



Field Induced Transitions in Quantum Magnets



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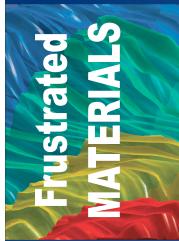


Motivation

Study quantum magnets as gases of interacting bosons

Why?

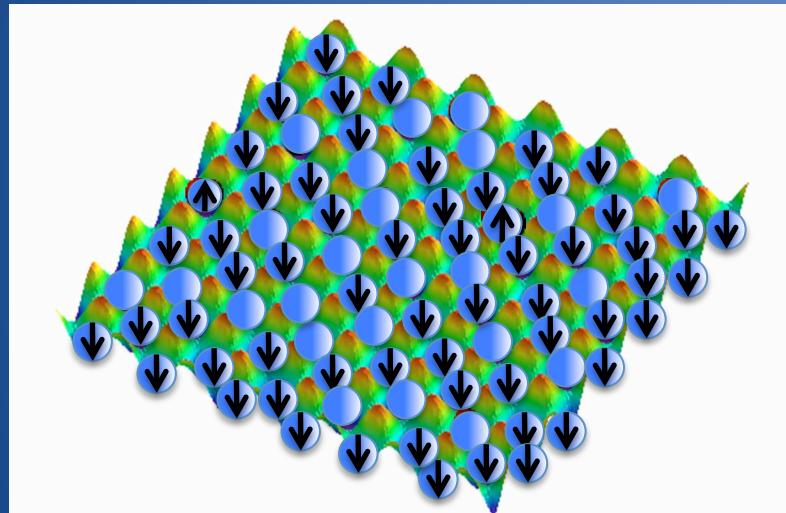
- We can **expand in the lattice gas parameter** for solving the spin Hamiltonian in regimes that correspond to a **dilute gas of particles** (near field induced transition).
- It adds a **new perspective of the same problem** that helps our physical intuition for finding unusual states of matter.
- It opens the possibility of finding magnetic realizations of models of interacting bosons that are difficult to realize in optical lattices.



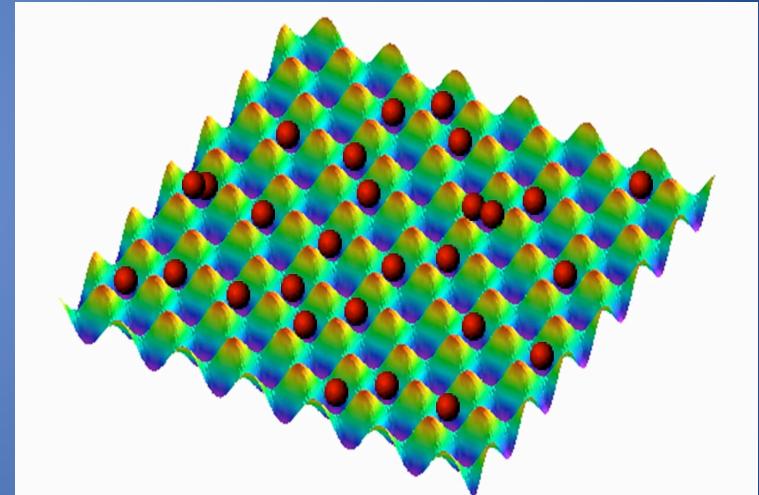
Spin-Particle Mapping



S=1 Spin Lattice



Lattice Gas of Bosons



$$S^z = 1$$



$$S^z = 0$$



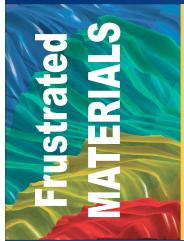
$$S^z = -1$$



$$n = 2$$

$$n = 1$$

$$n = 0$$



Spin-Particle Mapping

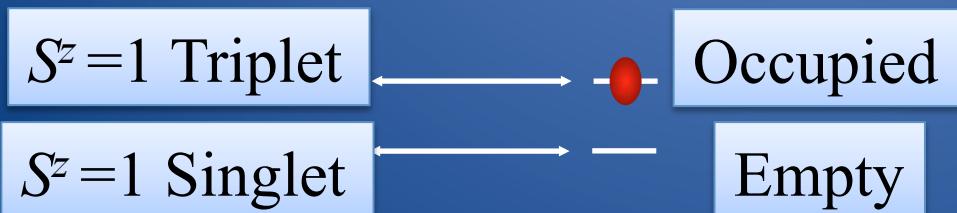
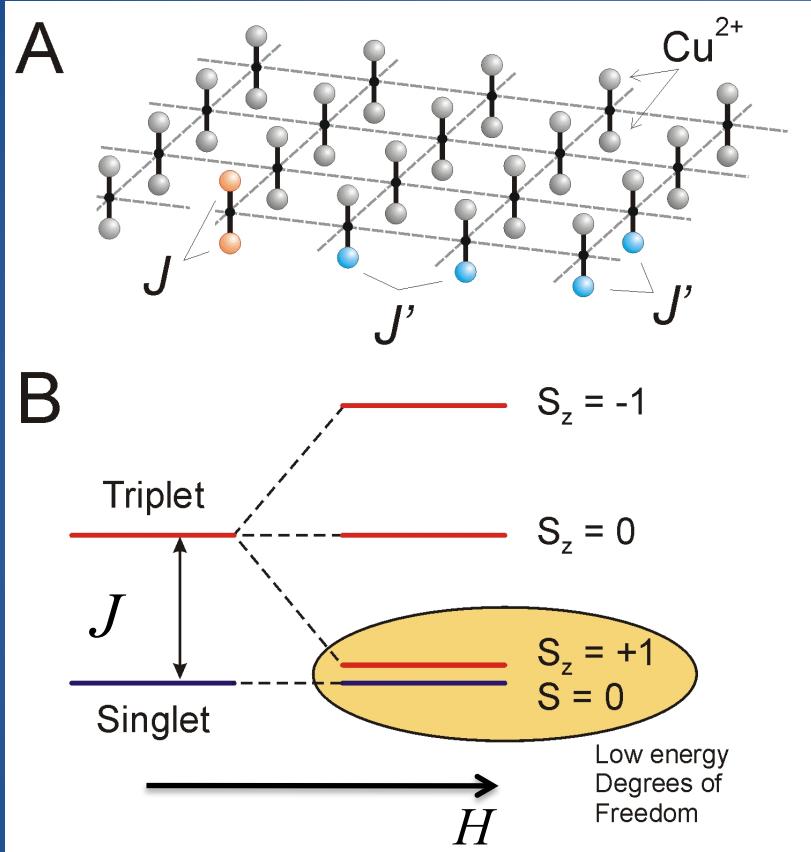


Matsubara-Matsuda Transformation
 $s=1/2 \longleftrightarrow$ Hard core bosons

$$s_j^+ = b_j^\dagger, \quad s_j^- = b_j, \quad s_j^z = n_j - \frac{1}{2}$$



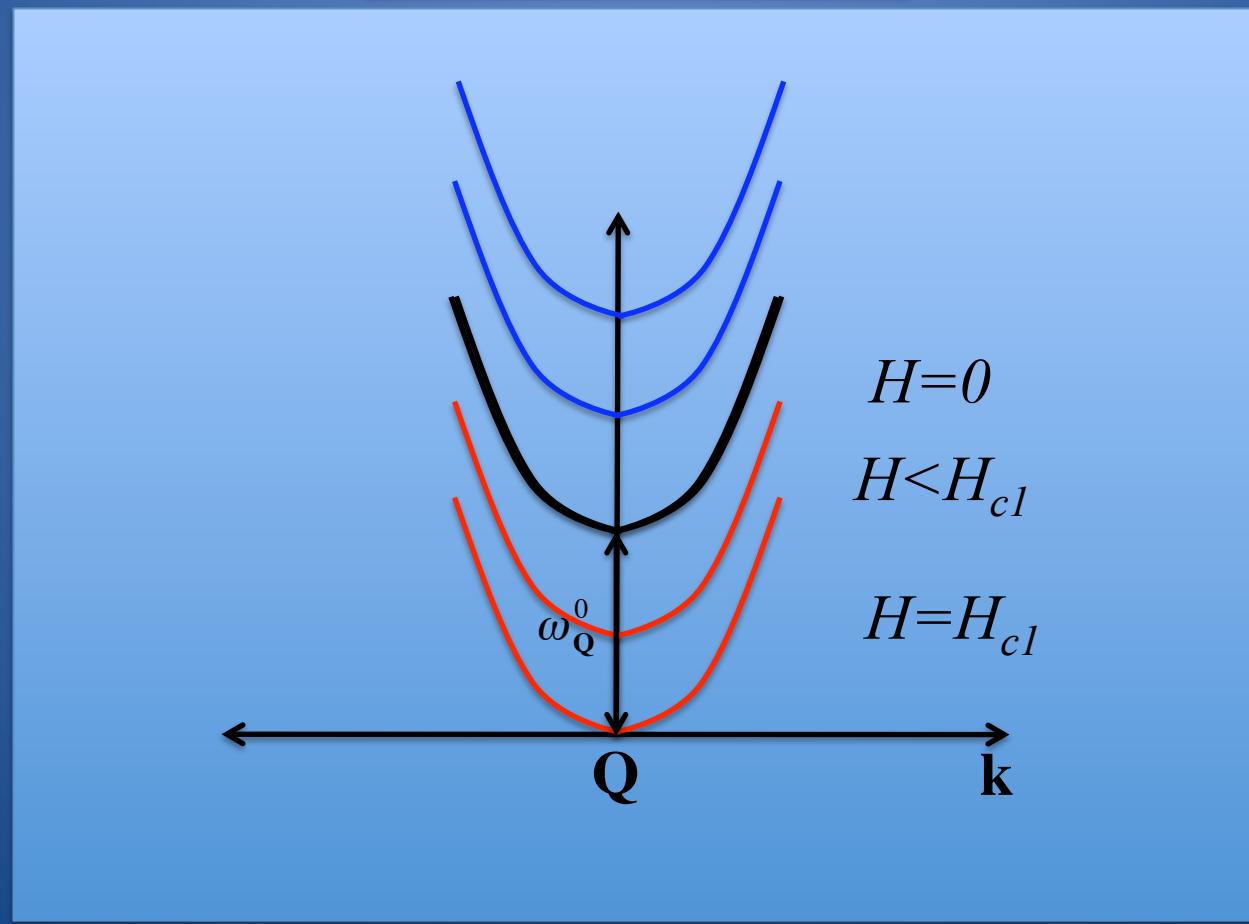
Weakly Coupled Dimers



TiCuCl₃
KCuCl₃
(CH₃)₂ (CHNH₃CuCl₃)
Ba₃Cr₂O₈
Sr₃Cr₂O₈
Pb₂V₃O₉
(CuCl)LaNb₂O₇
Ba₃Mn₂O₈
F₂PNNNO
AgVOAsO₄
Ag₂VOP₂O₇

