ENTANGLEMENT, DECOHERENCE & QUANTUM ISING SYSTEMS

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Physics & Astronomy
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for
Theoretical Physics

We want to understand:

(i) Multipartite Entanglement & Decoherence
(ii) Dynamics of Quantum Ising Systems
(iii) Dynamics of real systems like Fe-8, $LiHo_xY_{1-}F_4$

TALK in THREE PARTS

PART A: Multipartite Entanglement, Q Ising (T Cox, PCE Stamp)

PART B: Real World Q Ising & Q Computation (T Cox, PCE Stamp)

PART C: Dynamics of $LiHo_xY_{1-}F_4$ System (RD McKenzie, PCE Stamp)

NSERC CRSNG

SIMONS FOUNDATION

N-PARTICLE QUANTUM STATES

Here are two interesting questions

QUESTION 1

What is multiparticle entanglement – how do we characterize it, & what is its dynamics?

QUESTION 2

What do the low-energy states of a quantum computer look like? In particular, an adiabatic quantum computer?

STATES

A pure state has a density matrix operator $\hat{\rho} = |\psi\rangle\langle\psi|$ where $|\psi\rangle$ is the pure state vector

For some system *S* the 'reduced density matrix' is: $\bar{\rho}_S = Tr_E\{\hat{\rho}\}$ where $\hat{\boldsymbol{\rho}}$ describes 'the universe', & trace is over 'environmental' modes.

QUBITS

Consider a system of N such qubits; ρ has general form

$$\rho_{12\ldots N} = \frac{1}{2^N}\left(I + \langle\sigma_1^{\mu_1}\sigma_2^{\mu_2}\ldots\sigma_N^{\mu_N}\rangle\sigma_1^{\mu_1}\sigma_2^{\mu_2}\ldots\sigma_N^{\mu_N}\right)$$

We'll be dividing these into 'correlated' and uncorrelated parts:

2 qubits: $\rho_S \equiv \rho_{12} = \bar{\rho}_1\bar{\rho}_2 + \rho_{12}^C$

3 qubits: $\rho_S = \bar{\rho}_1\bar{\rho}_2\bar{\rho}_3 + \rho_{123}^C + \bar{\rho}_1\bar{\rho}_{23}^C + \bar{\rho}_2\bar{\rho}_{13}^C + \bar{\rho}_3\bar{\rho}_{12}^C$

Let's see how this works....

EXAMPLE: PAIR of QUBITS

NB: for 1 qubit

$$\rho = \frac{1}{2}(1 + \langle \boldsymbol{\sigma} \rangle \cdot \boldsymbol{\sigma})$$

For 2 qubits: $$\rho_{12} = \frac{1}{4}\Big(1 + \sum_{j=1,2} \langle \sigma_{j\mu} \rangle {\sigma_j}^{\mu} + \langle \sigma_{1\mu}\sigma_{2\nu} \rangle {\sigma_1}^{\mu}{\sigma_2}^{\nu}\Big)$$

$$= \frac{1}{4}\prod_j (1 + \langle \sigma_{j\mu} \rangle {\sigma_j}^{\mu}) + \frac{1}{4}\langle\langle \sigma_{1\mu}\sigma_{2\nu} \rangle\rangle {\sigma_1}^{\mu}{\sigma_2}^{\nu} \qquad = \rho_1\rho_2 + \rho_{12}^C$$

where $\langle\langle \sigma_{1\mu}\sigma_{2\nu} \rangle\rangle = \langle \sigma_{1\mu}\sigma_{2\nu} \rangle - \langle \sigma_{1\mu} \rangle \langle \sigma_{2\nu} \rangle$ (Correlated part)

Example 1: Cat state $|\Psi_2^C\rangle \equiv \frac{1}{\sqrt{2}}\left(|\uparrow\uparrow\rangle + e^{i\phi_{\downarrow\downarrow}}|\downarrow\downarrow\rangle\right)$ pure entangled state

$$|\Psi_2^C\rangle\langle\Psi_2^C| = \frac{1}{4}\Big(1 + \cos\phi_{\downarrow\downarrow}[\sigma_1^x\sigma_2^x - \sigma_1^y\sigma_2^y] + \sin\phi_{\downarrow\downarrow}[\sigma_1^y\sigma_2^x + \sigma_1^x\sigma_2^y] + \sigma_1^z\sigma_1^z\Big)$$ density matrix

Example 2: Incoherent mixture (of $|\uparrow\uparrow\rangle$ and $|\rightarrow\rightarrow\rangle$ states)

$$\rho_{12} = \frac{1}{2}(|\uparrow\uparrow\rangle\langle\uparrow\uparrow| + |\rightarrow\rightarrow\rangle\langle\rightarrow\rightarrow|) = \frac{1}{4}\left[1 + \tfrac{1}{2}(\hat{x} + \hat{z}) \cdot (\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) + \tfrac{1}{2}(\sigma_1^x\sigma_2^x + \sigma_1^z\sigma_2^z)\right]$$

Now – how entangled are these states? The cat state looks pretty entangled – what about the mixture? Note we have for this state that

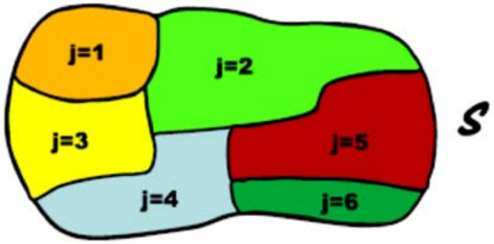
$$\langle\langle \sigma_1^x\sigma_2^x \rangle\rangle = \langle\langle \sigma_1^z\sigma_2^z \rangle\rangle = -\langle\langle \sigma_1^x\sigma_2^z \rangle\rangle = -\langle\langle \sigma_1^z\sigma_2^x \rangle\rangle = \frac{1}{4}.$$ (non-zero correlations)

'Measures of Entanglement' (concordance, entanglement cost, entanglement of formation, relative entropy of entanglement, etc., etc.) Entanglement witnesses, etc, are no use – they don't necessarily agree.

So – let's go with the correlators instead !

