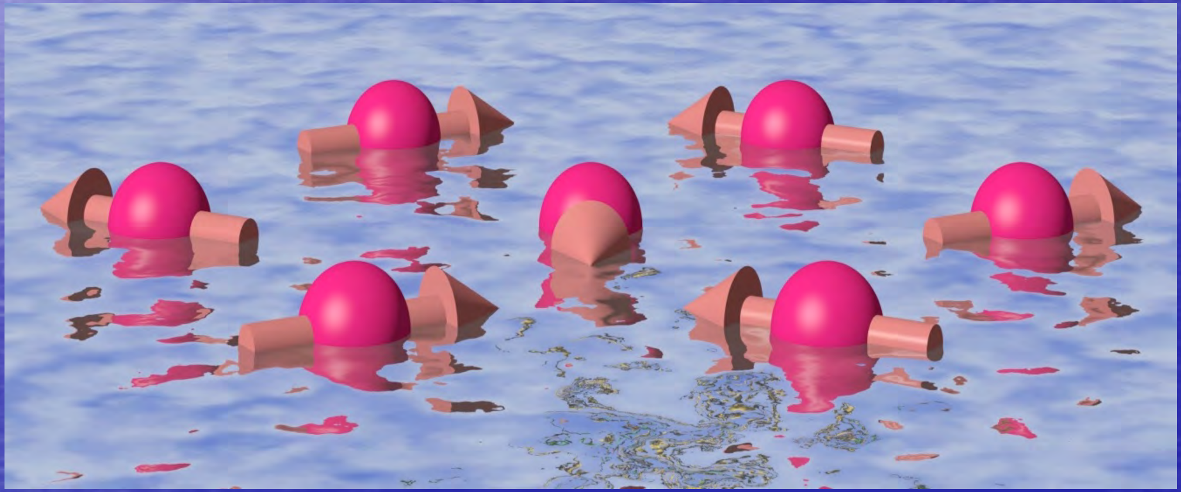
Unconventional ordered states in anisotropic triangular antiferromagnets

Andrey Chubukov
University of Minnesota

Oleg Starykh
University of Utah



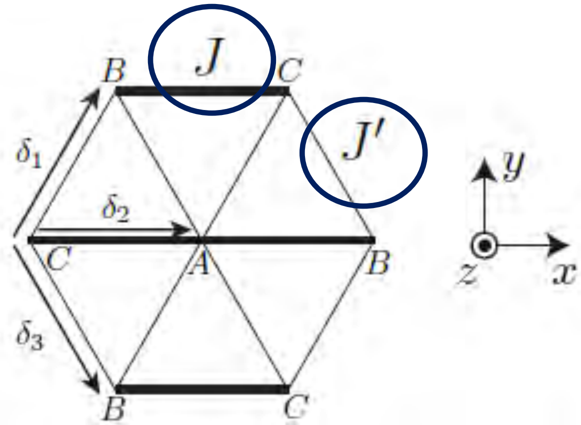
SPICE Workshop on Computational Quantum Magnetism, May 23, 2015

My goal:

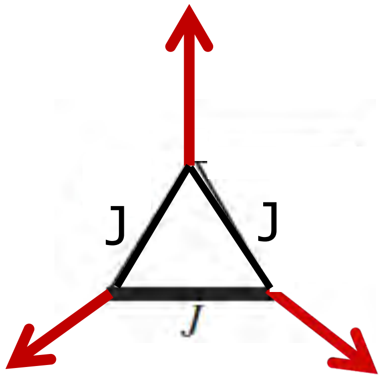
To get workshop participants, particularly those specializing in numerical calculations, interested in looking at unconventional ordered state in triangular AFM

And also to show that there is interesting physics not falling under the umbrella of a “spin liquid”

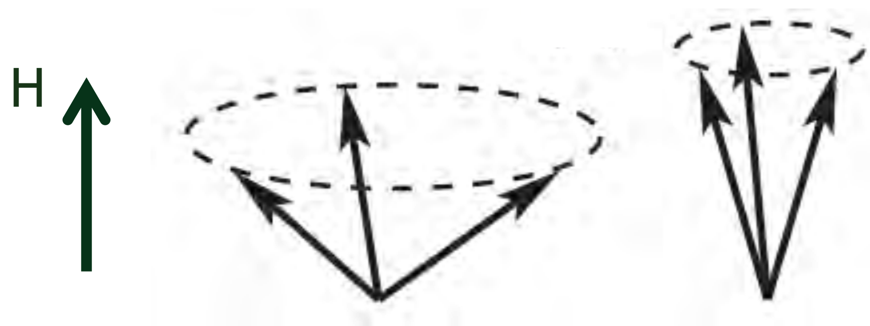
I consider a rather simple 2D system of localized spins on a triangular lattice



If J=J', at zero field spins form a 120° configuration



Now apply a field

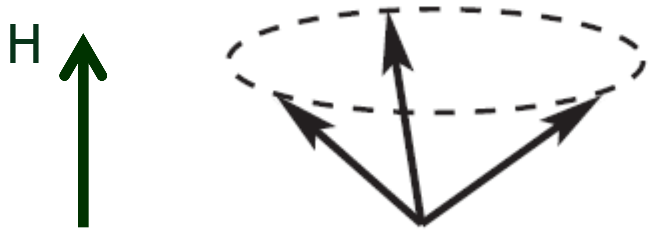


A seemingly obvious choice: a non-co-planar state with all three spins in a triad equally rotating towards a field

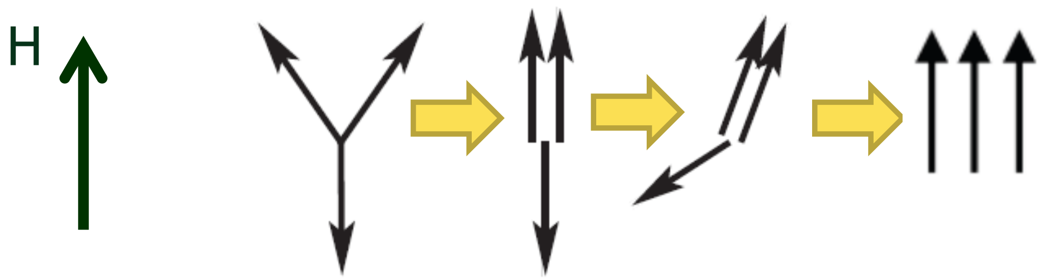
Such an order breaks U(1) * Z_2

Is this the right result for the 2D model?

Classical degeneracy in 2D: for classical spins, an infinite number of different spin configurations at a given H have the same energy at T=0



One “end point” of the set is the non-co-planar cone state (umbrella)



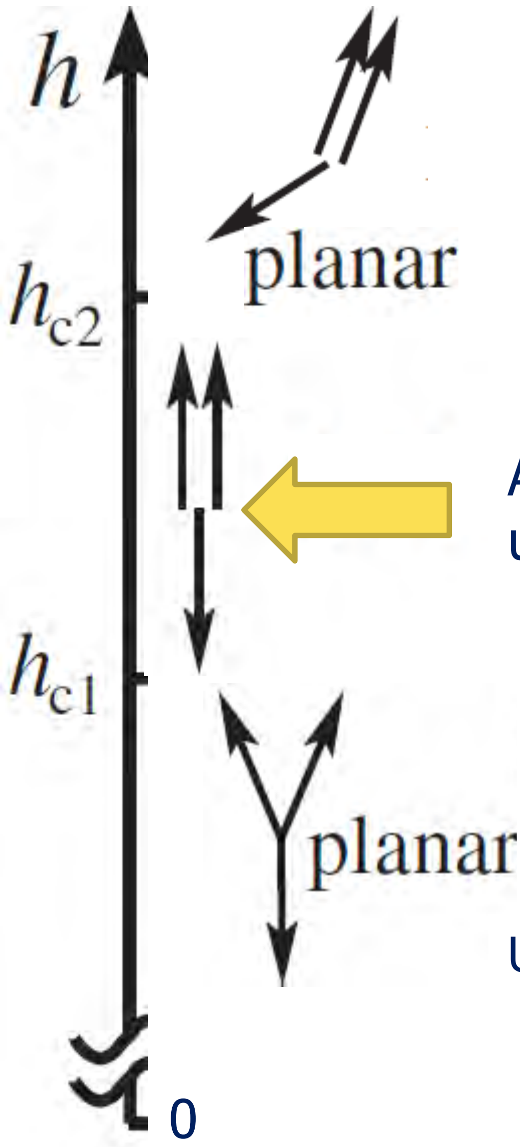
The other “end point” is the co-planar state

The co-planar state breaks the discrete Z_3 symmetry by selecting which of the three spins in a triad is opposite to H

The degeneracy is broken by thermal and quantum fluctuations

Quantum phase diagram (J=J′): co-planar state wins!

