Quantum Criticality and Frustration in Columbite

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and
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Layout

- INTRODUCTION
- ISING CHAIN
- PERFECT TRIANGLES
- ISOSCELES TRIANGLES
- EXPERIMENT
- SUMMARY

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QCP's in Nature

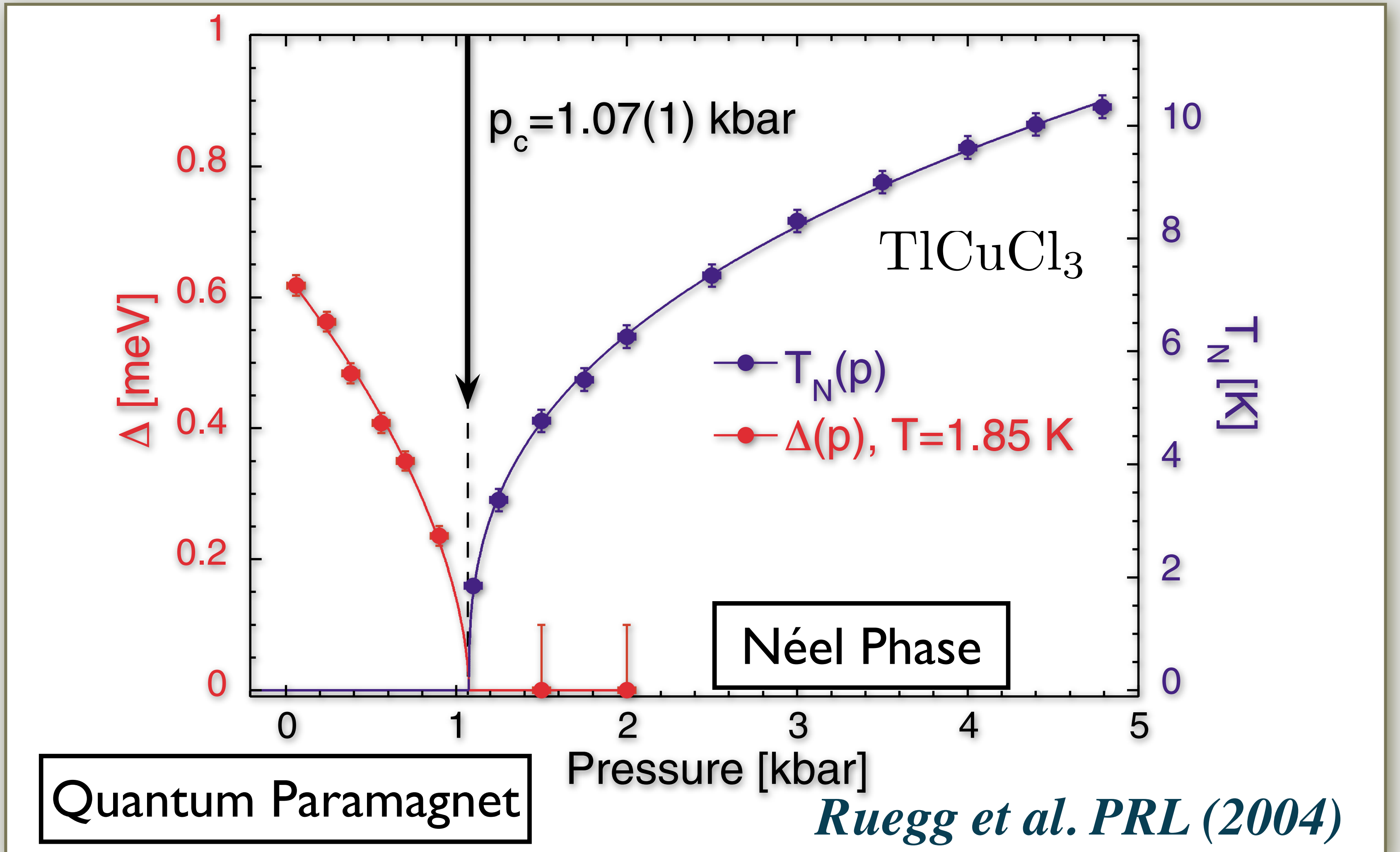
Important:

Confrontation of theory and experiment
for quantum phase transitions (criticality)

	Th.	Exp.
Metallic/Non-stoichiometric QCP	??	✓
QCP in stoichiometric insulators	✓	??

"Clean" Insulating QCPs

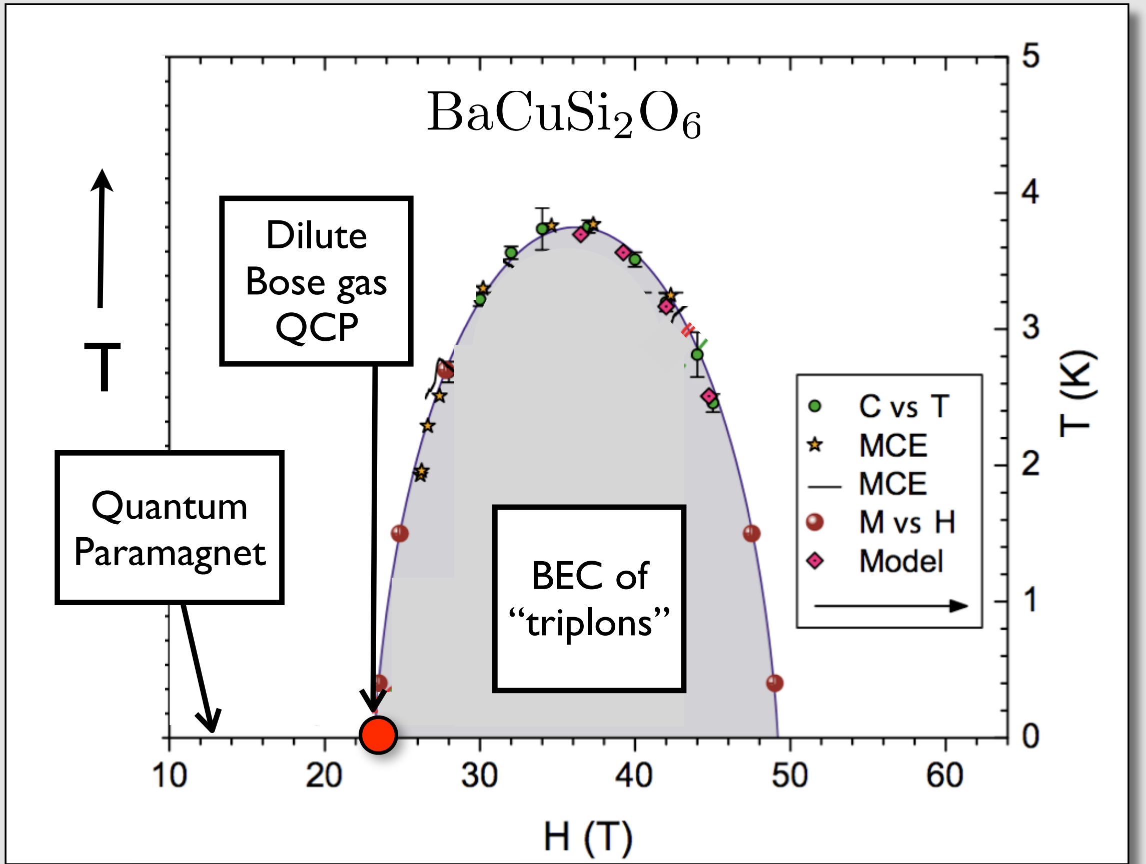
"Han Purple" family -- Dimerized AFM under pressure



Ruegg et al. PRL (2004)

"Clean" Insulating QCPs

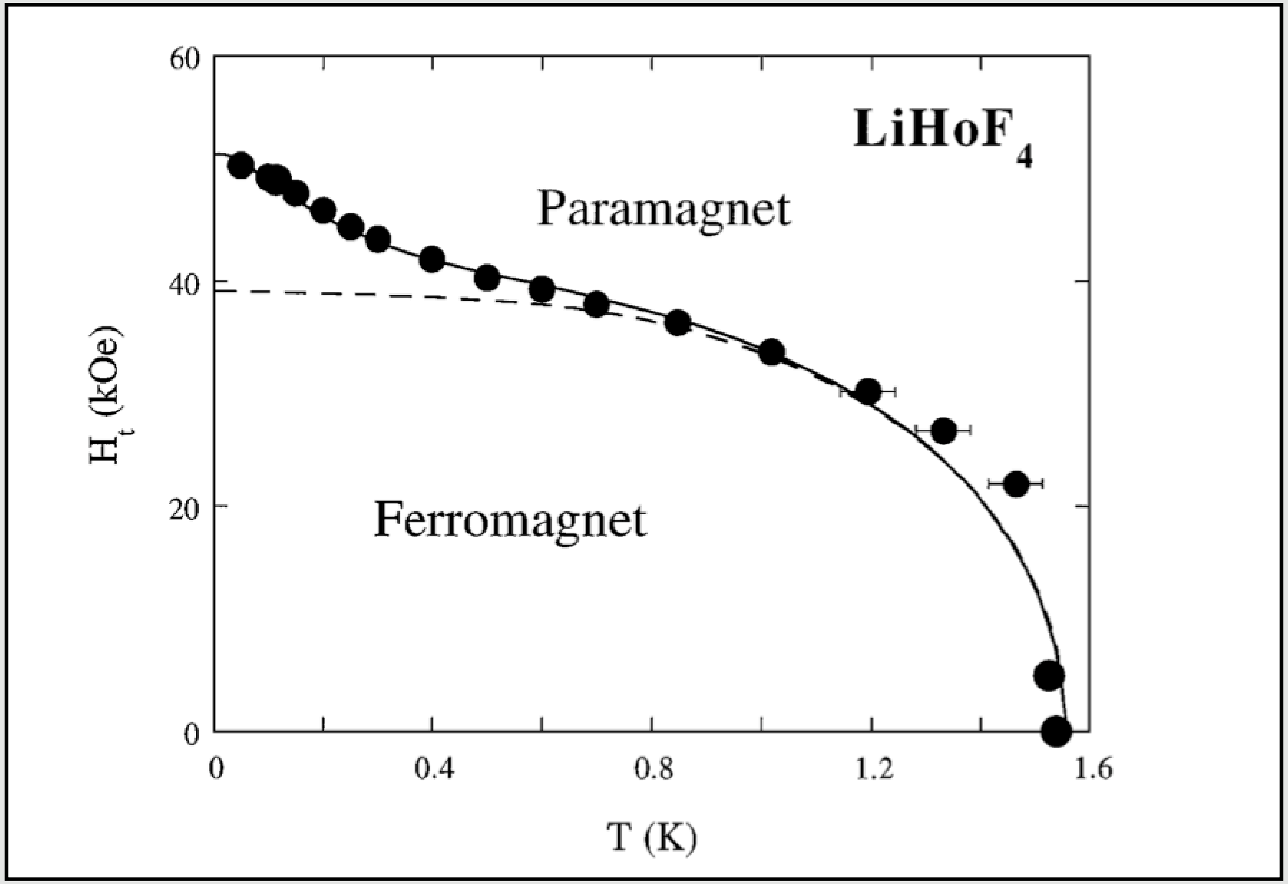
"Han Purple" family -- Dimerized AFM in a H-field



Jaime et al. PRL (2004)

"Clean" Insulating QCPs

Dipolar Ising. in transverse field.

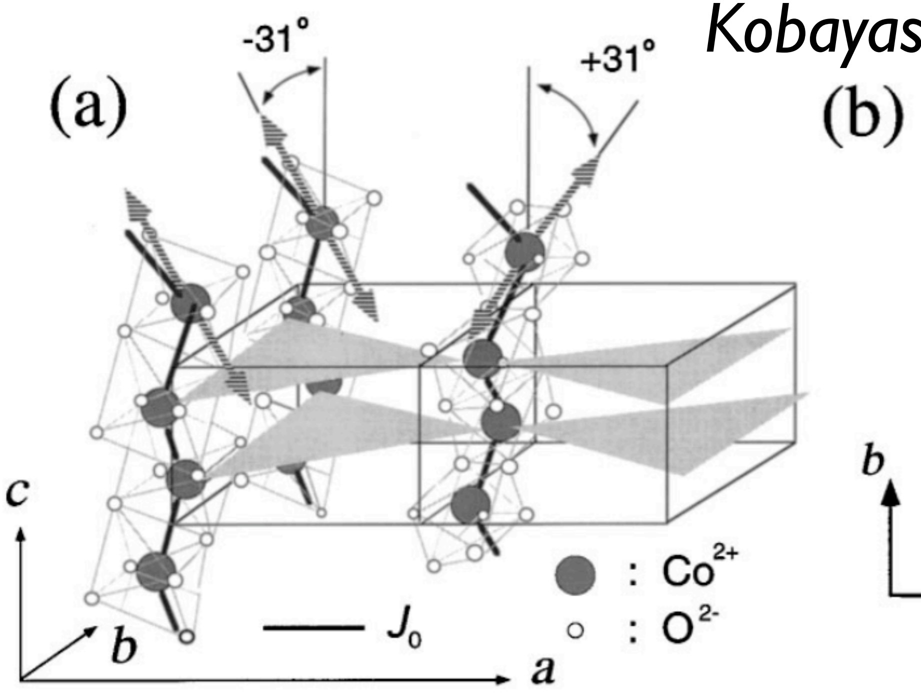


Bitko et al. PRL (1996)

$CoNb_2O_6$: Experimentalist's View

Co^{2+} form ferro-Ising chains along c-axis.
isosceles triangular lattice in the basal a-b plane

Kobayashi et al., PRB (2001)