PARTITIONS & SUBSETS

Consider a set S made from N distinguishable 'cells'

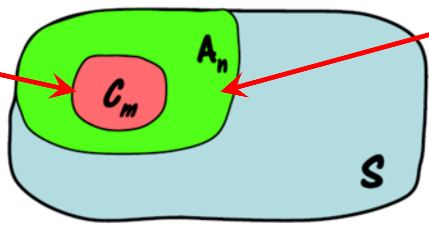


'Power set' P_S (set of all subsets): 2^N members
'Partition Set' $\mathcal{P}_S$ of all partitions: B_N members

(Bell number $B_n \sim n^n$ for large n).

GOAL: To define the full density matrix for S in terms of all the subsidiary density matrices (for either P_S, or for $\mathcal{P}_S$).

$$\rho_S = \sum_{\mathcal{A} \subseteq \mathcal{S}} \left(\prod_{j \notin \mathcal{A}} \bar{\rho}_j \right) \bar{\rho}^C_{\mathcal{A}}$$

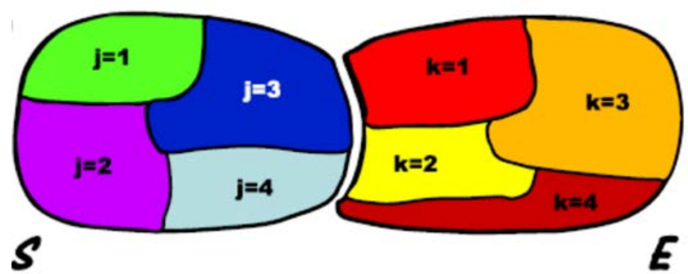


where we have

$$\bar{\rho}^C_{\mathcal{A}^{(n)}_\alpha} = \sum_{m=2}^{n} (-1)^{(n-m)} \sum_{\mathcal{C}^{(m)}_\mu \subseteq \mathcal{A}^{(n)}_\alpha} \left(\bar{\rho}_{\mathcal{C}_m} \prod_{j \in \mathcal{A}^{(n)}_\alpha \setminus \mathcal{C}^{(m)}_\mu} \bar{\rho}_j \right) - (-1)^n (n-1) \prod_{j \in \mathcal{A}^{(n)}_\alpha} \bar{\rho}_j$$

"Entanglement Correlators"

Can do same analysis for system S coupled to an 'environment' E.
(Can integrate out the environment – or look at system-bath correlations and/or entanglement).

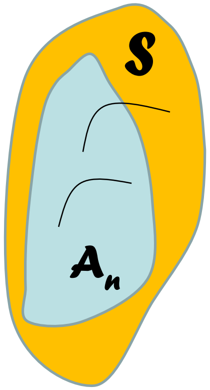


T. Cox, PCE Stamp, Phys Rev A98, 062110 (2018)

DYNAMICS of ENTANGLEMENT CORRELATORS

‘Schwinger-Dyson’ hierarchy of eqtns of motion for all the correlators

Start from the general result: $i\hbar\partial_t \rho_S = [H_S, \rho_S]$



Now suppose a Hamiltonian of ‘pairwise cell interaction’ form

$$\bar{H}_{\mathcal{A}_n} = \sum_{j\in\mathcal{A}_n}\left(H_i^0 + \frac{1}{2}\sum_{i\neq j\in\mathcal{A}_n} V_{ij}\right)$$

so that: $$i\hbar\partial_t \bar{\rho}_{\mathcal{A}_n} = [\bar{H}_{\mathcal{A}_n}, \bar{\rho}_{\mathcal{A}_n}] + \sum_{\ell\notin\mathcal{A}_n} \operatorname{tr}_\ell\left(\sum_{j\in\mathcal{A}_n}[V_{j\ell},\ \bar{\rho}_{\mathcal{A}_n\cup\{\ell\}}]\right)$$

Application to QUBITS

Hamiltonian: $$H = \sum_i \frac{1}{2}\mathbf{h}_i\cdot\boldsymbol{\sigma}_i + \sum_{i=1}^{N}\sum_{j<i}\frac{1}{2}V_{ij}^{\mu\nu}\sigma_i^\mu\sigma_j^\nu$$

We then get a hierarchy of eqtns of motion for the entanglement correlators:

$$\frac{d}{dt}\left\langle\prod_{i\in\mathcal{A}}\sigma_i^{\mu_i}\right\rangle = \sum_{i\in\mathcal{A}}\varepsilon^{\mu_i\alpha\nu}h_i^\alpha\left\langle\sigma_i^\nu\prod_{j\in\mathcal{A}\setminus\{i\}}\sigma_j^{\mu_j}\right\rangle + \sum_{i\in\mathcal{A}}\sum_{\ell\notin\mathcal{A}}\varepsilon^{\mu_i\alpha\nu}V_{i\ell}^{\alpha\lambda}\left\langle\sigma_\ell^\lambda\sigma_i^\nu\prod_{j\in\mathcal{A}\setminus\{i\}}\sigma_j^{\mu_j}\right\rangle$$
$$+\sum_{i\in\mathcal{A}}\sum_{j\in\mathcal{A}\setminus\{i\}}\varepsilon^{\mu_i\alpha\nu}V_{ij}^{\alpha\mu_j}\left\langle\sigma_i^\nu\prod_{k\in\mathcal{A}\setminus\{i,j\}}\sigma_k^{\mu_k}\right\rangle$$

Like any such hierarchy (Schwinger-Dyson, BBGKY, etc.) this is awfully intimidating.

NB – All Entanglement Witnesses can be written as f^{ns} of these correlators !

We get a little intuition by looking at the lowest orders:

1-qubit dynamics: $\frac{d}{dt}\langle\boldsymbol{\sigma}_1\rangle = (\mathbf{h}_1 + \tilde{\mathbf{V}}_1) \times \langle\boldsymbol{\sigma}_1\rangle$ with $\tilde{V}_1^{\alpha} = \sum_{\ell\neq 1} V_{1\ell}^{\alpha\lambda}\langle\sigma_\ell^\lambda\rangle$ Interaction with other qubits

2-qubit dynamics: This couples pairs of qubits to triplets of them

$$\frac{d}{dt}\langle\sigma_1^{\mu_1}\sigma_2^{\mu_2}\rangle = \sum_{j\neq j'=1,2} \varepsilon^{\mu_j\alpha\beta}\left[h_j^\alpha\langle\sigma_j^\beta\sigma_{j'}^{\mu_{j'}}\rangle + V_{12}^{\alpha\mu_{j'}}\langle\sigma_j^\beta\rangle + \sum_{\ell\neq 1,2} V_{j\ell}^{\alpha\lambda}\langle\sigma_\ell^\lambda\sigma_j^\beta\sigma_{j'}^{\mu_{j'}}\rangle\right]$$

ENTANGLEMENT CORRELATOR SUPERVECTOR: The components of this vector are ALL POSSIBLE correlation functions for a system.