J=J′

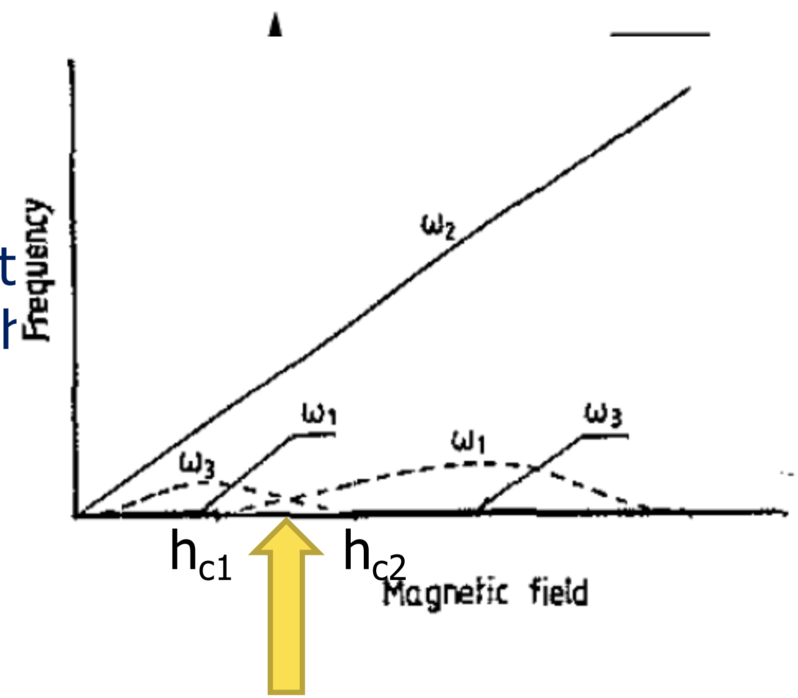


0

U(1) x Z_3

An intermediat
up-up-down ph
Only Z_3
M = $M_{sat}/3$

U(1) x Z_3

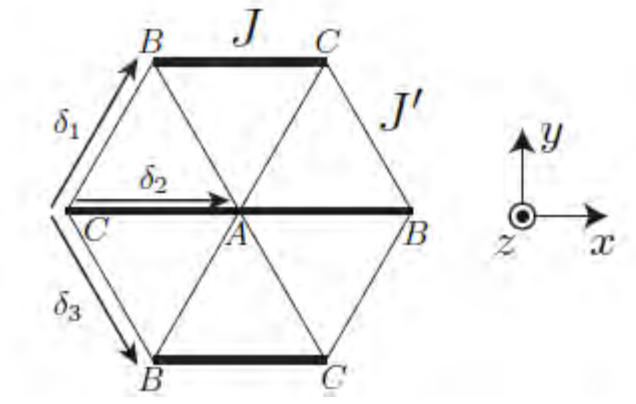


All 3 branches of spin-wave excitations are gapped

Experiment:

The two mostly studied antiferromagnets on a triangular lattice are Cs_2CuCl_4 and Cs_2CuBr_4

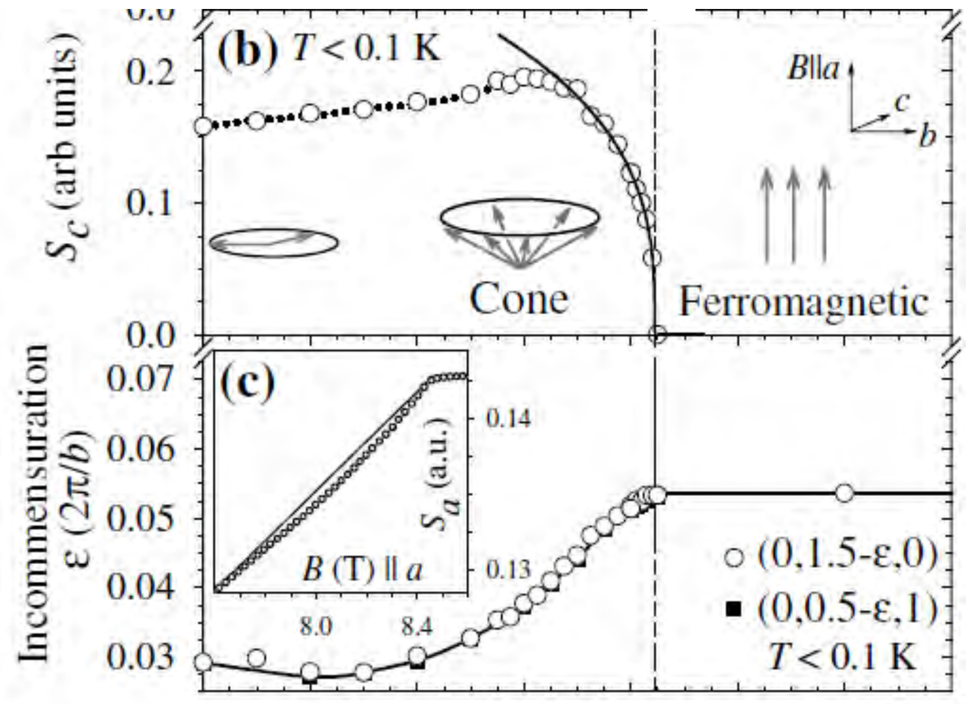
They do have non-equal exchange interactions



For both systems J > J′ (anisotropy towards 1D chains)

Cs_2CuCl_4 (J' =0.3-0.35 J)

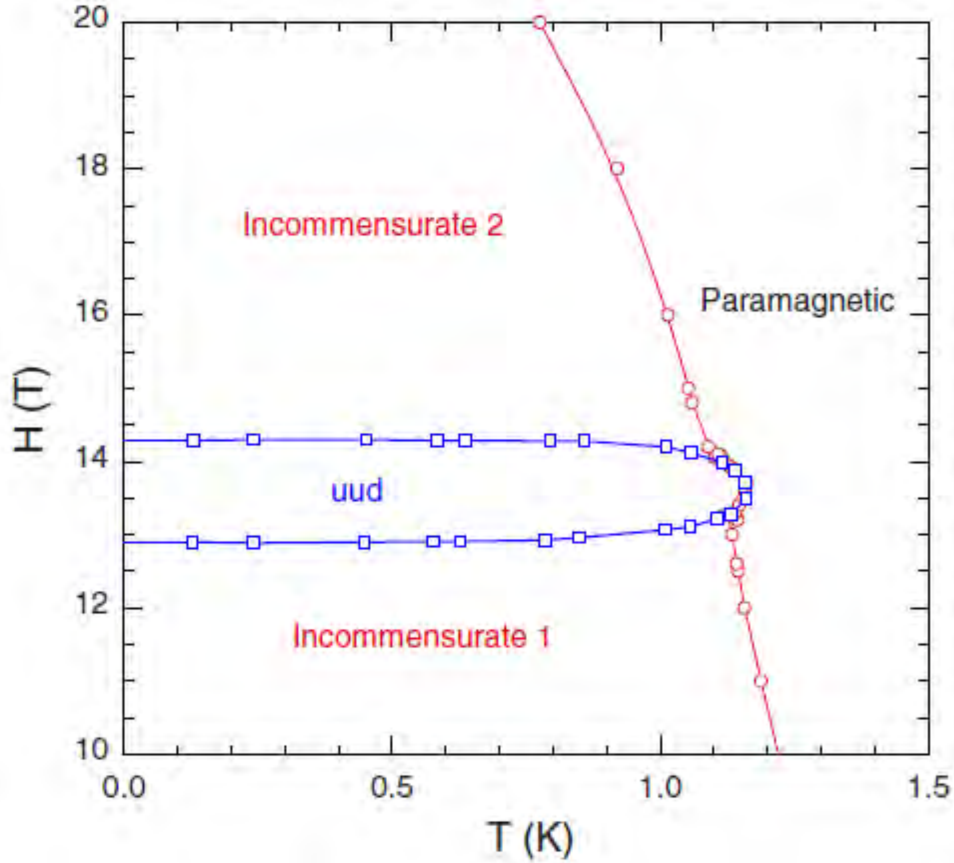
No magnetization plateau



Magnetic field

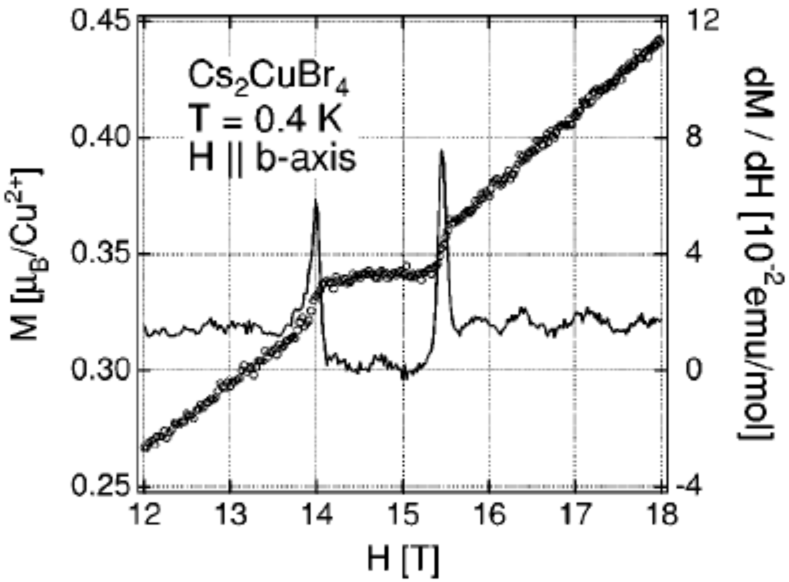
R. Coldea et al, 2002

Cs_2CuBr_4 (J' =0.7 J)

