Physics 220: Advanced Statistical Mechanics

Spring 2012

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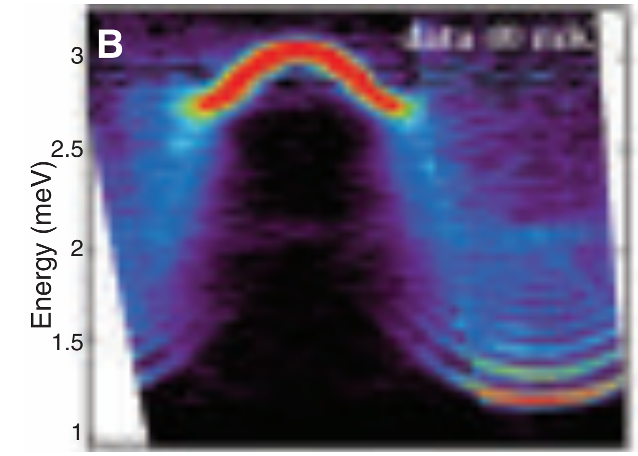
Plan

- General subject: statistical methods and phenomena in many-body systems
  - Phases and phase transitions
  - Critical phenomena - classical and quantum
  - Elementary excitations and topological defects
  - Models
  - Statistical field theory
  - Monte Carlo methods

Plan

- Cover subjects through illustrative topical examples from recent research such as
  - <u>Quantum criticality in an Ising chain</u>
  - Spin ice
  - Order by disorder

Ising Chain

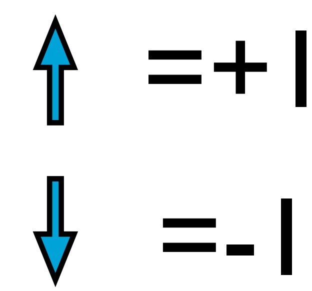


- Very beautiful paper from R. Coldea (Oxford), experimentally studying the *quantum transverse field Ising chain*, a canonical model of statistical mechanics
- We can learn about:
    - Ising models
    - Ordered and paramagnetic phases
    - Quantum and classical phase transitions
    - Elementary excitations and domain walls

Ising model

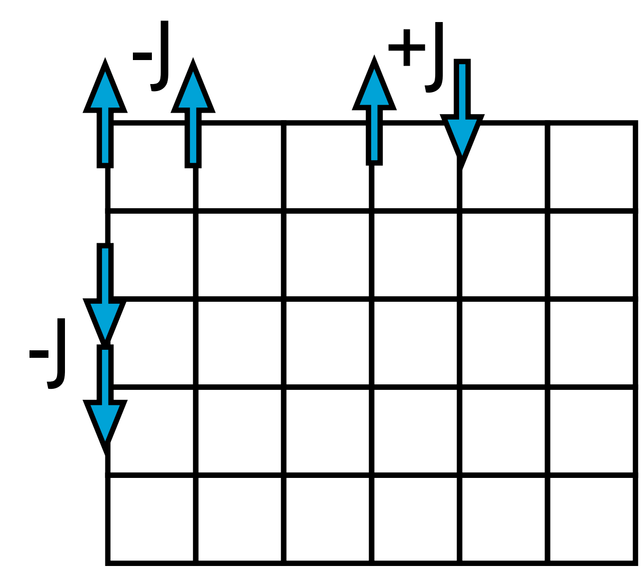
- Classical model of "spins" $\sigma_i = \pm 1$ which interact

$$H = -\frac{1}{2}\sum_{ij} J_{ij}\sigma_i\sigma_j$$



- Usually put them on a regular lattice and make them couple *locally*, e.g. by nearest-neighbors

$$H = -J\sum_{\langle ij\rangle} \sigma_i\sigma_j$$



J>0: "ferromagnetic"
J<0: "antiferromagnetic"

Thermal fluctuations

- Boltzmann

$$p[\sigma_1, \sigma_2, \cdots, \sigma_N] = \frac{1}{Z} e^{-\beta H} \qquad\qquad \beta = 1/k_\mathrm{B}T$$

- High temperature $\beta J \ll 1$
  - Spins are basically random and equally likely to take any value: *paramagnetic* phase
- Low temperature $\beta J \gg 1$
  - Spins are highly correlated and neighbors are almost always parallel: ?? *ordered, ferromagnetic* phase??

Phases

- A *phase* is a set of states of a system whose properties vary *smoothly* when varying control parameters continuously
  - Usually we say that the free energy is analytic within a phase
- Two systems are in the same phase if all their properties are *qualitatively* the same
- Distinct phases exist only in systems with (1) an infinite number of degrees of freedom and/or (2) at zero temperature
  - Why??? fluctuations etc.

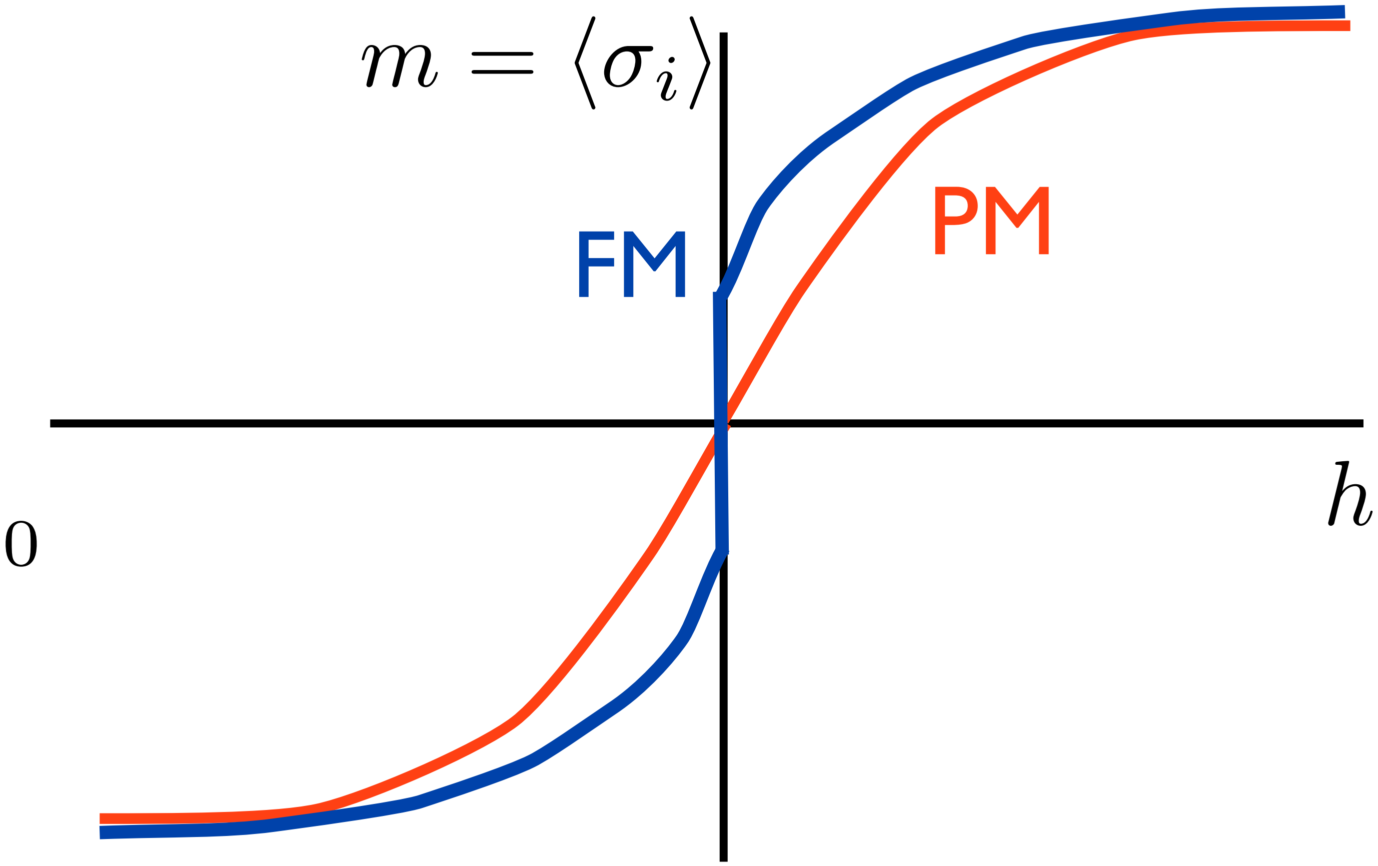
Symmetry Breaking

- The difference between the paramagnetic and ferromagnetic phases is *broken Ising symmetry*
  - High T: paramagnetic $\langle \sigma_i \rangle = 0$
    - What does this mean (guaranteed by symmetry?)
    - Consider infinitesimal applied field
  - Low T: ferromagnetic $\langle \sigma_i \rangle \neq 0$
    - Infinitesimal field
    - Long range order

Susceptibility and LRO

- Susceptibility

$$\chi = \frac{\partial \langle \sigma_i \rangle}{\partial h}\bigg|_{h=0}$$



- Linear response

$$\frac{\partial \langle \sigma_i \rangle}{\partial h} = \beta \sum_j \left(\langle \sigma_i \sigma_j \rangle - \langle \sigma_i \rangle \langle \sigma_j \rangle \right)$$

  - diverges when spins become long-range correlated

Define magnetization

- Infinitesimal field

$$m = \lim_{h \to 0^+} \langle \sigma_i \rangle_h$$

- Long-range order

$$m^2 = \lim_{|i-j| \to \infty} \langle \sigma_i \sigma_j \rangle_{h=0}$$

Correlation Length

- In the paramagnet, there is a finite length beyond which spins are uncorrelated

$$\langle \sigma_i \sigma_j \rangle \sim e^{-|i-j|/\xi} \qquad\qquad |i-j| \gg \xi$$

- The correlation length must go from finite to infinite to enter the FM: defines *critical temperature* T_c
  - Either it jumps to infinity: "first order transition"
  - Or it diverges continuously: "second order" or "continuous" transition
    - In the latter case, there can be non-analytic features on approaching T_c (why??)

Mean field theory

- The simplest approximation to describe a phase transition is MFT
  - There are many types of MFT, and if one wants to be more precise, this is "Curie-Weiss MFT"
- Idea: replace interaction between spins by an effective "exchange field"
  - Then solve the stat. mech. of this spin, and make the field self-consistent

MFT

- Decoupling

$$J_{ij}\sigma_i\sigma_j \to J_{ij}\left[\langle\sigma_i\rangle\sigma_j + \sigma_i\langle\sigma_j\rangle - \langle\sigma_i\rangle\langle\sigma_j\rangle\right]$$

- Exchange field

$$-\frac{1}{2}\sum_{ij} J_{ij}\sigma_i\sigma_j \to -\sum_i h_i^{\text{eff}}\sigma_i + \text{const.}$$

$$h_i^{\text{eff}} = \sum_j J_{ij}\langle\sigma_j\rangle$$

- Self-consistency (for a classical Ising spin)

$$\langle\sigma_j\rangle = \tanh\beta h_j^{\text{eff}}$$

MFT: solution

- For Ising Ferromagnet, on lattice with *z* nearest neighbors

$$m = \tanh z\beta J m$$

- For $k_B T > zJ$, only solution is m=0 (PM)
- For $k_B T < zJ$, get spontaneous m≠0 (FM)

$$m \sim (T_c - T)^{1/2}\Theta(T_c - T) \qquad |T - T_c|/T_c \ll 1$$

  - non-analytic behavior characteristic of *continuous* transition

Other MFT predictions

- Susceptibility

$$\chi \sim \frac{A}{T - T_c} \qquad\qquad T > T_c$$

- Specific heat

$$c_v \sim A - B\Theta(T - T_c)$$

- These kinds of predictions often work qualitatively and sometimes semi-quantitatively
  - We expect MFT works best when z is large

Ising Chain

- Coldea: $$H = \sum_i \left[-J S_i^z S_{i+1}^z - h_\perp S_i^x \right]$$

  $\boxed{\mathbf{S}_i = \boldsymbol{\sigma}_i/2 \ \text{Pauli matrices}}$

- Zero transverse field: effectively classical

$$H = -J_{\text{eff}} \sum_i \sigma_i^z \sigma_{i+1}^z$$

- What is the transition like?
  - exactly solvable by "transfer matrix"

Transfer matrix

- Partition function

$$Z = \sum_{\{\sigma_i\}} e^{\beta J_{\text{eff}} \sum_{i=1}^N \sigma_i \sigma_{i+1}} \qquad \text{(PBCs)}$$

$$= \sum_{\{\sigma_i\}} \prod_{i=1}^N e^{K \sigma_i \sigma_{i+1}}$$

$$\equiv \sum_{\{\sigma_i\}} \prod_{i=1}^N \langle \sigma_i | \hat{T} | \sigma_{i+1} \rangle = \mathrm{Tr}\left(\hat{T}^N\right)$$

- Transfer matrix

$$\hat{T} = \begin{pmatrix} e^K & e^{-K} \\ e^{-K} & e^K \end{pmatrix} \qquad K = \beta J$$

Transfer Matrix (2)

- Solution

$$Z = \lambda_1^N + \lambda_2^N$$

$$\lambda_1 = 2\cosh K \;\; > \;\; \lambda_2 = 2\sinh K$$

- Large system

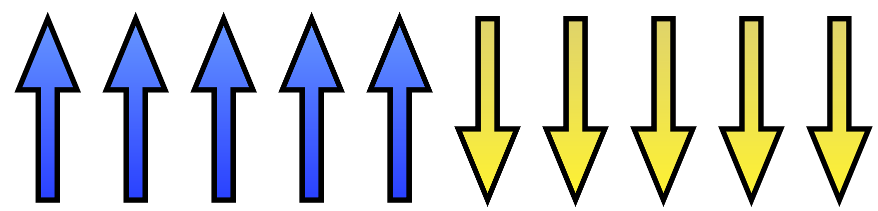
$$Z \approx (2\cosh K)^N$$

$$F = -\beta^{-1} \ln Z \approx -N\beta^{-1} \ln(2\cosh K)$$

- This is a smooth function with no singularity at finite, non-zero K = J/k_BT: no phase transition!

Why no transition?

- This is because of *domain walls*



$\Delta E=2J$

- Correlation length = distance between domain walls: finite for any $T>0$

$$\xi \sim e^{2\beta J}$$

- Can verify this from transfer matrix

Fluctuations

- So *thermal* fluctuations have a drastic effect in 1d - destroy the phase transition entirely
  - In fact this is a general phenomena: d=1 is the "lower critical dimension" for discrete symmetry breaking at T>0
  - more on this theme later
- What about quantum fluctuation effects at T=0, or thermal fluctuations for d>1?
  - Even when they do not destroy the ordered phase, they alter critical properties and lead to other effects

Quantum Ising chain

- Coldea $H = \sum_i \left[-J S_i^z S_{i+1}^z - h_\perp S_i^x\right]$
- This can be exactly solved by *Jordan-Wigner transformation*
- First we will reformulate it slightly

$$S_i^z = T_i^x \qquad\qquad S_i^x = -T_i^z$$

$$H = \sum_i \left[-J\, T_i^x T_{i+1}^x + h_\perp T_i^z\right]$$

Jordan-Wigner

- Idea: spin-1/2 are similar to fermions

$$\{T_i^-, T_i^+\} = 1 \qquad (T_i^+)^2 = (T_i^-)^2 = 0$$

- Transformation

$$T_i^z = \hat{n}_i - 1/2 = c_i^\dagger c_i - 1/2$$

$$T_i^- = U_i c_i \qquad T_i^+ = c_i^\dagger U_i^\dagger$$

$$U_i = e^{i\pi \sum_{j<i} \hat{n}_j} = U_i^\dagger = U_i^{-1}$$

- The "string operator" U_i ensures that spins on different sites *commute*

Jordan-Wigner

- Exchange term

$$
\begin{aligned}
T_i^x T_{i+1}^x &= \tfrac{1}{4}(T_i^+ + T_i^-)(T_{i+1}^+ + T_{i+1}^-) \\
&= \tfrac{1}{4}(c_i + c_i^\dagger)U_i U_{i+1}(c_{i+1} + c_{i+1}^\dagger) \\
&= \tfrac{1}{4}(c_i + c_i^\dagger)e^{i\pi\hat{n}_i}(c_{i+1} + c_{i+1}^\dagger) \\
&= \tfrac{1}{4}(c_i^\dagger - c_i)(c_{i+1}^\dagger + c_{i+1})
\end{aligned}
$$

- Hamiltonian

$$
H = \sum_i \left[-\frac{J}{4}(c_i^\dagger - c_i)(c_{i+1}^\dagger + c_{i+1}) + h_\perp(c_i^\dagger c_i - 1/2) \right]
$$

$\boxed{\text{quadratic!}}$

Solution

- Fourier $c_j = \frac{1}{\sqrt{L}} \sum_{k \in 2\pi\mathbb{Z}/L} e^{-ikx_j} c_k$
- Hamiltonian

$$H = \sum_k \left[-\tfrac{J}{4}(c_k^\dagger c_{-k}^\dagger e^{-ik} - c_{-k} c_k e^{-ik} + c_k^\dagger c_k e^{-ik} + c_k^\dagger c_k e^{ik}) + h_\perp c_k^\dagger c_k \right]$$

$$= \sum_{k>0} \left[-\tfrac{J}{4}(-2i \sin k \,(c_k^\dagger c_{-k}^\dagger - c_{-k} c_k) + 2\cos k \,(c_k^\dagger c_k + c_{-k}^\dagger c_{-k})) + h_\perp (c_k^\dagger c_k + c_{-k}^\dagger c_{-k}) \right]$$

- Particle-hole

$$c_{-k} = d_k^\dagger \qquad\qquad k > 0$$

Solution (2)

- Hamiltonian

$$H = \sum_{k>0} \Big[\frac{iJ}{2} \sin k \, (c_k^\dagger d_k - d_k^\dagger c_k) + (h_\perp - 2J \cos k\,)(c_k^\dagger c_k - d_k^\dagger d_k)\Big]$$

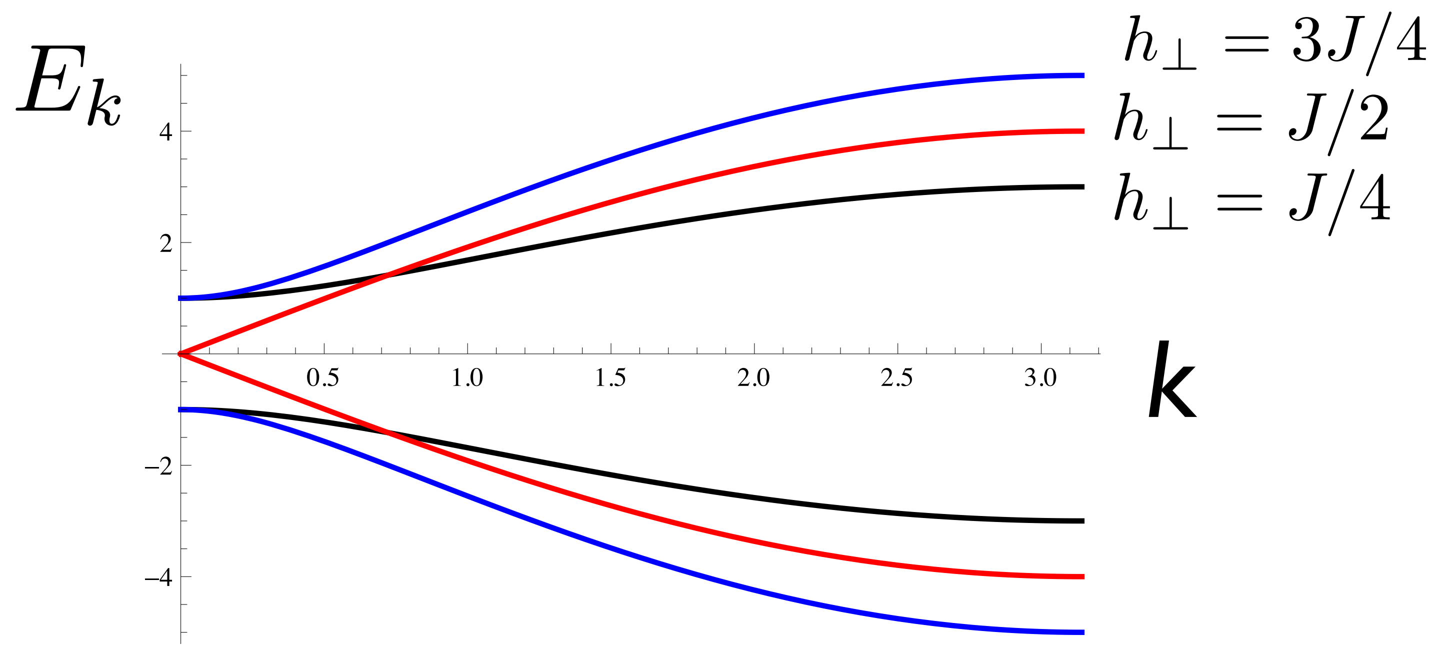
- Spinor $\quad \psi_k = \begin{pmatrix} c_k \\ d_k \end{pmatrix}$

$$H = \sum_{k>0} \psi_k^\dagger \begin{pmatrix} h_\perp - \frac{J}{2} \cos k & i\frac{J}{2} \sin k \\ -i\frac{J}{2} \sin k & -(h_\perp - \frac{J}{2} \cos k) \end{pmatrix} \psi_k$$

Solution (3)

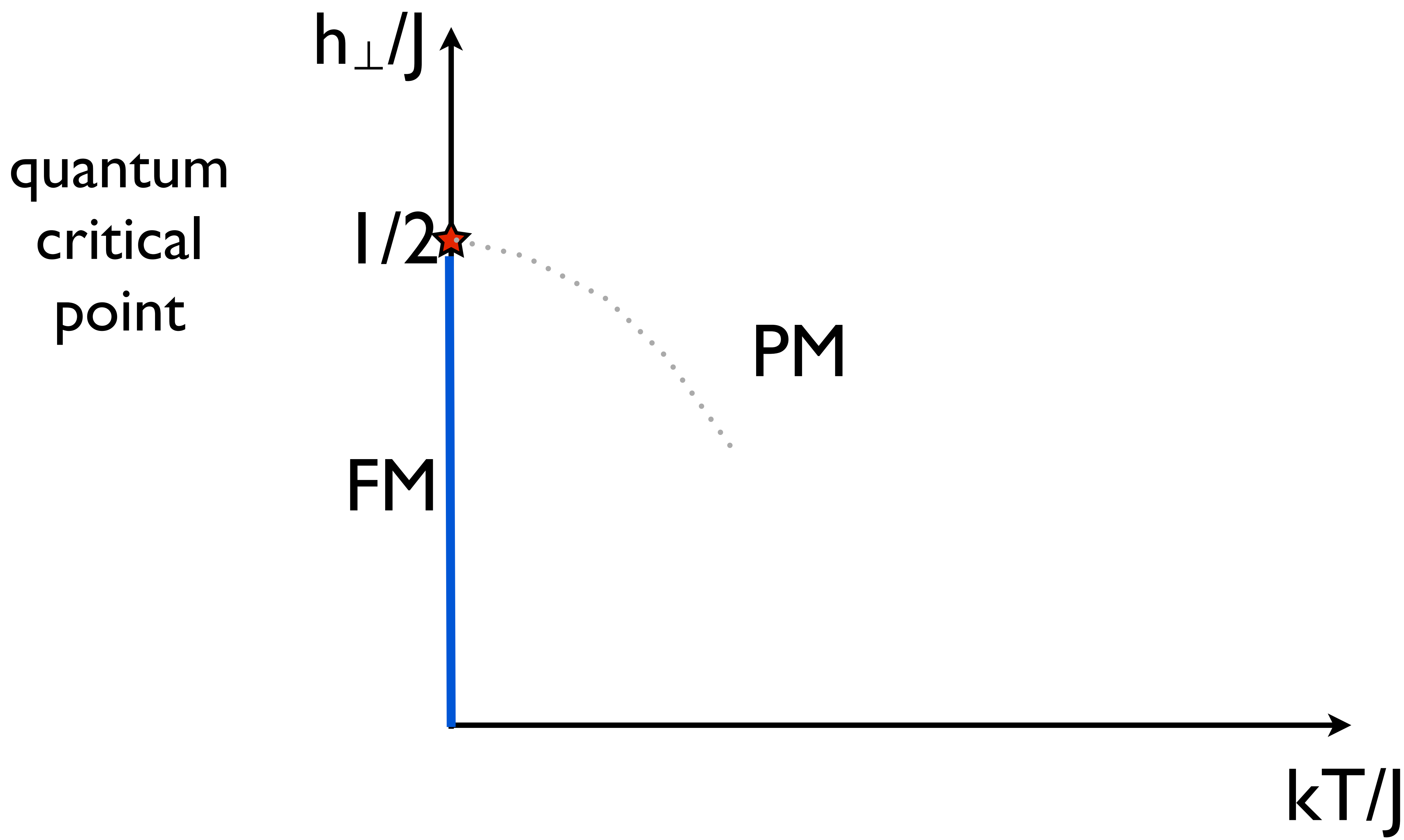
- Two "bands": 0 < k < π

$$E_k = \pm\left[(h_\perp - \tfrac{J}{2}\cos k)^2 + (\tfrac{J}{2}\sin k)^2\right]^{1/2}$$



- States evolve smoothly *except* at $h_\perp$=J/2, which is qualitatively different: this is the *quantum critical point*

Phase Diagram



Phase transition

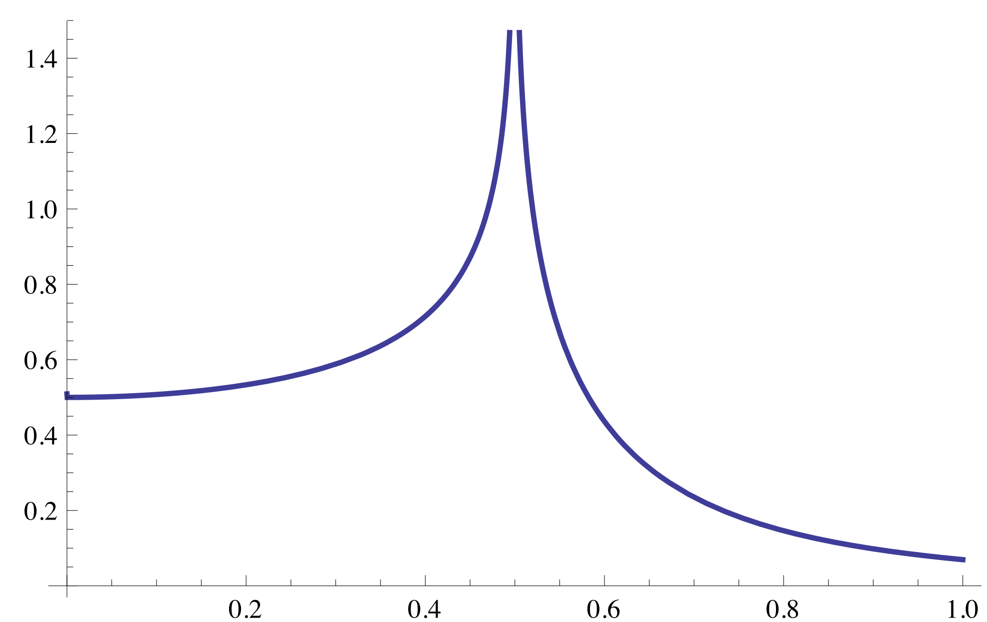
- Ground state energy

$$E = -\sum_k |E_k| = -L \int_0^\pi \frac{dk}{2\pi} |E_k|$$

- Second derivative

$$-\frac{1}{L}\frac{\partial^2 E}{\partial h_\perp^2} = \int_0^\pi \frac{dk}{2\pi} \frac{2J^2 \sin^2 k}{(J^2 + 4h_\perp^2 - 4h_\perp J \cos k)^{3/2}}$$

"transverse susceptibility" diverges!



this is analogous to specific heat divergence at a classical phase transition

Correlation Length

- Singularity implies *continuous* transition
  - Can focus on *long-distance* physics

$$
\begin{aligned}
E_k &= \pm\left[(h_\perp - \tfrac{J}{2}\cos k)^2 + (\tfrac{J}{2}\sin k)^2\right]^{1/2} \\
&\approx \pm\left[(h_\perp - \tfrac{J}{2})^2 + \tfrac{1}{2}h_\perp J k^2\right]^{1/2} \\
&= \pm\left[\Delta^2 + v^2 k^2\right]^{1/2}
\end{aligned}
$$

$$\Delta = h_\perp - J/2 \qquad\qquad v = \sqrt{h_\perp J/2} \approx J/2$$

$$\xi = v/\Delta = \frac{\sqrt{2h_\perp J}}{2h_\perp - J} \sim (h_\perp - h_\perp^c)^{-\nu} \qquad\qquad \nu = 1$$

Time scale

- Correlation time scales with ξ

$$\tau \sim \xi/v \sim (h_\perp - h_\perp^c)^{-\nu}$$

- This is consistent with energy-time scaling in quantum mechanics

$$\Delta \sim \hbar/\tau \sim v/\xi$$

- n.b. in general, at a critical point, can have a *dynamical critical exponent z*

$$\tau \sim \xi^z \qquad\qquad z \geq 1$$

Power laws

- Notice that everything appears to be described by power laws near the QCP
    - This is a general property - "scaling" - of second order phase transitions
- How to understand it?
    - Scale invariance

Majorana

$$H = \sum_i \left[-\frac{J}{4}(c_i^\dagger - c_i)(c_{i+1}^\dagger + c_{i+1}) + h_\perp (c_i^\dagger c_i - 1/2) \right]$$

- Majorana = real fermions

$$\gamma_j = c_j + c_j^\dagger \qquad \eta_j = i(c_j - c_j^\dagger)$$

- Anticommutators $\{\gamma_i, \gamma_j\} = 2\delta_{ij}$ etc.

$$H = \sum_j \left[-\tfrac{iJ}{4} \eta_j \gamma_{j+1} + \tfrac{i}{2} h_\perp \eta_j \gamma_j \right]$$

$$\approx \int dx \ \left[\tfrac{i\Delta}{2} \eta\gamma - \tfrac{iJ}{4} \eta \partial_x \gamma \right]$$

Majorana magic

- Rotation $\eta = \frac{1}{\sqrt{2}}(\eta_R + \eta_L)$ $\gamma = \frac{1}{\sqrt{2}}(\eta_R - \eta_L)$
- 1d Majorana Hamiltonian

$$\boxed{H = \int dx \; \Big[\underbrace{-\frac{iv}{4}(\eta_R \partial_x \eta_R - \eta_L \partial_x \eta_L)}_{\text{critical theory}} + \underbrace{\frac{i\Delta}{2}\eta_L \eta_R}_{\text{deviation from criticality}}\Big]}$$

- Δ=0: no intrinsic length scale

$$\eta_{R/L} \sim L^{-1/2}$$

$$H \sim v/L$$

"scaling dimension" of η: d_η = 1/2

Effective field theory

$$H = \int dx \, \left[-\frac{iv}{4}(\eta_R \partial_x \eta_R - \eta_L \partial_x \eta_L) + \frac{i\Delta}{2} \eta_L \eta_R \right]$$

- A critical point is described by a *scale invariant* effective field theory
- *Dimensionless* effective action

$$\mathcal{S} = \int dt dx \, \left\{ \frac{i}{4} \left[\eta_R(\partial_t - v\partial_x)\eta_R + \eta_L(\partial_t + v\partial_x)\eta_L \right] + \frac{i\Delta}{2} \eta_L \eta_R \right\}$$

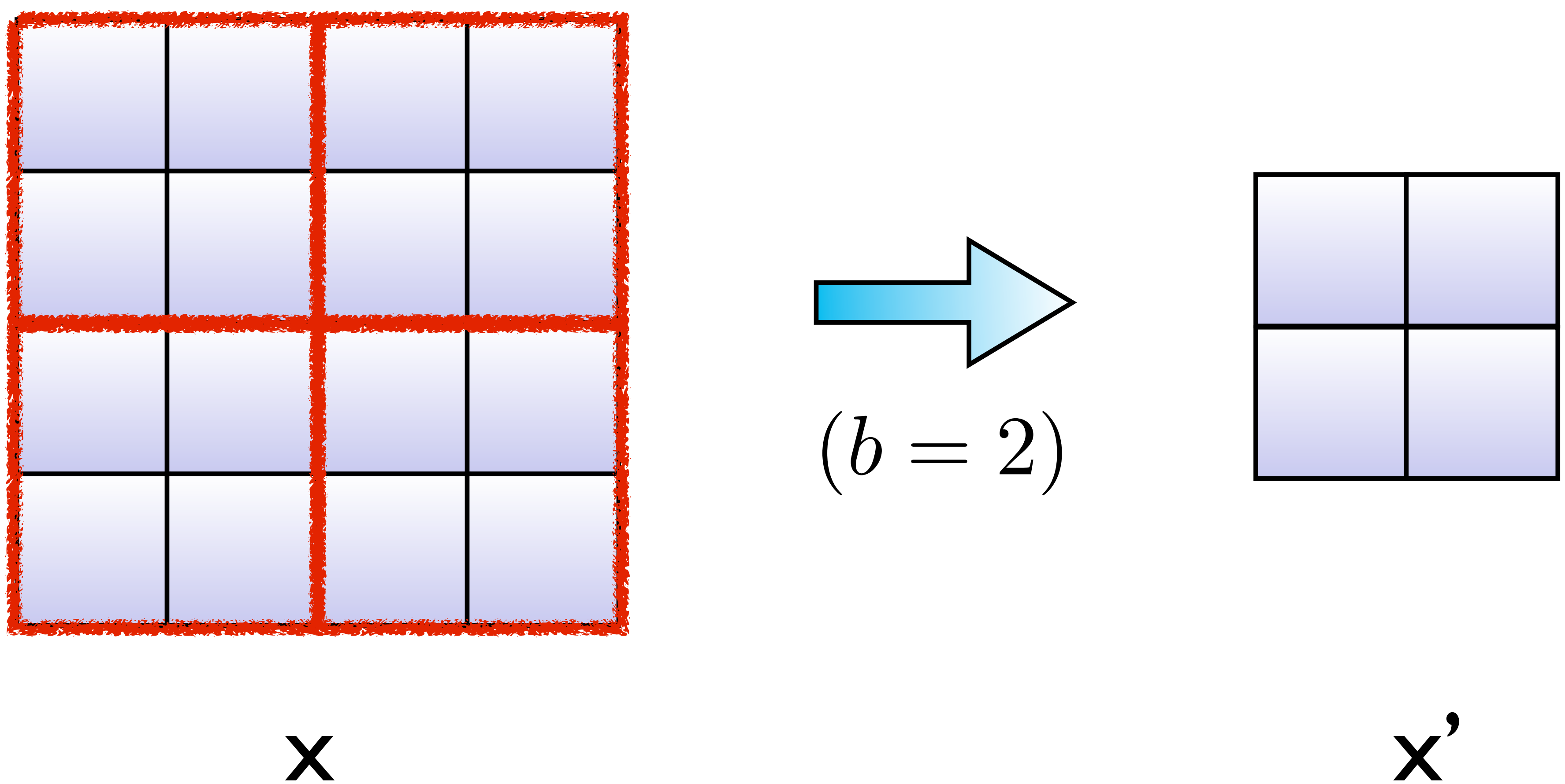
$$t \to b\,t$$
$$x \to b\,x$$
$$\eta_{R/L} \to b^{-1/2}\,\eta_{R/L}$$

critical theory (Δ=0) is invariant under this!

