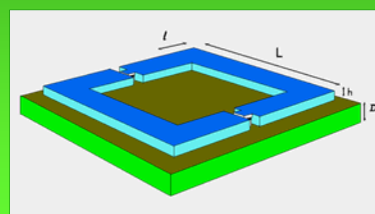
SUPPRESSION of DECOHERENCE in MAGNETS & SUPERCONDUCTORS

P.C.E. STAMP
I.S. TUPITSYN



This is a tutorial guide to our recent work, with some discussion of what it was built on, and the relevant experiments.

For theorists there is also a summary of some of the derivations (slide 16, & slides 21-24).



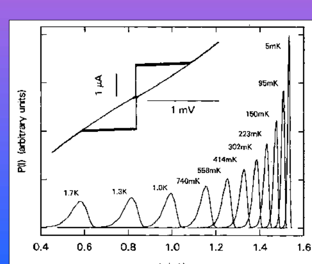
Macroscopic Quantum Tunneling (MQT) in SQUIDs

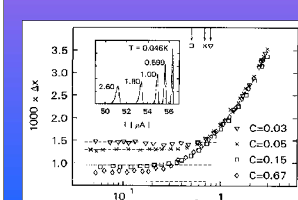
It was shown by Leggett that essentially all previous arguments against large-scale Quantum phenomena were flawed, because (i) matrix elements between macroscopically different states can be controlled by microscopic energies, and (ii) Because what really matters is the behaviour in time of

$$O_{AB}(t) = \langle \Psi(R_A; r_1, r_2, ..) | e^{iHt} | \Psi(R_B; r_1, r_2, ..) \rangle \qquad \text{(transition matrix)}$$

and that in particular, "Macroscopic Quantum Tunneling" between 2 different Flux states of a SQUID should be possible- a QUANTATIVE THEORETICAL PREDICTION was given.

Experimental confirmation came very quickly





Caldeira & Leggett: Ann. Phys. 149, 374 (1983) [THEORY]
Voss & Webb: PRL 47, 265 (1981)
Clarke et al: Science 239, 992 (88)

MQT in Magnets

Actually one can get MQT under more general circumstances

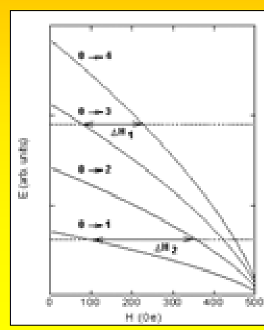
It was later pointed out that any QUANTUM SOLITON should show large-scale quantum properties. Quantitative predictions could also be made here- indicating that in some situations magnetic domain walls containing up to 10^{10} spins should be able to tunnel.

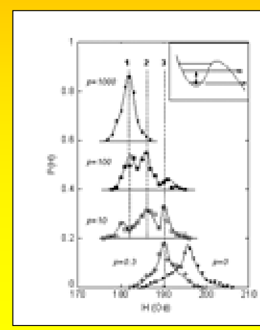
Experiments in Ni wires and in large particles bore out the theory

Example:

P.C.E. Stamp, PRL 66, 2802 (1991)
M.Dube, P.C.E.Stamp, JLTP 110, 779 (1998) [THEORY]

K. Hong,N. Giordano, Europhys. Lett.36, 147 (1996) [EXPT]

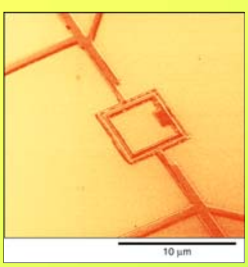


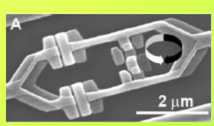


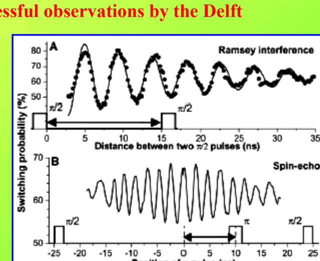
Experiments on SQUIDs

J.E. Mooij et al, Science 285, 1036 (1999)
C. Van der Wal et al., Science 290, 773 (2000)
I. Chiorescu et al., Science 299, 1869 (2003)

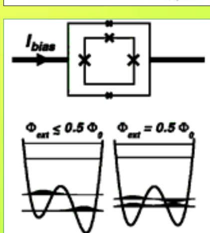
The attempt to produce coherent tunneling in SQUIDs finally culminated, after 15 yrs, in the successful observations by the Delft group

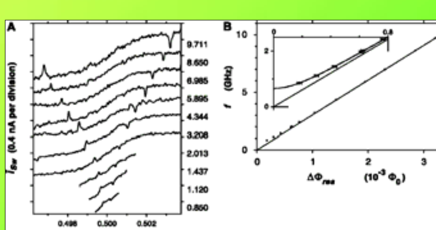






However decoherence rates are Much higher than the rates predicted by Caldeira-Leggett theory.

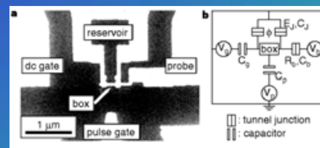


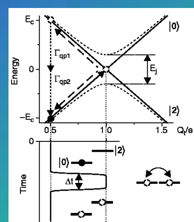


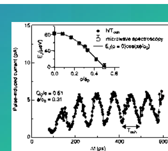
Experiments on COOPER PAIR BOXES

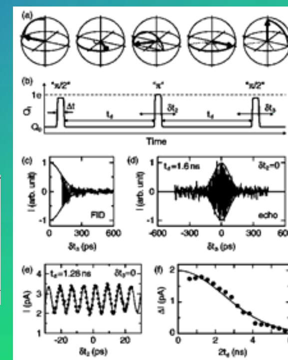
A Cooper pair box is just a very small superconductor connected to a SQUID. It is so small that the capacitative charging energy associated with a single electron, $E_c = e^2/2C$ is similar to the Josephson Energy E_J.

