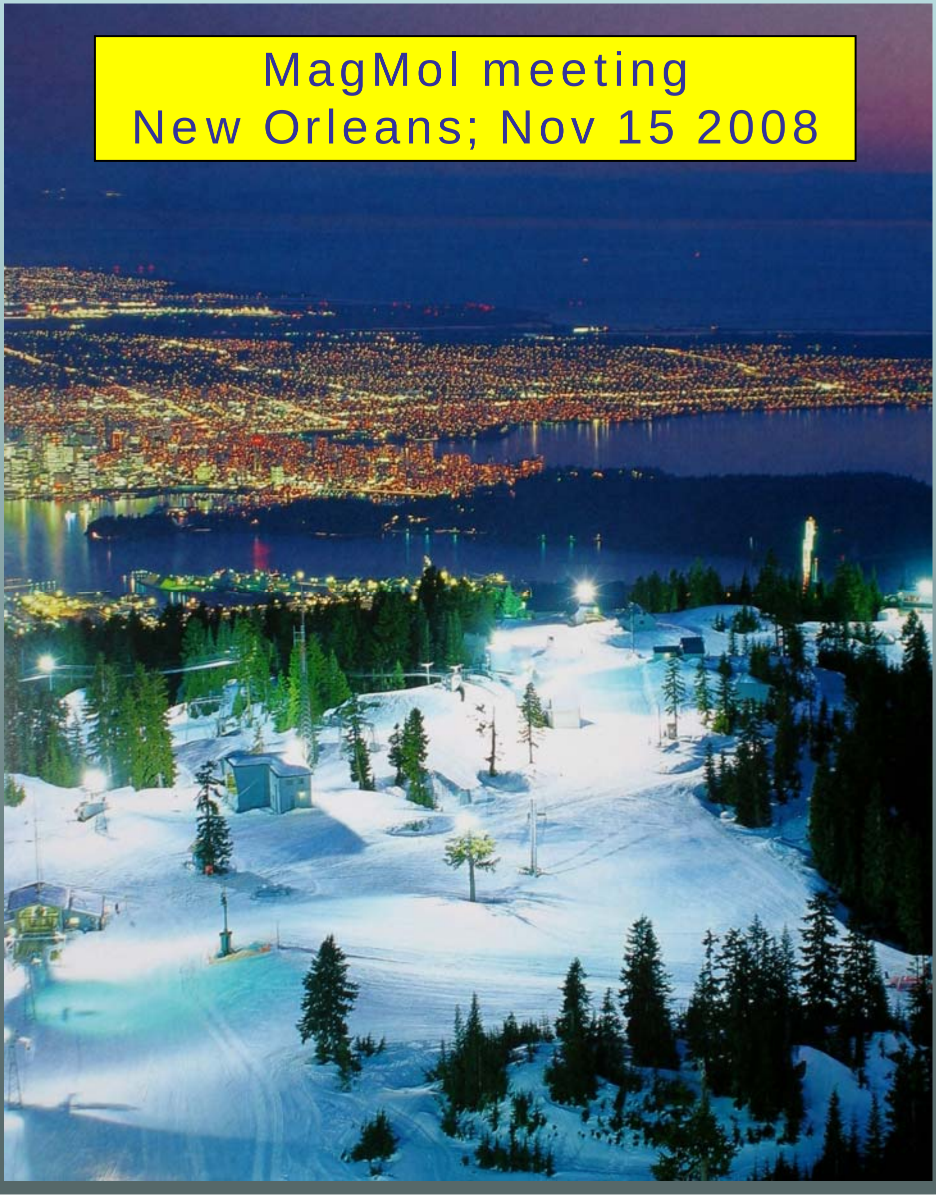
PCE STAMP

REMARKS on COHERENCE & DECOHERENCE in Chemistry-based spin qubit systems



MagMol meeting
New Orleans; Nov 15 2008

Physics & Astronomy
UBC
Vancouver

Pacific Institute
for
Theoretical Physics

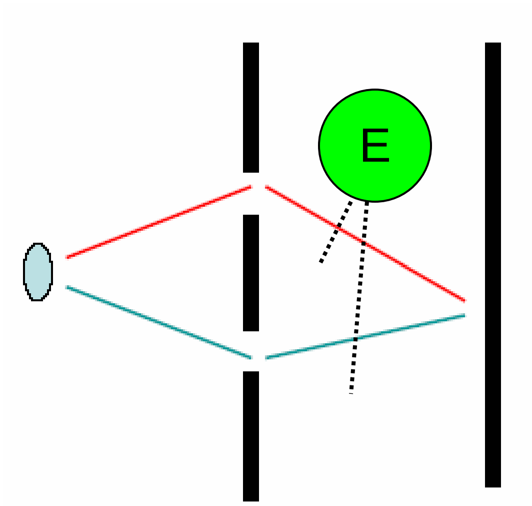
WELL, HERE
WE ARE in
New Orleans

Lots of
TASTES
SIGHTS
&
SOUNDS

PART 1

SOME REMARKS
on
DECOHERENCE

Question: WHAT DO WE MEAN BY "DECOHERENCE" ?



When some quantum system with coordinate Q interacts with any other system (with coordinate x) , the result is typically that they form a combined state in which there is some entanglement between the two systems.

Example: **In a 2-slit expt., the particle coordinate Q couples to photon coordinates, so that we have the following possibility:**

$$\Psi_o(Q) \;\; \Pi_q \, \phi_q^{in} \;\; \rightarrow \;\; [a_1 \Psi_1(Q) \, \Pi_q \, \phi_q^{(1)} \;\; + \;\; a_2 \Psi_2(Q) \, \Pi_q \, \phi_q^{(2)} \,]$$

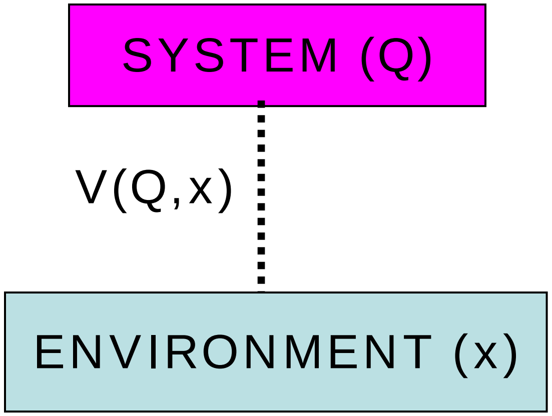
But now suppose we do not have any knowledge of, or control over, the photon states- we must then average over these states, in a way consistent with the experimental constraints. In the extreme case this means that we lose all information about the PHASES of the coefficients a_1 & a_2 (and in particular the relative phase between them). This process is called DECOHERENCE

NB 1: **In this interaction between the system and its "Environment" E (which is in effect performing a measurement on the particle state), there is no requirement for energy to be exchanged between the system and the environment- only a communication of phase information.**

NB 2: **Nor is it the case that the destruction of the phase interference between the 2 paths must be associated with a noise coming from the environment- what matters is that the state of the environment be CHANGED according to the what is the state of the system.**

Question: How do we describe this for a 'COMPLEX' SYSTEM ?

DECOHERENCE – The 'Standard Model'



SYSTEM (Q)

V(Q,x)

ENVIRONMENT (x)

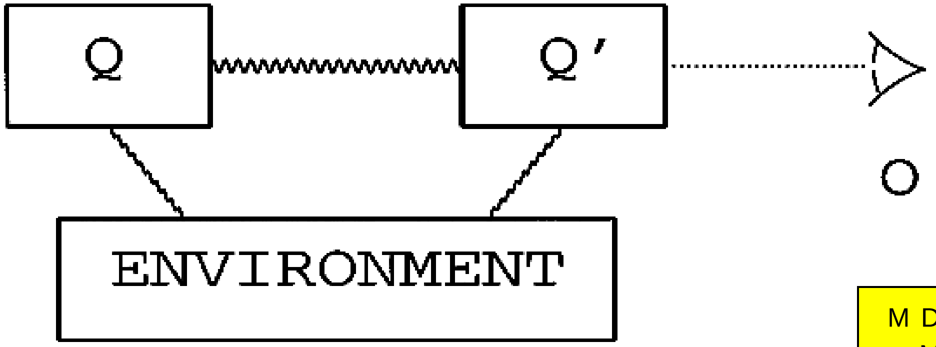
As discussed very clearly by Feynman, we can start any discussion in quantum field theory in terms of a Model in which a the system of interest is coupled to an environment of some kind, as shown.

The appropriate effective Hamiltonian is

$$\mathcal{H} = H_o(Q) + V(Q,x) + H_{env}(x)$$

where the environmental variables range over the 'rest of the universe'.

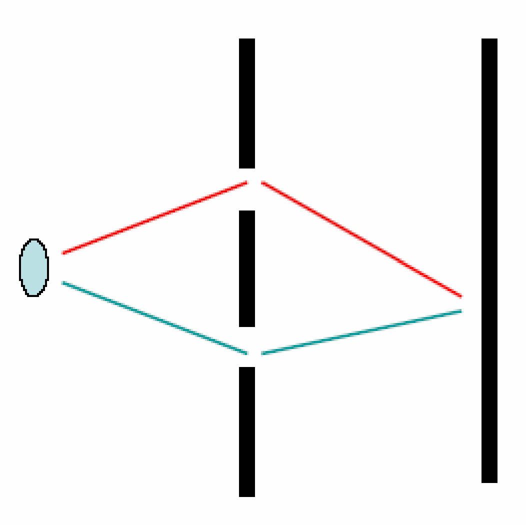
The standard idea is then that we 'integrate out' (ie., average over) the environmental variables to calculate the statistical behaviour (in the form of a reduced density matrix) of the system. This averaging generates interactions. If the dynamics of system and environment are entangled, this produces decoherence in the system dynamics.