Scale Invariance

- What does it mean?

$x \to b\,x$ **??** $\qquad x = b\,x' \qquad b > 1$



Effective field theory

$$\mathcal{S}_c = \int dt\, dx \left\{ \frac{i}{4} \left[\eta_R(\partial_t - v\partial_x)\eta_R + \eta_L(\partial_r + v\partial_x)\eta_L \right] \right\}$$

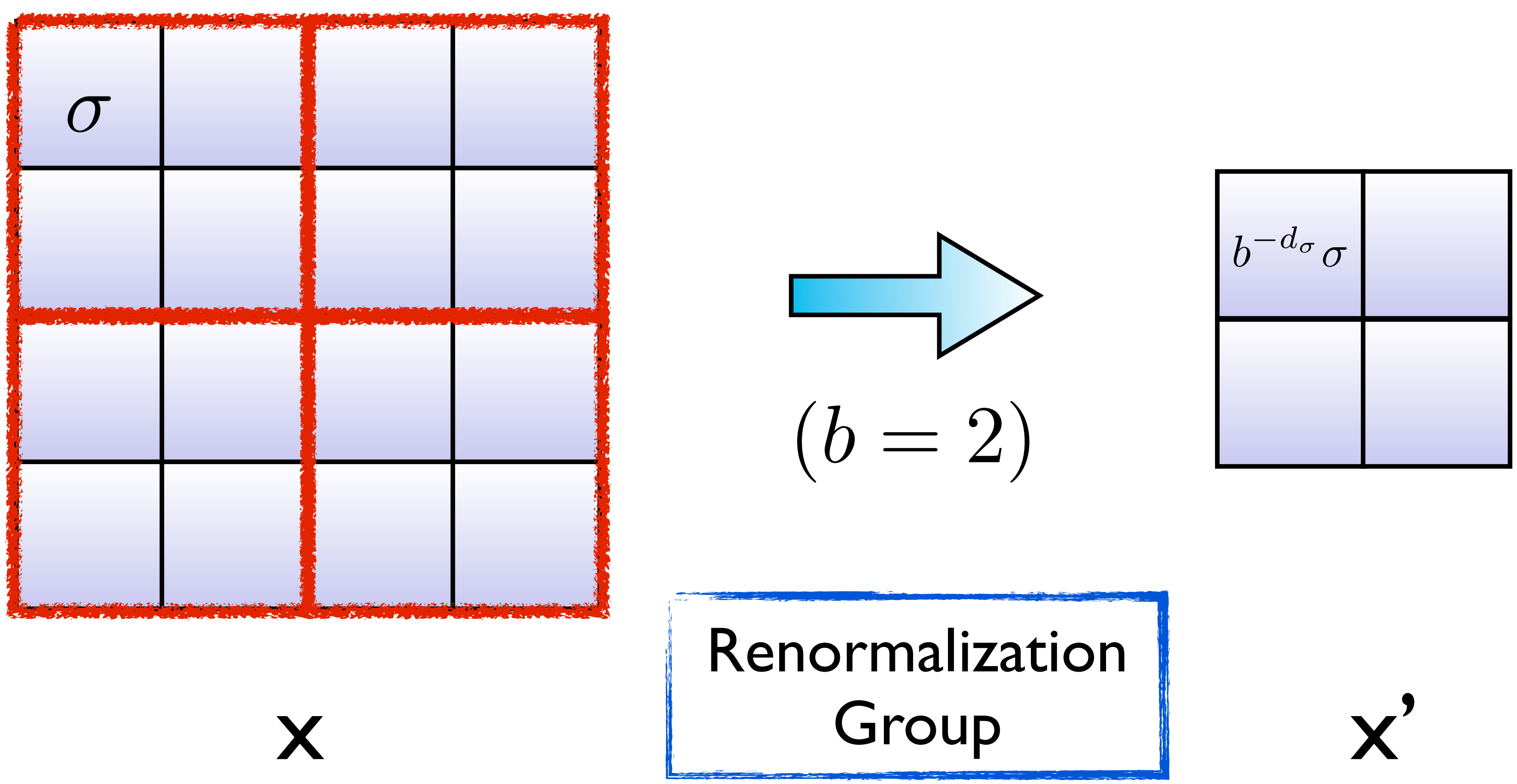
- A critical point is described by a *scale invariant* effective field theory
    - Perturbations are described by *local operators* carrying *scaling dimensions*

Fermion		d_η = 1/2
Transverse spin	$\Delta S^x \sim \varepsilon \sim \eta_L \eta_R$	d_ε = 1
Ising spin	$S^z \sim \sigma \sim ??$	d_σ = 1/8!!

Scale Invariance

- What does it mean?

$$x \to b\,x \;\; ?? \qquad\qquad x = b\,x' \qquad\qquad b > 1$$



Renormalization Group

- Perturbations

$$\Delta\mathcal{S} = \int dt\, dx\, \left\{\Delta h_\perp\, \varepsilon + h_\parallel\, \sigma\right\}$$

- Under RG

$$\Delta h_\perp \to b^{2-d_\varepsilon} h_\perp = b\, h_\perp$$

$$\Delta h_\parallel \to b^{2-d_\sigma} h_\parallel = b^{15/8}\, h_\parallel$$

relevant perturbations

- After rescaling, physical quantities with new and old perturbations should be the same

RG

- e.g. Correlation function

$$C(x_i - x_j) = \langle S_i^z S_j^z \rangle \ \sim \langle \sigma(x_i)\sigma(x_j) \rangle$$

$$C(x, h_\perp, h_\parallel) = b^{-2/8} C(x/b, b\, h_\perp, b^{15/8} h_\parallel)$$

- Can choose *b*=*x*

$$C(x, h_\perp, h_\parallel) = x^{-1/4} C(1, h_\perp\, x, h_\parallel\, x^{15/8})$$

- Or b=1/h$_\perp$= ξ

$$C(x, h_\perp, h_\parallel) = \xi^{-1/4} C(x/\xi, 1, h_\parallel\, \xi^{15/8})$$

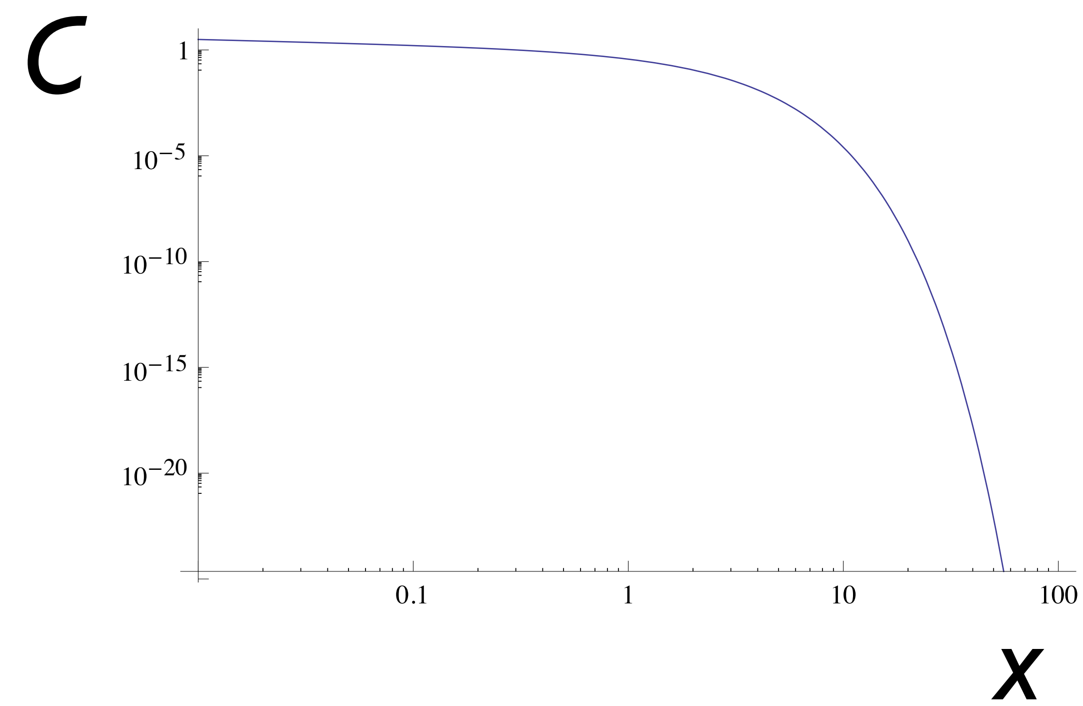
Correlation function

- In zero longitudinal field ($h_{\parallel}=0$)

$$C(x, h_\perp) = x^{-1/4}\mathsf{C}(x/\xi)$$

$$\mathsf{C}(0) = \mathsf{C}_0$$

$$h_\perp > h_\perp^c$$



$$\mathsf{C}(X) \sim X^{-\alpha}e^{-X} \qquad h_\perp > h_\perp^c \quad X \gg 1$$

$$\sim X^{1/4} \qquad h_\perp < h_\perp^c \quad X \gg 1$$

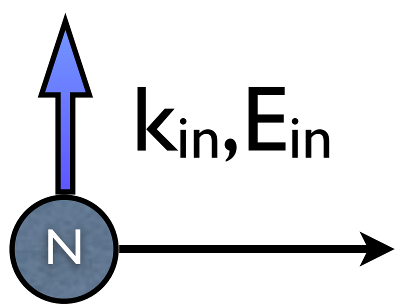
$$\beta = 1/8$$

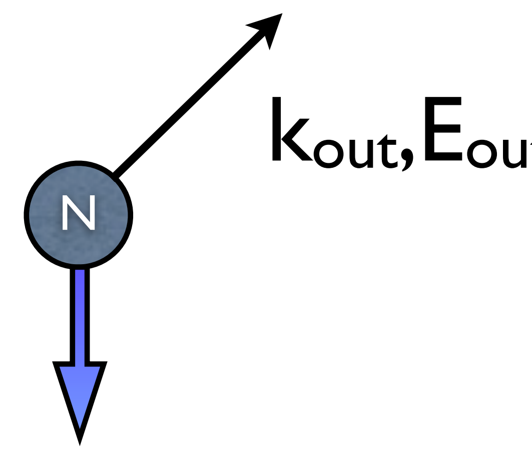
Summary

- 1d TFIM has a QCP (like *all* continuous phase transitions) described by a *scale invariant continuum field theory*
  - The critical point is characterized by scaling operators (ε,σ) with scaling dimensions d_σ etc., and by a dynamical critical exponent z
- Perturbations to the QCP can be analyzed by RG, or scaling theory
  - Usually the *relevant* ones (which grow under rescaling) are most important
  - Scaling analysis can be applied to correlation functions, free energy, excitation energies,...you name it!

Back to Coldea

- Coldea studies $CoNb_2O_6$ via *inelastic neutron scattering*





$E = E_{in} - E_{out}$

$k = k_{in} - k_{out}$

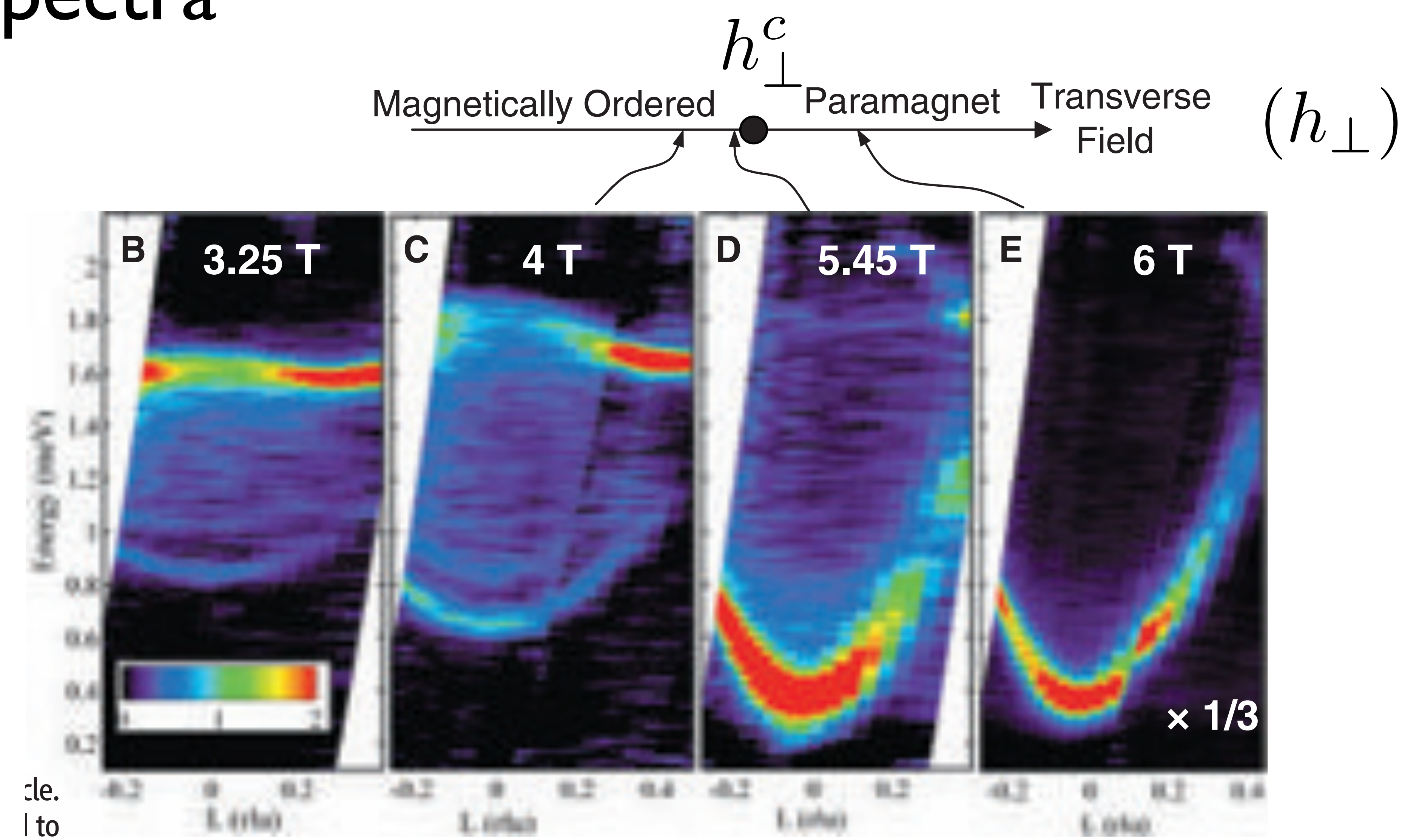
$\Delta S = 1$

measure

$$A(k,E) \sim \sum_n |\psi_n|^2 \delta(E - \epsilon_n(k))$$

Coldea

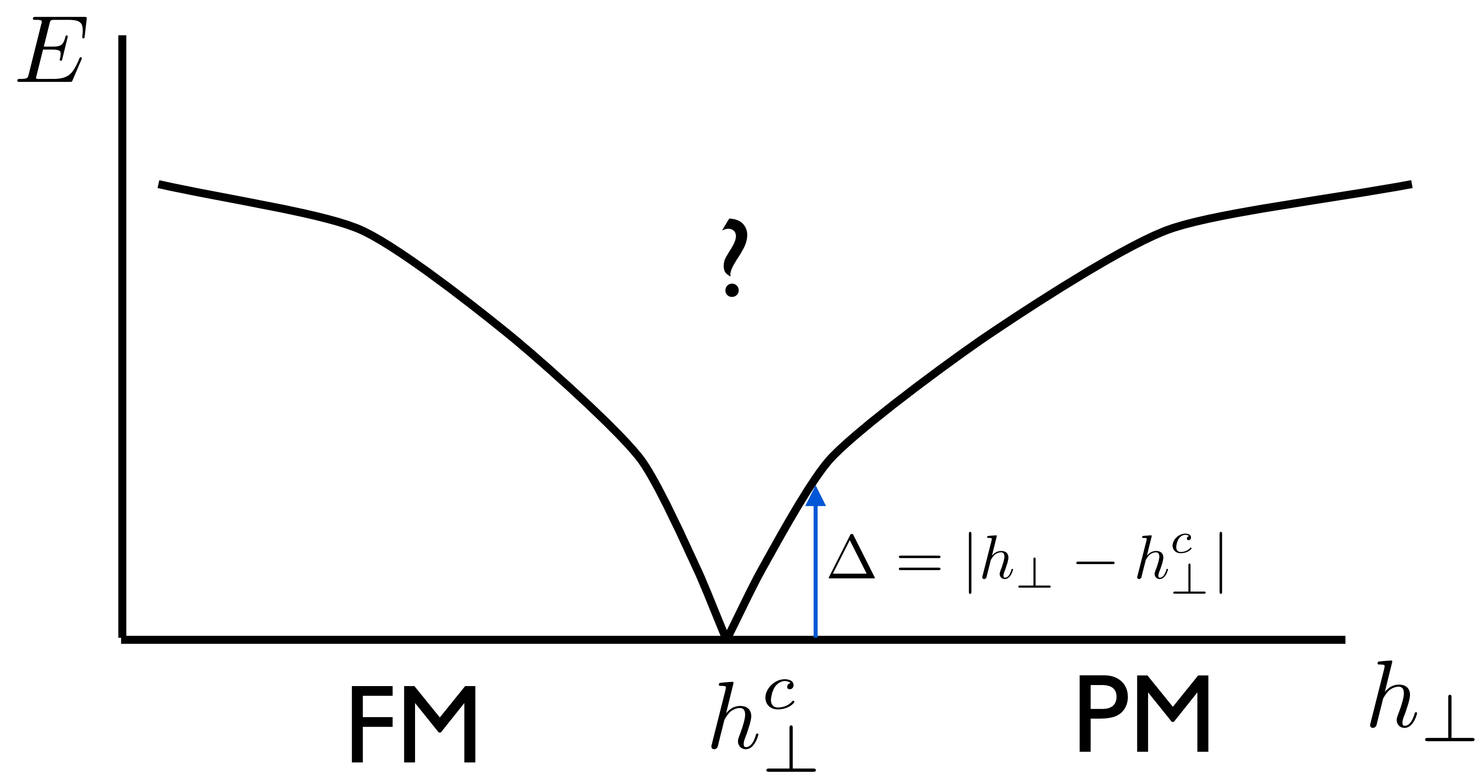
- Spectra



continuum broken into many small dispersion curves

sharply peaked dispersion

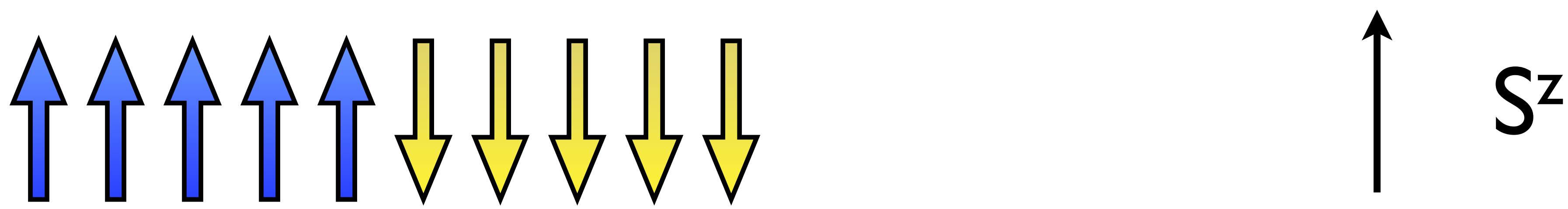
Excitations



- From scaling: expected excitation gap except at QCP
  - what is the nature of the excitations?

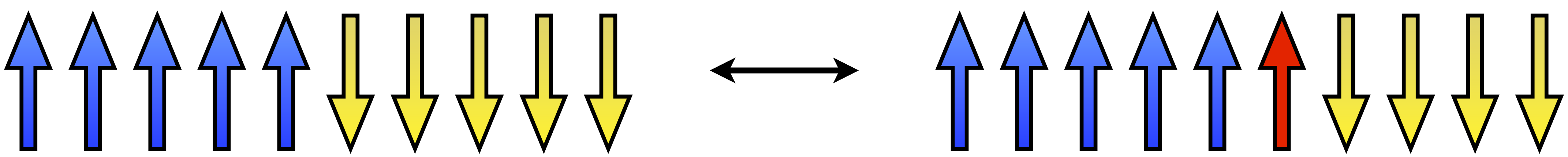
FM phase

- Domain walls



ΔE=J/2 $\quad (h_\perp = 0)$

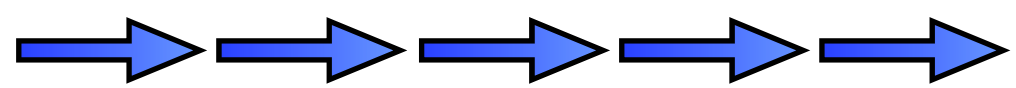
- Hopping



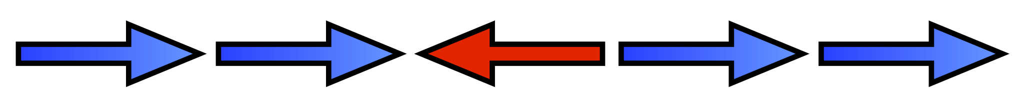
$$\epsilon_{dw}(k) \sim J/2 - h_\perp \cos k$$

PM phase

- J=0: ground state is spins polarized along x



- Excitations are single spin flips

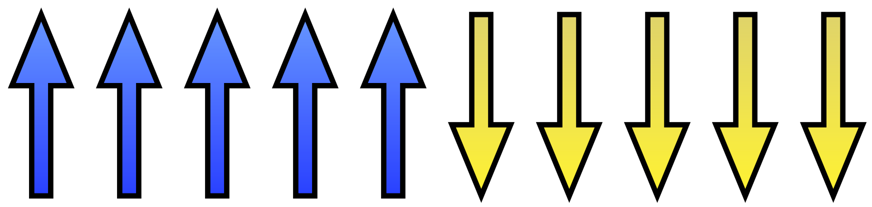


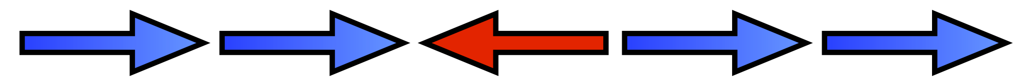
$$\epsilon = h_\perp$$

- Hopping

$$\epsilon_{sf}(k) \sim h_\perp - \frac{J}{2}\cos k$$

Local vs Non-local





- Domain wall is *non-local*: a semi-infinite number of spins must be flipped to generate it from the ground state
- The misaligned spin in the x-polarized state is *local*: only one spin needs to be flipped to generate it
  - A neutron can excite a single spin flip, but *not* a single domain wall

Scattering Intensity

- Recall

$E = E_{in} - E_{out}$

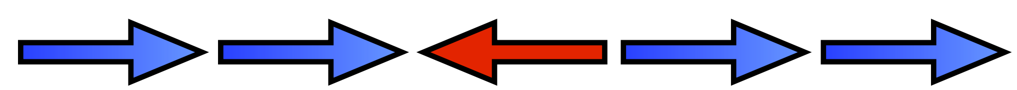
$k = k_{in} - k_{out}$

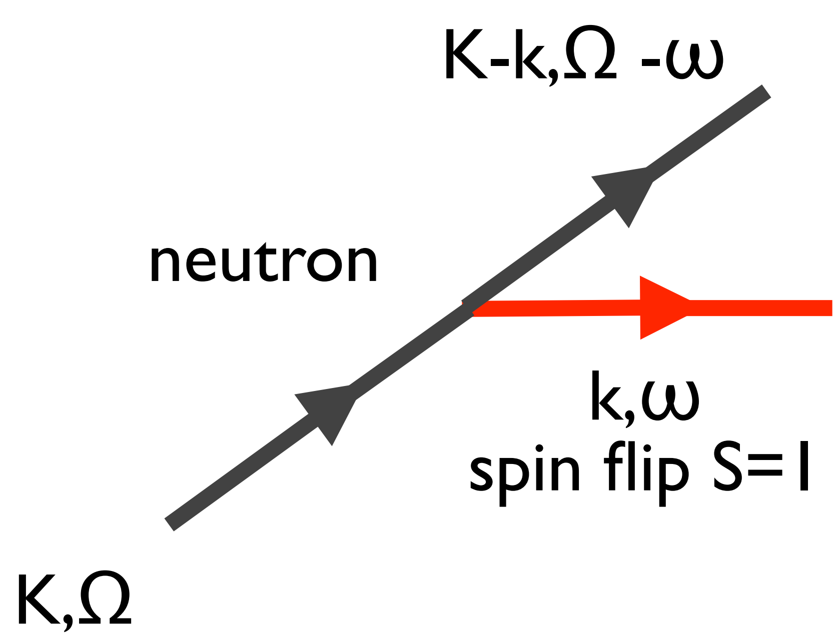
$\Delta S = 1$

measure

$$A(k, E) \sim \sum_n |\psi_n|^2 \delta(E - \epsilon_n(k))$$

- In the paramagnet: neutron creates one spin flip:





$\omega = \varepsilon(k)$

Scattering Intensity

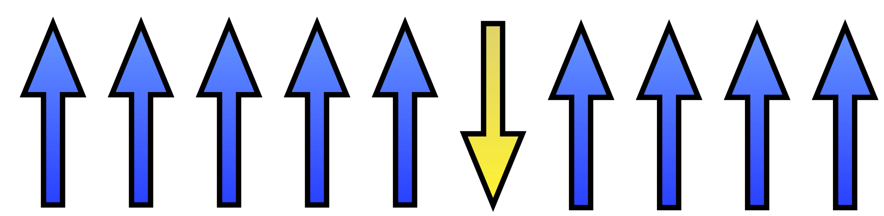
- Recall

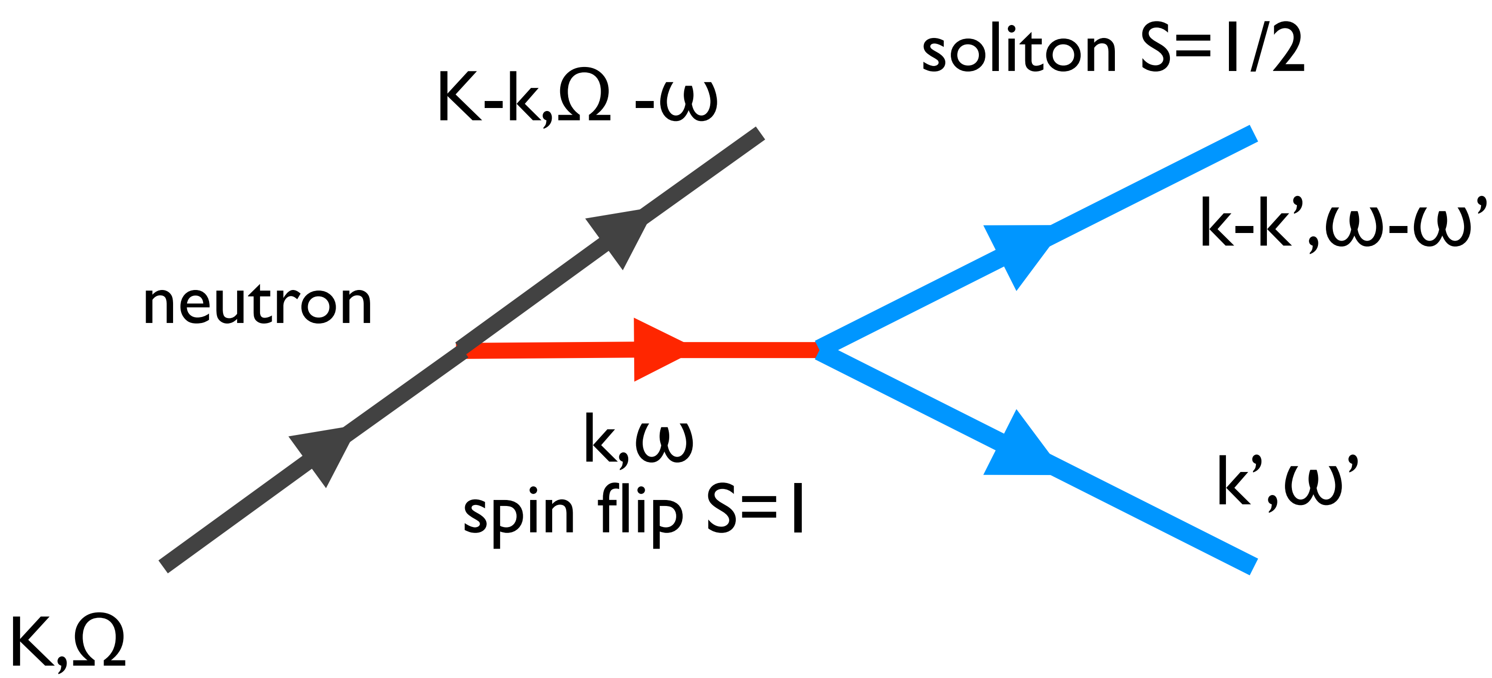
$$E = E_{in} - E_{out}$$
$$k = k_{in} - k_{out}$$
$$\Delta S = 1$$

measure

$$A(k, E) \sim \sum_n |\psi_n|^2 \delta(E - \epsilon_n(k))$$

- In the ferromagnet: neutron creates two domain walls:





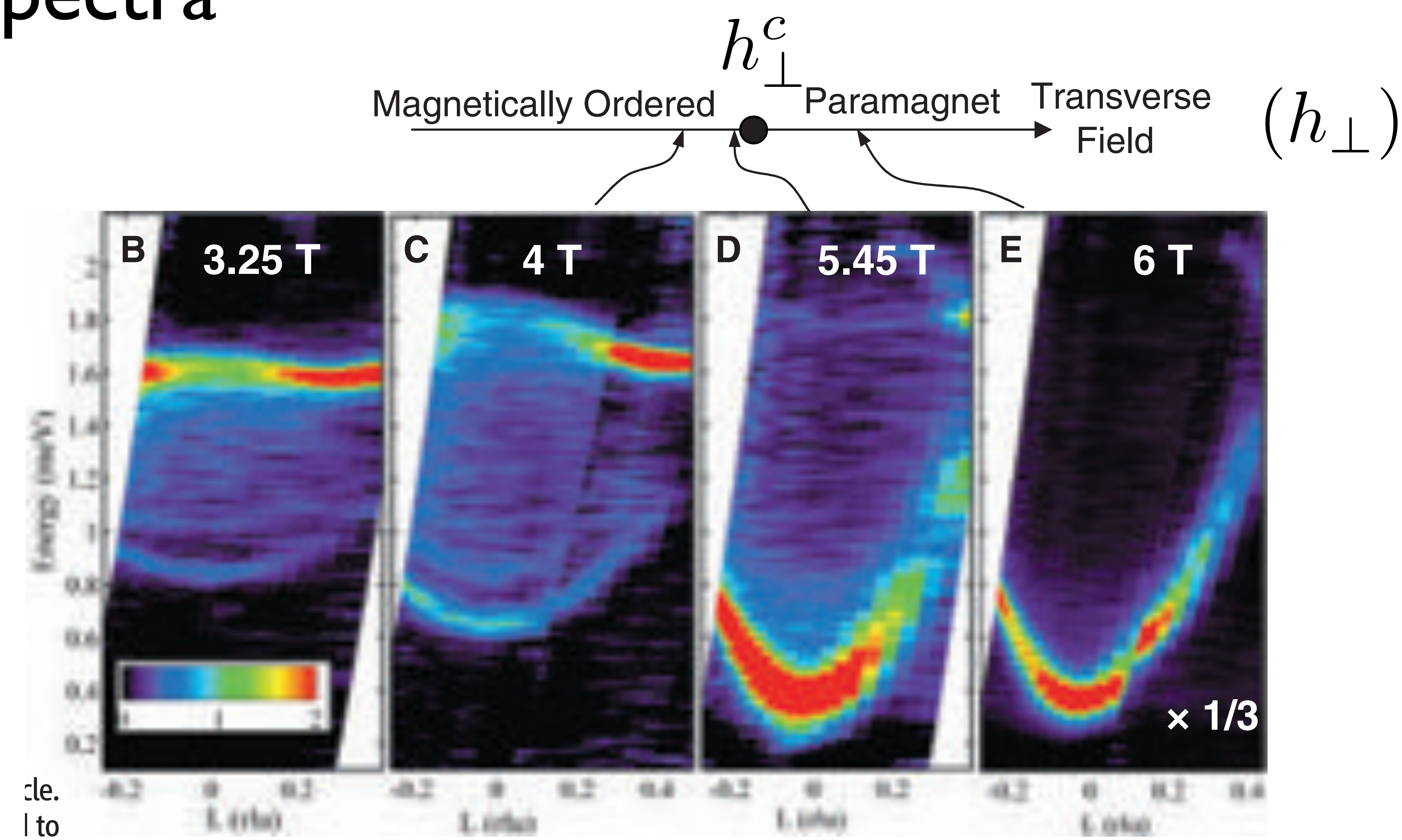
$$\omega = \varepsilon(k') + \varepsilon(k - k')$$

$$A(k, \omega) \sim \int dk' \, f(k') \delta(\omega - \epsilon(k') - \epsilon(k - k'))$$

2-particle continuum

Coldea

- Spectra



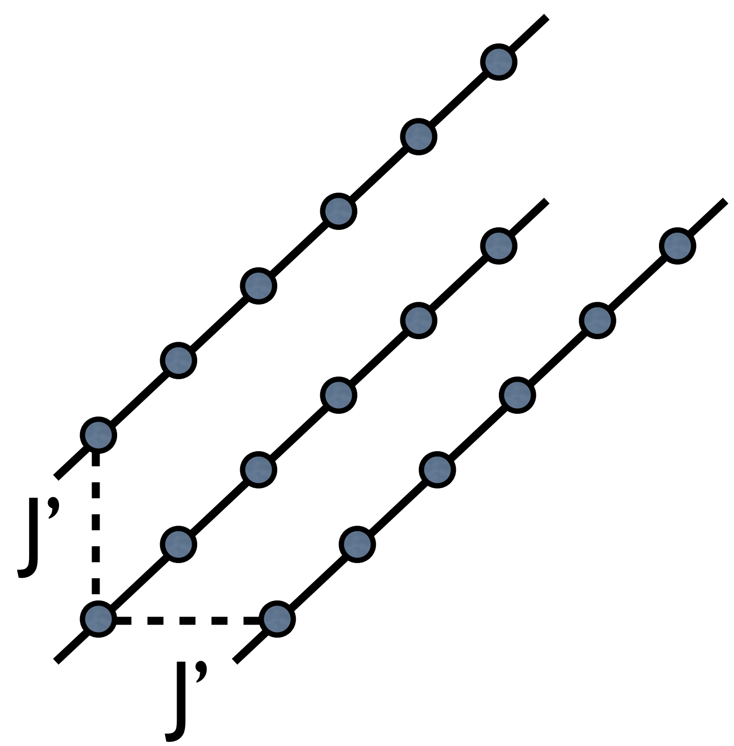
2 soliton continuum
?? why the fine structure ??

single spin flip

Fine structure

- This is due to *three dimensional coupling* between the Ising chains

$$H' = -J' \sum_{n} \sum_{\langle ij \rangle} S^z_{i,n} S^z_{j,n}$$

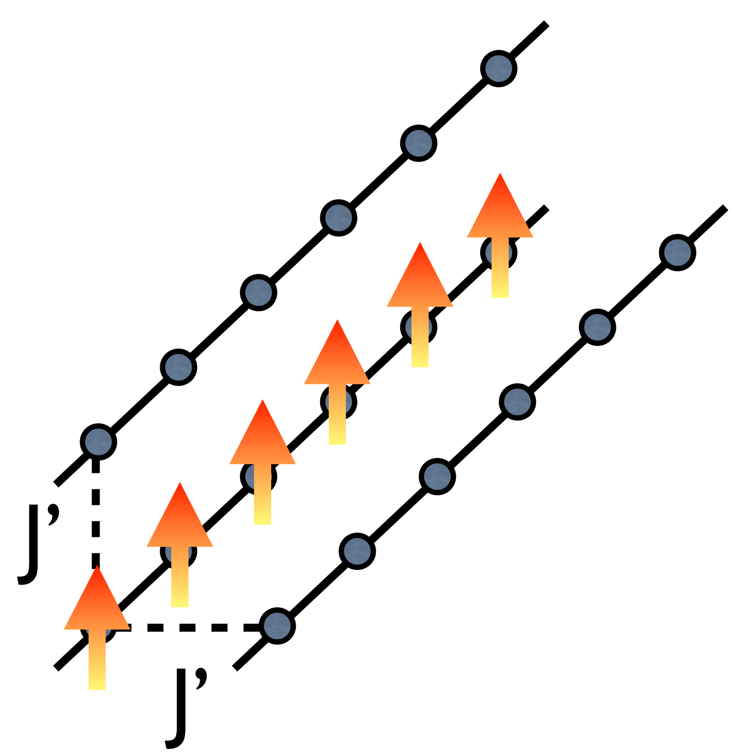


Does very small J’ have an effect?

Fine structure

- This is due to *three dimensional coupling* between the Ising chains

$$H' = -J' \sum_{n} \sum_{\langle ij \rangle} S^z_{i,n} S^z_{j,n}$$

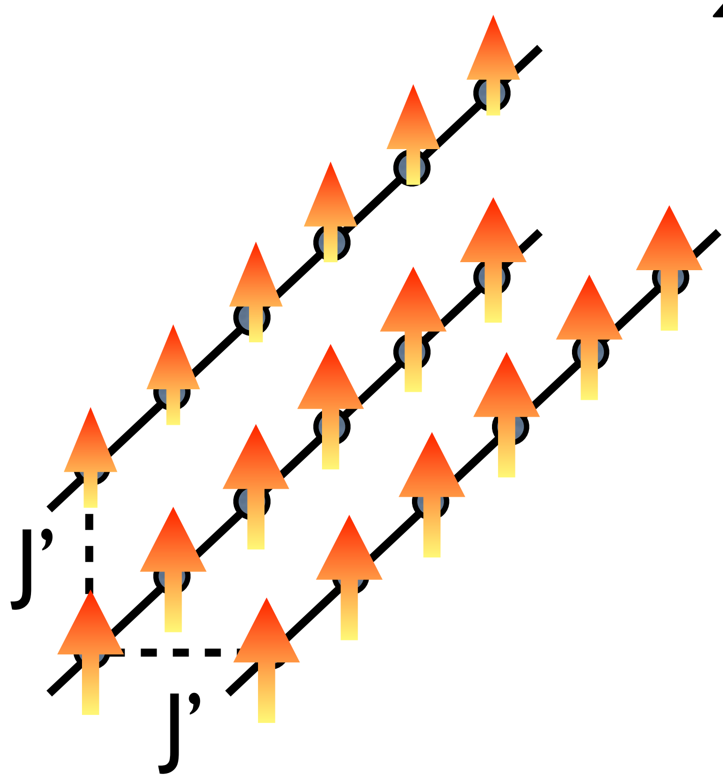


Suppose chains are ferromagnetic

Fine structure

- This is due to *three dimensional coupling* between the Ising chains

$$H' = -J' \sum_{n} \sum_{\langle ij \rangle} S^z_{i,n} S^z_{j,n}$$

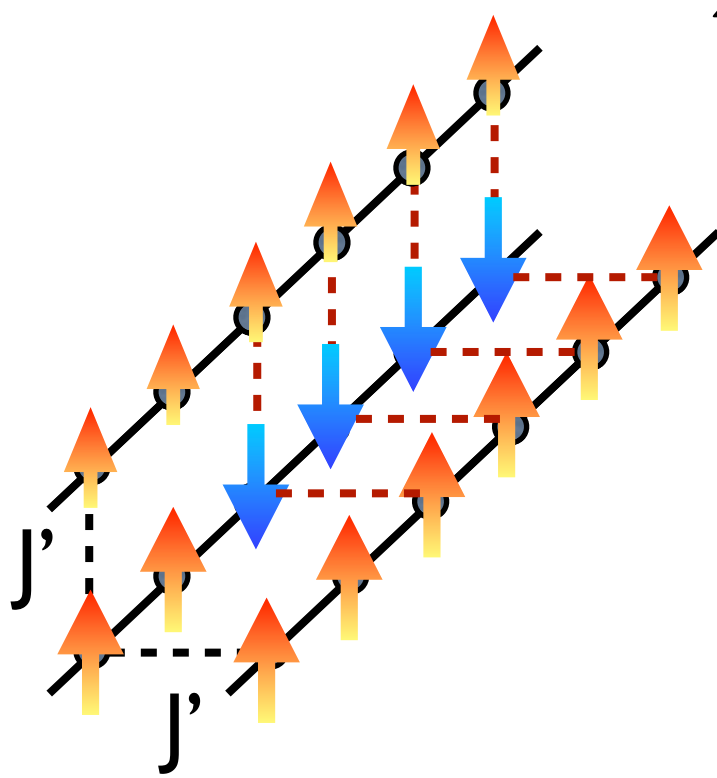


J' prefers they align

Fine structure

- This is due to *three dimensional coupling* between the Ising chains

$$H' = -J' \sum_n \sum_{\langle ij \rangle} S^z_{i,n} S^z_{j,n}$$

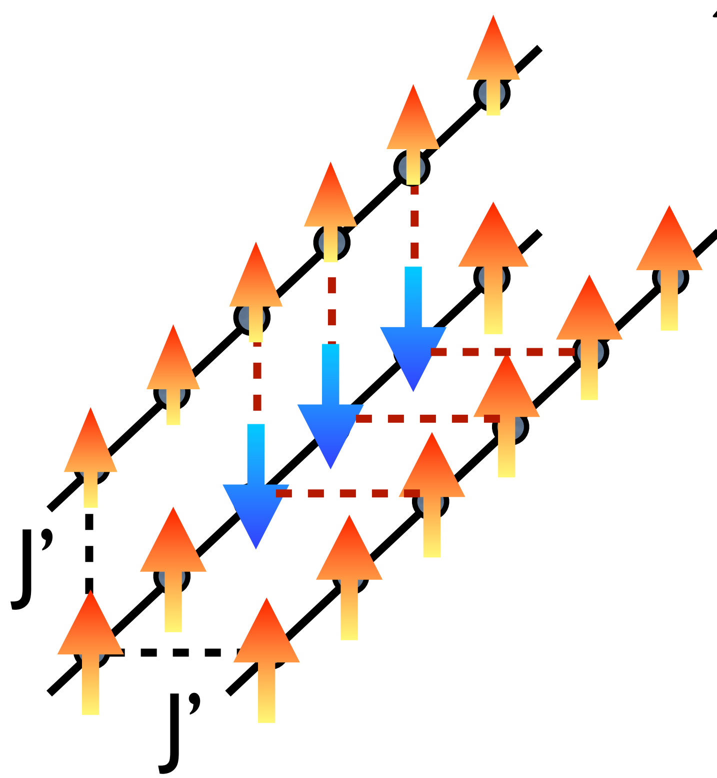


O(J') energy cost *per misaligned bond*: infinite in thermodynamic limit!

Fine structure

- This is due to *three dimensional coupling* between the Ising chains

$$H' = -J' \sum_n \sum_{\langle ij \rangle} S^z_{i,n} S^z_{j,n}$$



pair of domain walls separated by x on the same chain costs an energy ∝ J' |x|: *linear confinement*

Confinement

- Mean field

$$H' \to -h_{\parallel} \sum_{i,n} S^z_{i,n} \qquad h_{\parallel} \propto J' \langle S^z_{i,n} \rangle = J' m$$

- Confining potential

$$V(x) = \lambda |x| \qquad \lambda = h_{\parallel} m$$

- Two particle quantum mechanics

$$H_{\text{eff}} = 2\epsilon_{\text{dw}} - \frac{1}{2\mu}\frac{\partial^2}{\partial x_1^2} - \frac{1}{2\mu}\frac{\partial^2}{\partial x_1^2} + \lambda |x_1 - x_2|$$

Confinement

- Relative coordinate

$$H_{\text{eff}} = 2\epsilon_{\text{dw}} - \frac{1}{\mu}\frac{\partial^2}{\partial x^2} + \lambda|x|$$

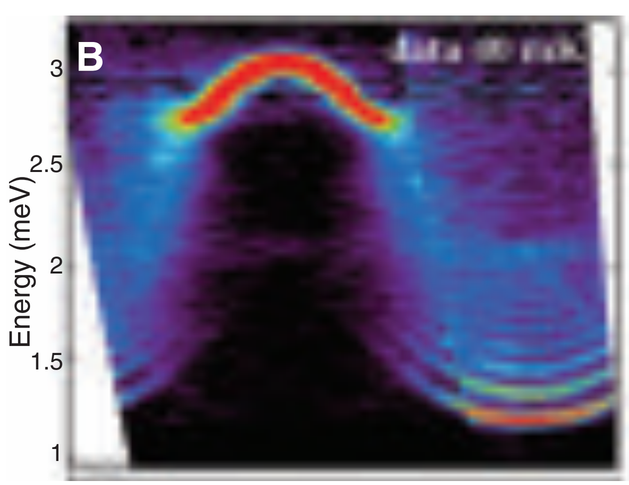
- Standard problem in WKB theory: Airy functions

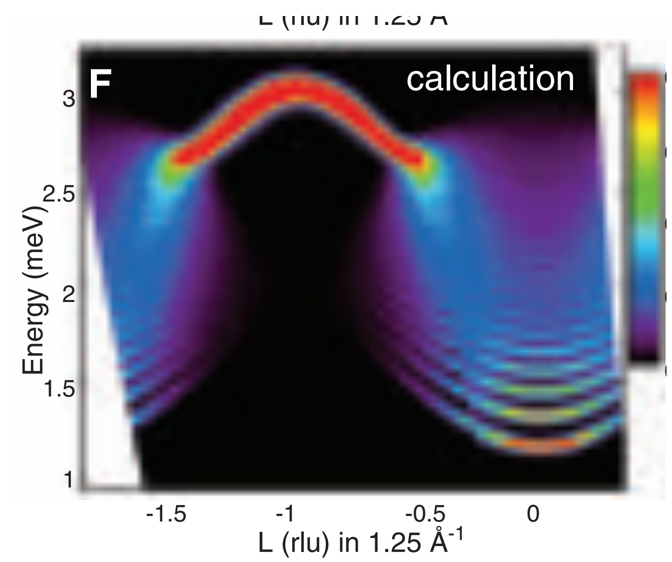
$$E_n = 2\epsilon_{\text{dw}} + z_j(\lambda^2/\mu)^{2/3}$$

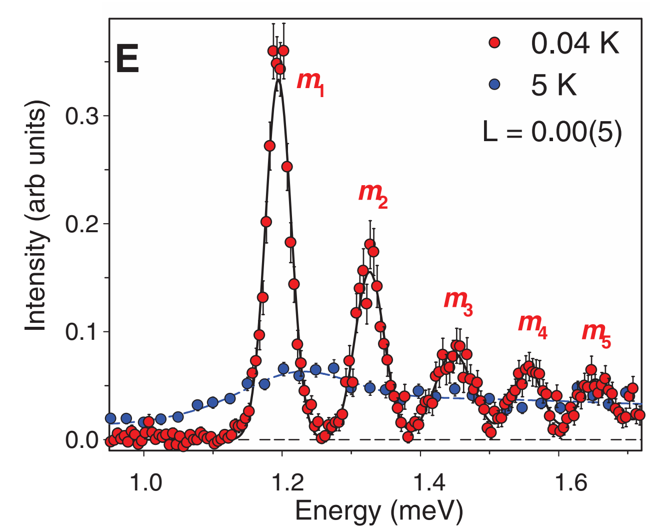
  - z_j = 2.33, 4.08, 6.78.. zeros of Airy function
  - apart from z_j, get this from scaling...

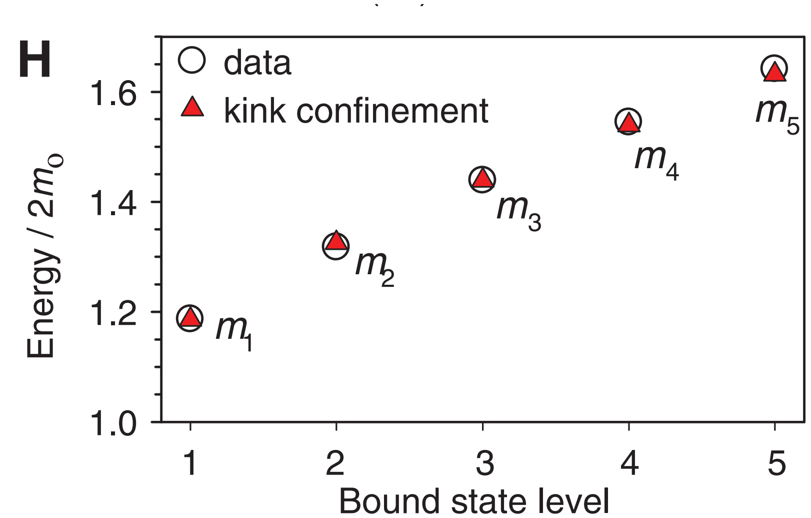
Experiment

- Airy function levels are very beautifully seen!



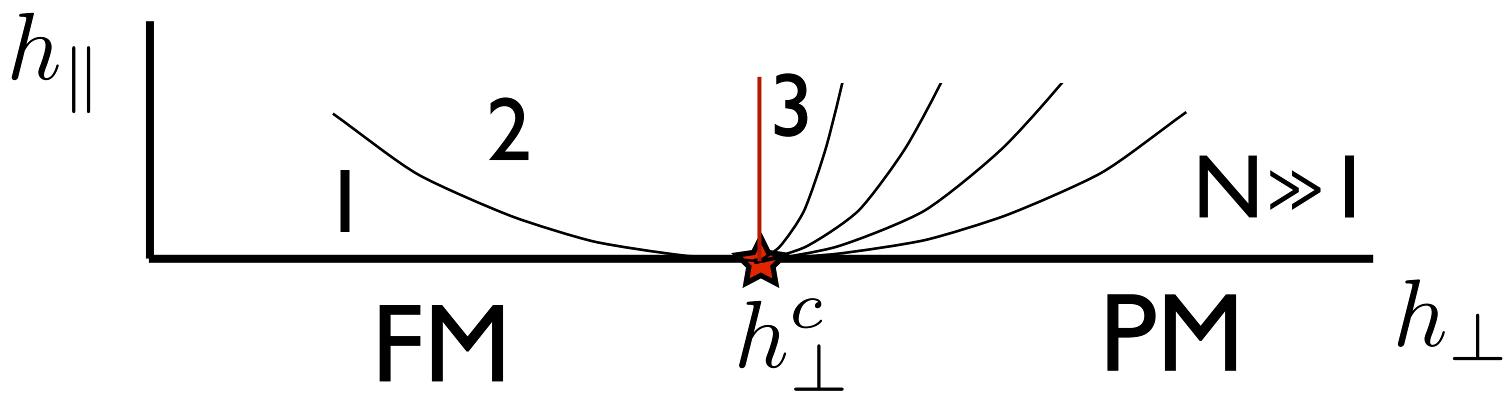


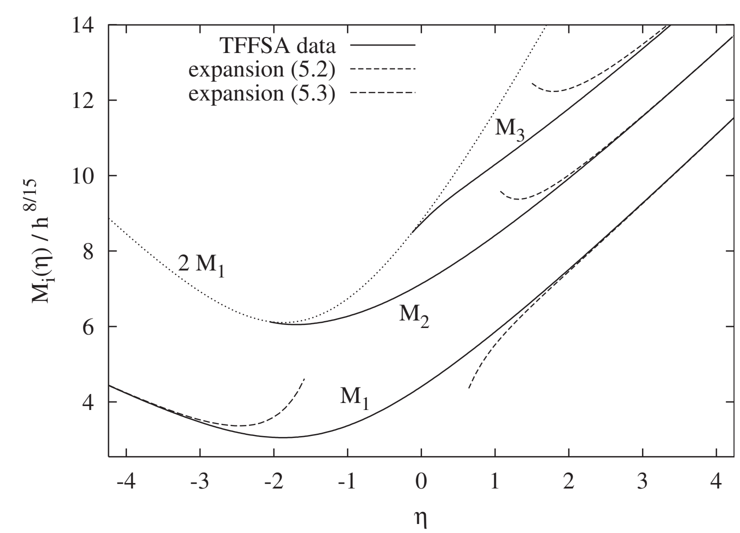




Field evolution?

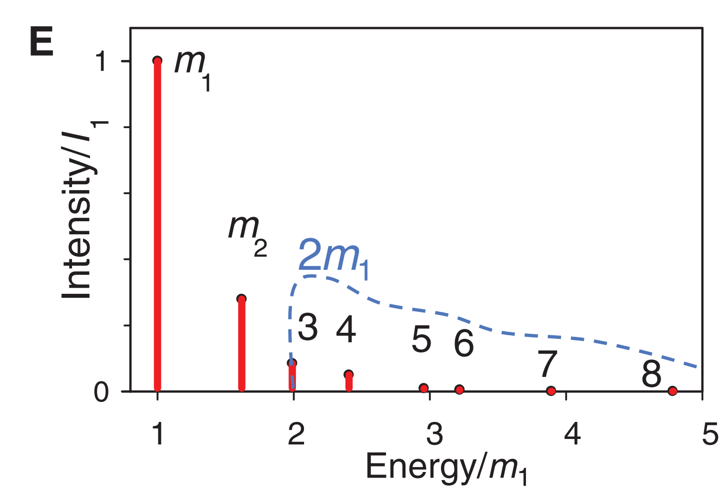
- Number of bound states evolves with $h_\perp$





Fonseca + Zamolodchikov, 2002

- Precisely at $h_\perp = h_\perp^c$, there is an exact solution
  - Scaling $\quad \epsilon_n \sim c_n (h_{\|}/v)^{8/15}$



$$\epsilon_2/\epsilon_1 = (1+\sqrt{5})/2\,!!$$

Ising Model - Parting Shots

- We discussed continuous phase transitions in this specific context, but the lessons are much broader
- There is an important notion of *universality*:
  - the critical properties (exponents etc.) of continuous transitions depend on very few things - symmetry, dimensionality being the main ones
  - otherwise, transitions involving the same symmetries, even in completely different physical systems, show the same critical behavior - examples??

Universality

- One explanation: Landau theory
  - Near criticality, the order parameter is small, and one can Taylor expand the free energy in it. This gives a form which depends only on symmetries
- Renormalization group provides a more refined explanation

Antiferromagnets

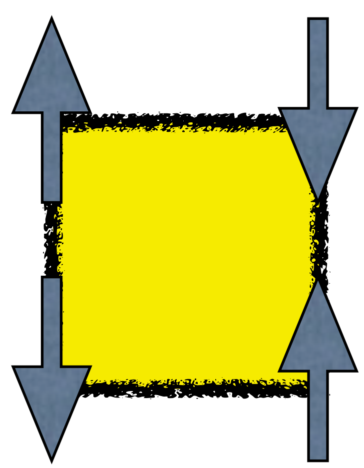
- So far, we have talked about the Ising ferromagnet, which is about the simplest model of statistical mechanics
- Often much complex interactions and/or more complex ordering arises and the statistical mechanics becomes much more involved - and more interesting!
- In the case of magnetic systems, *antiferromagnets* show this kind of richness

Antiferromagnets

- Antiferromagnet: 2 definitions
  - A magnet which orders but has no net magnetization
  - A material with exchange interactions which prefer anti-aligned spins
- Could be both, either, or neither, but both is common

Bipartite AFs

- A lattice is bipartite if it can be divided into two sets of sites, A and B, with A sites neighboring B sites *only*, and vice-versa
- Then AF exchange is easily satisfied with A and B spins antiparallel

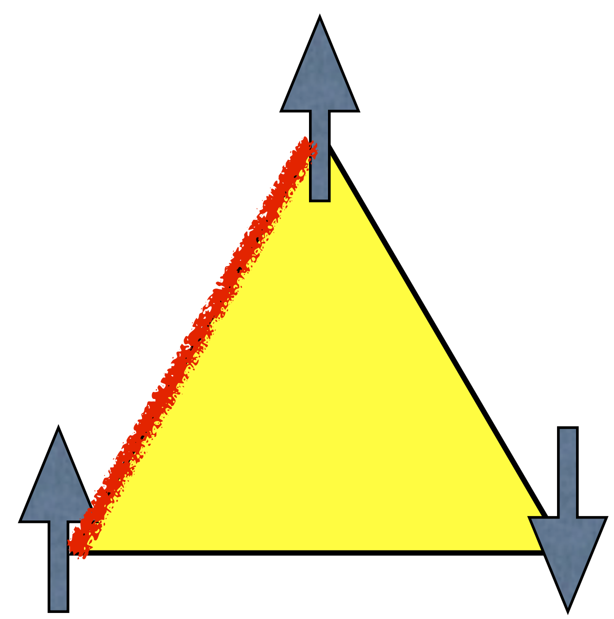


In this case, classical problem can be mapped back to the FM one by $S_B \to -S_B$

Frustration

- Competing interactions generate degenerate ground states

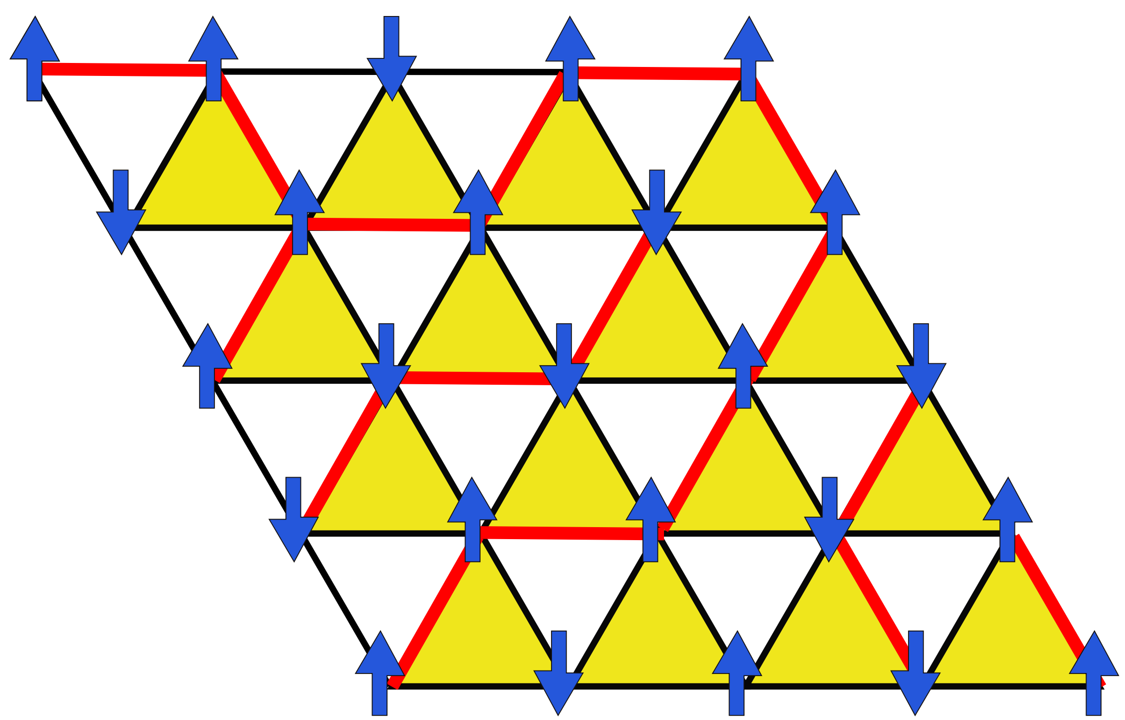
Ising spins



"geometric frustration"

Degeneracy

- Ideally: frustration induces ground state degeneracy, and spins fluctuate amongst those ground states down to low temperature
- e.g. triangular lattice Ising antiferromagnet

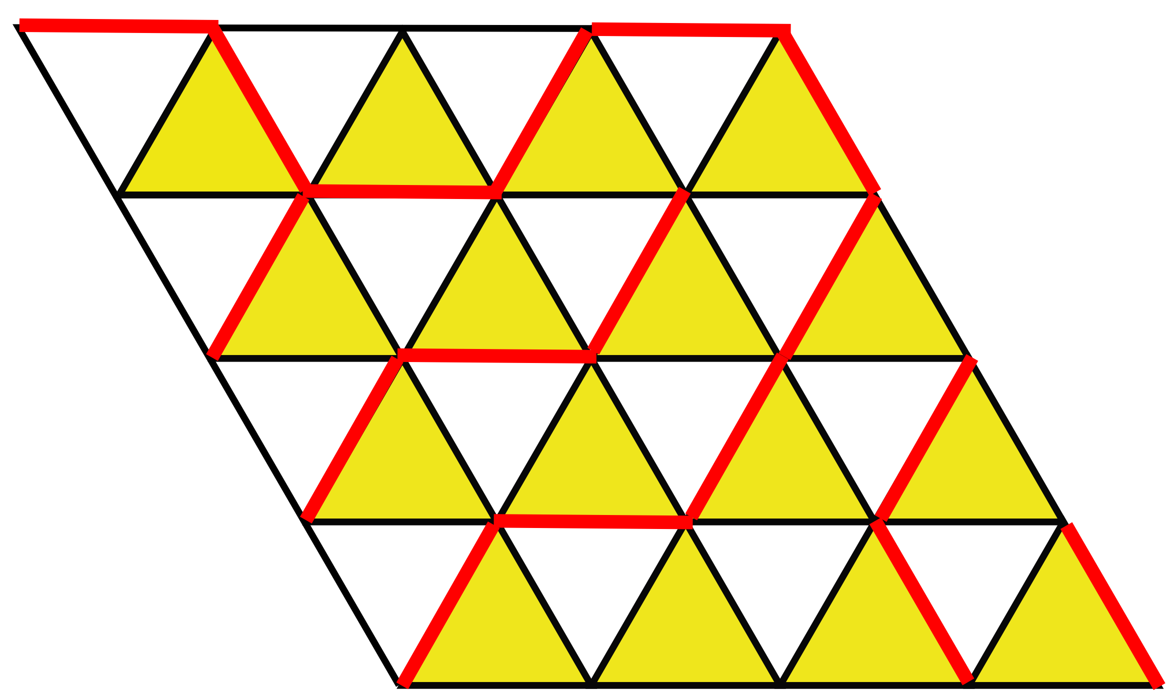


1 frustrated bond per triangle

Wannier (1950): $\Omega = e^{S/k_B}$ $S \approx 0.34 N k_B$

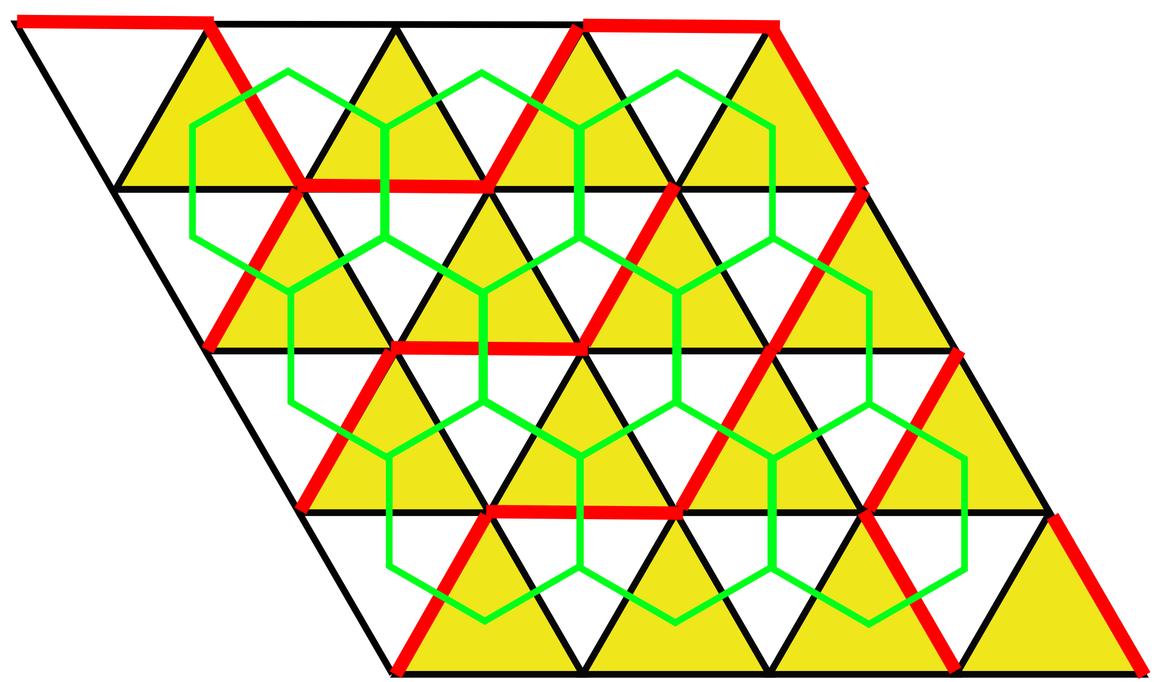
Estimate degeneracy?