Field Induced Transition

$$\left[\mathcal{H}, g\mu_B H \sum_{\mathbf{r}} S_{\mathbf{r}}^z \right] = 0$$



Effective Action

$$S = \int dr^d d\tau \left(\phi^* \partial_\tau \phi + |\nabla \phi|^2 - \mu |\phi|^2 + u |\phi|^4 \right)$$

$$D = d + z = d + 2$$



$d = 2$ is the upper critical dimension

For $d \leq 2$: $\frac{1}{\xi^z} \propto \Delta \propto \mu \propto \frac{1}{\xi^{1/\nu}}$

$\nu = 1/2$ for $d \geq 2$
(Mean Field)

$\nu = 1/z = 1/2$

$\nu = 1/2$ for any spatial dimension!



Elisabeth West FitzHugh & Lynda A. Zycherman
Studies in Conservation **37**, 145 (1992)

Heinz Berke
Angew. Chem. Int. Ed. **41**, 2483 (2002)

$\text{BaCuSi}_2\text{O}_6$



Calcite - CaCO_3
Weddellite - $\text{Ca}(\text{CO}_3)_2(\text{OH})_2$
Hydrocerussite – $2\text{Pb}(\text{CO}_3)_2 \cdot \text{Pb}(\text{OH})_2$



Soot - carbon black

Han Purple - $\text{BaCuSi}_2\text{O}_6$



Cinnabar - HgS

Hematite - Fe_2O_3

Minium – Pb_3O_4

Malachite – $\text{Cu}_2\text{CO}_3(\text{OH})_2$

Han Blue – $\text{BaCuSi}_4\text{O}_{10}$
(cuprorivaite)

J. Zuo et al., *J. Raman Spectrosc.* **34**, 121 (2003)
H. Langhals & D. Bathelt, *Angew. Chem. Int. Ed.* **42**, 5676 (2003)

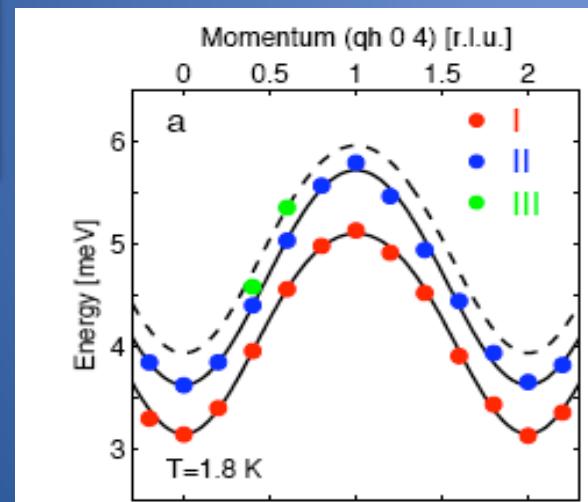
BaCuSi₂O₆

$$\mathcal{H} = J_1 \sum_{\mathbf{r} \in A} \mathbf{S}_{\mathbf{r}1} \cdot \mathbf{S}_{\mathbf{r}2} + J_2 \sum_{\mathbf{r} \in A} \mathbf{S}_{\mathbf{r}1} \cdot \mathbf{S}_{\mathbf{r}2} + J' \sum_{\mathbf{r}, \mathbf{v}=\mathbf{x}, \mathbf{y}; \eta=1,2} \mathbf{S}_{\mathbf{r}\eta} \cdot \mathbf{S}_{\mathbf{r}+\mathbf{e}_v\eta} + J_f \sum_{\mathbf{r}, \mathbf{v}} \mathbf{S}_{\mathbf{r}2} \cdot \mathbf{S}_{\mathbf{r}+\mathbf{u}_v1} - g\mu_B H \sum_{\mathbf{r}} S_{\mathbf{r}}^z$$

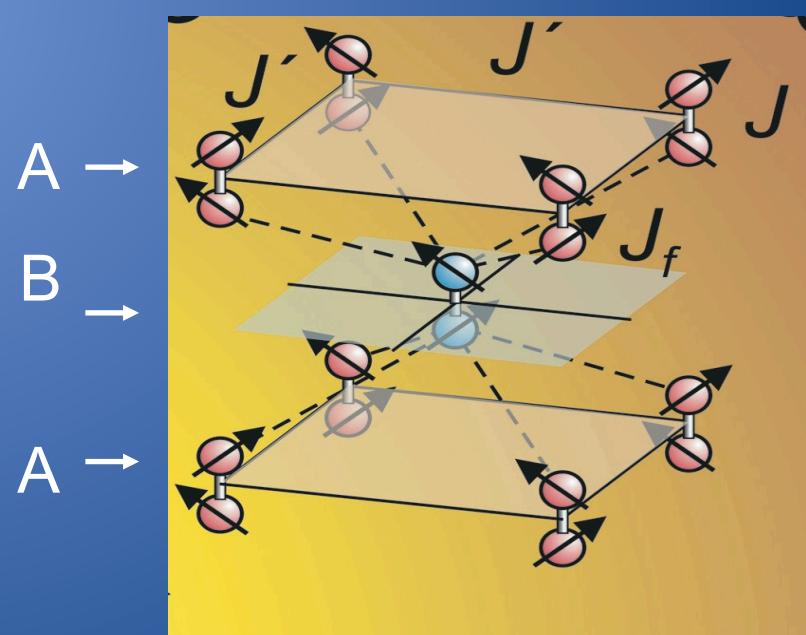
$$J_1 = 4.27 \text{ meV}$$

$$J_2 = 4.72 \text{ meV}$$

$$J' = 0.5 \text{ meV}$$

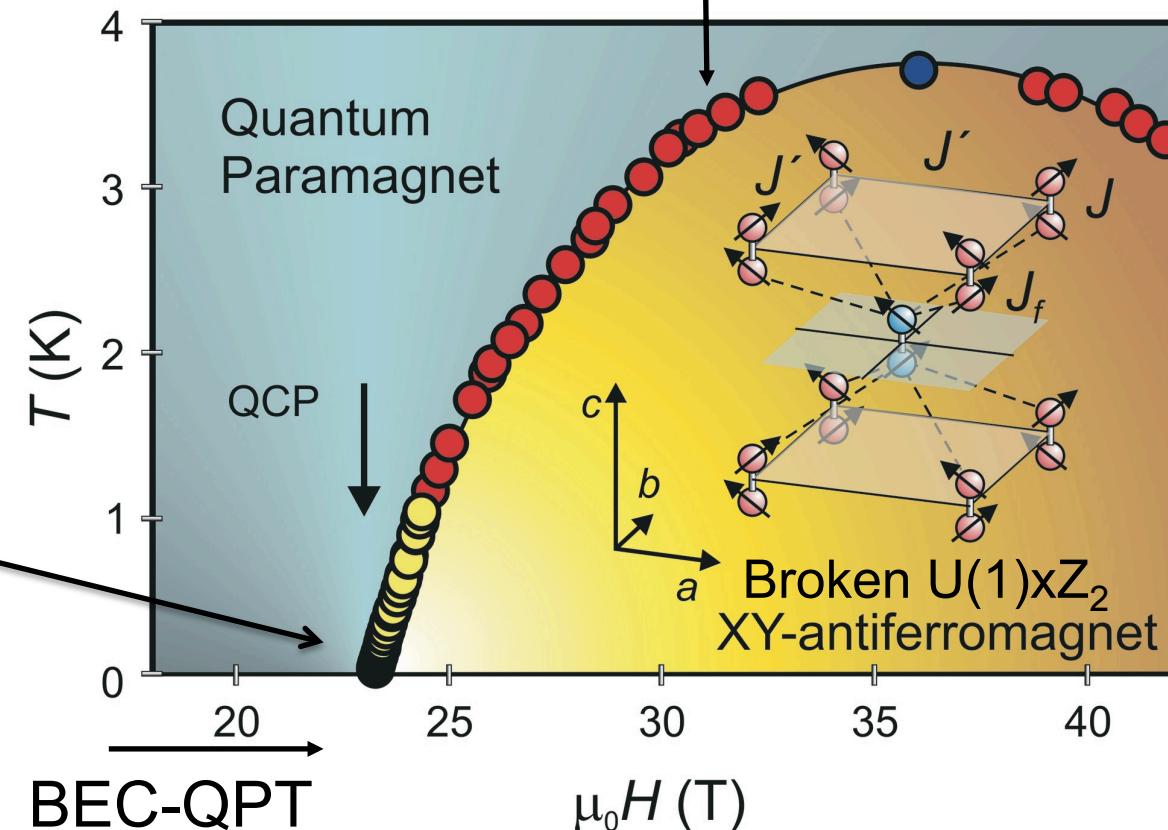


Ch. Ruegg et al,
PRL 98, 017202
(2007).