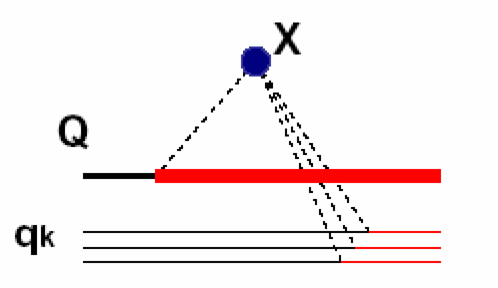


One can do the same analysis of the dynamics of a system plus measuring apparatus; or more generally for any number of 'systems'; averaging generates interactions

M Dube PCE Stamp, Int J Mod Phys B12, 1191 (1998)
M Dube, PCE Stamp, Chem Phys 268, 257 (2001)

WARNING: 3rd PARTY DECOHERENCE





This is fairly simple- it is decoherence in the dynamics of a system A (coordinate Q) caused by *indirect* entanglement with an environment E- the entanglement is achieved via a 3rd party B (coordinate X).

Ex: Buckyball decoherence

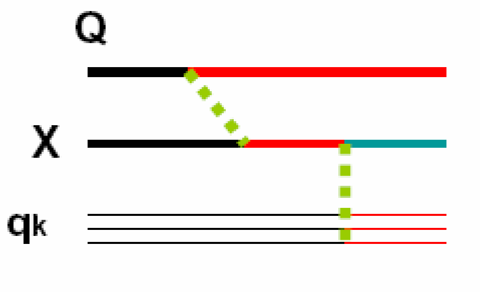
Consider the 2-slit expt with buckyballs. The COM coordinate Q of the buckyball does not couple directly to the vibrational modes $\{q_k\}$ of the buckyball- by definition. However BOTH couple to the slits in the system, in a distinguishable way.

Note: the state of the 2 slits, described by a coordinate X, is irrelevant- it does not need to change at all. We can think of it as a scattering potential, caused by a system with infinite mass (although recall Bohr's response to Einstein, which includes the recoil of the 2 slit system). It is a PASSIVE 3rd party.

PCE Stamp, Stud. Hist Phil Mod Phys **37**, 467 (2006)

ACTIVE 3rd PARTY: **Here the system state correlates with the 3rd party, which then goes on to change the environment to correlate with Q. We can also think of the 3rd party X as PREPARING the states of both system and environment. Alternatively we can think of the system and the environment as independently measuring the state of X. In either case we see that system and environment end up being correlated/entangled.**

Note the final state of X is not necessarily relevant- it can be changed in an arbitrary way after the 2nd interaction of X. Thus X need not be part of the environment. Note we could also have more than one intermediary- ie., X, Y, etc.- with correlations/entanglement are transmitted along a chain (& they can wiped out before the process is finished).

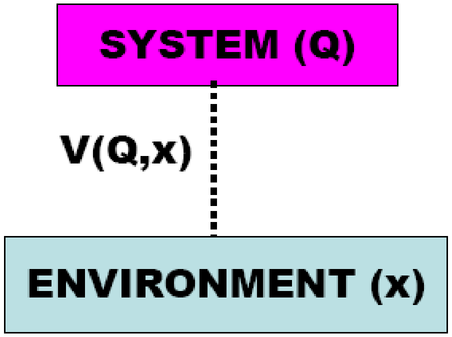


ENVIRONMENTAL DECOHERENCE

Typically we will be concerned with a system where a set of interactions (which may try to freeze the system) competes with quantum fluctuations – for example:

$$H_o = \Sigma_j \Delta_j \tau_j^x + \Sigma_{ij} V_{ij} \tau_i^z \tau_j^z$$

However this is not enough to properly understand the system – it will give results which badly misrepresent its true behaviour. The dynamics at low T depends essentially on what sort of environment the system variables couple to. The question of how to treat the environment must not be treated lightly.



SYSTEM (Q)

V(Q,x)

ENVIRONMENT (x)

Quite generally we are interested in $\mathcal{H} = H_o(Q) + V(Q,x) + H_{env}(x)$

However there are two kinds of environment:

OSCILLATOR BATH: $H_{\text{eff}}^{\text{osc}} = H_0 + H_{\text{int}} + H_{\text{env}}^{\text{osc}}$

where $H_{osc} = \sum_{q=1}^{N_o} \left(\frac{p_q^2}{m_q} + m_q \omega_q^2 x_q^2 \right)$ and $H_{\text{int}}^{\text{osc}} = \sum_{q=1}^{N} [F_q(Q) x_q + G_q(P) p_q]$

Feynman & Vernon, Ann. Phys. 24, 118 (1963)

Caldeira & Leggett, Ann. Phys. 149, 374 (1983)
AJ Leggett et al, Rev Mod Phys 59, 1 (1987

SPIN BATH: $H_{\text{eff}}^{\text{sp}}(\Omega_0) = H_0 + H_{\text{int}}^{\text{sp}} + H_{\text{env}}^{\text{sp}}$

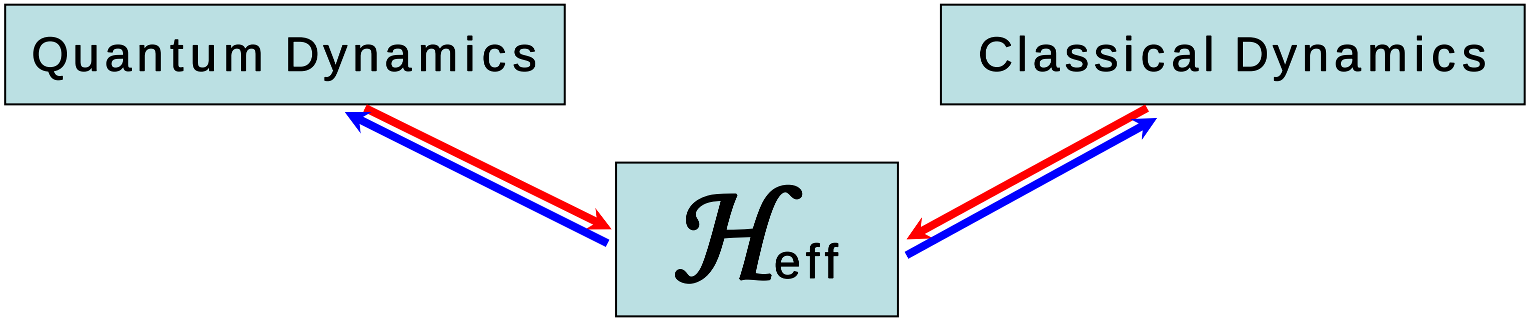
where $H_{\text{env}}^{\text{sp}} = \sum_k^{N_s} \mathbf{h}_k \cdot \boldsymbol{\sigma}_k + \sum_{k,k'}^{N_s} V_{kk'}^{\alpha\beta} \sigma_k^{\alpha} \sigma_{k'}^{\beta}$

and $H_{\text{int}}^{\text{sp}} = \sum_k^{N_s} \boldsymbol{F}_k(P,Q) \cdot \boldsymbol{\sigma}_k$

Defects, TLS, dislocations, Nuclear & PM spins, Charge fluctuators..

(1) P.C.E. Stamp, PRL 61, 2905 (1988)
(2) NV Prokof'ev, PCE Stamp, J Phys CM5, L663 (1993)
(3) NV Prokof'ev, PCE Stamp, Rep Prog Phys 63, 669 (2000)

REDUCTION to a LOW-ENERGY OSCILLATOR BATH FORM



Quantum Dynamics

Classical Dynamics

$\mathcal{H}_{\text{eff}}$

Suppose we want to describe the dynamics of some quantum system in the presence of decoherence. As pointed out by Feynman and Vernon, if the coupling to all the environmental modes is WEAK, we can map the environment to an 'oscillator bath, giving an effective Hamiltonian like:

$$H_{\text{eff}}(\Omega_0) = H_0(P,Q) + \sum_{q=1}^{N} [F_q(P,Q)x_q + G_q(P,Q)p_q] + \frac{1}{2}\sum_{q=1}^{N}\left(\frac{p_q^2}{m_q} + m_q\omega_q^2 x_q^2\right)$$

A much more radical argument was given by Caldeira and Leggett- that for the purposes of TESTING the predictions of QM, one can pass between the classical and quantum dynamics of a quantum system in contact with the environment via H_{eff}. Then, it is argued, one can connect the classical dissipative dynamics directly to the low-energy quantum dynamics, even in the regime where the quantum system is showing phenomena like tunneling, interference, coherence, or entanglement; and even where it is MACROSCOPIC.

This is a remarkable claim because it is very well-known that the QM wave-function is far richer than the classical state- and contains far more information.

