LECTURES – COLLEGE de FRANCE, MAY 2016
3rd LECTURE

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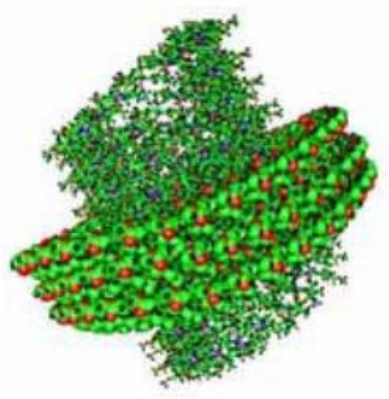
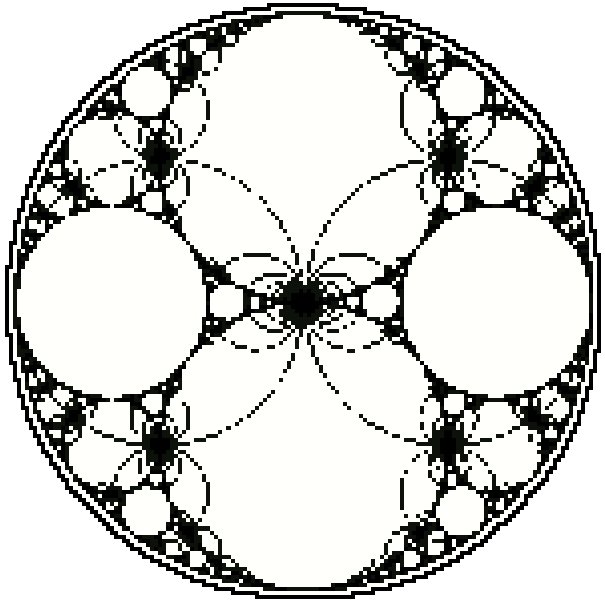
LECTURE 3

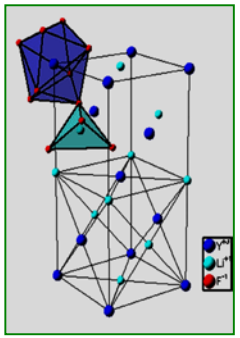
FROM QUBITS

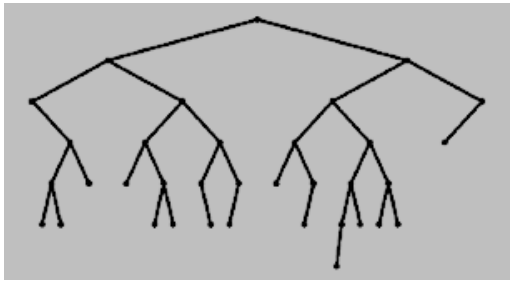
to

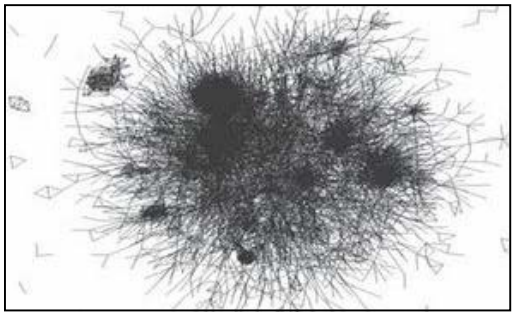
SPIN NETS - 2











QUANTUM NETWORKS – WHAT ARE WE INTERESTED IN?

In what follows, I will be looking at the following questions:

(i) What sort of quantum networks are particularly important?
(ii) How should we try and understand their dynamics?
(iii) How should we be trying to understand quantum computation?
(iv) How can we engage experimentally with all of this?

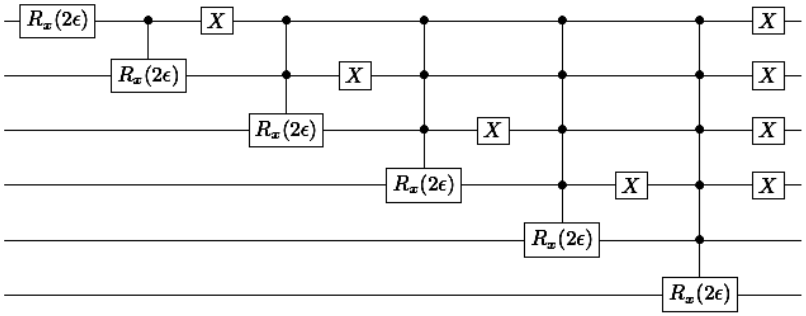
There will be less formal theory in this lecture – the emphasis will be more on examples. We will look at

(A) Numerical simulations on a "capricious voter model" (simulates elections but is actually a dissipative Q Ising model); & analytic solutions for quantum diffusion on a hypercube

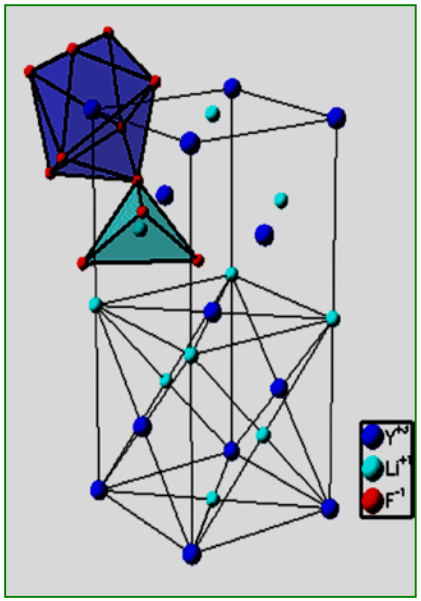
(B) As usual, I will discuss a real world example – in fact I will actually discuss THREE real world examples in this lecture, these being

- Quantum Ising network of Fe-8 molecular spins
- Quantum Ising network of Ho ions
- Polaronic dynamics in chains – metals, insulators, & biomolecules

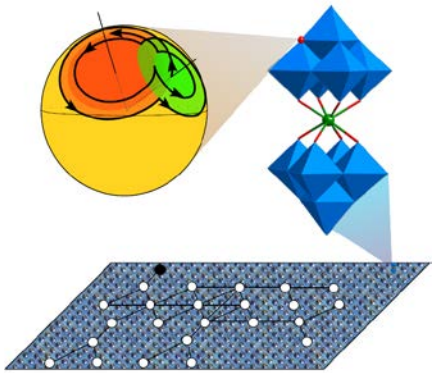
GEOMETRY of the NETWORKS



ABOVE: structure in a gated Q Computer



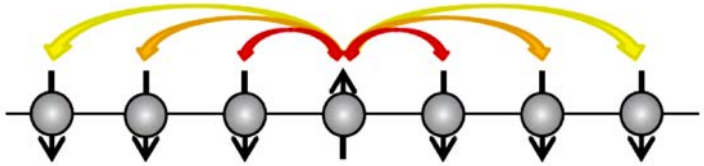
ABOVE: LiHoF, unit cell



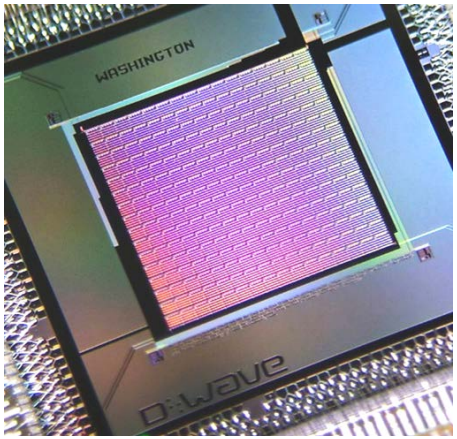
ABOVE: The pthalocyanine idea for Quantum computation

As noted in the last lecture, one can discuss many different networks using the same language, by transforming between them.

Their topology then becomes important – some examples of key cases are shown here. One has 1-d chains, surfaces of varying structure, & 3-d lattices.

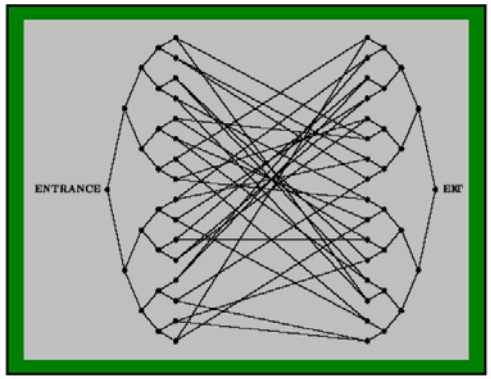


ABOVE: Interactions in $^{40}Ca^{+}$ ion spin chain

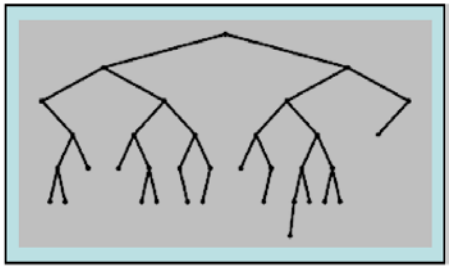


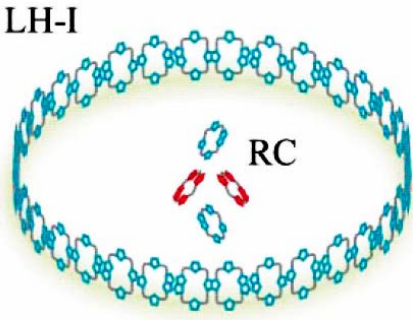
ABOVE: d-wave Q annealing chip

In the 'Q information space' of equivalent graphs, the topology is crucial – the presence of closed rings plays a big role, as do hierarchical 'tree' structures, and the connectivity between "in" and "out" networks.



LEFT & BELOW: graphs for quantum info nets – "in-out" and "inverted tree"





ABOVE: Geometry of a Light-Harvesting Molecule

NETWORK HAMILTONIANS

We will be looking for the most part at 2 kinds of effective Hamiltonian (recall that these Hamiltonians are usually the result of some elaborate truncation procedure):

(i) HOPPING MODEL: We have $$H_o = \sum_{ij} \left[t_{ij} c_i^\dagger c_j \, e^{iA^o_{ij}} + H.c. \right] + \sum_j \varepsilon_j c_j^\dagger c_j + H_{int}^{env}$$

This is not the most general model. In a quantum computer the parameters will typically be time-dependent; and an important generalization of this model is to the "composite" Hamiltonian:

$$\hat{H}_C = -\sum_{ij} [F_{ij}(\mathcal{M}_{ij};t)\hat{c}_i^\dagger \hat{c}_j + \text{H.c.}] + \sum_j G_j(\mathcal{L}_j;t)\hat{c}_j^\dagger \hat{c}_j + \hat{H}_o(\{\mathcal{M}_{ij},\mathcal{L}_j\}) + H_{int}^{env}$$

where we attach supplementary variables to each node and link. These could be extra spin variables (ie, internal nodes); we can also organize things so that these variables are activated only when the node or link is occupied, which is one way of generating a dynamical network, which can grow with time.

We will not discuss these more general Hamiltonians here.

(ii) QUANTUM ISING MODEL: The standard Q Ising model has the form

$$\mathcal{H} = \sum_j \Delta_o \hat{\tau}_j^x + \sum_{ij} V_{ij} \hat{\tau}_i^z \hat{\tau}_j^z + H_{int}^{env}$$

This is the simplest possible form – more general one has a different transverse field at each site, one also has a longitudinal field at each site, and one can have transverse as well as longitudinal interactions at each site.

We also have coupling of the network variables to an environment

COUPLING to an ENVIRONMENT for QUANTUM WALKS

Oscillator bath

The oscillators couple to both nodes & links (often called "diagonal" and "non-diagonal" terms:

$$H_{osc} = \sum_{q=1}^{N_o} \left(\frac{p_q^2}{m_q} + m_q \omega_q^2 x_q^2 \right)$$

$$V_{int} = \sum_{q=1}^{N_o} \left[\sum_{ij} (U_j(q) \hat{c}_i^\dagger \hat{c}_j + H.c.) + \sum_j V_j(q) \hat{c}_j^\dagger \hat{c}_j \right] x_q$$

Spin Bath

The same happens when we couple the walker to a spin bath (here written for a bath of 2-level systems):

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

$$V_{int} = \sum_k^{N_s} \left[\sum_{ij} (\boldsymbol{F}_j(k) \hat{c}_i^\dagger \hat{c}_j + H.c.) + \sum_j \boldsymbol{G}_j(k) \hat{c}_j^\dagger \hat{c}_j \right] \cdot \boldsymbol{\sigma}_k$$

COUPLING to an ENVIRONMENT for QUANTUM ISING SYSTEM

We write the coupling of a quantum Ising system to a combination of oscillator & spin baths as

$$V_{int} = \sum_{j=1}^{N} \left[\sum_k \omega_{jk}^{\alpha\beta} \tau_j^\alpha \sigma_k^\beta + \sum_q [U_j^\alpha(q) \tau_j^\alpha x_q + V_j^\alpha(q) \tau^\alpha p_q] \right]$$

Coupling to spin bath

Coupling to oscillator bath

We can resolve these into transverse and longitudinal processes – the latter usually dominate after renormalization.

Just as with the case of quantum gates, we can transform the quantum Ising system (and its environmental couplings) to a quantum walk form.