BaCuSi₂O₆

3d-XY classical phase transition (driven by phase fluctuations)



$$\varepsilon_k = \frac{k^2}{2m^*}$$

$$z = 2$$

D=d+z (driven by amplitude fluctuations)

S. E. Sebastian, N. Harrison², CDB, L. Balicas, M. Jaime, P. A. Sharma, N. Kawashima & I. R. Fisher, Nature **441**, 04732 (1 June 2006)

BaCuSi₂O₆

$$H = \sum_{\mathbf{q}} (\varepsilon_{\mathbf{q}} - \mu) b_{\mathbf{q}}^\dagger b_{\mathbf{q}} + v_0 \sum_{\mathbf{r}} n_{\mathbf{r}}^2$$

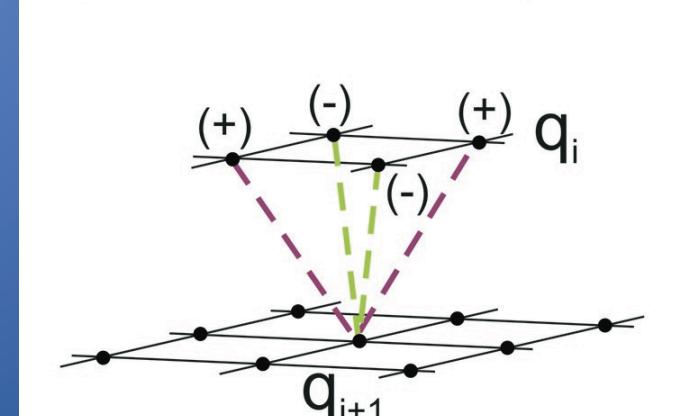
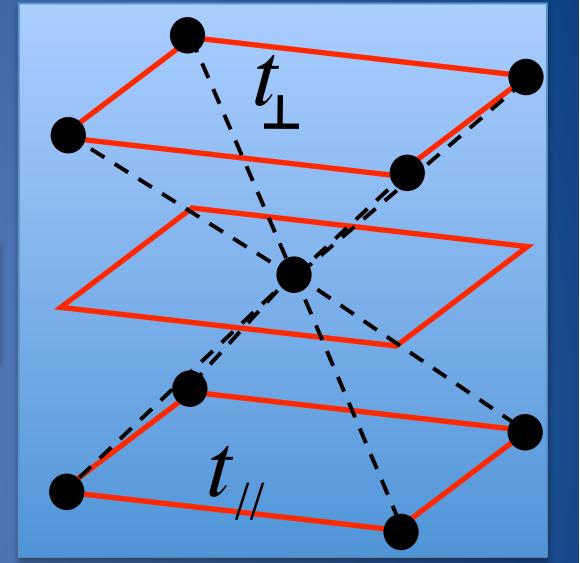
$$\varepsilon_{\mathbf{q}} = 2t_{||}(2 + \cos q_x + \cos q_y) + 8t_{\perp} \cos q_z \cos(q_x/2) \cos(q_y/2)$$

The minimum of $\varepsilon_{\mathbf{q}}$ is at $q_x = q_y = \pi$ if $t_{\perp} < t_{||}$.

In the long wave-length limit:

$$\mathbf{k} = \mathbf{q} - \mathbf{Q} \text{ with } \mathbf{Q} = (\pi, \pi, 0)$$

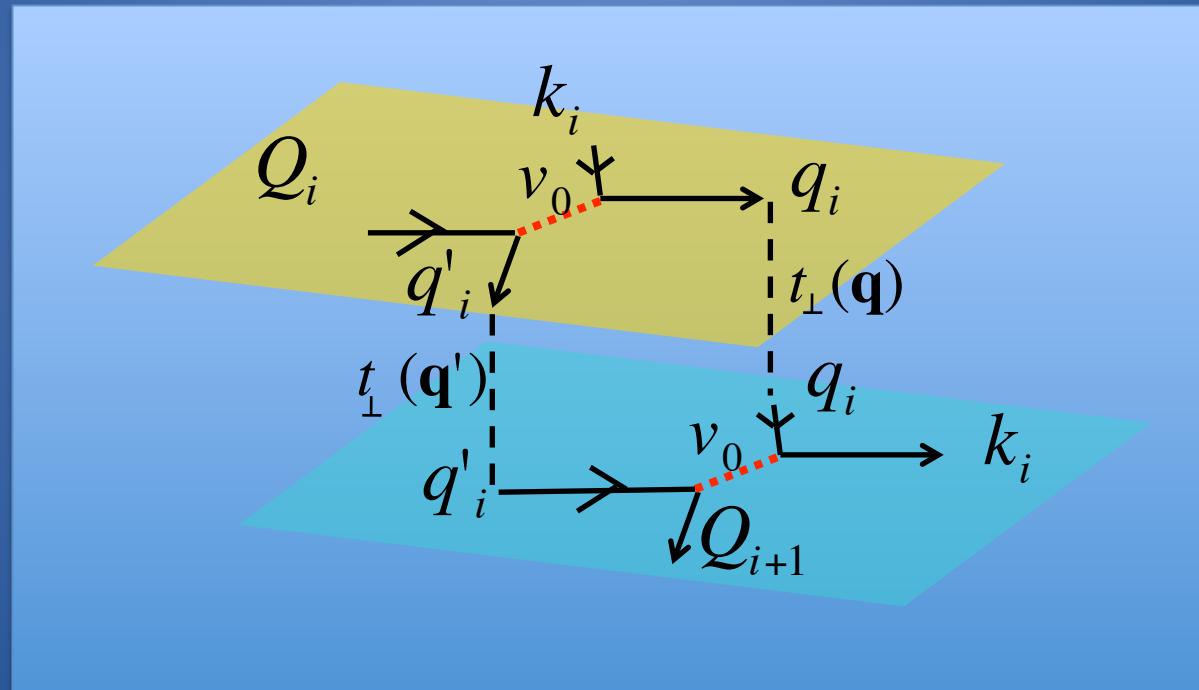
$$\varepsilon_{\mathbf{k}} \approx t_{||}(k_x^2 + k_y^2) + t_{\perp} k_x k_y (2 - k_z^2)$$



No coupling between layers for the single-particle ground state!

BaCuSi₂O₆

Although a single boson with parallel momentum $Q_i = (\pi, \pi)$ cannot hop to another layer, it can do it when it is assisted by a second boson via the interaction term, v_0 :



$$\tilde{t}_{z2} = R\rho$$

$$\rho = \langle b_{\mathbf{r}}^\dagger b_{\mathbf{r}} \rangle$$

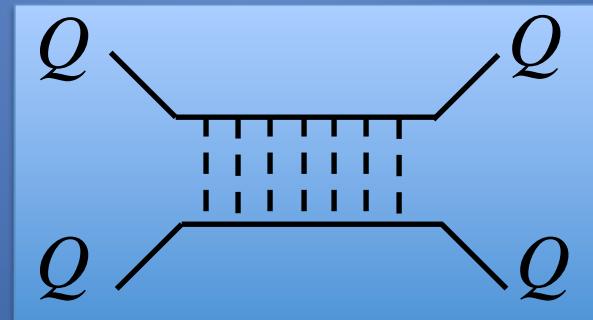
BaCuSi₂O₆

For hard-core bosons, $u_0 \rightarrow \infty$, the effective long-wavelength interaction constant, v_0 , corresponds to the pair-vertex (sum of ladder diagrams) with an heuristic infra-red cut-off:

$$\frac{1}{v_0} = \frac{1}{2} \int_{k_0}^{\pi} \frac{d^2 k_{\parallel}}{4\pi} \frac{1}{\epsilon_{k_{\parallel}}} \propto \frac{\ln \frac{t_{\parallel}}{\mu}}{t_{\parallel}}$$

$$k_0 = \sqrt{\mu/t_{\parallel}}$$

V. N. Popov, Theor. Math. Phys.
11, 565 (1972). D. Fisher and P. C.
Hohenberg, PRB 37, 4936 (1988).



Ladder Diagrams

$$\epsilon_{\mathbf{k}}^* = \epsilon_{\mathbf{k}} + 2R\rho \cos 2k_z$$

$$\mu^* = \mu - 2v_0\rho$$

BaCuSi₂O₆

$$\varepsilon_{\mathbf{k}}^* = \varepsilon_{\mathbf{k}} + 2R\rho \cos 2k_z$$

$$\mu^* = \mu - 2v_0\rho$$

$$x_0 \propto t_{||} \frac{k_0^2}{k_B T} \approx - \frac{\rho t_{||}}{k_B T} \frac{2}{\ln(\mu/t_{||})}$$

$$\rho(\mu, T) \propto \frac{1}{2\pi^2} \int_{-\pi}^{\pi} dk_z \int_{k_0}^{\infty} \frac{k_{||} dk_{||}}{e^{\beta(\varepsilon_{\mathbf{k}}^* - \mu^*)} - 1}$$



$$\frac{\rho(\mu^* = 0, T_c)}{k_B T_c} \propto \frac{1}{2\pi^2} \frac{1}{t_{||}} \int_0^{\pi} dk_z \int_{x_0}^{\infty} \frac{dx}{e^{\frac{x + \frac{2R\rho}{k_B T_c} \cos(2k_z)}{\mu^*}} - 1}$$

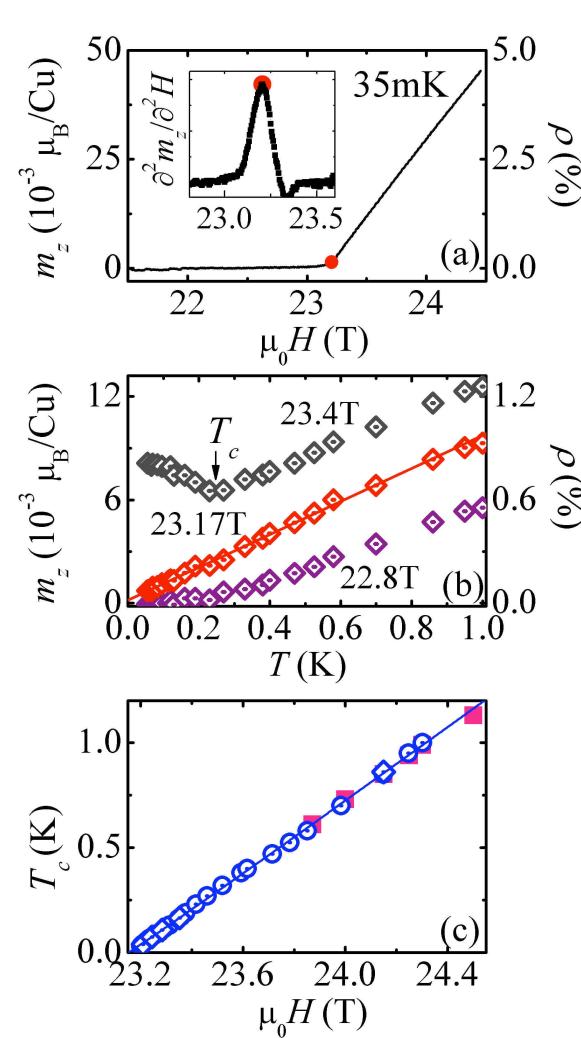
$$\mu \propto \frac{T_c}{\ln(t_{||}/T_c)}$$

$$T_c \propto -t_{||} \frac{\rho}{\ln \ln \rho}$$

$$\rho(\mu = 0, T) \propto T \ln \ln \frac{t_{||}}{T}$$

Dimensional reduction!