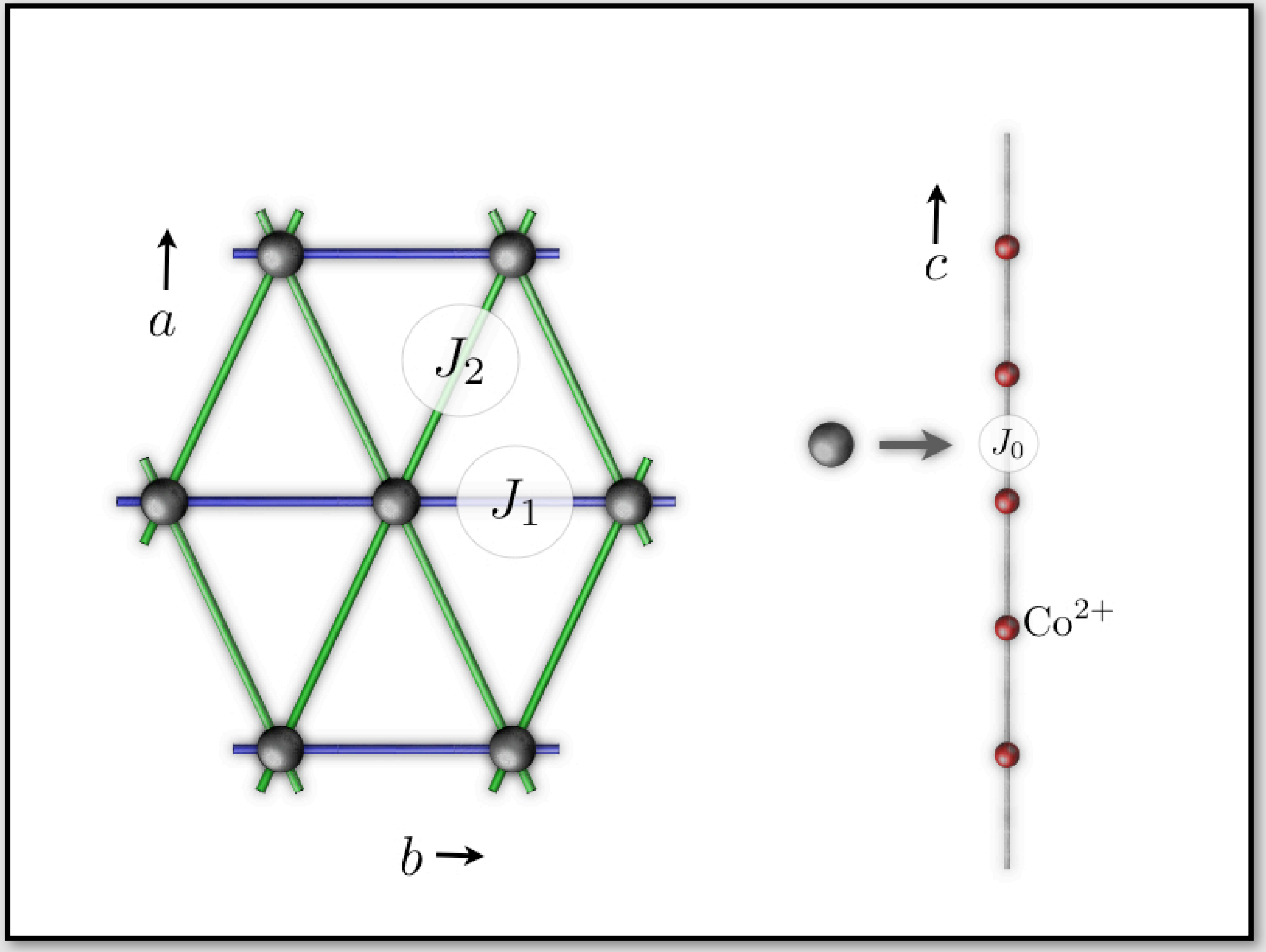
$CoNb_2O_6$: Neutrons

Amazing single crystal inelastic neutron scattering experiment by Coldea 2009. To appear in Science soon.

Phase Diagram & Spectrum of $CoNb_2O_6$
with external field in b-direction

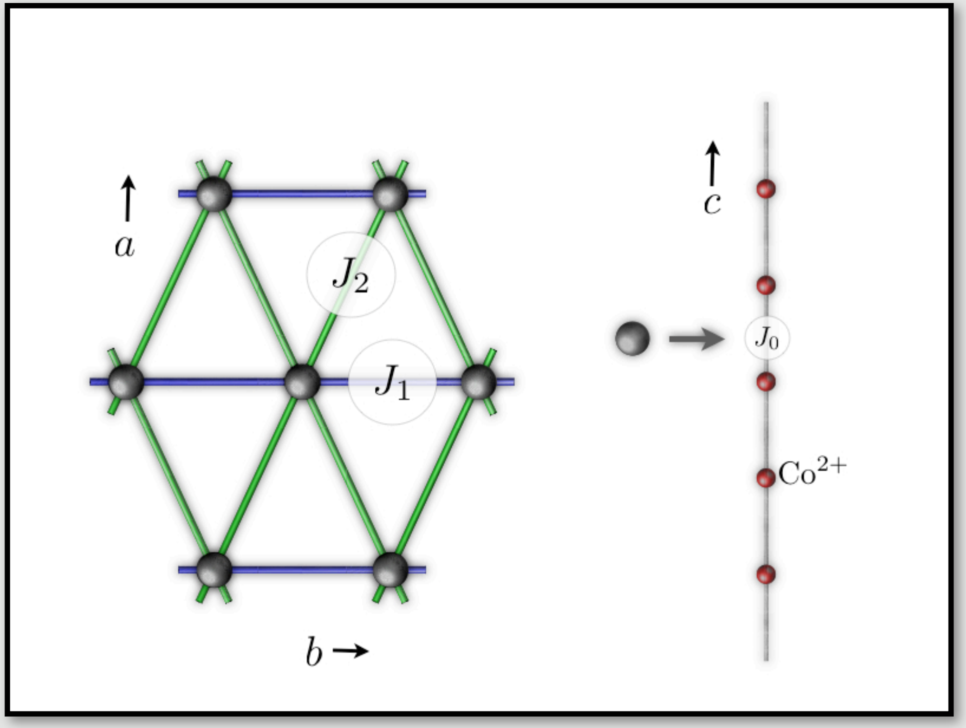
Goal here:
Address these experiments

$CoNb_2O_6$: Theorist's View



$CoNb_2O_6$: Theorist's View

$$H = J_0 \sum S^z_{z;\mathbf{r}} S^z_{z+1;\mathbf{r}} - h_\perp \sum S^x_{z;\mathbf{r}}$$
$$+ J_1 \sum_{\mathbf{r}} S^z_{z;\mathbf{r}} S^z_{z;\mathbf{r}+\mathbf{a_1}} + J_2 \sum_{\mathbf{r}} S^z_{z;\mathbf{r}} S^z_{z;\mathbf{r}+\mathbf{a_2}} + J_2 \sum_{\mathbf{r}} S^z_{z;\mathbf{r}} S^z_{z;\mathbf{r}+\mathbf{a_3}}$$



$J_0 < 0$

$J_1 > 0$

$J_2 > 0$

$|J_0| \gg J_1, J_2$

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Isolated Chains

$$H_{\mathrm{TFIC}} = J_0 \sum_i S_i^z S_{i+1}^z - h_\perp \sum_i S_i^x$$

$h_\perp$

Isolated Chains

$$H_{\mathsf{TFIC}} = J_0 \sum_i S_i^z S_{i+1}^z - h_\perp \sum_i S_i^x$$

$h_\perp$ $|\rightarrow\rightarrow\rightarrow\rightarrow \ldots\rangle$

PM

FM

$|\uparrow\uparrow\uparrow\uparrow \ldots\rangle$

Isolated Chains

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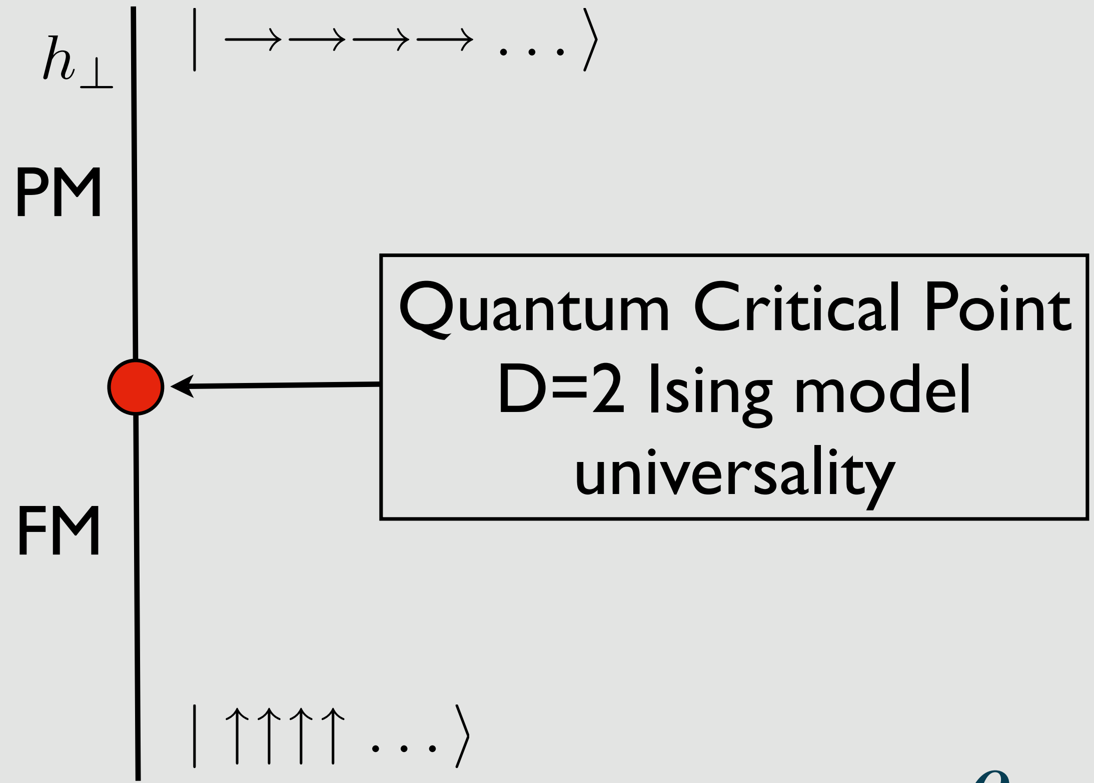

Quantum Phase Transitions, S. Sachdev (1999).

Isolated Chains

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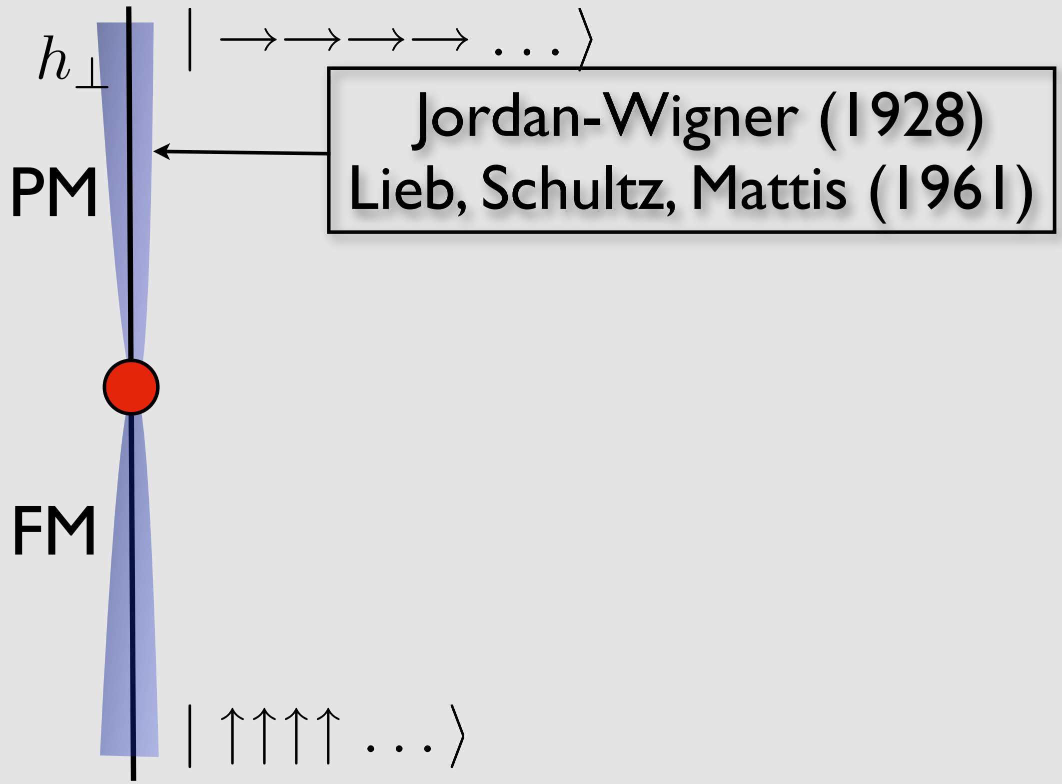
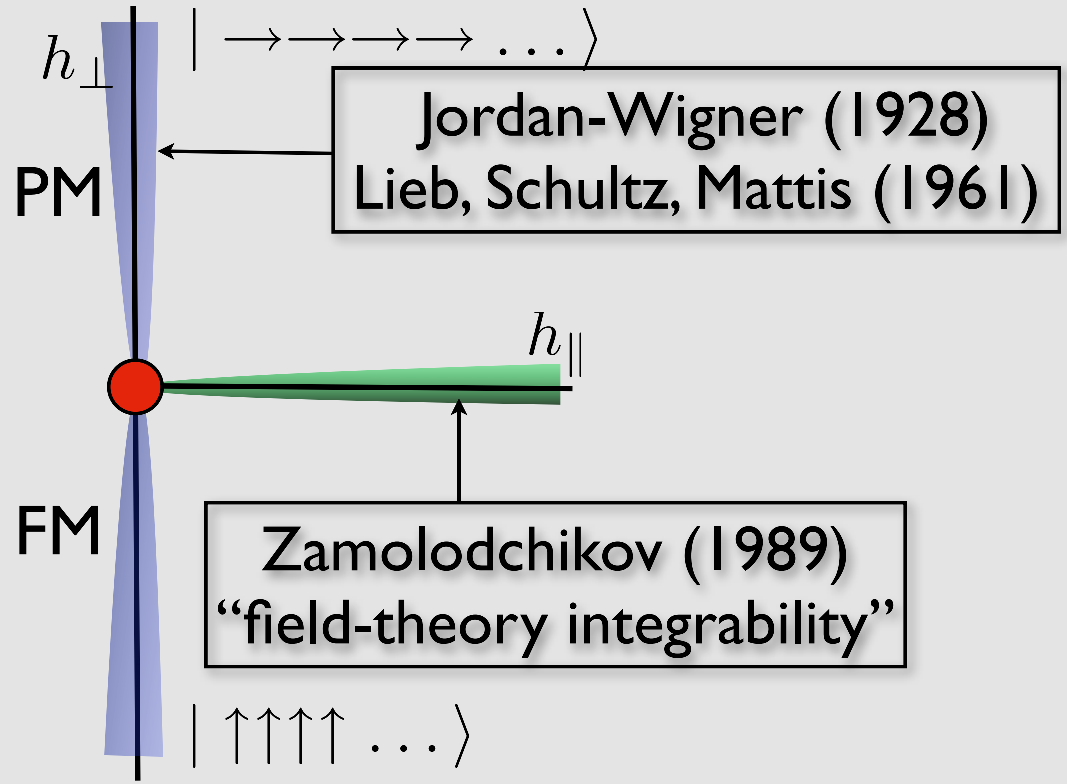


