1
→ this material where ObD takes place is $Er_2Ti_2O_7$

2
→ Er is a rare-earth (~~...~~

Er^{3+} is magnetic $4f^{11}$ will return to this below

Ti ~~is~~ unimportant

O "mediates" the interactions between the Er moments

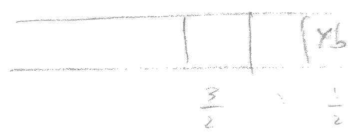
3
→ Er sits on a pyrochlore lattice

↳ recall spin ice · same chemical stoechiometry.

4
→ this means there are unpaired electrons (unfilled shell).

→ $L = 6$?

$S = \frac{3}{2}$?



→ Er is heavy (bottom of the periodic table)

⇒ large spin-orbit coupling $= \vec{L}\cdot\vec{S}$ (relativistic effect)

↳ good QN "is" $\vec{J} = \vec{L} + \vec{S}$

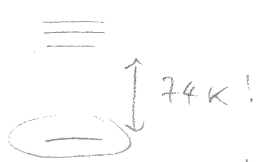
$^4I_{15/2}$

→ manifold selected by $\underbrace{\text{Hund's rules}}_{\text{215 or 223 class}}$: $J = \frac{15}{2}$ $L^2 =$ $S^2 =$

6
→ crystal fields i.e. electric fields of the ~~elect~~ atoms (protons mostly) split (oxygens are important) the degeneracy of the manifold (acts on the orbital part.  etc.)

∝ different for each.

5
→ doublets · Kramer's degeneracy (half integer J)
result (ugly Electron paramagnetic resonance).



effective
2 state system : "spin" $\frac{1}{2}$ ← call that spin & use $\vec{S}$.

7
→ now we want to ask: what's the Hamiltonian? ← need it to make progress (specific to ETO at least).

↙ ep. 1M. 20-3

→ 2-spin interactions (most important contributions & allowed by symmetry)

$\sum_{i,j \atop \mu,\nu} J_{ij}^{\mu\nu} S_i^\mu S_j^\nu$

\+ consider $\vec{S} = (\cos\alpha\, \hat{a}_i + \sin\alpha\, \hat{b}_i) = \mathrm{Re}[\Phi^*(\hat{a}_i + i\hat{b}_i)]$ ← definition

↳ meaning: for well chosen basis

\+ write $F = b|\Phi|^2 + a\Phi^2 + a^*\Phi^{*2}$ completely general for two spin interactions assuming the Ansatz (*)

BUT :

3-fold

$\frac{2\pi}{3}$

↑ takes bonds into one another.

\+ 6 fold terms ↙ allowed can come from 6-spin interactions (tiny) 10^{-9} meV or fluctuations

→ ... be able to write low-en theory which depends on the gradient of the angle only.

↳ ... spin wave mode.

→ continuous deg. ROBUST Used only symmetries. Estimate S^6 term → tiny

& turns out ground state for Er.

↳ Goldstone mode

↳ low en.

→ NN interactions dominate (exchange decays exponentially w/ distance of orbital overlap & orbital $\sim e^{-\lambda r}$)

↳ consider just those

→ know one of them! spin ice term $J_{zz} S_i^z S_j^z$

→ other terms: $J_\pm (S_i^+ S_j^- + S_i^- S_j^+)$ ...

→ know (+ experimental evidence) that mostly classical → should remind you of the ObD description did earlier today

write the terms using what's called "Holstein-Primakoff" expansion.

$\vec{S} =$

→ have oscillators which have subject to quantum fluctuations.

→ what are the ω's ?

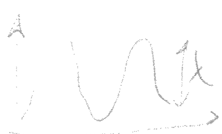
↑ what we need to know

$e^{-\beta E}$

↳ need to know H & then compute ω.

write H + HP expansion

low en theory.

→  depend on α (num. calc)

↖ ~~fixed~~ analytic approx if have time.

→ excitations in S.

→ gap → consequences for C_v ... T^3 write down expansion.