In the Nakamura expts, this was made to operate as a qubit.





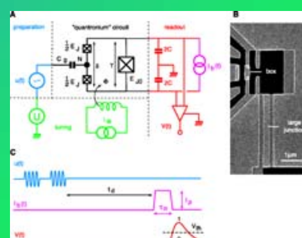


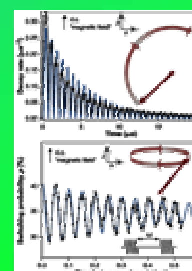


In a more recent experiment by the Saclay group, the "decoherence Q-factor" was raised to a value of 25,000. This value is high enough to allow error correction routines to work.

Y. Nakamura et al., Nature 398, 786 (1999), and PRL 88, 047901 (2002)

D. Vion et al., Science 296, 886 (2002)





A qubit coupled to a bath of delocalised excitations: the SPIN-BOSON Model

Feynman & Vernon, Ann. Phys. 24, 118 (1963)
PW Anderson et al, PR B1, 1522, 4464 (1970)
Caldeira & Leggett, Ann. Phys. 149, 374 (1983)
AJ Leggett et al, Rev Mod Phys 59, 1 (1987)

U. Weiss, "Quantum Dissipative Systems" (World Scientific, 1999)

Suppose we have a system whose low-energy dynamics truncates to that of a 2-level system τ. In general it will also couple to DELOCALISED modes around (or even in) it. A central feature of many-body theory (and indeed quantum field theory in general) is that

(i) under normal circumstances the coupling to each mode is WEAK (in fact ~ O $(1/N^{1/2})$), where N is the number of relevant modes, just BECAUSE the modes are delocalised; and

(ii) that then we map these low energy "environmental modes" to a set of non-interacting Oscillators, with canonical coordinates $\{x_q, p_q\}$ and frequencies $\{\omega_q\}$.

It then follows that we can write the effective Hamiltonian for this coupled system (assuming orthodox theory) in the form:

$$H(\Omega_o) = \{[\Delta_o \tau_x + \varepsilon_o \tau_z] \quad \text{qubit}$$
$$+ \tfrac{1}{2} \Sigma_q (p_q^2/m_q + m_q \omega_q^2 x_q^2) \quad \text{oscillator}$$
$$+ \Sigma_q [c_q \tau_z + (\lambda_q \tau_+ + H.c.)] x_q \} \quad \text{interaction}$$

Where Ω_o is a UV cutoff, and the $\{c_q, \lambda_q\} \sim N^{-1/2}$.

WHAT ARE THE LOW-ENERGY EXCITATIONS IN A SOLID ?

DELOCALISED

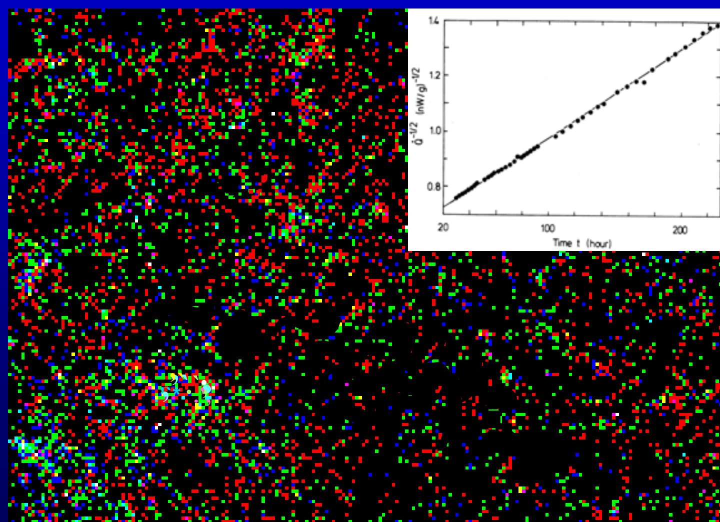
Phonons, photons, magnons, electrons, ………

LOCALISED .

Defects,
Dislocations,
Paramagnetic impurities,
Nuclear Spins,
…….

At right- artist's view of energy distribution at low T in a solid- at low T most energy is in localised states.

INSET: heat relaxation in bulk Cu at low T

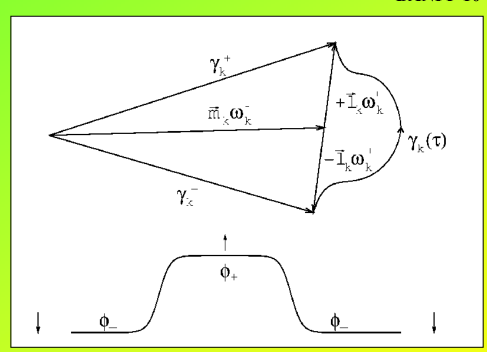


Derivation of Effective hamiltonian

This is done using instanton methods- but can be explained in pictures. To be definite do this for a SQUID and a "spin bath".

(i) Start with the k-th bath spin, and define the field

$$\gamma_k(\tau) = \omega_k^{\perp} m_k + \omega_k^{\parallel} l_k(\tau)$$



which varies in (imaginary) time as shown, during the transitions of the SQUID qubit.

(ii) Define the "transfer matrix"

$$T_k = \exp\{- i/h \int d\tau\, \omega_k\, l_k^{\parallel}(\tau) \cdot \sigma_k(\tau) \}$$
$$= \exp\{- i (\phi_k + \alpha_k \cdot \sigma_k)\}$$

where ϕ_k and the vector α_k are complex.

(iii) Add to this the intrinsic dynamics of the bath spin.