Example: pick a 2-qubit system - there are 15 such correlators.

The supervector $\underline{X}$ is

$$\underline{X} = \begin{pmatrix} X_1 \\ X_2 \\ X_3 \\ X_5 \\ X_6 \\ X_7 \\ X_8 \\ \vdots \end{pmatrix} = \begin{pmatrix} \langle\tau_1^x\rangle \\ \langle\tau_1^y\rangle \\ \langle\tau_1^z\rangle \\ \langle\tau_2^x\rangle \\ \langle\tau_2^y\rangle \\ \langle\tau_2^z\rangle \\ \langle\tau_1^x\tau_2^x\rangle \\ \langle\tau_1^x\tau_2^y\rangle \\ \vdots \end{pmatrix} \equiv \begin{pmatrix} \langle\boldsymbol{\tau}_1\rangle \\ \langle\boldsymbol{\tau}_2\rangle \\ \langle\boldsymbol{\tau}_1\otimes\boldsymbol{\tau}_2\rangle \end{pmatrix}$$

Eqtn. of motion: $\frac{d}{dt}\underline{X} = \mathbb{M}\underline{X}$ (linear ODE!)

written out: $\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} \langle\boldsymbol{\tau}_1\rangle \\ \langle\boldsymbol{\tau}_2\rangle \\ \langle\boldsymbol{\tau}_1\otimes\boldsymbol{\tau}_2\rangle \end{pmatrix}$

$$= \begin{pmatrix} \mathbb{L}_1 & 0 & \mathbb{U}_{1,p} \\ 0 & \mathbb{L}_2 & \mathbb{U}_{2,p} \\ \mathbb{U}_{p,1} & \mathbb{U}_{p,2} & \mathbb{L}_p \end{pmatrix}\begin{pmatrix} \langle\boldsymbol{\tau}_1\rangle \\ \langle\boldsymbol{\tau}_2\rangle \\ \langle\boldsymbol{\tau}_1\otimes\boldsymbol{\tau}_2\rangle \end{pmatrix}$$

Crucial Point: the matrix M is in general extremely SPARSE

→ Solution to eqtns of motion

EXACTLY SOLVABLE EXAMPLE

A really simple show some of what happens (later on we look at a more complex 'Real World' example).

We pick the Hamiltonian (a dumbed down 'central spin model'):

$$H = \tfrac{1}{2}\Delta_0 \tau^x + \sum_{i \in \mathcal{B}} \tfrac{1}{2}\omega_i \sigma_i^z \tau^z$$

with initial condition:

$$\rho(0) = \tfrac{1}{2}(1 + \tau^x)\mathbf{I}_{\mathcal{B}}$$

and look at the n+1 spin correlator:

$$\left\langle \vec{\tau} \prod_{i=1}^{n} \sigma_i^z \right\rangle$$

Parameters are:

$$\omega_i = 0.05\Delta_0, \; N = 100$$

Colour coding:

$$\langle \tau^x \ldots \rangle \quad \langle \tau^y \ldots \rangle \quad \langle \tau^z \ldots \rangle$$

The results show correlations 'cascading' towards higher numbers of entangled spins.