BaCuSi₂O₆



$d \geq 2$

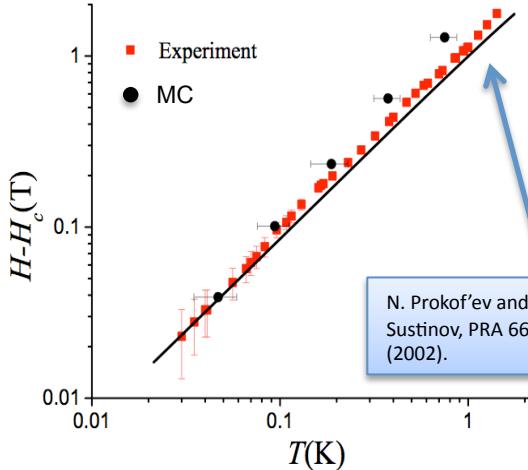
$$m_z(T = 0) \propto (H - H_c)$$

$$m_z(H = H_c) \propto T^{d/2}$$

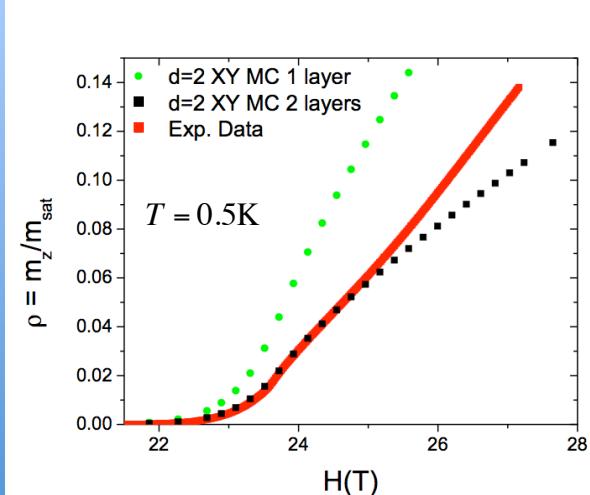
$$T_c \propto (H - H_c)^{2/d}$$

C. D. B., J. Schmalian, N. Kawashima, P. Sengupta, S. Sebastian, N. Harrison, M. Jaime, I. Fisher, PRL **98**, 257201 (2007).

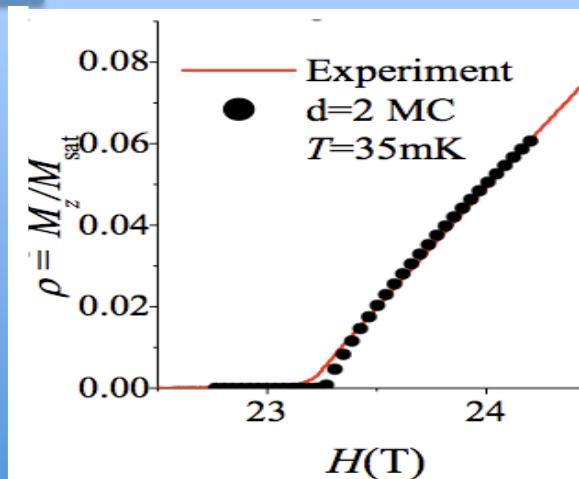
MC simulation of d=2 gas of hard-core bosons



$$t_{\parallel} = \frac{J'}{2} = 3\text{K}$$

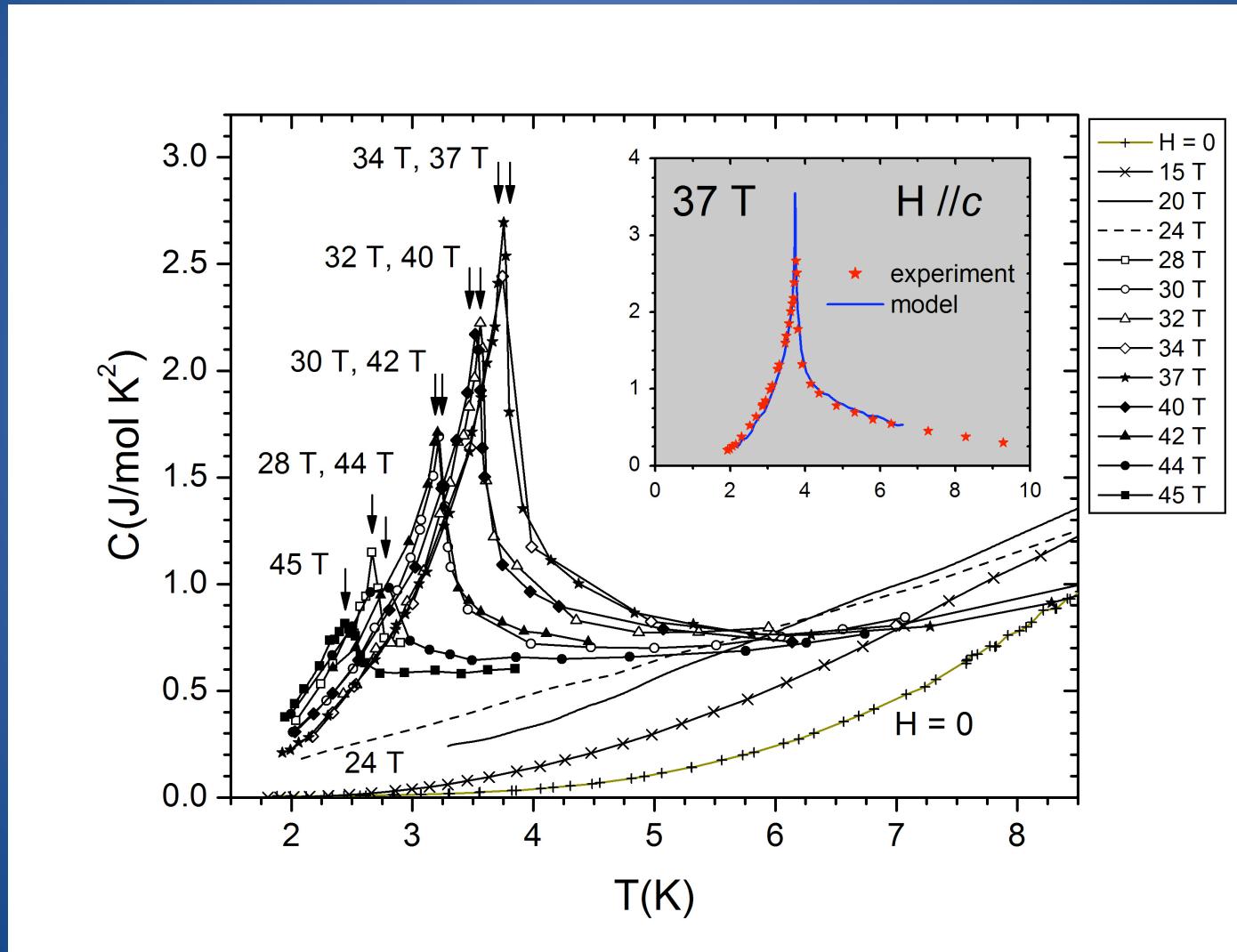


No free parameters!