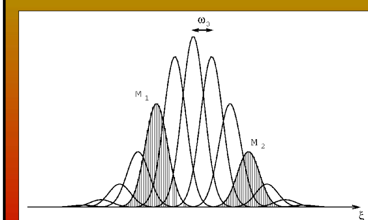
A qubit coupled to a bath of localised excitations: the CENTRAL SPIN Model

P.C.E. Stamp, PRL 61, 2905 (1988)
AO Caldeira et al., PR B48, 13974 (1993)
NV Prokof'ev, PCE Stamp, J Phys CM5, L663 (1993)
NV Prokof'ev, PCE Stamp, Rep Prog Phys 63, 669 (2000)

Now consider the coupling of our 2-level system to LOCALIZED modes. These have a Hilbert space of finite dimension, in the energy range of interest- in fact, often each localised excitation has a Hilbert space dimension 2. From this we see that our central Qubit is coupling to a set of effective spins; ie., to a "SPIN BATH". Unlike the case of the oscillators, we cannot assume these couplings are weak.

For simplicity assume here that the bath spins are a set $\{\sigma_k\}$ of 2-level systems. Now actually these interact with each other very weakly (because they are localised), but we cannot drop these interactions. What we then get is the following low-energy effective Hamiltonian (recall previous slide):

$$H(\Omega_o) = \{ [\Delta\tau_+ \exp(-i \Sigma_k \alpha_k.\sigma_k) + H.c.] + \varepsilon_o\tau_z \quad \text{(qubit)}$$
$$+ \tau_z\omega_k.\sigma_k + h_k.\sigma_k \quad \text{(bath spins)}$$
$$+ \text{ inter-spin interactions}$$



The crucial thing here is that now the couplings ω_k, h_k to the bath spins- the first between bath spin and qubit, the second to external fields- are often very strong (much larger than either the inter-spin interactions or even than Δ).

Decoherence in SQUIDs

A.J. Leggett et al., Rev. Mod Phys. 59, 1 (1987)
AND
PCE Stamp, PRL 61, 2905 (1988)
Prokof'ev and Stamp Rep Prog Phys 63, 669 (2000)

A very detailed analysis of couplings to the oscillator bath modes (these being mainly electrons, phonons, photons) shows, as one might expect, that their effects are worse at higher energy (ie., if either Δ_o or kT is large). In fact the decoherence rate goes like

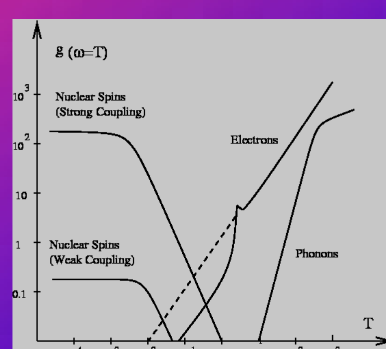
$$\tau_\phi^{-1} \sim \Delta_o \; g(\Delta,T) \coth(\Delta/2kT)$$

With the spectral function $g(\omega,T)$ as shown.

On the other hand paramagnetic spin impurities (particularly in the Josephson junctions), and nuclear spins have a Zeeman coupling to the SQUID flux which peaks at low energies- at energies below E_o, this typically causes complete incoherence. In the more interesting regime when $\Delta_o >> E_o$, the decoherence rate turns out to be:

$$1/\tau_\phi = \Delta_o \; (E_o/8\Delta_0)^2$$

(we will see later where this comes from).

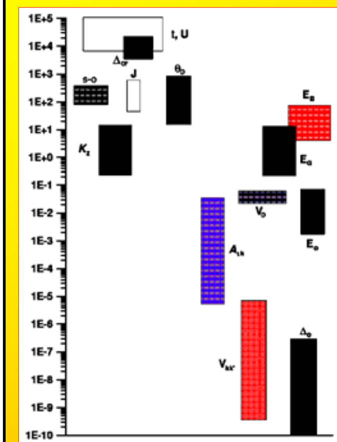


BANFF 13

Quantum Dynamics of an isolated Nanomagnet

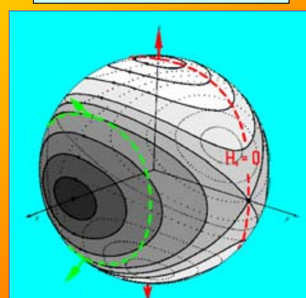
Magnetic systems are complex because there are many different interactions at different energy scales. However things simplify at low energy- the strong exchange interactions lock the electronic spins into a "Giant Spin" of spin S.

In a typical nanomagnet, one has an "easy axis" spin anisotropy potential. At low T, the only way the system can move quantum-mechanically from one well to another is by tunneling. It is very helpful to think of this in path integral language- the system looks very much like the well-known "double slit" set-up (including a tunneling amplitude which oscillates as one changes the tunneling paths using an external field). Below ~ 1K, the system behaves like a QUBIT:

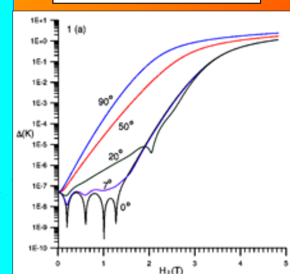


Energy scales in a magnetic System. At left, bulk system. At right, a nanomagnet.