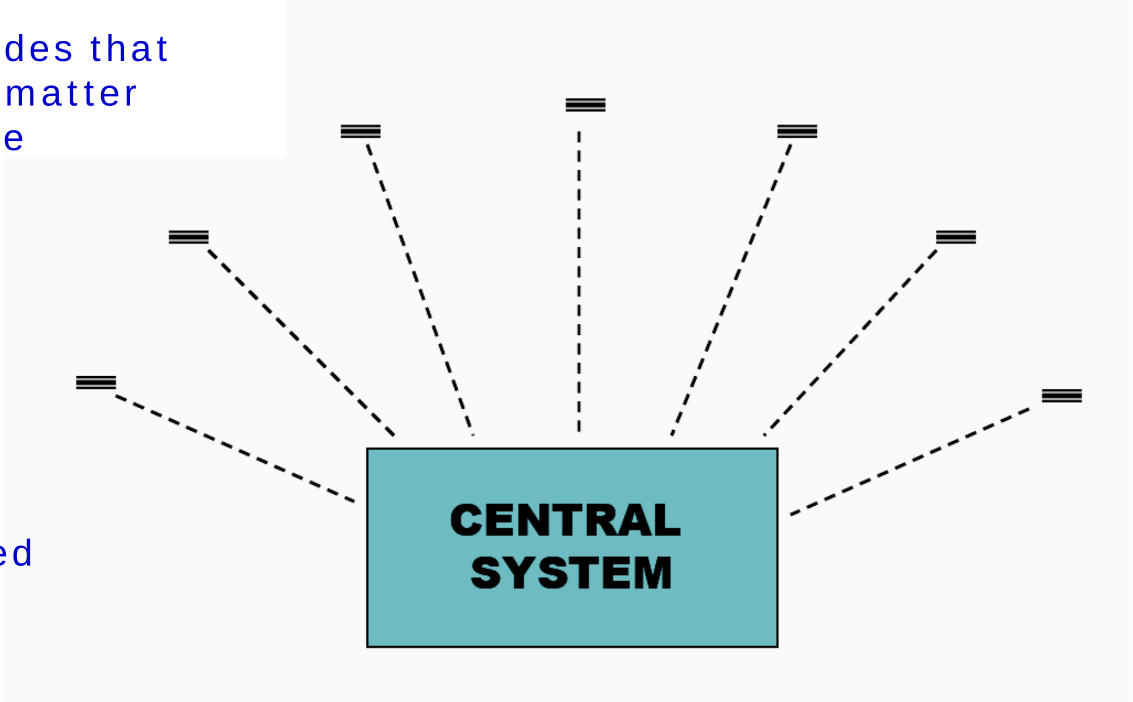
Feynman & Vernon, Ann. Phys. 24, 118 (1963)

Caldeira & Leggett, Ann. Phys. 149, 374 (1983)
AJ Leggett et al, Rev Mod Phys 59, 1 (1987

QUANTUM ENVIRONMENTS of LOCALISED MODES

Consider now the set of localised modes that exist in all solids (and all condensed matter systems except the He liquids). As we saw before, a simple description of these on their own is given by the 'bare spin bath Hamiltonian'

$$H_{env}^{sp} = \sum_{k}^{N_s} \mathbf{h}_k \cdot \boldsymbol{\sigma}_k + \sum_{k,k'}^{N_s} V_{kk'}^{\alpha\beta} \sigma_k^{\alpha} \sigma_{k'}^{\beta}$$



where the 'spins' represent a set of discrete modes (ie., having a restricted Hilbert space). These must couple to the central system with a coupling of general form:

$$H_{int}^{sp} = \sum_{k}^{N_s} \boldsymbol{F}_k(P,Q) \cdot \boldsymbol{\sigma}_k$$

$$H = H_0(P,Q) + H_{\text{int}}(P,Q;\{\hat{\vec{\sigma}}\}) + H_{\text{env}}(\{\hat{\vec{\sigma}}\})$$

$$H_{\text{int}}(P,Q;\{\hat{\vec{\sigma}}\}) = \sum_{k=1}^{N} [F_k^{\parallel}(P,Q)\hat{\sigma}_k^z + [F_k^{\perp}(P,Q)\hat{\sigma}_k^- + \text{h.c.}]]$$

$$H_{\text{env}}(\{\hat{\vec{\sigma}}\}) = \sum_{k=1}^{N} \vec{h}_k \hat{\vec{\sigma}}_k + \sum_{k=1}^{N}\sum_{k'=1}^{N} V_{kk'}^{\alpha\beta}\hat{\sigma}_k^{\alpha}\hat{\sigma}_{k'}^{\beta}$$

We are thus led to a general description of a quantum system coupled to a 'spin bath', of the form shown at right. This is not the most general possible Hamiltonian, because the bath modes may have more than 2 relevant levels.

P.C.E. Stamp, PRL 61, 2905 (1988)
NV Prokof'ev, PCE Stamp, J Phys CM5, L663 (1993)
NV Prokof'ev, PCE Stamp, Rep Prog Phys 63, 669 (2000)

A NOTE on the FORMAL NATURE of the PROBLEM

We want the density matrix

$$K(Q_2, Q_2'; Q_1, Q_1'; t, t') = \int_{Q_1}^{Q_2} \mathscr{D}q \int_{Q_1'}^{Q_2'} \mathscr{D}q' \, \mathrm{e}^{-\mathrm{i}/\hbar(S_0[q]-S_0[q'])} \mathscr{F}[q, q'],$$

with $$\mathcal{F}[Q, Q'] = \prod \langle \hat{U}_k(Q, t) \hat{U}_k^\dagger(Q', t) \rangle$$

Here the unitary operator $\hat{U}_k(Q, t)$ describes the evolution of the kth environmental mode, given that the central system follows the path $Q(t)$ on its 'outward' voyage, and $Q'(t)$ on its 'return' voyage; and $\mathcal{F}[Q, Q']$ acts as a weighting function, over different possible paths $(Q(t), Q'(t'))$.

Easy for oscillator baths (it is how Feynman set up field theory). We write:

$$\mathcal{F}[Q,Q'] \;=\; \prod_q^{N_o} \int \mathcal{D}x_q(\tau) \int \mathcal{D}x_q(\tau') \; \exp\left[\frac{i}{\hbar} \int d\tau \frac{m_q}{2}[\dot{x}_q^2 - \dot{x}_q'^2 + \omega_q^2(x_q^2 - x_q'^2)] \;+\; [F_q(Q)x_q - F_q(Q')x_q']\right]$$

For the simplified bilinear 'Caldeira-Leggett' form, $F_q(P,Q)\,x_q = v_q x_q Q$ we get

$$F[q,q'] \;=\; \exp\left[-\frac{1}{\hbar} \int_{t_o}^{t} d\tau_1 \int_{t_o}^{\tau_1} d\tau_2 [q(\tau_1) - q'(\tau_2)][\mathcal{D}(\tau_1 - \tau_2) q(\tau_2) - \mathcal{D}^*((\tau_1 - \tau_2) q'(\tau_2)]\right]$$

where $$\mathcal{D}(\tau) \;=\; \sum_q \frac{|v_q|^2}{2m_q\omega_q} \left[e^{i\omega_q\tau} \;+\; 2\frac{\cos\omega_q\tau}{e^{\beta\omega_q} - 1}\right]$$

For a spin bath it is not so simple. We have:

$$\mathcal{F}[Q,Q'] \;=\; \prod_k^{N_s} \int \mathcal{D}\boldsymbol{\sigma}_k(\tau) \int \mathcal{D}\boldsymbol{\sigma}_k(\tau') \; \exp\left[\frac{i}{\hbar}(S_{int}[Q,\boldsymbol{\sigma}_k] - S_{int}[Q',\boldsymbol{\sigma}_k'] \;+\; S_E[\boldsymbol{\sigma}_k] - S_E[\boldsymbol{\sigma}_k'])\right]$$

where

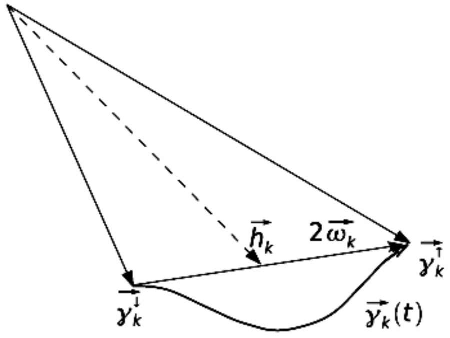
$$S_{int}^{sp}(Q,\boldsymbol{\sigma}_k) \;=\; -\int d\tau \sum_k^{N_s} \boldsymbol{F}_k(P,Q) \cdot \boldsymbol{\sigma}_k \qquad \& \qquad S_{env}^{sp} \;=\; \int d\tau \left[\sum_k^{N_s} (\mathcal{A}_k \cdot \frac{d\boldsymbol{\sigma}_k}{dt} \;-\; \mathbf{h}_k \cdot \boldsymbol{\sigma}_k) \;-\; \sum_{k,k'}^{N_s} V_{kk'}^{\alpha\beta} \sigma_k^\alpha \sigma_{k'}^\beta\right]$$

Integrating out the spin bath is then non-trivial (see Appendix)

RESULTS: DECOHERENCE

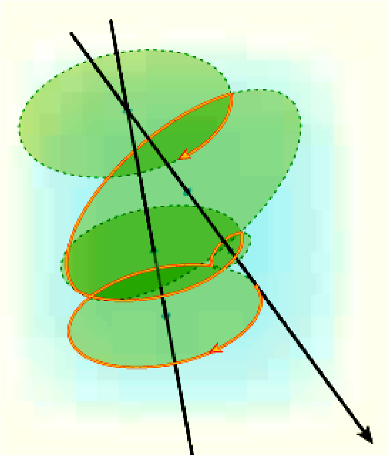
Considerable success has been achieved for some problems – eg., a qubit coupled to a spin bath, or a set of dipolar interacting qubits coupled to a spin bath.