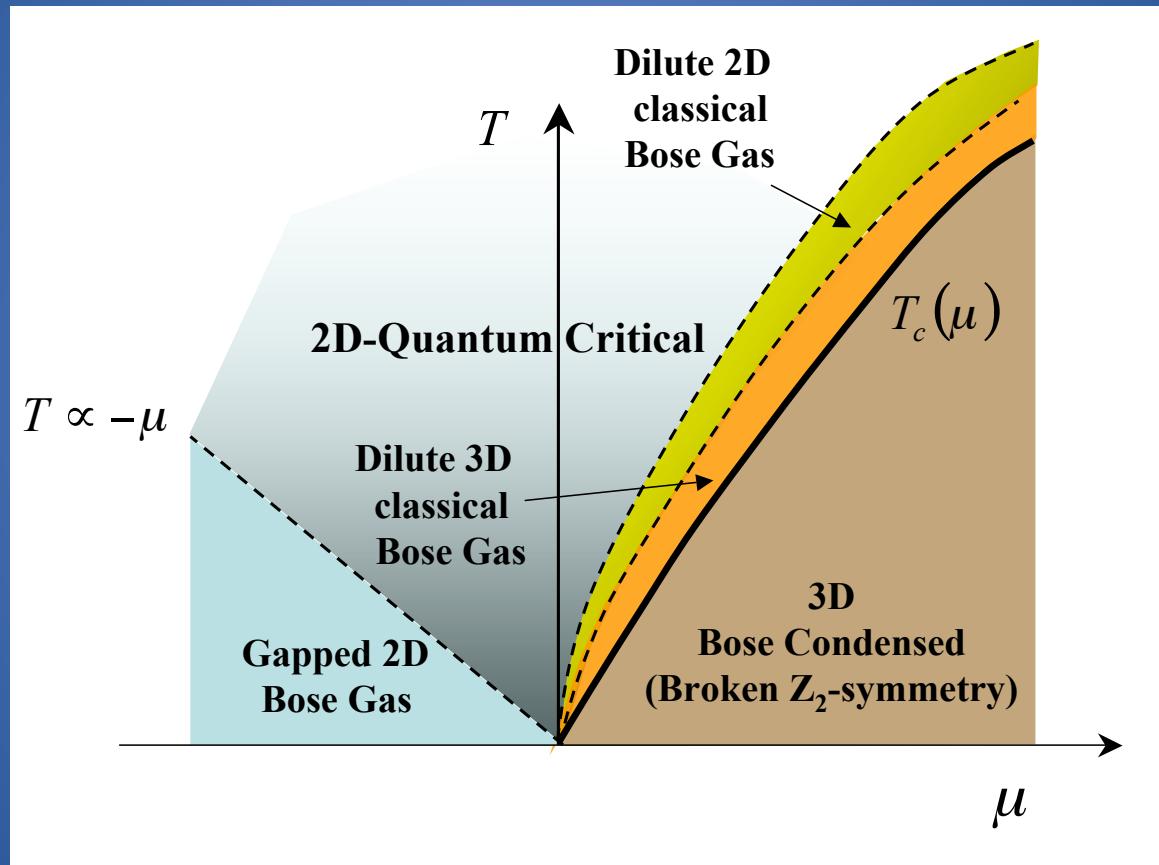


Since there are two non-equivalent layers, the agreement is very good as long as:

$$H - H_c \ll \frac{J_1 - J_2}{g\mu_B} = 3.75\text{T}$$

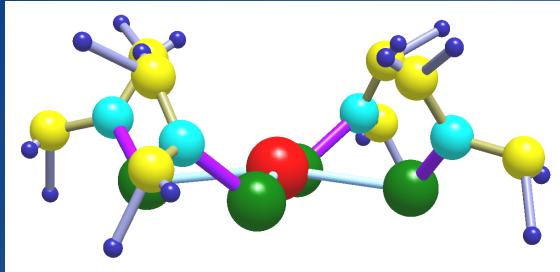


Phase Diagram

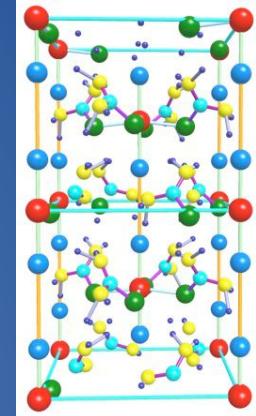


J. Schmalian and C. D. B., Phys. Rev. B 77, 094406 (2008).

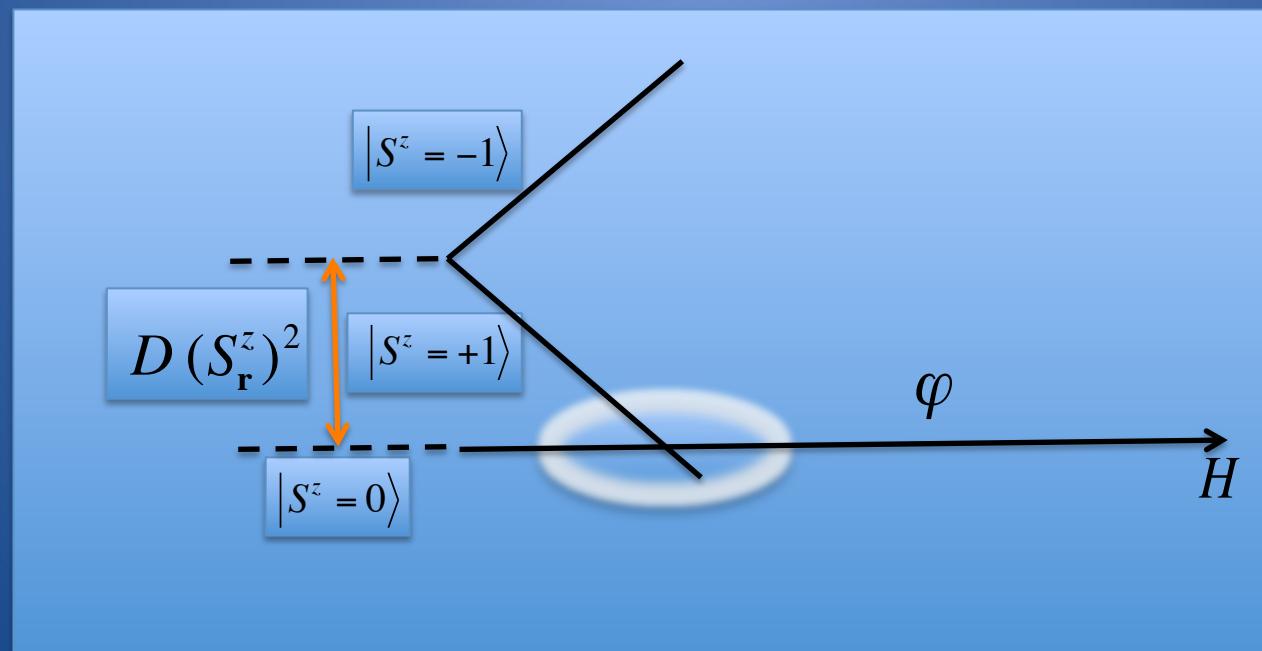
DTN: $\text{NiCl}_2\text{-}4\text{SC}(\text{NH}_2)_2$



$$\mathcal{H}_{ion} = D \sum_{\mathbf{r}} (S_{\mathbf{r}}^z)^2 - g\mu_B H \sum_{\mathbf{r}} S_{\mathbf{r}}^z$$



Ni
Cl





DTN: Phase Diagram

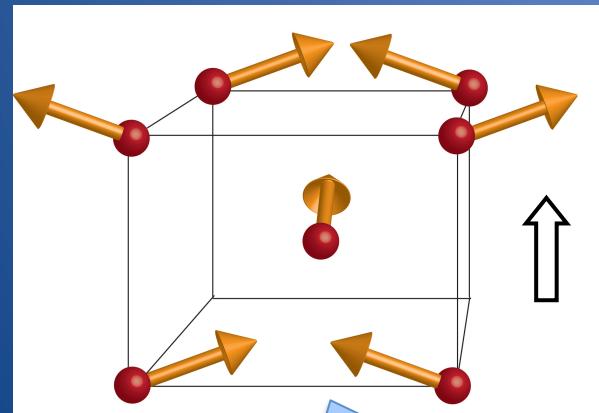


$$\mathcal{H} = \sum_{\mathbf{r}, \nu} J_\nu \mathbf{S}_{\mathbf{r}} \cdot \mathbf{S}_{\mathbf{r} + \mathbf{e}_\nu} + D \sum_{\mathbf{r}} (S_{\mathbf{r}}^z)^2 - g\mu_B H \sum_{\mathbf{r}} S_{\mathbf{r}}^z$$