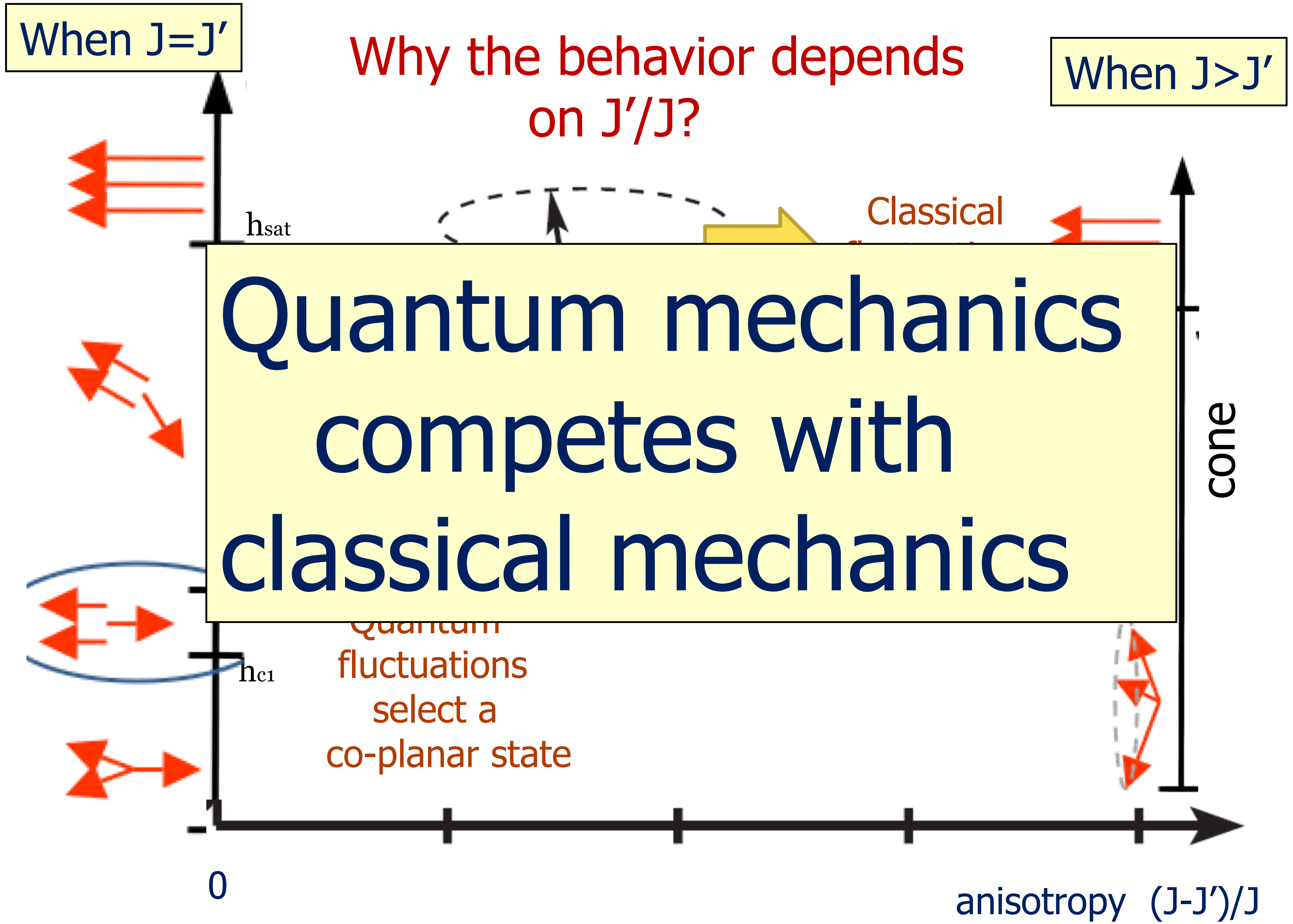


Tsujii et al, 2007

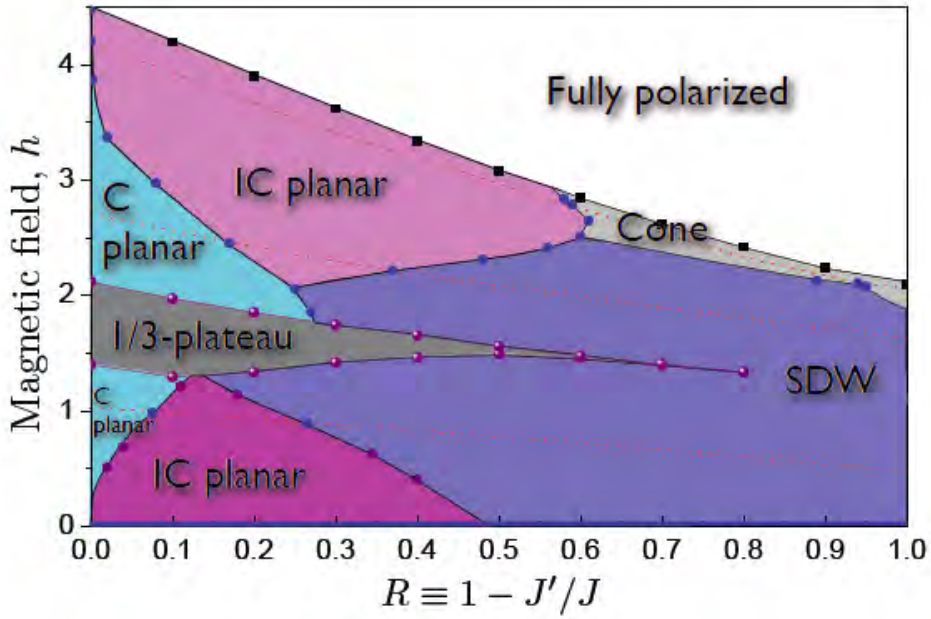
Magnetization plateau



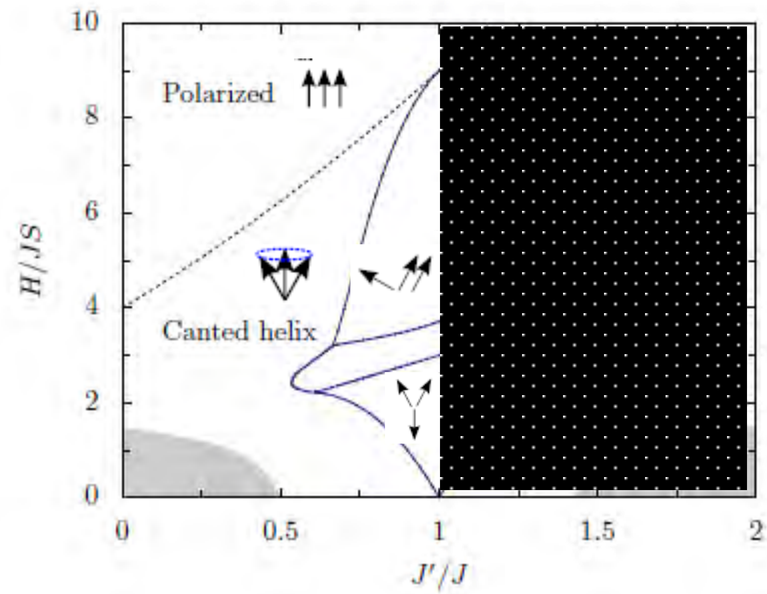
Ono et al, 2002



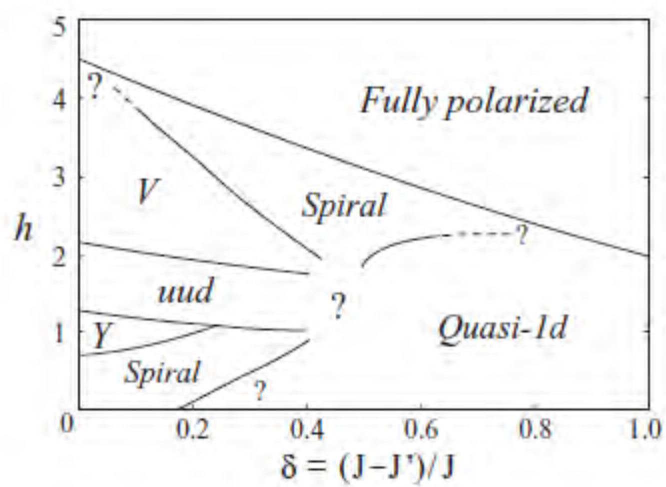
When J=J′
Why the behavior depends on J′/J?
When J>J′
Classical
hsat
Quantum mechanics competes with classical mechanics
cone
Quantum
hc1
fluctuations
select a
co-planar state
0
anisotropy (J-J′)/J