Isolated Chains

$$H_{\mathsf{TFIC}} = J_0 \sum_i S_i^z S_{i+1}^z - h_\perp \sum_i S_i^x - h_\parallel \sum_i S_i^z .$$



Isolated Chains

$$H_{\mathsf{TFIC}} = J_0 \sum_i S_i^z S_{i+1}^z - h_\perp \sum_i S_i^x - h_\| \sum_i S_i^z .$$

$$E_{\mathrm{TFIC}} = \frac{J_0}{2} \mathcal{E}_{\mathrm{IFT}} \left(\frac{h_\perp - J_0/2}{J_0/2}, \frac{c_h h_\|}{J_0/2} \right) .$$

$$\mathrm{c}_h = \sqrt{\frac{e^{1/4} 2^{1/12}}{4A^3}} \approx 0.4016$$

Isolated Chains

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$\bar{h}_\perp$ $\bar{h}_\parallel$

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Isolated Chains

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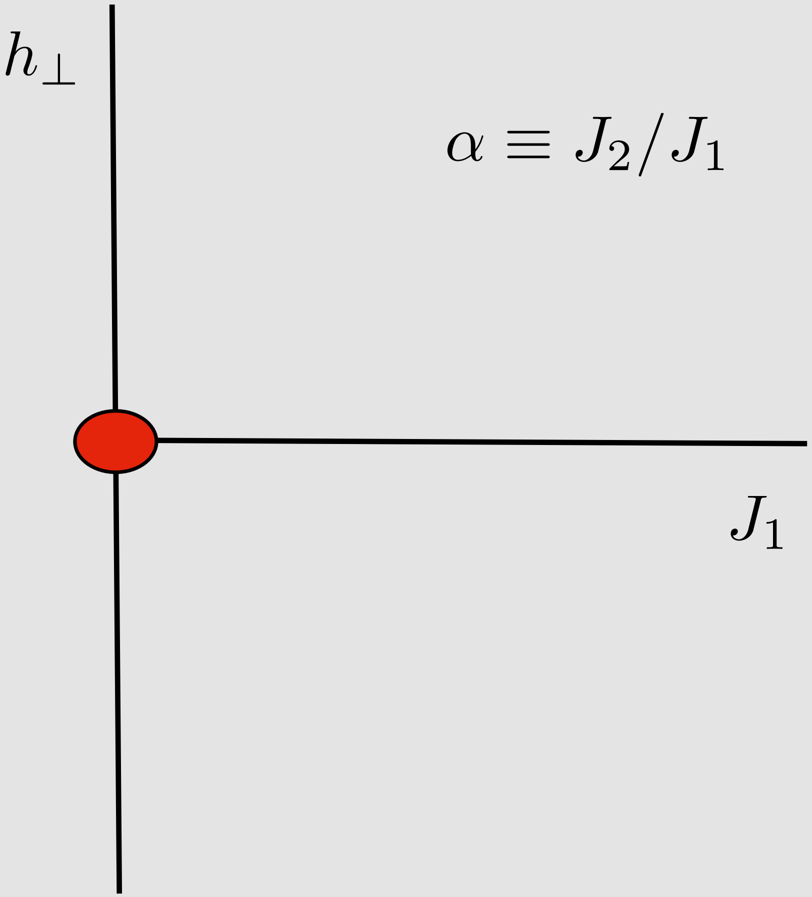
$$\begin{aligned}
\mathcal{E}_{\mathrm{IFT}}^{\bar{h}_\perp > 0}(\bar{h}_\perp, \bar{h}_\parallel) &= \frac{\bar{h}_\perp^2}{8\pi} \log \bar{h}_\perp^2 + \bar{h}_\perp^2 \left(G_2 \xi^2 + G_4 \xi^4 + G_6 \xi^6 \ldots \right) , \\
\mathcal{E}_{\mathrm{IFT}}^{\bar{h}_\perp < 0}(\bar{h}_\perp, \bar{h}_\parallel) &= \frac{\bar{h}_\perp^2}{8\pi} \log \bar{h}_\perp^2 + \bar{h}_\perp^2 \left(\tilde{G}_1 |\xi| + \tilde{G}_2 |\xi|^2 + \ldots \right) , \\
\mathcal{E}_{\mathrm{IFT}}(\bar{h}_\perp, \bar{h}_\parallel) &= \frac{\bar{h}_\perp^2}{8\pi} \log \bar{h}_\perp^2 + \bar{h}_\parallel^{16/15} \left[-\frac{\eta^2}{8\pi} \log \eta^2 + \left(\Phi_0 + \Phi_1 \eta + \Phi_2 \eta^2 + \ldots \right) \right] ,
\end{aligned}$$

$$\xi = \bar{h}_\parallel / \bar{h}_\perp^a \qquad \eta = -\bar{h}_\perp / \bar{h}_\parallel^{1/a}$$

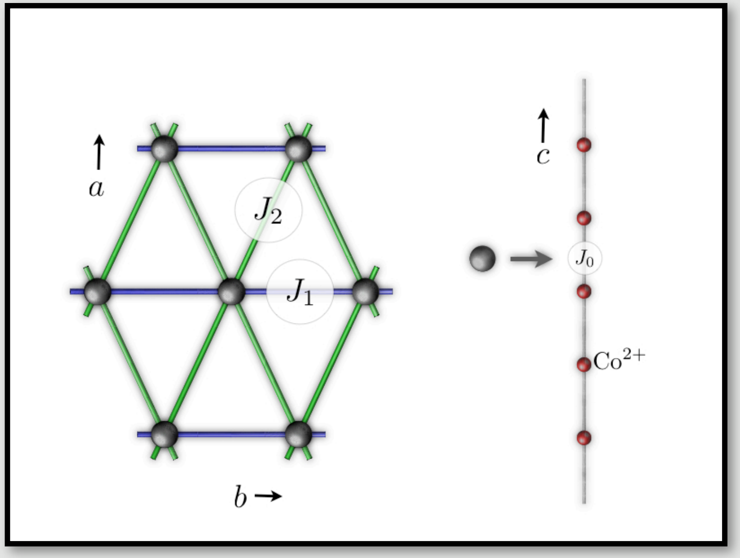
Fonseca & Zamolodchikov. J. Stat. Phys. (2003)

Main Question: Phase Diagram?

$$
\begin{aligned}
H &= J_0 \sum S^z_{z;\mathbf{r}} S^z_{z+1;\mathbf{r}} - h_\perp \sum S^x_{z;\mathbf{r}} \\
&+ J_1 \sum_{\mathbf{r}} S^z_{z;\mathbf{r}} S^z_{z;\mathbf{r}+\mathbf{a_1}} + J_2 \sum_{\mathbf{r}} S^z_{z;\mathbf{r}} S^z_{z;\mathbf{r}+\mathbf{a_2}} + J_2 \sum_{\mathbf{r}} S^z_{z;\mathbf{r}} S^z_{z;\mathbf{r}+\mathbf{a_3}}
\end{aligned}
$$



$$\alpha \equiv J_2/J_1$$



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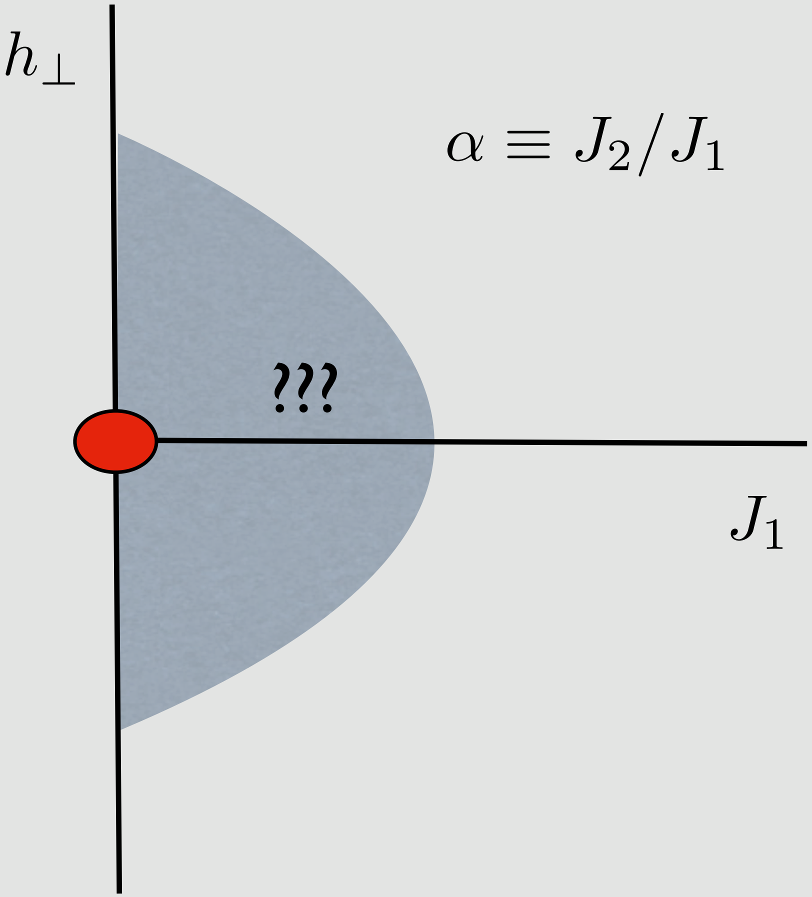
\end{aligned}
$$



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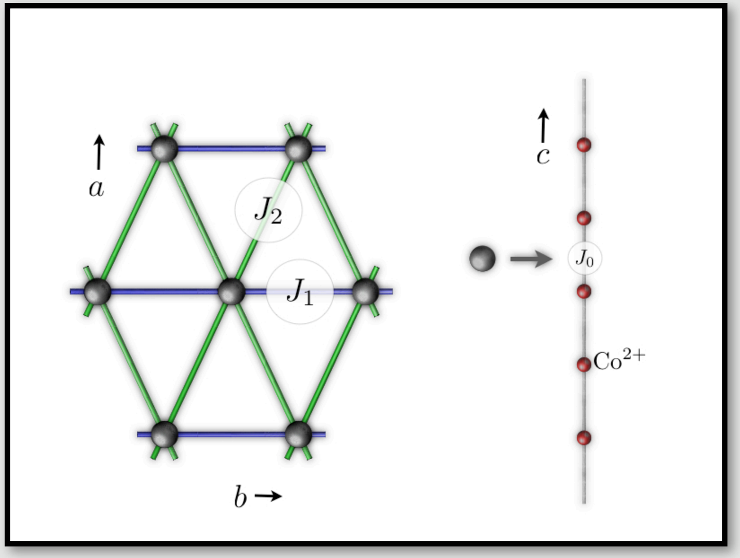

Mean-Field Theory

wavefunction with $\bar{h}_i = \bar{h}_{\|}$ variational parameters:

$$|\Psi\rangle = \prod_i |\bar{h}_i\rangle$$

$$E_{\rm mf} \quad = \quad \sum_i \mathcal{E}_{\rm IFT}(\bar{h}_\perp, \bar{h}_i) + \bar{h}_i \bar{m}_i + \sum \bar{m}_i \frac{\bar{J}_{ij}}{2} \bar{m}_j$$

(work in units of $J_0/2$)

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(work in units of $J_0/2$)

Main Strategy:

What are the optimum values of the $\bar{h}_i$?