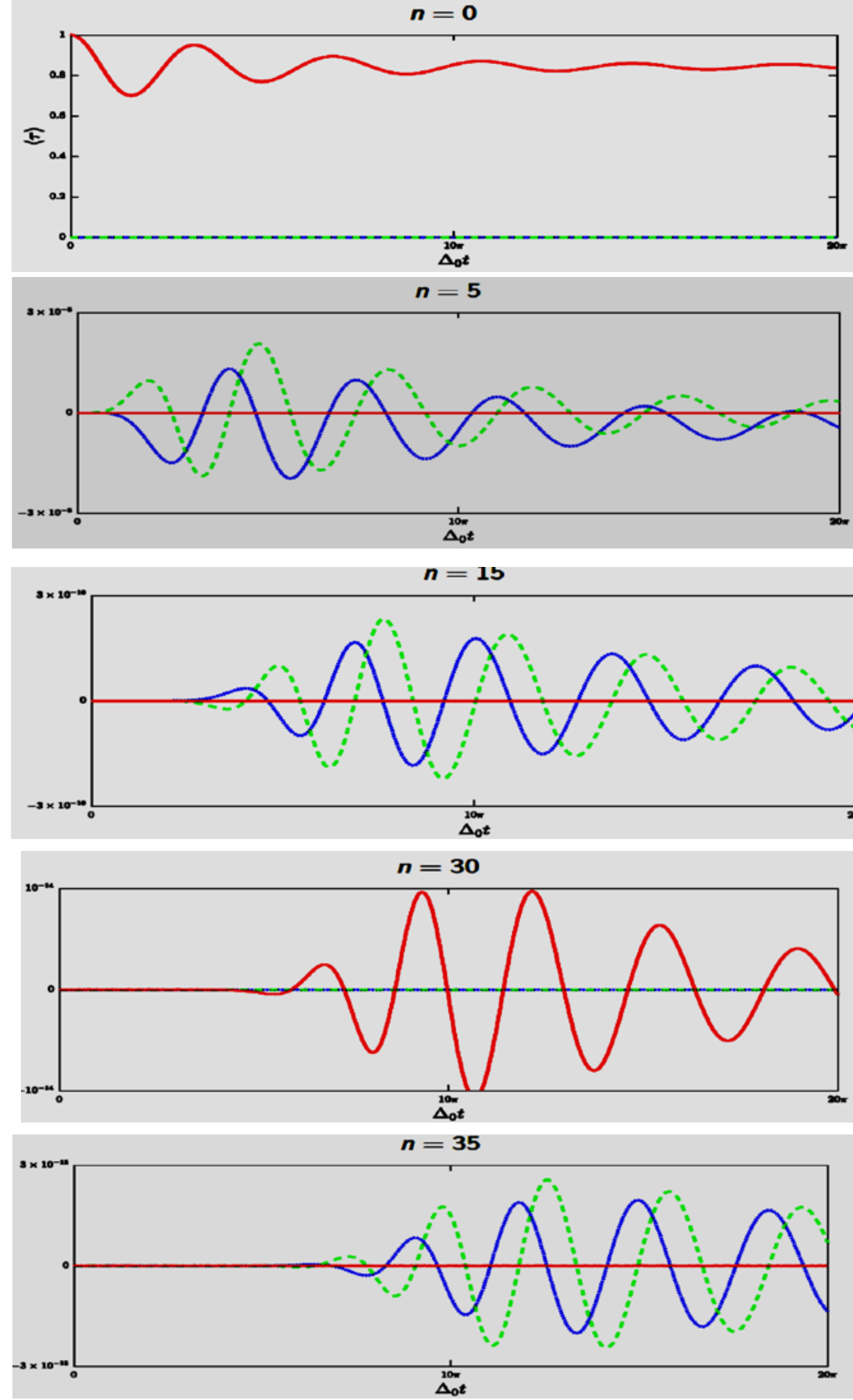
n=0

n=5

n=15

n=30

n=35



The REAL WORLD

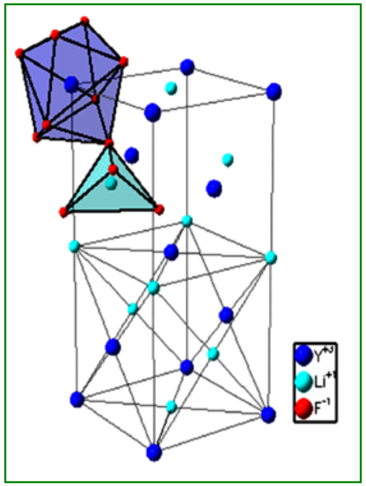
"A theory is not a theory until it produces a number" R.P. Feynman (Lectures on Physics, 1965)

Only wimps specialize in the general case. Real scientists pursue examples. **MV Berry: Ann NY Acad Sci 755, 303 (1995)**

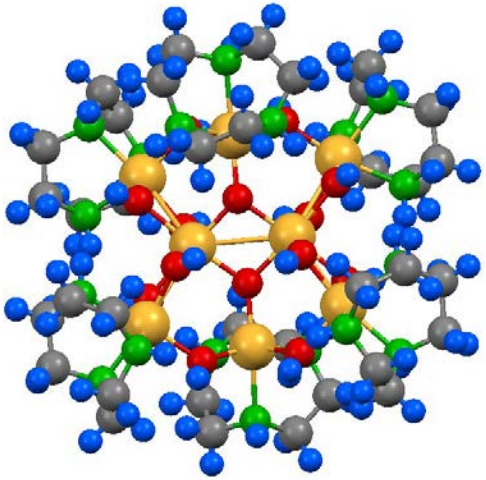
We will look at

QUANTUM ISING SYSTEMS

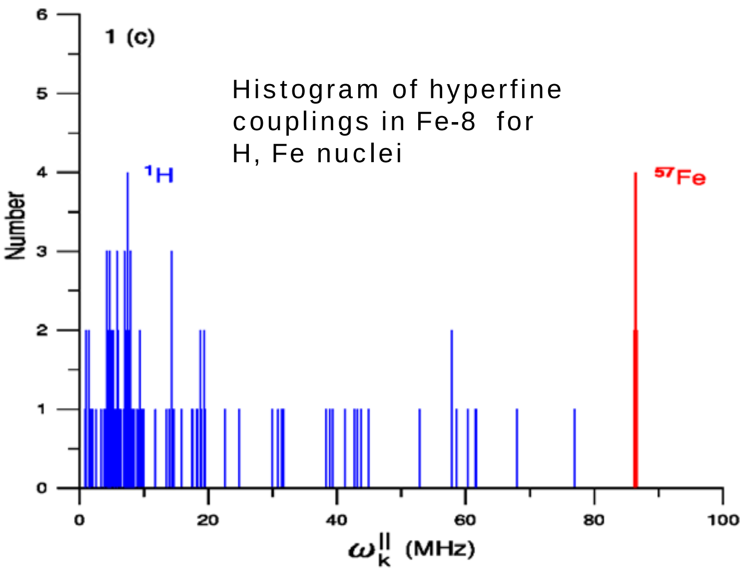
$LiHo_xY_{1-x}F_4$



Fe_8 MOLECULE



CORRELATIONS in Fe-8



Below 0.3K this entire molecule behaves like a qubit, with effective Hamiltonian

$$\mathcal{H}_o(\hat{\tau}) = (\Delta_o \hat{\tau}_x + \epsilon_o \hat{\tau}_z)$$

However the qubit couples to 215 nuclear spins inside the molecule (H, O, Br, N, Fe)

Coupling strengths: 1-100 MHz (50 μK-5 mK)

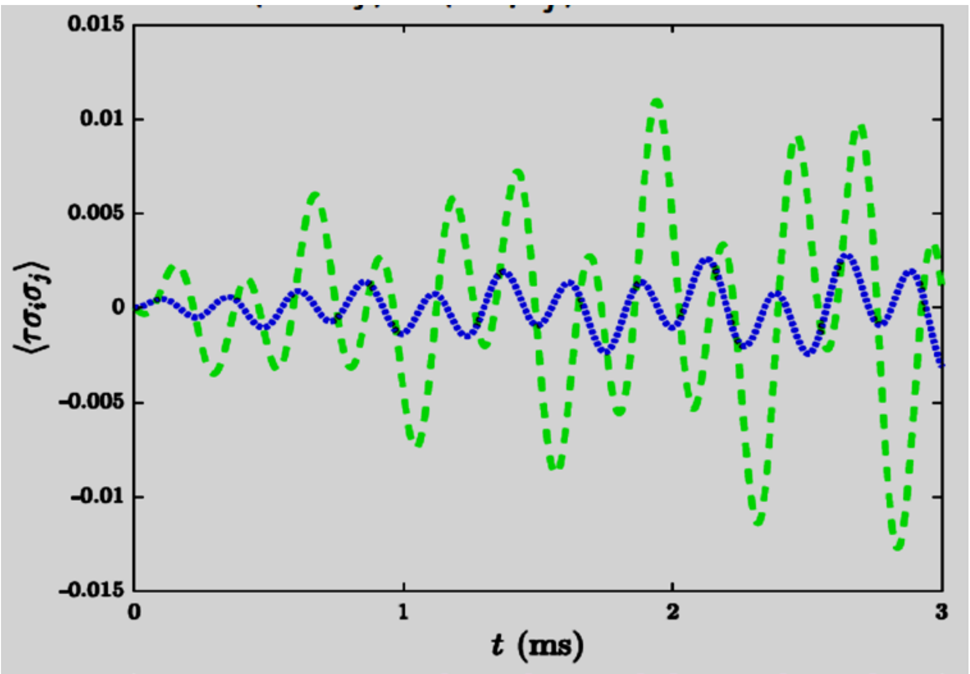
PREDICTIONS for entanglement correlators in the Fe-8 molecule