- Dual representation
  - honeycomb lattice



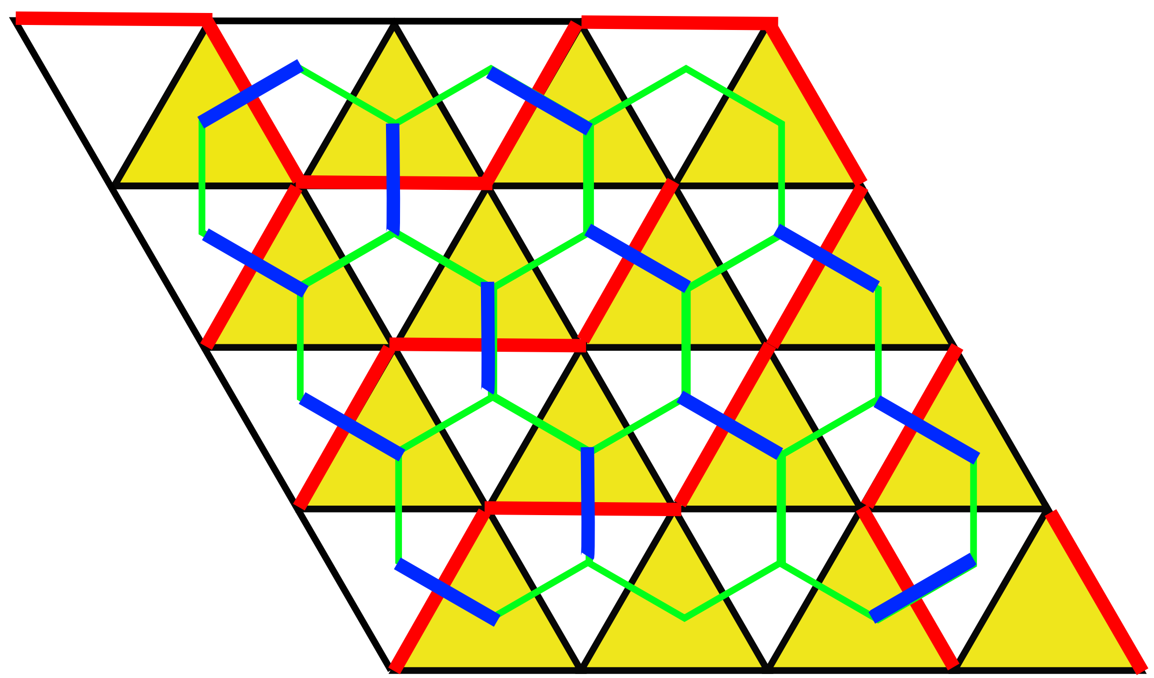
Estimate degeneracy?

- Dual representation
  - focus on the frustrated bonds



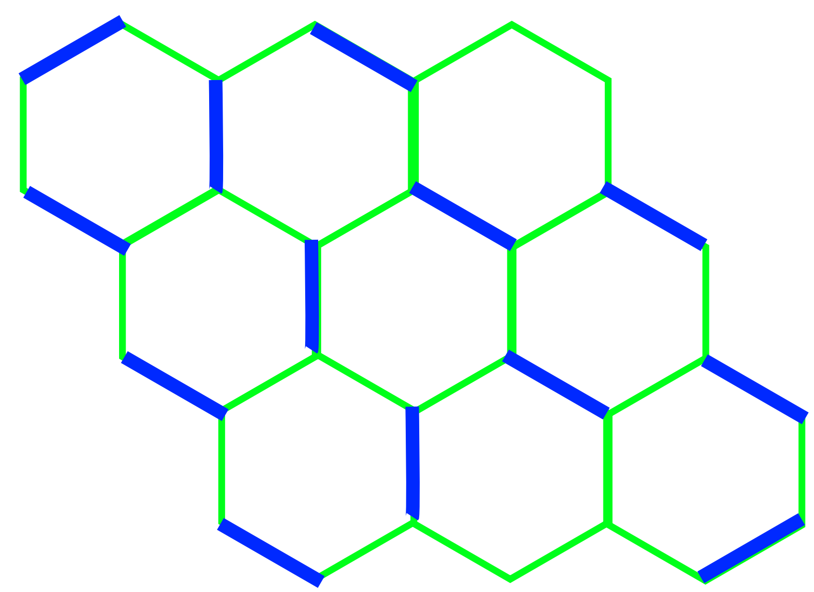
Estimate degeneracy?

- Dual representation
  - color “dimers” corresponding to frustrated bonds
    - “hard core” dimer covering



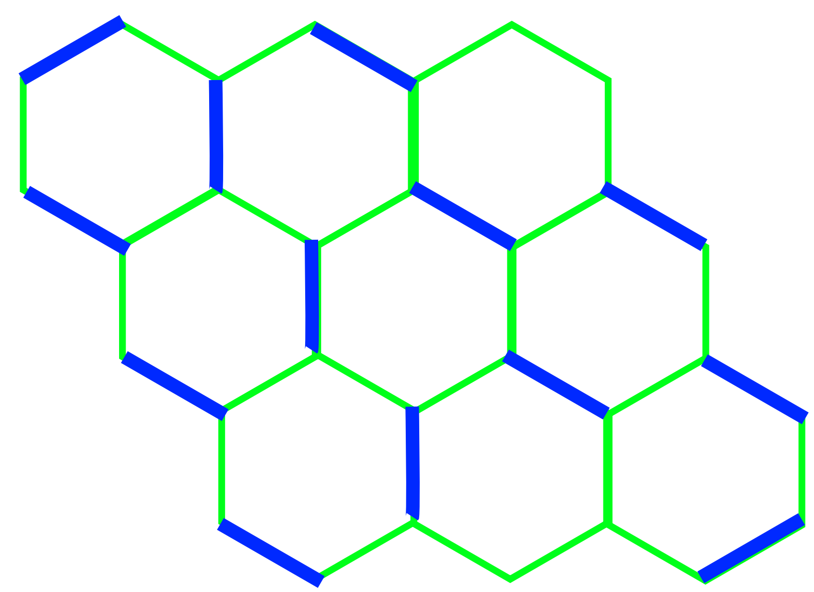
Estimate degeneracy?

- Dual representation
  - A 2:1 mapping from Ising ground states to dimer coverings

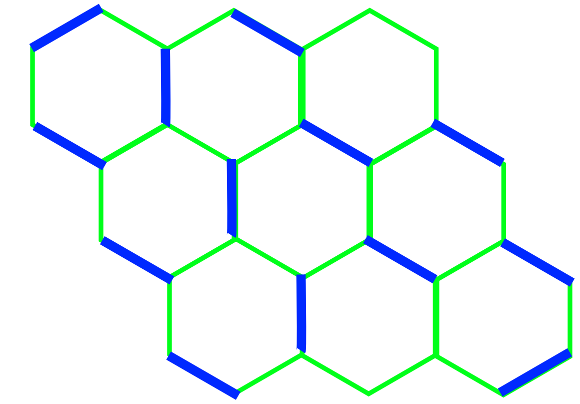


Dimer states

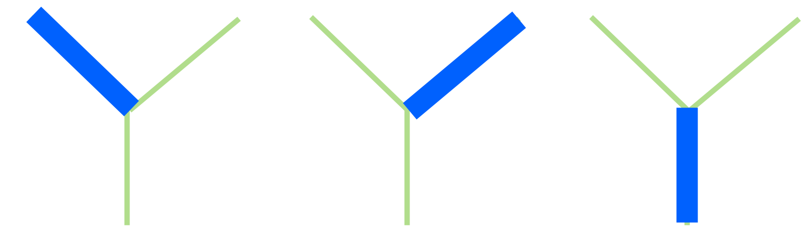
- First exercise: can we understand Wannier's result?
  - count the dimer coverings



Dimer states



- Consider the "Y" dual sites
  - each has 3 configurations
  - this choice fully determines the dimer covering



- But we have to make sure the Y^{-1} sites are singly covered. Make a crude approximation:
  - Prob(dimer) = 1- Prob(no dimer)= 1/3
  - Prob(good Y^{-1}) = 2/3 * 2/3 * 1/3 * 3 = 4/9
- Hence

$$\Omega \approx 3^N \left(\frac{4}{9}\right)^N = e^{N \ln(4/3)}$$

$S \approx 0.29 \text{ N } k_B$

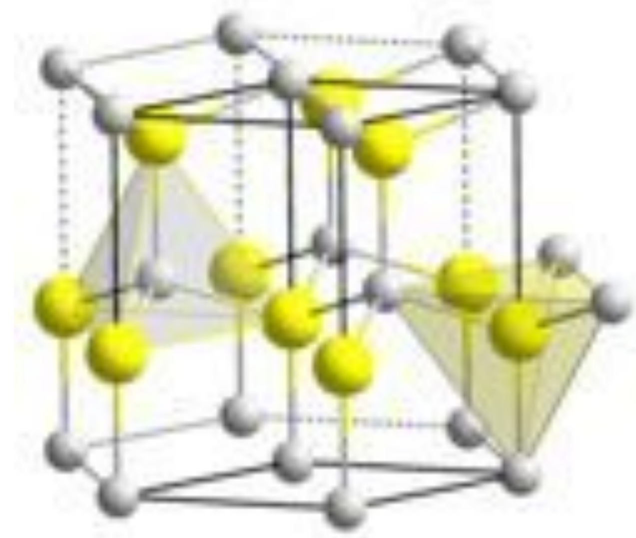
Wannier $S \approx 0.34 \text{ N } k_B$

Spin (and water) Ice

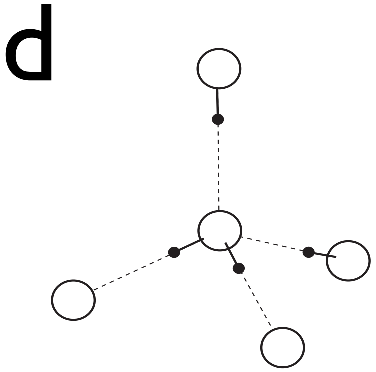
- This simple NN AF Ising model is rather idealized
  - You may expect that there are always perturbations that split this degeneracy and change the physics
- BUT...turns out that something similar happens in spin ice, which really seems to be an almost ideally simple material - by accident!

Water ice

- Common "hexagonal" ice: tetrahedrally coordinated network of O atoms - a wurtzite lattice

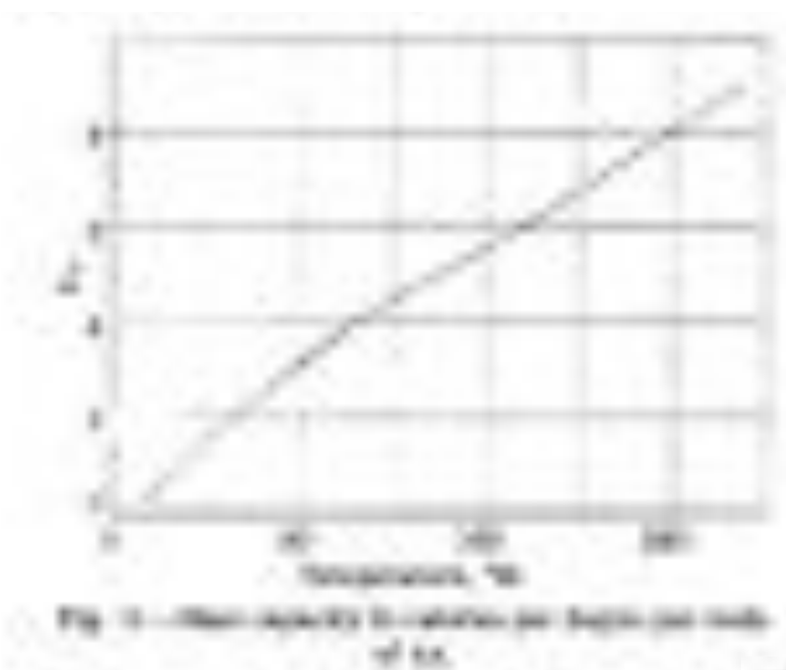


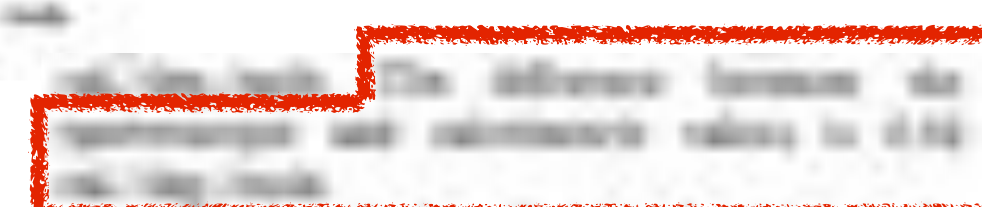
- Must be two protons in each H_2O molecule - but they are not ordered



Ice entropy

- Giauque 1930's measured the "entropy deficit" by integrating C/T from low T and comparing to high T spectroscopic measurements

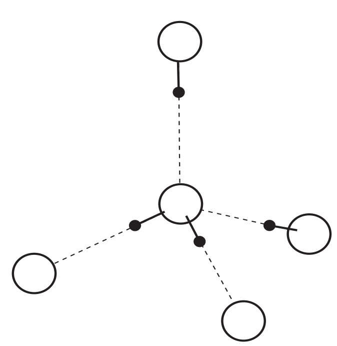




Pauling argument

- Pauling made a simple "mean field" estimate of the entropy due to randomness of the protons, which turns out to be quite accurate

$$\Omega = e^{S/k_B} =$$



$$\underbrace{2^{2N}}_{\text{each bond}} \times \underbrace{\left(\frac{6}{16}\right)^N}_{\text{O constraints}} = \left(\frac{3}{2}\right)^N$$

$$\binom{4}{2} = 6$$

allowed configurations each O

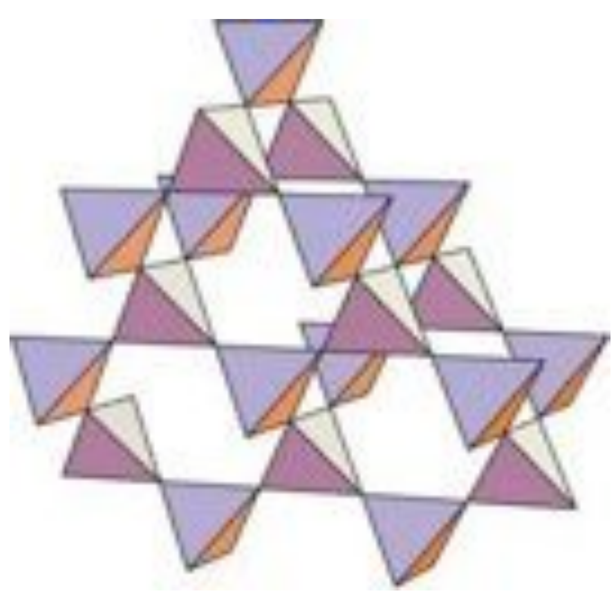
$$S = k_B \ln(3/2) = 0.81 \mathrm{Cal/deg \cdot mole}$$

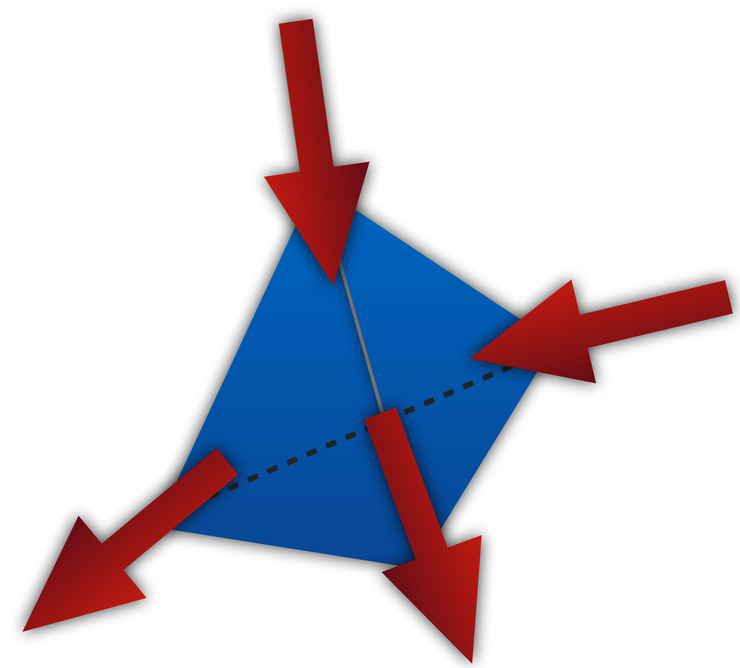
$$\text{c.f. } S_{\text{exp}} = 0.82 \pm 0.05 \mathrm{Cal/deg \cdot mole}$$

Classical realization: spin ice

- Rare earth pyrochlores $Ho_2Ti_2O_7$, $Dy_2Ti_2O_7$: spins form *Ising doublets*, behaving like classical vectors of fixed length, oriented along *local* easy axes

$$\vec{S}_i = \hat{e}_i \sigma_i$$





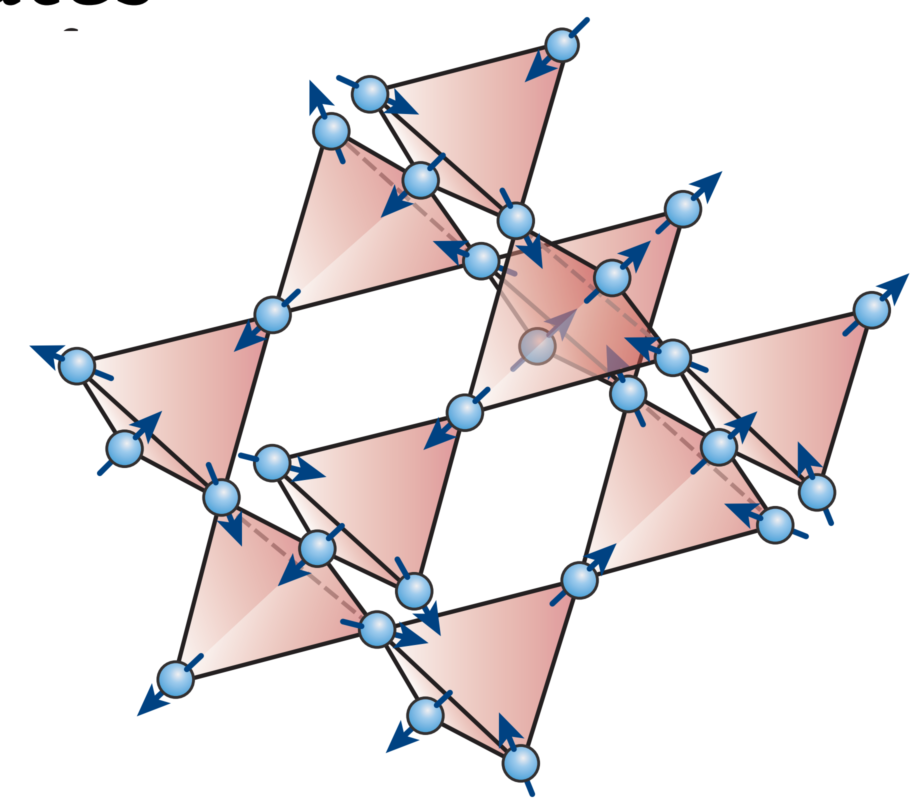
$\hat{e}_0 = (1,1,1)/\sqrt{3}$ $\hat{e}_1 = (1,-1,-1)/\sqrt{3}$ $\hat{e}_2 = (-1,1,-1)/\sqrt{3}$ $\hat{e}_3 = (-1,-1,1)/\sqrt{3}$

Spin Ice (simplified)

- Exchange (due largely to dipolar interactions) is *ferromagnetic*
  - Prefers "2 in - 2 out" states

$$-J\vec{S}_i \cdot \vec{S}_j = \frac{J}{3}\sigma_i\sigma_j$$

same as Ising antiferromagnet

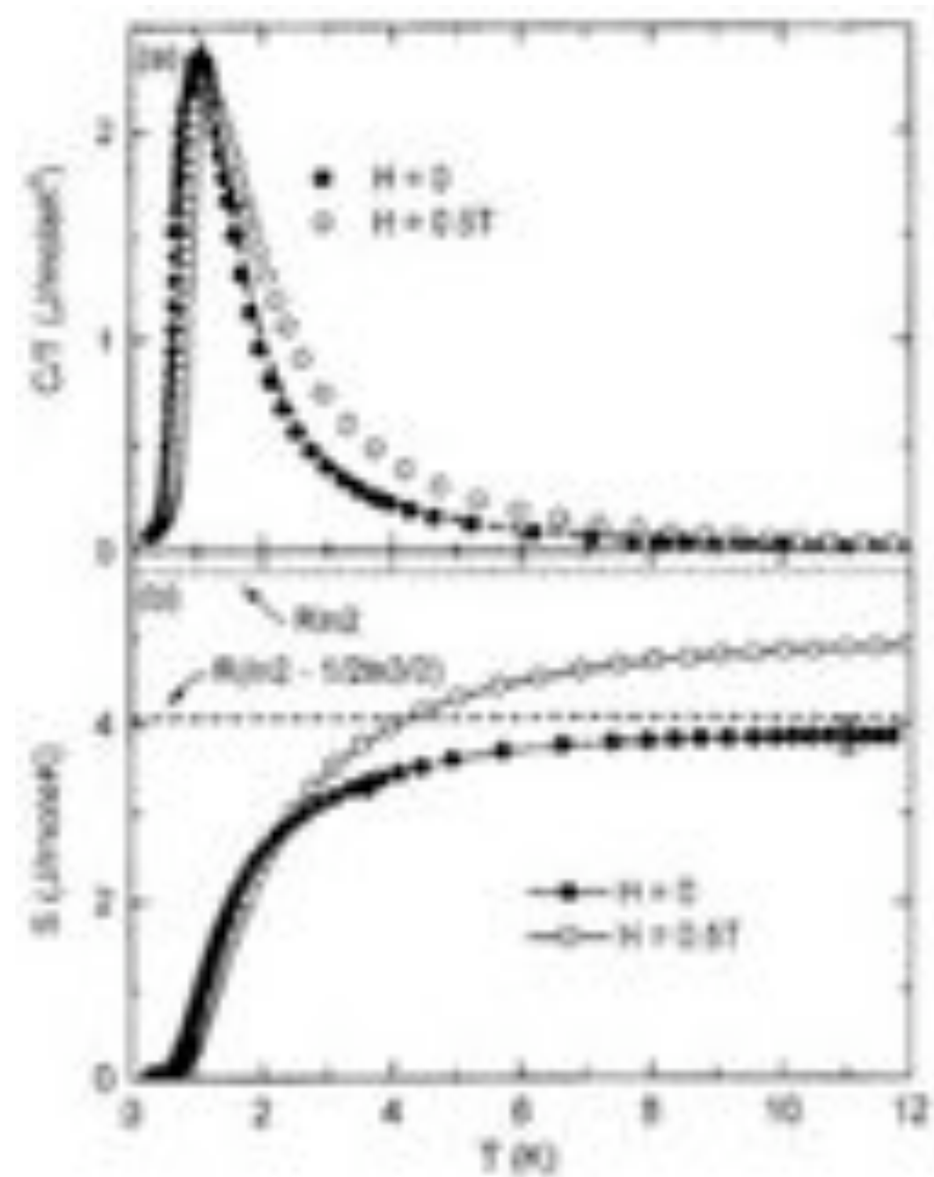


"ice rules"

$\hat{e}_i \cdot \hat{e}_j = -1/3 \qquad i \neq j$

Entropy

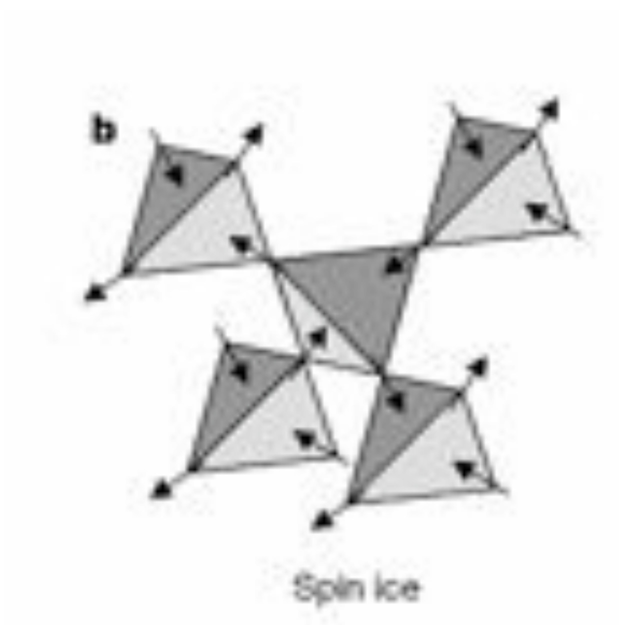
- The integrated specific heat of $Dy_2Ti_2O_7$ showed explicitly that the entropy did not vanish at low temperature
  - quantitative agreement with Pauling's 1935 estimate
- We call this situation, with spins fluctuating for kT<<J, a classical *spin liquid*



A.P. Ramirez *et al*, 1999

Spin liquid physics

- The spin liquid fluctuations are a form of "artificial magnetostatics" (classical)
  - ice rules: divergence free condition

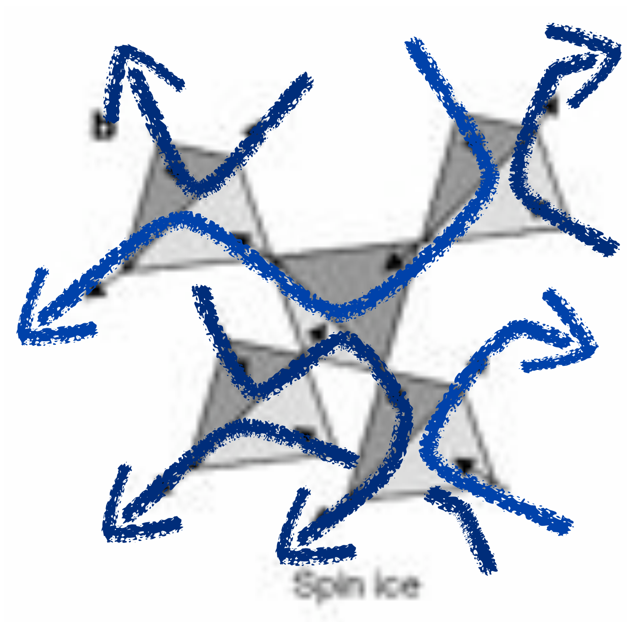


$$\vec{S} \sim \vec{b}$$

$$\vec{\nabla} \cdot \vec{b} = 0$$

Spin liquid physics

- The spin liquid fluctuations are a form of "artificial magnetostatics" (classical)
  - ice rules: divergence free condition



$$\vec{S} \sim \vec{b}$$

$$\vec{\nabla} \cdot \vec{b} = 0$$

field lines = loops or strings tracing spin configurations
Can we see effects in long-distance correlations?

Structure Factor

- Static neutron structure factor

$$\mathcal{S}_{\mu\nu}(k) = \sum_{i,j} \langle S_i^\mu S_j^\nu \rangle e^{i\mathbf{k}\cdot(\mathbf{r}_i - \mathbf{r}_j)}$$

- Typically, S(k) is used to distinguish *ordered* and paramagnetic states via *Bragg peak*
  - Long range order: |i-j|≫ξ

$$\langle \vec{S}_i \cdot \vec{S}_j \rangle \to \langle \vec{S}_i \rangle \cdot \langle \vec{S}_j \rangle \sim |M_Q|^2 \cos[\mathbf{Q} \cdot (\mathbf{r}_i - \mathbf{r}_j)]$$

$$S(k) \sim |M_Q|^2 \delta(k - Q)$$

  - Short range order

$$S(k) \sim \frac{A}{(k-Q)^2 + \xi^{-2}}$$

Structure Factor

- In spin ice, there is no incipient ordered state: feature in correlations is more subtle than a peak
- Coarse-graining argument: correlations are governed by *effective free energy*

$$H_{\mathrm{eff}} = \int d^3r \, \frac{c}{2} |\vec{b}|^2$$

- Need to calculate

$$\langle b_\mu(r) b_\nu(r') \rangle = \frac{1}{Z} \int [d\vec{b}(r)] \boxed{\delta[\vec{\nabla} \cdot \vec{b}]} b_\mu(r) b_\nu(r') \, e^{-\beta H_{\mathrm{eff}}[\vec{b}]}$$

Structure factor

- Fourier $$H_{\text{eff}} = \sum_k \frac{c}{2}|\vec{b}_k|^2$$
- Constraint $\vec{\nabla} \cdot \vec{b} = 0 \qquad b_z = -(k_x b_x + k_y b_y)/k_z$

$$H_{\text{eff}} = \sum_k \frac{c}{2} B_k^\dagger \begin{pmatrix} 1 + \frac{k_x^2}{k_z^2} & \frac{k_x k_y}{k_z^2} \\ \frac{k_x k_y}{k_z^2} & 1 + \frac{k_y^2}{k_z^2} \end{pmatrix} B_k\,, \quad B_k = \begin{pmatrix} b_x \\ b_y \end{pmatrix}$$

- Structure factor

$$\langle b_\mu(r) b_\nu(r') \rangle = \frac{1}{N} \sum_k \langle b_\mu^*(k) b_\nu(k) \rangle e^{ik\cdot(r-r')}$$

Gaussian integrals

- General rule

$$\beta H = \frac{1}{2} \sum_{ij} K_{ij} x_i x_j$$

$$\langle x_i x_j \rangle = \frac{1}{Z} \int [\prod_k dx_k] x_i x_j e^{-\beta H}$$

$$= \left[K^{-1}\right]_{ij}$$

- Proved in many many references...