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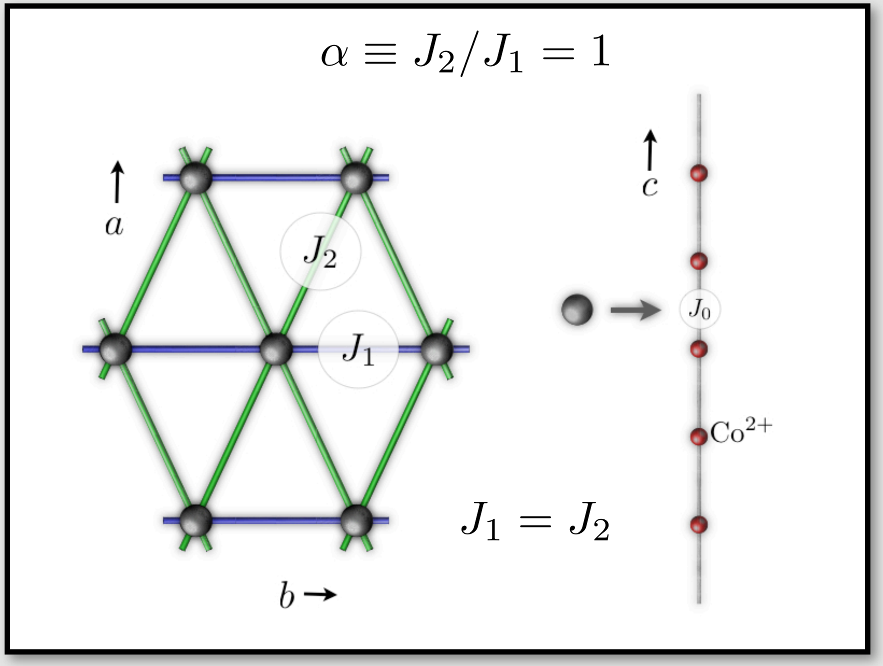
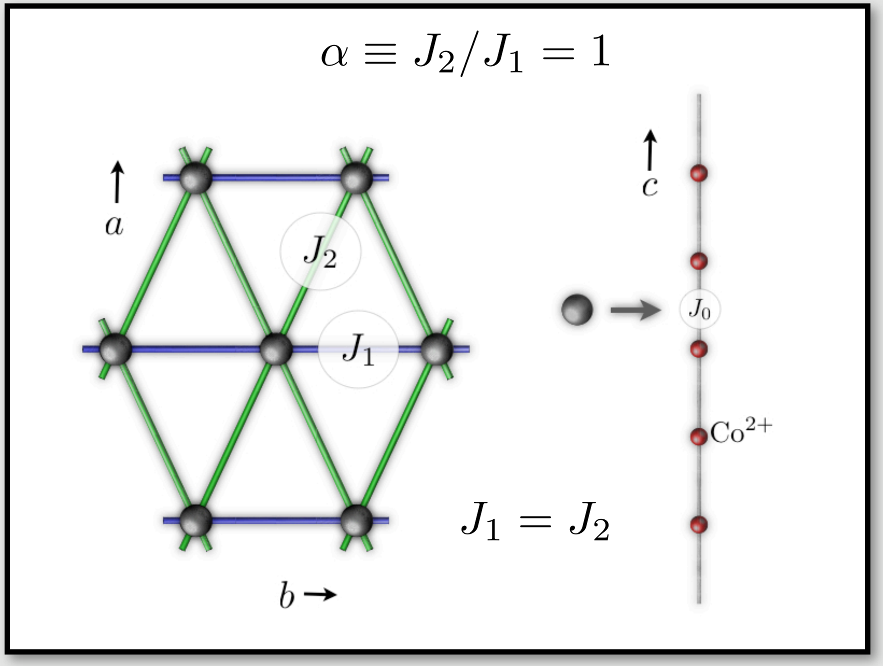
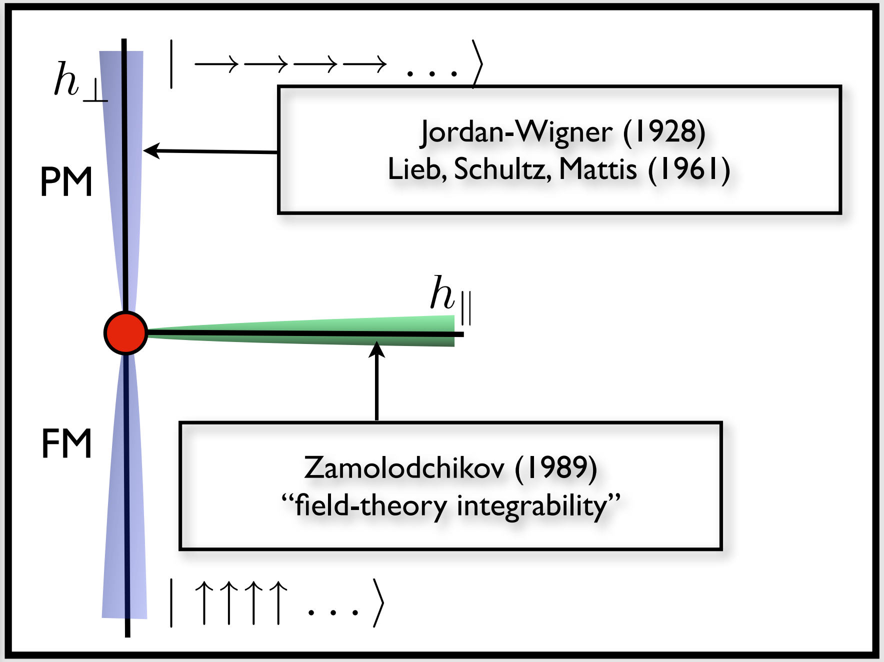
Perfect Triangles



Perfect Triangles





... 3 expansions.

Perfect Triangles

(I) $\bar{h}_\perp > 0$

$$E_{\rm mf} \quad = \quad \sum_i \mathcal{E}_{\rm IFT}(\bar{h}_\perp, \bar{h}_i) + \bar{h}_i \bar{m}_i + \sum \bar{m}_i \frac{\bar{J}_{ij}}{2} \bar{m}_j$$

$$\mathcal{E}^{\bar{h}_\perp>0}_{\rm IFT}(\bar{h}_\perp, \bar{h}_\parallel) \quad = \quad \frac{\bar{h}_\perp^2}{8\pi} \log \bar{h}_\perp^2 + \bar{h}_\perp^2 \left(G_2 \xi^2 + G_4 \xi^4 + G_6 \xi^6 \ldots \right),$$

$$\xi = \bar{h}_\parallel / \bar{h}_\perp^a$$

Landau theory:
Which momenta gets negative mass first?

Perfect Triangles

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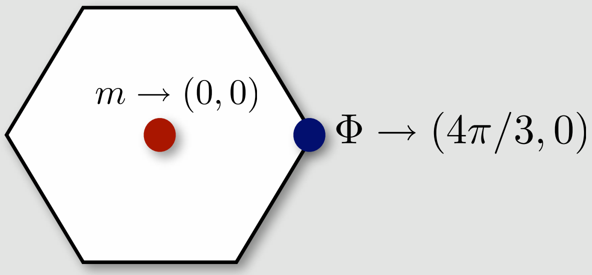
$\xi = \bar{h}_\parallel / \bar{h}_\perp^a$

$\alpha = 1 (J_1 = J_2) \Rightarrow \mathbf{Q_c} = (4\pi/3, 0)$



$$h_i = \Phi e^{\mathbf{i Q_c \cdot r}} + \Phi^* e^{-\mathbf{i Q_c \cdot r}} + m$$

condensation causes SDW

Perfect Triangles

(I) $\bar{h}_{\perp} > 0$

$$\epsilon_{\rm L} = \alpha_\Phi |\Phi|^2 + \beta_\Phi |\Phi|^4 + \alpha_m m^2 + \lambda_3 m(\Phi^3 + \Phi^{*3}) + \lambda_6(\Phi^6 + \Phi^{*6})$$

$$h_i = \Phi e^{\mathbf{i Q_c \cdot r}} + \Phi^* e^{-\mathbf{i Q_c \cdot r}} + m$$

Landau theory.

Optimize over Φ and m .

What is resulting state of matter?

Perfect Triangles

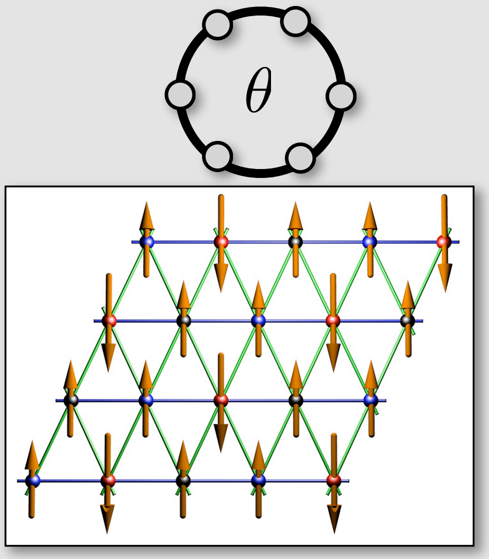
(I) $\bar{h}_\perp > 0$

$$\epsilon_{\rm L} = \alpha_\Phi|\Phi|^2 + \beta_\Phi|\Phi|^4 + \alpha_m m^2 + \lambda_3 m(\Phi^3 + \Phi^{*3}) + \lambda_6(\Phi^6 + \Phi^{*6})$$

$$\Phi = |\Phi|e^{i\theta}$$

Ferri-magnet (FR)

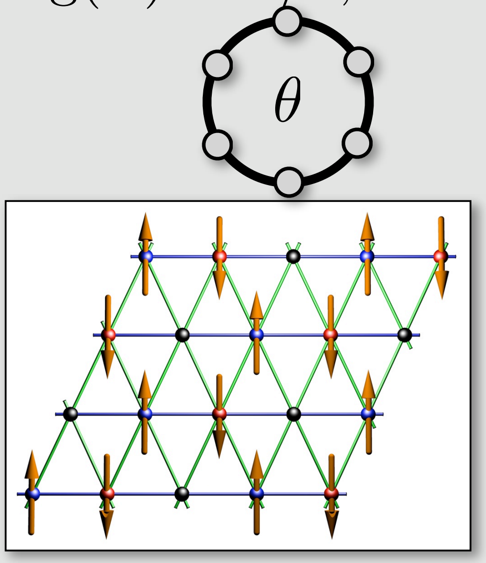
$\arg(\Phi) = 0, m \neq 0$



$$\lambda_6 - \frac{\lambda_3^2}{4\alpha_{\rm m}} < 0$$

Anti-ferro (AF)