Feynman Paths on the spin sphere for a biaxial potential. Application of a field pulls the paths towards the field



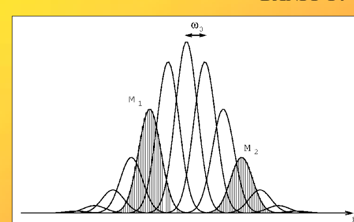
Typical tunneling splitting as a function of the magnitude and direction of the field



BANFF 14

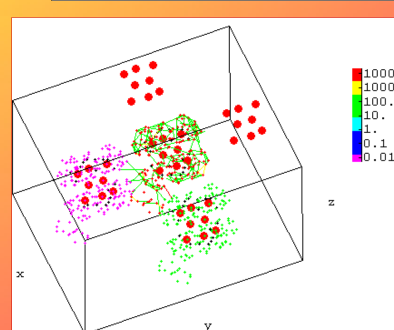
Quantum Relaxation of a single NANOMAGNET

Structure of Nuclear spin Multiplet →



When the characteristic magbit energy (the tunneling splitting Δ) is small- much less than the spread E_o in the nuclear multiplet states around each magbit level), the system relaxes via incoherent tunneling. The bias on the magbit coming from the time-fluctuating nuclear spin bath field acts like a rapidly varying noise field, causing the magbit to move rapidly in and out of resonance, PROVIDED the static field acting on the qubit satisfies

$$|g\mu_B S H_o| < E_o$$



Otherwise the fluctuations cannot bring the qubit to resonance. Notice that tunneling now proceeds over a wide range of bias, governed by the NUCLEAR SPIN multiplet. The relaxation rate is given by

$$\Gamma \sim \Delta^2/E_o$$ **for a single qubit.**

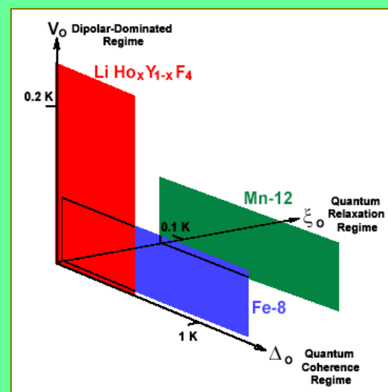
NV Prokof'ev, PCE Stamp, J Low Temp Phys 104, 143 (1996)

DYNAMICS of the DIPOLAR SPIN NET

The dipolar spin net is of great interest to solid-state theorists because it represents the behaviour of a large class of systems with "frustrating" interactions (spin glasses, ordinary dipolar glasses). It is also a fascinating toy model for quantum computation:

$$H = \sum_j (\Delta_j \tau_j^x + \varepsilon_j \tau_j^z) + \sum_{ij} V_{ij}^{dip} \tau_i^z \tau_j^z + H_{NN}(I_k) + H_\phi(x_q) + \text{interactions}$$

For magnetic systems this leads to the picture at right.



Almost all experiments so far are done in the region where Δ_o is small- whether the dynamics is dipolar-dominated or single molecule, it is incoherent. However one can give a theory of this regime.

The next great challenge is to understand the dynamics in the quantum coherence regime, with or without important inter-molecule interactions

Derivation of Kinetic Eqtn. For Q. Relaxation Regime

The kinetic eqtn for the magnetic qubit distribution $P_\alpha(\xi, r)$ is a BBGKY one, coupling it to the 2-qubit distribution P_2. Here r is the position of the qubit, $\alpha = +,-$ is the polarisation of the qubit along the z-axis, and ξ is the longitudinal field at r.

$$\dot{P}_\alpha(\xi,\vec{r}) = -\tau_N^{-1}(\xi)[P_\alpha(\xi,\vec{r}) - P_{-\alpha}(\xi,\vec{r})] - \sum_{\alpha'} \int \frac{d\vec{r}\,'}{\Omega_0} \int \frac{d\xi'}{\tau_N(\xi')} \left[P^{(2)}_{\alpha\alpha'}(\xi,\xi';\vec{r},\vec{r}\,') - P^{(2)}_{\alpha\alpha'}(\xi - \alpha\alpha'\tilde{U}(\vec{r}-\vec{r}\,'),\xi';\vec{r},\vec{r}\,') \right]$$

In this kinetic equation the interaction $U(r-r')$ is dipolar, and the relaxation rate τ^{-1}_N is the inelastic, nuclear spin-mediated, single qubit tunneling flip rate, as a function of the local bias field. As discussed before, this relaxation operates over a large bias range ξ_o where typically $\xi_o \sim E_o$ (and E_o is the width of the nuclear spin muliplet introduced before)

$$\tau_N^{-1}(\xi) \approx \tau_0^{-1} e^{-|\xi|/\xi_o}.$$

$$\tau_N^{-1}(\xi = 0) \equiv \tau_0^{-1} \approx \frac{2\Delta_{10}^2}{\pi^{1/2}\Gamma_2}.$$

$$\tilde{U}_{ij}^{zz} = \sum_{\mu_i \nu_j} \gamma_\mu \gamma_\nu \left[\frac{\mathbf{s}_{\mu_i} \cdot \mathbf{s}_{\nu_j}}{|\mathbf{r}_{\mu_i} - \mathbf{r}_{\nu_j}|^3} - 3\frac{(\mathbf{r}_{\mu_i} - \mathbf{r}_{\nu_j}) \cdot \mathbf{s}_{\mu_i} (\mathbf{r} - \mathbf{r}_k) \cdot \mathbf{s}_{\nu_j}}{|\mathbf{r}_{\mu_i} - \mathbf{r}_{\nu_j}|^5} \right]$$

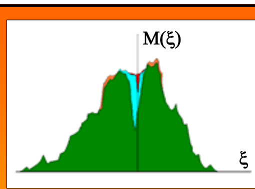
The BBGKY hierarchy can be truncated with the kinetic equation above if the initial 2-qubit distribution factorizes (see right). This happens if the system is initially (i) polarized or (ii) strongly annealed.

$$P_{\alpha\alpha'}(\xi,\xi',r,r';t) = P_\alpha(\xi,r,t) P_{\alpha'}(\xi',r',t) \ \text{at} \ t = 0$$

The kinetic equation can then be solved, and gives the square root short-time behaviour:

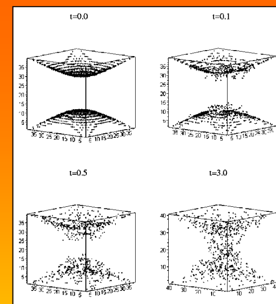
$$M(t) = M_o[1 - (t/\tau_Q)^{1/2}]$$

$$\Gamma_{sqrt} \equiv \tau_Q^{-1} \sim (\Delta_o^2/V_o)\xi_o N(\epsilon_o)$$



Quantum Relaxation in a "Spin Net" of Interacting MAGBITS

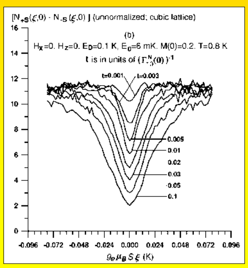
$V_{ij} >> E_o > \Delta$



IS Tupitsyn, PCE Stamp

At first glance the problem of a whole net of magbits, with long-range "frustrating" dipole interactions between them, looks insuperable. But actually the short-time dynamics can be solved analytically! This is because the dipole fields around the sample vary slowly in time compared to the fluctuating hyperfine fields. This leads to universal analytic predictions:

NV Prokof'ev, PCE Stamp, PRL 80, 5794 (1998)



(1) Only magbits near resonance make incoherent flips
As tunneling occurs, the resonant surfaces move & disintegrate- then, for ANY sample shape

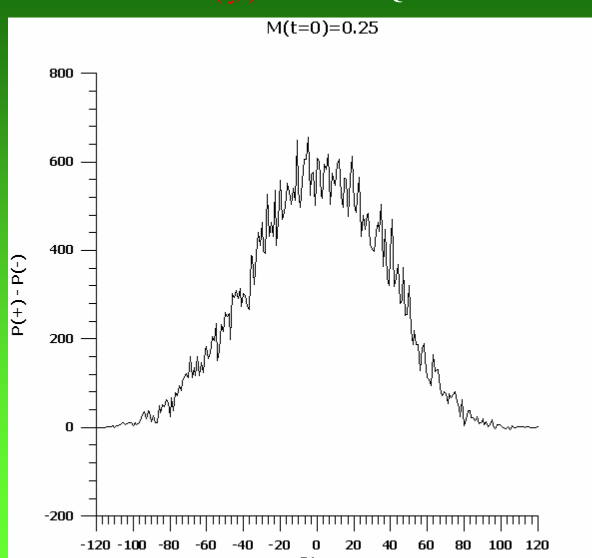
$$\delta M(t) \sim [t/\tau_Q]^{1/2} \qquad \tau_Q \sim (\Delta^2 T_2) E_o^2 N(\xi=\varepsilon_H)/W$$

where W is the width of the dipolar field distribution, and $N(\xi)$ is the density of the distribution over bias.

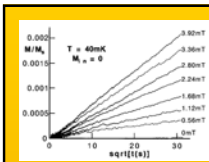
(2) Tunneling digs a "hole" in this distribution, with initial width E_o, and a characteristic spreading with time- so it depends again on the nuclear hyperfine couplings.

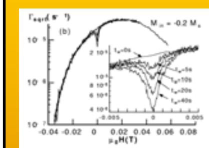
Monte Carlo simulation of relaxation dynamics (Tupitsyn)

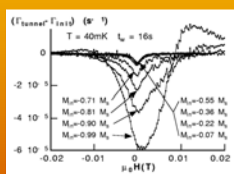
This is a movie simulation of $M(\xi,t)$ shown in SQUARE ROOT TIME.

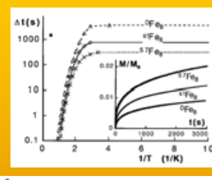


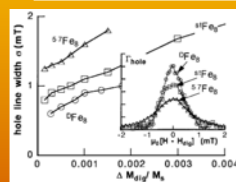
Quantum Relaxation Experiments in Magnetic Molecules

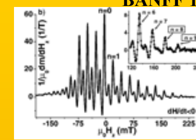










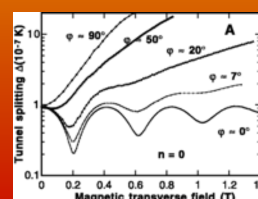


R. Giraud et al., PRL 87, 057203 (2001)

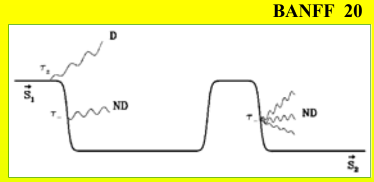
In the rare earth compound $\text{LiHo}_x\text{Y}_{1-x}\text{F}_4$ the hyperfine coupling on the Ho sites is so strong that one sees the hyperfine structure directly in the quantum relaxation rate. For dilute spins (x <<1) one looks at the relaxation of individual Ho ions- and sees the nuclear multiplet structure directly!

Experiments by 4 different groups have verified these predictions. These results on Fe-8 (of the Wernsdorfer group) show the square root relaxation, and the hole digging in the internal field distribution, Inferred from the square root relaxation rate. The hole width, and its variation with isotopes, agrees with theory. Finally, the relaxation rate oscillates with transverse field as expected for the Aharonov-Bohm oscillations in spin space.

Wernsdorfer et al, PRL 82, 3903 (1999); and PRL 84, 2965 (2000); and Science 284, 133 (1999)



DECOHERENCE In NANOMAGNETS

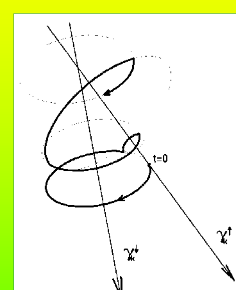


Now suppose that we have a very BIG energy scale for the qubit operation, so that $\Delta >> E_o$.
We can get coherence, but there is residual decoherence

(i) From the noise discussed before

(ii) From transitions INDUCED in the spin bath by the transitions of the qubit- this imparts an extra random topological phase to the spins in the bath. This exchange of phase causes "topological decoherence".

(iii) From precession of the bath spins in the field of the qubit- how this precession goes depends on which state the qubit is in. Thus by distinguishing the 2 qubit states, one causes decoherence.