THEORETICAL METHODS

The theory is significantly more complex than before – so I will not go into too many details; instead, the general lines of what is done will be indicated.

(1) Let us recall that for a classical N-particle system, the dynamics is described by the BBGKY hierarchy – this is a set of N-1 integrodifferential eqtns relating the N different s-particle distribution functions (with s = 1,2,...N), given in terms of the full N-particle density matrix by

$$\rho_s(\mathbf{X}_1,\ldots,\mathbf{X}_s,t) = \int\cdots\int d\mathbf{X}_{s+1}\ldots d\mathbf{X}_N\ \rho(\mathbf{X}_1,\ldots,\mathbf{X}_N,t)$$

To remove the dependence on volume, we define: $F_N(\mathbf{X}_1,\ldots,\mathbf{X}_N,t) \equiv V^N\rho(\mathbf{X}_1,\ldots,\mathbf{X}_N,t)$

The BBGKY eqtns are then

$$\boxed{\frac{\partial F_s}{\partial t} + i\hat{L}^s F_s = \frac{1}{\nu}\sum_{i=1}^{s}\int d\mathbf{X}_{s+1}\hat{\Theta}_{i,s+1}F_{s+1}(\mathbf{X}_1,\ldots,\mathbf{X}_{s+1},t)}$$

where the Liouville operator L^N and the scattering operator θ depend on the form of the Hamiltonian; thus, eg., for the 2-body form

$$H^N(\mathbf{X}^N) = \sum_{i=1}^{N}\frac{p_i^2}{2m} + \sum_{i<j}^{N(N-1)/2}\phi(|\mathbf{q}_i-\mathbf{q}_j|)$$

we have

$$\hat{L}^N = -i\sum_{i=1}^{N}\frac{\mathbf{p}_i}{m}\cdot\frac{\partial}{\partial\mathbf{q}_i} + i\sum_{i<j}^{N(N-1)/2}\hat{\Theta}_{ij} \qquad \text{and} \qquad \hat{\Theta}_{ij} = \frac{\partial\phi_{ij}}{\partial\mathbf{q}_i}\cdot\frac{\partial}{\partial\mathbf{p}_i} + \frac{\partial\phi_{ij}}{\partial\mathbf{q}_j}\cdot\frac{\partial}{\partial\mathbf{p}_j}$$

and the first member of the hierarchy is just the Boltzmann eqtn

$$\frac{\partial F_1}{\partial t} + \frac{\mathbf{p}_1}{m}\cdot\frac{\partial F_1}{\partial\mathbf{q}_1} = \frac{1}{\nu}\int d\mathbf{X}_2\hat{\Theta}_{12}F_2(\mathbf{X}_1,\mathbf{X}_2,t)$$

(2) For a quantum N-particle/N-spin system, we set up a similar set of equations, in terms of the s-particle correlation functions. Likewise, for a quantum field, we set up the 'Schwinger-Dyson" hierarchy of equations for the m-point correlators.

Thus, eg., for a scalar field we have the definitions

$$G_n(x_1,\cdots,x_n) \;=\; \langle 0|\hat{T}\{\phi(x_1),\cdots,\phi(x_n)\}|0\rangle \;=\; \frac{\oint D\phi\, e^{i/\hbar S[\phi]}\,\phi(x_1)\cdots\phi(x_n)}{\oint D\phi\, e^{i/\hbar S[\phi]}}$$

and the action

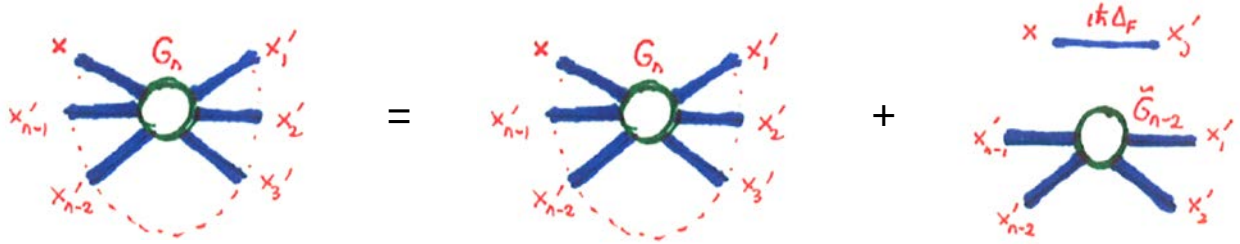
$$S \;=\; \int d^4x\,\left[\frac{1}{2}(\partial^\mu\phi\partial^\mu\phi - m^2\phi^2) \;-\; \frac{g}{4!}\phi^4\right]$$

We then find that

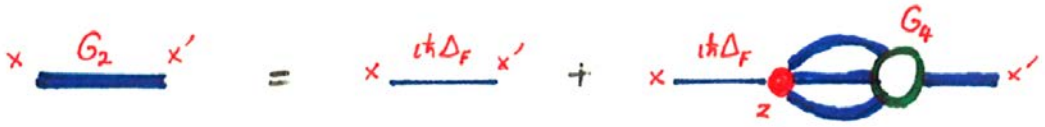
$$G_n(x,x_1'\ldots,x_{n-1}') \;-\; \frac{g}{6}\int d^4z\,\Delta_F(x-z)\,G_{n-2}(z\,z\,z\,,x_1'\ldots,x_{n-1}') \;-\; i\hbar\sum_{j=1}^{n-1}\Delta_F(x-x')\tilde{G}_{n+2}(\{x_j'\}) \;=\; 0$$

where we have defined $\tilde{G}_{n-2}(\{x_j'\}) \;\equiv\; G_{n-2}(x_1',x_2',\ldots,x_{j-1}',x_{j+1}',\ldots,x_{n-1}',)$

Equations like these are best understood diagrammatically – our main result reads



The lowest member is just Dyson's eqtn



(the quantum analogue to Boltzmann's eqtn)

(3) When we deal directly with the qubits (written here as spin-1/2 systems) we have to adapt the Schwinger-Dyson or BBGKY calculus to these systems. Thus, eg., for a set of interacting spin-1/2 degrees of freedom, with Hamiltonian

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

we get a hierarchy of eqtns of form

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

which can be extended to include a coupling to a spin bath or an oscillator bath. It is of considerable interest that this allows us to define a set of correlators which completely define the entanglement properties of the interacting qubit system.

If we decide to represent the interacting qubit system in the form a quantum walker, then the formalism is actually much simpler (but the interactions more complicated). Consider, eg., the 1-d walk around a ring, with Hamiltonian

$$H_o = \sum_{ij}\left[t_{ij} c_i^\dagger c_j\, e^{iA_{ij}^o} + H.c.\right] \qquad \text{such that} \qquad A_{ij}^o = \frac{e}{2}\mathbf{H}\cdot\mathbf{R}_i \times \mathbf{R}_j = \Phi/N$$

Then the density matrix for the walker in a site representation evolves according to

$$\rho_{jj'}(t) = \sum_{l,l'} \mathcal{K}_{jj',ll'}(t)\rho_{l,l'}^{(\mathrm{in})} \qquad \text{with propagator} \qquad \mathcal{K}_{jj',ll'}(t) = \sum_{pp'} K_{jj',ll'}^o(p,p';t) F_{jj'}^{ll'}(p,p')$$

with a sum over winding numbers involving a (calculable) influence functional

Z Zhu, A Aharony, O Entin, PCE Stamp, PR A81, 062127 (2010)

THEORY EXAMPLE # 1
CAPRICIOUS VOTER MODEL

$$\mathcal{H} = \sum_j \Delta_o \hat{\tau}_j^x + \sum_{ij} V_{ij} \hat{\tau}_i^z \hat{\tau}_j^z + H_{int}^{env}$$

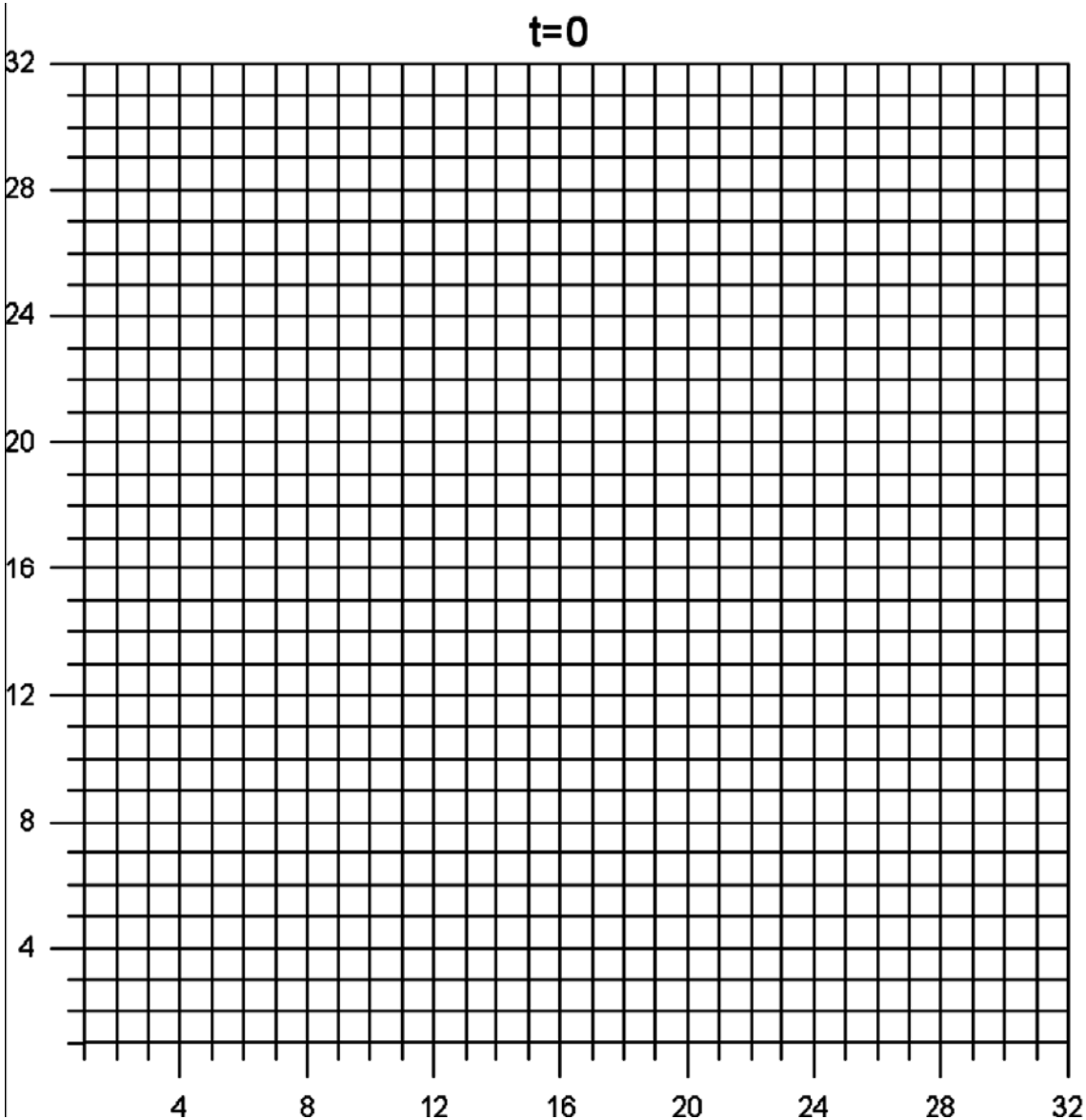
This is actually a Quantum Ising model with coupling to an environment; here we will look at the case of long-range interactions.