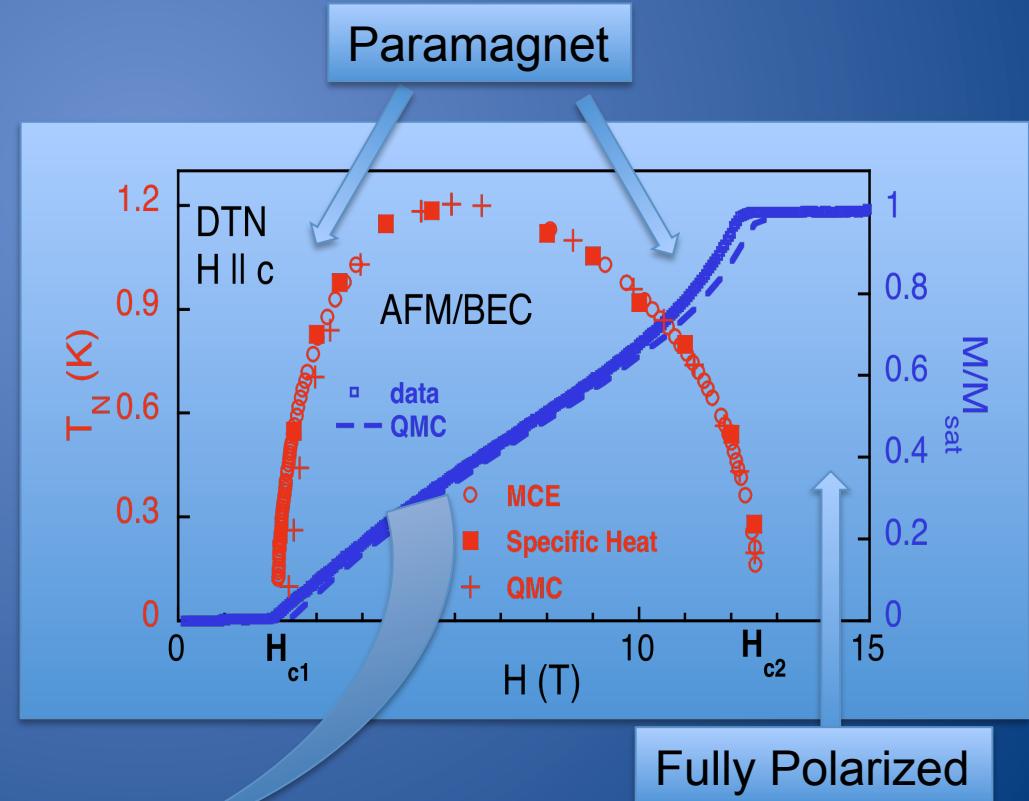
$$D = 9 \text{ K}$$

$$\begin{aligned} J_c &= 2.2 \text{ K} \\ J_a &= 0.18 \text{ K} \end{aligned}$$

$$2 < H < 12 \text{ T}$$



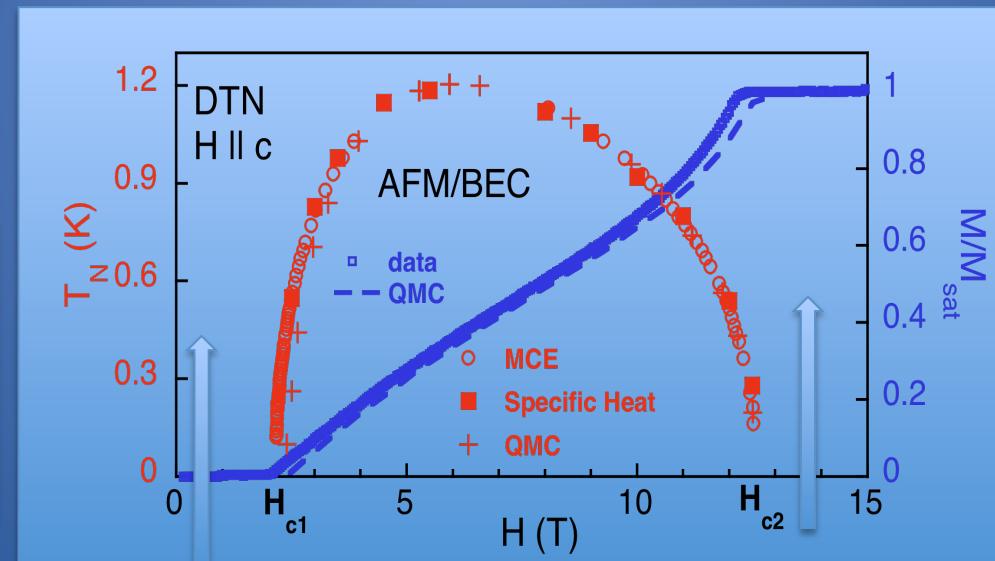
↑
b
a
c



DTN: Phase Diagram

$$\mathcal{H} = \sum_{\mathbf{r}, \nu} J_\nu \mathbf{S}_{\mathbf{r}} \cdot \mathbf{S}_{\mathbf{r} + \mathbf{e}_\nu} + D \sum_{\mathbf{r}} (S_{\mathbf{r}}^z)^2 - g\mu_B H \sum_{\mathbf{r}} S_{\mathbf{r}}^z$$

The ground state for $H > H_{c1}$ has strong inter-site quantum fluctuations



The ground state for $H > H_{c2}$ has no inter-site quantum fluctuations

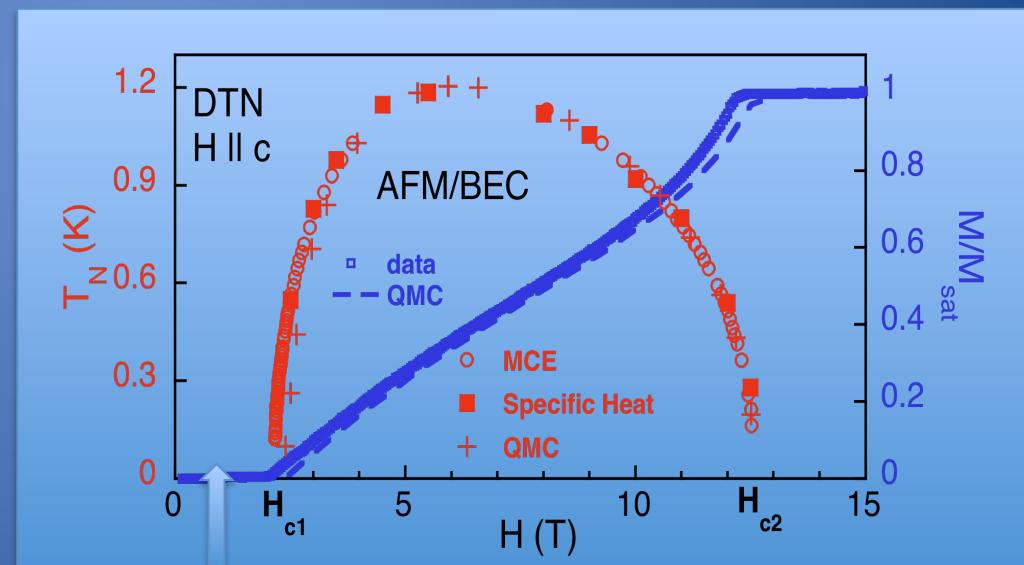
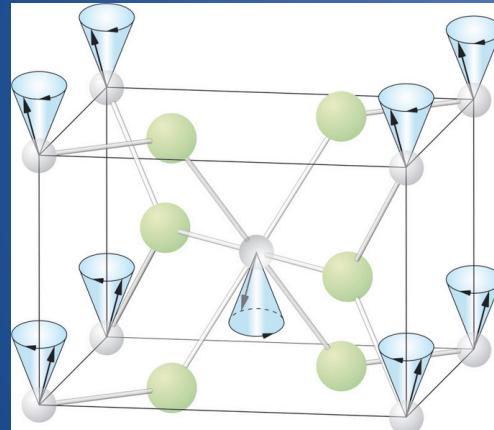
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↑↑↑↑↑↑↑↑

Quantum Paramagnet

The usual spin-wave approach cannot be applied to our low-field quantum paramagnet.

$$\langle S^z = 0 | S^x | S^z = 0 \rangle = \langle S^z = 0 | S^y | S^z = 0 \rangle = \langle S^z = 0 | S^z | S^z = 0 \rangle$$



000000000000

SU(3) Spin-Waves



Magnetic moment

$$S_{\mathbf{r}}^\eta$$

Spin Nematic

$$S_{\mathbf{r}}^\eta S_{\mathbf{r}}^\mu + S_{\mathbf{r}}^\mu S_{\mathbf{r}}^\eta$$

$$\eta = x, y, z$$

$$\mu = x, y, z$$

$$b_{\mathbf{r}\uparrow}^+ b_{\mathbf{r}\uparrow} + b_{\mathbf{r}0}^+ b_{\mathbf{r}0} + b_{\mathbf{r}\downarrow}^+ b_{\mathbf{r}\downarrow} = 1$$

Constraint of only one boson per site

$$\begin{aligned} S_{\mathbf{r}}^+ &= \sqrt{2}(b_{\mathbf{r}\uparrow}^+ b_{\mathbf{r}0} + b_{\mathbf{r}0}^+ b_{\mathbf{r}\downarrow}) \\ S_{\mathbf{r}}^- &= \sqrt{2}(b_{\mathbf{r}\downarrow}^+ b_{\mathbf{r}0} + b_{\mathbf{r}0}^+ b_{\mathbf{r}\uparrow}) \\ S_{\mathbf{r}}^z &= b_{\mathbf{r}\uparrow}^+ b_{\mathbf{r}\uparrow} - b_{\mathbf{r}\downarrow}^+ b_{\mathbf{r}\downarrow} \end{aligned}$$

Spin operators as a function of SB operators

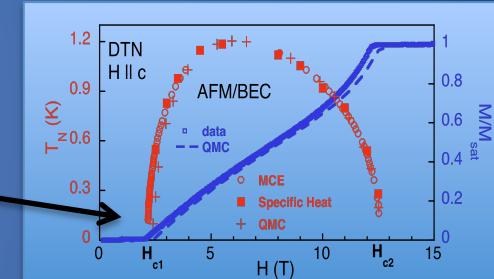
SU(3) Spin-Waves

We enforce the constraint at the mean field:

$$\hat{\mathcal{H}} \rightarrow \hat{\mathcal{H}} = \mathcal{H} + \mu \sum_{\mathbf{r}} (b_{\mathbf{r}\uparrow}^+ b_{\mathbf{r}\uparrow} + b_{\mathbf{r}0}^+ b_{\mathbf{r}0} + b_{\mathbf{r}\downarrow}^+ b_{\mathbf{r}\downarrow} - 1)$$

We condense the $S^z=0$ boson ($0 \leq H \leq H_{c1}$),

$$b_{\mathbf{r}0}^+ = b_{\mathbf{r}0}^- = s,$$



and keep terms up to quadratic order in the other two, $S^z=\pm 1$, boson operators:

$$\hat{\mathcal{H}}_{sw} = E_0 + \sum_{\mathbf{k};\sigma=\uparrow,\downarrow} \left[(\mu + s^2 \epsilon_{\mathbf{q}} - h_{\sigma}) b_{\mathbf{q}\sigma}^+ b_{\mathbf{q}\sigma} + \frac{s^2 \epsilon_{\mathbf{k}}}{2} (b_{\mathbf{q}\sigma}^+ b_{-\mathbf{q}-\sigma}^+ + b_{\mathbf{q}\sigma} b_{-\mathbf{q}-\sigma}) \right]$$