Proof

- Generating function

$$\langle e^{\sum_i q_i x_i} \rangle = \frac{1}{Z} \int [\prod_k dx_k] e^{-\frac{1}{2}\sum_{ij} K_{ij} x_i x_j + \sum_i q_i x_i}$$

- Shift

$$x_i \to x_i + \sum_j [K^{-1}]_{ij} q_j$$

- Result

$$\langle e^{\sum_i q_i x_i} \rangle = e^{\frac{1}{2}\sum_{ij}[K^{-1}]_{ij} q_i q_j}$$

- Differentiating twice gives $\langle x_i x_j \rangle = \left[K^{-1}\right]_{ij}$

Gaussian integrals

- General rule: invert the quadratic form

$$\langle b_\mu^*(k) b_\nu(k)\rangle = \frac{k_B T}{c}\begin{pmatrix} 1+\frac{k_x^2}{k_z^2} & \frac{k_x k_y}{k_z^2} \\ \frac{k_x k_y}{k_z^2} & 1+\frac{k_y^2}{k_z^2}\end{pmatrix}^{-1}$$

- With some algebra

$$\langle b_\mu^*(k) b_\nu(k)\rangle = \frac{k_B T}{c}\left(\delta_{\mu\nu} - \frac{k_\mu k_\nu}{k^2}\right)$$

- We could have guessed this!

$$\sum_\mu k_\mu \langle b_\mu^*(k) b_\nu(k)\rangle = 0$$

Power law correlations

- Neutrons

$$\mathcal{S}(k) = \sum_{\mu\nu} (\delta_{\mu\nu} - \frac{k_\mu k_\nu}{k^2}) \mathcal{S}_{\mu\nu}(k)$$

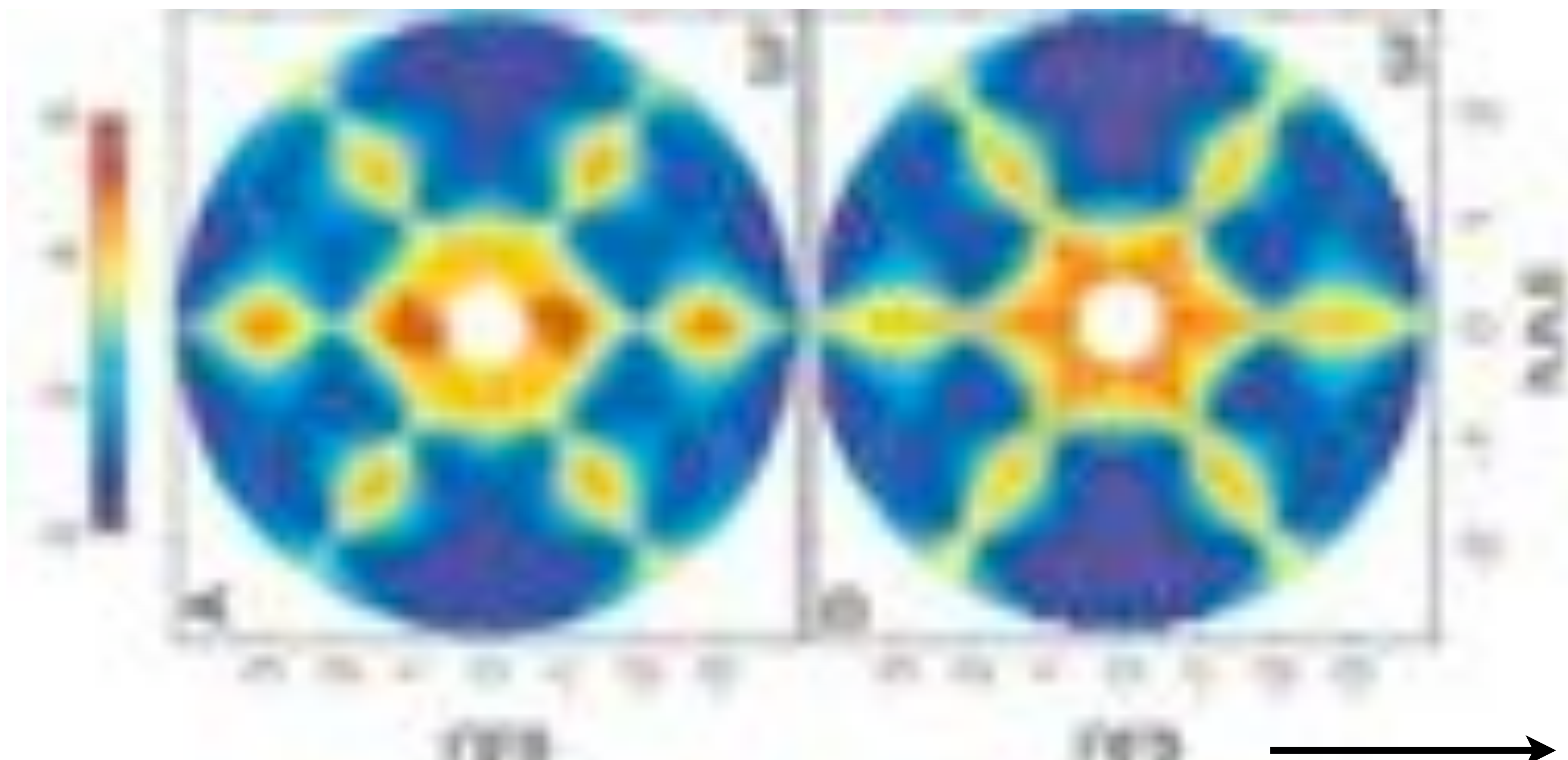
- Measured near a reciprocal lattice vector

$$\mathcal{S}(K_{002} + k) = \mathcal{S}_{xx}(K + k) + \mathcal{S}_{yy}(K + k)$$

$$\approx 2 - \frac{k_x^2 + k_y^2}{k^2} = 1 + \frac{k_z^2}{k^2}$$

- Not a peak but a singularity

pinch points in $Ho_2Ti_2O_7$



experiment theory

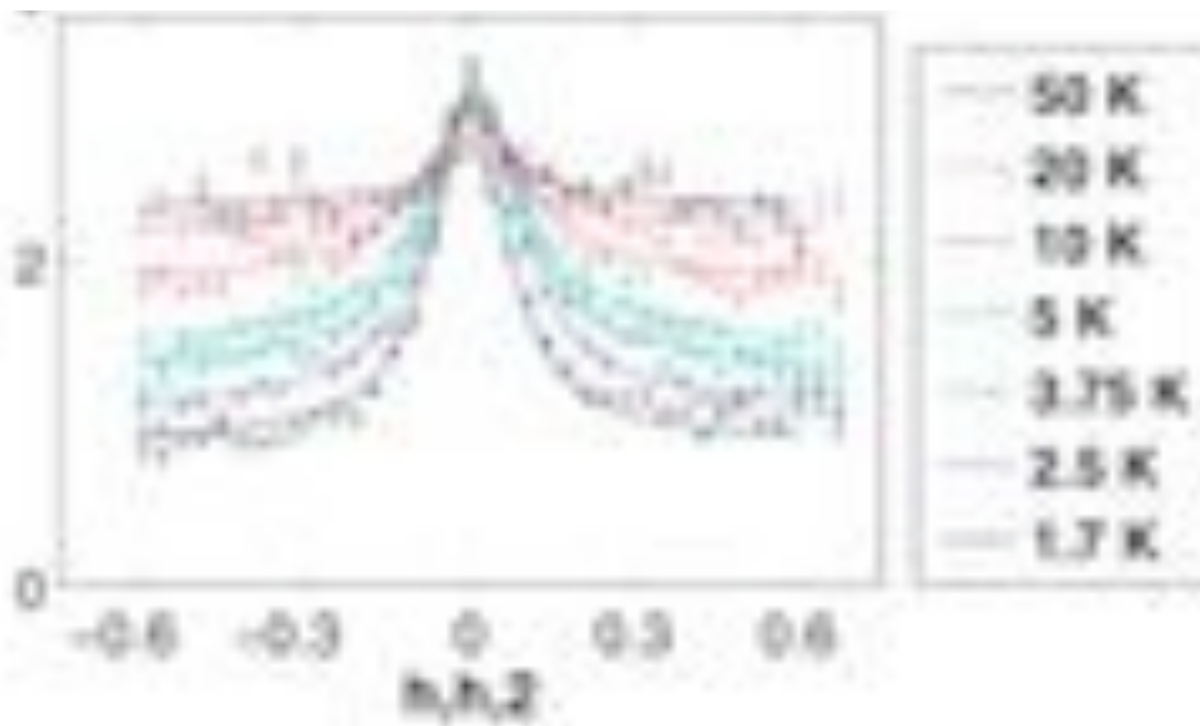
k_z

T. Fennell *et al*, 2009

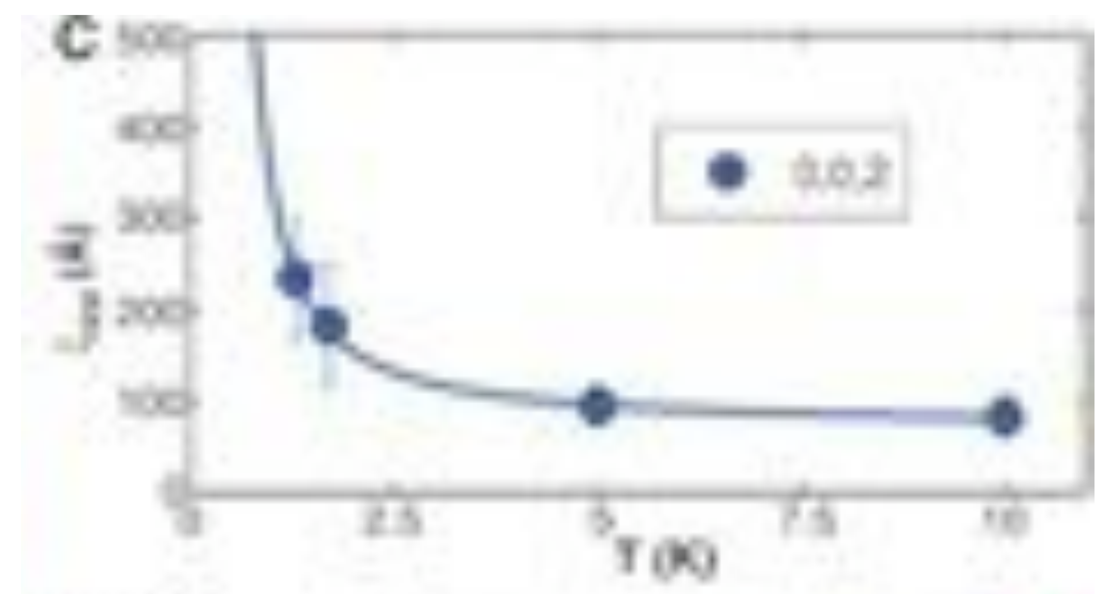
$$\mathcal{S}(K_{002}+k) \sim \frac{k_z^2}{k^2}$$

vanishes for k_z=0

Quality of singularity



pinch point sharpens with lower T

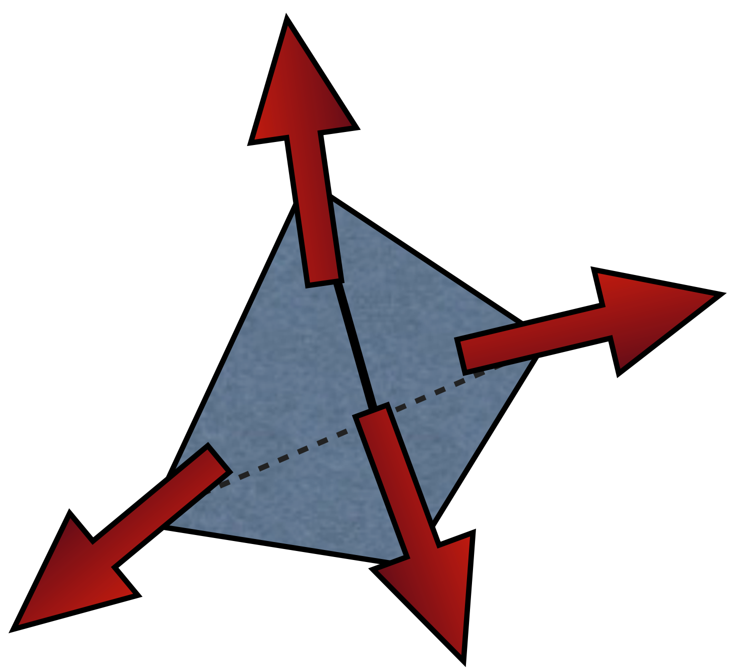


"Correlation length" for rounding of pinch point

Roughly $\xi \sim e^{1.8K/T}$

Defects

- The ice rules constraint is not perfectly enforced at T>0
- Primitive defect is a "charged" tetrahedron with $\sum_i \sigma_i = \pm 1$.



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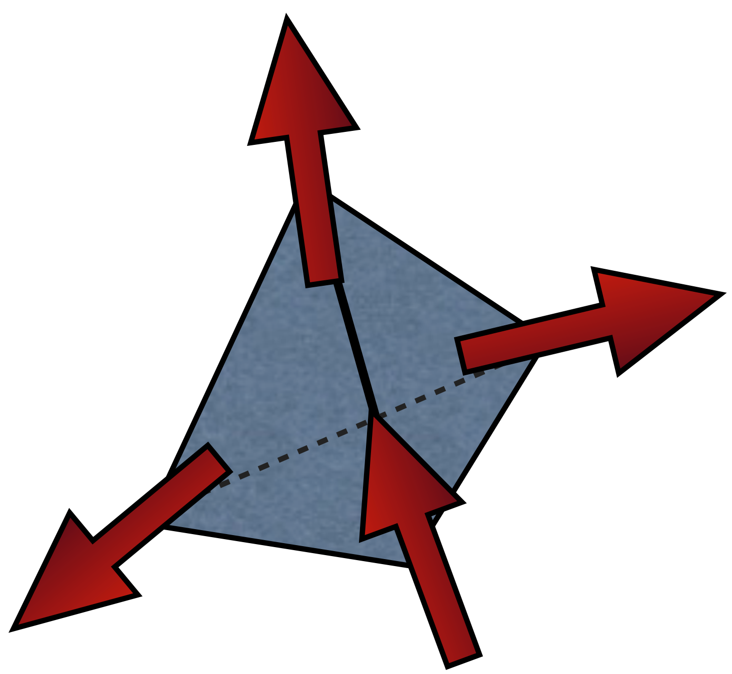


costs energy $2J_{eff}$

What to call it?

- Consider Ising "spin"

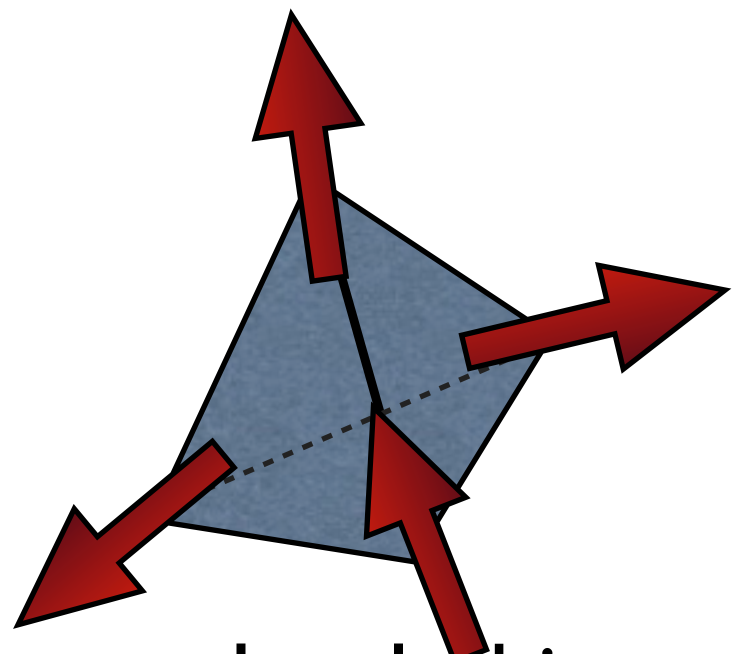
$$S^z_{\mathrm{TOT}} = \sum_i \sigma_i = \frac{1}{2}\sum_t S^z_t$$

- Single flipped tetrahedron has $S^z_{\mathrm{TOT}} = \pm 1/2$
  - "spinon"? (M. Hermele *et al*, 2004)
  - But S^z is not very meaningful in spin ice
- Use magnetic analogy: *magnetic monopole*

Magnetic monopoles

Castelnovo *et al*, 2008

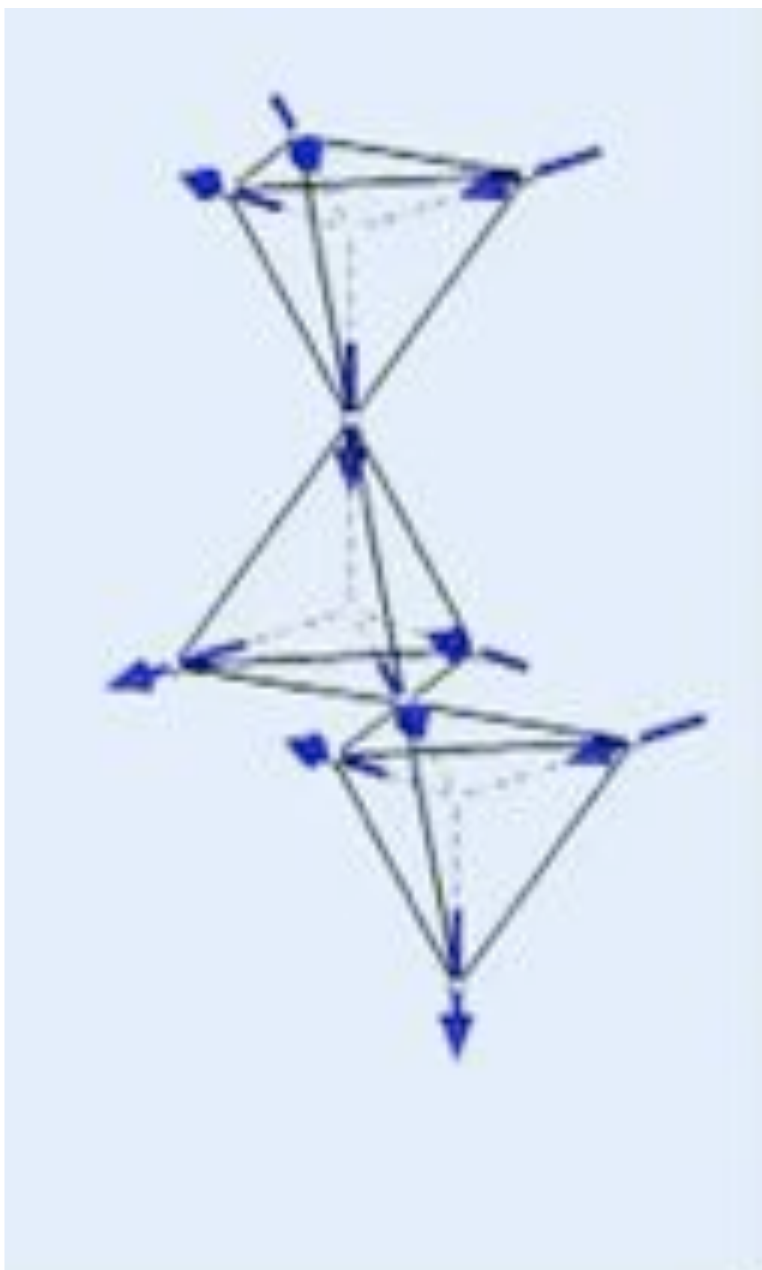
- Defect tetrahedra are sources and sinks of "magnetic" flux



div b = 1

- It is a somewhat non-local object
  - Must flip a semi-infinite string of spins to create a single monopole
  - Note similarity to 1d domain wall

String



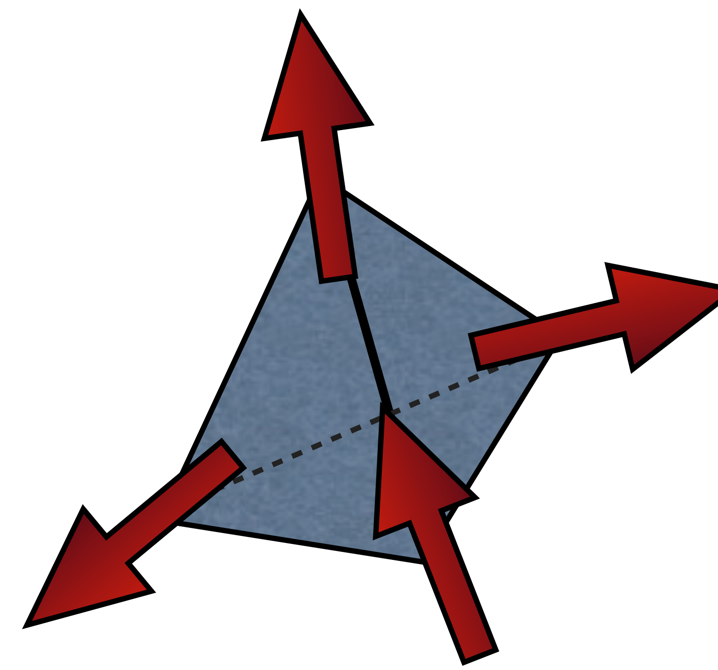
stolen (by somebody else on youtube) from Steve Bramwell

- Note that the string is tensionless because the energy depends only on $\sum_i \sigma_i$ on each tetrahedra
    - In an ordered phase, this would cost energy
- Once created, the monopole can move by single spin flips

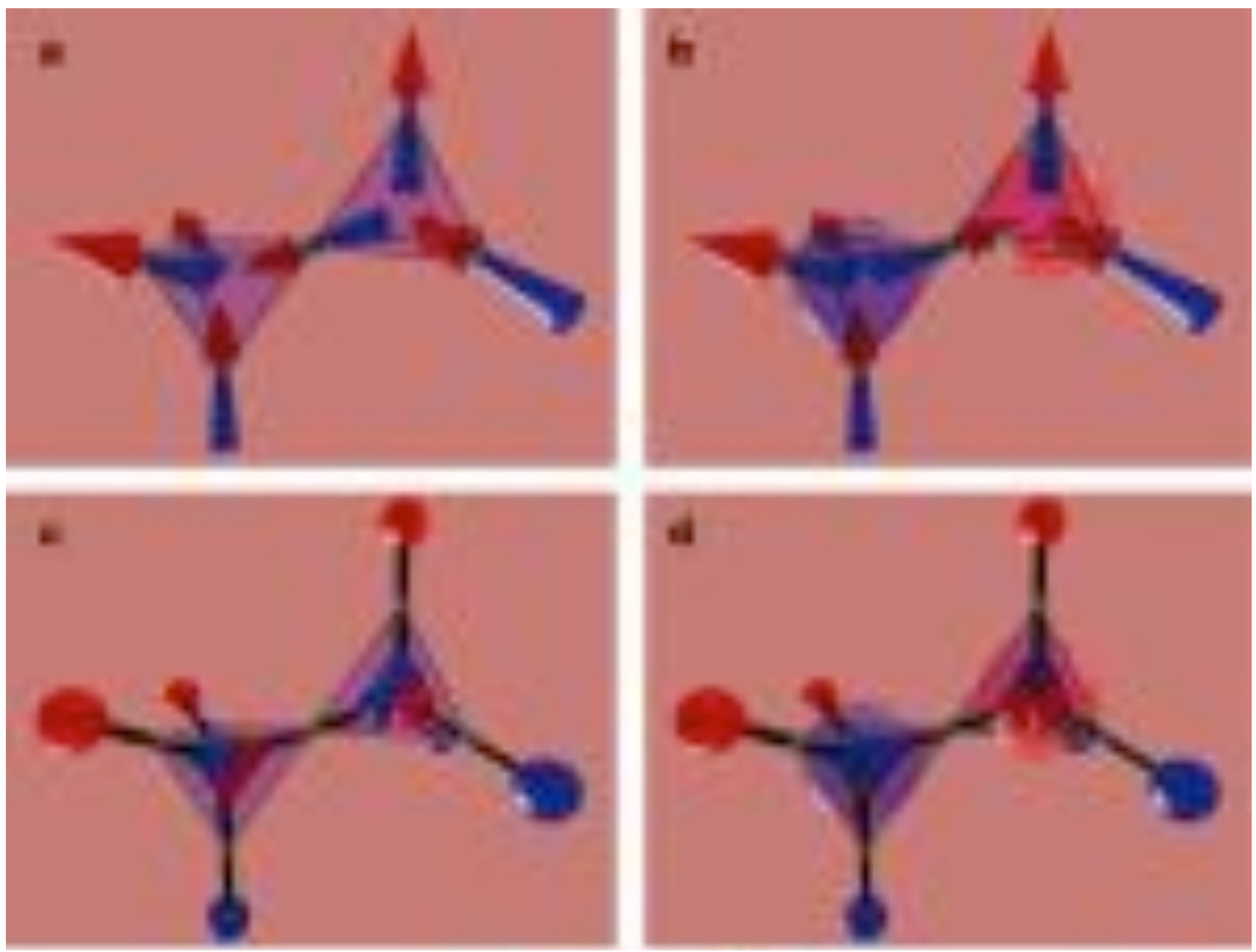
Monopoles are “real”

Castelnovo *et al*, 2008

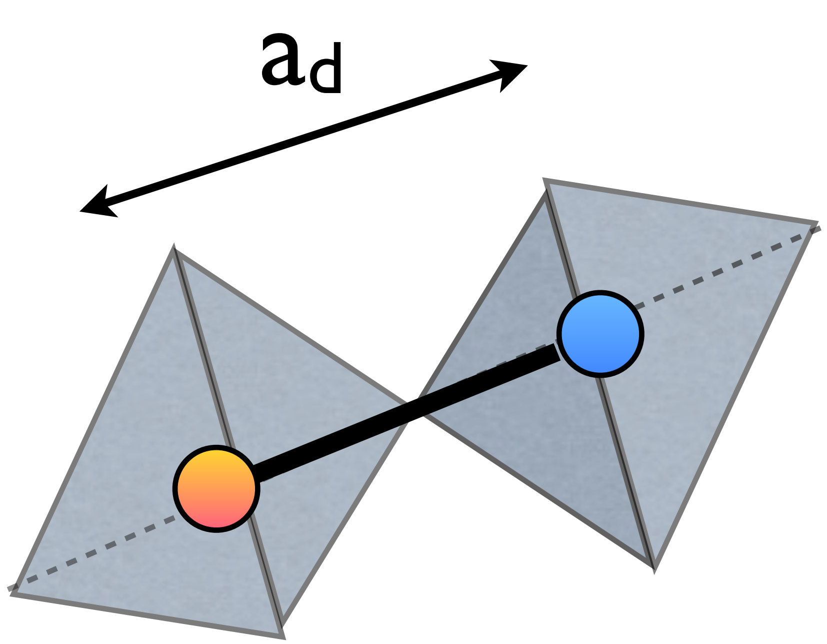
- Monopoles actually are sources for (internal) magnetic field
  - Magnetization M $\propto$ b
  - hence div M ~ div H ~ q δ(r)
- Actual magnetic charge is small



Monopoles for dumbbells



Dumbbell model



magnetic charge ±q $\quad q = \mu / a_d$

Dy, Ho $\quad \mu \approx 10 \mu_B$

potential

$$V_{qq} = \frac{\mu_0}{4\pi} \frac{q_a q_b}{r_{ab}}$$

$$= \frac{\mu_0}{4\pi} \frac{\mu^2}{a_d^2} \frac{1}{r_{ab}}$$

Coulomb

$$V_{ee} = \frac{1}{4\pi\epsilon_0} \frac{e^2}{r}$$

Dumbbell model

ratio

$$V_{ee}/V_{qq} = \frac{e^2}{\mu^2}\frac{a_d^2}{\epsilon_0\mu_0} = \frac{e^2c^2a_d^2}{\mu^2} \qquad \left(\frac{1}{\epsilon_0\mu_0} = c^2\right)$$

$$= \frac{e^2c^2a_d^2}{100\mu_B^2} = \frac{e^2c^2a_d^2(2m_e)^2}{100e^2\hbar^2} \qquad \left(\mu_B^2 = \frac{e\hbar}{2m_e}\right)$$

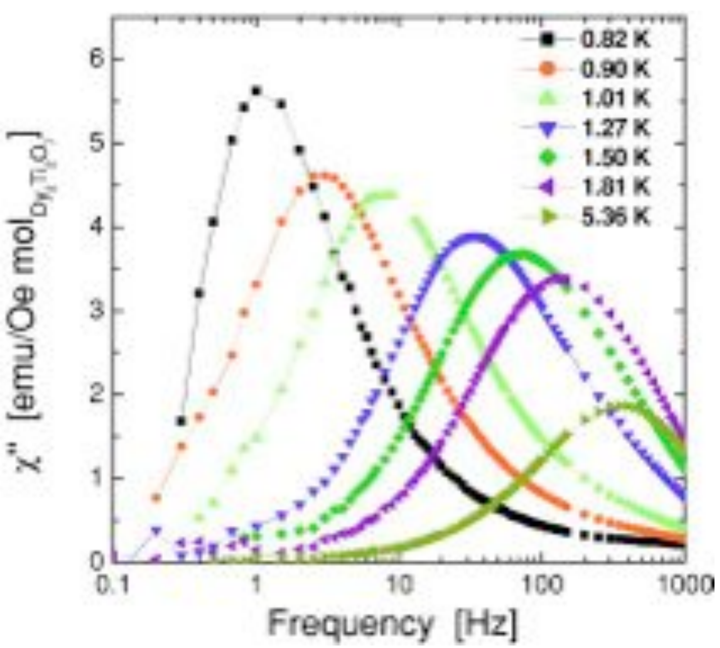
$$= \frac{a_d^2}{25\alpha^2a_0^2} \qquad \left(a_0 = \frac{\hbar}{m_ec\alpha}\right)$$

$$\approx 56000$$

Magnetic Coulomb interaction is *very* weak, but comparable to k_BT at T ~ 1K

Experiment/Theory

- Some nice evidence from magnetic relaxation



Snyder *et al*, 2004

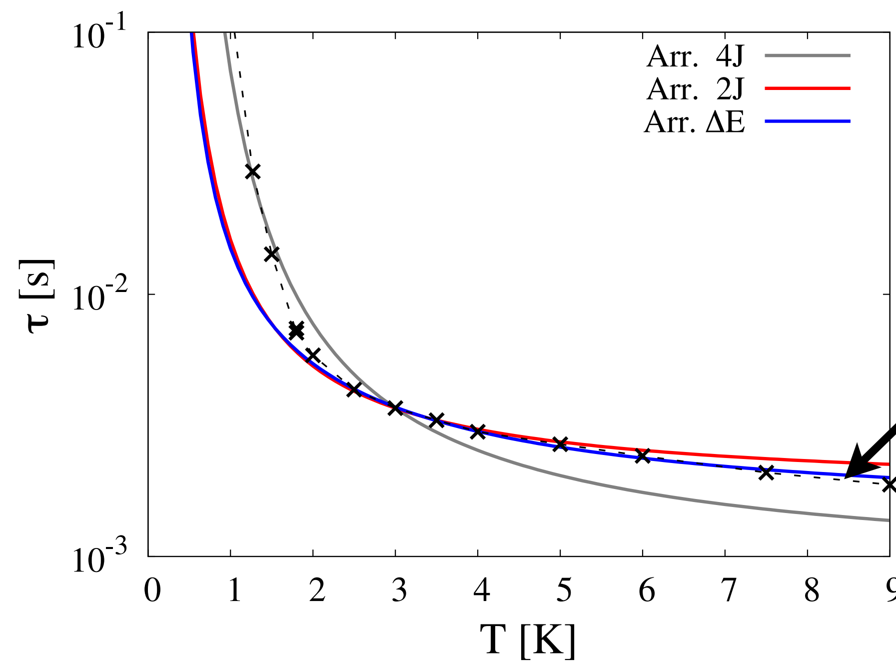


Figure from L. Jaubert's thesis

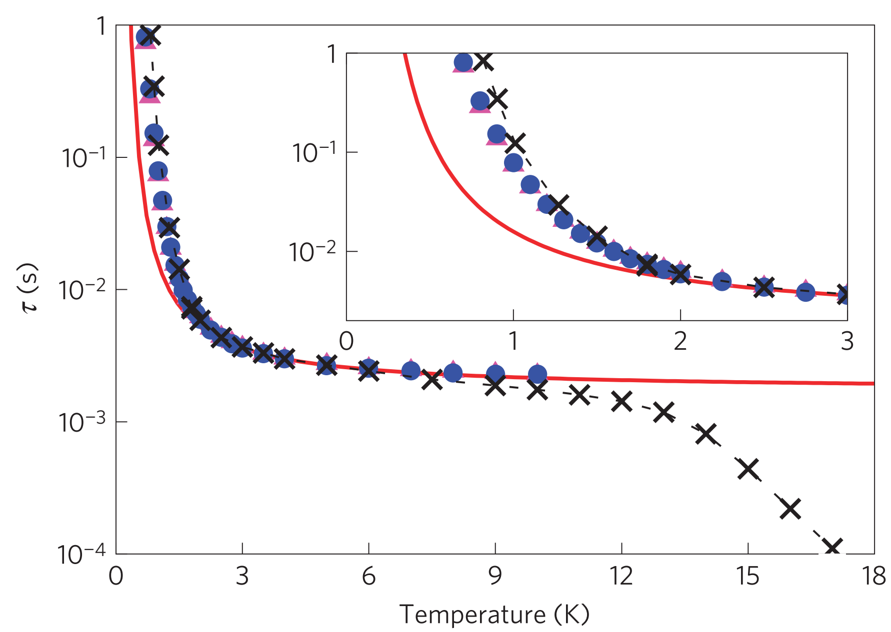
reasonable fit of activated monopoles

$$\tau \sim e^{E_m/k_B T}$$

- Rapid rise below 2K due to Coulomb!