What follows is a depiction of the time evolution of correlated errors in quantum information processing

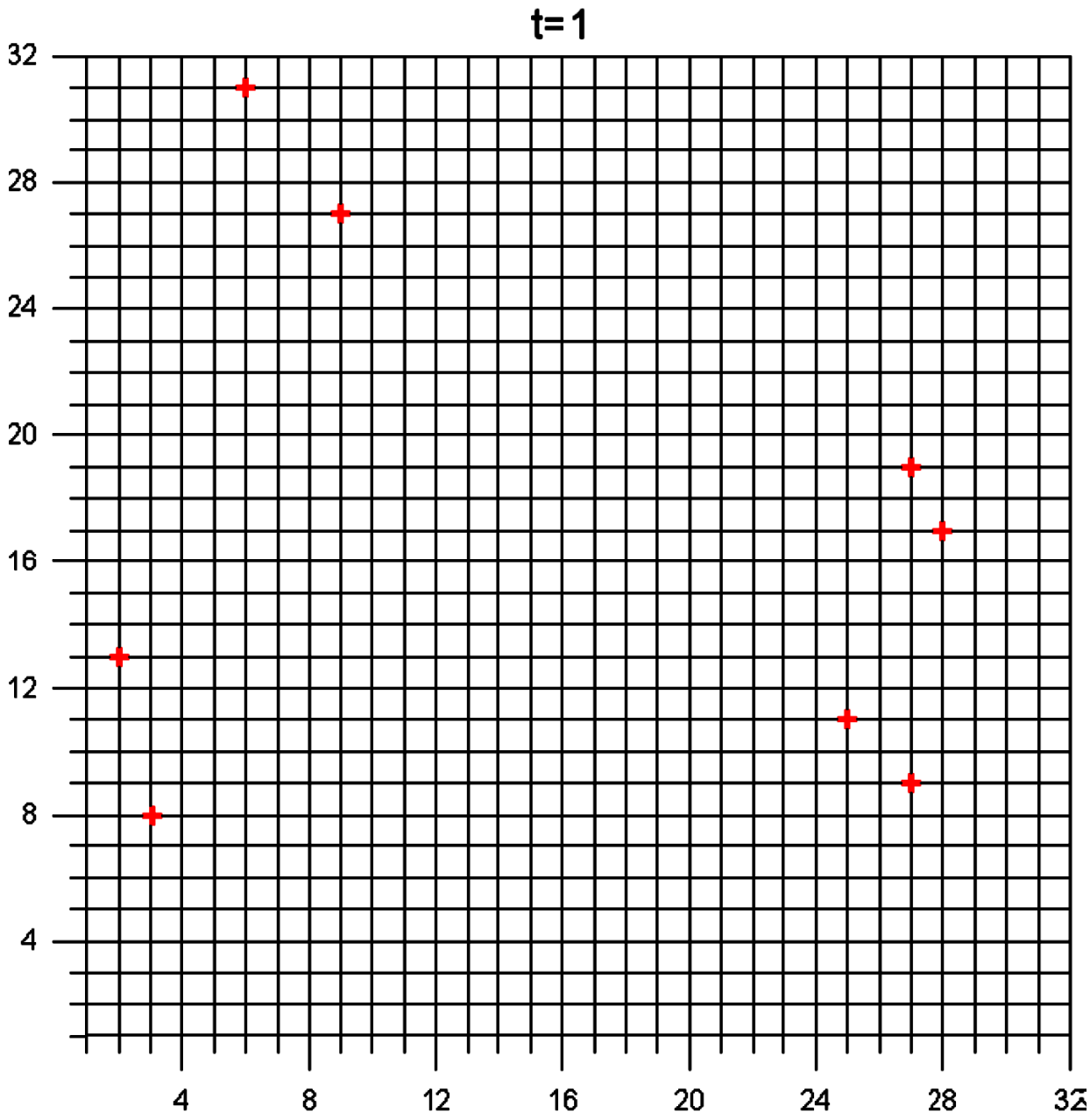
At t=0, start with an unpolarized array of spins (qubits) with random orientations (half up, half down).

In what follows we show which spins have flipped after a time t

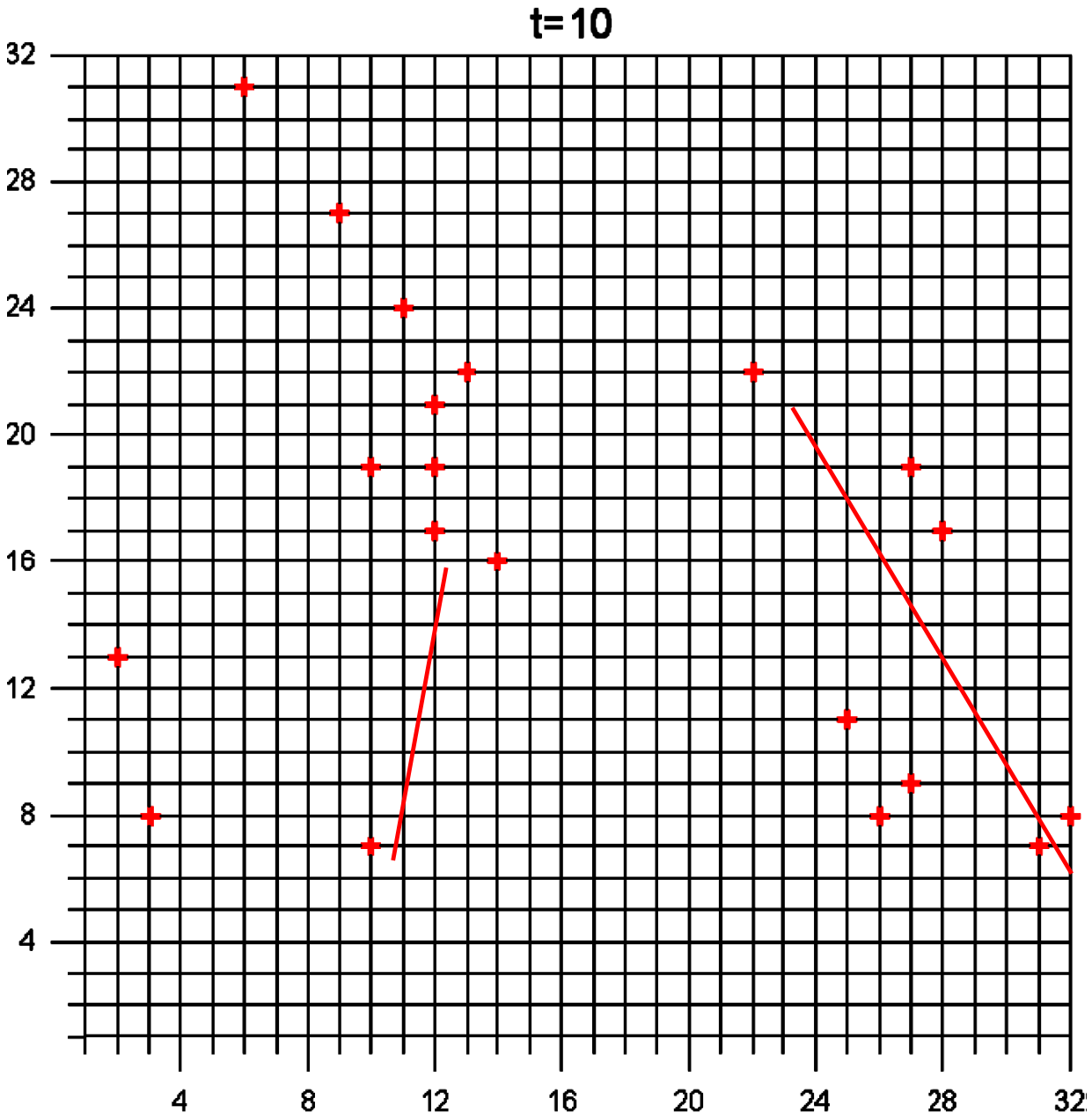
Thus, at t=0, no spins have yet flipped



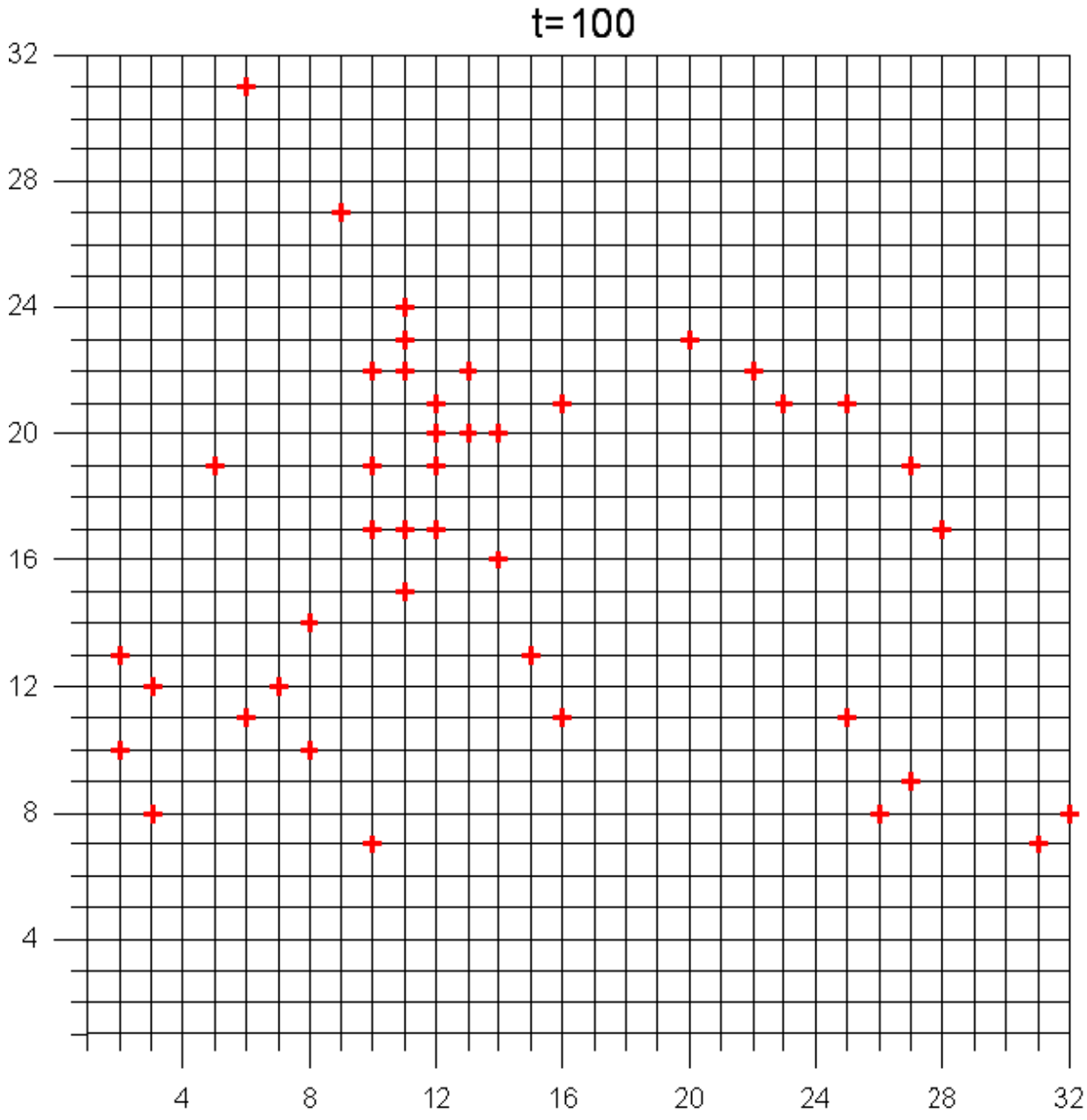
The spins flip in pairs. At t=1, 4 pairs of spins have flipped (8 flipped spins)



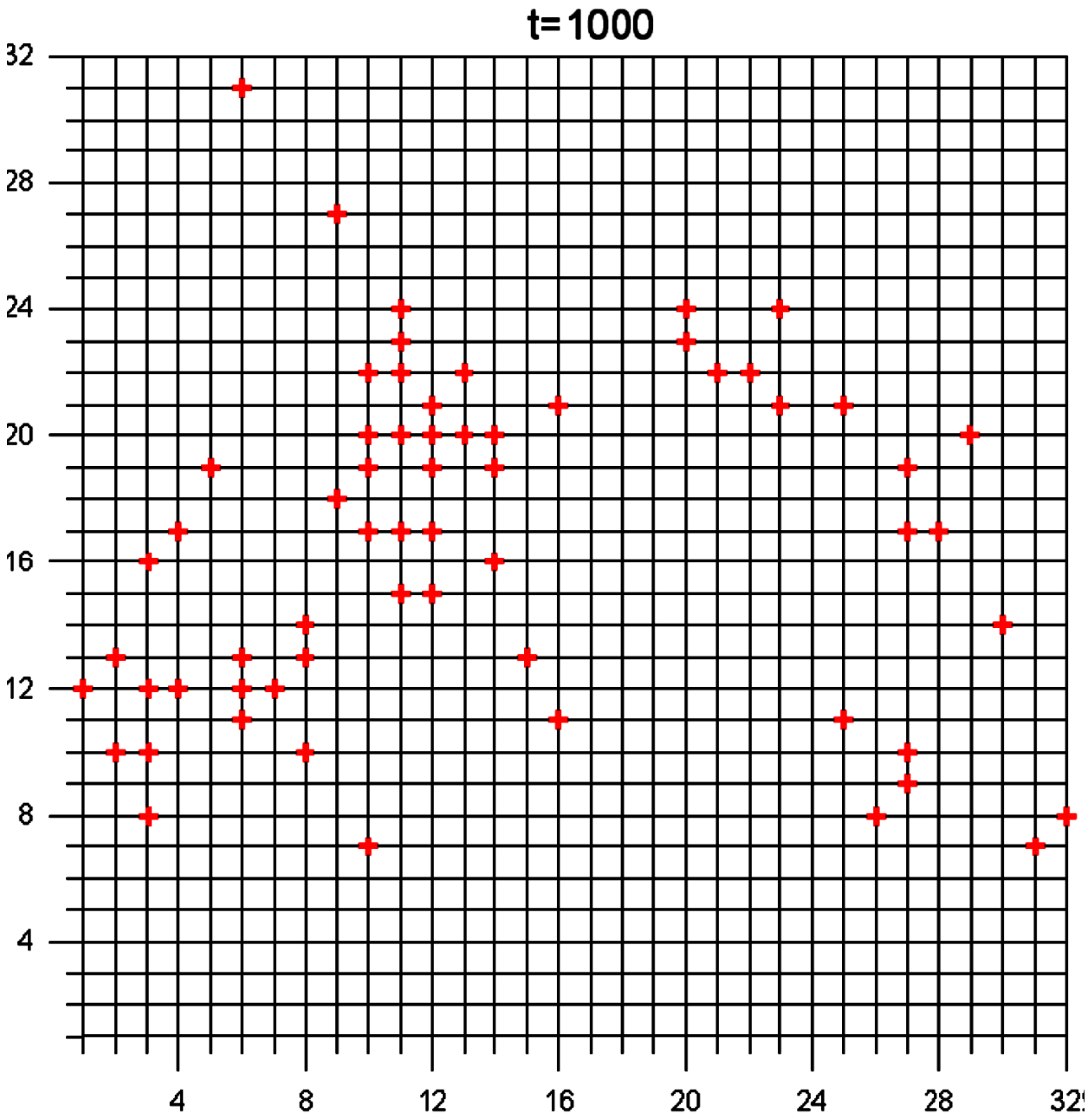
At t=10, 10 pairs of spins have flipped. (20 flipped spins) Note that a few of these are ‘outliers’, far from the others.