$\arg(\Phi) = \pi/2, m = 0$

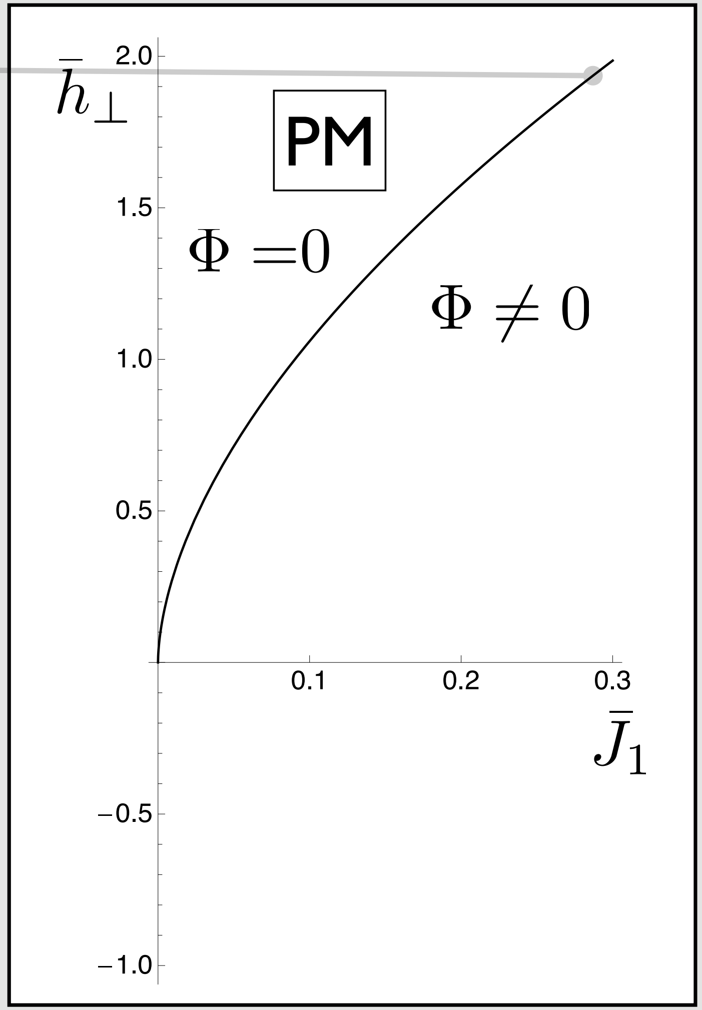


$$\lambda_6 - \frac{\lambda_3^2}{4\alpha_{\rm m}} > 0$$

Perfect Triangles

$$\alpha = 1(J_1 = J_2) \qquad \bar{h}_\perp > 0$$

$$\bar{J}_1^c = \frac{1}{6|G_2|}\bar{h}_\perp^{2a-2}$$



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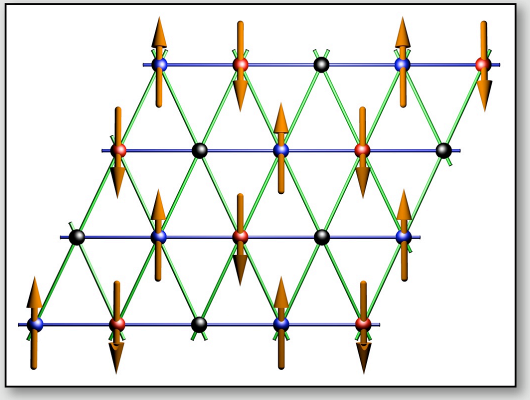
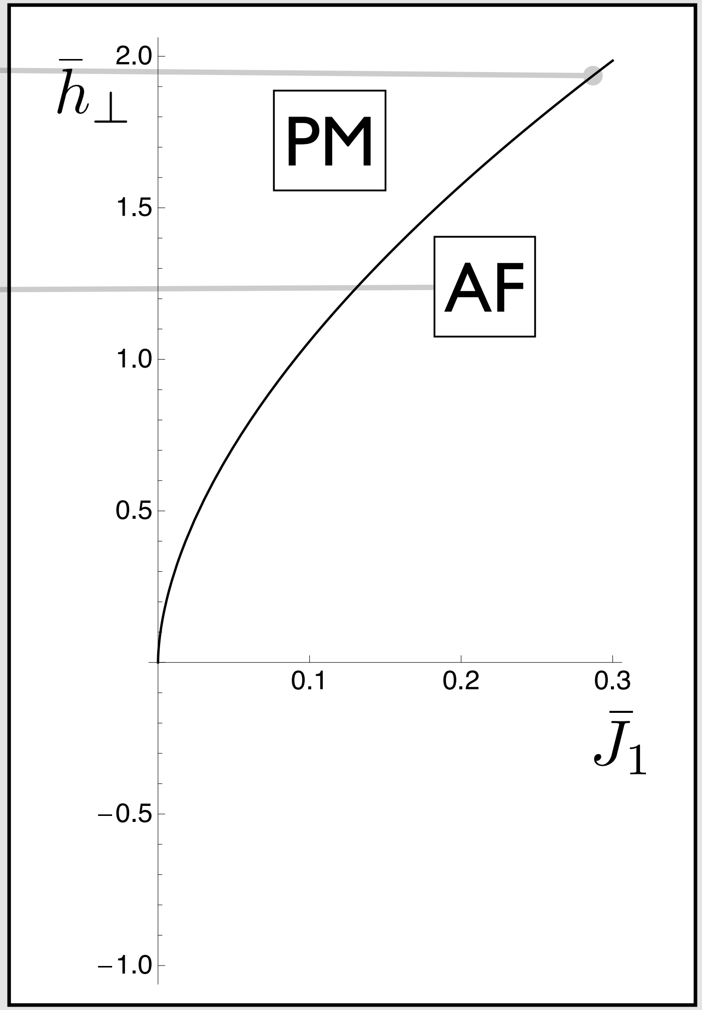


$$\lambda_6 - \frac{\lambda_3^2}{4\alpha_m}$$

$$= \frac{3G_2G_6 - 8G_4^2}{3G_2}\bar{h}_\perp^{2-6a} > 0$$



Perfect Triangles

(2) $\bar{h}_\perp < 0$

$$E_{\rm mf} \;=\; \sum_i \mathcal{E}_{\rm IFT}(\bar{h}_\perp, \bar{h}_i) + \bar{h}_i \bar{m}_i + \sum \bar{m}_i \frac{\bar{J}_{ij}}{2} \bar{m}_j$$

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$$\xi = \bar{h}_\parallel / \bar{h}_\perp^a$$

Ising chains ordered. Magnetization finite.
"degenerate perturbation theory". Effective hamiltonian:

$$H = \bar{J} \sum_{\langle ij \rangle} \sigma_i \sigma_j - K \sum_i \left(\sum_a \sigma_{i+e_a} \right)^2$$

$$K \sim O(\bar{J}^2)$$

Perfect Triangles

(2) $\bar{h}_\perp < 0$

$$H = \bar{J} \sum_{\langle ij \rangle} \sigma_i \sigma_j - K \sum_i \left(\sum_a \sigma_{i+e_a} \right)^2$$

Which Ising conf. minimizes K term?

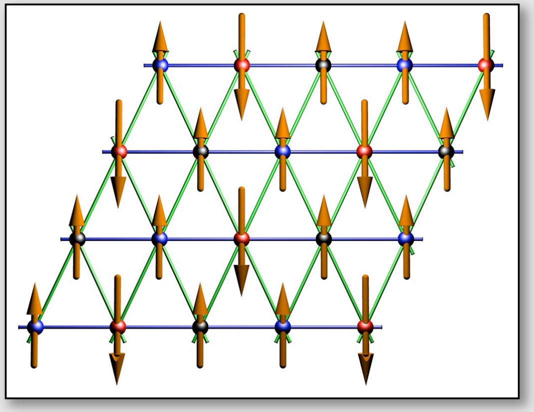
Perfect Triangles

(2) $\bar{h}_\perp < 0$

$$H = \bar{J} \sum_{\langle ij \rangle} \sigma_i \sigma_j - K \sum_i \left(\sum_a \sigma_{i+e_a} \right)^2$$

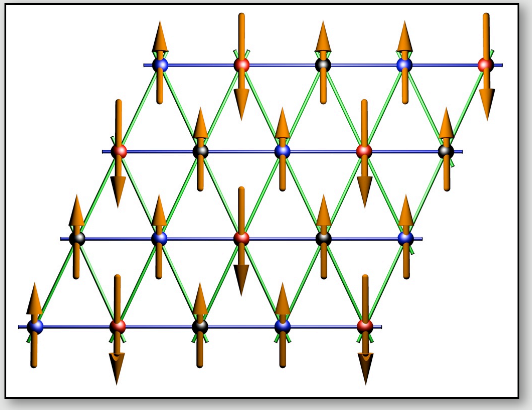
Which Ising conf. minimizes K term?

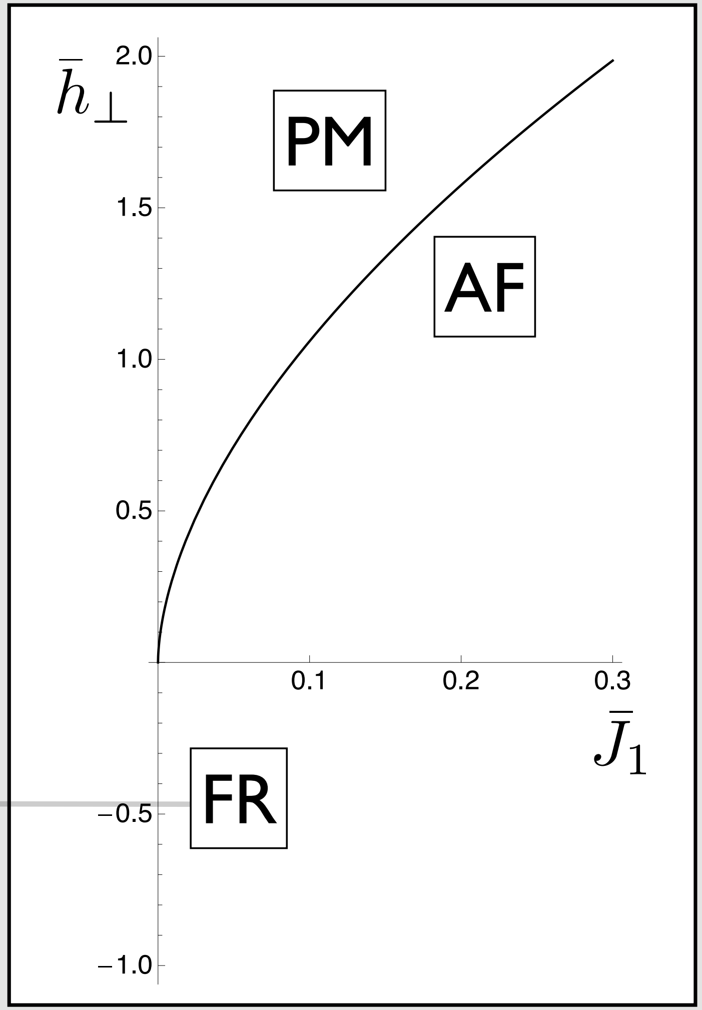
Ferri-magnet



Perfect Triangles

(2) $\bar{h}_\perp < 0$





Perfect Triangles

(3) $\bar{h}_\perp = 0$

$$E_{\mathrm{mf}} = \sum_i \mathcal{E}_{\mathrm{IFT}}(\bar{h}_\perp, \bar{h}_i) + \bar{h}_i \bar{m}_i + \sum \bar{m}_i \frac{\bar{J}_{ij}}{2} \bar{m}_j$$

$$\mathcal{E}_{\mathrm{IFT}}(\bar{h}_\perp, \bar{h}_\parallel) = \frac{\bar{h}_\perp^2}{8\pi} \log \bar{h}_\perp^2 + \bar{h}_\parallel^{16/15} \left[-\frac{\eta^2}{8\pi} \log \eta^2 + \left(\Phi_0 + \Phi_1 \eta + \Phi_2 \eta^2 + \ldots \right) \right],$$

$$\eta = -\bar{h}_\perp / \bar{h}_\parallel^{1/a}$$

Perfect Triangles

$$\bar{h}_\perp = 0$$

$$E_{\rm mf} = \sum_i \mathcal{E}_{\rm IFT}(\bar{h}_\perp, \bar{h}_i) + \bar{h}_i \bar{m}_i + \sum \bar{m}_i \frac{\bar{J}_{ij}}{2} \bar{m}_j$$

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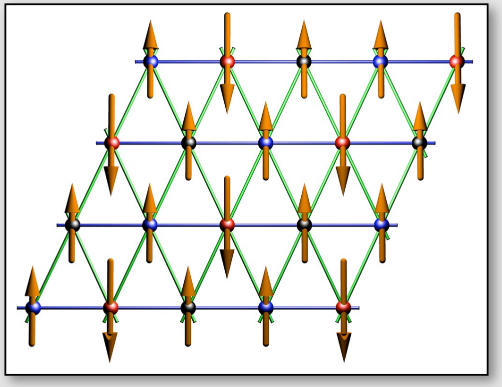
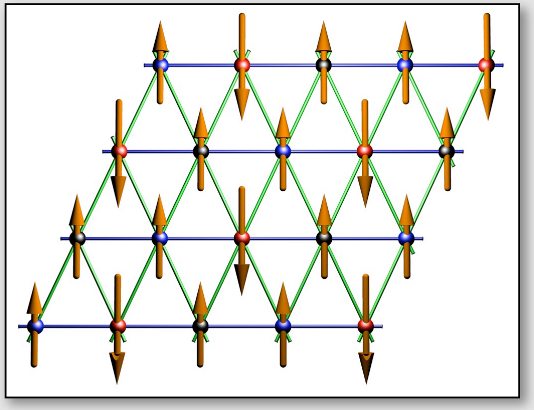
$$\eta = -\bar{h}_\perp / \bar{h}_\parallel^{1/a}$$

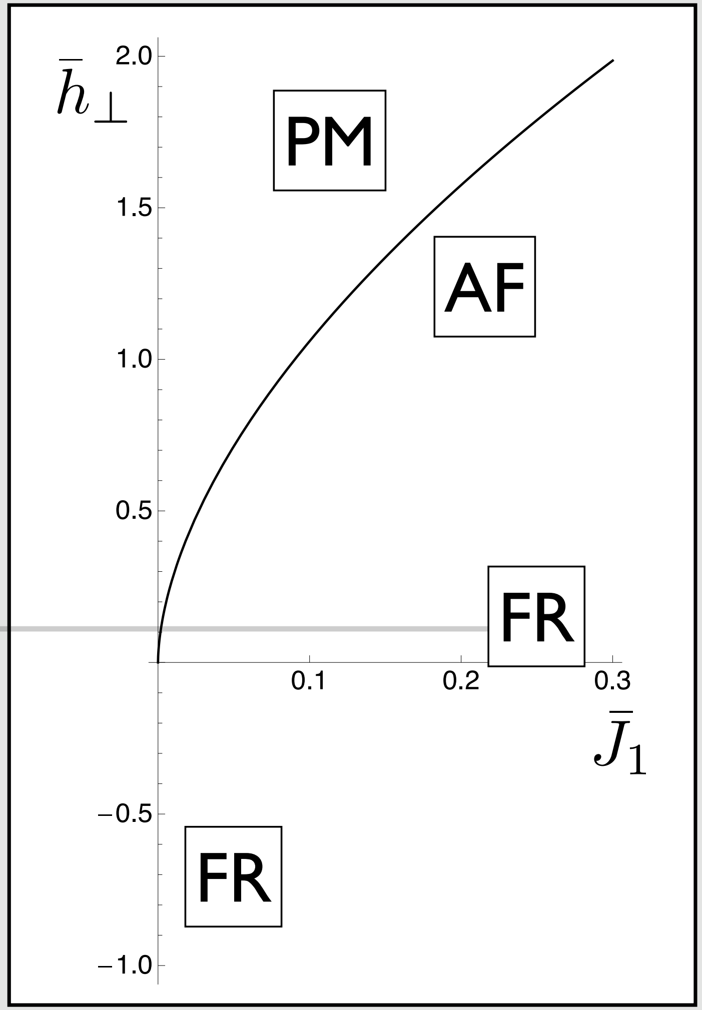
Magnetization finite in field
minimize energy, Ferri-magnet