The most important problem is to find the decoherence ratesfor experiments on real systems. This has been very successful recently. A general feature of the results is that one can have extremely strong decoherence with almost no dissipation – the spin bath is almost invisible in energy relaxation, but causes massive Decoherence (largely PRECESSIONAL DECOHERENCE)



For a qubit write:

$$\hat{H}_{QB} = H^0_{QB}(\vec{\tau}) + \sum (\vec{\gamma}_k + \xi_k) \cdot \vec{\sigma}_k$$



Precessional decoherence

where

$$\gamma_k^\alpha = h_k^\alpha + \sum_\beta \omega_k^{\beta\alpha} \tau_\beta$$

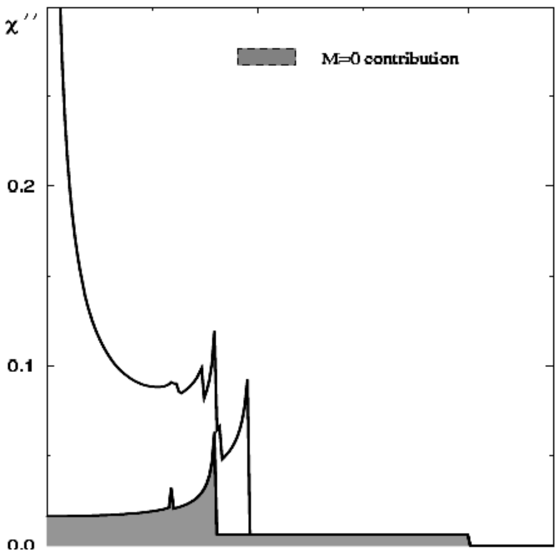
$$\xi_k^\alpha = \sum_{k'} \sum_\beta V_{kk'}^{\alpha\beta} \sigma_{k'}^\beta$$

Then decoherence rates are

$$\Gamma_\phi^P \sim 1/2 \sum_k (\omega_k / h_k)^2 ; \omega_k \ll h_k$$

$$\Gamma_\phi^P \sim 1/2 \sum_k (h_k / \omega_k)^2 ; h_k \ll \omega_k$$

However the lineshape is not conventional at all:



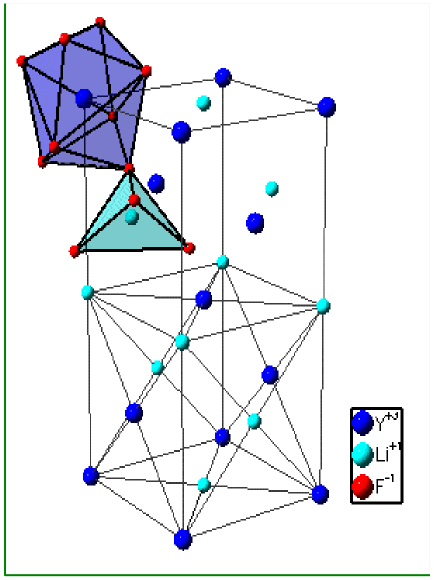
PART 2

BRIEF REMARKS
on
EXPERIMENTAL SYSTEMS

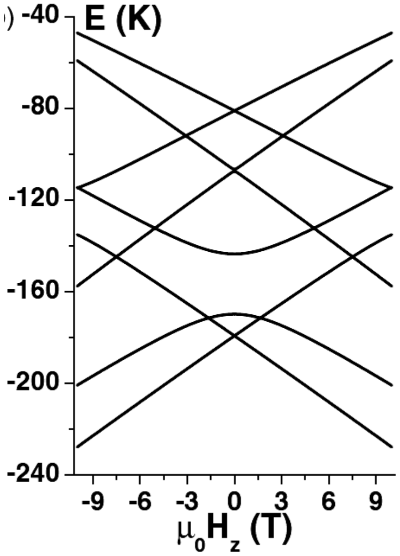
NUCLEAR SPIN BATH in MAGNETIC SYSTEMS

(1) $LiHo_xY_{1-x}F_4$

Q Ising $H = -\sum_{i,j} V_{ij}^{zz} \tau_i^z \tau_j^z - \Delta_0(H_\perp) \sum_i \tau_i^x$



The single spin has $J = 8$ and
a 1-spin crystal-field Hamiltonian $H_{cf} = \alpha_J B_2^0 O_2^0 + \beta_J (B_4^0 O_4^0 + B_4^4 O_4^4) + \gamma_J (B_6^0 O_6^0 + B_6^4 O_6^4),$



$B_2^0 = 273.9$ K

$B_4^0 = -97.7$ K $B_4^4 = -1289.1$ K $B_6^4 = -631.6$ K

$B_6^0 = -6.5$ K

In zero field there is a low-energy doublet, which we call $|\Uparrow\rangle$ $|\Downarrow\rangle$

This is separated from a 3rd state $|\Gamma_2^l\rangle$ by a gap $\Omega_0 = 10.5$ K

2nd-order perturbation theory gives $\Delta_0 \sim 9(\mu_B H_\perp)^2/\Omega_0$

Dipolar interactions have nearest neighbour strength $|V_{ij}^{zz}| \sim 0.3$ K

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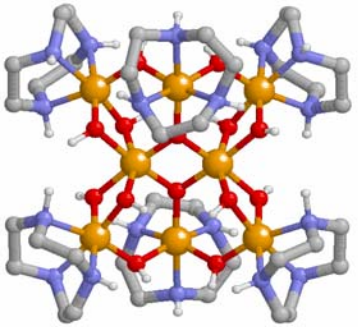
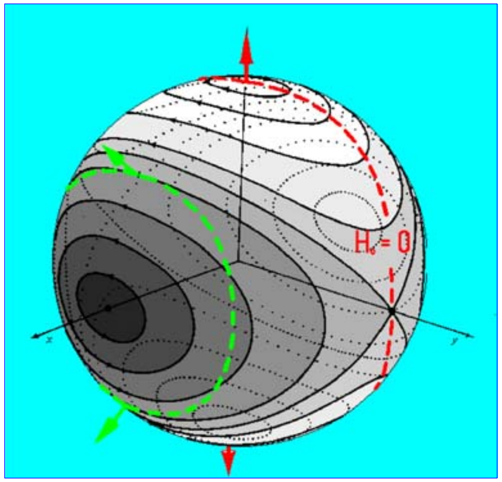
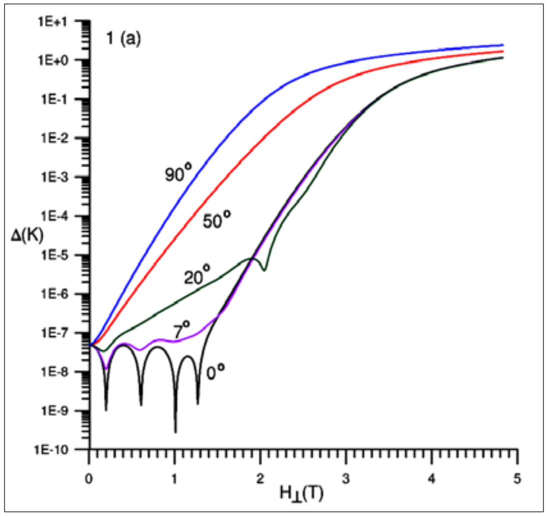
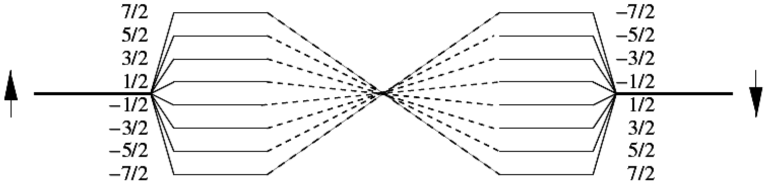
(2) Fe-8 molecule







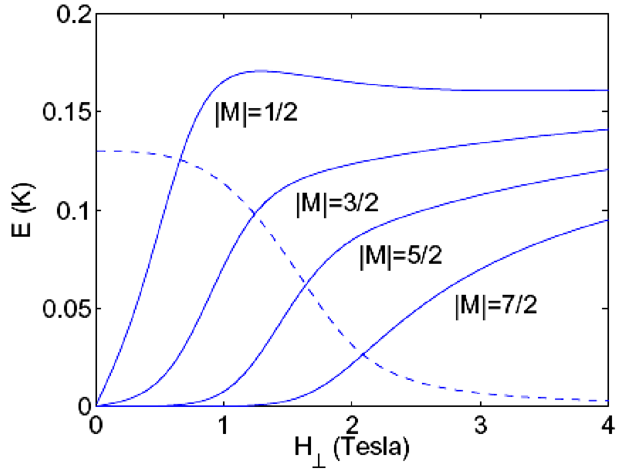
LiHo SYSTEM: THEORY



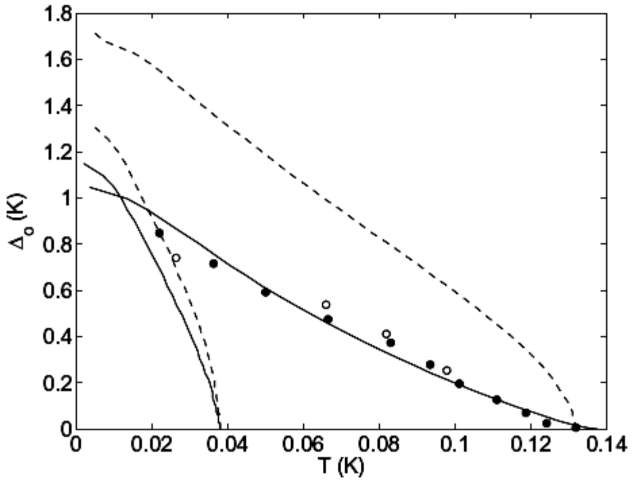
M Schechter, PCE Stamp, PRL **95**, 267208 (2005)
“ “ J Phys CM19, 145218 (2007)
“ “ /condmat 0801.2889