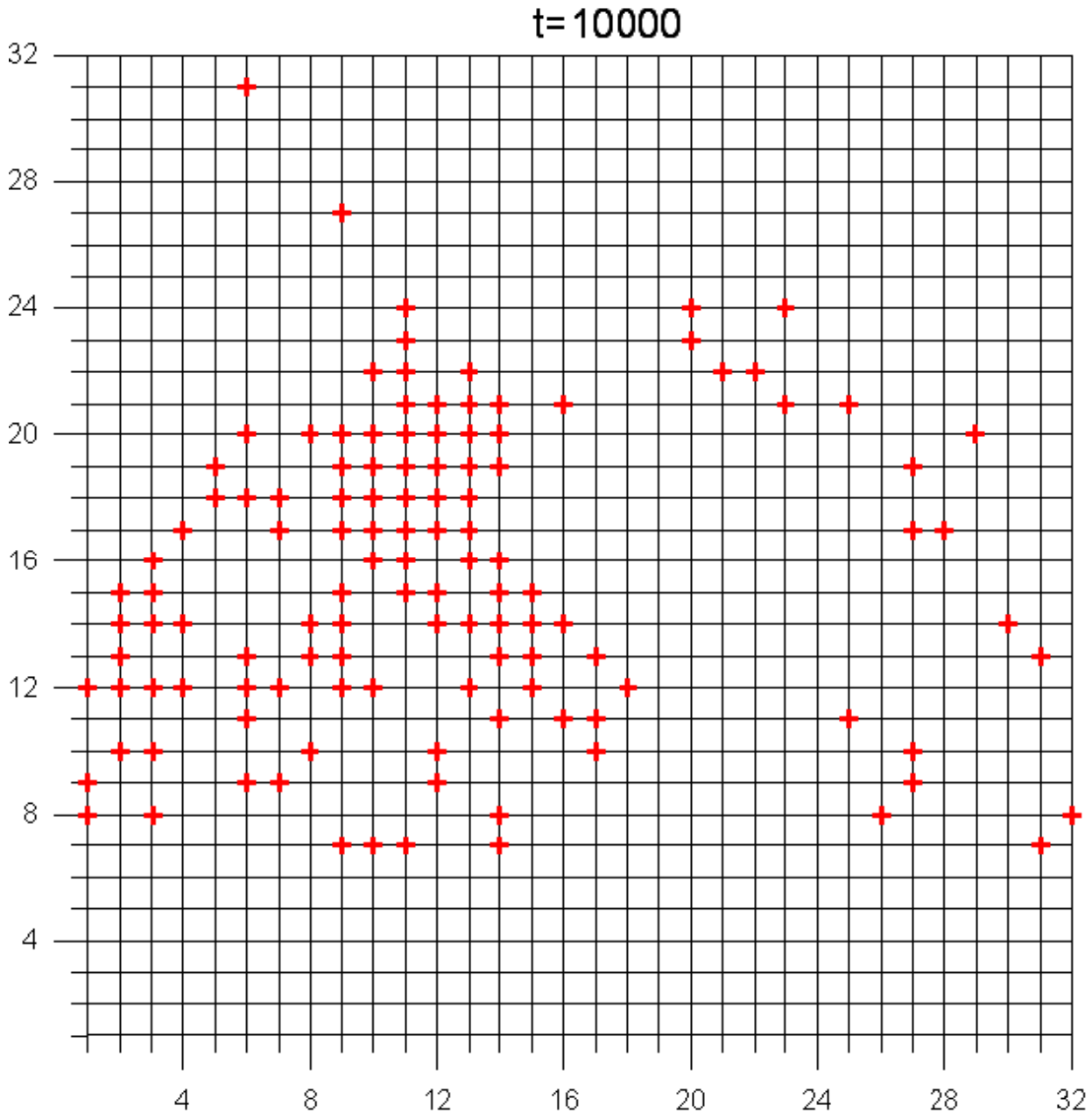
At t=100, 42 spins have flipped. Although it is hard to see, a complex pattern is building up, both in real space and in energy space.



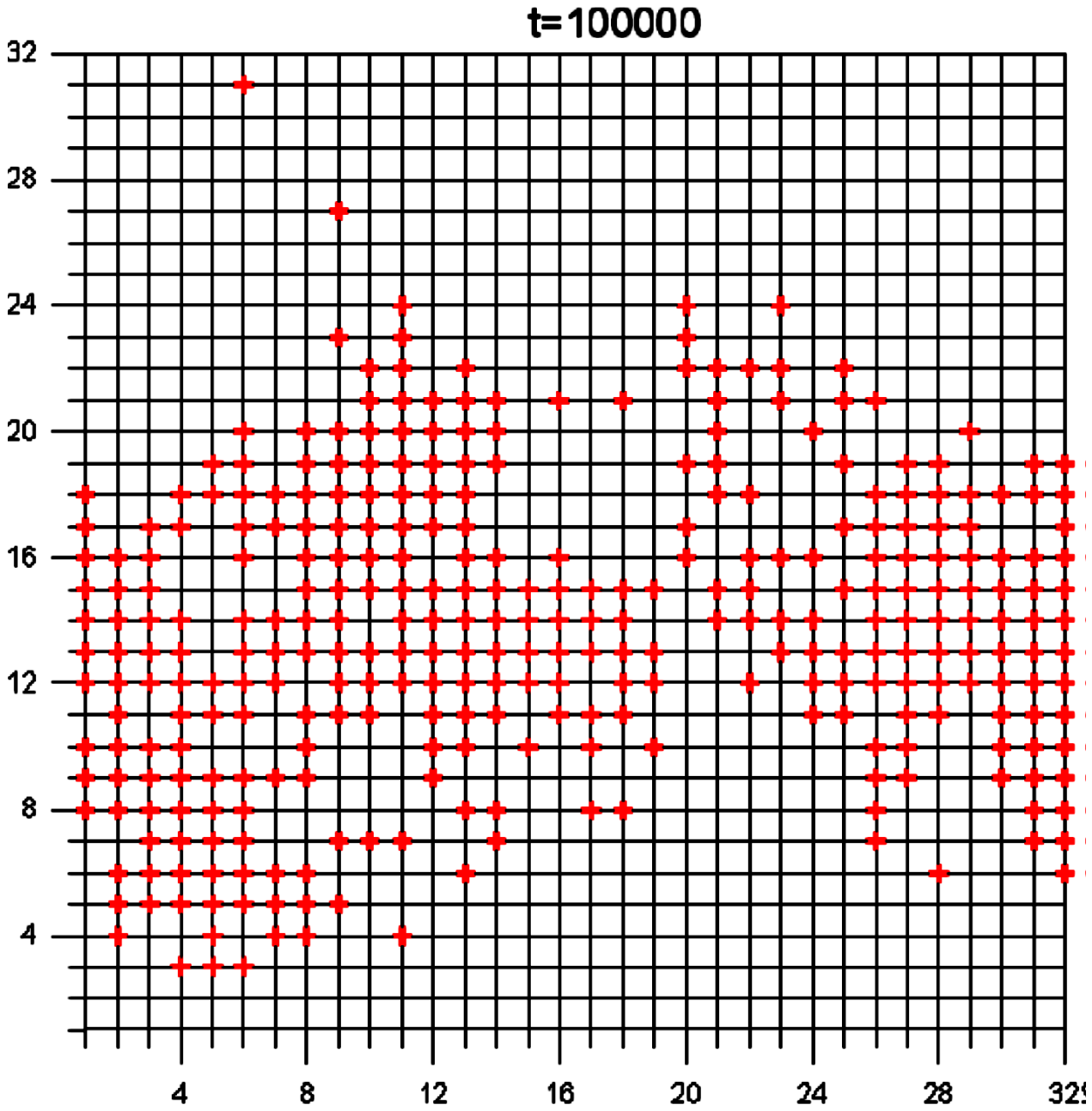
At t=1000, we now have 62 flipped spins.



At t=10,000, there are now 132 flipped spins



At t=100,000, we have 320 flipped spins. A spatial pattern is somewhat discernable.



RESULTS

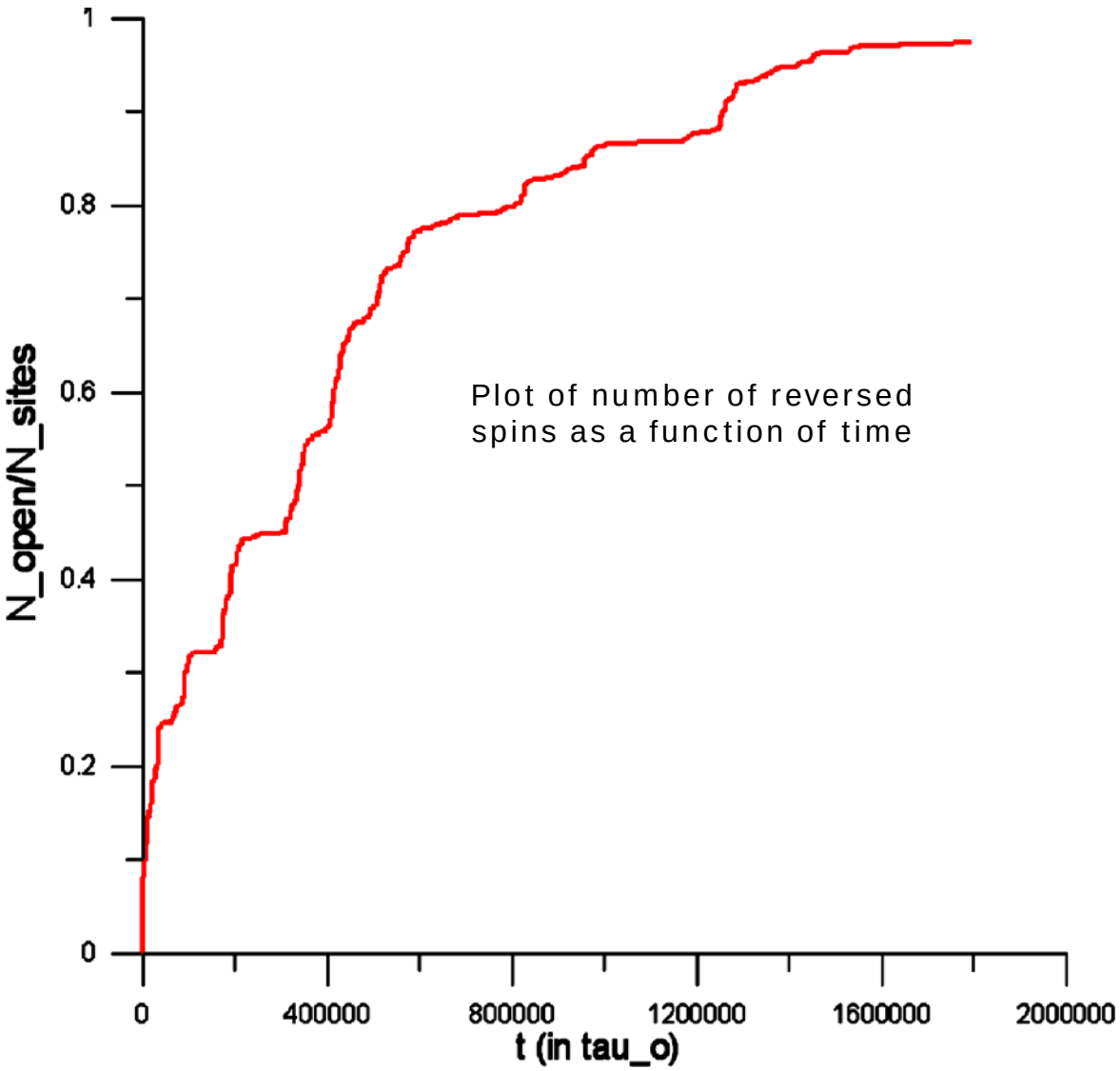
Regions of flipped spins grow in fits and starts – Physicists call this 'anomalous diffusion', characterized by Levy flights. Biologists call this 'punctuated equilibrium'.

CONCLUSIONS:

(1) No localization – the flipped regions will grow indefinitely (problem for error correction)

(1) Pattern formation in energy space (and it turns out, in real space), even for long-range interactions

This model also describes voting patterns (eg., in modern USA !)