$$\epsilon_{\mathbf{q}} = 2J_a(\cos q_x + \cos q_y) + 2J_c \cos q_z$$



SU(3) Spin-Waves

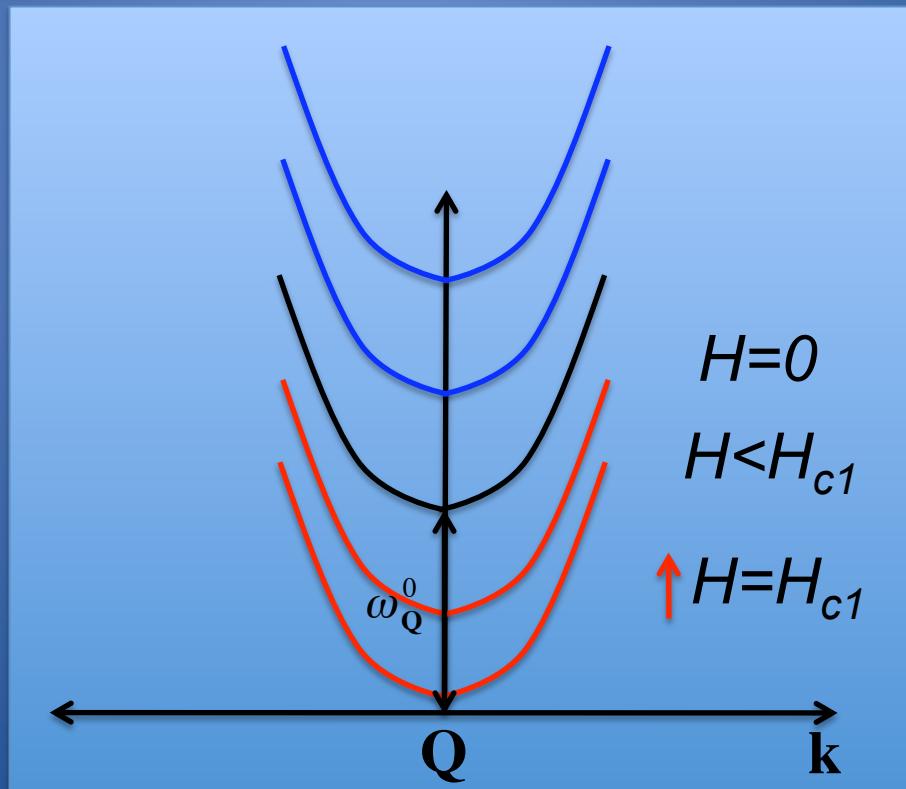


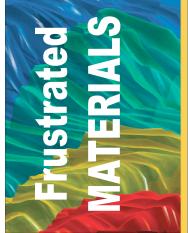
$$\hat{\mathcal{H}}_{sw} = E_0 + \sum_{\mathbf{q}} \left[(\omega_{\mathbf{k}}^0 - g\mu_B H) \beta_{\mathbf{q}\uparrow}^+ \beta_{\mathbf{q}\uparrow}^- + (\omega_{\mathbf{k}}^0 + g\mu_B H) \beta_{\mathbf{q}\downarrow}^+ \beta_{\mathbf{q}\downarrow}^- \right].$$

$$\omega_{\mathbf{q}}^0 = \sqrt{\mu^2 + 2\mu s^2 \varepsilon_{\mathbf{q}}} \approx \sqrt{\mu^2 - 4\mu s^2 (2J_a + J_c) + 2\mu s^2 \left[J_a (k_x^2 + k_y^2) + J_c k_z^2 \right]}$$

$$g\mu_B H_{c1} = \omega_{\mathbf{Q}}^0,$$

$$\mathbf{Q} = (\pi, \pi, \pi)$$





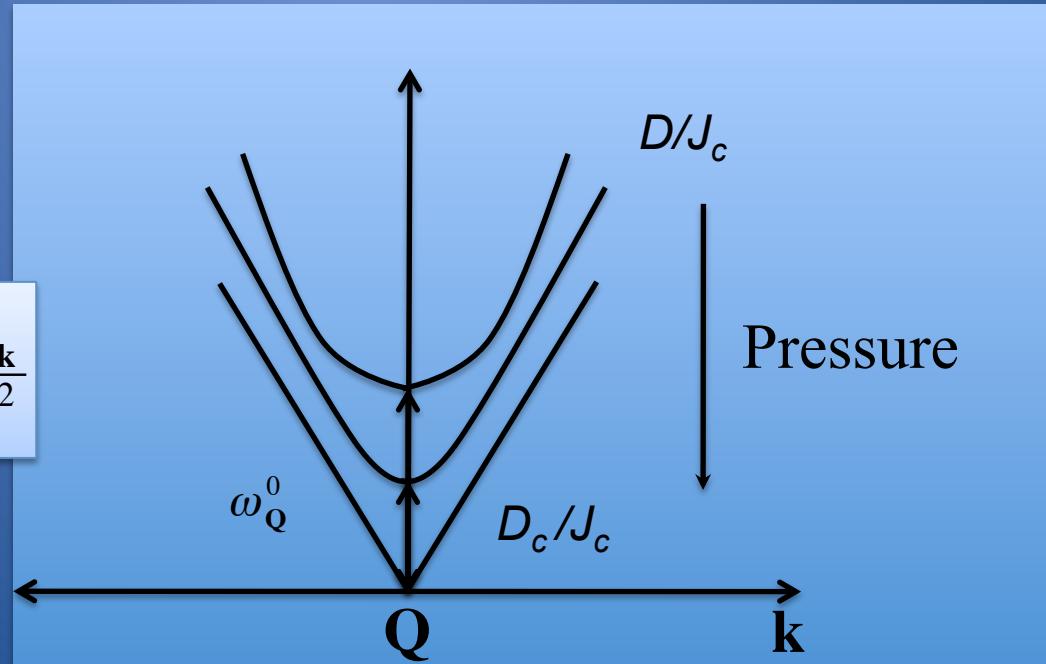
SU(3) Spin-Waves



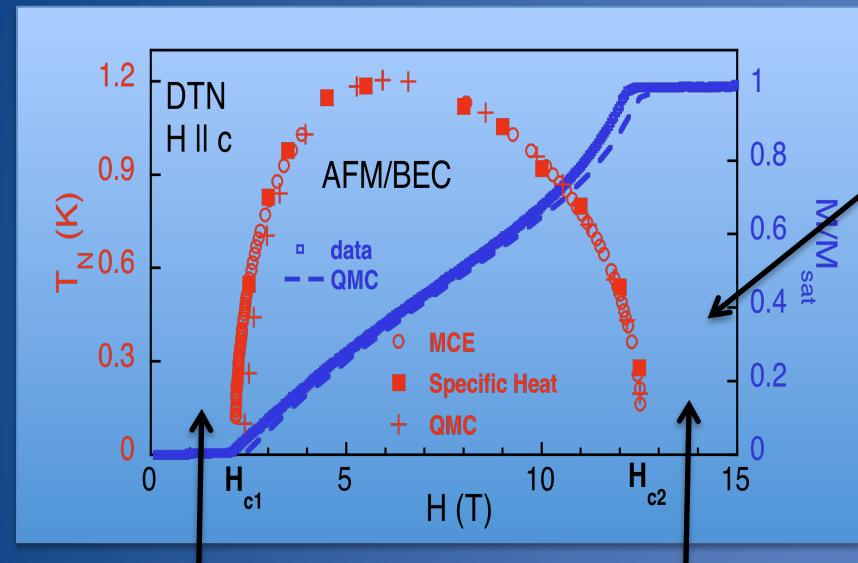
$$\hat{\mathcal{H}}_{sw} = E_0 + \sum_{\mathbf{q}} \left[(\omega_{\mathbf{k}}^0 - g\mu_B H) \beta_{\mathbf{q}\uparrow}^+ \beta_{\mathbf{q}\uparrow}^- + (\omega_{\mathbf{k}}^0 + g\mu_B H) \beta_{\mathbf{q}\downarrow}^+ \beta_{\mathbf{q}\downarrow}^- \right].$$

$$\omega_{\mathbf{q}}^0 = \sqrt{\mu^2 + 2\mu s^2 \epsilon_{\mathbf{q}}} \approx \sqrt{\mu^2 - 4\mu s^2 (2J_a + J_c) + 2\mu s^2 \left[J_a (k_x^2 + k_y^2) + J_c k_z^2 \right]}$$

$$\frac{1}{m_{vv}^*} = \frac{\partial^2 \omega_{\mathbf{k}}^0}{\partial k_v^2} = \frac{\mu s^2}{\omega_{\mathbf{k}}^0} \frac{\partial^2 \epsilon_{\mathbf{k}}}{\partial k_v^2}$$



Specific Heat and Thermal Transport



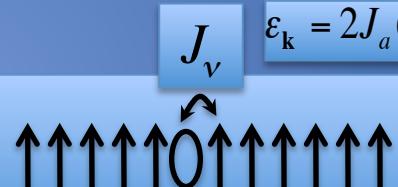
m_{vv}^*

m_{vv}

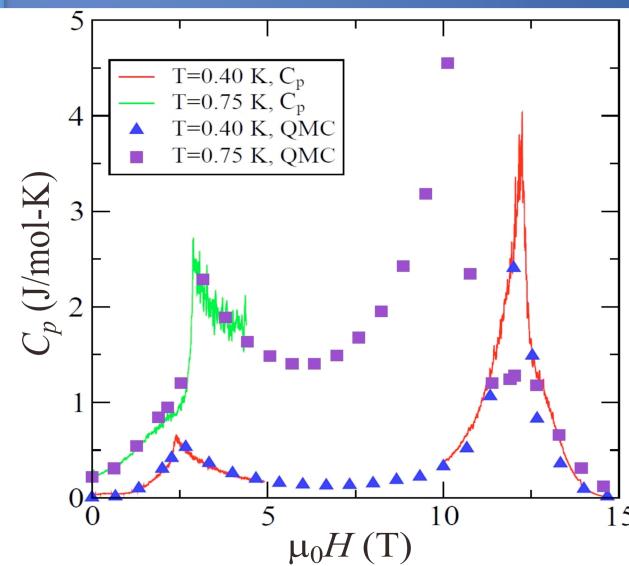
$$\frac{m_{vv}}{m_{vv}^*} \approx \frac{H_{c2}}{4H_{c1}} \left(1 + \sqrt{1 + \frac{8H_{c1}^2}{H_{c2}^2}} \right) \approx 3.2$$