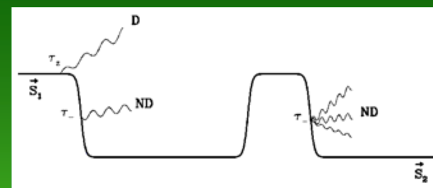
It is the precessional decoherence (which is related to the idea of motional narrowing in NMR) which causes the worst decoherence- at a rate

$$\tau_\phi^{-1} \sim (E_0/\Delta_o)^2 \Delta_o$$

So- this is where we should look for coherence in magbits. No experiments yet…..

Dynamics of Central Spin Model- some key points

The easiest way to solve for the dynamics of problems like this (going back to the Kondo problem) is a path integral formulation. The effective Hamiltonian has both diagonal (D) and non-diagonal (ND) couplings in the qubit variables. A typical path is shown at right.



The standard way of doing such path integrals assumes a weak coupling to each environmental mode, assumed to be an oscillator- one then writes it as an integral over an "influence functional" (a la Feynman).

$$P_{11}(t) = \sum_{nm}^{\infty} (\mathrm{i}\Delta_0)^{2(n+m)} \int_0^t \mathrm{d}t_1 \cdots \int_{t_{2n-1}}^t \mathrm{d}t_{2n} \int_0^t \mathrm{d}t_1' \cdots \int_{t_{2m-1}'}^t \mathrm{d}t_{2m}' \mathcal{F}[Q_{(n)}, Q_{(m)'}].$$

The problem when one couples a qubit to a spin bath is that this assumption is no longer generally true- very often the coupling between the qubit and each bath spin is quite strong (indeed, with magnets, it can be much bigger even than Δ_o). Thus with a Hamiltonian like the Central spin model (we recall again the Hamiltonian here), we cannot use the influence functional technique.

$$H_{CS}(\Omega_0) = \left\{ 2\tilde{\Delta}\hat{\tau}_- \cos\left[\Phi - \sum_k \vec{V}_k \cdot \hat{\vec{\sigma}}_k\right] + \mathrm{H.c.} \right\} + \hat{\tau}_z \sum_{k=1}^N \omega_k^{\parallel} \vec{l}_k \cdot \hat{\vec{\sigma}}_k + \sum_{k=1}^N \omega_k^{\perp} \vec{m}_k \cdot \hat{\vec{\sigma}}_k + \sum_{k=1}^N \sum_{k'=1}^N V_{kk'}^{\alpha\beta} \hat{\sigma}_k^{\alpha} \hat{\sigma}_{k'}^{\beta}$$

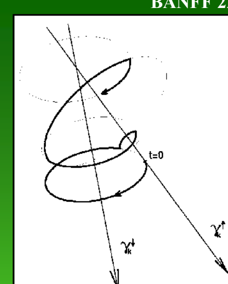
Precessional Decoherence- derivation

$$H_{\mathrm{eff}} = 2\Delta_0 \tau_x + \hat{\tau}_z \omega_0^{\parallel} \sum_{k=1}^N \vec{l}_k \cdot \hat{\vec{\sigma}}_k + \sum_{k=1}^N \omega_k^{\perp} \vec{m}_k \cdot \hat{\vec{\sigma}}_k .$$

The most important physical effects are contained in the above reduced Hamiltonian. To handle this we introduce a unitary rotation between the 2 field directions

$$|\{\vec{\sigma}_k^f\}\rangle = \prod_{k=1}^N \hat{U}_k |\{\vec{\sigma}_k^{\mathrm{in}}\}\rangle = \hat{U}|\{\vec{\sigma}_k^{\mathrm{in}}\}\rangle.$$

$$|\vec{\sigma}_k^f\rangle = \hat{U}_k |\vec{\sigma}_k^{\mathrm{in}}\rangle = \mathrm{e}^{-\mathrm{i}\beta_k \hat{\sigma}_k^x} |\vec{\sigma}_k^{\mathrm{in}}\rangle.$$



The 2 qubit fields

The constraint of long nuclear T_1 means polarisation group M does not change- implemented in a path integral with a projection operator Π_M

$$\hat{\Pi}_M = \delta\left(\sum_{k=1}^N \hat{\sigma}_k^z - M\right) = \int_0^{2\pi} \frac{\mathrm{d}\xi}{2\pi} \mathrm{e}^{\mathrm{i}\xi(\sum_{k=1}^N \hat{\sigma}_k^z - M)}.$$

The dynamics of the qubit reduced density matrix are found by summing over paths, using the angle β_k (the angle between the fields γ_k^+ and γ_k^-) as expansion parameter.

Physically, the bath spins precess around the 2 qubit fields, and the integration picks up the precessional phase (top right)

$$P_{M_0,M}(t) \equiv \langle R^*_{M_0,M}(t) R_{M_0,M}(t)\rangle = \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} \frac{(\mathrm{i}\Delta_0(\Phi)t)^{2(n+m)}}{(2n)!(2m)!} \prod_{i=1}^{2n}\prod_{j=1}^{2m} \int \frac{\mathrm{d}\xi_i}{2\pi} \times \int \frac{\mathrm{d}\xi_j'}{2\pi} \mathrm{e}^{-\mathrm{i}M_0(\sum_i^{2n}\xi_i - \sum_j^{2m}\xi_j')} \mathrm{e}^{2\mathrm{i}M(\sum_{i=\mathrm{odd}}^{2n-1}\xi_i - \sum_{j=\mathrm{odd}}^{2m-1}\xi_j')} \langle \hat{T}_{2m}^{\dagger} \hat{T}_{2n}\rangle.$$