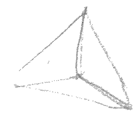
* 2-spin interactions (6-spin interactions are also allowed by symmetry & come from excited doublets, but are completely negligible)

i.e. $\frac{1}{2}\sum_{\substack{i,j\\ \mu\nu}} J_{ij}^{\mu\nu} S_i^\mu S_j^\nu = H$

* consider (informed choice) w/ translational invariance

$\vec{S} = \cos\alpha\, \hat{a}_i + \sin\alpha\, \hat{b}_i = \mathrm{Re}\left[\Phi^*(\hat{a}_i + i\hat{b}_i)\right]$ ← defines Φ $\qquad \Phi = \rho e^{i\alpha}$

drawn on the picture



* write $F = a\Phi^2 + a^*\Phi^{*2} + b|\Phi|^2$ nothing else one can write
F will be of the form b/c of TR.

→ there is not just TR, but also geometric symmetries

e.g.

C_3 3-fold rotation

$\alpha \to \alpha + \frac{2\pi}{3}$ easy to see for $\vec{S}_0$ here

→ true (not easy to see!) for the others

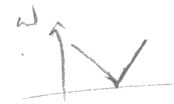
↳ $\Phi = \rho e^{i\alpha} \to \rho e^{i(\alpha + \frac{2\pi}{3})} \Rightarrow \Phi \to \Phi e^{i\frac{2\pi}{3}}$

$\Rightarrow \quad a = a^* = 0$

F is independent of α!

i.e. "U(1)" symmetry
↓
circle

consequences: "Goldstone mode" (C^0 sym)



← excitation spectrum

gapless

→ can write Landau free energy in terms of gradients of α only

→ $S = \int d^3r\, d\tau \left[\frac{\kappa}{2}(\partial_\tau \alpha)^2 + \frac{\kappa_\mu}{2}(\partial_\mu \alpha)^2\right]$

* 6^{th} order terms will come in as $\frac{1}{2}\underbrace{\cos 6\alpha}_{\text{symmetries}}$ $\sim(\Phi^6 + \Phi^{*6})$

note: * used only discrete symmetries to prove C^0 degeneracy

= "accidental" degeneracy

* symmetry-protected degeneracy, did not use any specific coefficients. need to calculate the ω's

higher-order allowed terms: Φ^6 etc but negligible when not from fluctuational origin. ⇑

↳ ObD quantum here

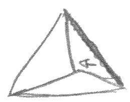
* indeed ground (& stable) state.

Σ for this need the specific Hamiltonian

→ said 2-spin int. $J_{ij}^{\mu\nu} S_i^\mu S_j^\nu$

→ constrained by symmetry i.e. not $\underbrace{3\times3}_{9}\times\underbrace{4\times4}_{16} = 144$ by just 4!

$16 \times 9 = 144$ $\quad 5 \quad 12\times12$!



symmetries turn the bonds into one another

need to work out the details. Can think of 2 sites too but complicated.

so: know one term already: cf studied w/ Leon

spin ice: $H = J_{zz} \sum_{\langle ij \rangle} S_i^z S_j^z$ local bases.

→ get the coefficients by fits to neutron scattering, will return to this later

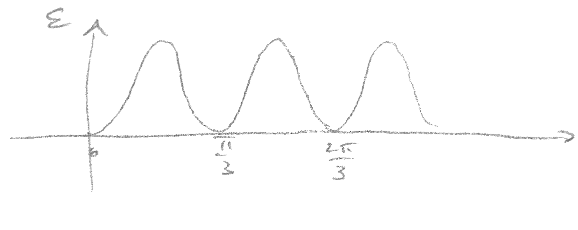
→ get the ω's using spin wave theory → HP other sheet.

the $\omega(k)$'s
→ ~~they~~ depend on α (just like in the previous example where $A_k(\underline{\phi})$

⇒ the zero point energy $= \sum_k \frac{\hbar \omega_k(\alpha)}{2}$

$\varepsilon \sim \frac{\lambda}{2} \cos 6\alpha$

$\lambda > 0$



→ domains

* can write a "low-energy (effective) action for the system at $T=0$

$\updownarrow$

→ assume slow time & space variations of α:

$$S = \int \frac{d^3 r}{v_{uc}} d\tau \left[\sum_\mu \frac{\kappa_\mu}{2} (\partial_\mu \alpha)^2 + \frac{\eta}{2} (\partial_\tau \alpha)^2 - \frac{\lambda}{2} \cos 6\alpha \right]$$

← note can build characteristic length & velocity

$$\xi_\mu = \sqrt{\frac{\kappa_\mu}{18\lambda}} \quad v_\mu = \sqrt{\frac{\kappa_\mu}{\eta}}$$

$$\mathcal{E}_0^{sw} = \frac{1}{V_{BZ}} \sum_{i=1}^{4} \int_{k \in BZ} \frac{\omega_k^i}{2} = \frac{-\lambda}{2} \cos 6\alpha$$

* what's the gap?