Chen, Ju, Jiang, Starykh, Balents



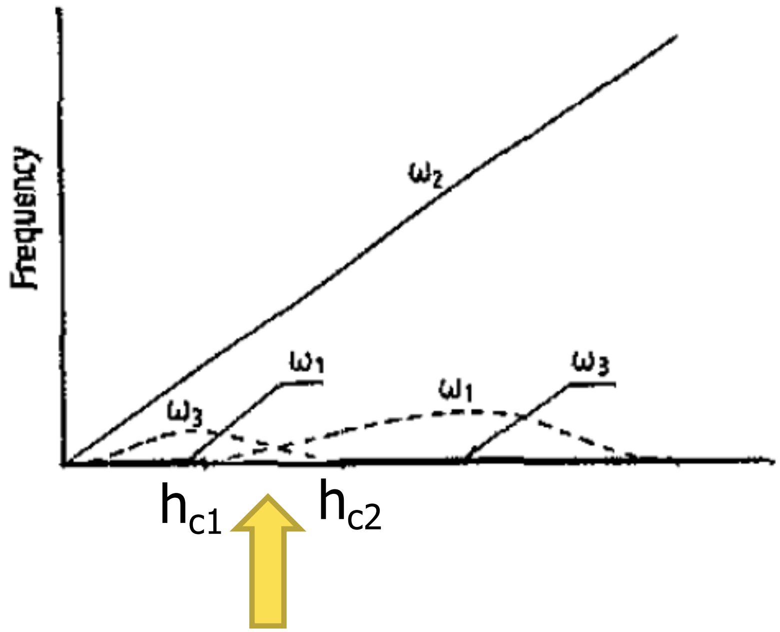
Coletta, Zhitomirsky, Mila



Tay, Motrunich

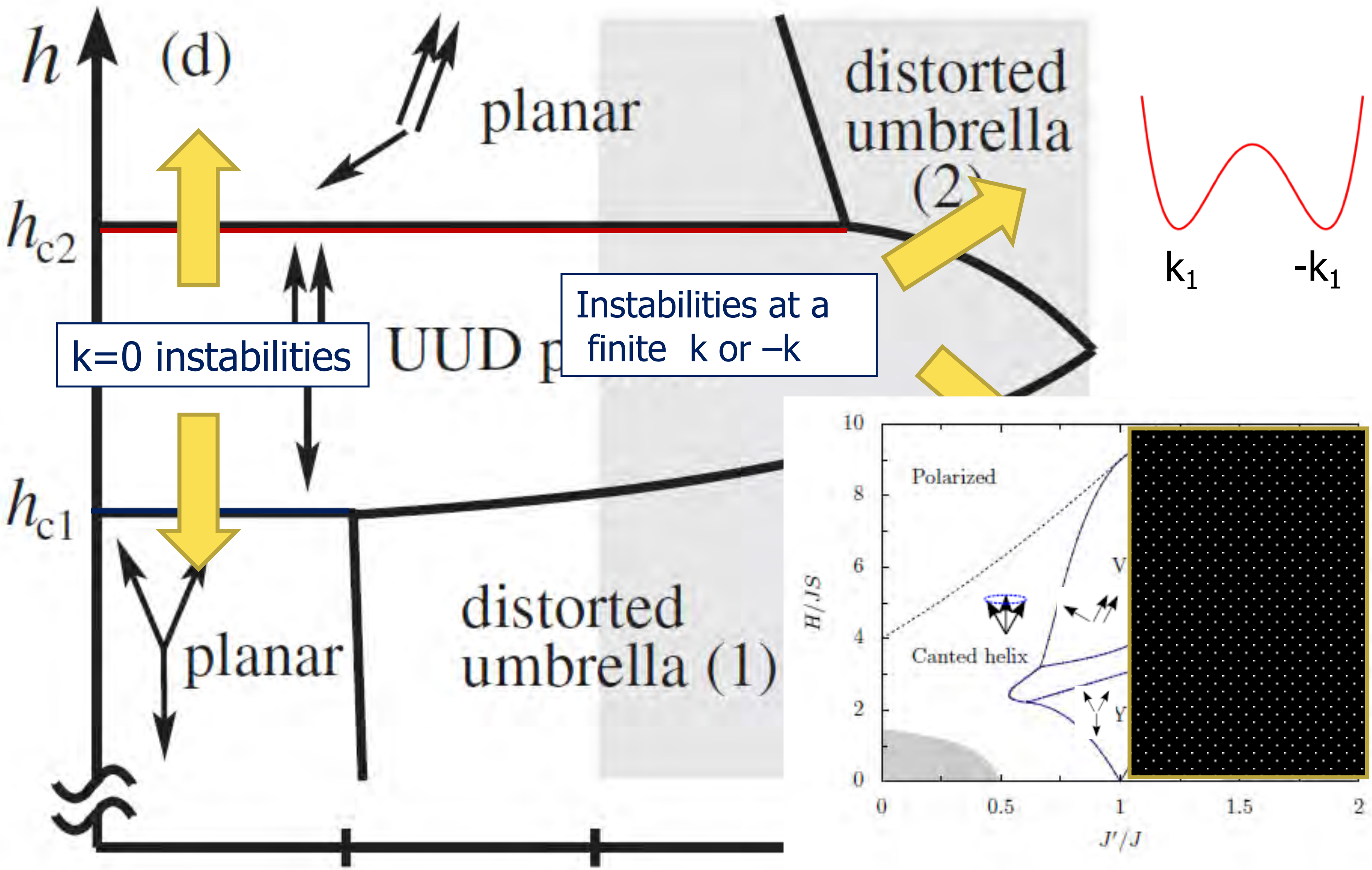
Part I

To see how classical mechanics competes with quantum mechanics, let's start with up-up-down phase and do spin-wave calculations



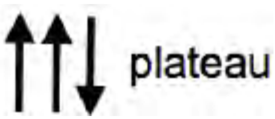
All 3 branches of spin-wave excitations are gapped

“Spin-wave” analysis



J. Alicea, O. Starykh, A.C

anisotropy $(J-J')/J/S^{1/2}$



?

Once there is a spin-wave instability at a finite momentum |k|, there are two options for a system:

It can develop condensates ψ simultaneously at +k and –k

$$S_x (r) = \psi (\text{Cos } k\, r + \text{Cos } (-k\, r)) = 2 \text{ Cos } k\, r$$

$$S_y (r) = \psi (\text{Sin } k\, r + \text{Sin } (-k\, r)) = 0$$

A co-planar state (spins in XZ plane)

Or, it can develop a condensate ψ at +k OR at –k

$$S_x (r) = \psi \text{ Cos } k\, r, \quad S_y (r) = \psi \text{ Sin } k\, r$$

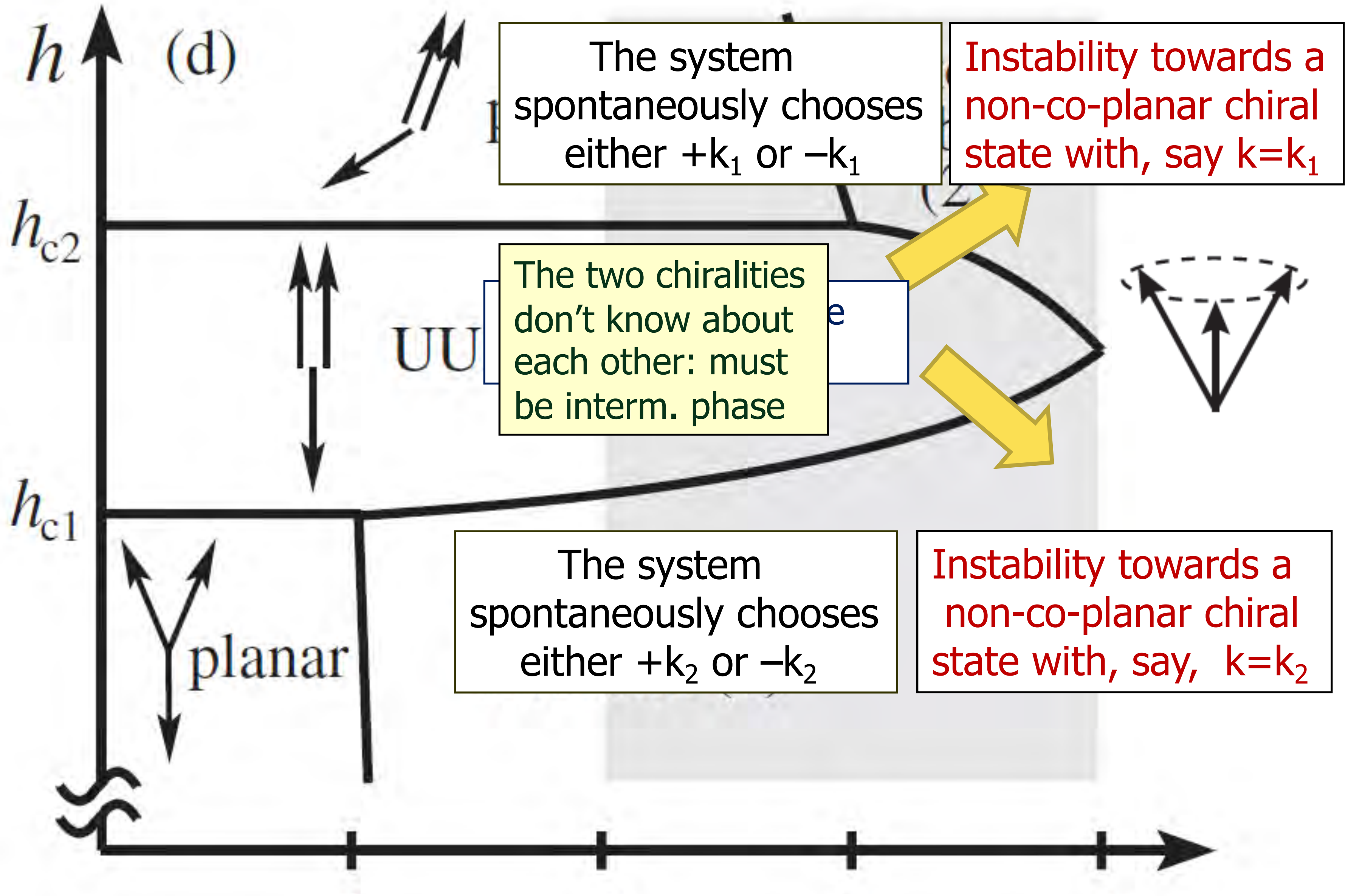
A non-coplanar state (spins have all 3 components)

How to distinguish? One has to derive Landau functional

$$F = \alpha\, (\psi^2_k + \psi^2_{-k}) + \beta_1(\psi^4_k + \psi^4_{-k}) + 2\, \beta_2\, \psi^2_k \psi^2_{-k}$$

A non co-planar state if $\beta_2 > \beta_1$, and a co-planar state if $\beta_1 > \beta_2$

We derived Landau functional. The results:



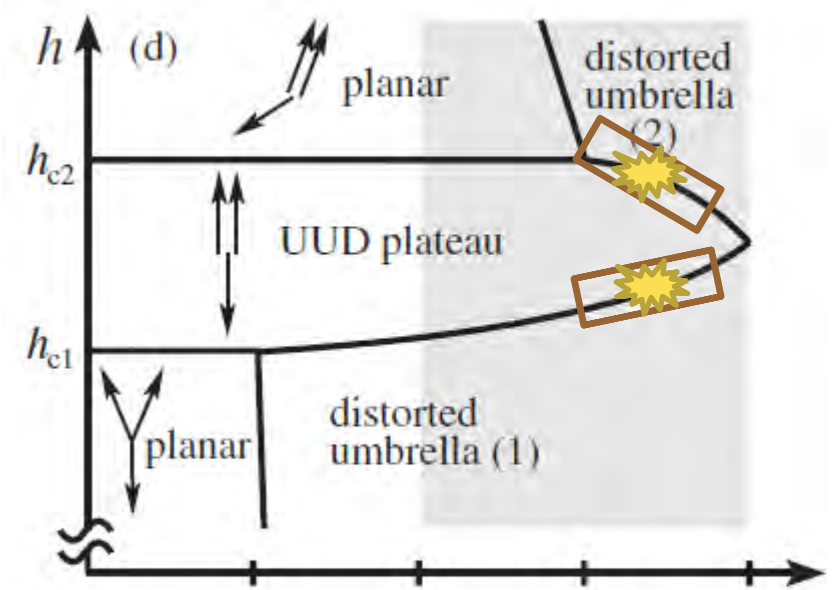
J. Alicea, O. Starykh, A.C

We decided to do one thing at a time and search for a potential pre-emptive two-magnon instability

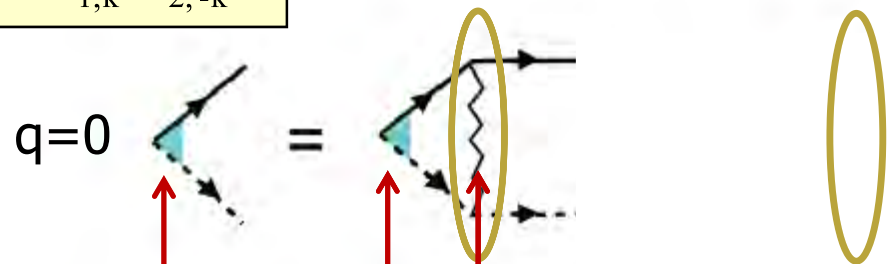
At a first glance, this is waist of time:
magnon-magnon interaction is repulsive in an antiferromagnet,
so no reasons to expect a two magnon bound state

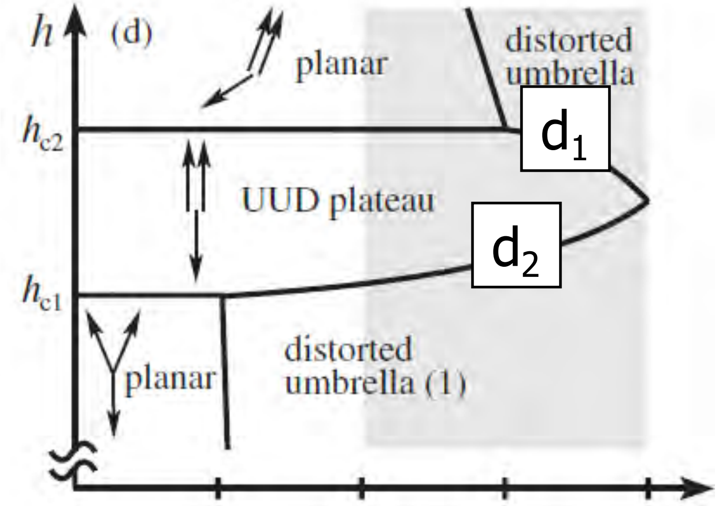
Indeed, we considered interaction between magnons within one branch and found only repulsion.

But a conventional reasoning does not work when the two magnons, which we try to pair, belong to different spin-wave branches



$$\Delta(k) = \langle d^{+}_{1,k}\ d^{+}_{2,-k} \rangle$$





$\delta = (J-J')^2/(J^2\ S)$

Linearized gap equation

$$\Delta(k) = \int (\Delta(q) - \Delta^{*}(q))\, K(k,q)\, d^2q$$

$$\Delta(k) = \Delta\, f(k)$$

$$\Delta = \frac{1}{S} I(\delta)\,(\Delta - \Delta \quad 0$$

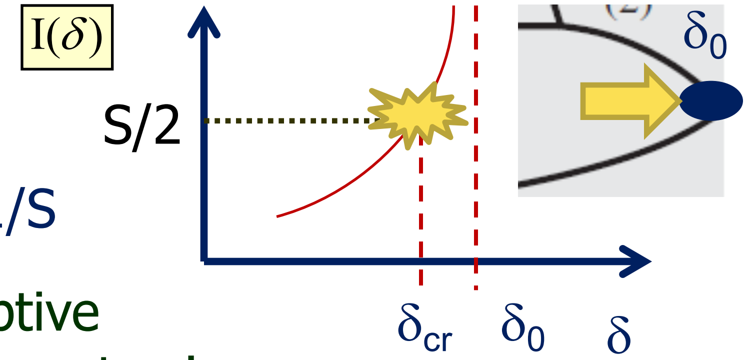
$I(\delta) > 0$, attraction!

Real Δ -- no instability

If we choose an imaginary solution $\Delta(k) = i\,\Phi(k)$

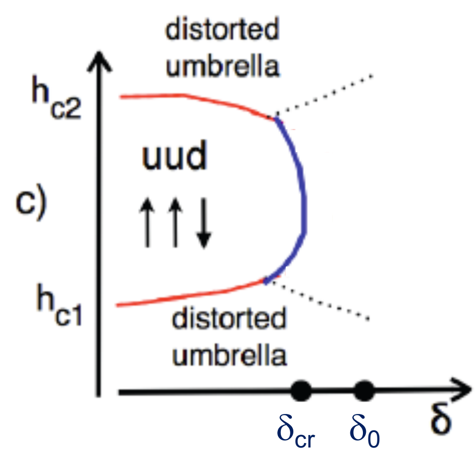
$$\Phi = \frac{2}{S}\,\Phi\, I(\delta) \qquad I(\delta) > 0$$

$$\Phi = \frac{2}{S}\Phi\ \ I(\delta), \quad I(\delta) > 0$$



One needs to check that I(δ) can overcome 1/S

As a result, the system develops a pre-emptive instability, in which two magnons from different spin-wave branches form a q=0 bound state with an imaginary order parameter

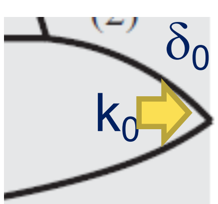


Math:

$$\delta_{cr} = \delta_0\,(1 - O(1/S^2))$$

2-magnon instability condition is at δ_{cr}

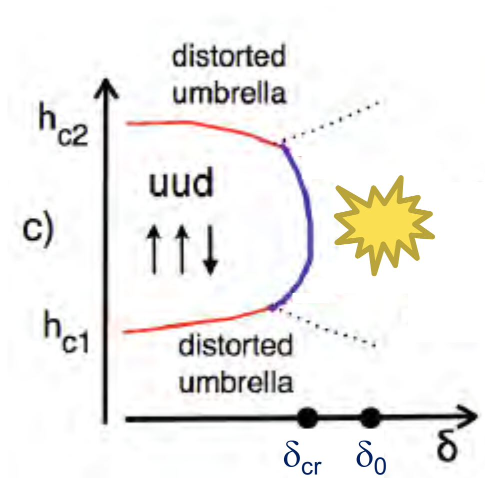
$$1 = \frac{2}{S} I(\delta) = \frac{1}{S}\frac{3}{N}\sum_p \frac{k_0}{(p^2 + (1-\delta_{cr}/\delta_0)k_0^2)^{3/2}}$$



k_0 – momentum of spin-wave instability at $\delta = \delta_0$ (same for both branches)

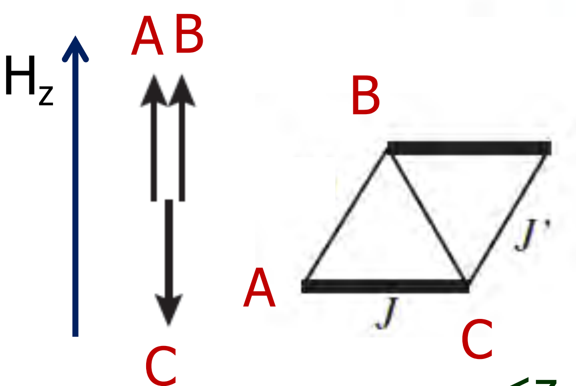
$$\delta_0 : (1 - J'/J)^2 = 3/10S$$

What is the spin configuration in this state?



$$< d^{+}_{1,k} > = < d^{+}_{2,k} > = 0$$

$$< d^{+}_{1,k} d^{+}_{2,-k} > = i\,\Phi\, f(k)$$



$$<\mathbf{S}_{A,perp}> = <\mathbf{S}_{B,perp}> = <\mathbf{S}_{C,perp}> = 0$$

$$<\mathbf{S}_A\,\mathbf{S}_B> = <\mathbf{S}_B\,\mathbf{S}_C> = <\mathbf{S}_C\,\mathbf{S}_A> = 0$$

$$<z\,(\mathbf{S}_A \times \mathbf{S}_C)> = <z\,(\mathbf{S}_C \times \mathbf{S}_B)> = <z\,(\mathbf{S}_B \times \mathbf{S}_A)> \sim \Phi$$

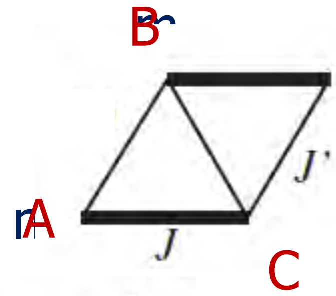
Vector chirality

$< \mathbf{S}_A\,(\mathbf{S}_B \times \mathbf{S}_C)> \sim \Phi$ Scalar chirality

N.B. No non-collinear incommensurate spin order!