$$\hat{T}_{2n}^{(k)}|\uparrow_k\rangle = \mathrm{e}^{\mathrm{i}\xi_{2n}\hat{\sigma}_k^z}\mathrm{e}^{-\mathrm{i}\beta_k\hat{\sigma}_k^x}\ldots\mathrm{e}^{-\mathrm{i}\beta_k\hat{\sigma}_k^x}\mathrm{e}^{\mathrm{i}\xi_1\hat{\sigma}_k^z}\mathrm{e}^{\mathrm{i}\beta_k\hat{\sigma}_k^x}|\uparrow_k\rangle = \mathrm{e}^{\mathrm{i}\sum_{i=1}^{2n}\xi_i}\Big[(1-n\beta_k^2)|\uparrow_k\rangle + \mathrm{i}\beta_k|\downarrow_k\rangle \sum_{l=1}^{2n}(-1)^{l+1}\mathrm{e}^{-2\mathrm{i}\sum_{i=l}^{2n}\xi_i} - \beta_k^2|\uparrow_k\rangle \sum_{l'=l+1}^{2n}\sum_{l=1}^{2n-1}(-1)^{l'-l}\mathrm{e}^{-2\mathrm{i}\sum_{i=l}^{l'-1}\xi_i} + \mathrm{O}(\beta_k^3)\Big],$$

The path integral splits into contributions for each M. They have the effective action of a set of interacting instantons

$$P_M(t) = \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} \frac{(\mathrm{i}\Delta_0(\Phi)t)^{2(n+m)}}{(2n)!(2m)!} \prod_{i=1}^{2n}\prod_{j=1}^{2m} \int \frac{\mathrm{d}\xi_i}{2\pi} \times \int \frac{\mathrm{d}\xi'_j}{2\pi} \exp\{2\mathrm{i}M(\xi_{2n-1}+\xi_{2n-3}+\cdots+\xi_1) - K^{\mathrm{eff}}_{nm}(\xi_i,\xi'_j)\}.$$

$$\chi_\alpha = \sum_{\alpha'=\alpha}^{2(n+m)} 2\xi_{\alpha'} + \pi\alpha,$$

$$P_M(t) = \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} \frac{(\mathrm{i}\Delta_0(\Phi)t)^{2(n+m)}}{(2n)!(2m)!} \left(\prod_{\alpha=1}^{2(n+m)} \int \frac{\mathrm{d}\chi_\alpha}{2\pi}\right) \times \exp\left\{\mathrm{i}M\sum_{\alpha}(-1)^{\alpha+1}\chi_\alpha - 2\kappa\left[(n+m) + \sum_{\alpha'>\alpha}\cos(\chi_\alpha - \chi_{\alpha'})\right]\right\}.$$

The effective interactions can be mapped to a set of fake charges to produce an action having the structure of a "spherical model" involving a spin S

$$\vec{\mathcal{S}} = \sum_{\alpha=1}^{2(n+m)} \vec{s}_\alpha, \qquad \sum_{\alpha',\alpha}\cos(\chi_\alpha - \chi_{\alpha'}) = \vec{\mathcal{S}}^2.$$

$$G(\vec{\mathcal{S}}) = \left(\prod_{\alpha=1}^{2(n+m)} \int \frac{\mathrm{d}\chi_\alpha}{2\pi} \mathrm{e}^{\mathrm{i}M(-1)^{\alpha+1}\chi_\alpha}\right) \exp\left\{-\kappa\sum_{\alpha',\alpha}\cos(\chi_\alpha - \chi_{\alpha'})\right\} = \left(\prod_{\alpha=1}^{2(n+m)} \int \frac{\mathrm{d}\chi_\alpha}{2\pi} \mathrm{e}^{\mathrm{i}M(-1)^{\alpha+1}\chi_\alpha}\right)\mathrm{e}^{-\kappa\vec{\mathcal{S}}^2}.$$

The key step is to then reduce this to a sum over Bessel functions associated with each polarisation group.

$$G(\vec{\mathcal{S}}) = \int \mathrm{d}\vec{\mathcal{S}}\mathrm{e}^{-\kappa\vec{\mathcal{S}}^2} \prod_{\alpha=1}^{2(n+m)} \int \frac{\mathrm{d}\chi_\alpha}{2\pi} \mathrm{e}^{\mathrm{i}M(-1)^{\alpha+1}\chi_\alpha} \delta\left(\vec{\mathcal{S}} - \sum_\alpha \vec{s}_\alpha\right)$$
$$= \int \frac{\mathrm{d}\vec{z}}{2\pi} \int \mathrm{d}\vec{\mathcal{S}}\mathrm{e}^{-\kappa\vec{\mathcal{S}}^2 + \mathrm{i}\vec{z}\cdot\vec{\mathcal{S}}} \left(\int_0^{2\pi} \frac{\mathrm{d}\chi_\alpha}{2\pi} \mathrm{e}^{-\mathrm{i}\vec{z}\vec{s}_\alpha + \mathrm{i}M\chi_\alpha}\right)^{2(n+m)}$$
$$= \frac{1}{2\kappa}\int \mathrm{d}z z \mathrm{e}^{-z^2/4\kappa} J_M^{2(n+m)}(z),$$

We can now reduce the time evolution of the qubit density matrix to a sum over independently relaxing polarisation groups. The interesting thing here is that each group has its own effective tunneling matrix element $\Delta_M(x)$.

$$P_M(t) = 2\int_0^\infty \mathrm{d}x x \mathrm{e}^{-x^2} \frac{1}{2}\left(1 + \sum_{s=0}^{\infty} \frac{[2\mathrm{i}t\Delta_0(\Phi)J_M(2x\sqrt{\kappa})]^{2s}}{(2s)!}\right)$$
$$= P_M(t) = \int_0^\infty \mathrm{d}x x \mathrm{e}^{-x^2}(1 + \cos[2\Delta_0(\Phi)J_M(2x\sqrt{\kappa})t])$$
$$\equiv 2\int_0^\infty \mathrm{d}x x \mathrm{e}^{-x^2} P_{11}^{(0)}(t, \Delta_M(x)),$$

a *superposition of non-interacting* correlation functions for effective tunnelling rates $\Delta_M(x)$

