MODELING COHERENCE, DECOHERENCE and QUANTUM RELAXATION: Some Questions

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My own support:

SOME TYPICAL MODELS for DECOHERENCE, Q. RELAXATION

Here are 2 generic models used to discuss these topics, by physicists:

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

Oscillator Bath model

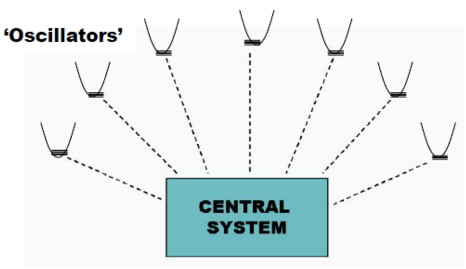
Central system — Coupling to bath — Bath/Environment

$$H_{\text{eff}} = H_o(P,Q) + \mathcal{F}(P,Q;\{\boldsymbol{\sigma}_\mu\}) + \sum_{\mu}^{N_s} \mathbf{h}_\mu \cdot \boldsymbol{\sigma}_\mu + \sum_{\mu,\mu'}^{N_s} V_{\mu\mu'}^{\alpha\beta} \sigma_\mu^\alpha \sigma_{\mu'}^\beta$$

Spin Bath model

KEY DIFFERENCES

Couplings here very small (~ $O(N^{-1/2})$)



Osc Bath

Phonons, photons, magnons, spinons, Holons, Electron-hole pairs, gravitons,..

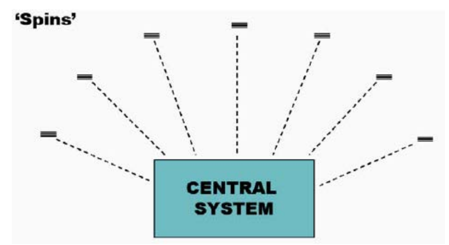
Feynman & Vernon, Ann. Phys. 24, 118 (1963)

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

DELOCALIZED BATH MODES
↓
OSCILLATOR BATH

Couplings NOT SMALL (~ $O(1)$)

Spin Bath



Defects, dislocation modes, vibrons, Localized electrons, spin impurities, nuclear spins, ...

LOCALIZED BATH MODES
↓
SPIN BATH

(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)

A SIMPLE EXAMPLE: the 'QUBIT'

Here the central system is just a 2-level system, or 'qubit', written as a Pauli spin

(i) The "Spin-Boson" Model

The qubit is coupled to a bath of oscillators

$$H_{\mathrm{SB}} = \mathbf{b}_o \cdot \boldsymbol{\tau} + \sum_{q=1}^{N} c_q^{\alpha} \hat{\tau}^{\alpha} x_q + \frac{1}{2} \sum_{q=1}^{N} \left(\frac{p_q^2}{m_q} + m_q \omega_q^2 x_q^2 \right)$$

Again – the couplings here are assumed VERY SMALL: in other words, we have

$$c_q^{\ 2} \sim \omega_q / N$$

the point here being that if the couplings are not small, we cannot necessarily assume either linear couplings or that the environment can be mapped to oscillators

(ii) The "Central Spin" model

The qubit is coupled to a bath of 2-level systems

$$H_{CS} = \mathbf{b}_o \cdot \boldsymbol{\tau} + \sum_{\mu} \omega_{\mu}^{\alpha\beta} \tau^{\alpha} \sigma_{\mu}^{\beta} + \sum_{\mu} \mathbf{h}_{\mu} \cdot \boldsymbol{\sigma}_{\mu} + \sum_{\mu\mu'} V_{\mu\mu'}^{\alpha\beta} \sigma_{\mu}^{\alpha} \sigma_{\mu'}^{\beta}$$

Now, the ratio between the coupling ω_{μ} and the characteristic bath energy h_{μ} can be ARBITRARY .

It turns out that for a large parameter range, one can get more or less exact ANALYTIC solutions to this model.

The model is only meaningful if the environmental modes can be mapped to 2-level systems (or to some m-level systems, where m is small), and where the internal bath couplings are small.

QUESTION 1: How can we understand decoherence intuitively?

(i) Oscillator Bath

Each oscillator (labelled by q), feels a total force: $\Upsilon_q(t) = m_q \omega_q^2 x_q - F_q(Q(t))$

Eg., for spin-boson model: $\Upsilon_q(t) = m_q \omega_q^2 x_q - c_q^\alpha \hat{\tau}^\alpha(t)$

V. weak force from central system

Effect of this weak force on bath oscillator: it simultaneously weakly excites it (dissipation) and causes it to very weakly entangle with the central system (decoherence).