However the real Hamiltonian is quite different

$$H = -\sum_{i,j,m,m'} \tilde{V}^{zz}_{ij,m,m'}(H_\perp)\, n_{im} n_{jm'} s^z_{im} s^z_{jm'} - \sum_{i,m} n_{im}[\epsilon_m + \tilde{\Delta}_m(H_\perp) s^x_{im}] .$$



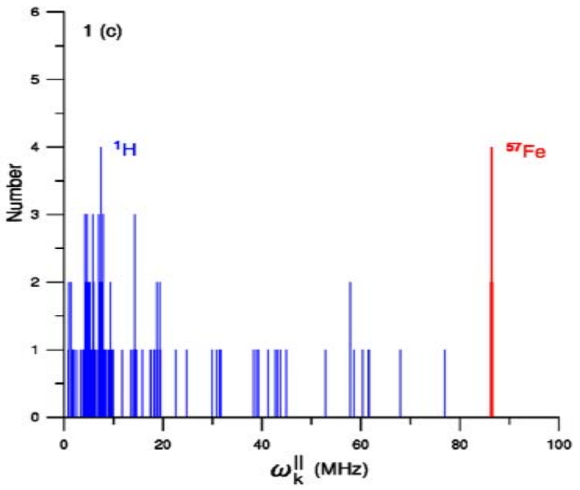
A full treatment also includes the transverse dipolar interactions. The thermodynamics & Quantum phase transition depend essentially on the nuclear spins. This has been very successful in treating the LiHo system



Fe-8 SYSTEM: THEORY

$$H^{CS}_{eff} = [\Delta_o \hat{\tau}_+ e^{-i\sum_k \boldsymbol{\alpha}_k\cdot\boldsymbol{\sigma}_k} + H.c.] + \hat{\tau}^z(\epsilon_o + \sum_k \boldsymbol{\omega}_k\cdot\boldsymbol{\sigma}_k) + H^{sp}_{env}([\boldsymbol{\sigma}_k])$$

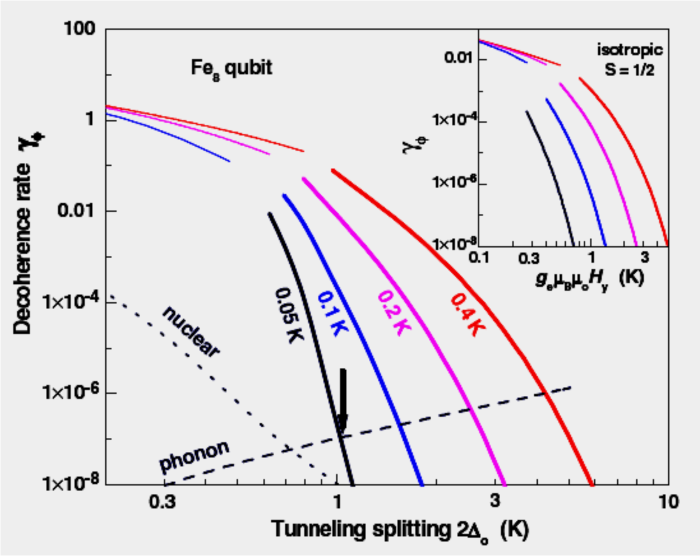
The hyperfine couplings of all 213 nuclear spins are well known (as are spin-phonon and dipolar couplings). Theory works quantitatively on real systems, even in predictions of decoherence rates.



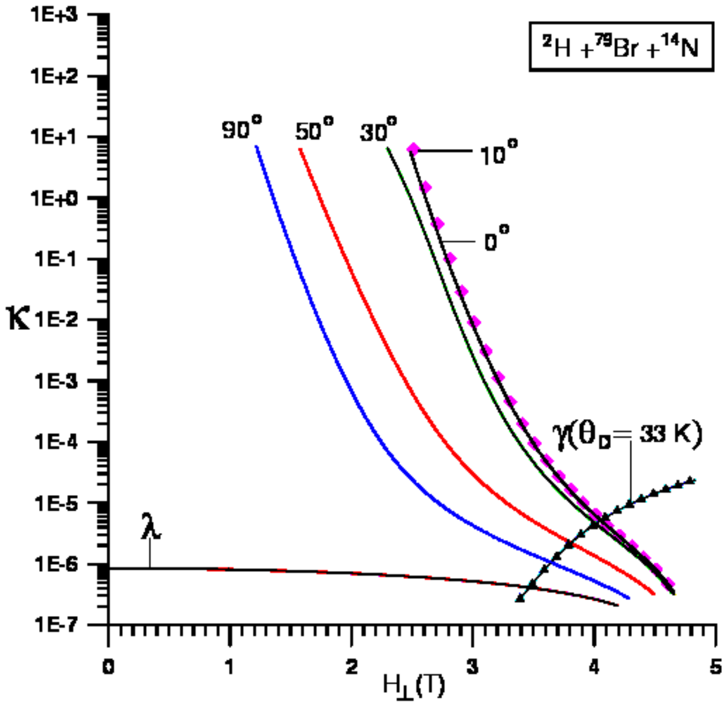
A full theory of the dynamics now exists

DECOHERENCE in the Fe-8 Molecule

There is a 'coherence window' operating for a single Fe-8 'qubit' which can be probed in large transverse fields (RIGHT)



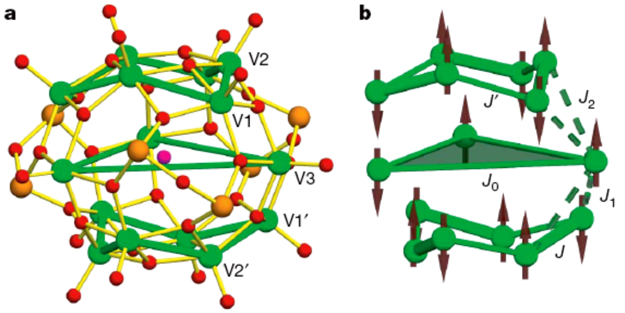
Adding dipolar interactions makes things a lot more Complex (see LEFT)

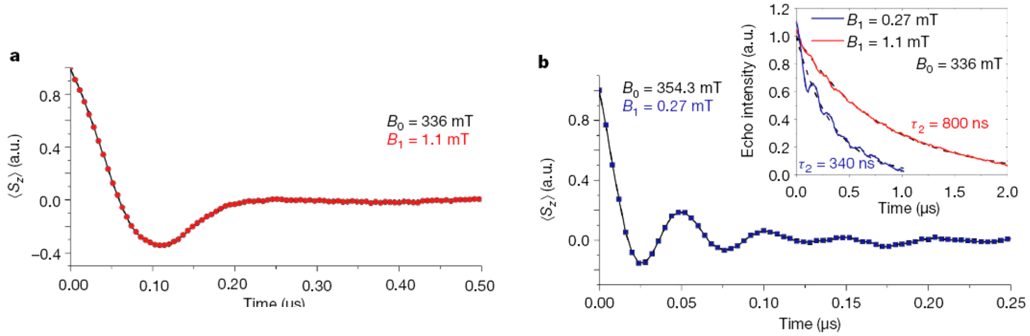


Stamp, P.C.E., Tupitsyn, I.S., Phys Rev **B69**, 014401 (2004)
Morello A, Stamp PCE, Tupitsyn IS, Phys Rev Lett 97, 207206 (2006)

DECOHERENCE in V-15 MOLECULE

S Bertaina et al, Nature 453, 203 (2008)





PART 3

SOMETHING COMPLETELY DIFFERENT: QUANTUM PHASE TRANSITIONS

QUANTUM SPIN GLASSES

The naïve description of a QSG is

$$H = -\sum_{i,j} V_{ij}^{zz} \tau_i^z \tau_j^z - \Delta_0 \sum_i \tau_i^x$$

Where the interactions are often anisotropic dipolar

A much better description is

$$\mathbf{H} = \Sigma_j (\Delta_j \tau_j^x + \varepsilon_j \tau_j^z) + \Sigma_{ij} V_{ij}^{dip} \tau_i^z \tau_j^z + \mathbf{H}_{NN}(I_k) + \mathbf{H}_{\phi}(x_q) + \text{interactions}$$