But.. $\Delta_M(x)$ has to be phase-averaged over a phase variable x. This variable represents the accumulated precessional phase of the spin bath. The total dephasing effect of this average is parametrised by the dimensionless κ.

$$\Delta_M(x) = \Delta_0(\Phi)J_M(2x\sqrt{\kappa}).$$

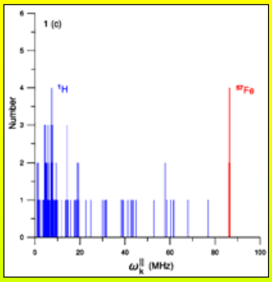
This parameter tells us the total effect of the mismatch between the 2 fields from the qubit on the bath spins (which is parametrised for each bath spin by the angle β_k). The total effect is reminiscent of the reduction of transition rates embodied in the Frank-Condon or Anderson orthogonality reduction factors.

$$\mathrm{e}^{-\kappa} = \prod_{k=1}^{N}\cos\beta_k \sim \mathrm{e}^{-(1/2)\sum_k \beta_k^2}.$$

Finally, we have to perform a thermal average over different polarisation groups.

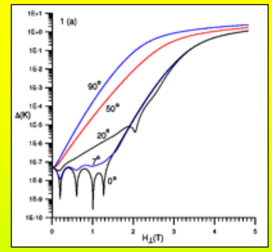
$$P_{11}(t;T) = \sum_{M=-N}^{N} w(T,M)P_M(t),$$

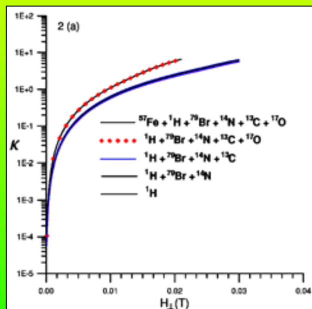
DECOHERENCE in the Fe-8 Molecule



Hyperfine couplings for H,^{57}Fe

This remarkable molecule cannot only be well-characterised in experiments, it also can be given a very accurate theoretical analysis. All nuclear spin interactions can be determined theoretically, with reasonable accuracy.

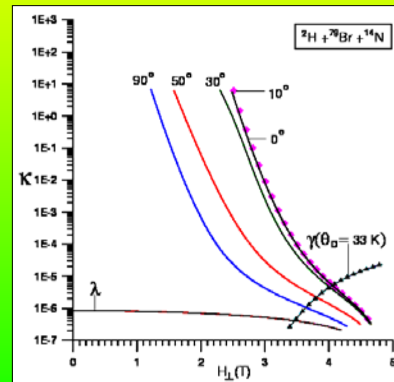




Shown here is the dimensionless decoherence rate

$$\kappa = (\Delta_o \tau_\phi)^{-1}$$

coming from the precessional decoherence mechanism for low & high transverse fields (see STAMP & TUPITSYN, Condmat 0302015)



Decoherence in SQUIDs

A.J. Leggett et al., Rev. Mod Phys. 59, 1 (1987)
AND
PCE Stamp, PRL 61, 2905 (1988)
Prokof'ev and Stamp Rep Prog Phys 63, 669 (2000)

We recall from the earlier slides that the oscillator bath decoherence rate goes like

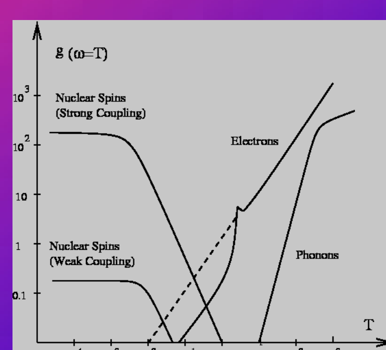
$$\tau_\phi^{-1} \sim \Delta_o \; g(\Delta,T) \coth(\Delta/2kT)$$

with the spectral function $g(\omega,T)$ shown below for an Al SQUID (contribution from electrons & phonons). All of this is well known and leads to a decoherence rate $\tau_\phi^{-1} \sim \pi\alpha\Delta_o$ once $kT < \Delta_o$. By reducing the flux change $\delta\phi = (\phi_+ - \phi_-) \sim 10^{-3}$, it has been possible to make $\alpha \sim 10^{-7}$ (Delft expts), ie., a decoherence rate for electrons ~ O(100 Hz). This is v small!

On the other hand paramagnetic spin impurities (particularly in the junctions), & nuclear spins have a Zeeman coupling to the SQUID flux peaking at low energies- at energies below E_o, this will cause complete incoherence. Coupling to charge fluctuations (also a spin bath of 2-level systems) is not shown here, but also peaks at very low frequencies.

However when $\Delta_o >> E_o$, the spin bath decoherence rate is:

$$1/\tau_\phi = \Delta_o \; (E_o/8\Delta_0)^2 \qquad \text{as before}$$



CONCLUSIONS & SUMMARY

GENERAL: The spin bath decoherence effects dominate at low energy, whereas oscillator baths dominate at high energy. Both can be reduced in various ways, leaving an "opportunity window" in frequency, where decoherence is v small. This decoherence window is generic to solid-state qubit designs, & of practical importance.

SQUIDS: Very low coupling to oscillator bath excitations has now been achieved in expts. This has opened up the opportunity window but the decoherence from low-energy excitations (attributed in the expts to noise from charge fluctuations and spin impurities) is still a serious problem. We suggest that it will be important to purify spins from the system.

MAGNETS: The incoherent relaxation regime is now well understood, both for single nanomagnetic systems, and for interacting dipolar arrays. Applying strong transverse fields will take some systems to a very low decoherence regime. By far the worst obstacle to getting qubit nets is nuclear spin decoherence- this is obvious in expts as well as in the theory. Better probing and control of the nuclear spin dynamics is required.