Plot of number of reversed spins as a function of time

THEORY EXAMPLE # 2
DIFFUSIVE QUANTUM WALK

We consider a d-dimensional hyperlattice, with a non-diagonal coupling to a spin bath; Here we look at a cubic hyperlattice:

The Hamiltonian is $$\mathcal{H} = \Delta_o \sum_{<ij>} \left\{ c_i^\dagger c_j \cos\left(\sum_k \alpha_k \sigma_k^x \right) + H.c. \right\} + H_{int}^{env}$$

which actually describes pure phase (precessional) decoherence.

QUESTION 1: WHAT BEHAVIOUR DO WE EXPECT?

(A) Free (ballistic) Quantum Propagation: One possibility, when the system is decoupled from the bath, is free (band) propagation:

(i) Localized initial state: $\psi \mathbf{n}(t=0) = \delta_{\mathbf{n}0}$
with probability distribution $P_{\mathbf{n}}^0(t) = |\psi_{\mathbf{n}}(t)|^2$

One gets $$P_{\mathbf{n}}^0(t) = \prod_{\mu=1}^{d} J_{n_\mu}^2(z) \; ; \quad z = 2\Delta_o t$$

(ii) Initial wave-packet: $$\psi_{\mathbf{n}}(t=0) \approx \left(\frac{1}{\sqrt{\pi} R} \right)^{d/2} e^{-n^2/2R^2}$$

gives $$P_{\mathbf{n}}^0(t) \approx \left(\frac{R^2}{\pi (R^4 + z^2)} \right)^{d/2} e^{-n^2 R^2/(R^4+z^2)}$$

Thus, quite generally one has

$$P_0^0(t) \propto 1/t^d$$

$$\langle R^2 \rangle \propto t^2$$

(ballistic propagation)

(B) Quantum Diffusive Propagation: In the "pointer basis" picture of quantum measurements made by quantum environments, one has the classical limiting behaviour of diffusion:

$$P_0^{(cl)}(t) \propto 1/t^{d/2} \quad \text{so that} \quad \langle R^2 \rangle \propto t$$

So - what is the actual behaviour?

Q2: DECOHERENCE DYNAMICS – What is the answer ?

For an initially localized state one has $P_{\mathbf{n}}(t) = \int_0^{2\pi} \frac{d\varphi}{2\pi} \prod_{\mu=1}^{d} J_{n_\mu}^2(z\cos\varphi)$

&, for an initial wave-packet $P_{\mathbf{n}}(t) \approx \int_0^{2\pi} \frac{d\varphi}{2\pi} \frac{R^d\, e^{-n^2R^2/(R^4+z^2\cos^2\varphi)}}{\left[\pi(R^4+z^2\cos^2\varphi)\right]^{d/2}}$ (can be written in terms of special functions)

Now these solutions produce a very surprising result:

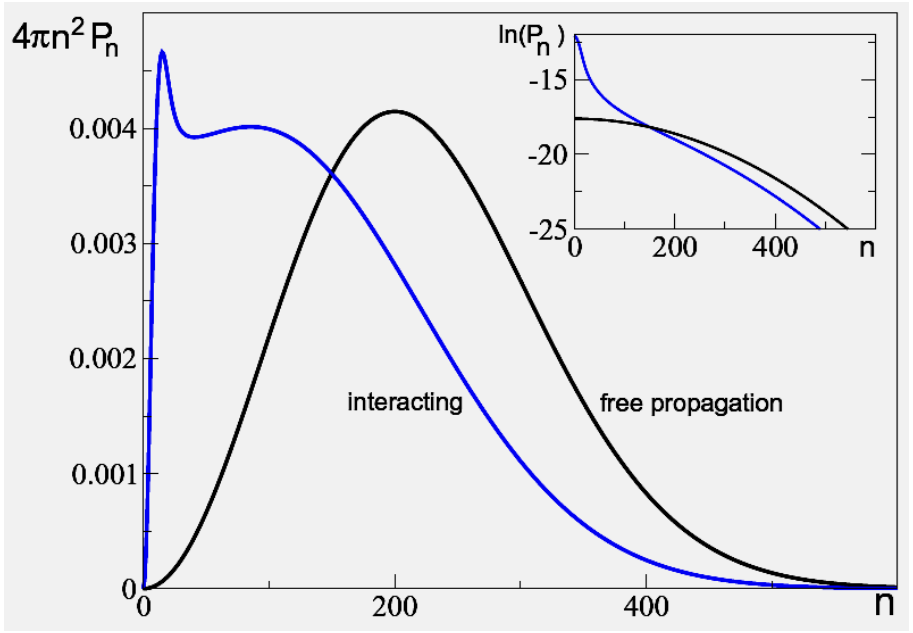
$P_0(z\to\infty) \approx \frac{A_d R^{2-d}}{\Delta_o t}$ BUT.... $< (\mathbf{n}(t)-\mathbf{n}(0))^2 >= 12\sum_n \mathbf{n}^2 P_{\mathbf{n}}(z) = \frac{d}{2}(\Delta_o t)^2$

In other words, the particle spends more time near the origin than classical diffusion would predict (weak localization in fact), BUT it also has a BALLISTIC part (even in the long-time limit !!).

Note the quite extraordinary implications of this result: ballistic diffusion combined with sub-diffusive behaviour!

Note that this schizophrenic behaviour persists even for very strong coupling to the bath (figure at right: dimensionless coupling = 100)

NB: can also happen with an oscillator bath with certain kinds of coupling



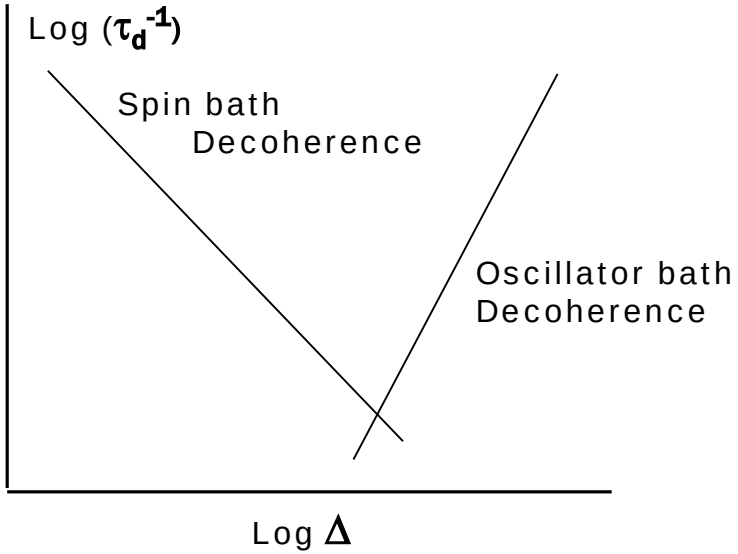
Density matrix after time t such that $z=2\Delta t >> R^2$, with z = 2000 and R=10. Long-range part is ballistic, short-range part is sub-diffusive.

NV Prokof'ev, PCE Stamp, Phys Rev A74, 020102 (2006)

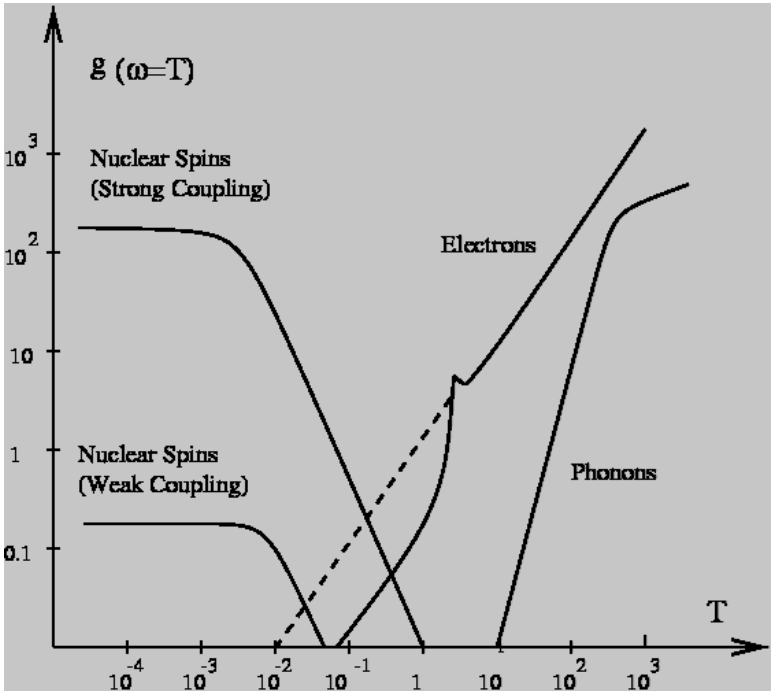
OTHER THEORETICAL REMARKS

In ANY solid-state qubit system, the spin bath dominates at low energies, the oscillator bath at high energies. A coherence window arises at intermediate energies because of the large separation of energy scales existing between spin and oscillator baths.

If we now fix the operating frequency Δ of the qubits to lie well below the high oscillator bath frequencies, but well above the characteristic spin bath frequencies (given by hyperfine couplings, couplings to defects and paramagnetic spins, etc.) then the oscillators are too fast to cause decoherence, & the bath spins are too slow. This is where the coherence window lies.



Above we see the general idea. At right we see some of the main contributions to decoherence in superconductors.



REAL WORLD PROBLEMs #3

QUANTUM DYNAMICS
of

(i) QUANTUM ISING NETS

- in Fe-8 Lattices
- in $LiHo_xY_{1-x}F_4$ Lattices

(ii) 1-d POLARONS

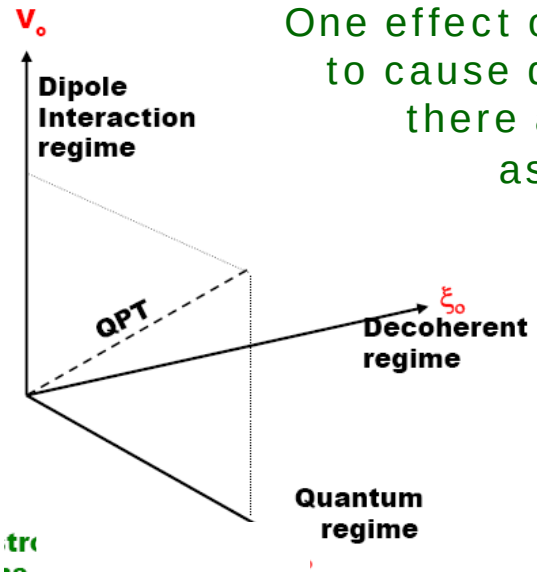
QUANTUM ISING SYSTEMS – some general features

Nature provides a wide variety of Quantum Ising systems, as do physics labs. In most of these we must consider coupling to both oscillator and spin baths

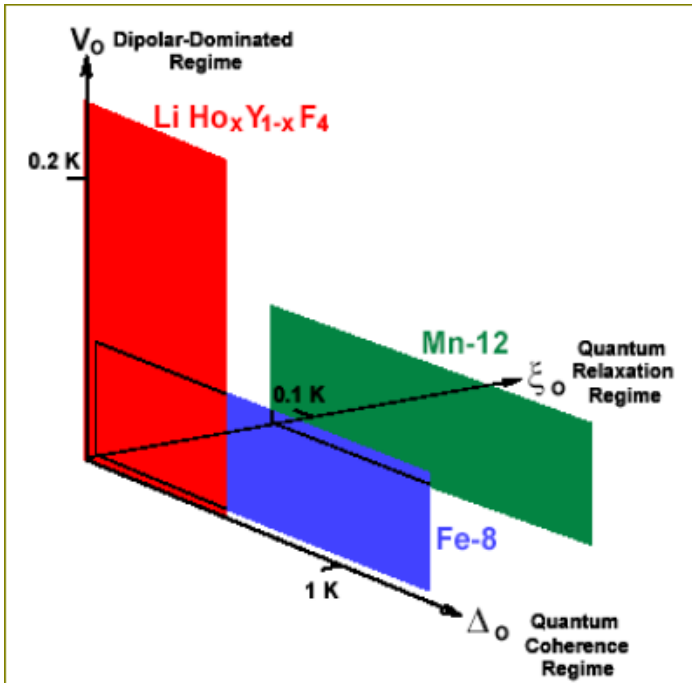
We then have the effective Hamiltonian:

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

Without anticipating too much the results to come, we can say that the presence of the bath introduces a new parameter characterizing the effects of the bath (the temperature is of course another).

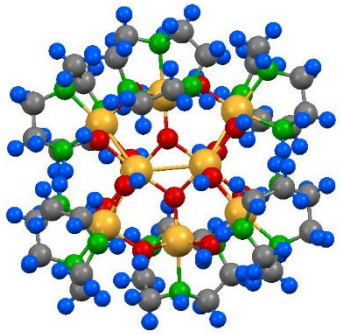


One effect of this parameter is to cause decoherence – but there are many other effects as well.