where we couple to a nuclear spin bath, and to a phonon oscillator bath

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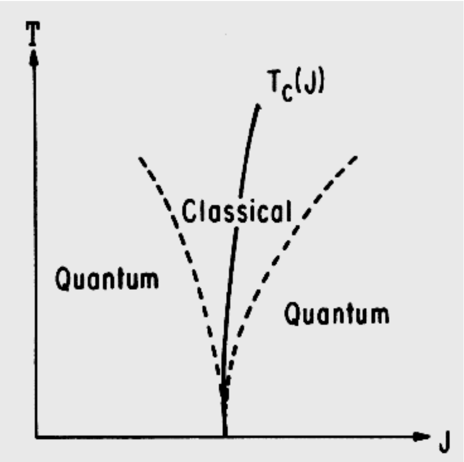
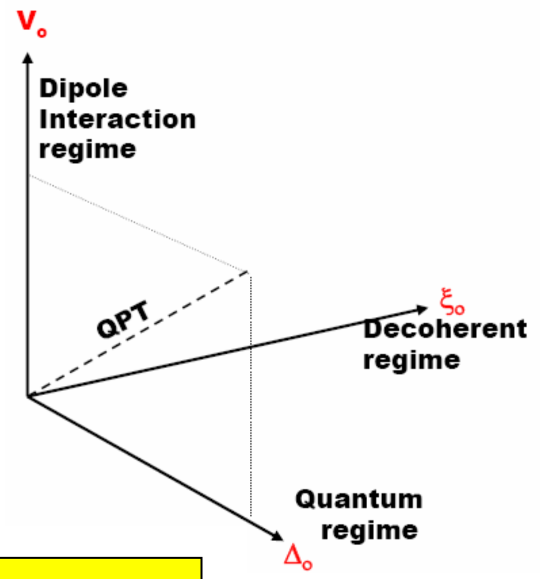
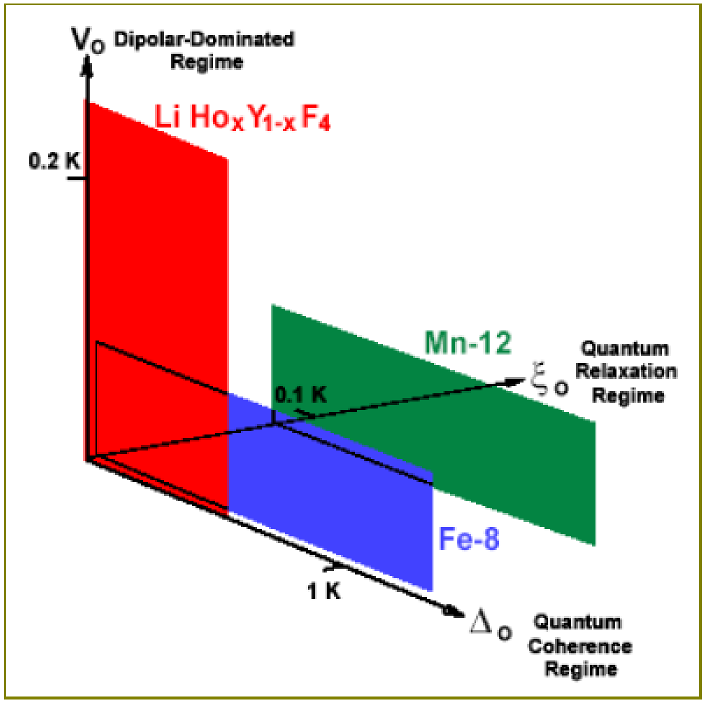
The usual 'quantum critical' scenario



What we now have



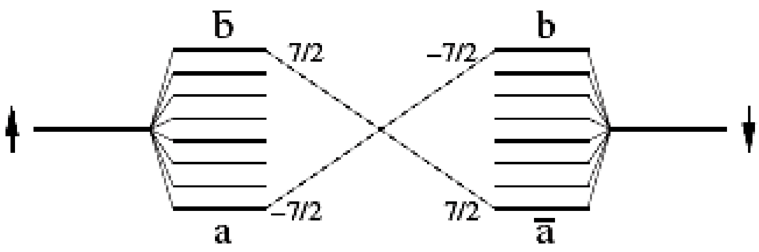
Some experimental examples



KEY QUESTIONS
(1) What controls the phase diagram now?
(2) What drives dynamics?

HYPERFINE COUPLING to the NUCLEAR SPIN BATH

We have a simple interaction $H_{\rm hf} = A_J \sum_i \vec{I}_i \cdot \vec{J}_i$ with $I = 7/2$



The hyperfine splitting between nuclear levels is roughly 0.25K

This interaction has a profound effect on the dynamics & on the effective Hamiltonian at low energy – electronic spins cannot flip unless multiple nuclear transitions also take place.

$a \equiv |\Uparrow, -7/2\rangle$ $\bar{a} \equiv |\Downarrow, 7/2\rangle$

$\bar{b} \equiv |\Uparrow, 7/2\rangle$ etc

Consider first what happens in low transverse field; we single out the 4 important states shown in the diagram. This problem is easily solved without the transverse hyperfine coupling; we get eigenstates

$$|+\rangle = c_1|a\rangle + c_2|b\rangle; \qquad |-\rangle = c_1|\bar{a}\rangle + c_2|\bar{b}\rangle$$

where $c_1 = \alpha\Delta_0$ & $c_2 = \alpha[A - \sqrt{A^2 + \Delta_0^2}]$

with mixing coefficient $\alpha = [\Delta_0^2 + (A - \sqrt{A^2 + \Delta_0^2})^2]^{-1/2}$ & $2A \approx 1.4$ K

At low transverse field this just produces a classical Ising system:

$$H_{\rm eff}^{\parallel} = -\sum_{i,j} \tilde{V}_{ij}^{zz} s_i^z s_j^z$$

with $\tilde{V}_{ij}^{zz} = \eta^2 V_{ij}^{zz}$

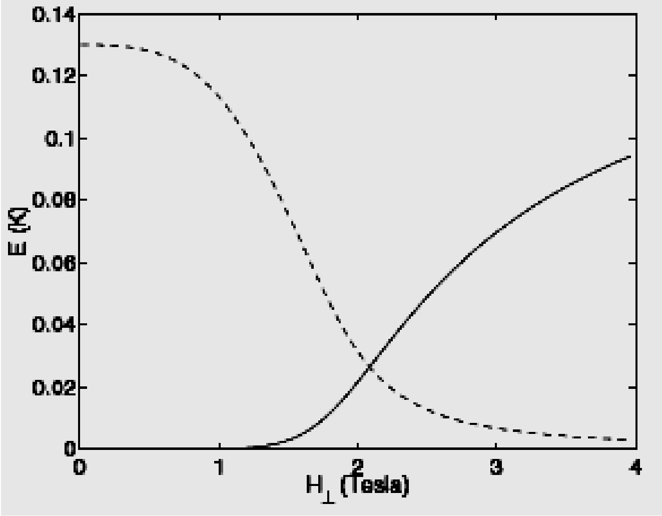
and $\eta \equiv (c_1^2 - c_2^2)$ & renormalised spin $\langle \sigma_+^z \rangle = \eta \langle \sigma_+^z(0) \rangle$

The transverse hyperfine term $H_{\rm hf}^{\perp} = A_J(I_+J_- + I_-J_+)/2$

only becomes effective when $\langle \Uparrow | \mu_B H_\perp | \Gamma_2^l \rangle \sim \Omega_0$

We then have a renormalised Hamiltonian:

$$H = -\sum_{i,j} \tilde{V}_{ij}^{zz}(H_\perp, A) s_i^z s_j^z - \tilde{\Delta}(H_\perp, A, \Omega_0) \sum_i s_i^x$$



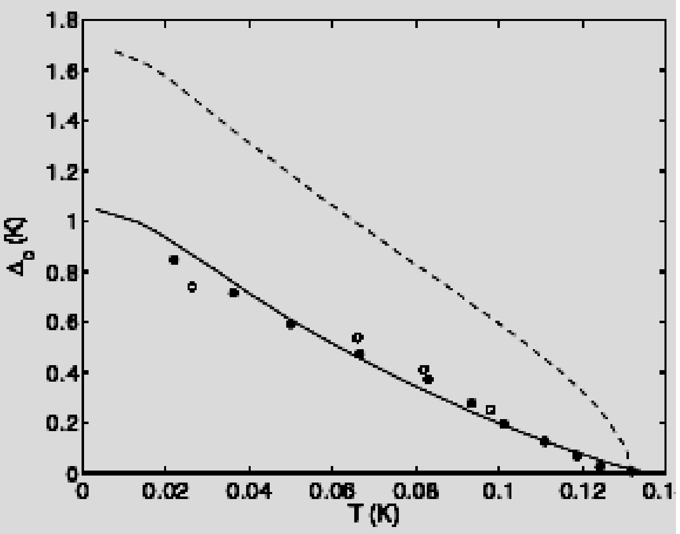
Dealing with the Phase Diagram

We have seen that the hyperfine interactions radically modify the energetics of the single ions – so the simplest way to them attack the phase diagram is to deal with the single ion properties exactly and then treat the longitudinal dipole interactions using mean field theory.

This amounts to finding the phase diagram for the effective Hamiltonian

$$H_{\mathrm{MF}} = H_{\mathrm{cf}} - \sum_j g_J \mu_B H_\perp J_j^x + A_J \sum_j \vec{I}_j \cdot \vec{J}_j + \sum_j V_0 \langle J_j^z \rangle J_j^z.$$

Actually this already solves most of the huge discrepancy between theory and experiment (cf. hatched line in figure at right).



However there is still one more important physical effect that has been left out. Unless x=1, there are strong random transverse dipolar fields in the system. It is not sufficient to treat these by adding them directly to the MF Theory above – it makes more physical sense to add them as an extra term of form

$$\tilde{H}_\perp = H_\perp + H_\perp^d.$$

And if we adjust this so that $H_\perp^d = 0.65\ \mathrm{T}$ then we get good agreement with experiment.