Experiment/Theory

- Theory including Coulomb interactions (Monte Carlo):



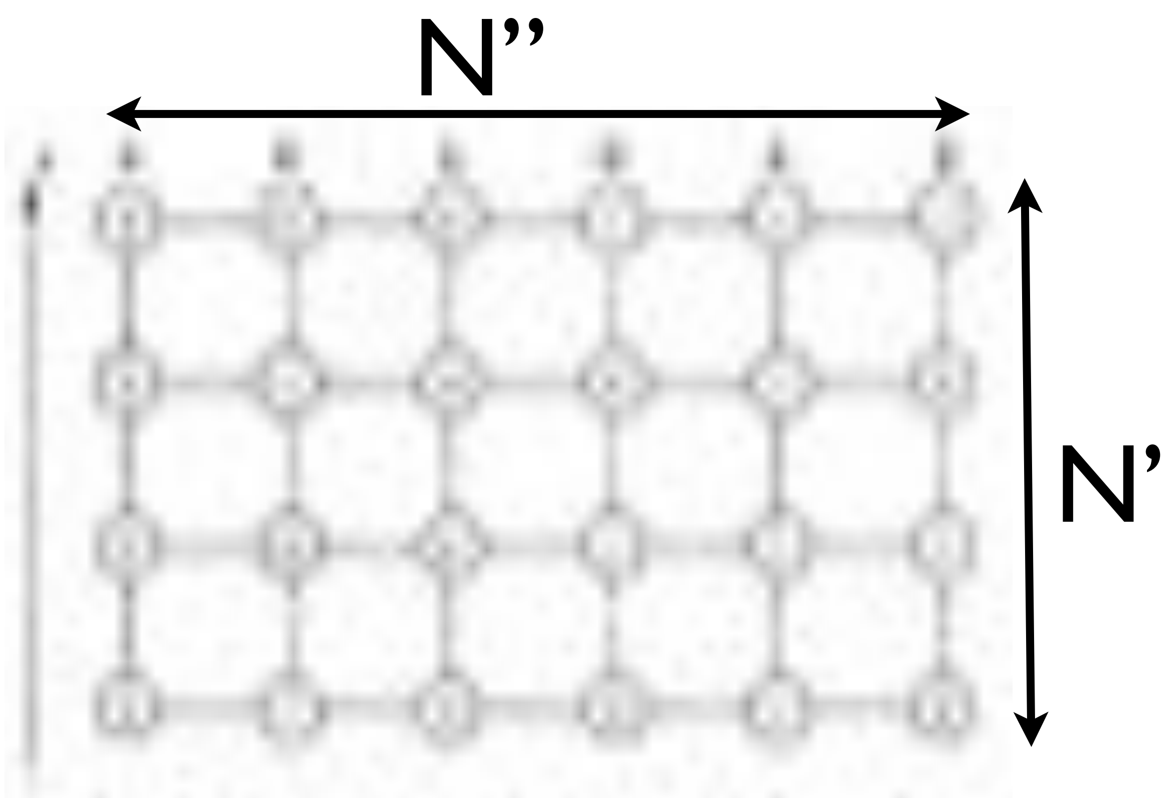
- Rise is due to *binding* of monopole-antimonopole pairs

Order by Disorder

- In spin ice, the ground state degeneracy seems to prevent an ordered phase forming
- Actually, this is not so obvious at low but non-zero temperature
- In fact, many models with ground state degeneracy *break* that degeneracy at $T>0$ due to fluctuations
  - "Order by disorder", due to J. Villain
  - Idea: *free* energy of states is generally different once fluctuations are included

J. Villain *et al*, J. Physique **41**, 1263 (1980).

Domino Model



$$H = -\frac{1}{2}\sum_{ij} J_{ij}\sigma_i\sigma_j$$

J_{AA}, J_{AB} ferromagnetic

J_{BB} antiferromagnetic

$0 < J_{AB} < |J_{BB}| < J_{AA}$

- Ground states are FM A chains and AF B chains, with $2^{N''}$ degeneracy

Order

- However, one can show that the model has a phase transition (by exact solution)
- Evidently it is ordered at low T despite the degeneracy - this is due to fluctuations.
- Let's understand this in some simple limits

Very low T

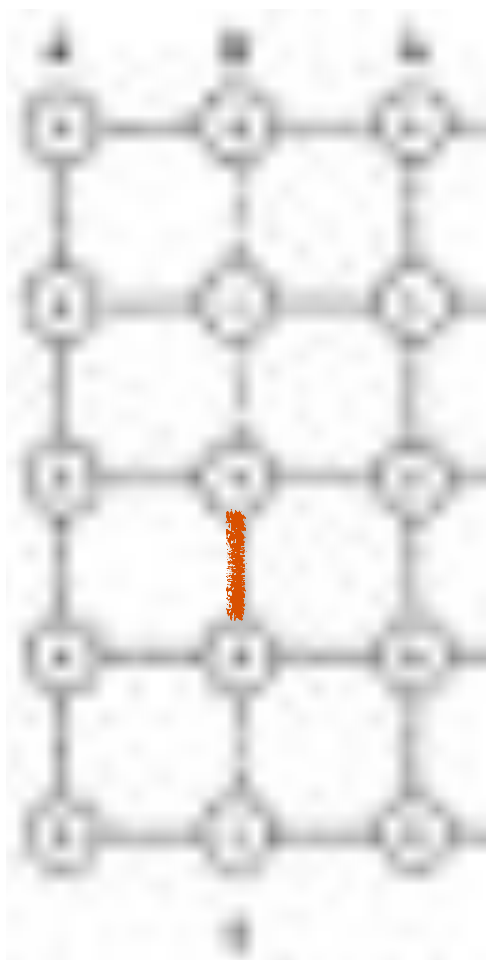
- $k_B T \ll J_{AA}, |J_{BB}|, J_{AB}$: only rare excitations within each chain
  - Ask: is there any preference for successive A chains to be aligned vs anti-aligned?
  - Do this by "integrating out" B chain between each pair of A chains

$$P[\{\sigma_{i\in A}\}] = \frac{1}{Z}\sum_{\sigma_j\in B} e^{-\beta H}$$

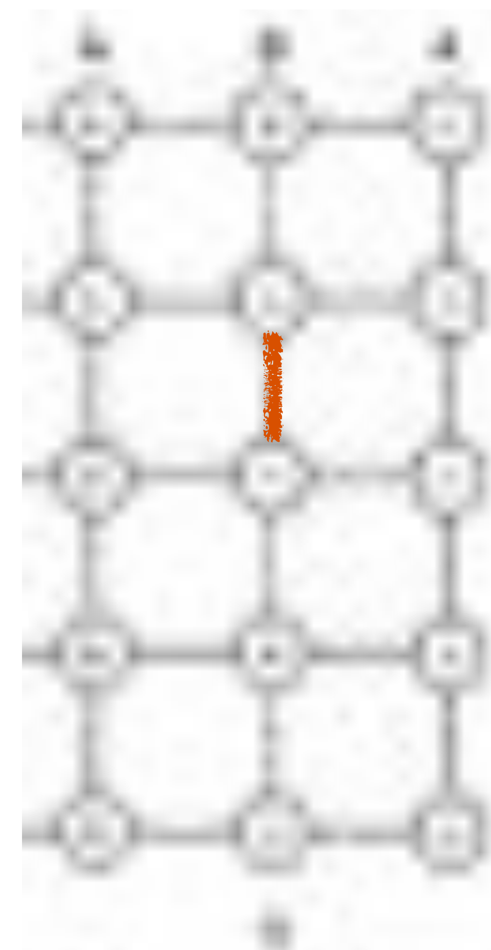
Very low T

- Two cases:

domain wall



excitation lowers J_{AB} energy

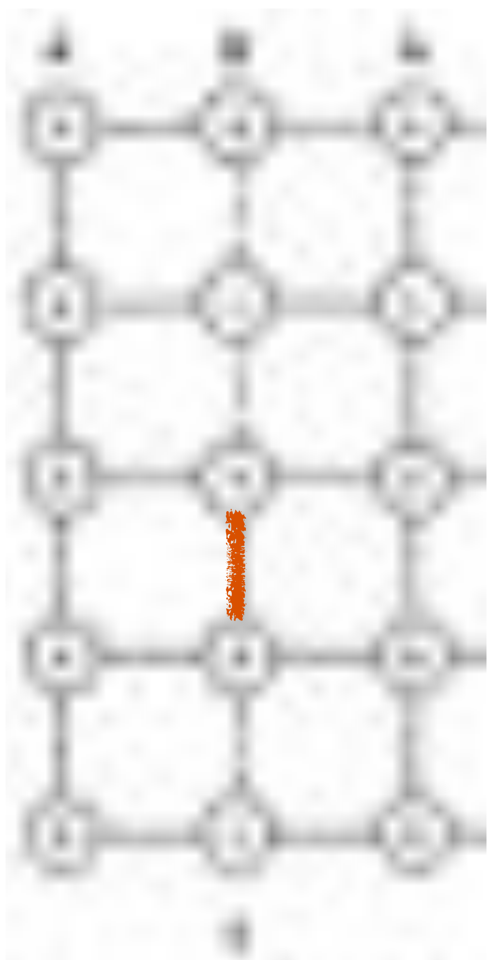


excitation does not lower J_{AB} energy

Very low T

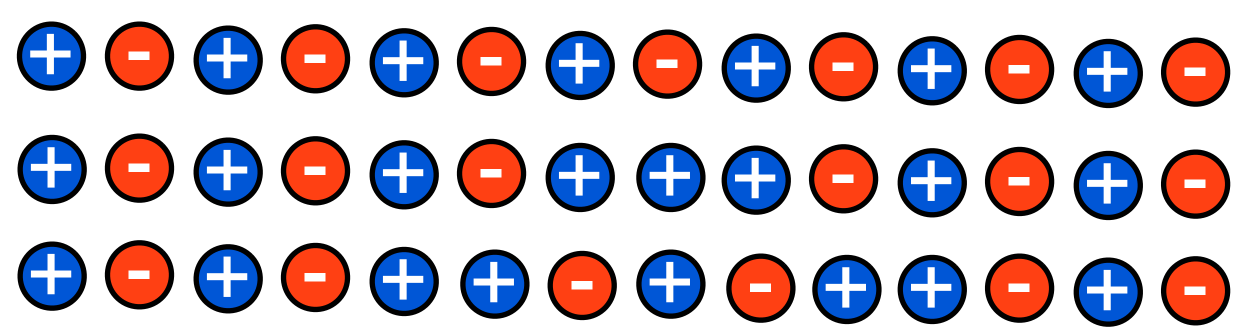
- Two cases:

domain wall



$$H_B = \sum_i \{|J_{BB}|\,\sigma_i\sigma_{i+1} - 2J_{AB}\,\sigma_i\}$$

$$\Delta E_B = 2|J_{BB}| - 2J_{AB}M_{DW}$$

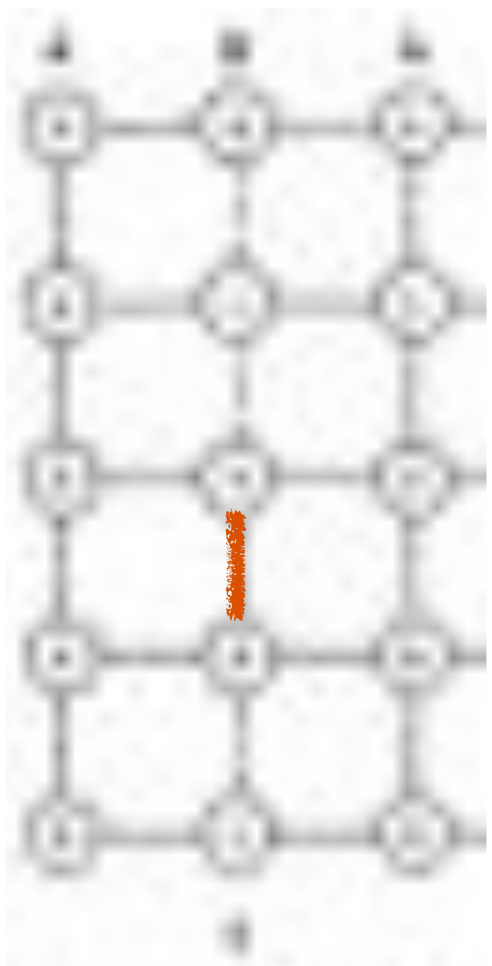


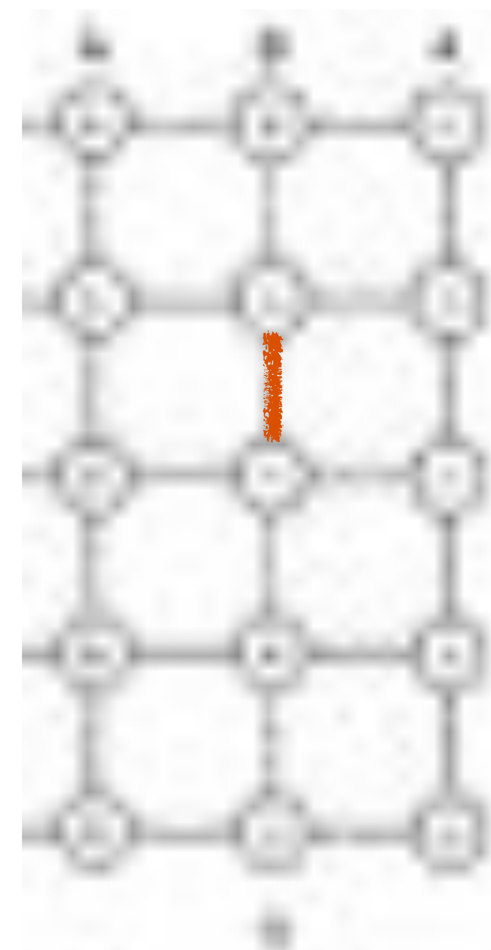
M=2=1+1

Very low T

- Two cases:

domain wall





energy $\Delta E = 2|J_{BB}| - 2J_{AB}$

$\Delta E = 2|J_{BB}|$

note: factor of 2 difference from Villain paper

B partition function

- We can place the domain wall in N'/2 places

$$Z_B \approx Z_{B0}\left(1+\frac{N'}{2}e^{-\beta\Delta E}\right) \approx Z_{B0}e^{\frac{N'}{2}e^{-\beta\Delta E}}$$

- This prefers ferromagnetic ordering

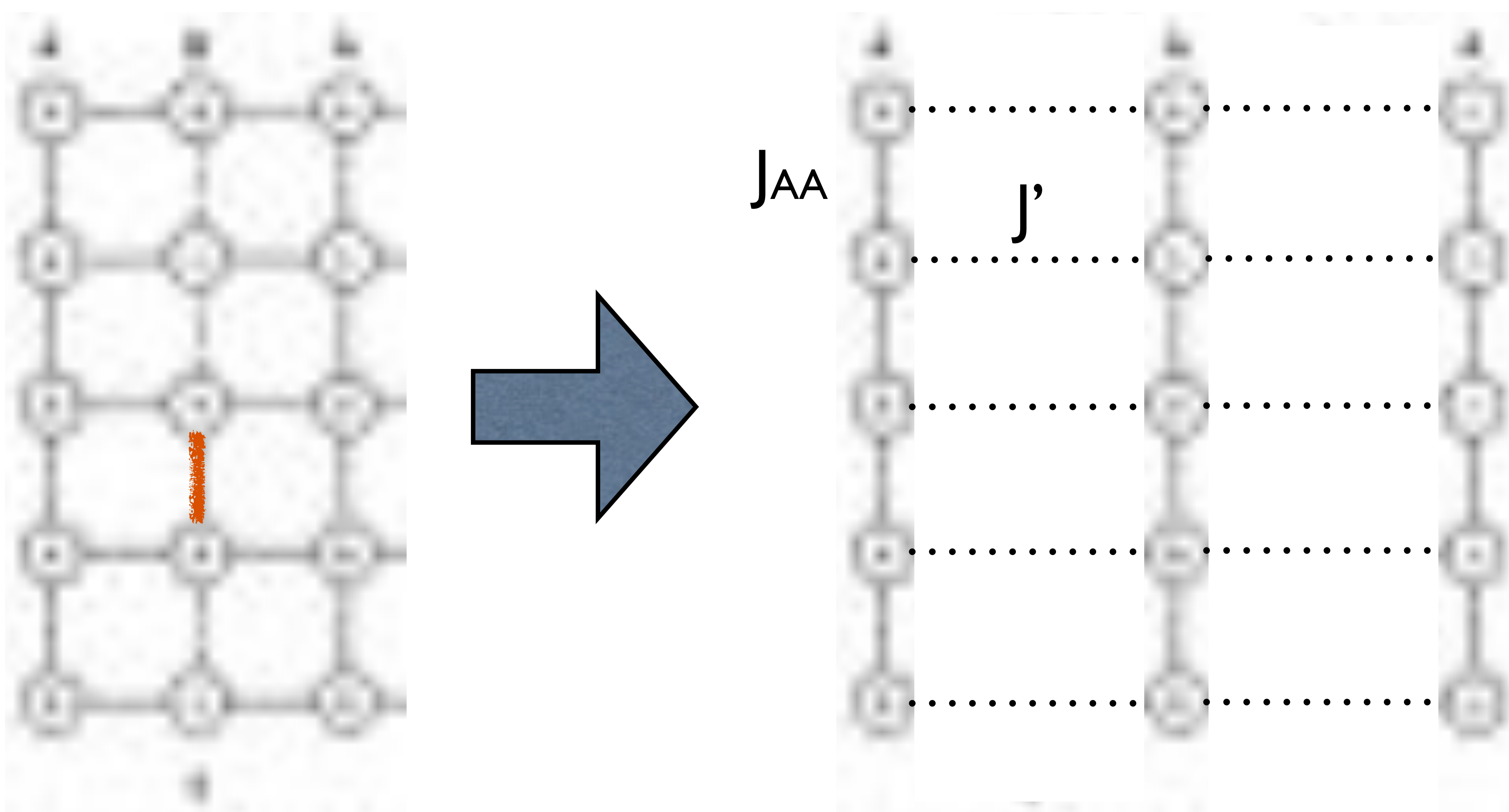
$$\frac{P(++)}{P(+-)} \approx e^{\frac{N'}{2}e^{-2\beta(|J_{BB}|-J_{AB})}}$$

- Effectively this is like a FM exchange

$$2\beta J' = \frac{1}{2}e^{-2\beta(|J_{BB}|-J_{AB})}$$

Order?

- Effective rectangular lattice



J' is shrinking fast at low T

but correlation length of A chains is growing very fast

- Orders if $J'\xi_A \sim k_B T$

Order?

- Estimate
  - 1d Ising $\xi_A \sim e^{2\beta J_{AA}}$
  - Entropy $2\beta J' = \frac{1}{2} e^{-2\beta(|J_{BB}| - J_{AB})}$
- Together

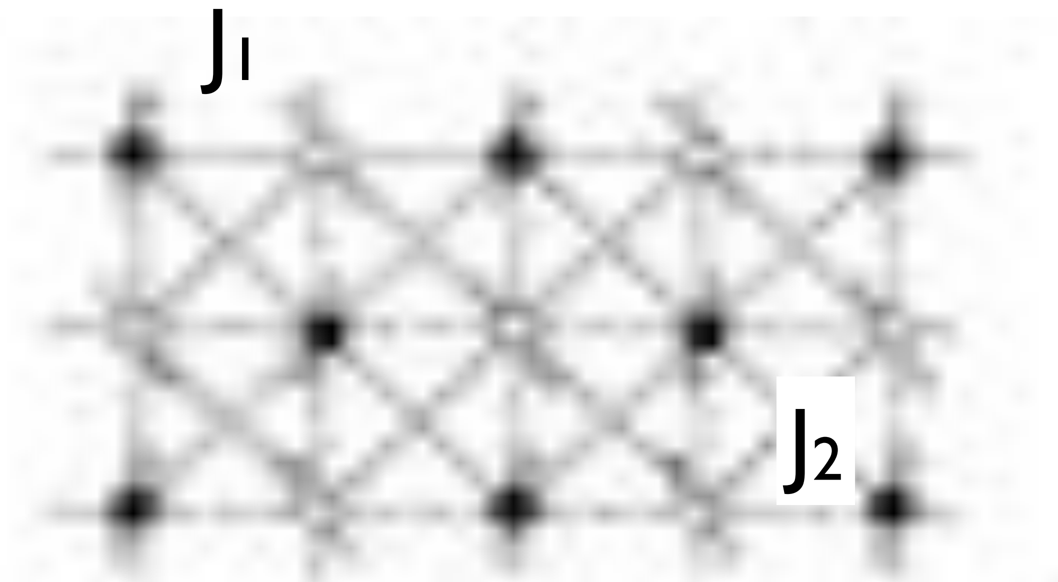
$$\beta J' \xi_A \sim e^{-2\beta(|J_{BB}| - J_{AB}|)} e^{2\beta J_{AA}}$$

$$\gg 1 \qquad\qquad J_{AA} > |J_{BB}| - J_{AB}$$

$\boxed{\text{Thus the A spins are ferromagnetically ordered!}}$

Continuous Spins

- Actual strictly Ising systems are rather rare in magnets, but similar phenomena can occur for continuous spins
- Example: frustrated square lattice "XY" AF - spins are unit vectors in the plane



$J_2 > J_1/2$

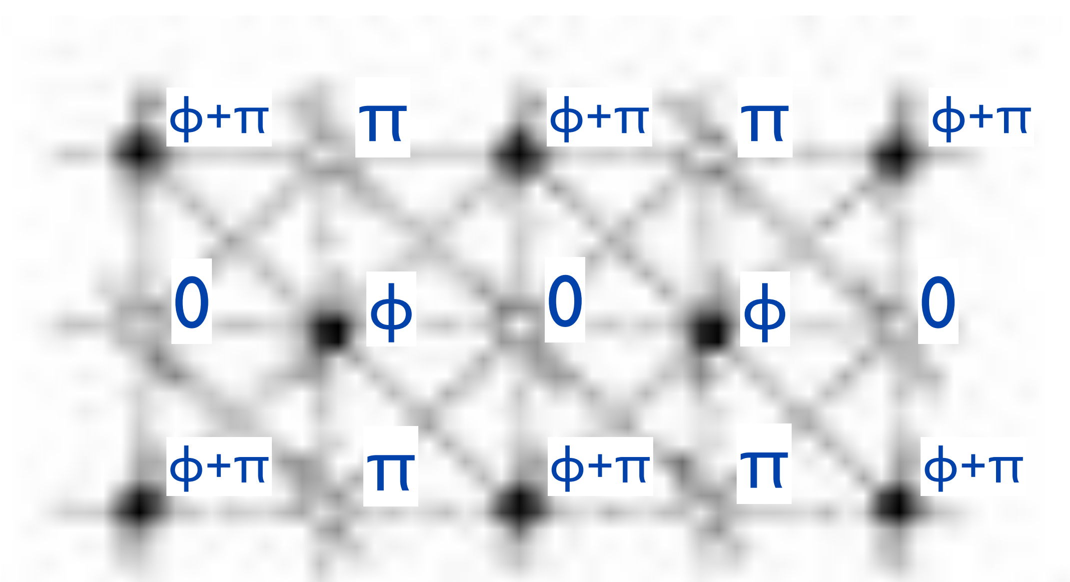
C. Henley, 1989

Thermal fluctuations

- Consider expansion around an arbitrary ground state

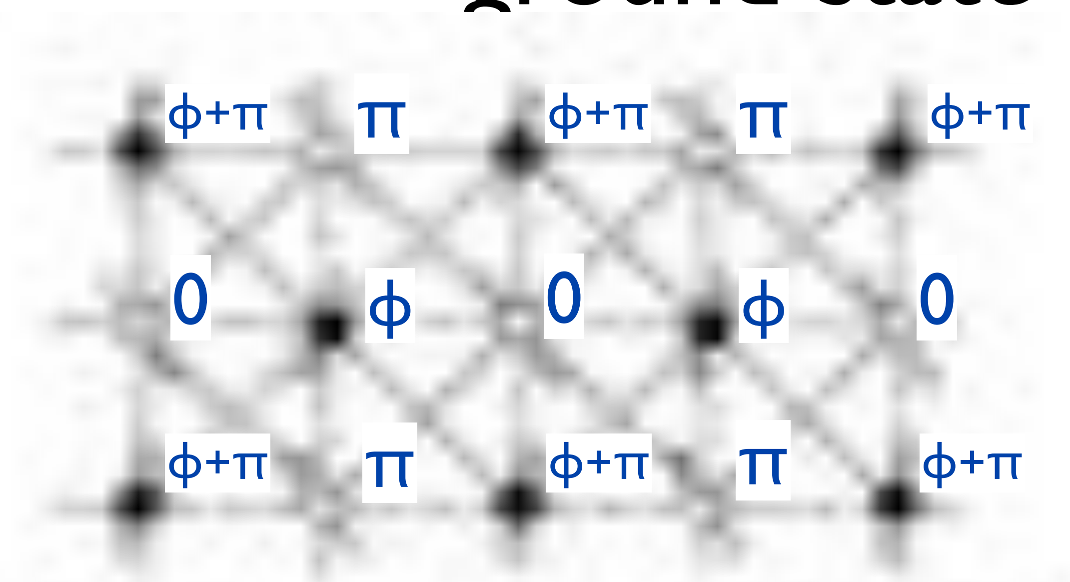
$$H = -\frac{1}{2}\sum_{ij} J_{ij}\cos(\theta_i - \theta_j)$$

$$\approx E_0 + \frac{1}{4}\sum_{ij} J_{ij}\cos(\theta_{ij}^{(0)})(\delta\theta_i - \delta\theta_j)^2$$



Thermal fluctuations

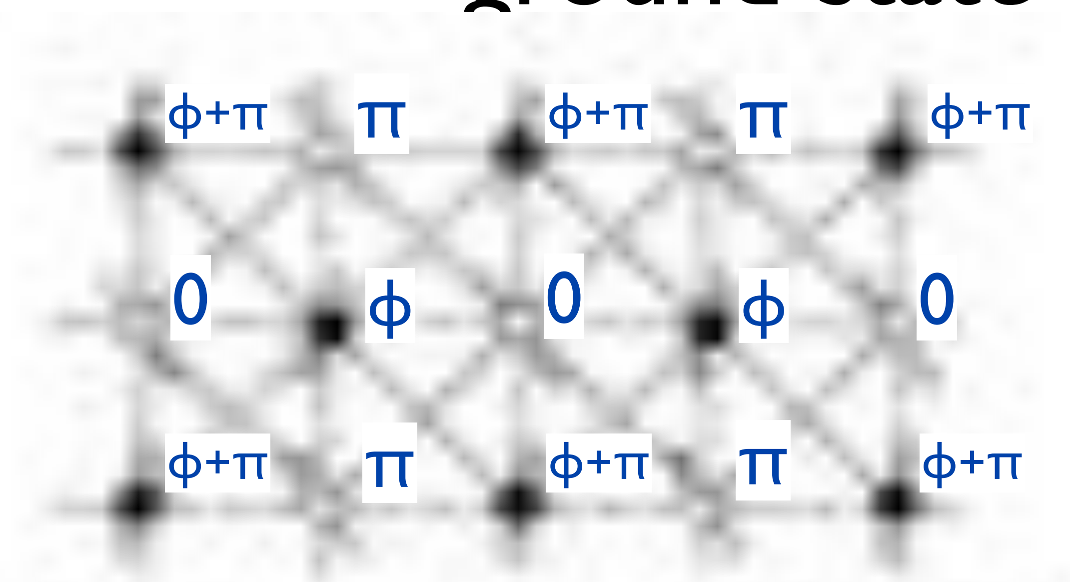
- Consider expansion around an arbitrary ground state



$$H \approx \frac{J_1}{2}\sum_{xy}\cos\phi\left[(\delta\theta_{xy}-\delta\theta_{x+1,y})^2-(\delta\theta_{xy}-\delta\theta_{x,y+1})^2\right]$$
$$-\frac{J_2}{2}\sum_{xy}\left[(\delta\theta_{xy}-\delta\theta_{x+1,y+1})^2+(\delta\theta_{xy}-\delta\theta_{x+1,y-1})^2\right]$$

Thermal fluctuations

- Consider expansion around an arbitrary ground state



$$\delta\theta_{xy} = \frac{1}{\sqrt{N}} \sum_k e^{i\mathbf{k}\cdot\mathbf{r}} \delta\theta_{\mathbf{k}}$$

$$H \approx \frac{J_1}{2} \sum_{\mathbf{k}} 2\cos\phi(\cos k_y - \cos k_x)|\delta\theta_{\mathbf{k}}|^2$$

$$-\frac{J_2}{2} \sum_{\mathbf{k}} \left[4 - 2\cos(k_x + k_y) - 2\cos(k_x - k_y)\right]\right] |\delta\theta_{\mathbf{k}}|^2$$

Thermal Fluctuations

- Collecting terms

$$\delta H \approx \frac{1}{2} \sum_{\mathbf{k}} A_{\mathbf{k}}(\phi) |\delta\theta_{\mathbf{k}}|^2$$

$$A_{\mathbf{k}}(\phi) = 4J_2(1 - \cos k_x \cos k_y) - 2J_1 \cos\phi(\cos k_x - \cos k_y)$$

- Gaussian integral

$$Z \approx e^{-\beta E_0} \int [\prod_{\mathbf{k}} d\delta\theta_{\mathbf{k}}] e^{-\delta H} \sim e^{-\beta E_0} \prod_{\mathbf{k}} \frac{1}{\sqrt{A_{\mathbf{k}}}}$$

Entropy

- Free energy

$$F = -k_B T \ln Z \approx E_0 + \frac{k_B T}{2} \sum_{\mathbf{k}} \ln A_{\mathbf{k}}$$

$$\equiv E_0 - T S_0$$

$$S_0 = -N \frac{k_B}{2} \int \frac{d^2\mathbf{k}}{(2\pi)^2} \ln A_{\mathbf{k}}$$

more entropy if A_k is smaller

$$\ln A_{\mathbf{k}} = \ln[4J_2(1 - \cos k_x \cos k_y)] + \ln[1 - \frac{J_1 \cos\phi}{2J_2} \frac{\cos k_x - \cos k_y}{1 - \cos k_x \cos k_y}]$$

indep. of ϕ

Entropy

- Up to a constant

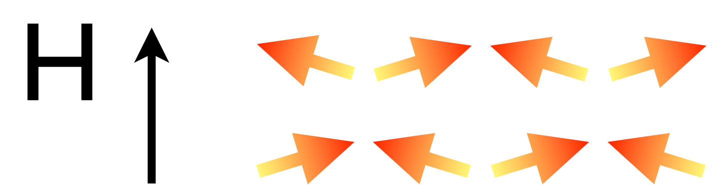
$$S_0(\phi) = \text{const} - \frac{Nk_B}{2}\int \frac{d^2\mathbf{k}}{(2\pi)^2} \ln\left[1 - X\frac{\cos k_x - \cos k_y}{1 - \cos k_x \cos k_y}\right]$$

$$X = \frac{J_1 \cos\phi}{2J_2}$$

- This is an *increasing* function of |X|, so minimized when ϕ=0 or π: *collinear state*
  - See this, e.g. by expanding in X using $\ln(1\text{-}\varepsilon) = \text{-}\varepsilon\ \text{-}\varepsilon^2 + \ldots$

Collinear states

- Why collinear states?
- Think about each sublattice as an antiferromagnet in a fluctuating field due to the other sublattice
  - An antiferromagnet likes to “flop” normal to an applied field



  - The fluctuating field from A sublattice on the B spins is normal to the A spins

Collinear states

- So...the normal to A spins should be normal to B spins, i.e. A and B should be collinear!
- It has been suggested (Henley) that this is rather general.