Fluctuation – dissipation - decoherence

(ii) Spin Bath

Now each bath spin feels the total force: $\Upsilon_\mu(t) = \mathbf{h}_\mu + \mathbf{F}_\mu(t) + \boldsymbol{\xi}_\mu(t)$

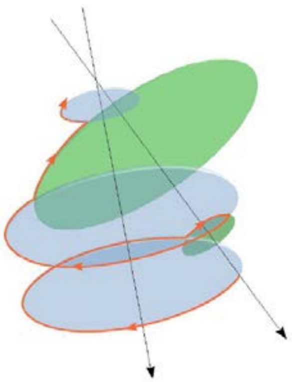
Force from central system (<u>NOT</u> small)

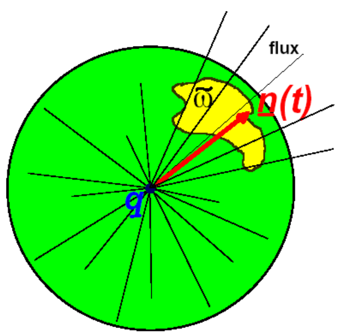
V weak force from other bath spins

Eg., for central spin model:

$$\gamma_\mu^\alpha(t) = h_\mu^\alpha + \sum_\beta \omega_\mu^{\alpha\beta} \tau_\beta(t)$$

The effect of the force is not to excite the bath spin, but to cause it to PRECESS – (accumulating a "Berry phase" in the process). This causes very large entanglement with the central system (hence, decoherence), but NO DISSIPATION.





The only dissipation is caused by the weak interaction between bath spins

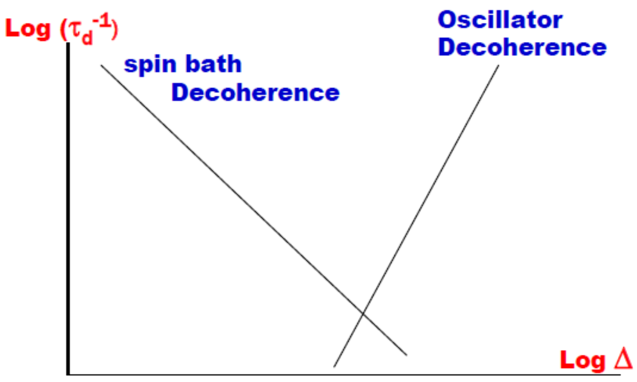
$$\xi_\mu^\alpha(t) = \sum_{\mu'} V_{\mu\mu'}^{\alpha\beta} \sigma_{\mu'}^\beta(t) \sim \sum_{\mu'} V_{\mu\mu'}^{\alpha\beta} \langle \sigma_{\mu'}^\beta(t) \rangle$$

WHAT ARE SOME OBSERVABLE CHARACTERISTICS OF THESE BATHS?

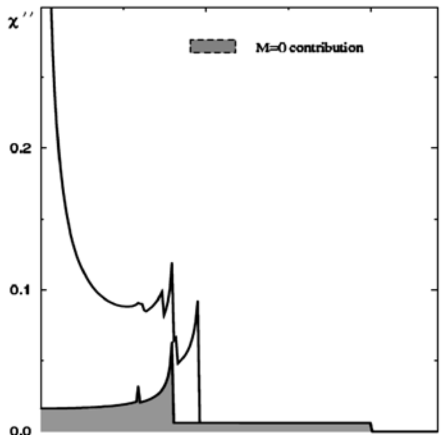
We have seen that localized environmental modes cause quite different behaviour from delocalized ones. How would this show up in measureable properties?

Here are 3 ways:

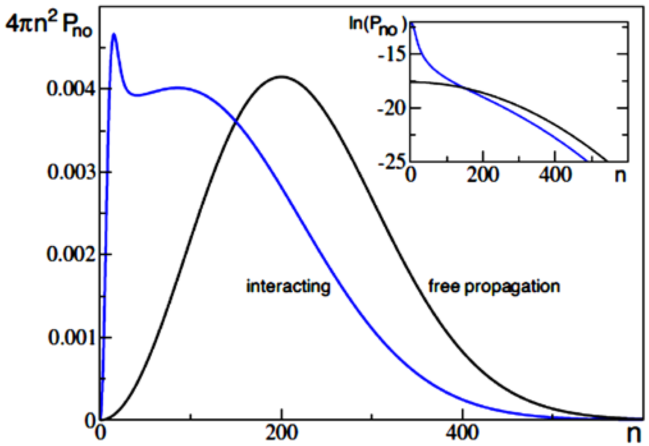
(1) Coherence Window: Very often (particularly in solid-state systems) there is a separation in frequency scale, which can lead to a 'coherence window'.



(2) Spectral signature: The spin bath/localized modes lead to unconventional lineshapes



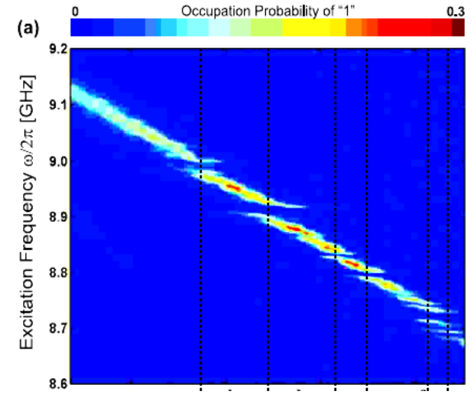
(3) Real Space Dynamics: Oscillator baths typically lead to straightforward decay. This is often not the case with spin baths- they can even show simultaneous superdiffusive + completely coherent dynamics.