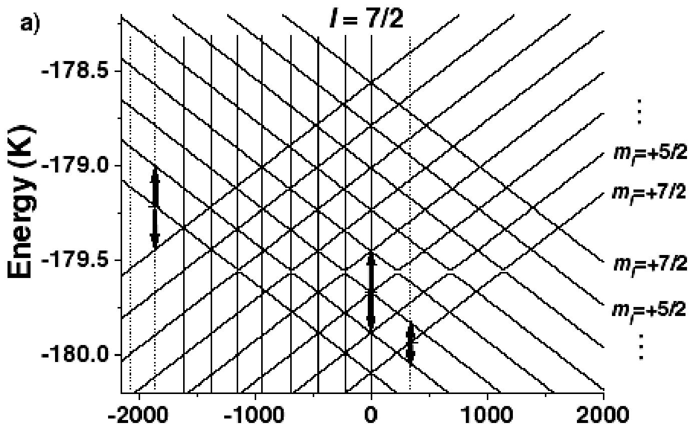
Finally, the size of the cusp in $\chi_3(T)$ can also be explained in this theory - because

$\sum_{ij} \langle S_i S_j \rangle^2 = S_0^4 \sum_{ij} \langle s_i s_j \rangle^2$ we expect $\mathrm{Max}(\chi_3(T)) \propto S_0^4.$

But this is what happens – reducing T increases H_c, reducing S_0 (it works quantitatively)

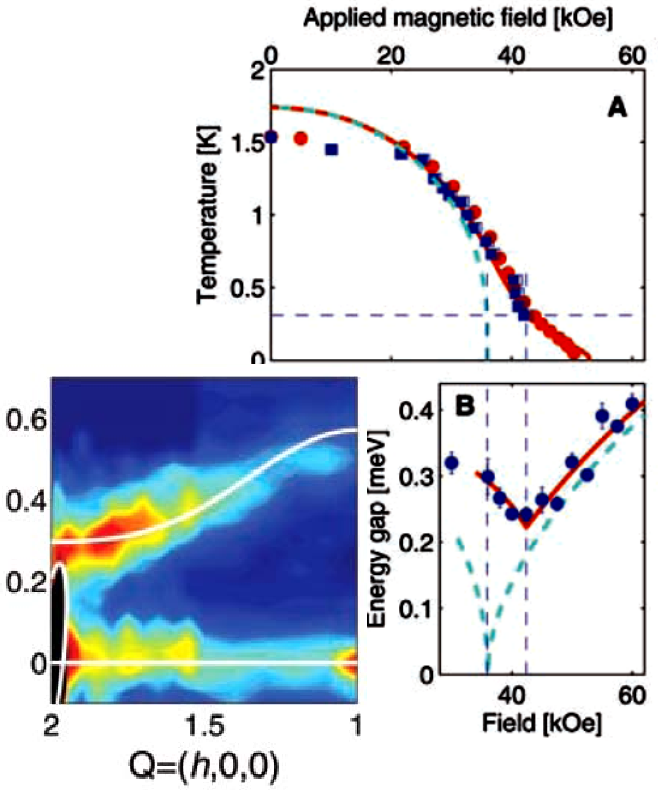
SOME EXPTS (LiHo)

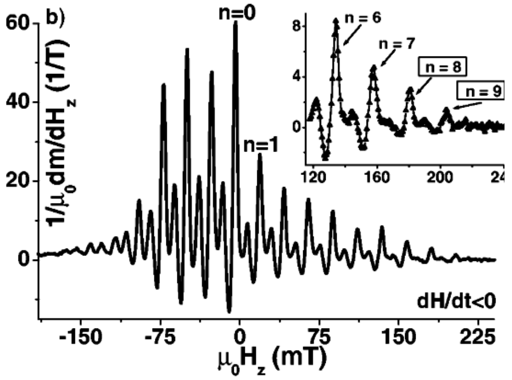
In the LiHo system there are no mmts yet of coherent dynamics – but there are mmts of the quantum relaxation, showing how the dynamics is switched on and off by the spin bath.

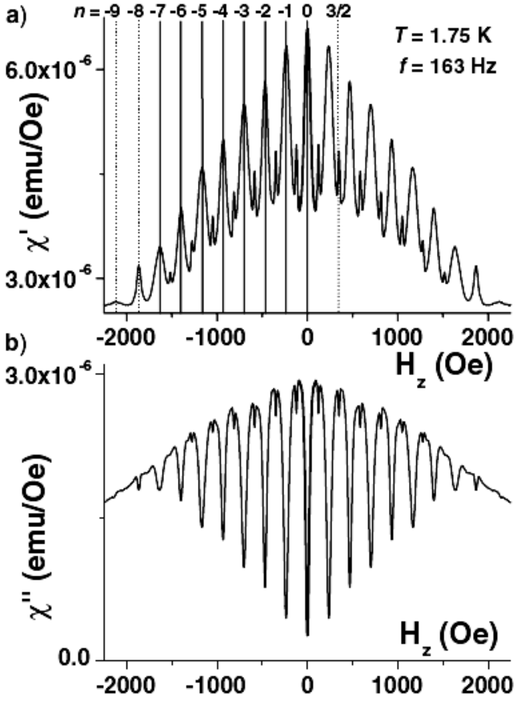


One also has a very interesting neutron scattering Experiments, showing a 'lifting' of the zero mode around H_c by the spin bath, in the case where x=1.

Then there are striking resonance experiments (again, in hysteresis) which directly show the role of the nuclear spins in the dynamics of these quantum spin glasses







H.M. Ronnow et al., Science 308, 389 (2005)

R. Giraud et al., PRL 87, 057203 (2001)
" PRL 91, 257204 (2003)

THE END

APPENDIX

TECHNICAL AFTERTHOUGHTS

CONDITIONS for DERIVATION of OSCILLATOR BATH MODELS

Starting from some system interacting with an environment, we want an effective low-energy Hamiltonian of form

$$H_{\text{eff}}(\Omega_0) = H_0(P,Q) + \sum_{q=1}^{N} [F_q(P,Q)x_q + G_q(P,Q)p_q] + \frac{1}{2}\sum_{q=1}^{N}\left(\frac{p_q^2}{m_q} + m_q\omega_q^2 x_q^2\right)$$

(1) PERTURBATION THEORY

Assume environmental states $\phi_\alpha(\mathbf{X})$ and energies ϵ_α

The system-environment coupling is $V(Q,\mathbf{X})$

Weak coupling: $|V_{\alpha\beta}| \ll |(\epsilon_\alpha - \epsilon_\beta)|$ where $V_{\alpha\beta} = \int d\mathbf{X}\, \phi^*_\alpha(\mathbf{X})\, V(Q,\mathbf{X})\, \phi_\beta(\mathbf{X})$

In this weak coupling limit we get oscillator bath with $\omega_q \equiv (\epsilon_\alpha - \epsilon_\beta)$

and couplings $F_q(Q) = V_q(Q)$

(2) BORN-OPPENHEIMER (Adiabatic) APPROXIMATION

Suppose now the couplings are not weak, but the system dynamics is SLOW, ie., Q changes with a characteristic low frequency scale E_o . We define slowly-varying environmental functions as follows:

Quasi-adiabatic eigenstates: $\tilde\phi_\alpha(\mathbf{X},Q)$ Quasi-adiabatic energies: $\tilde\epsilon_\alpha(Q)$

'Slow' means $E_o \ll \tilde\epsilon_\alpha$

Then define a gauge potential $iA_{\alpha\beta} = \int d\mathbf{X}\, \tilde\phi^*_\alpha(\mathbf{X})\, \partial/\partial Q\, \tilde\phi_\beta(\mathbf{X})$

We can now map to an oscillator bath if $|A_{\alpha\beta}| \ll |(\tilde\epsilon_\alpha - \tilde\epsilon_\beta)|$

Here the bath oscillators have energies $\omega_q \equiv (\tilde\epsilon_\alpha - \tilde\epsilon_\beta)$

and couplings $F_q(P,Q) = \omega_q^2 \int_0^Q dQ'\, Re A_q(P,Q')$

The oscillator bath models are good for describing delocalised modes; then usually $F_q(Q) \sim O(1/N^{1/2})$ (normalisation factor)

All this is fine except when either : (i) oscillators couple to solitons (ii) We have degenerate bath modes (iii) Environment contains localised modes

CONDITIONS for DERIVATION of SPIN BATH MODELS

We start again from a model of general form: $H_{\text{eff}}^{\text{sp}}(\Omega_0) = H_0 + H_{\text{int}}^{\text{sp}} + H_{\text{env}}^{\text{sp}}$

with interaction: $H_{\text{int}}^{\text{sp}} = \sum_k^{N_s} \boldsymbol{F}_k(P,Q)\cdot\boldsymbol{\sigma}_k$ and bath $H_{\text{env}}^{\text{sp}} = \sum_k^{N_s} \mathbf{h}_k \cdot \boldsymbol{\sigma}_k + \sum_{k,k'}^{N_s} V_{kk'}^{\alpha\beta}\sigma_k^{\alpha}\sigma_{k'}^{\beta}$

For this effective Hamiltonian to be valid we require that no other environmental levels couple significantly to the localised bath levels. We also require that the bath modes couple weakly to each other, satisfying the conditions:

(i) $|V_{kk'}| \ll |F_k(P,Q)| \quad \forall\, k,k'$ (intra-bath mode-mode coupling weak compared to the coupling to the central system); or failing this, that:

(ii) $|V_{kk'}| \ll |\underline{h}_k|$ The 'external fields' acting on the bath modes are much larger than the intra-bath couplings

There is no 'Born-Oppenheimer' requirement of 'slow' changes.