Quantum Fluctuations

- At T=0, we can imagine quantum zero point motions of the spins plays the role of thermal fluctuations
- Simple idea: quantize the normal mode frequencies corresponding to the modes $\delta\theta_k$:

$$\hbar\omega_{\mathbf{k}} = \sqrt{A_{\mathbf{k}}/m}$$

- This corresponds to the semi-classical "1/S" or spin-wave expansion

Zero point energy

- Harmonic oscillators

$$E_{0-\mathrm{pt}} = \sum_{\mathbf{k}} \frac{\hbar\omega_{\mathbf{k}}}{2} \sim \frac{1}{\sqrt{2m}} \sum_{\mathbf{k}} \sqrt{A_{\mathbf{k}}}$$

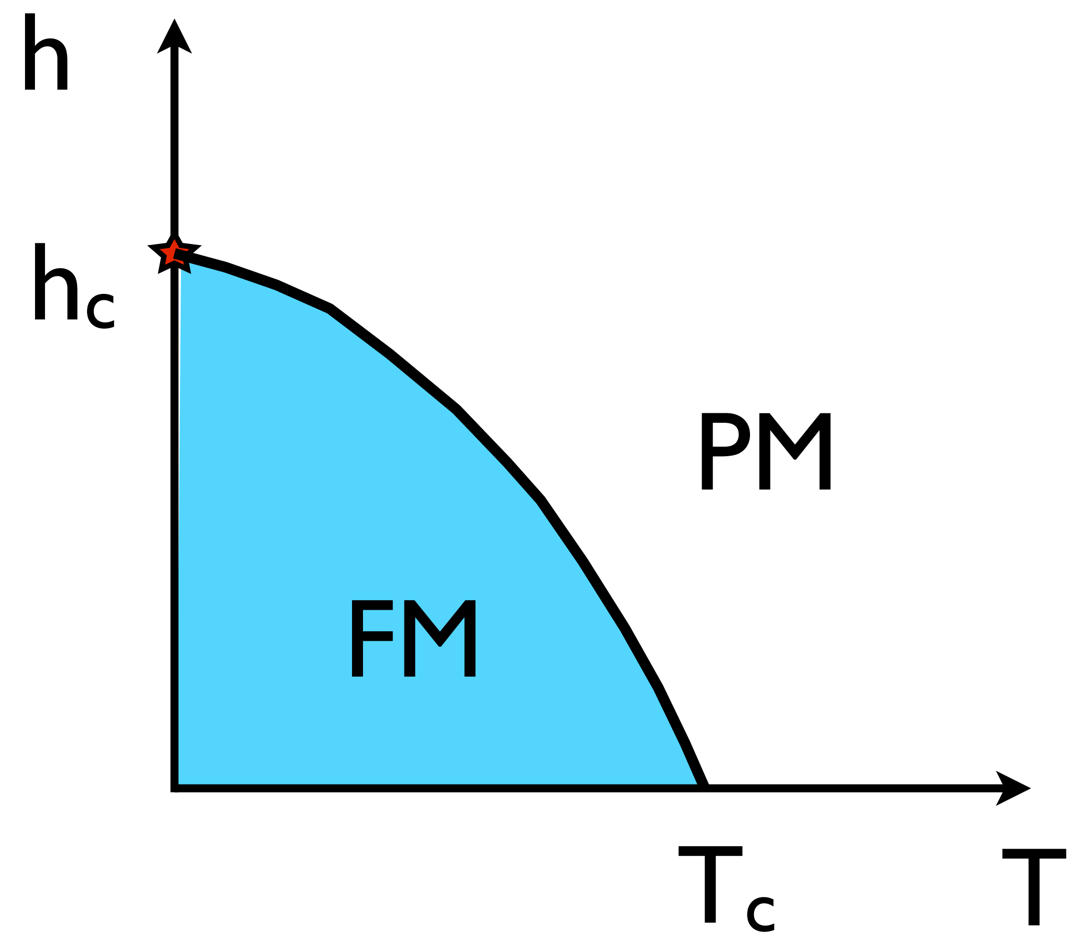
- The zero point energy is again minimized if A_k is smaller -
  - one can check that this is again $\phi=0,\pi$

Seeing ObD

- In models, this is a generic phenomena: small fluctuations break “accidental” degeneracies
- But...many other perturbations also remove the accidental degeneracies
  - e.g. explicit small J’ interaction
  - How can you ever really know - in an experiment - if order is due to disorder or just some interaction you missed?
- Lucile will tell you Thursday!

Quantum phase transitions in metals

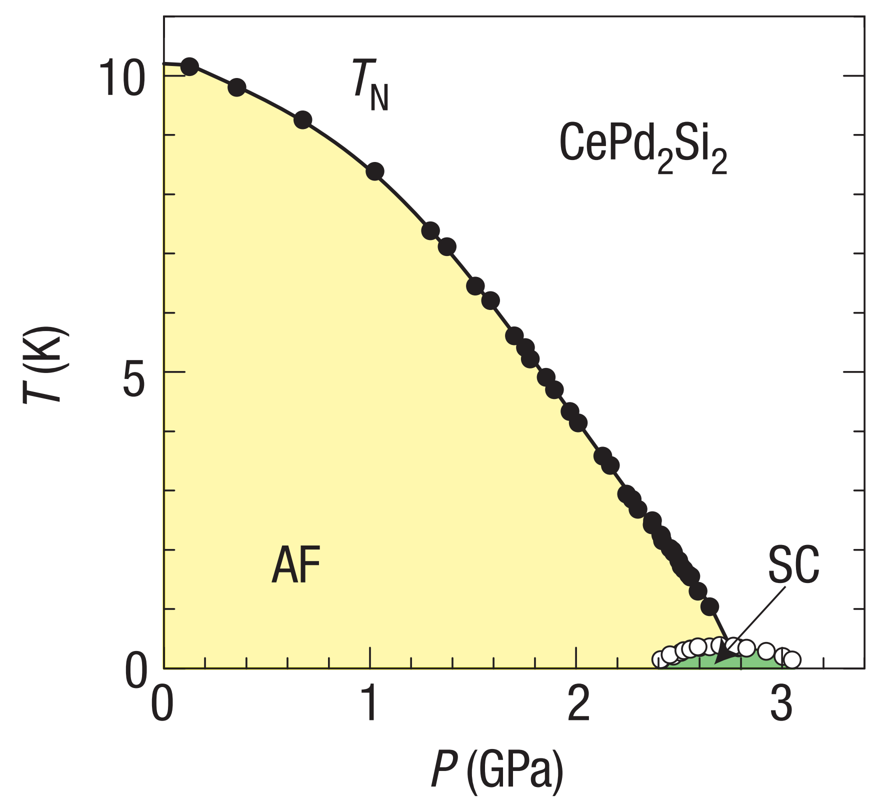
- Some quantum phase transitions are very similar to classical ones
  - recall TFIM



Actually the same field theory describes classical and quantum transitions in the Ising model

But some are not

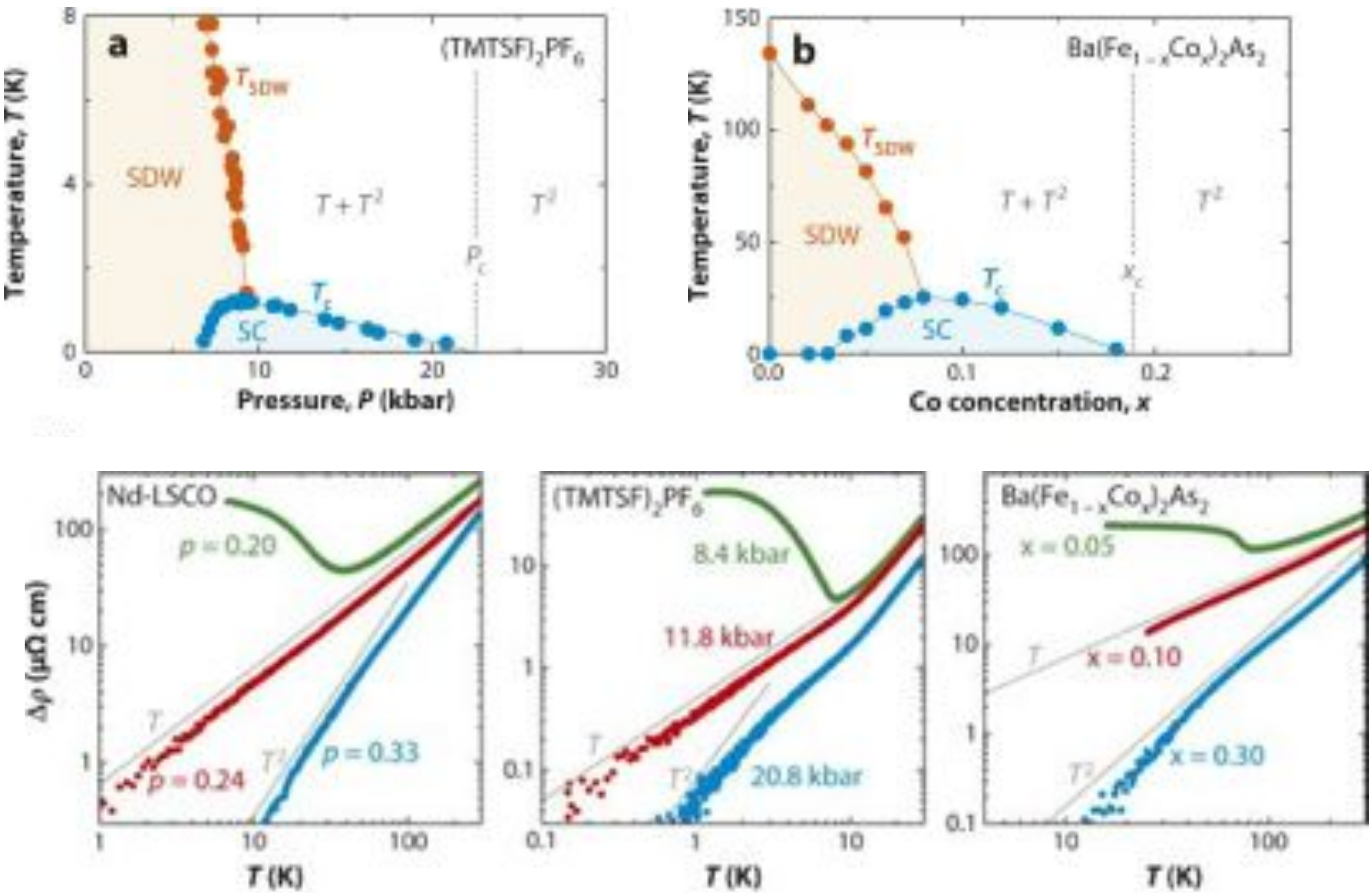
- Especially: quantum phase transitions in metals



"heavy fermion"

- Often superconducting state "covers" QCP
- Critical exponents non-classical
- Anomalous metallic behavior

Linear resistivity



Why does metal make a difference?

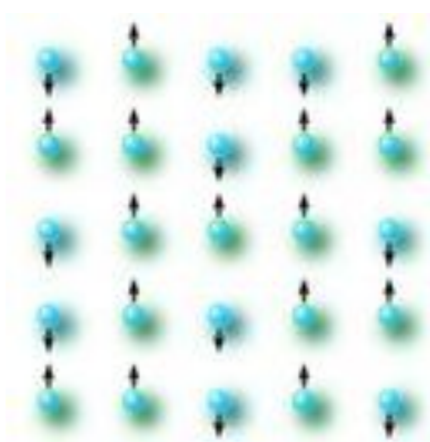
- These phase transitions are nominally similar to those in insulators

$$\langle \vec{S}(\mathbf{r}) \rangle = \vec{\Phi} e^{i\mathbf{Q}\cdot\mathbf{r}} + \text{c.c.}$$

- Might expect a Landau theory in Φ to apply
- But...usual assumption is that the only contributions to the critical behavior come from the ordering fluctuations, as *only these persist to long distances* (up to ξ)
- In a metal, there are other long-distance fluctuations and correlations which are due to low energy quasiparticles

Connection of quantum and classical stat. mech.

- In classical stat. mech., the partition function is a sum/integral over degrees of freedom in *d* dimensions



$$Z = \sum_{\{\sigma_{\mathbf{r}}\}} e^{-\beta \sum_{\mathbf{r}} \mathcal{H}_{\mathbf{r}}}$$

$$\sim \int [d\Phi(\mathbf{r})] e^{-\beta \int d^d\mathbf{r}\, \mathcal{H}[\Phi(\mathbf{r}), \nabla\Phi(\mathbf{r})]}$$

Connection of quantum and classical stat. mech.

- In quantum stat. mech., the partition function is a trace

$$Z = \mathrm{Tr}\,\left[e^{-\beta H}\right]$$

$$= \sum_{\{\sigma^z_{\mathbf{r}}\}} \langle \sigma^z_{\mathbf{r}_1}\sigma^z_{\mathbf{r}_2}\cdots|e^{-\beta H}|\sigma^z_{\mathbf{r}_1}\sigma^z_{\mathbf{r}_2}\cdots\rangle$$

- There is nothing local about the matrix elements of exp[-βH]

Connection of quantum and classical stat. mech.

- Trotter formula

$$Z = \mathrm{Tr}\,\left[e^{-\beta H}\right]$$

$$= \mathrm{Tr}\,\Big[\underbrace{e^{-\delta\tau H}e^{-\delta\tau H}\cdots e^{-\delta\tau H}}_{\text{N factors}}\Big] \qquad \delta\tau = \beta/N$$

$$= \sum_{\{\sigma^z_{\mathbf{r},\tau}\}} \langle\{\sigma^z_{\mathbf{r},\beta}\}|e^{-\delta\tau H}|\{\sigma^z_{\mathbf{r},\beta-\delta\tau}\}\rangle\langle\{\sigma^z_{\mathbf{r},\beta-\delta\tau}\}|e^{-\delta\tau H}\cdots\langle\{\sigma^z_{\mathbf{r},\delta\tau}\}|e^{-\delta\tau H}|\{\sigma^z_{\mathbf{r},0}\}\rangle$$

Connection of quantum and classical stat. mech.

- Trotter formula

$$Z = \mathrm{Tr}\left[e^{-\beta H}\right] = \sum_{\{\sigma^z_{\mathbf{r},\tau}\}} e^{-\sum_{\mathbf{r},\tau}\mathcal{L}_{\mathbf{r},\tau}}$$

$$\sim \int [d\Phi(\mathbf{r},\tau)] e^{-\int d^d\mathbf{r}\, d\tau\, \mathcal{L}[\Phi(\mathbf{r},\tau),\partial_\mu\Phi(\mathbf{r},\tau)]}$$

$$= \int [d\Phi(\mathbf{r},\tau)] e^{-S[\Phi(\mathbf{r},\tau)]}$$

"Euclidean action"

- So one expects there to be a relation between the *d* dimensional quantum problem and a classical-like problem in *d* space and *one* "time-like" direction

Degrees of freedom

- But...in a metal we do not just have spins
  - really the trace must include the states of the electrons

$$H = \frac{1}{2}\sum_{\mathbf{r},\mathbf{r}'} J_{\mathbf{r},\mathbf{r}'}\vec{S}_{\mathbf{r}}\cdot\vec{S}_{\mathbf{r}'} + \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k},\alpha} c_{\mathbf{k},\alpha}$$

$$+J_K \sum_{\mathbf{r},\mathbf{k},\mathbf{k}'} e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}}\vec{S}_{\mathbf{r}}\cdot c^{\dagger}_{\mathbf{k},\alpha}\frac{\vec{\sigma}_{\alpha\beta}}{2} c_{\mathbf{k}',\beta}$$

  - Trace includes S_r and c_k

Degrees of freedom

- But...in a metal we do not just have spins
  - really the trace must include the states of the electrons

$$H = \frac{1}{2}\sum_{\mathbf{r},\mathbf{r}'} J_{\mathbf{r},\mathbf{r}'} \vec{S}_{\mathbf{r}} \cdot \vec{S}_{\mathbf{r}'} + \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k},\alpha} c_{\mathbf{k},\alpha}$$

$$+ J_K \sum_{\mathbf{r}} \vec{S}_{\mathbf{r}} \cdot \vec{s}_{\mathbf{r}}$$

- Trace includes S_r and c_k - so does the action

Path integral

- Formally

$$Z = \int [d\Phi][dc\, dc^\dagger] e^{-S[\Phi, c, c^\dagger]}$$

- We can *try* to reduce this to a *d+1*-dimensional "classical" problem by integrating out c, $c^\dagger$

- How feasible is this?

Integrating out c,c†

- Formally

$$Z = \int [d\Phi][dc\, dc^\dagger] e^{-S[\Phi,c,c^\dagger]} = \int [d\Phi] e^{-S_{\rm eff}[\Phi]}$$

- Fermionic integral may be singular
  - It involves an infinite number of d.o.f.
  - Fermions are gapless: low energy electron/ hole excitations mean fermion correlation functions behave like power-laws at large x,τ

J.A. Hertz, PRB **14**, 1165 (1976)

Hertz Theory

- Formally

$$Z = \int [d\Phi] e^{-S_{\text{eff}}[\Phi]}$$

$$e^{-S_{\text{eff}}[\Phi]} = e^{-S_{\text{spin}}[\Phi]} \int [dc\, dc^\dagger] e^{-S_{\text{el}}[c,c^\dagger]} \underbrace{e^{-J_K \int d^d\mathbf{r} d\tau \left(\vec{\Phi}_{\mathbf{r},\tau} e^{i\mathbf{Q}\cdot\mathbf{r}} + \text{c.c.}\right)\cdot \vec{s}_{\mathbf{r},\tau}}}_{\text{expand this out}}$$

- Result:

$$S_{\text{eff}}[\Phi] = S_{\text{spin}}[\Phi] - \int \frac{d^d\mathbf{k} d\omega_n}{(2\pi)^{d+1}} \frac{\chi_0(\mathbf{Q}+\mathbf{k},\omega_n)}{2} \vec{\Phi}_{\mathbf{k},\omega_n} \cdot \vec{\Phi}_{-\mathbf{k},-\omega_n} + O(\Phi^4)$$

Hertz Theory

- The free electron susceptibility behaves like

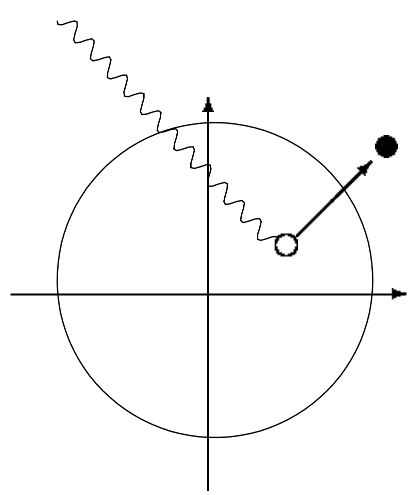
$$\chi_0(\mathbf{Q}+\mathbf{k},\omega_n) \approx c_0 + c_1 k^2 + c_2|\omega_n| \qquad Q \neq 0$$

$$\approx c_0 + c_1 k^2 + c_2 \frac{|\omega_n|}{v_F k} \qquad Q = 0$$

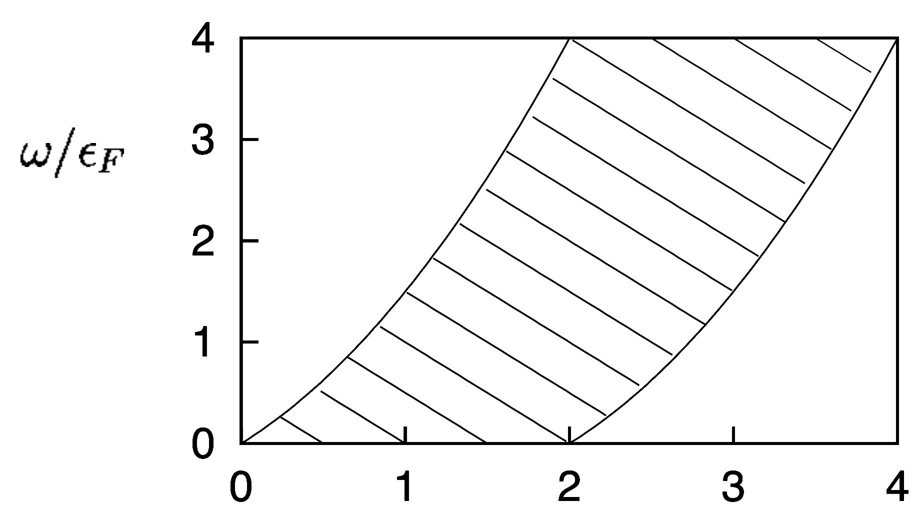
- Importantly, note the *non-analytic* $|\omega_n|$ dependence - this reflects *spin damping*. The spins can exchange energy (and spin) with the electron gas
    - Unfortunately deriving this is a bit complicated, but you would learn it, e.g., in Physics 217b.

Electron-hole pairs

- The non-analytic $|\omega_n|$ term arises because the spin fluctuation can decay into or mix with an electron hole pair at low energy



$Q = k_p - k_h$



Q/k_F

Landau expansion

- Add the fermion term to the Landau theory

$$S = \int \frac{d^d\mathbf{k}d\omega_n}{(2\pi)^{d+1}} \left\{ (k^2 + \frac{|\omega_n|}{k^a} + r)|\Phi_{\mathbf{k},\omega_n}|^2 \right\} + u \int d^d\mathbf{x} d\tau \, |\Phi_{\mathbf{r},\tau}|^4$$

$$= \int \frac{d^d\mathbf{k}d\omega_n}{(2\pi)^{d+1}} \left\{ (k^2 + \frac{|\omega_n|}{k^a} + r)|\Phi_{\mathbf{k},\omega_n}|^2 \right\}$$

$$+ u \int \frac{d^{3d}\mathbf{k}_i d^3\omega_{n,i}}{(2\pi)^{3d+3}} \, \Phi_{k_1,\omega_{n1}} \Phi_{k_2,\omega_{n2}} \Phi_{k_3,\omega_{n3}} \Phi_{-k_1-k_2-k_3,-\omega_{n1}-\omega_{n2}-\omega_{n3}}$$

a=0,1 (Q≠0, Q=0)

Power counting

- Rescaling: $k \to k/b \qquad \omega_n \to \omega_n/b^z$

$$\Phi_{k,\omega_n} \to b^{d+z-d_\Phi}\,\Phi_{bk,b^z\omega_n}$$

$$S = \int \frac{d^d\mathbf{k}\,d\omega_n}{(2\pi)^{d+1}} \Big\{ \boxed{(k^2 + \frac{|\omega_n|}{k^a}} + r)|\Phi_{\mathbf{k},\omega_n}|^2 \Big\} + u \int \frac{d^{3d}\mathbf{k}_i\,d^3\omega_{n,i}}{(2\pi)^{3d+3}}\, \Phi_{k_1,\omega_{n1}}\Phi_{k_2,\omega_{n2}}\Phi_{k_3,\omega_{n3}}\Phi_{-k_1-k_2-k_3,-\omega_{n1}-\omega_{n2}-\omega_{n3}}$$

$z = 2 + a$

$$-d - z - 2 + 2(d + z - d_\Phi) = 0$$

$$d + a - 2d_\Phi = 0$$

$$d_\Phi = \frac{d+a}{2}$$

k versus x scaling

- Note: Fourier transform

$$\Phi_{\mathbf{k},\omega_n} = \int d^d\mathbf{x}\, d\tau\, e^{-i\mathbf{k}\cdot\mathbf{x}-i\omega_n\tau}\,\Phi_{\mathbf{x},\tau}$$

- Space-time scaling

$$\Phi_{\mathbf{x},\tau} = \boxed{b^{-d_\Phi}}\,\Phi'_{\mathbf{x}/b,\tau/b^z}$$

- Hence

$$\begin{aligned}\Phi_{\mathbf{k},\omega_n} &= b^{-d_\Phi}\int d^d\mathbf{x}\, d\tau\, e^{-i\mathbf{k}\cdot\mathbf{x}-i\omega_n\tau}\,\Phi'_{\mathbf{x}/b,\tau/b^z} \\ &= b^{-d_\Phi+d+z}\int d^d\mathbf{x}\, d\tau\, e^{-ib\mathbf{k}\cdot\mathbf{x}-ib^z\omega_n\tau}\,\Phi'_{\mathbf{x},\tau} \\ &= \boxed{b^{-d_\Phi+d+z}}\,\Phi'_{b\mathbf{k},b^z\omega_n}\end{aligned}$$

note difference!

Power counting

- Rescaling: $k \to k/b \qquad \omega_n \to \omega_n / b^z$

$$\Phi_{k,\omega_n} \to b^{d+z-d_\Phi} \Phi_{bk, b^z \omega_n}$$

$$S = \int \frac{d^d\mathbf{k} d\omega_n}{(2\pi)^{d+1}} \left\{ (k^2 + \frac{|\omega_n|}{k^a} + r) |\Phi_{\mathbf{k},\omega_n}|^2 \right\} + u \int \frac{d^{3d}\mathbf{k}_i d^3\omega_{n,i}}{(2\pi)^{3d+3}} \Phi_{k_1,\omega_{n1}} \Phi_{k_2,\omega_{n2}} \Phi_{k_3,\omega_{n3}} \Phi_{-k_1-k_2-k_3,-\omega_{n1}-\omega_{n2}-\omega_{n3}}$$

$$z = 2 + a \qquad r \to b^2 r$$

$$d_\Phi = \frac{d+a}{2} \qquad u \to b^{2-d-a} u = b^{4-d-z} u$$

u is “irrelevant” when d+a>2

Aside: Classical Case

- Power counting $\quad x \to bx \qquad \Phi_x \to b^{-d_\Phi}\Phi_{x/b}$

$$F = \int d^d x \left\{ (\nabla\Phi)^2 + r\Phi^2 + u\Phi^4 \right\}$$

- Gradient term $\quad d_\Phi = \frac{d-2}{2}$
- RG:

$$\boxed{\begin{aligned} r &\to b^2 r \\ u &\to b^{4-d} u \end{aligned}}$$

u is irrelevant for d>4

Upper critical dimension

- It turns out that for $d>4$, one gets *mean field behavior*. We call $d_{u.c.}=4$ the *upper critical dimension*
  - This coincides with - and is a consequence of - the fact that *u* is irrelevant, i.e. that the Gaussian fixed point is stable.
  - Below the u.c.d., critical exponents are non-MF like

Classical scaling for d>4

- Correlation length: ν=1/2

$$\xi = b\, g(r\, b^2, u\, b^{4-d}) = |r|^{-1/2} g(\pm 1, u|r|^{(d-4)/2})$$

- Free energy

$$f = b^{-d}\mathcal{F}(r\, b^2, u\, b^{4-d}) = |r|^{d/2}\mathcal{F}(\pm 1, u\, |r|^{(4-d)/2})$$

  - r>0: $f \sim |r|^{d/2}$
  - r<0: u is necessary for stability

$$f \sim |r|^{d/2}[u\, |r|^{(4-d)/2}]^{-1} \sim r^2/u \qquad \alpha=0$$

$$\boxed{\text{u is a } \textit{dangerously irrelevant} \text{ operator}}$$

Classical scaling for d>4

- Order parameter

$$m \sim b^{-(d-2)/2}\mathcal{M}(\pm 1, u|r|^{(d-4)/2})$$

- m vanishes for r>0 and again is singular for r<0 (m ~ $u^{-1/2}$)

$$m \sim b^{-(d-2)/2}[u|r|^{(d-4)/2}]^{-1/2} \sim |r|^{1/2}$$

β=1/2

Back to Hertz

critical point is "trivial" ?