Here we show:

$$\langle \tau^y \sigma_i^x \sigma_j^x \rangle = \langle \tau^y \sigma_i^y \sigma_j^y \rangle :$$

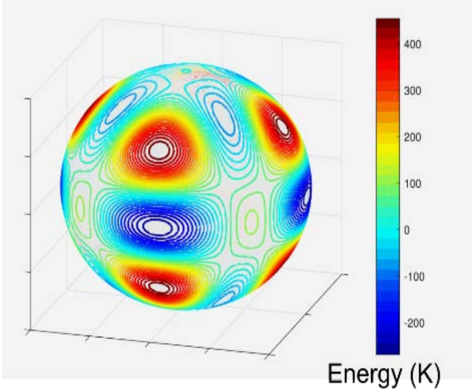
$$\langle \tau^z \sigma_i^x \sigma_j^x \rangle = \langle \tau^z \sigma_i^y \sigma_j^y \rangle :$$

for 2 of the 120 protons in Fe-8 (amongst the 213 nuclear spins)



Quantities like this will be a future topic for experimentalists – we are entering a new era of multipartite entanglement – aka quantum computation

The $LiHo_xY_{1-x}F_4$ System

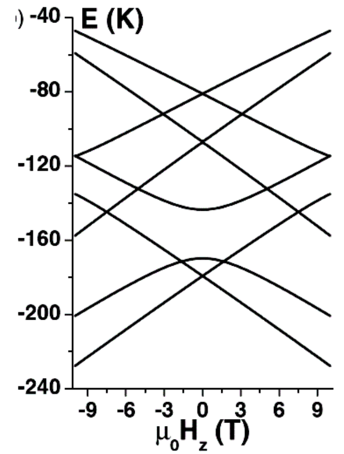


(1) KEY THEORETICAL FACTS

Ignoring Nuclear Spins & phonons, we have effective spin-8 Ho ions, with a very complicated crystal field (see figure).

At low energy (<< 10K) we can truncate to Ising doublet states, with Hamiltonian

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



Dipolar interaction strength: $|V_{ij}^{zz}| \sim 0.3$ K (for nearest neighbor pair)

Thus typical dipolar coupling energy scale is ~ 1-1.5K

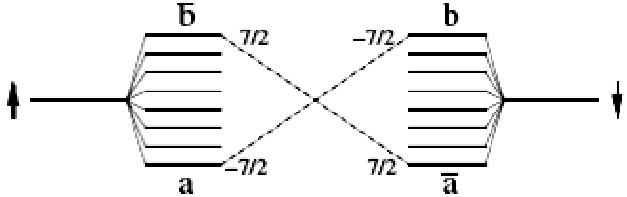
Without nuclear spins, 'tunneling' energy is $\Delta_0 \sim 9(\mu_B H_\perp)^2/\Omega_0$

with $\Omega_0 = 10.5$ K

Effect of nuclear spins is profound

Each Ho nuclear spin has $I = 7/2$

Each electronic Ising level split into 8 states.



One cannot flip an Ising spin without also flipping the nuclear spin through 6 intermediate states. This is very hard!

Should radically alter both phase diagram & the dynamics.

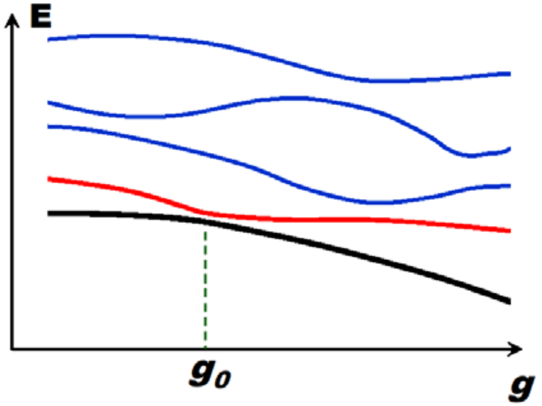
Bare hyperfine coupling: $H_{hf} = A_J \sum_i \vec{I}_i \cdot \vec{J}_i$

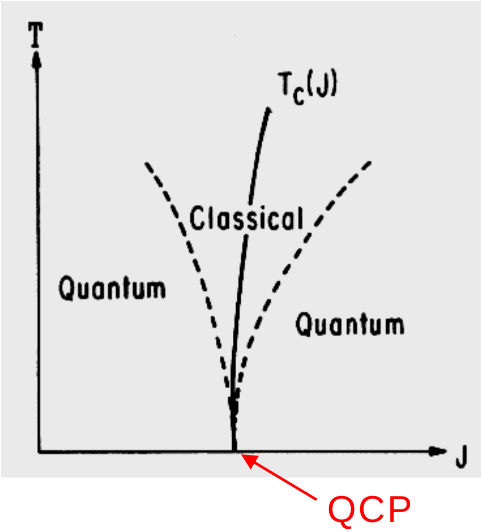
Bare hyperfine coupling is huge – separation between hyperfine levels is ~ 0.25 K.
Hyperfine energies span a range ~ 1.4K

M Schechter, PCE Stamp, PRL 95, 267208 (2005)
" " , Phys Rev B78, 054438 (2008)

(2) EXPECTED LOW-ENERGY PHYSICS

Imagine some finite quantum system, with a coupling constant g we can vary. We can get an 'avoided crossing', where the 1st excited state |1> and ground state |0> approach each other around $g = g_0$

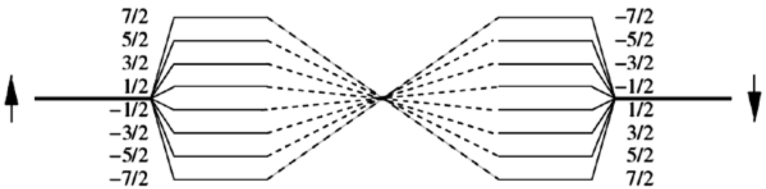




For some systems, this close approach between |1> & |0> persists as we go to the "thermodynamic limit". In this limit the gap goes to zero, at the "Quantum Critical Point" (QCP), where we have a Quantum Phase Transition.