If the system changes on a timescale *T*, so that:

$$\left|\frac{\partial_t F_k}{F_k}\right| T \sim O(1).$$

Then define:

$$u_k = \frac{1}{|F_k|T} \sim \left|\frac{\partial_t F_k}{F_k^2}\right|$$

The model is valid for all *u_k*:

$u_k \ll 1$ slow "adiabatic" limit

$u_k \gg 1$ fast "sudden" limit

INFLUENCE FUNCTIONAL

This is given by the standard form:

$$\mathcal{F}[Q,Q'] = \prod_k^{N_s} \int \mathcal{D}\boldsymbol{\sigma}_k(\tau) \int \mathcal{D}\boldsymbol{\sigma}_k(\tau') \exp\left[\frac{i}{\hbar}\left(S_{int}[Q,\boldsymbol{\sigma}_k] - S_{int}[Q',\boldsymbol{\sigma}'_k] + S_E[\boldsymbol{\sigma}_k] - S_E[\boldsymbol{\sigma}'_k]\right)\right]$$

With the interaction action $S_{int}^{sp}(Q,\boldsymbol{\sigma}_k) = -\int d\tau \sum_k \boldsymbol{F}_k(P,Q)\cdot\boldsymbol{\sigma}_k$

However now we have $S_{env}^{sp} = \int d\tau \left[\sum_k^{N_s}\left(\mathcal{A}_k \cdot \frac{d\boldsymbol{\sigma}_k}{dt} - \mathbf{h}_k\cdot\boldsymbol{\sigma}_k\right) - \sum_{k,k'}^{N_s} V_{kk'}^{\alpha\beta}\sigma_k^{\alpha}\sigma_{k'}^{\beta}\right]$

The bath action contains a topological term

DERIVATION of EFFECTIVE INTERACTIONS & INFLUENCE FUNCTIONAL (OSCILLATOR BATH)

(1) Consider an oscillator perturbed by some *t*-dependent force, so that

$$L = \frac{M}{2}\dot{x}^2 - \frac{M\omega^2}{2}x^2 - \gamma(t)x$$

Then the propagator is given by

$$G_{ba} = \sqrt{\frac{M\omega}{2\pi i\hbar \sin \omega T}}\, e^{(i/\hbar)S_{cl}}$$

where

$$\begin{aligned} S_{cl} = \frac{M\omega}{2\sin\omega T}\Big[&(\cos\omega T)(x_b{}^2 + x_a{}^2) - 2x_b x_a \\ &+ \frac{2x_b}{M\omega}\int_{t_a}^{t_b} \gamma(t)\sin\omega(t-t_a)\,dt \\ &+ \frac{2x_a}{M\omega}\int_{t_a}^{t_b} \gamma(t)\sin\omega(t_b-t)\,dt \\ &- \frac{2}{M^2\omega^2}\int_{t_a}^{t_b}\int_{t_a}^{t} \gamma(t)\gamma(s)\sin\omega(t_b-t)\sin\omega(s-t_a)\,ds\,dt \Big] \end{aligned}$$

RP Feynman, AR Hibbs,
"Quantum Mechanics & Path integrals",
McGraw-Hill (1965)

RP Feynman, FL Vernon,
Ann Phys 24, 118 (1963)

One also has matrix elements between oscillator states *m* and *n* given by

$$G_{mn} = \frac{G_{00}}{\sqrt{m!n!}}\sum_{r=0}^{l}\frac{m!}{(m-r)!r!}\frac{n!}{(n-r)!r!}r!(i\beta)^{n-r}(i\beta^*)^{m-r}$$

where

$$G_{00} = \exp\left[-\frac{1}{2m\omega\hbar}\int_0^T\int_0^t \gamma(t)\gamma(s)e^{-i\omega(t-s)}\,ds\,dt\right]$$

and

$$\beta = \frac{1}{M\sqrt{2\omega}}\int \gamma(t)e^{-i\omega t}\,dt$$

$$\beta^* = \frac{1}{M\sqrt{2\omega}}\int \gamma(t)e^{+i\omega t}\,dt$$

(2) Now we can write down an expression for the propagator of the reduced density matrix. We recall that

$$K(Q_2, Q_2'; Q_1, Q_1'; t, t') = \int_{Q_1}^{Q_2} \mathscr{D}q \int_{Q_1'}^{Q_2'} \mathscr{D}q' \, \mathrm{e}^{-\mathrm{i}/\hbar(S_0[q]-S_0[q'])} \mathscr{F}[q, q'],$$

with $$\mathcal{F}[Q, Q'] = \prod_k \langle \hat{U}_k(Q, t) \hat{U}_k^\dagger(Q', t) \rangle$$

Here the unitary operator $\hat{U}_k(Q, t)$ describes the evolution of the kth environmental mode, given that the central system follows the path $Q(t)$ on its 'outward' voyage, and $Q'(t)$ on its 'return' voyage; and $\mathcal{F}[Q, Q']$ acts as a weighting function, over different possible paths $(Q(t), Q'(t'))$.

In general for oscillator bath environments we have

$$H_{\text{eff}}(\Omega_0) = H_0(P, Q) + \sum_{q=1}^{N} [F_q(P, Q) x_q + G_q(P, Q) p_q] + \frac{1}{2} \sum_{q=1}^{N} \left(\frac{p_q^2}{m_q} + m_q \omega_q^2 x_q^2 \right)$$

We can typically get rid of the interaction with p_q using a canonical transformation, so that:

$$\mathcal{F}[Q, Q'] \;=\; \prod_q^{N_o} \int \mathcal{D}x_q(\tau) \int \mathcal{D}x_q(\tau') \; \exp\left[\frac{i}{\hbar} \int d\tau \frac{m_q}{2} [\dot{x}_q^2 - \dot{x}_q'^2 + \omega_q^2 (x_q^2 - x_q'^2)] \;+\; [F_q(Q) x_q - F_q(Q') x_q'] \right]$$

Then let's assume the simplified bilinear 'Caldeira-Leggett' form: $\boldsymbol{F_q(P,Q)\, x_q = v_q x_q Q}$

Then, by using the results derived on the last page for the propagator of an oscillator coupled to a t-dependent force, we get the influence functional for 2 paths *q(t) & q'(t)* :

$$F[q, q'] \;=\; \exp\left[-\frac{1}{\hbar} \int_{t_o}^{t} d\tau_1 \int_{t_o}^{\tau_1} d\tau_2 [q(\tau_1) - q'(\tau_2)] [\mathcal{D}(\tau_1 - \tau_2) q(\tau_2) - \mathcal{D}^*((\tau_1 - \tau_2) q'(\tau_2)] \right]$$

with bosonic propagator (effective interaction):

$$\mathcal{D}(\tau) \;=\; \sum_q \frac{|v_q|^2}{2 m_q \omega_q} \left[e^{i\omega_q \tau} \;+\; 2 \frac{\cos \omega_q \tau}{e^{\beta\omega_q} - 1} \right]$$

More complex couplings lead to non-Gaussian forms

INTEGRATING OUT THE SPIN BATH

Each individual bath spin has a Lagrangian

$$L(\boldsymbol{\sigma}_k) = \mathcal{A}_k \cdot \frac{d\boldsymbol{\sigma}_k}{dt} - \mathbf{h}_k \cdot \boldsymbol{\sigma}_k - \boldsymbol{F}_k(t) \cdot \boldsymbol{\sigma}_k - \sum_{k'}^{N_s} V_{kk'}^{\alpha\beta} \sigma_k^\alpha \sigma_{k'}^\beta$$

This is a nasty problem. We can begin to simplify by noticing that to a very good approximation, we can write

$$\sum_{k'}^{N_s} V_{kk'}^{\alpha\beta} \sigma_k^\alpha \sigma_{k'}^\beta \rightarrow \xi_k^\alpha(t)$$

(fluctuating local bath field)

Then we have: $L(\boldsymbol{\sigma}_k) = \mathcal{A}_k \cdot \frac{d\boldsymbol{\sigma}_k}{dt} - \mathbf{b}_k(t) \cdot \boldsymbol{\sigma}_k$ where the t-dependent field is

$$\mathbf{b}(t) = \mathbf{h}_k + \boldsymbol{F}_k(t) + \boldsymbol{\xi}_k(t)$$

Now one can write down a solution for this problem. Here is one way of doing it – we ask what is the propagator of the spin between 2 coherent states in a time *t*, and find

$$\begin{aligned} \mathcal{G}(\mathbf{n}_2, \mathbf{n}_1; t) = \; & A_+(t) \cos\frac{\theta_2}{2} \cos\frac{\theta_1}{2} e^{\frac{i}{2}(\phi_2 - \phi_1)} + A_+^*(t) \sin\frac{\theta_2}{2} \sin\frac{\theta_1}{2} e^{-\frac{i}{2}(\phi_2 - \phi_1)} \\ & + A_-(t) \cos\frac{\theta_2}{2} \sin\frac{\theta_1}{2} e^{\frac{i}{2}(\phi_2 + \phi_1)} - A_-^*(t) \sin\frac{\theta_2}{2} \cos\frac{\theta_1}{2} e^{-\frac{i}{2}(\phi_2 + \phi_1)} \end{aligned}$$

where $\dot{A}_\sigma(t) = -ib_z(t) A_\sigma(t) + i\sigma b_\perp(t) A^*_{-\sigma}(t)$ with $b_\perp(t) = b_x(t) - ib_y(t)$

and $\sigma = \pm$

However it turns out not to be terribly useful to do everything in a completely general way from now on. In the next lecture we will look at the solution of a particular problem to see better how this work.

The REAL END