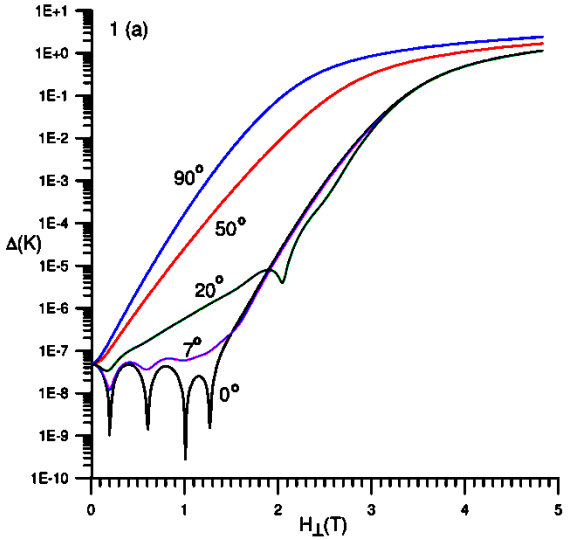
Some experimental examples

QUANTUM ISING, 1ST Example: Fe8 LATTICE



In lecture #2 we already looked at the behaviour of a single Fe-8 molecule coupled to its environment (phonons, photons, nuclear spins).

The key question: – what happens in a lattice (with long-range dipolar interactions between the Quantum Ising spins)?

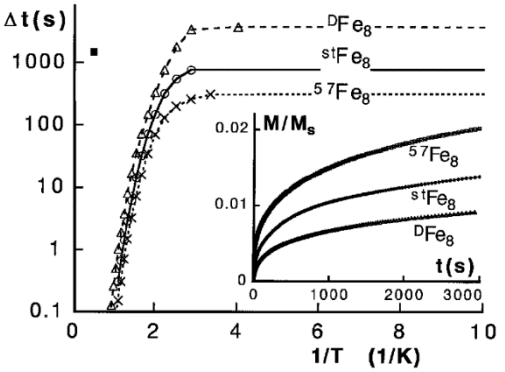


(A) QUANTUM RELAXATION DYNAMICS

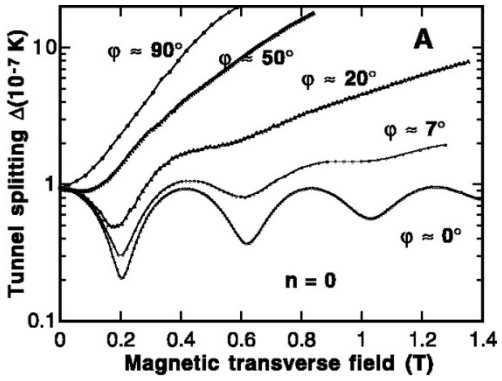
When the transverse field tunneling amplitude is small, one has inelastic tunneling-driven relaxation of the Q Ising system, described by a BBGKY eqtn with QUANTUM relaxation rates (which are controlled by the nuclear spins):

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

$$\times [P^{(2)}_{\alpha\alpha'}(\xi,\xi';\vec{r},\vec{r}') - P^{(2)}_{\alpha\alpha'}(\xi - \alpha\alpha' V_D(\vec{r}-\vec{r}'),\xi';\vec{r},\vec{r}')]$$



Experiments by many groups confirmed this theoretical picture – the predicted "sq. root time" scaling law, variation of relaxation rates with nuclear isotopes, shape dependence of relaxation rates, etc... (see figs at right)



THEORY: NV Prokof'ev, PCE Stamp, J Low Temp Phys 104, 143 (1996)
" " , Phys Rev Lett 80, 5794 (1998)

EXPT: W Wernsdorfer + al, Phys Rev Lett 82, 2903 (1999)
L Thomas + al, Phys Rev Lett 83, 2398 (1999)
R Sessoli, W Wernsdorfer, Science 284, 133 (2000)

(B) COHERENT DYNAMICS & DECOHERENCE MECHANISMS

The phonon & nuclear decoherence mechanisms show their usual face – but far more important is an entirely new mechanism, viz.:

Dipolar Decoherence and Correlated Errors

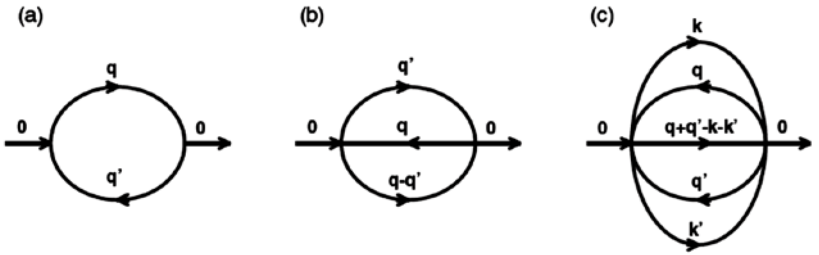
- The high-T (van Vleck) limiting form is $(\gamma_\phi^{\rm vV})^2 \approx \left[1 - \tanh^2\left(\frac{\Delta_0}{k_B T}\right)\right] \sum_{i \neq j} \left(\frac{\mathcal{A}_{yy}^{ij}}{\Delta_0}\right)^2,$

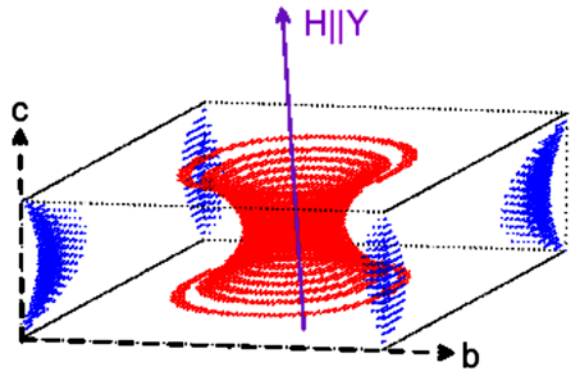
$$\mathcal{A}_{yy}^{ij} = \frac{U_d}{(2g_e S)^2}[(2\tilde{g}_y^2 + \tilde{g}_z^2)\mathcal{R}_{yy}^{ij} - (\tilde{g}_x^2 - \tilde{g}_z^2)\mathcal{R}_{xx}^{ij}],$$

$$\mathcal{R}_{\mu\nu}^{ij} = \mathcal{V}_c(|\mathbf{r}^{ij}|^2 \delta_{\mu\nu} - 3 r_\mu^{ij} r_\nu^{ij})/|\mathbf{r}^{ij}|^5$$

- At low T one gets a quite different form:

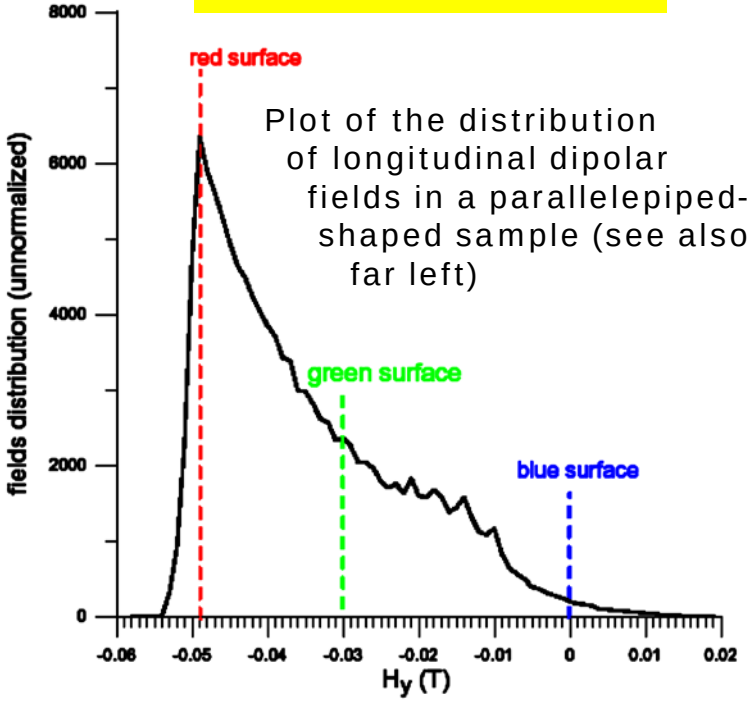
$$\gamma_\phi^m = \frac{2\pi}{\hbar \Delta_0} \sum_{\mathbf{q}\mathbf{q}'} |\Gamma_{\mathbf{q}\mathbf{q}'}^{(4)}|^2 \mathcal{F}[\bar{n}_\mathbf{q}] \delta(\omega_0 + \omega_\mathbf{q} - \omega_{\mathbf{q}'} - \omega_{\mathbf{q}-\mathbf{q}'}).$$





RESONANT SURFACES

Two qubits can only interact resonantly !!

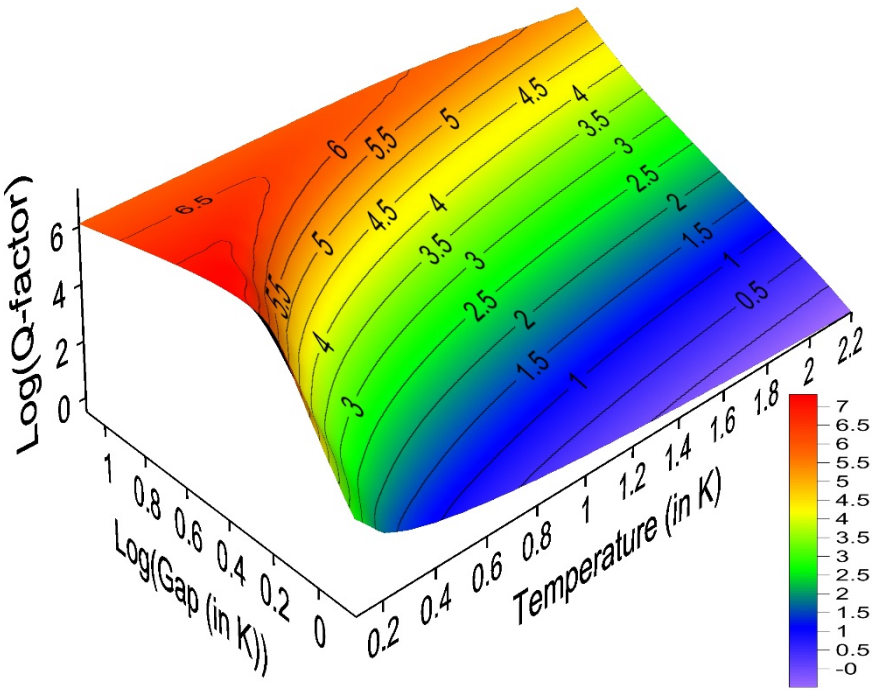


Plot of the distribution of longitudinal dipolar fields in a parallelepiped-shaped sample (see also far left)

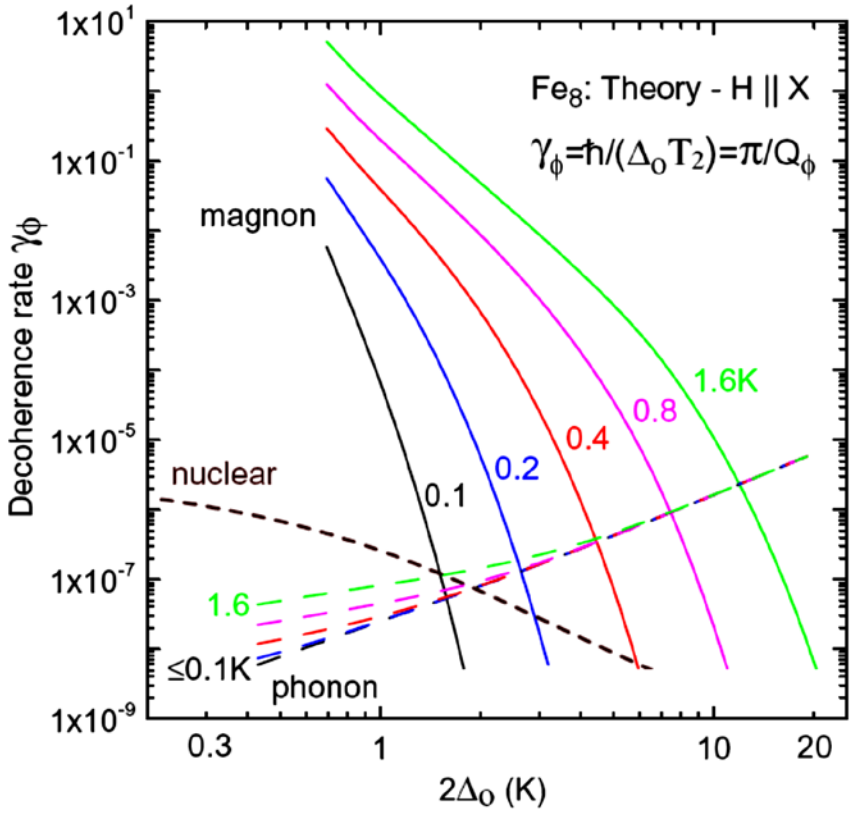
Suppose we now add all three forms of decoherence together; then we get the PREDICTION shown in Fig. at right:

Advantage of using Fe-8: it can be made very pure, with few defects in a crystal.

To raise the 'Q-factor' of this system it is very useful to go to high fields.