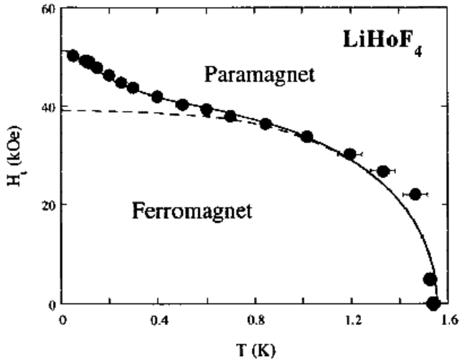
Quantum Annealing & Adiabatic Quantum Computation involve a slow passage through the QCP.

Classic Example: QUANTUM ISING MODEL



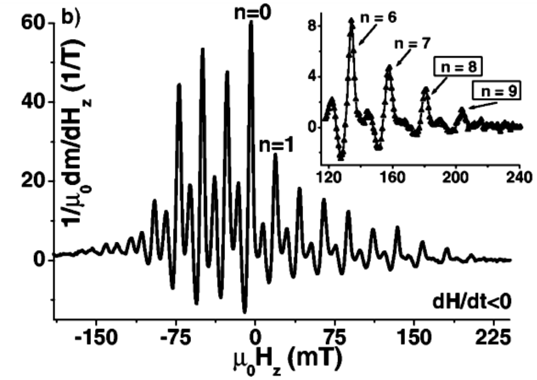
The big question is: will the coupling to the spin bath of nuclear spins mess up the Quantum Phase Transition?

(2) KEY EXPERIMENTAL FACTS



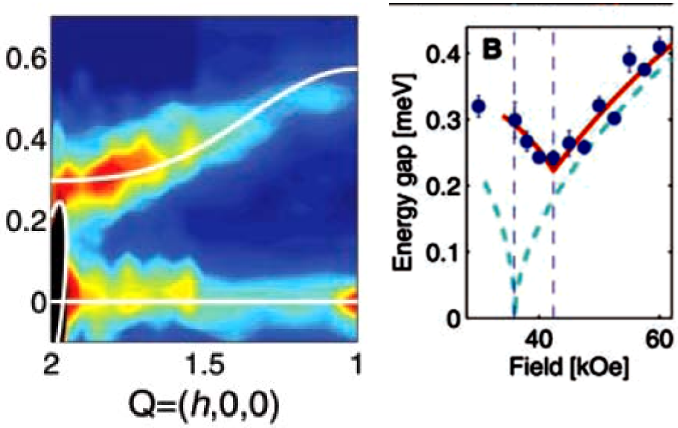
The quantum phase transition exists – transition line strongly influenced by nuclear spins.

In dilute systems ($LiHo_xY_{1-x}F_4$ with $x << 1$) the hysteresis & relaxation controlled by cross-relaxation via nuclear spins (with 13 different transitions



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

Looking for the soft mode

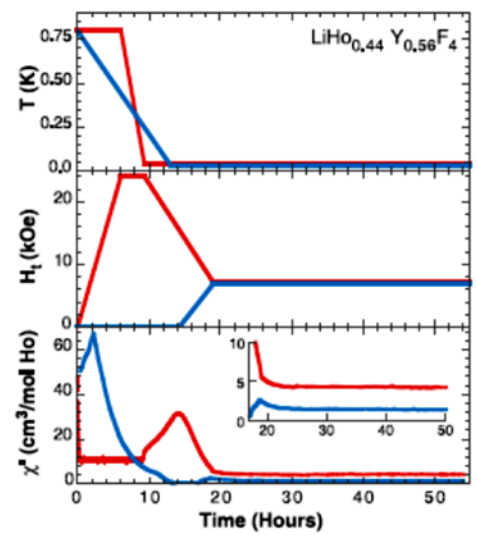


H.M. Ronnow et al., Science 308, 389 (2005)

Neutron scattering experiments are designed to see low-E excitations

But where is the soft mode? This one is GAPPED

Quantum Annealing is found – this was the 1st experimental observation of this



J. Brooke et al.,
Science 284, 779 (1999)

Preliminary conclusion from this expt – a spin bath gaps the soft mode, leads to new kind of transition

IN SEARCH OF THE SOFT MODE: LOW-ENERGY EXCITATIONS in $LiHoF_4$

The full effective low-energy Hamiltonian is

Crystal field potential

Transverse field Zeeman coupling

Dipolar coupling between Ho spins

$$\mathcal{H} = \sum_i V_c(\vec{J}_i) - g_L \mu_B \sum_i B_x J_i^x - \frac{1}{2} J_D \sum_{i \neq j} D_{ij}^{\mu\nu} J_i^\mu J_j^\nu$$

$$+ \frac{1}{2} J_{nn} \sum_{\langle ij \rangle} \vec{J}_i \cdot \vec{J}_j + A \sum_i \vec{I}_i \cdot \vec{J}_i$$

Exchange coupling between Ho spins

Hyperfine coupling to Ho nuclei

which we recall gives the truncated "interacting qubit" Hamiltonian

$$\mathcal{H}_{eff} = -\frac{1}{2} \sum_{i \neq j} V_{ij} \tau_i^z \tau_j^z - \Delta \sum_i \tau_i^x + \mathcal{H}_{hyp}$$