Spin current

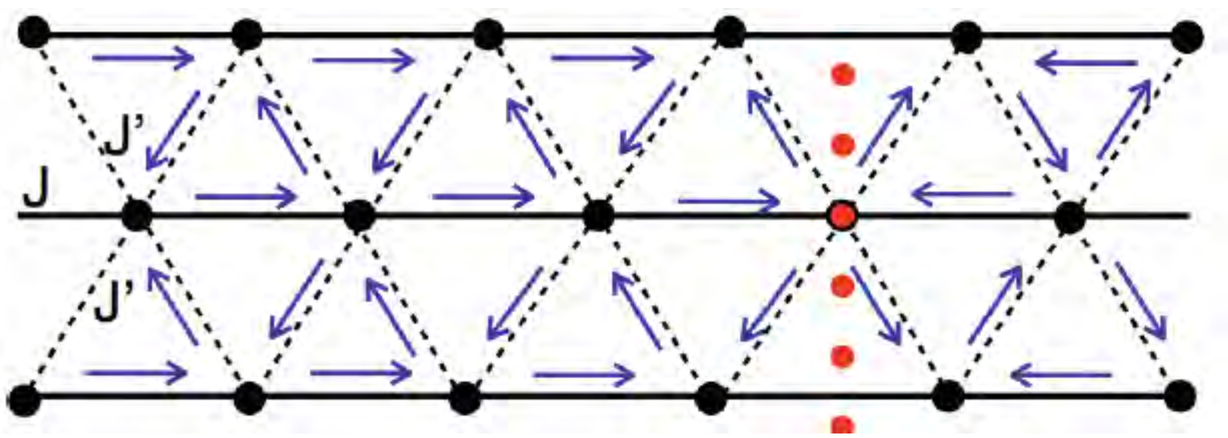
$$J^z_{nm} = \frac{1}{2i}(S^-_n S^+_m - S^+_n S^-_m)$$



$$J^z_{CA} = iS(c^+_{\mathbf{r}} a^+_{\mathbf{r}} - c_{\mathbf{r}} a_{\mathbf{r}}), J^z_{CB} = iS(c^+_{\mathbf{r}} b^+_{\mathbf{r}} - c_{\mathbf{r}} b_{\mathbf{r}})$$
$$J^z_{AB} = iS(b^+_{\mathbf{r}} a_{\mathbf{r}} - a^+_{\mathbf{r}} b_{\mathbf{r}}).$$

$$\langle c_r a_r \rangle = - \langle c_r b_r \rangle = \langle a^+_r b_r \rangle = i\,\Phi$$

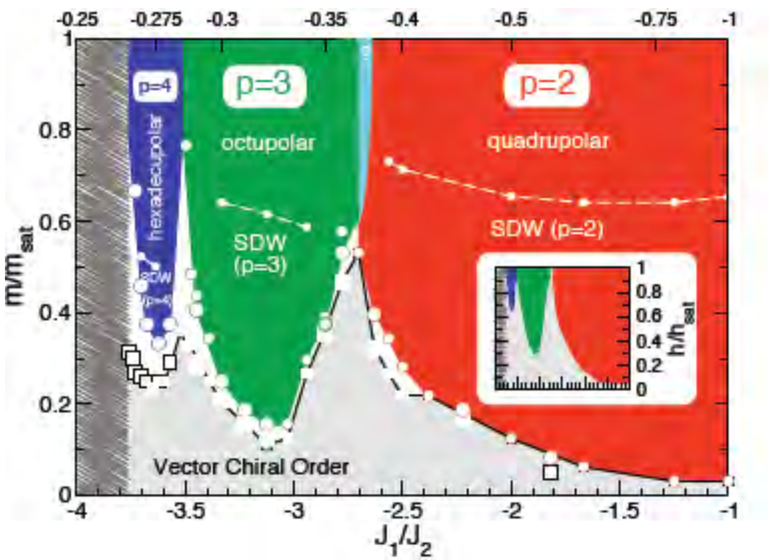
$\Phi>0$ $\Phi<0$



This may be the tip of the iceberg

The state we found may exist in a finite range of anisotropies and then become unstable towards multi-magnon condensation

An example of such behavior – 1D J_1/J_2 model

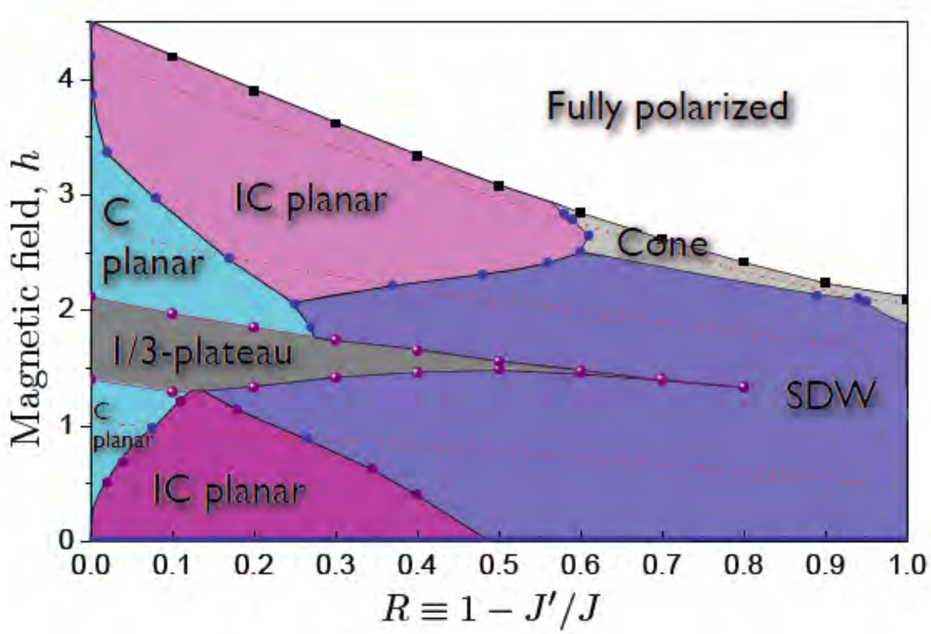


Sudan, Luscher, Lauchi
Hikihars, Kecke, Momoi, Furusaki
Shannon, Momoi, Sindzingre,
A.C., Balents….

Part II

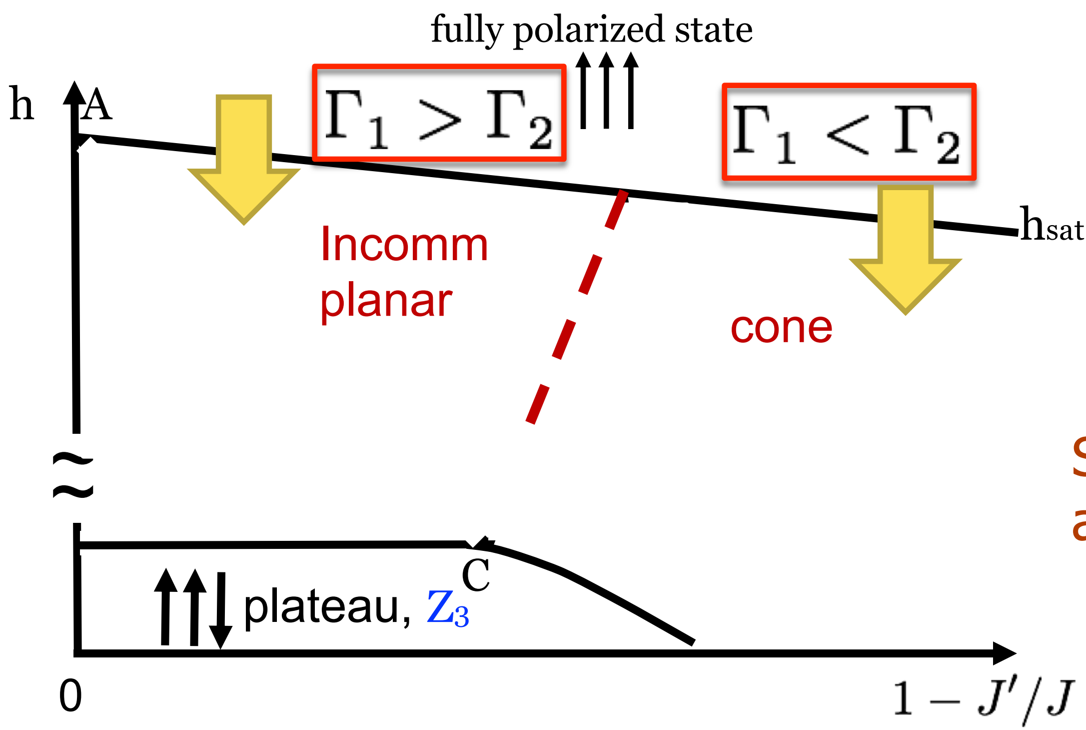
Phases of a triangular-lattice antiferromagnet near saturation:

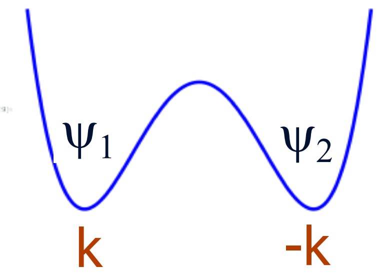
Earlier papers:



Chen, Ju, Jiang, Starykh, Balents

Do spin-wave calculations





Spin-wave instability at momenta k and -k

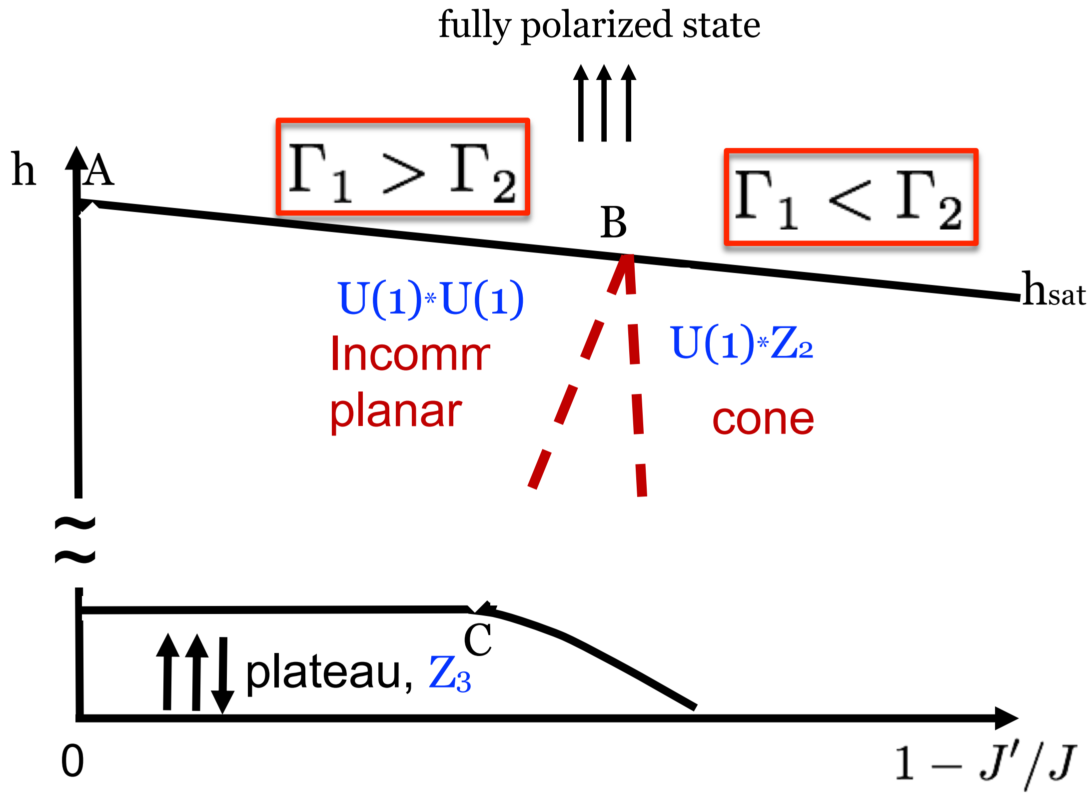
Low-density expansion $$E_0/N = -\mu(|\psi_1|^2 + |\psi_2|^2) + \frac{1}{2}\Gamma_1(|\psi_1|^4 + |\psi_2|^4) + \Gamma_2|\psi_1|^2|\psi_2|^2$$

$\Gamma_1 > \Gamma_2$: both condensates appear simultaneously, the result is co-planar state

$\Gamma_2 > \Gamma_1$: only one condensate emerges, this leads to cone state (chiral)

$$\Delta\Gamma = \Gamma_2 - \Gamma_1 = \Delta\Gamma^{(0)} + \Delta\Gamma^{(1)} = \frac{9(\delta J)^2}{J} - \frac{1.6J}{S}$$

Classical physics vs quantum physics



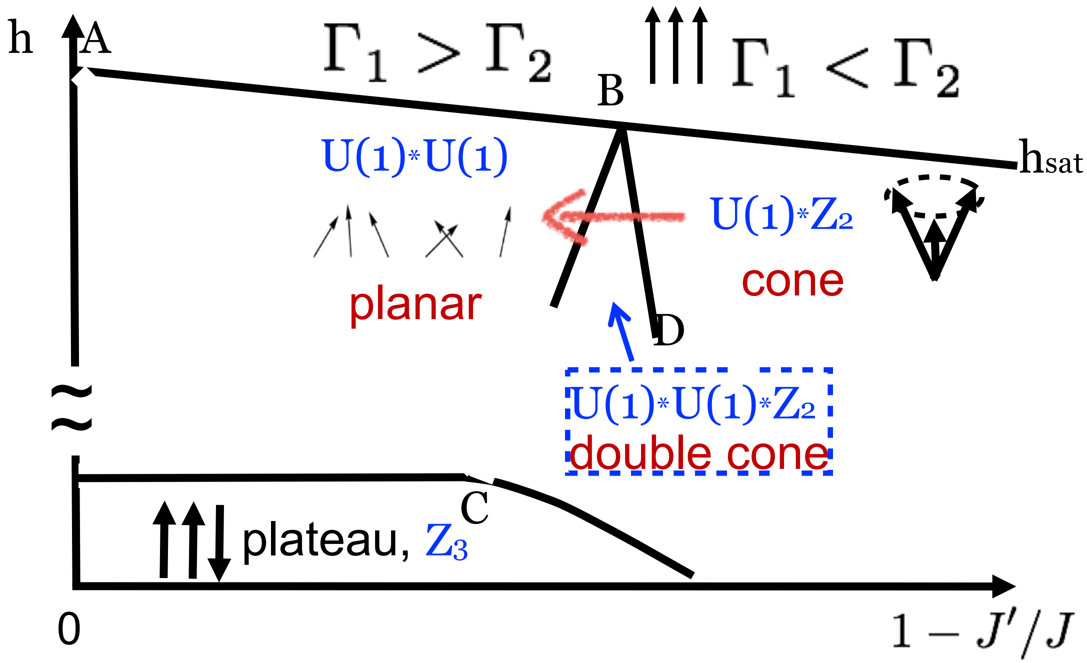
U(1)*U(1) == translational symmetry + the choice of the plane

U(1)*Z_2 == translational symmetry + chirality

How the transition between the two occurs?

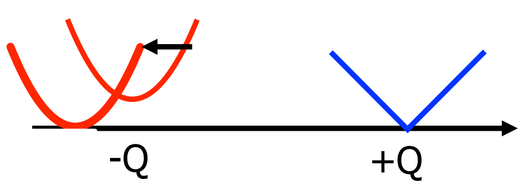
- direct, first order
- via an intermediate phase ★

Intermediate state is a double cone



Elementary excitation spectrum of the cone phase:
Goldstone mode at k = +Q, gapped at k = -Q

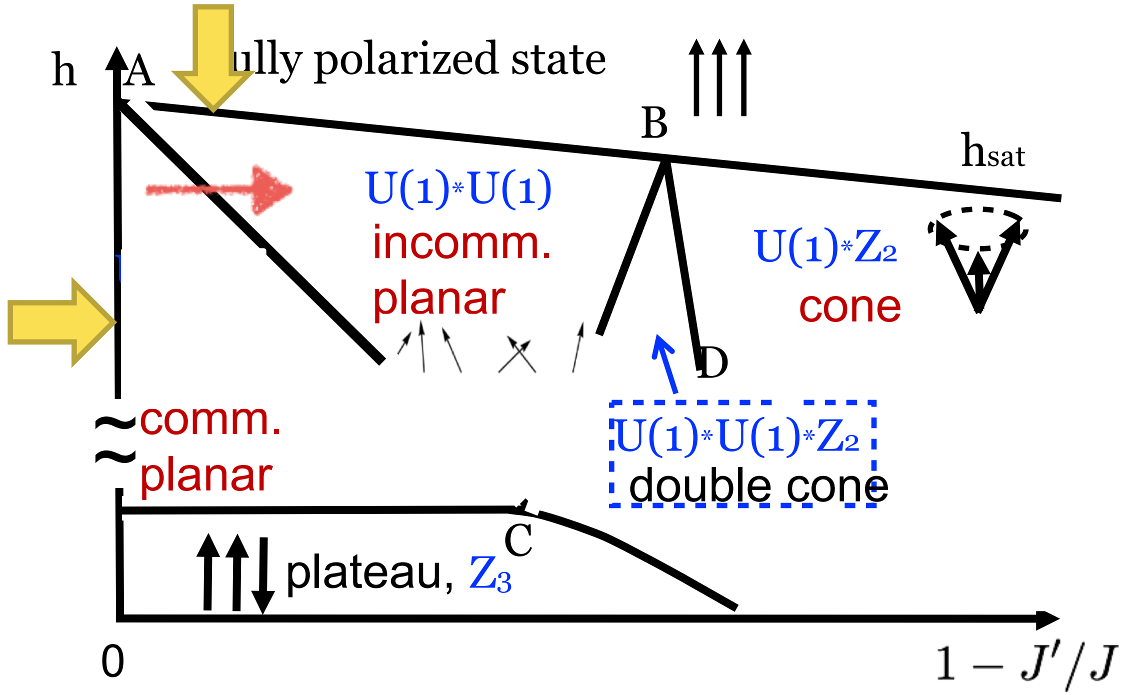
- Transition at **BD**: softening of the mode at -Q’



$$Q' = Q + \frac{1.45(h_{\text{sat}} - h)}{h_{\text{sat}}\sqrt{S}}$$

Double cone, one with Q, another with –Q’

Commensurate-incommensurate transition



This is NOT spin-wave driven transition

Rather, we have commensurate-incommensurate transition

Classical mechanics wants incommensuration,
quantum mechanics wants to keep state commensurate