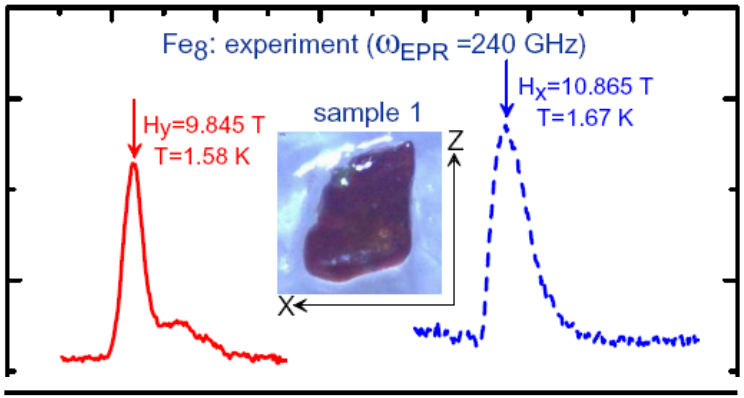
Decoherence Q-factor in Fe_8 crystal



Note the way in which these results allow us to optimize the design

NB: Can vary 3 decoherence mechanisms independently → experimental test

A. Morello, P.C.E. Stamp, I.S. Tupitsyn, Phys Rev Lett 97, 207206 (2006)



Using 'Hahn echo' ESR experiments, get good agreement with theory; no evidence for extrinsic decoherence sources.

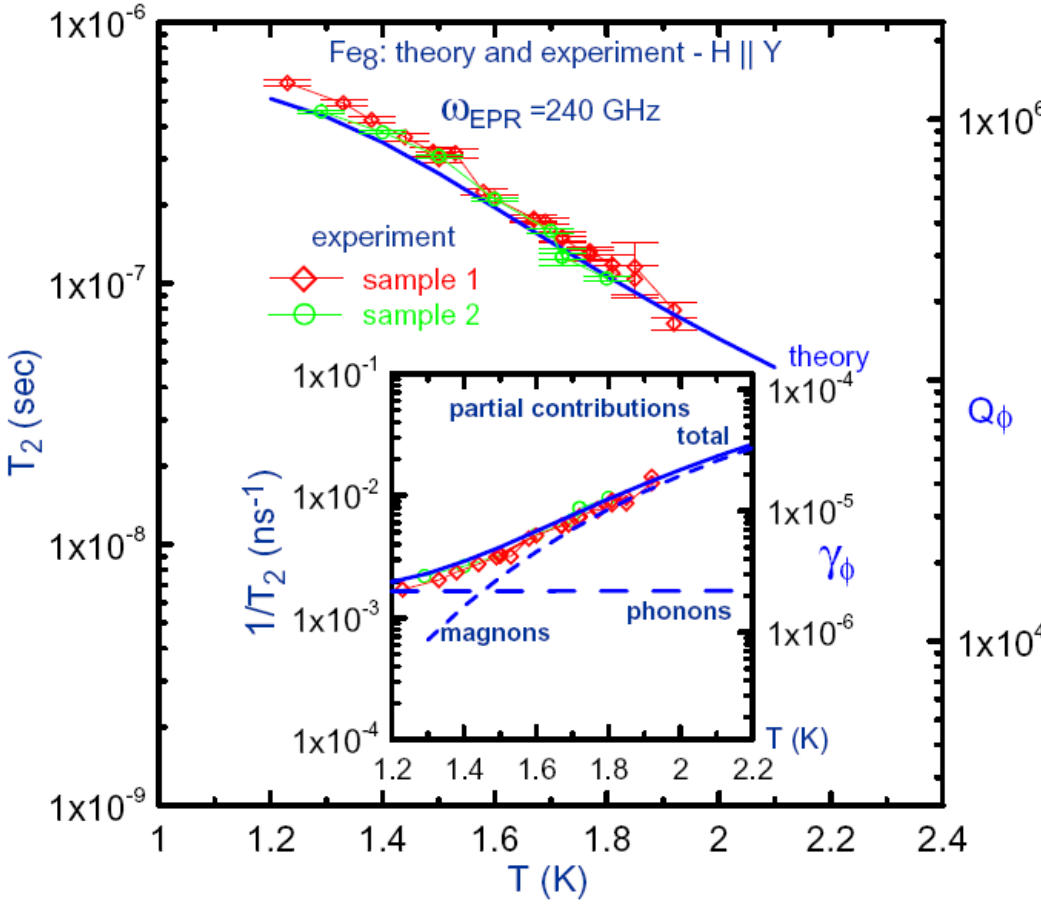
S. Takahashi + al., Nature 476, 76 (2011)

Used 2 different crystals, and 2 field orientations

SOME FIRSTS
in this EXPERIMENT

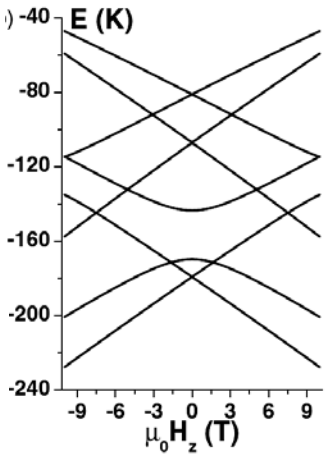
1. First detection of macroscopic spin precession of qubits
2. Lowest decoherence rate ever seen (at that time) in spin qubits.
3. First measurement of dipole decoherence in qubit array
4. First controlled measurement of decoherence rates from spin bath, oscillator bath, & dipolar interactions (with agreement with theory)

THEORIST'S REMARK: It was the first observation of the huge importance of correlated errors



QUANTUM ISING, 2nd Example: $LiHo_xY_{1-x}F_4$

The single spin has $J = 8$ and a 1-spin crystal-field Hamiltonian



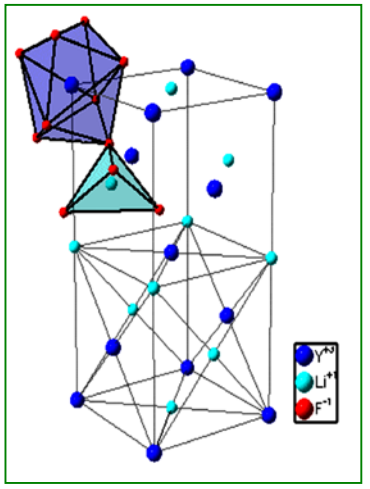
$$H_{\rm cf} = \alpha_J B_2^0 O_2^0 + \beta_J (B_4^0 O_4^0 + B_4^4 O_4^4) + \gamma_J (B_6^0 O_6^0 + B_6^4 O_6^4),$$

where: $B_2^0 = 273.9$ K

$B_4^0 = -97.7$ K $\quad B_4^4 = -1289.1$ K

$B_6^0 = -6.5$ K $\quad B_6^4 = -631.6$ K

which leads to the level structure shown at left.



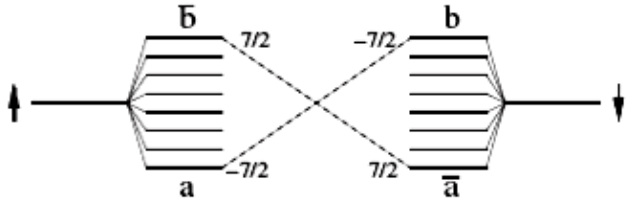
Crystal structure

Low-T EFFECTIVE HAMILTONIAN

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

Dipolar interactions: $|V_{ij}^{zz}| \sim 0.3$ K (nearest neighbours)

Without nuclear spins, we have $\Delta_0 \sim 9(\mu_B H_\perp)^2/\Omega_0$ with $\Omega_0 = 10.5$ K



$a \equiv |\uparrow, -7/2\rangle$ $\quad \bar{a} \equiv |\downarrow, 7/2\rangle$

$\bar{b} \equiv |\uparrow, 7/2\rangle$ $\quad$ etc...

The hyperfine term coupling to the Ho nuclear spins is

$$H_{\rm hf} = A_J \sum_i \vec{I}_i \cdot \vec{J}_i \quad \text{with} \quad I = 7/2$$

The hyperfine coupling is huge – the separation between hyperfine levels is ~ 0.25 K

(a) $LiHo_xY_{1-x}F_4$ is the canonical experimental system for Ising Q Phase transitions

(b) It was the original model for Q annealing/Adiabatic Q computation (now used by d-wave)

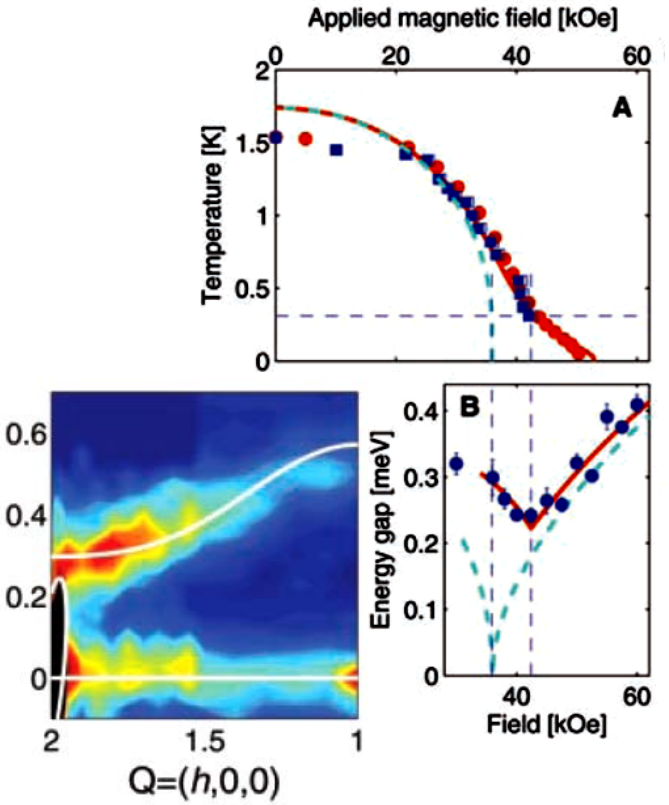
KEY EXPTS (LiHo)

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.

Neutron scattering experiments, show a 'lifting' of the zero mode around the quantum critical field H_c by the spin bath, in the case where x=1.

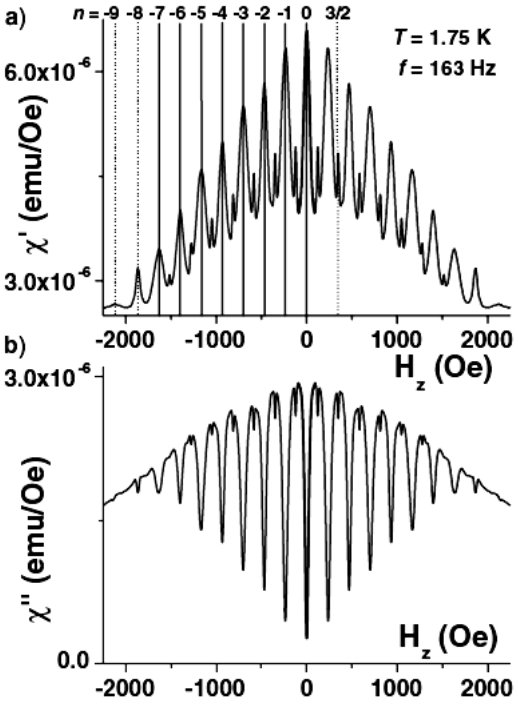
Ronnow et al., claim this indicates a new universality class for Q Phase transitions when a spin bath is present – a key unsolved problem

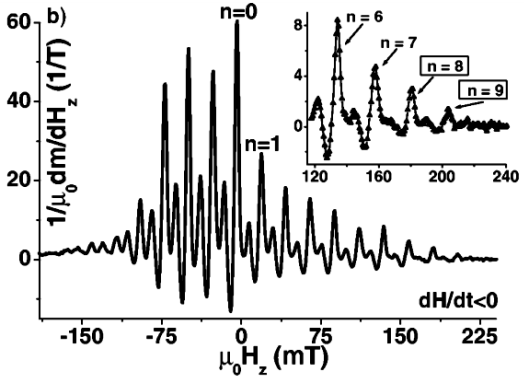
H.M. Ronnow et al., Science 308, 389 (2005)



Resonance experiments (in Q Relaxation, as seen in low-T hysteresis) directly show the role of the nuclear spins in the dynamics of the system – the hyperfine structure is scanned in the hysteresis curves !

The system also shows a quantum spin glass phase (not shown), and a Quantum Phase transition between FM and PM phases.





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

DYNAMIC QUANTUM PHASE TRANSITIONS IN Q ISING systems

Suppose we now have an effective Hamiltonian:

$$H(t) = -\sum_{j=1}^{N} [\mathbf{B}_o + \mathbf{H}(t)] \cdot \boldsymbol{\tau}_j - \sum_{i<j} V_{ij} \tau_i^z \tau_j^z + H_{\mathrm{HF}}$$ (Q Ising plus AC driving field)

We are now going to go to very high frequencies, such that: $|V_{ij}, |A_o| \ll \hbar\omega < \Lambda_o,$ where Λ is the UV cut-off for this theory.