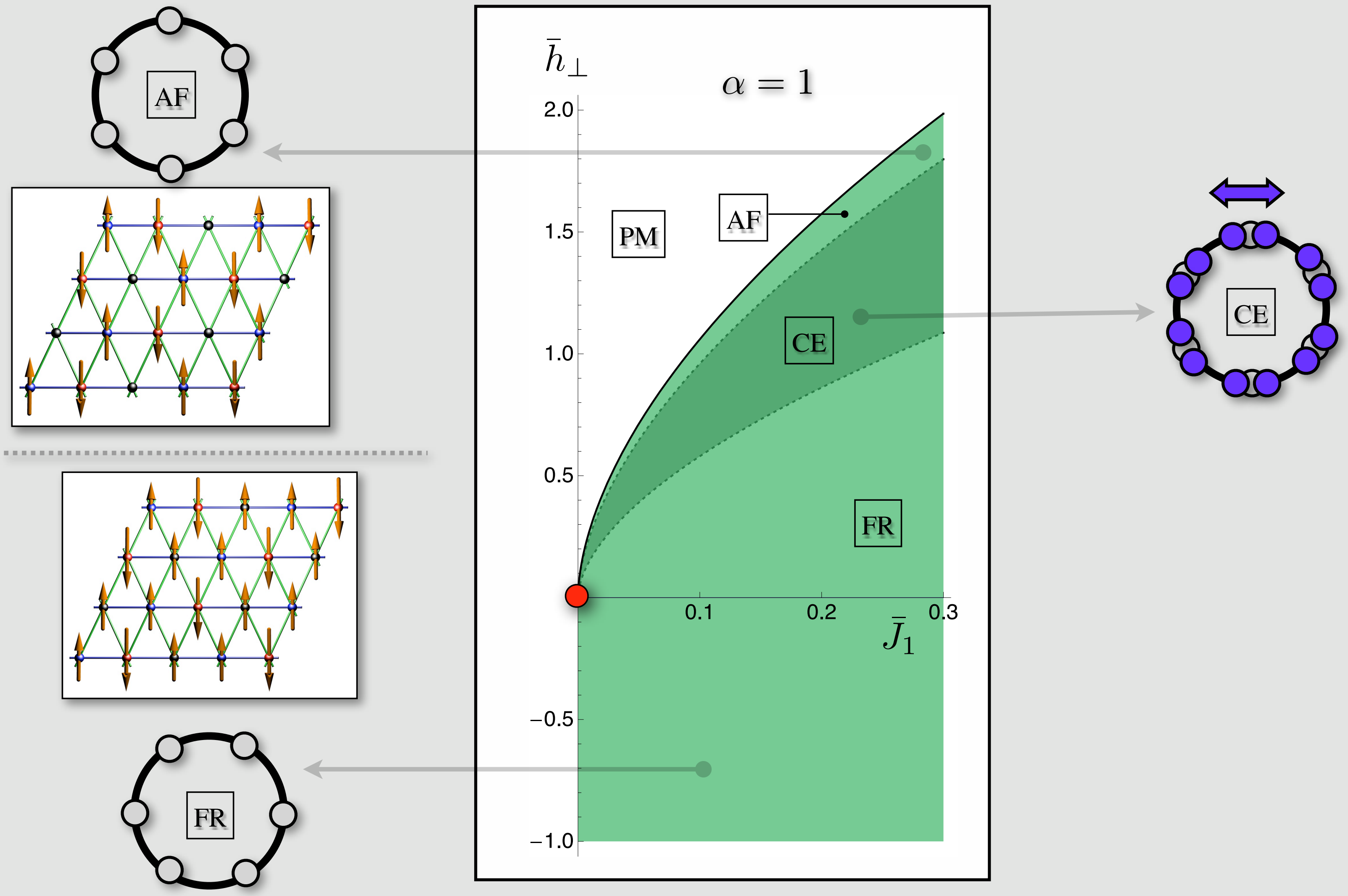
Perfect Triangles

Summary of phases obtained
from the three expansions





Perfect Triangles: Phase Diagram



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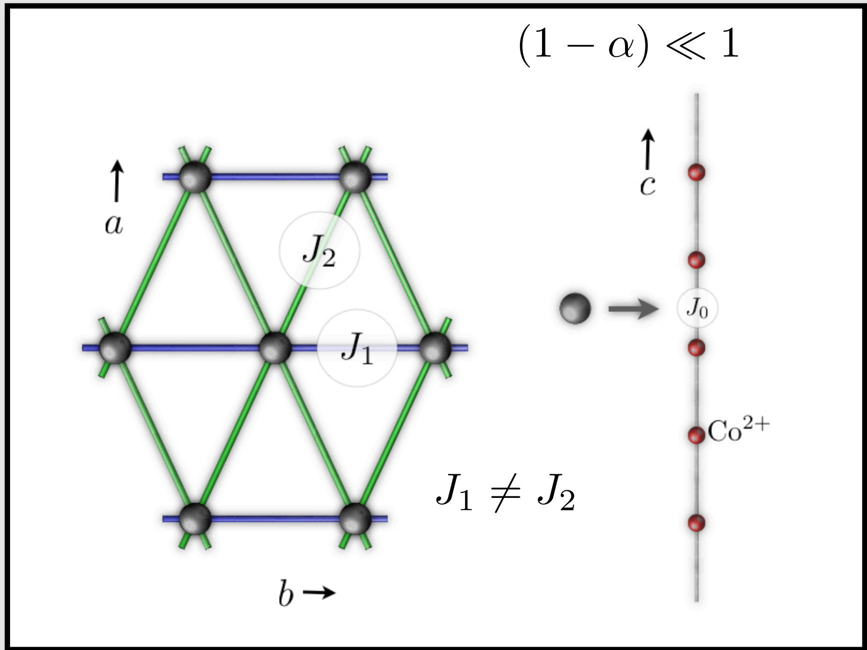
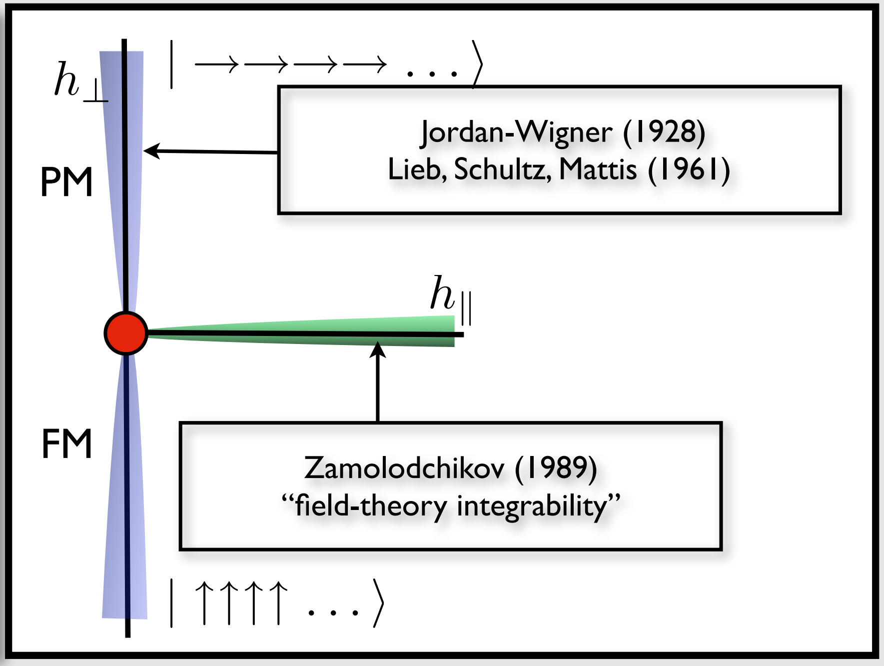
- SUMMARY

Isosceles Case





... 3 expansions.

Isosceles Triangles

$$\bar{h}_{\perp} > 0$$

$$E_{\mathrm{mf}} = \sum_i \mathcal{E}_{\mathrm{IFT}}(\bar{h}_{\perp}, \bar{h}_i) + \bar{h}_i \bar{m}_i + \sum \bar{m}_i \frac{\bar{J}_{ij}}{2} \bar{m}_j$$

$$\mathcal{E}_{\mathrm{IFT}}^{\bar{h}_{\perp}>0}(\bar{h}_{\perp}, \bar{h}_{\parallel}) = \frac{\bar{h}_{\perp}^2}{8\pi} \log \bar{h}_{\perp}^2 + \bar{h}_{\perp}^2 \left(G_2 \xi^2 + G_4 \xi^4 + G_6 \xi^6 \ldots \right),$$

Isosceles Triangles

$$\bar{h}_\perp > 0$$

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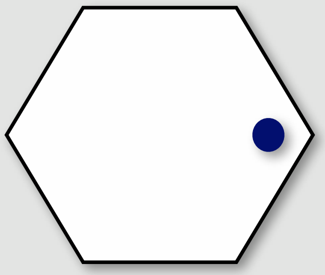
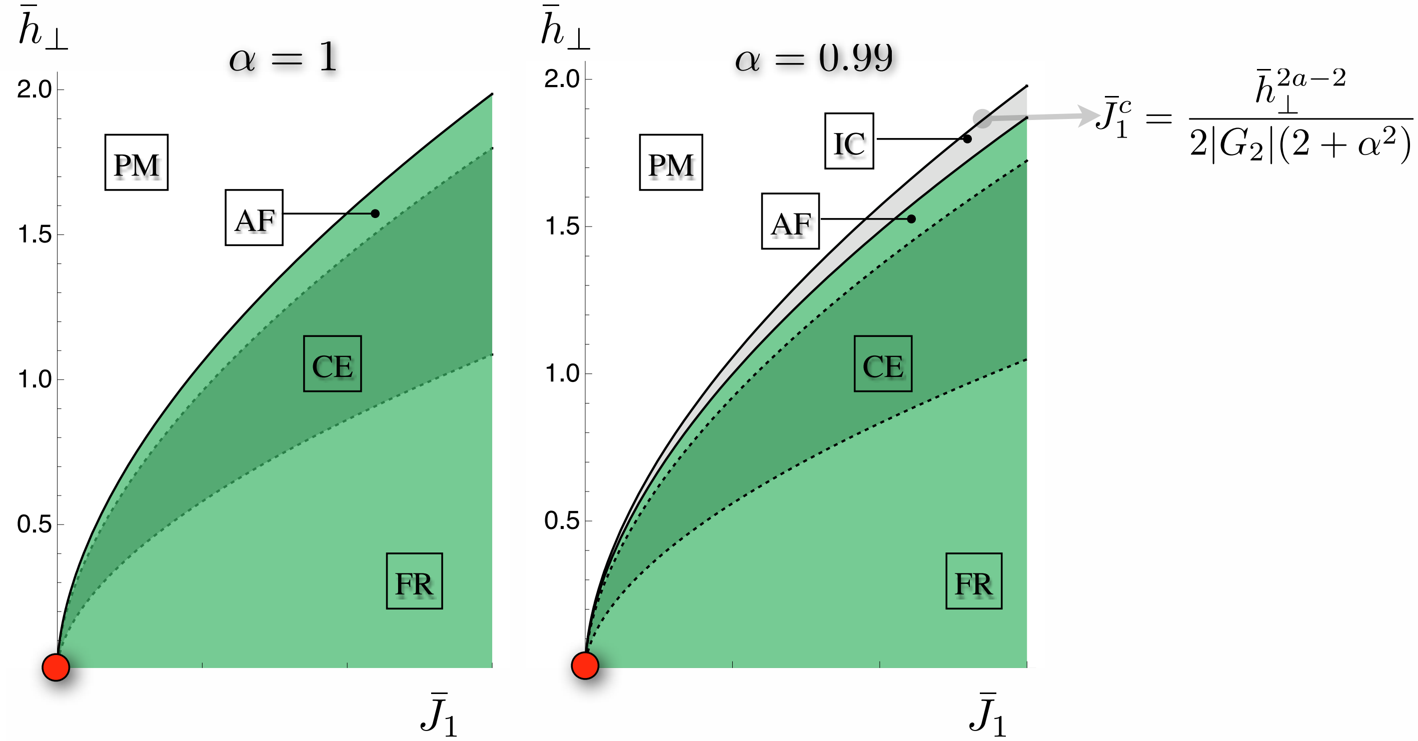
$\alpha \neq 1$ ⇨ $\mathbf{Q}^* = \left(2\cos^{-1}\left(-\frac{\alpha}{2}\right), 0\right)$



condensation causes incommensurate SDW

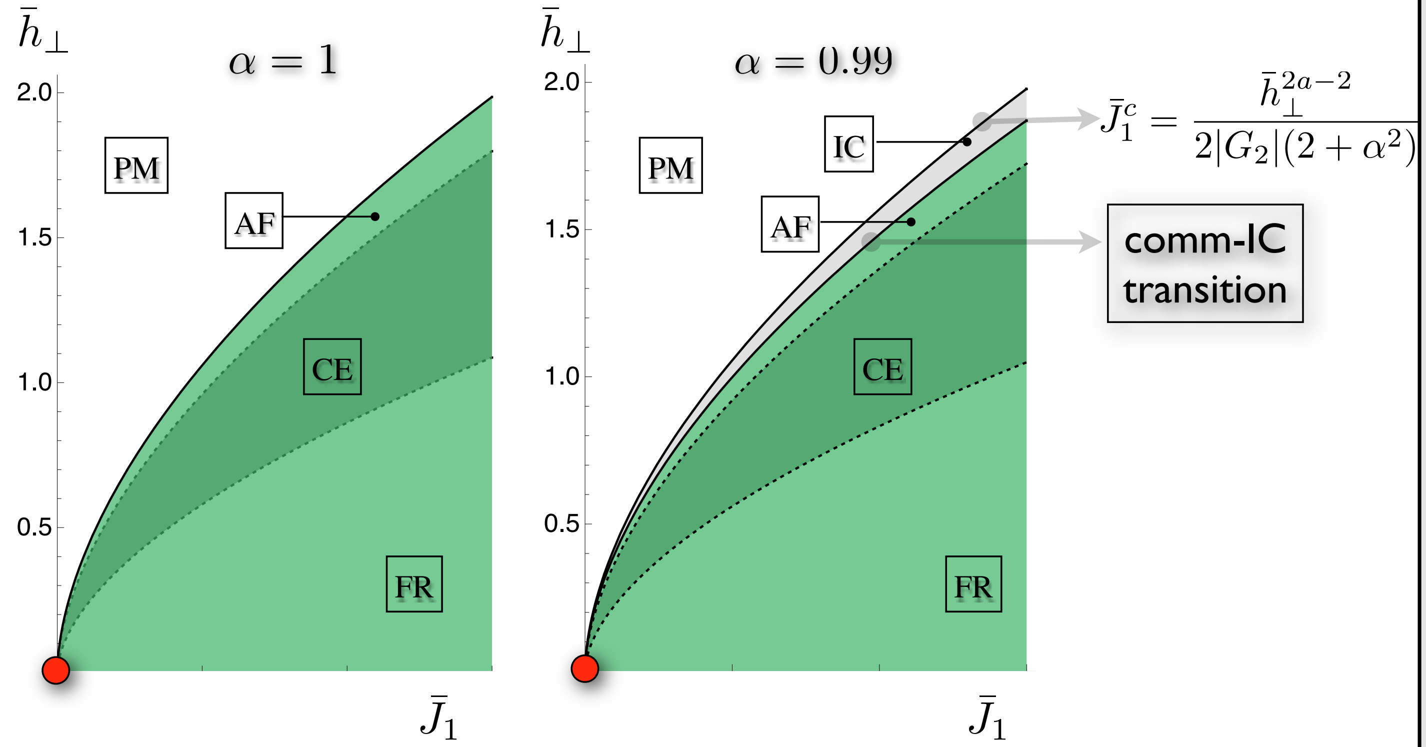
... infinitely many harmonics!