What I earlier called q=0 is actually $Q_0 = (4\pi/3, 0)$

In a generic case of order with |Q| we introduce condensates with Q and –Q: ψ_1 and ψ_2

$$E_0/N = -\mu(|\psi_1|^2 + |\psi_2|^2) + \frac{1}{2}\Gamma_1(|\psi_1|^4 + |\psi_2|^4)$$
$$+\Gamma_2|\psi_1|^2|\psi_2|^2 + \Gamma_3((\bar{\psi}_1\psi_2)^3 + \text{h.c.})\ldots$$

Γ_3 term is generally not allowed by momentum conservation, BUT is allowed if Q is commensurate (= Q_0)

$$\Gamma_3 = \frac{3}{32S^2}\sum_{\mathbf{k}\in\mathrm{BZ}}\left(\frac{(5J_\mathbf{k}+J_0)(5J_{\mathbf{Q}+\mathbf{k}}+J_0)J_{\mathbf{Q}-\mathbf{k}}}{(J_0-J_\mathbf{k})(J_0-J_{\mathbf{Q}+\mathbf{k}})} - \frac{(5J_\mathbf{k}+J_0)(J_\mathbf{k}+J_0)}{2(J_0-J_\mathbf{k})}\right) + \frac{3J_0}{64S^2} \approx -\frac{0.69J}{S^2}$$

quantum mechanics favors comm. order

$$\langle \mathbf{S}_\mathbf{r}\rangle = (S - 2\rho\cos^2[\mathbf{Q}\cdot\mathbf{r}+\theta])\hat{z} + \sqrt{4S\rho}\cos[\mathbf{Q}\cdot\mathbf{r}+\theta] \times(\cos\varphi\hat{x} + \sin\varphi\hat{y}),$$

generic expression for $\mathbf{S}_r$ in a co-planar phase

Make the phase θ coordinate-dependent

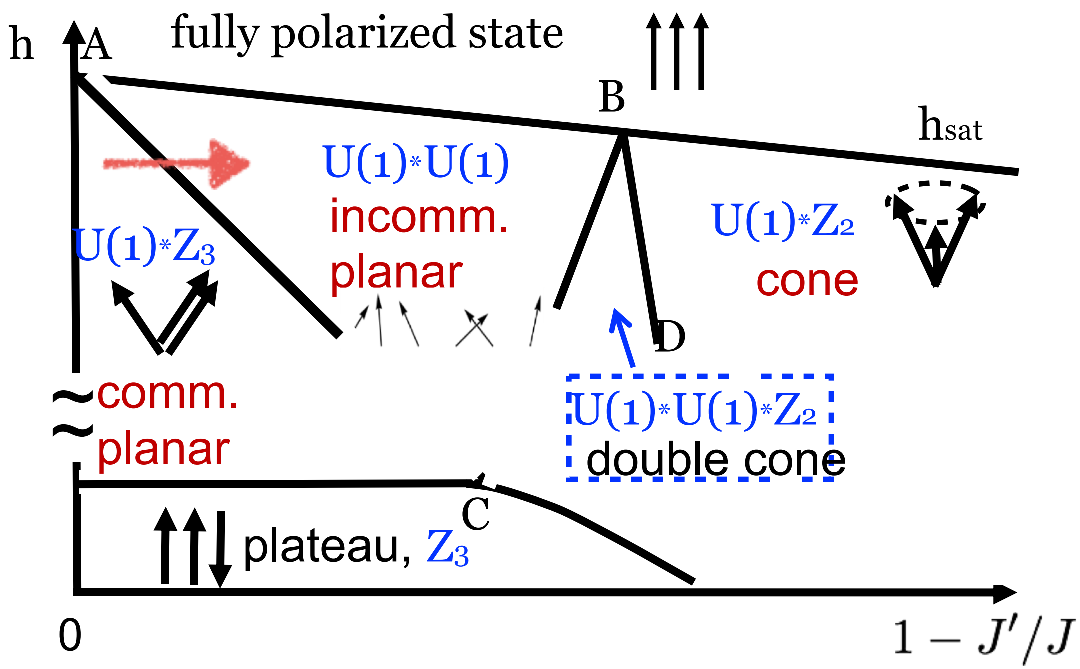
$$\mathcal{E}_\theta = \frac{3JS^2\mu}{4h_{\mathrm{sat}}}(\partial_x\theta)^2 + \frac{\sqrt{3}\delta JS^2\mu}{h_{\mathrm{sat}}}\partial_x\theta + S\frac{(\Gamma_3S^2)}{4}\frac{\mu^3}{h_{\mathrm{sat}}^3}\cos[6\theta]$$

$$\mu = (h_{\mathrm{sat}} - h)/h_{\mathrm{sat}}$$

classical mech

quantum mech

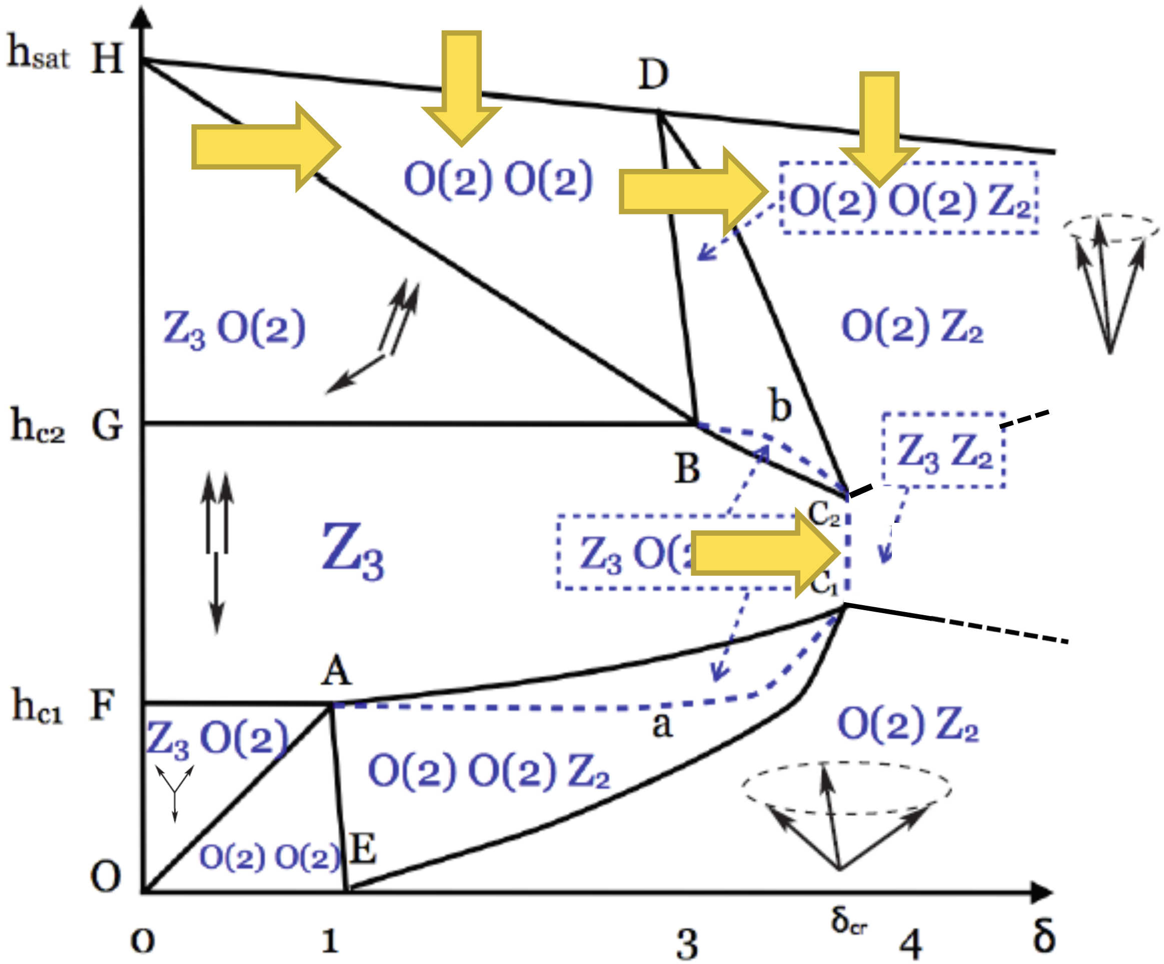
Phase diagram near saturation field: double cone and commensurate-incommensurate transition



$$\delta J_{c1} = 1.17(J/\sqrt{S})(\mu/h_{\text{sat}}) = 0.13\mu/S^{3/2}$$

$$\mu = (h_{\text{sat}} - h)/h_{\text{sat}}$$

The full phase diagram (our proposal)

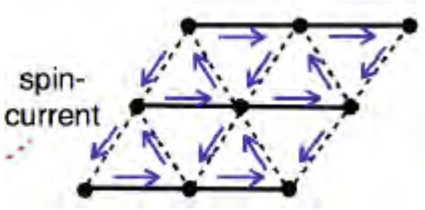


Need help from numerical studies

Conclusions

Anisotropic 2D triangular AFM has very rich physics

Spin-current order at fields near 1/3 of saturation

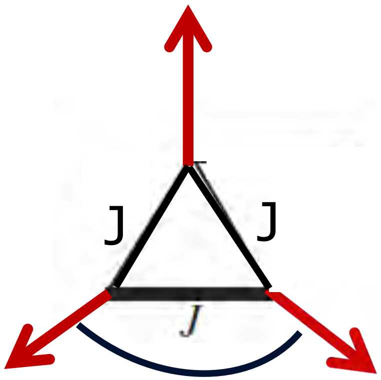


Incommensurate planar and cone states
near the saturation field

Double cone state in between

Commensurate-incommensurate transition
near the saturation field

And, there is indeed one more reason to consider 120^o structures



120^o

60 + 60 = 120

60

60

Dear Sasha and Igor:

Thank you