Interaction between Ising spins

Effective transverse field

Hyperfine coupling to Ising spins

with characteristic energies

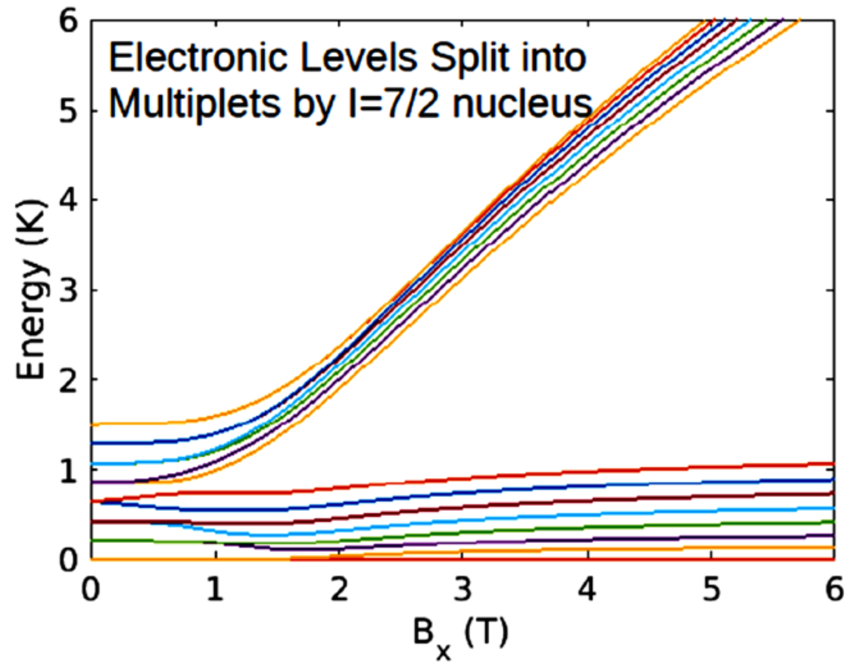
Typical dipolar coupling energy scale: ~ 1-1.5K

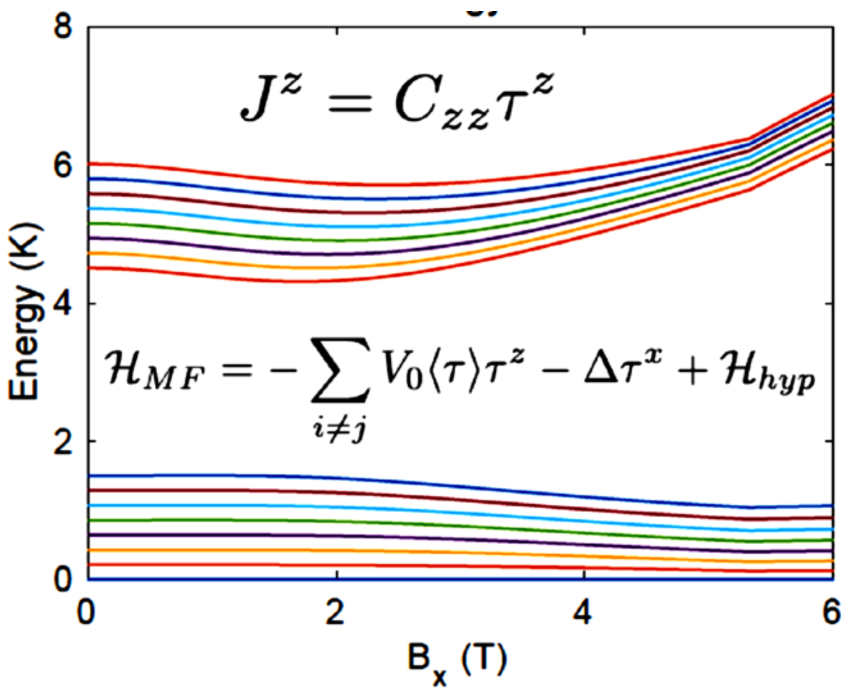
Hyperfine energies span a range ~ 1.4K

Effective transverse field Δ is varied in experiments

SINGLE ION EXCITATIONS

With the known crystal field Parameters and hyperfine couplings for the Ho ions in the system, we find the 15 lowest energy modes (Ising doublet split by hyperfine coupling





If we now add in the dipolar coupling between Ising spins in a very naive uniform mean field approximation, we get the picture shown at left

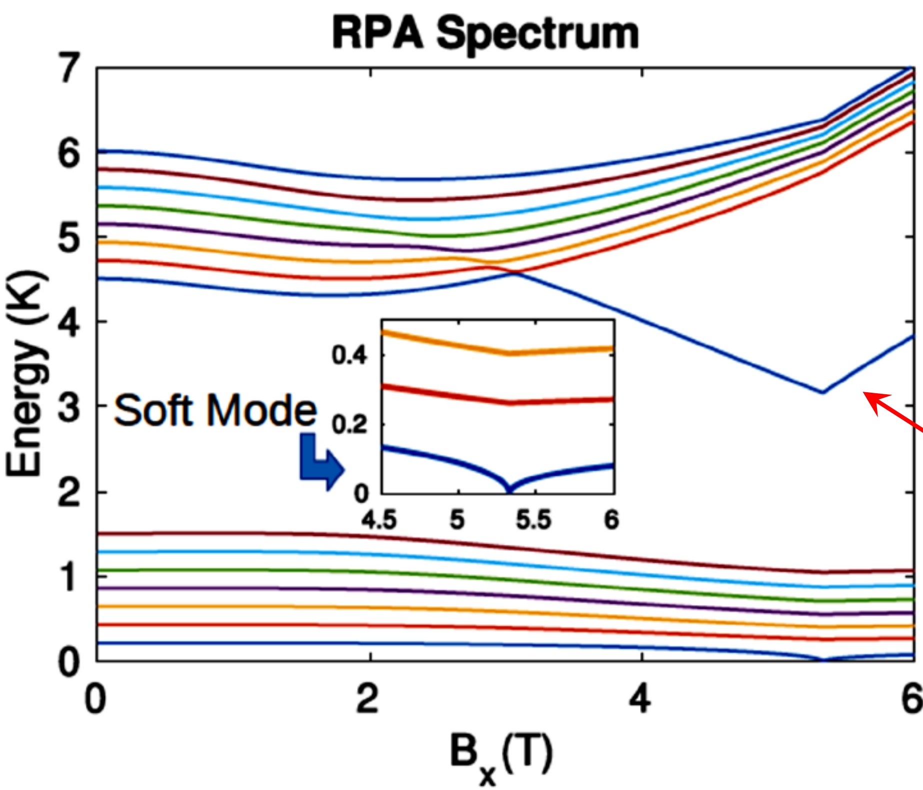
COLLECTIVE EXCITATIONS of ENTIRE SYSTEM

The true collective modes are coherent extended wave modes.
How do we find theoretical expressions for them?