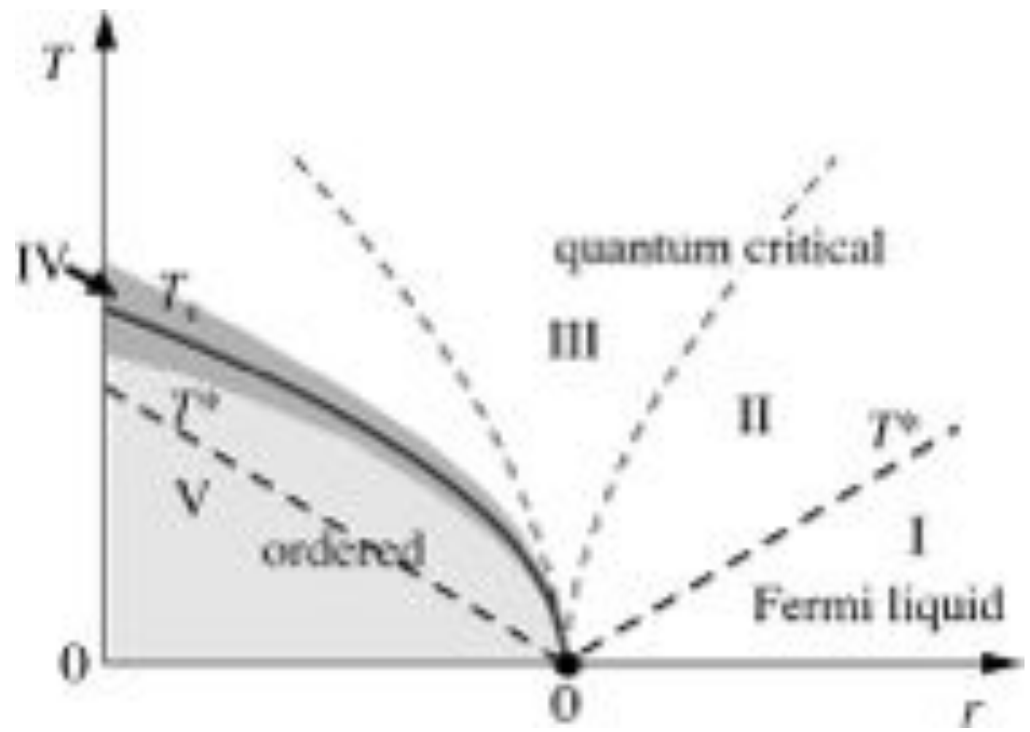
$$S = \int \frac{d^d\mathbf{k} d\omega_n}{(2\pi)^{d+1}} \left\{ (k^2 + \frac{|\omega_n|}{k^a} + r)|\Phi_{\mathbf{k},\omega_n}|^2 \right\} + u \int \frac{d^{3d}\mathbf{k}_i d^3\omega_{n,i}}{(2\pi)^{3d+3}} \Phi_{k_1,\omega_{n1}} \Phi_{k_2,\omega_{n2}} \Phi_{k_3,\omega_{n3}} \Phi_{-k_1-k_2-k_3,-\omega_{n1}-\omega_{n2}-\omega_{n3}}$$

- Additional ingredient for QCP: Temperature scaling:
  - relative to renormalized low energy scale, temperature *increases* under RG

$$k_B T \to b^z \, k_B T$$

  - Also seen from action $S = \displaystyle\int_0^\beta d\tau \cdots$

“Fan” diagram



- Two relevant perturbations of QCP
  - r: deviation from critical point at T=0
  - T: temperature

$$r \to b^2 r \qquad\qquad k_B T \to b^z \, k_B T$$

Quantum critical scaling

- Example: energy density

$$\varepsilon \sim b^{-(d+z)}\mathcal{E}(r\,b^2, k_B T\,b^z, u\,b^{4-d-z})$$

- Let's sit *at* the QCP (r=0) and raise temperature

$$\varepsilon \sim b^{-(d+z)}\mathcal{E}(0, k_B T\,b^z, u\,b^{4-d-z})$$

$$\sim (k_B T)^{\frac{d+z}{z}}\tilde{\mathcal{E}}(u\,(k_B T)^{\frac{d+z-4}{z}}) \;\; \sim (k_B T)^{\frac{d+z}{z}}$$

- Specific heat

$$c_v \sim \partial\varepsilon/\partial T \sim T^{d/z} \qquad \sim T^{3/2}$$ for 3d AF

Quantum critical scaling

- Thermal expansion coefficient

$$\alpha = \frac{1}{V} \left. \frac{\partial V}{\partial T} \right|_p = -\frac{1}{V} \left. \frac{\partial S}{\partial p} \right|_T$$

- We can deduce entropy scaling from specific heat

$$S \sim \int_0^T dT' \, \frac{C(T')}{T'} \sim T^{3/2}$$

- Hence

$$S \sim T^{3/2} \mathcal{S}(r T^{-2/z})$$

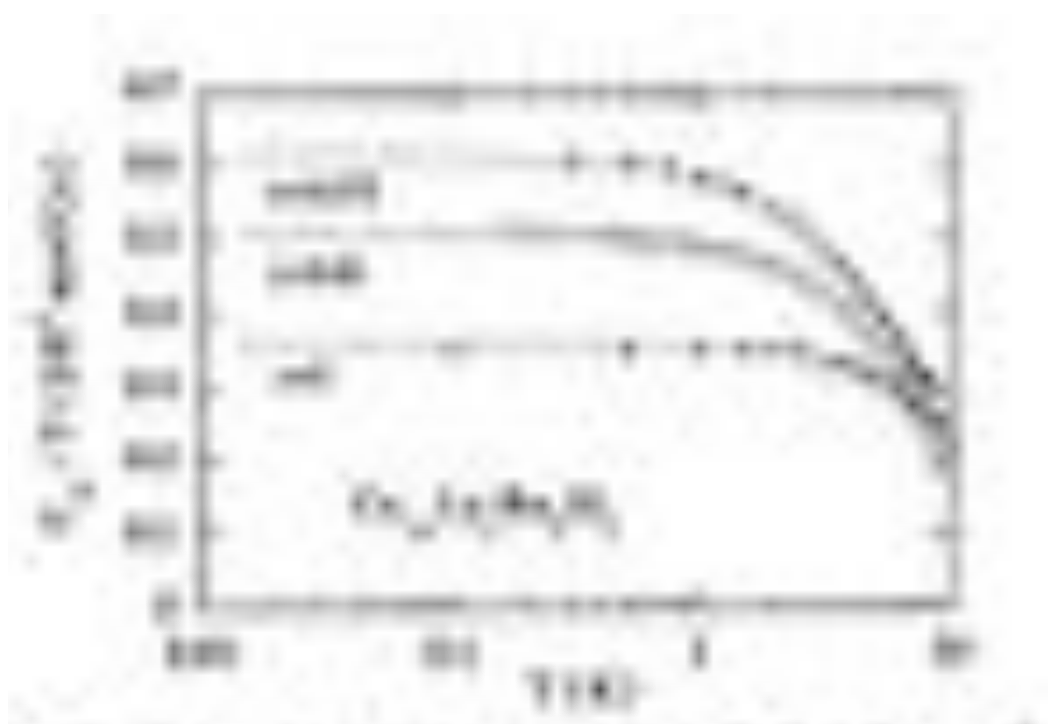
- For a pressure tuned transition then r ~ p

$$\alpha \sim \frac{\partial S}{\partial r} \sim T^{1/2}$$

(it is usually linear in a metal)

$Ce_{1-x}La_xRu_2Si_2$

- This seems to be one of the rare examples where Hertz theory works



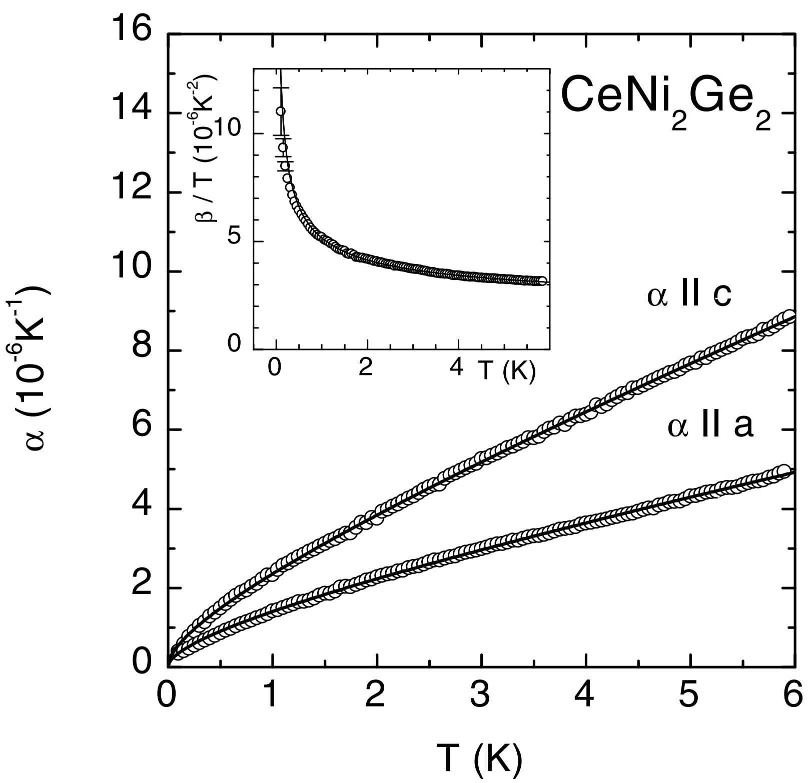
S. Kambe *et al*, JPSJ **65**, 3294 (1996)

$$c_v \sim \gamma T - cT^{3/2}$$

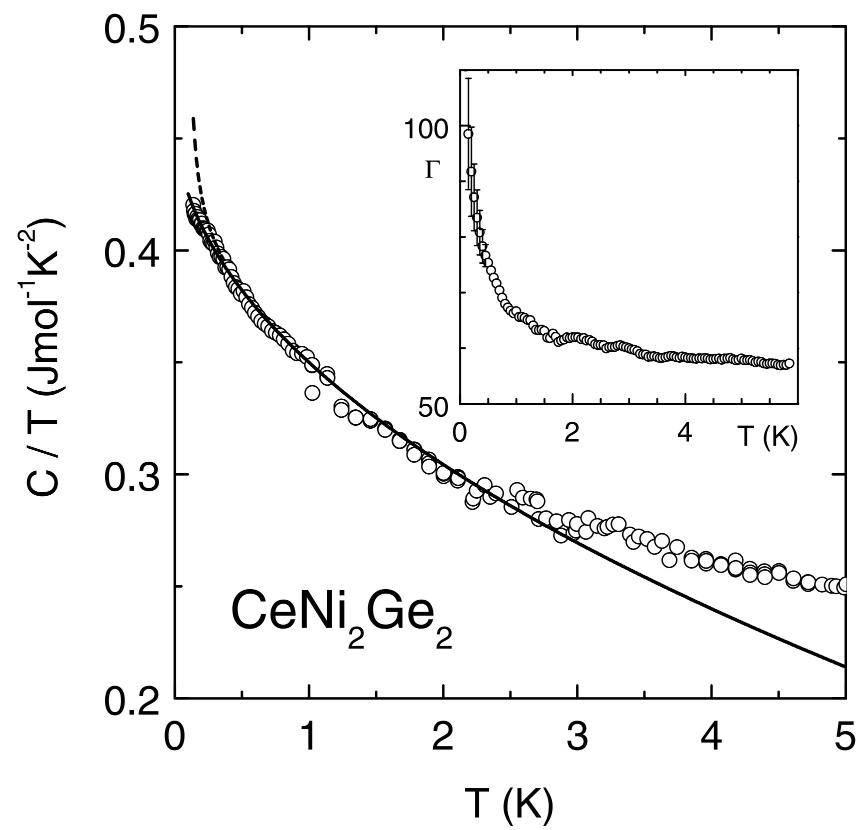
Fit is to a (slightly) more sophisticated theory which includes r $\neq 0$

$CeNi_2Ge_2$

- Believed to be "close" to an AF QCP at ambient pressure



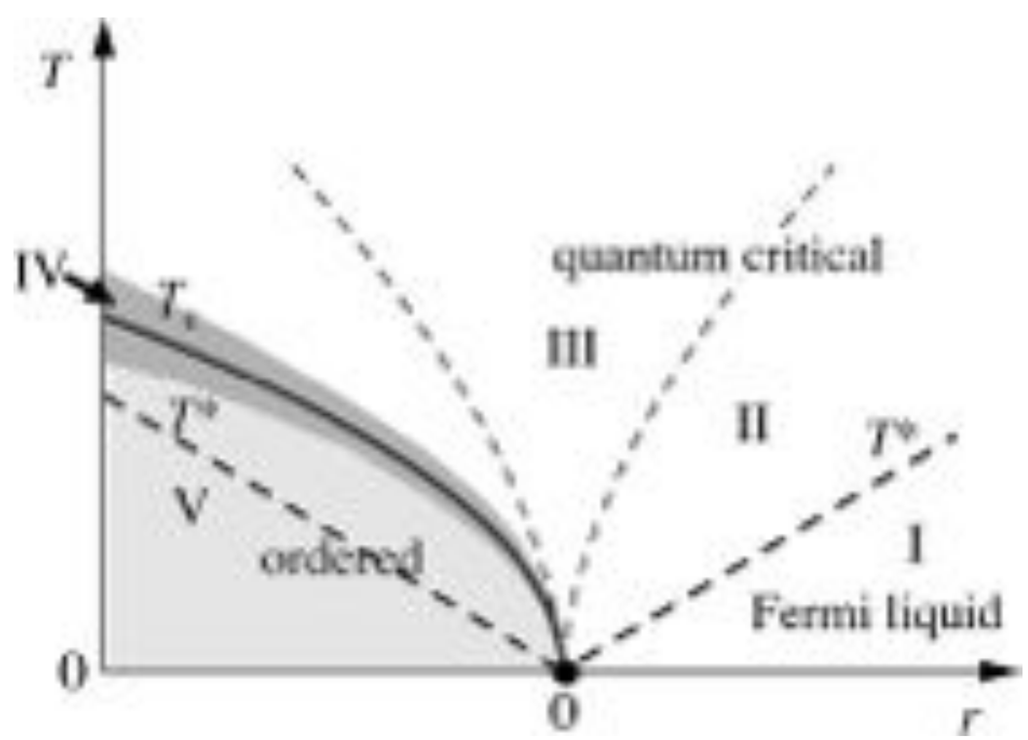
$$\alpha \sim aT^{1/2} + bT$$



$$c/T \sim \gamma - cT^{1/2}$$

Phase boundary

- What determines the shape of the phase boundary?
    - Physics: thermal fluctuations suppress order



Phase boundary

- Fluctuation correction to *location* of critical point

$$S = \int \frac{d^d\mathbf{k} d\omega_n}{(2\pi)^{d+1}} \left\{ (k^2 + \frac{|\omega_n|}{k^a} + r) |\Phi_{\mathbf{k},\omega_n}|^2 \right\} + u \int d^d\mathbf{x} d\tau \, |\Phi_{\mathbf{r},\tau}|^4$$

- "Mean-field"-like approximation (technically self-energy correction)

$$u\Phi^4_{\mathbf{x},\tau} \rightarrow 6u \left\langle (\Phi_{\mathbf{x},\tau})^2 \right\rangle (\Phi_{\mathbf{x},\tau})^2$$

$$\boxed{r_{\text{eff}} = r + 6u \left\langle (\Phi_{\mathbf{x},\tau})^2 \right\rangle}$$

shifts critical point to r<0

The shift

- Fourier (introduce "cutoff" ε)

$$\left\langle \Phi^2_{\mathbf{x},\tau} \right\rangle = \frac{1}{\beta} \sum_{\omega_n} \int_0^{\Lambda} \frac{d^d\mathbf{k}}{(2\pi)^d} \frac{1}{k^2 + |\omega_n| + \epsilon\, \omega_n^2}$$

- We want to extract the small temperature behavior of this. Poisson formula:

$$\frac{1}{\beta} \sum_{\omega_n} = \frac{2\pi}{\beta} \int \frac{d\omega_n}{2\pi} \sum_m \delta(\omega_n - 2\pi m/\beta) = \sum_m \int \frac{d\omega_n}{2\pi} e^{im\beta\omega_n}$$

The shift

- We obtain

$$\left\langle \Phi^2_{\mathbf{x},\tau} \right\rangle = \int_0^\Lambda \frac{d^d\mathbf{k}}{(2\pi)^d} \int \frac{d\omega_n}{2\pi} \sum_{m=-\infty}^{\infty} \frac{e^{im\beta\omega_n}}{k^2 + |\omega_n| + \epsilon\,\omega_n^2}$$

- Separate m=0 (T=0) term:

$$\left\langle \Phi^2_{\mathbf{x},\tau} \right\rangle = I_0 + 2\sum_{m=1}^{\infty} \underbrace{\int_0^\Lambda \frac{d^d\mathbf{k}}{(2\pi)^d} \int \frac{d\omega_n}{2\pi} \frac{\cos(m\beta\omega_n)}{k^2 + |\omega_n| + \epsilon\,\omega_n^2}}_{I_m}$$

Analyzing the integral

- Rotate contour $\omega_m = i\, y$

$$I_m = 2\mathrm{Re}\int_0^\Lambda \frac{d^d\mathbf{k}}{(2\pi)^d}\int_0^\infty \frac{d\omega_n}{2\pi}\,\frac{e^{im\beta\omega_n}}{k^2+\omega_n+\epsilon\,\omega_n^2}$$

$$= 2\mathrm{Re}\int_0^\Lambda \frac{d^d\mathbf{k}}{(2\pi)^d}\int_0^\infty \frac{dy}{2\pi}\,\frac{i\,e^{-m\beta y}}{k^2+iy-\epsilon\,y^2}$$

$$= 2\int_0^\Lambda \frac{d^d\mathbf{k}}{(2\pi)^d}\int_0^\infty \frac{dy}{2\pi}\,\frac{y e^{-m\beta y}}{y^2+(k^2-\epsilon\,y^2)^2}$$

Analyzing the integral

- Rescale: y = T u, k = $T^{1/2}$ q

$$I_m = 2\int_0^{\Lambda} \frac{d^3\mathbf{k}}{(2\pi)^3} \int_0^{\infty} \frac{dy}{2\pi} \frac{y e^{-m\beta y}}{y^2 + (k^2 - \epsilon\, y^2)^2}$$

$$= 2T^{3/2} \int_0^{\frac{\Lambda}{\sqrt{T}}} \frac{d^3\mathbf{q}}{(2\pi)^3} \int_0^{\infty} \frac{du}{2\pi} \frac{u e^{-mu}}{u^2 + (q^2 - \epsilon\, T^2 u^2)^2}$$

$$\approx 2T^{3/2} \int_0^{\infty} \frac{d^3\mathbf{q}}{(2\pi)^3} \int_0^{\infty} \frac{du}{2\pi} \frac{u e^{-mu}}{u^2 + q^4}$$

$$= c_m T^{3/2}$$

So finally...

- We obtain $\left\langle \Phi^2_{\mathbf{x},\tau} \right\rangle = I_0 + cT^{3/2}$
- Which implies

$$r_{\text{eff}} = r + 6u \left\langle \left(\Phi_{\mathbf{x},\tau}\right)^2 \right\rangle$$

$$= r_{\text{eff}}(T=0) + c\,u\,T^{3/2}$$

- So the critical point occurs when

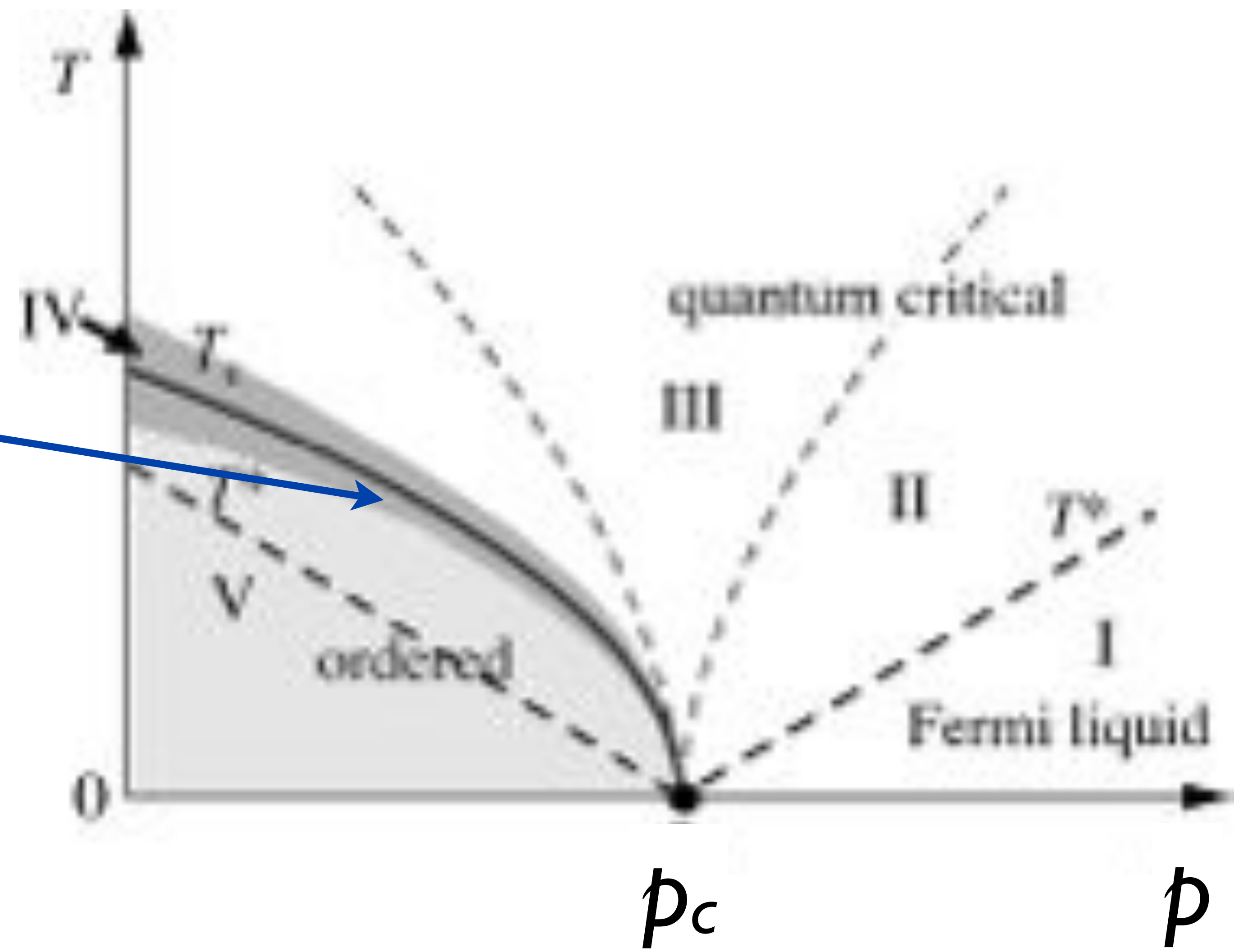
$$r_{\text{eff}}(T) = 0$$

$$\boxed{T_c = \left(\frac{-r_{\text{eff}}(T=0)}{cu} \right)^{2/3}}$$

Phase boundary

- This gives the shape:

$T_c \sim (p_c - p)^{2/3}$



Resistivity

- This is very complicated, even in Hertz theory above the upper critical dimension!
  - but...in general power-law behavior is expected, and usually different from that in an normal metal, i.e. away from the QCP
  - In the simplest approximation, for d=3, z=2, one obtains $\rho \sim \rho_0 + A\,T^{3/2}$ See von Löhneysen *et al*, RMP **79**, 1015, sec. IIIF
  - c.f. in a usual Fermi liquid, at low temperature $\rho \sim \rho_0 + A\,T^2$

Resistivity

- Behavior in $CeNi_2Ge_2$ seems consistent with the "simple" theory, which is expected to apply when the material is not too clean

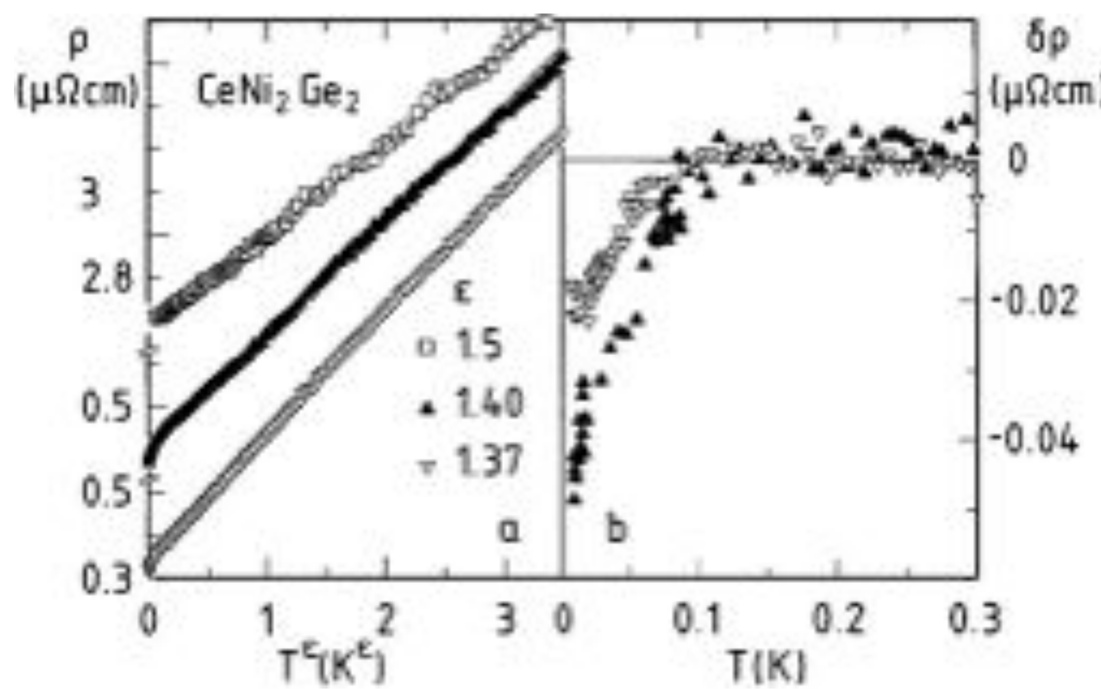


FIG. 2. Electrical resistivity as a function of temperature for three $CeNi_2Ge_2$ samples with $\rho_0 = 2.7\ \mu\Omega$ cm (□), 0.43 $\mu\Omega$ cm (▲), and 0.34 $\mu\Omega$ cm (▽) as ρ vs T^ε with differing exponents ε (a) and $\delta\rho = \rho - (\rho_0 + \beta T^\varepsilon)$ vs T (b).

When does it work?

- Not obvious: the assumption that integrating our electrons does nothing to higher order terms is questionable
- People have looked at these and it seems that it is OK when $Q \neq 0$ in d=3
- For Q=0 in d=2,3 and for $Q \neq 0$ in d=2 there are many singularities not captured by Hertz action
- In all these cases, one should try to study the QCP without integrating out fermions
    - This is much more complicated and still a matter of current research

Beyond LGW

- Driven partly by experiment and partly by theory, recent research in quantum criticality mostly focuses on situations *beyond* the Landau-Ginzburg-Wilson paradigm
- That is, situations in which an approach based on an order parameter alone is inadequate

When do we go beyond?

1. When a neighboring phase has lots of gapless excitations (like in metals!)

2. When a neighboring phase is not described by an order parameter

3. Sometimes even if both the neighboring phases and their excitations are ordinary, unconventional behavior can emerge at the QCP

When do we go beyond?

1. **When a neighboring phase has lots of gapless excitations (like in metals!)**
    1. Failure of Hertz theory for most such QCPs motivates other approaches
    2. Conservation approach: strongly-coupled fermion-boson criticality
    3. Radical approach: "Kondo breakdown"

Kondo effect

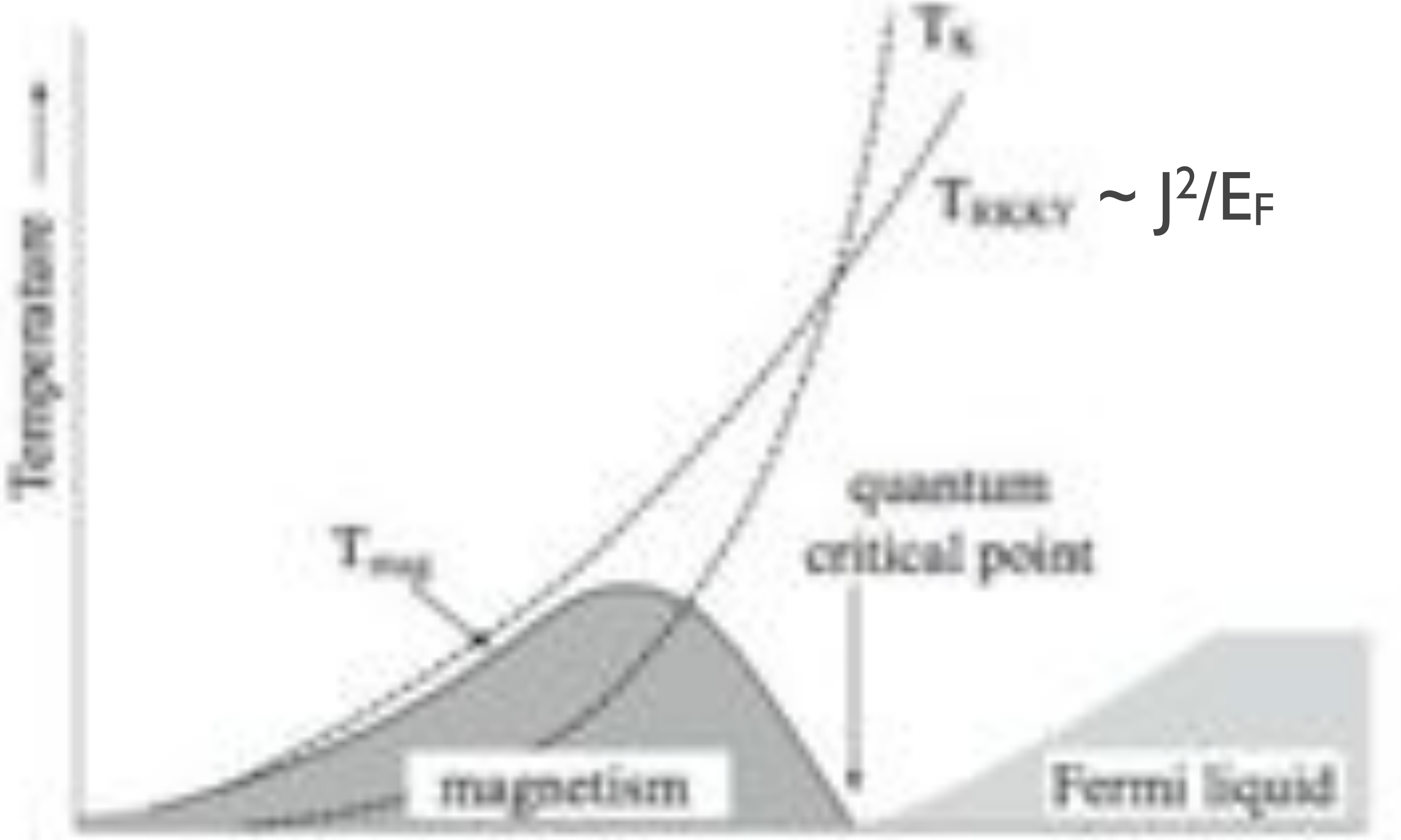
- Kondo effect:
  - a spin can be *screened* by coupling to conduction electrons
  - this happens with a "binding energy" which is exponentially small

$$k_B T_K \sim \epsilon_F e^{-\epsilon_F / J_K}$$

  - When there are many spins, the Kondo effect competes with the tendency of spins to order - RKKY interaction

Doniach diagram

?? Is the QCP a Kondo breakdown transition ??



$T_{RKKY} \sim J^2/E_F$

"heavy fermion": spins included in the carriers

"light" carriers

J/E_F

When do we go beyond?

1. When a neighboring phase has lots of gapless excitations (like in metals!)
2. **When a neighboring phase is not described by an order parameter**
3. Sometimes even if both the neighboring phases and their excitations are ordinary, unconventional behavior can emerge at the QCP

Phases without order parameters

- Phases are more fundamental - and more important - than phase transitions
- Usually, they are distinguished by symmetry
- But phases may differ even with the same symmetry
  - Excitations or other properties may be qualitatively different in two phases

Phases without order parameters

- Example: metal versus insulator
  - both are possible with the same symmetry, but excitations differ qualitatively, as does conductivity
  - but at $T>0$, they are the same phase
  - one can still have a $T>0$ *first order* "Mott transition", e.g. VO_2, V_2O_3,...
  - still not known if $T=0$ transition could be continuous
- There are other types of "quantum order" that can distinguish a phase

Mott transitions

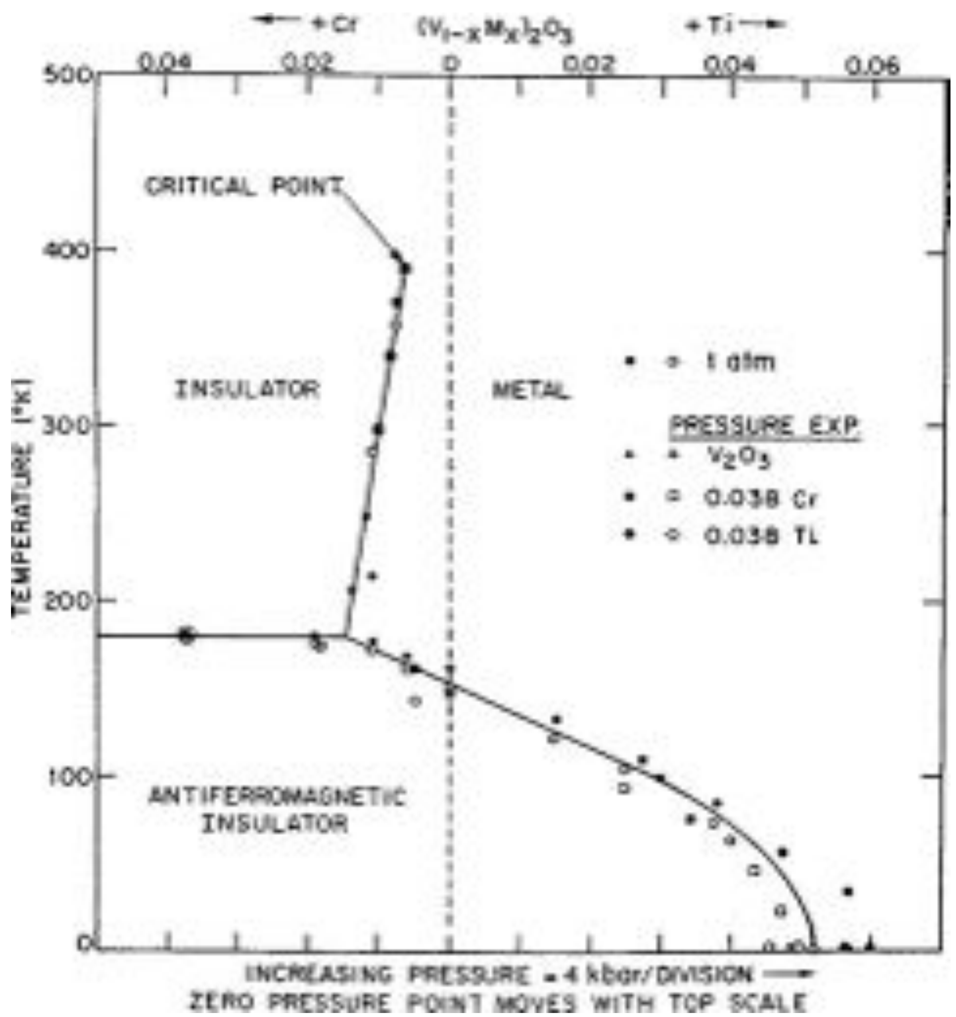


FIG. 70. Phase diagram for doped V_2O_3 systems, $(V_{1-x}Cr_x)_2O_3$ and $(V_{1-x}Ti_x)_2O_3$. From McWhan *et al.*, 1971, 1973.

Quantum orders

- Simplest cases are quantum phases in which there is a gap to all (bulk) excitations
- In this situation, there are "topological orders"
  - e.g. "Topological Insulators" : just non-interacting band insulators which are distinct from usual ones by "twisting" of wavefunctions of occupied bands
  - more interesting are "topological phases" : ground states of interacting electrons that host exotic excitations with fractional (or nonabelian) statistics (Q)

Examples?

- quantum Hall state (TI)
- toric code
- quantum spin liquid (RVB)
- entanglement entropy
- deconfined quantum critical points