Phase Boundary



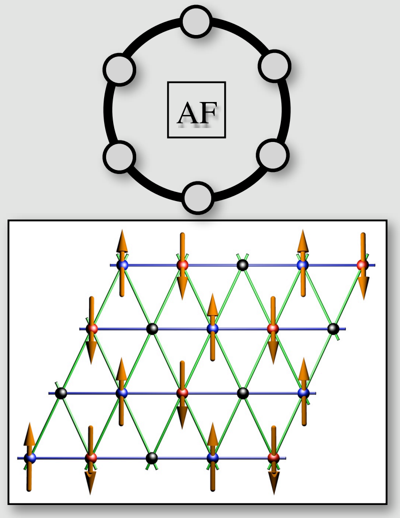
$$\bar{h}_\perp > 0$$

Phase Boundary



$$\bar{h}_\perp > 0$$

Comm-IC Transition



Energy for a domain wall

$$\bar{h}_i = |\Phi| \left[e^{i(\mathbf{Q_c} \cdot \mathbf{r_i} + \theta(\mathbf{r_i}))} + \text{c.c.} \right] + m$$

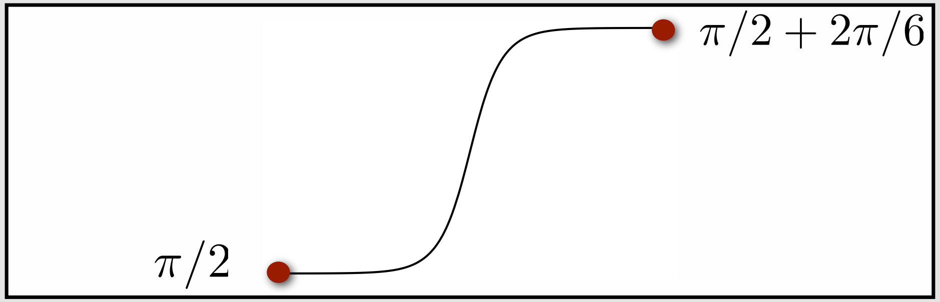
$$E_{\text{sg}} = A_{yz} \int dx \left[\frac{\kappa}{2} (\partial_x \theta)^2 + \delta_x \partial_x \theta + \lambda \cos(n_{\text{sg}} \theta) \right]$$

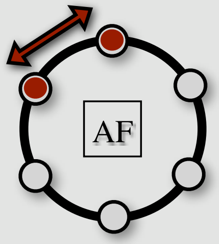
Sine-Gordon model

CIT

$$E_{\rm sg} = A_{yz}\int dx\left[\frac{\kappa}{2}(\partial_x\theta)^2 + \delta_x\partial_x\theta + \lambda\cos(n_{\rm sg}\theta)\right]$$

$$\theta(x) = \frac{4}{n}\tan^{-1}\left(e^{\pm n_{\rm sg}\sqrt{\frac{\lambda}{\kappa_x}}(x-x_0)}\right)$$





$$E_{\rm sg} \approx \left(\frac{8\sqrt{\kappa\lambda}}{n_{\rm sg}} - \frac{2\pi\delta_x}{n_{\rm sg}}\right)$$

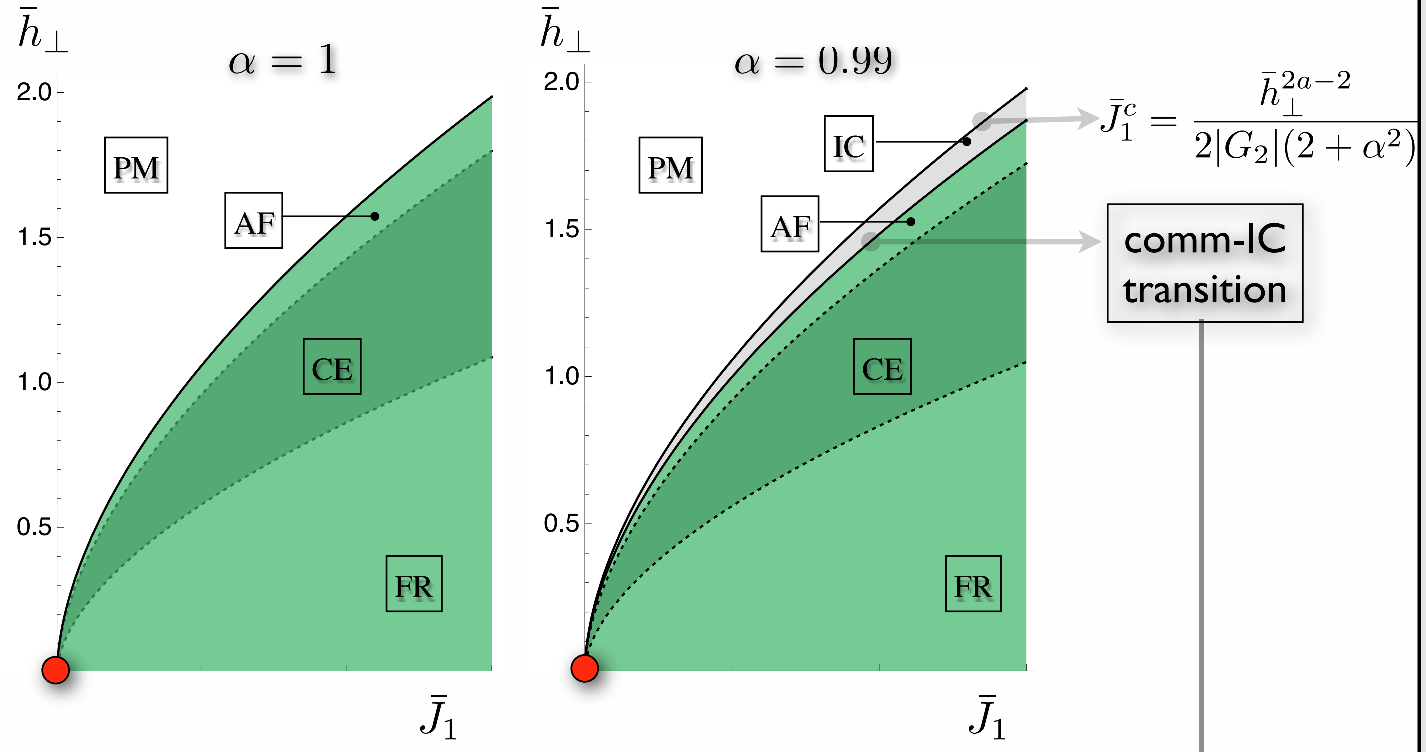
CIT

$$\delta_x > \delta_c = 4\sqrt{\kappa\lambda}/\pi$$

$$\begin{aligned}
\lambda_6 &= \frac{-8G_4^2 + G_2G_6}{G_2}\bar{h}_\perp^{2-6a}, \\
\lambda_3 &= -8G_4\bar{h}_\perp^{2-4a}, \\
\alpha_{\rm m} &= -3G_2\bar{h}_\perp^{2-2a}, \\
\lambda &= 2|\Phi|^6\left(\lambda_6 - \frac{\lambda_3^2}{4\alpha_{\rm m}}\right), \\
\kappa_x &= -|\Phi|^2G_2\bar{h}_\perp^{2-4a}, \\
\delta_x &= -|\Phi|^2\frac{2G_2(1-\alpha)}{\sqrt{3}}h_\perp^{2-2a}.
\end{aligned}$$

$$E_{\rm sg} = A_{yz}\int dx\left[\frac{\kappa}{2}(\partial_x\theta)^2 + \delta_x\partial_x\theta + \lambda\cos(n_{\rm sg}\theta)\right]$$

Phase Boundary



$$\bar{h}_\perp > 0$$

$$\bar{J}_1^{\mathrm{CIT}} = \bar{J}_1^c + \mathcal{A}_{\mathrm{CIT}} \bar{h}_\perp^{2a-2}(1-\alpha)$$

$$\mathcal{A}_{\mathrm{CIT}} = \frac{G_4 \pi}{-2G_2\sqrt{16G_4^2 - 6G_2G_6}}$$

Isosceles Triangle

$$\bar{h}_\perp < 0$$

$$E_{\rm mf} \quad = \quad \sum_i \mathcal{E}_{\rm IFT}(\bar{h}_\perp, \bar{h}_i) + \bar{h}_i \bar{m}_i + \sum \bar{m}_i \frac{\bar{J}_{ij}}{2} \bar{m}_j$$

$$\mathcal{E}^{\bar{h}_\perp < 0}_{\rm IFT}(\bar{h}_\perp, \bar{h}_\parallel) \quad = \quad \frac{\bar{h}_\perp^2}{8\pi} \log \bar{h}_\perp^2 + \bar{h}_\perp^2 \left(\tilde{G}_1 |\xi| + \tilde{G}_2 |\xi|^2 + \ldots \right),$$

$$\xi = \bar{h}_\parallel / \bar{h}_\perp^a$$

Ising chains ordered. Magnetization finite.

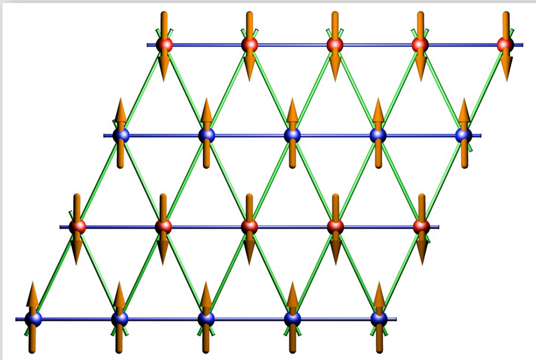
"degenerate perturbation theory"

$$H = \sum_{\langle ij \rangle} \bar{J}_{ij} \sigma_i \sigma_j - \sum_i \left(\sum_a \bar{J}_{ij} \sigma_{i+e_a} \right)^2$$

Isosceles

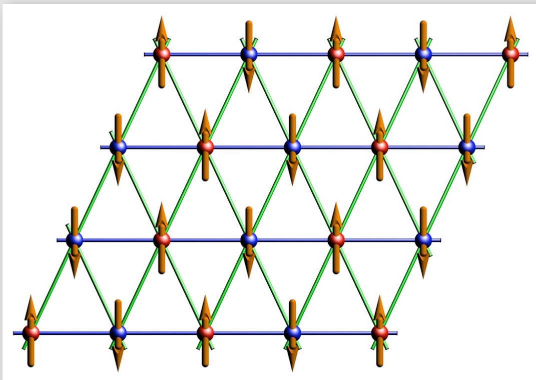
$$H = \sum_{\langle ij \rangle} \bar{J}_{ij}\sigma_i\sigma_j - \sum_i \left(\sum_a \bar{J}_{ij}\sigma_{i+e_a} \right)^2$$

$\mathbf{N1} : J_1 < J_2$



Degeneracy lifted at leading order

$\mathbf{N2} : J_1 > J_2$

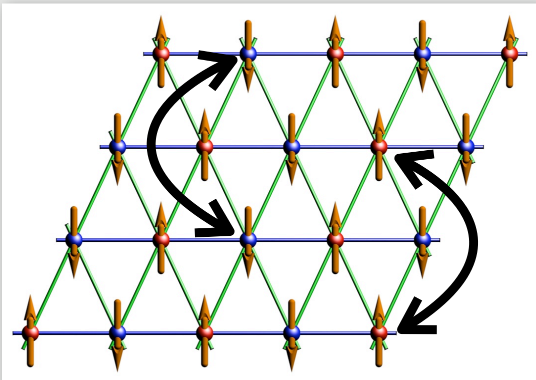


Degeneracy not lifted at any order in MFT!