We then go to a rotating frame, ie., make the transformation:

$$H(t) \rightarrow \tilde{H}(t) = U_1 H(t) U_1^{\dagger} - i U_1 \dot{U}_1^{\dagger}$$

with $$U_1 = e^{i \int dt \sum_j \mathbf{H}(t) \cdot \boldsymbol{\tau}_j}$$

Now at high frequencies, we can make a "Magnus expansion" in the dimensionless ratio of the characteristic energies in H divided by the frequency:

$$H(t) = \tilde{H}_0 + \frac{1}{\omega} \sum_{n=1}^{\infty} \frac{1}{n} \left[\tilde{H}_n, \tilde{H}_{-n}\right]$$

$$+ \frac{1}{\omega} \sum_{n=1}^{\infty} \frac{1}{n} \left\{ \left[\tilde{H}_0, \tilde{H}_n\right] e^{in\omega\tau_o} - \left[\tilde{H}_0, \tilde{H}_{-n}\right] e^{-in\omega\tau_o} \right\}$$

The last set of terms can be dropped if we have 'adiabatic launching' boundary conditions. We also drop higher order terms in inverse frequency.

Moreover, if we apply a LINEAR AC field, ie., $\mathbf{H}(t) = (H_x \cos(\omega t), 0, 0);$

Then we have $[\tilde{H}_n, \tilde{H}_{-n}] = 0$ leaving only the time-independent part.

FLOQUET effective Hamiltonian

We now have the 'time-independent' effective Hamiltonian

$$\tilde{\mathcal{H}}^{o}_{eff} = -\sum_{j}^{N} B_o \tau_j^x - \sum_{l\neq j}^{N} \left[\tilde{V}_{jl}^{zz} \tau_j^z \tau_l^z + \tilde{V}_{jl}^{yy} \tau_j^y \tau_l^y \right]$$

where

$$\tilde{V}_{jl}^{zz}(\alpha) = V_{jl}\left[1 + \mathcal{J}_0(2\alpha)\right]/4.$$
$$\tilde{V}_{jl}^{yy}(\alpha) = V_{jl}\left[1 - \mathcal{J}_0(2\alpha)\right]/4,$$

with $\alpha \equiv 2H_x/\omega,$

Performing the further unitary transformation $\mathcal{U}(\gamma) = \exp\left(i\gamma \sum_j \tau_j^x/2\right)$

and fixing $\gamma(\alpha) = \sqrt{-\tilde{V}_{jl}^{yy}/\tilde{V}_{jl}^{zz}},$

we finally get the new effective Ising system:

$$\mathcal{H}^{o}_{eff} = -\sum_{j}^{N} B_x \tau_j^x - \sum_{j\neq l}^{N} \mathcal{V}_{jl} \tau_j^z \tau_l^z \qquad \text{with} \qquad \mathcal{V}_{jl} = \tilde{V}_{jl}^{zz} + \tilde{V}_{jl}^{yy}$$

EFFECT of HYPERFINE INTERACTIONS

We can now go through exactly the same sort of manoeuvres with an added hyperfine coupling, to get a renormalized interaction, in the AC field, of

$$\tilde{H}_{\mathrm{HF}} = \sum_{j,\mu} \tilde{A}_\mu I_j^\mu \tilde{\tau}_j^\mu \qquad \text{where} \qquad \tilde{A}_\mu = \left(A_x, A_y \mathcal{J}_0(\alpha), A_z \mathcal{J}_0(\alpha)\right)$$

KEY RESULT: The renormalized interspin interaction has a different dependence on α from that of the hyperfine coupling

ENGINEERING the EFFECTIVE HAMILTONIAN

We use a hierarchy of Schwinger-Dyson coupled equations (in finite T Zubarev form) to analyze the dynamics. Decoupling at 2nd order we get the magnetization, in a finite transverse field, as

$$m_\mu^{(0)} = \frac{B_\mu + 2\mathcal{V}_0^{\mu\mu} m_\mu^{(0)}}{\tilde{\omega}} \tanh\left(\frac{\beta\tilde{\omega}}{2}\right) \qquad \text{with} \qquad (\mu = x, y, z)$$

$$\text{and} \quad \tilde{\omega} = \sqrt{\sum_\mu \left(\tilde{B}_\mu + 2\mathcal{V}_0^{\mu\mu} m_\mu^{(0)}\right)^2}$$

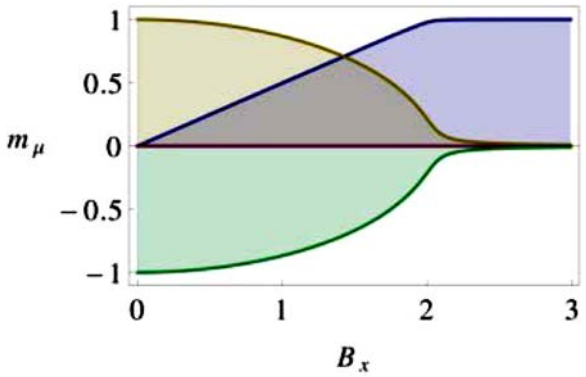
SOLUTIONS:

- For $B_x < 2\mathcal{V}_0$:

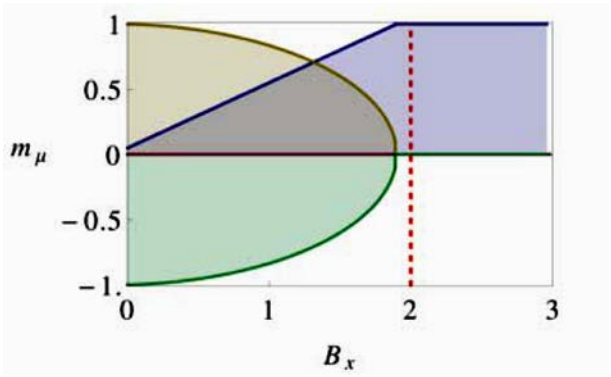
$$m_x^{(0)} = \frac{B_x}{2\mathcal{V}_0}, \quad m_y^{(0)} = 0, \quad m_z^{(0)} = \pm\frac{\sqrt{4\mathcal{V}_0^2 - B_x^2}}{2\mathcal{V}_0}$$

- For $B_x > 2\mathcal{V}_0$:

$$m_x^{(0)} = 1, \quad m_{y,z}^{(0)} = 0$$



No AC Field



AC Field with magic α

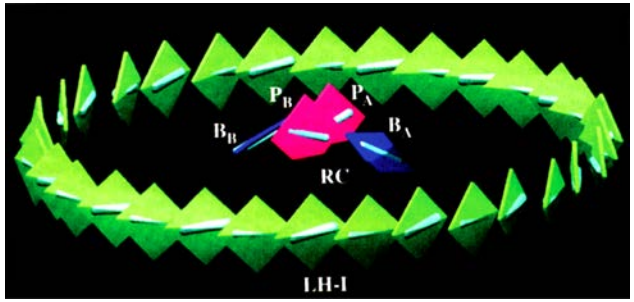
We can manipulate the amplitude and/or frequency of the field to suppress the hyperfine interaction, ie., suppress spin bath effects.

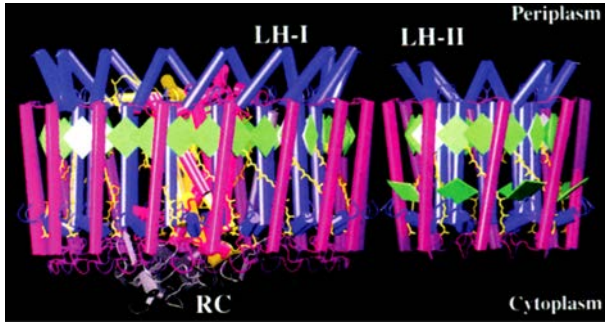
M Schechter, PCE Stamp, PRL 95, 267208 (2005)
" " , Phys Rev B78, 054438 (2008)
A Gomez, PCE Stamp, /arXiv 1512.08315 (2015)

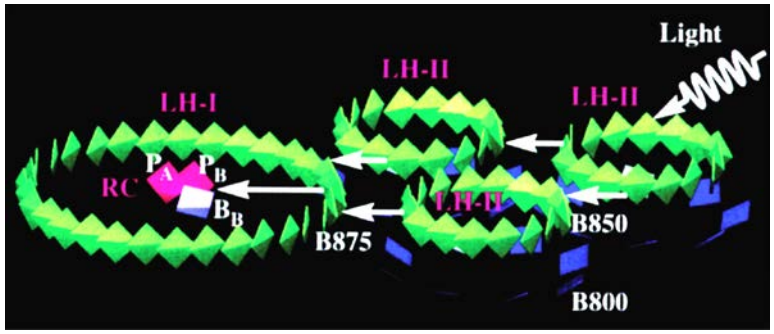
LIGHT HARVESTING MOLECULES – some general features

These are typical giant ring-shaped molecules (over 10nm across); light is absorbed in many chromophores at a time, in a coherent superposition of states – a typical LHM may contain 24 or 48 chromophores, which are also rather large, but for our purposes can be treated as 2-level systems.

Energy travels around between the chromophores as excitons (bound particle-hole pairs) and can even be transferred between different rings – but eventually is absorbed by a "reaction centre". The quantum efficiency of this process is an astonishing 99%







One can study the dynamics of coherent propagation around such rings. The main decoherence mechanism are

(i) coupling to defects & localized modes
(ii) coupling to phonons

P Trebentrost et al New J Phys 11, 033003 (2009)
M Plenio, SF Huelga New J Phys 10, 113019 (2008)

Z Zhu, A Aharony, O Entin, PCE Stamp, PR A81, 062127 (2010)

However there turns out to be a surprise in the coupling to phonons....

NON-DIAGONAL COUPLINGS TO PHONONS

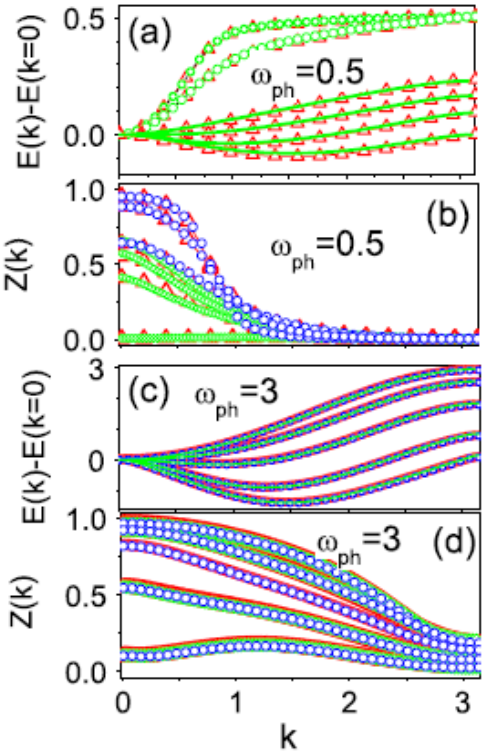
A key question in these studies, and in the physics of polaron and exciton dynamics, is the coupling to phonons. There is an important non-diagonal coupling:

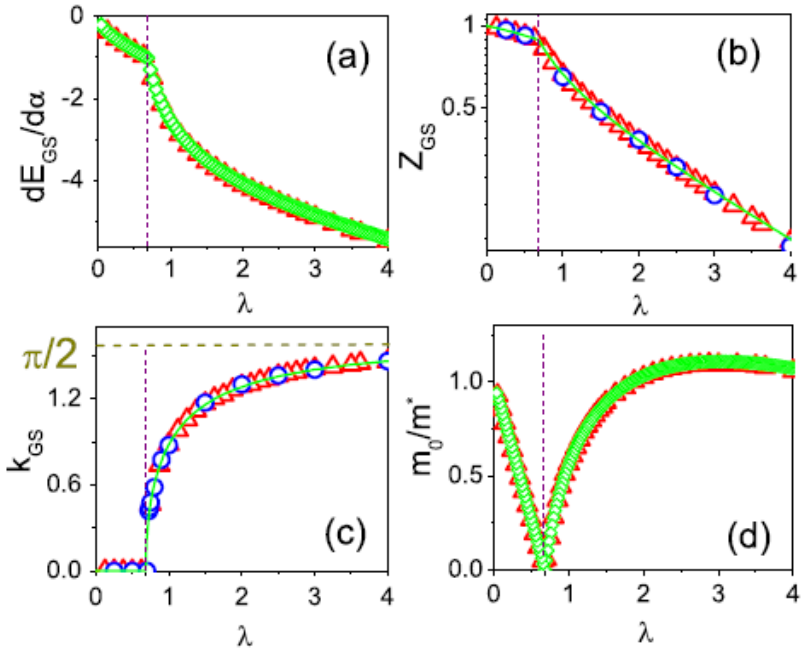
$$V = -\tilde{\alpha} t_0 \sum_i (\hat{X}_i - \hat{X}_{i+1})(c_i^\dagger c_{i+1} + \text{H.c.})$$

$$= N^{-1/2} \sum_{k,q} M(k,q) c_{k+q}^\dagger c_k (b_{-q}^\dagger + b_q),$$

where $M(k,q) = 2i\alpha[\sin(k+q) - \sin(k)]$

$$= i(2\lambda\omega_{\text{ph}} t_0)^{1/2}[\sin(k+q) - \sin(k)].$$





But non-diagonal interactions radically change the dynamics of these charge carriers. In fact they can cause what looks like a phase transition (something impossible for diagonal interactions) as a function of the dimensionless coupling

$$\lambda = 2\alpha^2/(t_0\omega_{\text{ph}})$$

Is this the key to the low decoherence rates??

DJ Marchand et al., PRL 105, 266605 (2010)