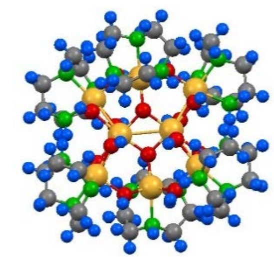
HOW GOOD are these MODELS for PREDICTING DECOHERENCE?

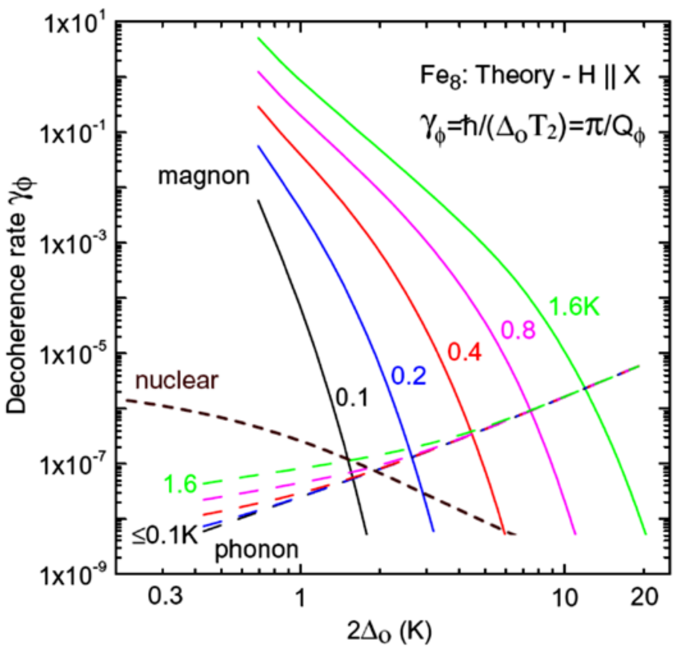
(1) Example 1: SQUIDs The first experiments (van der Wals et al., Science 290, 773 (2000)) found a decoherence rate 10^6 times greater than the oscillator bath predictions.

That this was caused by the spin bath (defects TLS) was confirmed in 2004, by the UCSB group.



(2) Example 2: Magnetic Molecules Single crystals of large magnetic molecules have 3 sources of decoherence – phonons (osc bath), Nuclear spins (spin bath), and long-range dipolar couplings. Here all the couplings are known, and so one can directly compare expt and theory, for a STRONGLY-COUPLED ENVIRONMENT.



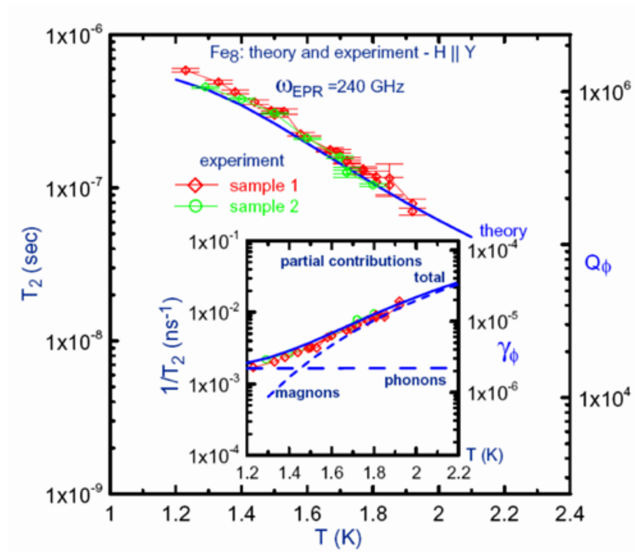


The predictions (made for this system in 2006) actually work (expts in 2011).

But – this illustrates 2 things

(i) Huge decoherence can arise from almost invisible modes.

(ii) Need to know what they are!



WHAT ABOUT POLARONS & EXCITONS –> BIOLOGICAL SYSTEMS?

For a theorist, this boils down to the 'hyperlattice' model:

$$H_o = \sum_{ij} \left[t_{ij} c_i^\dagger c_j \, e^{iA^o_{ij}} + H.c. \right] + \sum_j \epsilon_j c_j^\dagger c_j$$

Hopping amplitude — Site energy

Typically we might couple this object (polaron, exciton) to both localized phonons (vibrons) and delocalized phonons (acoustic, etc).

There are 2 important points I want to address here:

(a) In a system like this there is a large variety of diagonal & non-diagonal couplings to phonons – both localized and delocalized. The behaviour caused by non-diagonal couplings is totally different from that caused by diagonal couplings – almost all calculations done so far on these systems have assumed only diagonal couplings. (cf M BERCIU TALK)

(b) If one allows either kind of coupling to LOCALIZED modes, the results can be highly counter-intuitive, and show almost no resemblance to what would be given by a standard Feynman-Vernon oscillator bath model. This can be shown numerically for vibrons (DQMC – Prokof'ev et al; MA – Zhu, Berciu, Stamp), and by analytic work on spin bath models (Zhu, Stamp).

QUESTIONS

(1) How can we find ways of testing some of the theoretical ideas on these biosystems (and this is HARD)

(2) What about similar kinds of coherence elsewhere – particularly in the brain?