Degenerate perturbation theory

$$\frac{Z}{Z_0} = \frac{\int e^{-S_{1\text{d}} - S_\text{c}}}{\int e^{-S_{1\text{d}}}} = \langle e^{-S_\text{c}} \rangle$$

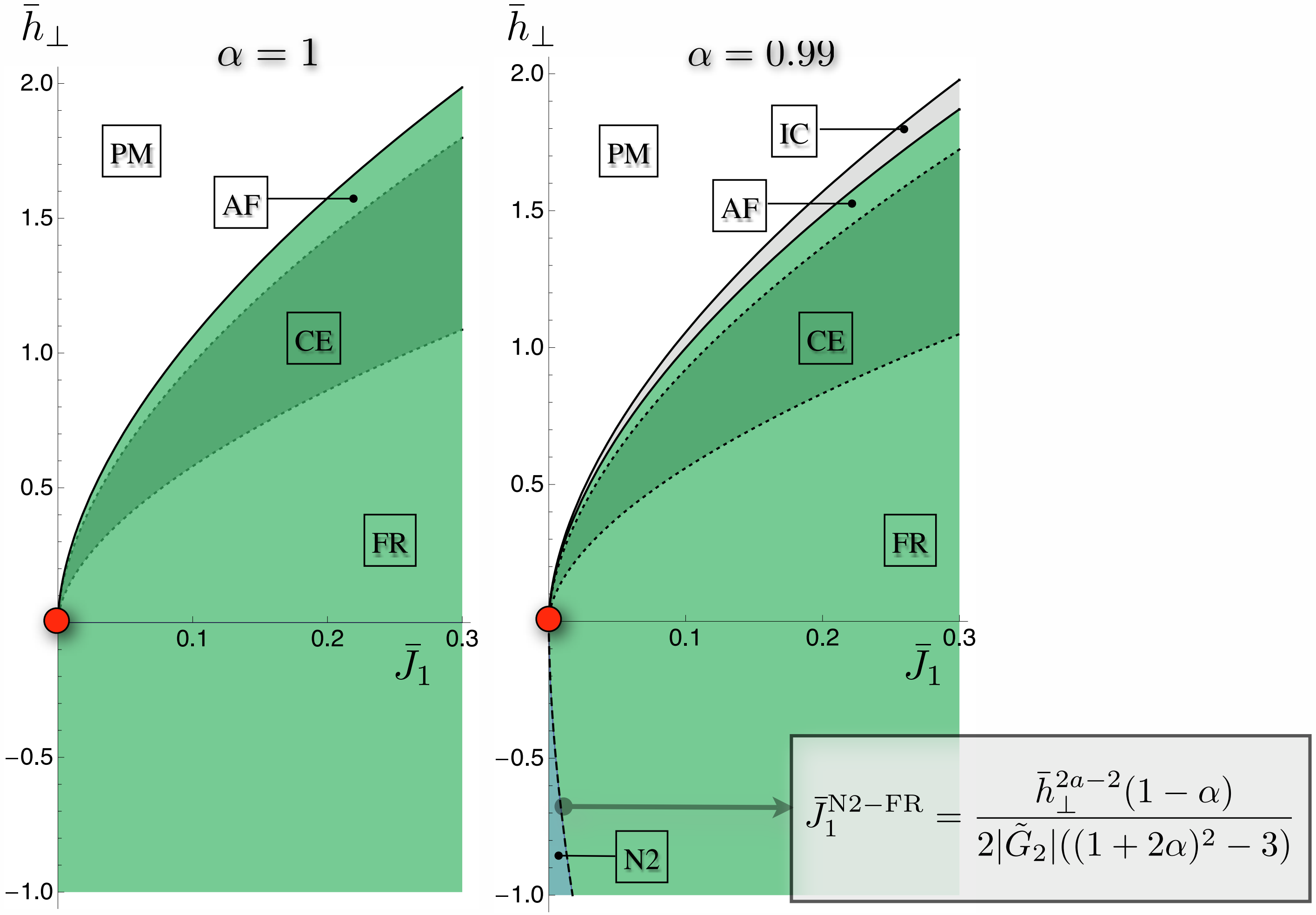
$$\langle e^{-S_\text{c}} \rangle = e^{-\left[\langle S_\text{c} \rangle - \frac{1}{2!}\langle S_\text{c}^2 \rangle_\text{con} + \frac{1}{3!}\langle S_\text{c}^3 \rangle_\text{con} - \frac{1}{4!}\langle S_\text{c}^4 \rangle_\text{con} + \dots\right]}$$



At fourth order,
effective ferro interaction!

4-fold degeneracy.

Phase Diagram



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q-vector in IC from PM

$$E_{\mathrm{mf}} = \sum_i \mathcal{E}_{\mathrm{IFT}}(\bar{h}_\perp, \bar{h}_i) + \bar{h}_i \bar{m}_i + \sum \bar{m}_i \frac{\bar{J}_{ij}}{2} \bar{m}_j$$

$$\bar{h}_i = \Phi_k e^{ik\cdot r_i} + \Phi_{3k} e^{i3k\cdot r_i} + \mathrm{c.c.}$$

$$e = \alpha_k |\Phi_k|^2 + u_k |\Phi_k|^4 + \alpha_{3k} |\Phi_{3k}|^2 + \lambda_k (\Phi_k^3 \Phi_{3k}^* + \mathrm{c.c.})$$

q-vector in IC from PM

$$E_{\rm mf} \quad = \quad \sum_i \mathcal{E}_{\rm IFT}(\bar{h}_\perp, \bar{h}_i) + \bar{h}_i \bar{m}_i + \sum \bar{m}_i \frac{\bar{J}_{ij}}{2} \bar{m}_j$$

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$$e = \alpha_k |\Phi_k|^2 + u_k |\Phi_k|^4 + \alpha_{3k} |\Phi_{3k}|^2 + \lambda_k (\Phi_k^3 \Phi_{3k}^* + \text{c.c.})$$

What is shift from $\mathbf{Q}^* = \left(2\cos^{-1}\left(-\frac{\alpha}{2}\right), 0\right)$

$$\delta q_x = \frac{32(2a-2)^2}{9\sqrt{3}} (1-\alpha) \left(\frac{\bar{h}_\perp - \bar{h}_\perp^c}{\bar{h}_\perp^c} \right)^2$$

q-vector in IC from AF

$$E_{\rm sg} \approx \left(\frac{8\sqrt{\kappa\lambda}}{n_{\rm sg}} - \frac{2\pi\delta_x}{n_{\rm sg}} \right)$$

finite density of domain walls,

$$\frac{E_{\rm sg}(n_d)}{A_{yz}} \approx \left(\frac{8\sqrt{\kappa\lambda}}{n_{\rm sg}} - \frac{2\pi\delta_x}{n_{\rm sg}} \right) n_d + U n_d e^{-\frac{1}{w n_d}},$$

$$w = \frac{1}{n_{\rm sg}}\sqrt{\frac{\kappa}{\lambda}}$$

q-vector in IC from AF

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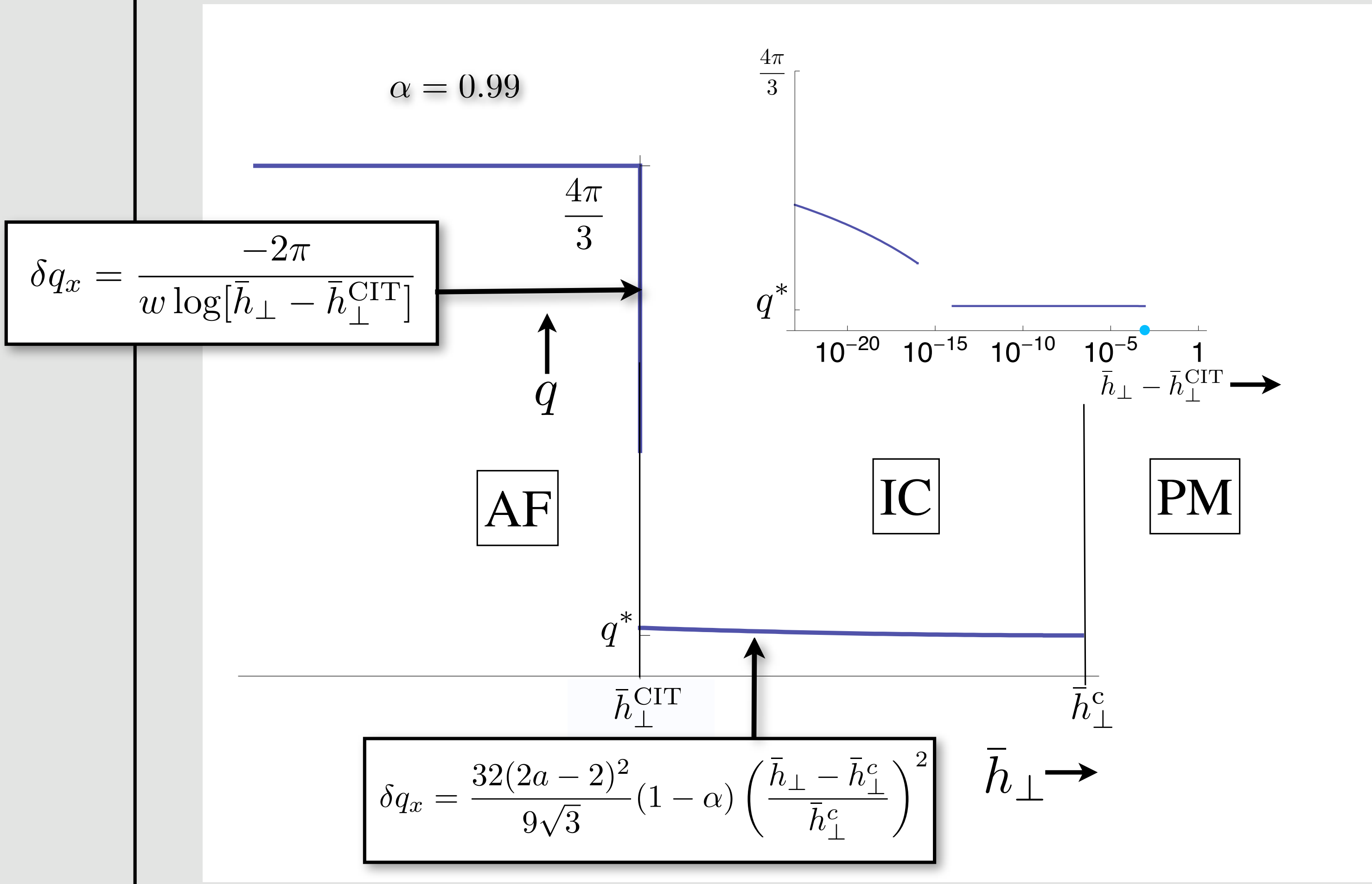
$$w = \frac{1}{n_{\rm sg}} \sqrt{\frac{\kappa}{\lambda}}$$

shift from $4\pi/3$

$$\delta q_x = \frac{-2\pi}{w \log[\bar{h}_\perp - \bar{h}_\perp^{\rm CIT}]}$$

q-vector summary



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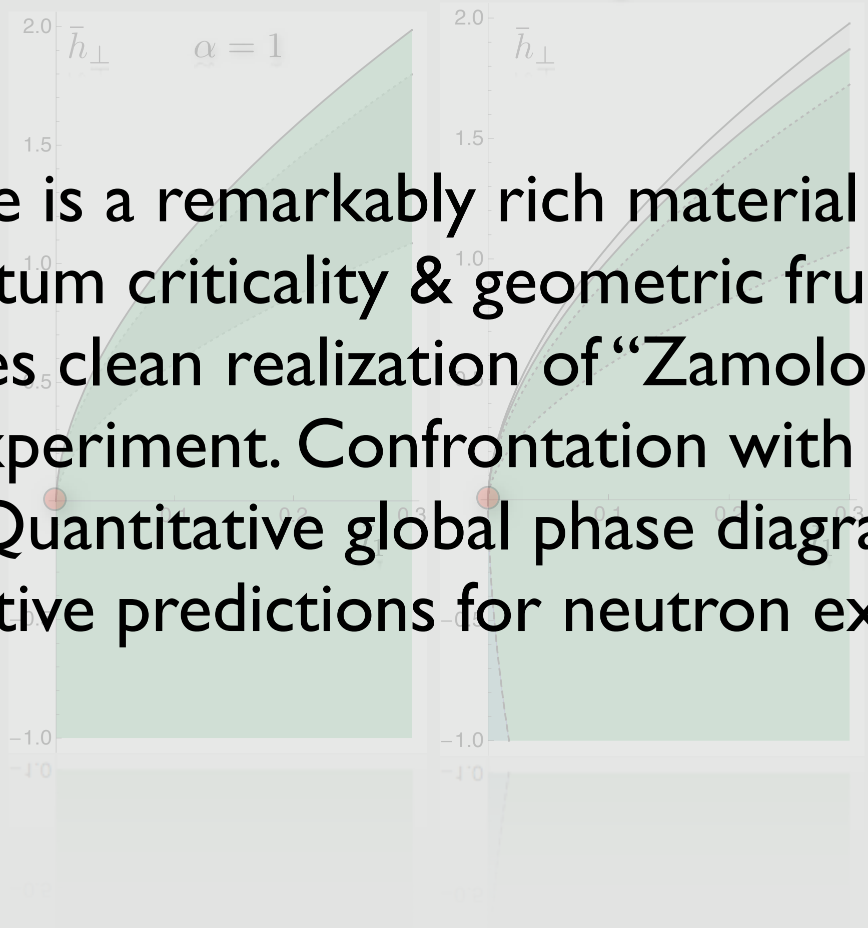

★ Columbite is a remarkably rich material -- interplay of quantum criticality & geometric frustration

★ Provides clean realization of "Zamolodchikov" physics in experiment. Confrontation with experiment!

★ Quantitative global phase diagram

★ Quantitative predictions for neutron experiments

Please look at:

S. Lee, R.K. Kaul & L. Balents

http://arxiv.org/abs/0911.0038