The Random Phase Approximation (RPA) does this by ignoring interactions between collective modes – to give a propagator:

$$\widetilde{G}(\mathbf{k}, i\omega_r) = \frac{C_{zz}^2 \sum_{n>m} |c_{mn}|^2 p_{mn} 2E_{nm} \prod_{t>s\neq nm} (E_{ts}^2 - (i\omega_r)^2)}{\prod_{n>m} (E_{nm}^2 - (i\omega_r)^2) - V_{\mathbf{k}} \sum_{n>m} |c_{mn}|^2 p_{mn} 2E_{nm} \prod_{ts\neq mn} (E_{ts}^2 - (i\omega_r)^2)}$$

Sums are over all the different mean field single ion states



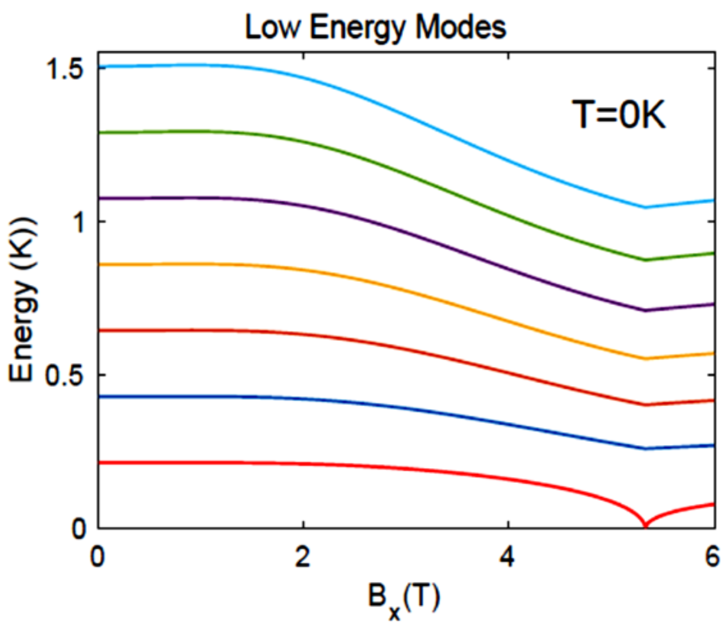
Q: Why should RPA work?

A: Renormalization group calculations show that intermode coupling is weak at low energies

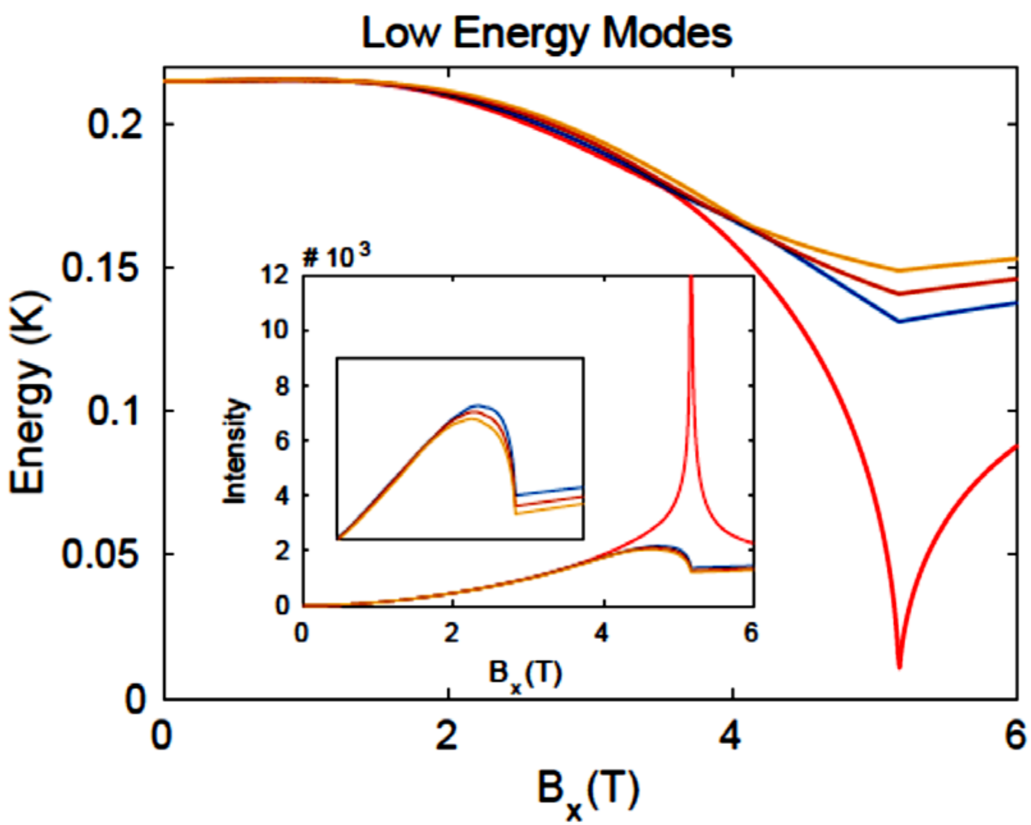
The mode seen by neutron Scattering experiments !

RD McKenzie, PCE Stamp, Phys Rev B97, 214430 (2018)

LOW-ENERGY COLLECTIVE MODES



Now let's focus on low energies.
At right, the zero temperature modes



We show the frequencies & spectral weights for the different low energy transitions, as they would be seen in experiment.

These have now been seen in experiment (see talk of Silevitch)

CONCLUSIONS

- One can characterize Multiparticle states & multi-qubit entanglement

- One can solve for their dynamics – this opens up a new way of doing many-body physics

- Application to real world systems like Fe-8 and $LiHo_xY_{1-x}F_4$ is feasible

- $LiHo_xY_{1-x}F_4$ is the archetypal quantum critical system (showing quantum annealing). But where is the soft mode?

- RPA theory shows it should be there, as one of 15 different ‘electronuclear’ modes.

- Experiments have now found them

This will have important implications for real world quantum computers – which also couple to spin baths