$\alpha(x_i, \tau) \rightsquigarrow$

→ go to Fourier space:

$$\frac{-\lambda}{2} \cos 6\alpha \approx -\frac{\lambda}{2} + 9\lambda\alpha^2 \qquad \cos x \sim 1 - \frac{x^2}{2} + \frac{1}{4!} x^4$$

$$S = \frac{1}{2\beta} \sum_n \sum_k \alpha_{-k, -\omega_n} \alpha_{k, \omega_n} \left[\kappa_x k_x^2 + \kappa_y k_y^2 + \kappa_z k_z^2 - \eta (i\omega_n)^2 + 18\lambda \right]$$

→ the "gap" is the lowest energy → $\sqrt{\frac{18\lambda}{\eta}} = \Delta$

from $\mathcal{E}=0$

$\xRightarrow{\text{analytic continuation}}$ $\omega = \sqrt{\frac{\kappa_x k_x^2}{\eta} + \frac{\kappa_y k_y^2}{\eta} + \frac{\kappa_z k_z^2}{\eta} + \frac{18\lambda}{\eta}}$

↳ for theorists: it's the "mass" i.e. coefficient of the α^2 term.

↳ note: periodicity of cosine unimportant here since look at low energies

* Holstein - Primakoff:

- need spin polarization for this to be reasonable
- assume "translational invariance"
- write fluctuations as follows:

$\hat{u}$ is along the classical (or MF) direction (select by the energy or the free energy

$(\hat{u}_i, \hat{v}_i, \hat{w}_i)$ is an orthonormal basis ($\neq (\hat{a}_i, \hat{b}_i, \hat{e}_i)$)

$$\begin{cases} \vec{S} \cdot \hat{u}_i = s - n_i \\ \vec{S} \cdot \hat{v}_i = \sqrt{s}\, x_a \\ \vec{S} \cdot \hat{w}_i = \sqrt{s}\, y_a \end{cases} \qquad \begin{array}{l} x_i^{+} = x_i \\ y_i^{+} = y_i \end{array} \qquad [x_i, y_i] = i \qquad n_i = \frac{x_i^2 + y_i^2}{2} - \frac{1}{2}$$

4 bosons → note: 8×8 matrices will be involve

→ expand in large s & $s = \frac{1}{2}$ but it usually works really well!

Classical
Energy $E = \sum_{ij} \vec{S}_i \cdot \vec{\vec{J}}_{ij} \cdot \vec{S}_j$

↑ involves the J_{zz}, $J_{\pm}$, $J_{z\pm}$ etc

e.g. $J_{01} = \begin{pmatrix} J_2 & J_4 & J_4 \\ -J_4 & J_1 & J_3 \\ -J_4 & J_3 & J_1 \end{pmatrix}$

$J_1 =$
$J_2 =$
$J_3 =$
$J_4 =$

→ go to Fourier space

get $H = \sum_k \begin{pmatrix} X_{-k}^T & Y_{-k}^T \end{pmatrix} \underbrace{\begin{pmatrix} A_k & C_k \\ C_k^T & B_k \end{pmatrix}}_{= G_k} \begin{pmatrix} X_k \\ Y_k \end{pmatrix}$

⇝ use path integral formulation (action)

→ modes are found by solving the zero eigenvalue equation

of $G_k + (i\omega_n)\Gamma$ w/ $\Gamma = \begin{pmatrix} 0 & -i\mathbb{1}_4 \\ i\mathbb{1}_4 & 0 \end{pmatrix}$ only 4 are physical ($\omega \times \delta_{?}$)