$$\omega_k^> = \epsilon_k - \epsilon_Q + (H - H_{c2}) / g\mu_B$$

J_v



$$\epsilon_k = 2J_a(\cos k_x + \cos k_y) + 2J_c \cos k_z$$



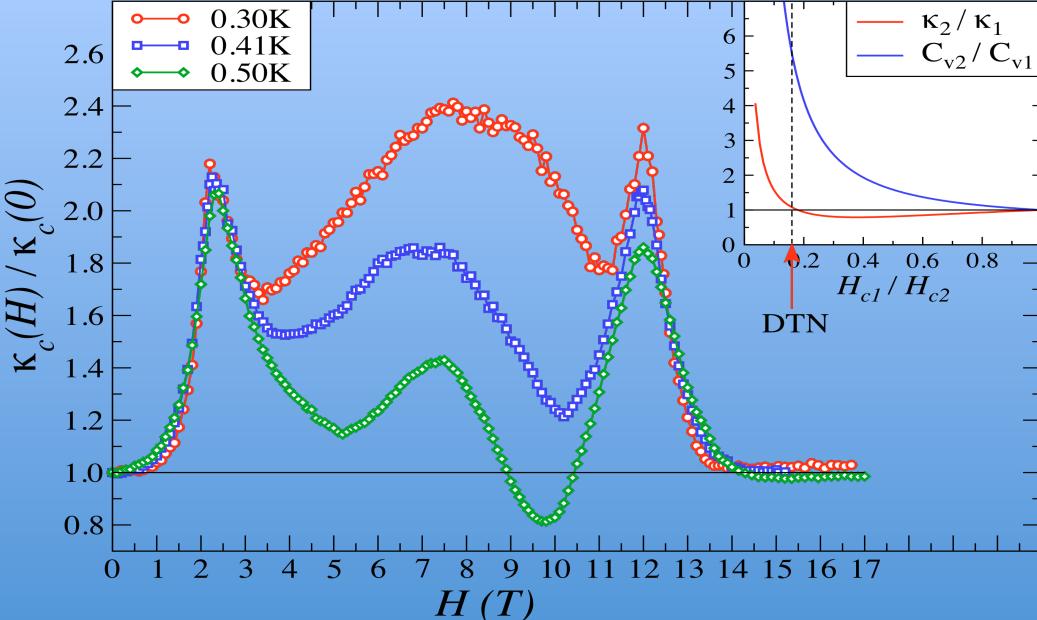
$$C_p \propto m^{3/2}$$

for $T < J_a$



$$C_{p2}/C_{p1} = m^{3/2}/m^{*3/2} \approx 5.7$$

Specific Heat and Thermal Transport



$$\kappa = l \int dk^3 \omega_k \frac{dn_B}{dT} v_k$$

Mean free path due to scattering by impurities:

$$l^{-1} = \frac{n_i}{2\pi} |V|^2 m^2$$

$$H_{imp}^D = \delta D (S_{\mathbf{R}}^z)^2 \Rightarrow \delta D \sum_{\sigma, \mathbf{k}, \mathbf{k}'} e^{i\mathbf{R}(\mathbf{k}-\mathbf{k}')} b_{\mathbf{k}\sigma}^+ b_{\mathbf{k}'\sigma} = \delta D \sum_{\sigma, \mathbf{k}, \mathbf{k}'} e^{i\mathbf{R}(\mathbf{k}-\mathbf{k}')} (u_{\mathbf{k}} u_{\mathbf{k}'} + v_{\mathbf{k}} v_{\mathbf{k}'}) \beta_{\mathbf{k}\sigma}^+ \beta_{\mathbf{k}'\sigma}$$

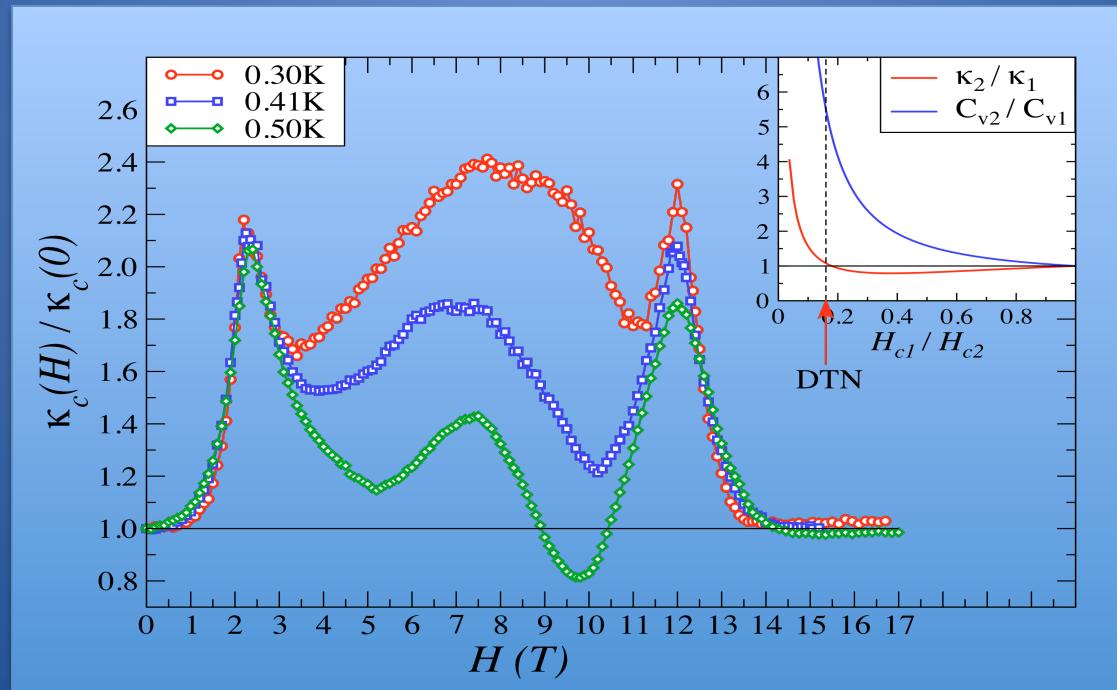
$$|V|^2 = \delta D^2 (u_{\mathbf{Q}}^2 + v_{\mathbf{Q}}^2)^2$$



DTN: Thermal Transport



$$\frac{\kappa_1}{\kappa_2} = \frac{ml_2}{m^*l_1} = \left(\frac{m}{m^*}\right) \frac{1}{4s^2} \left(1 + s^4 \left(\frac{m^*}{m}\right)^2\right)^2 \approx 1.2$$

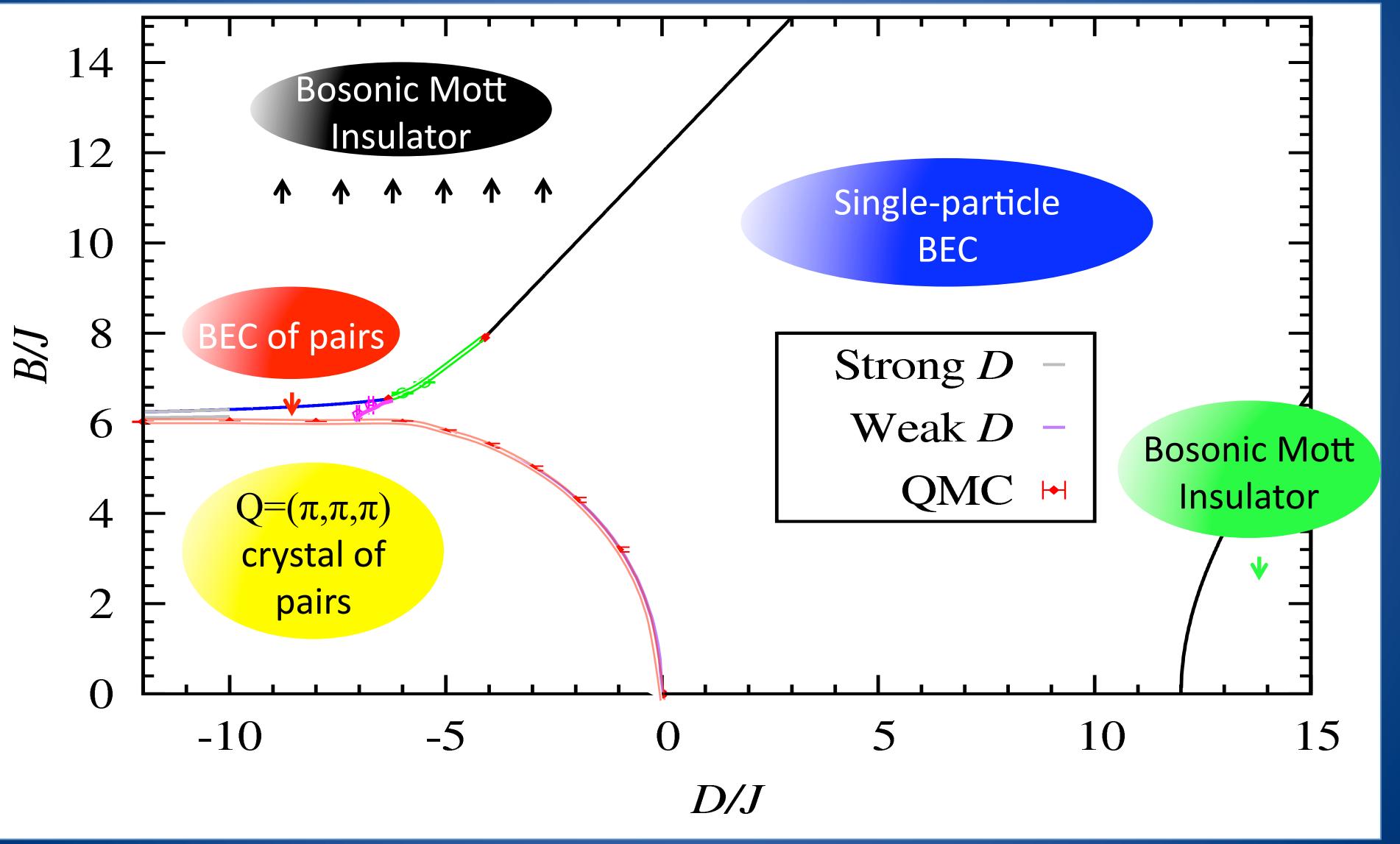


Easy-Axis Single-Ion Anisotropy

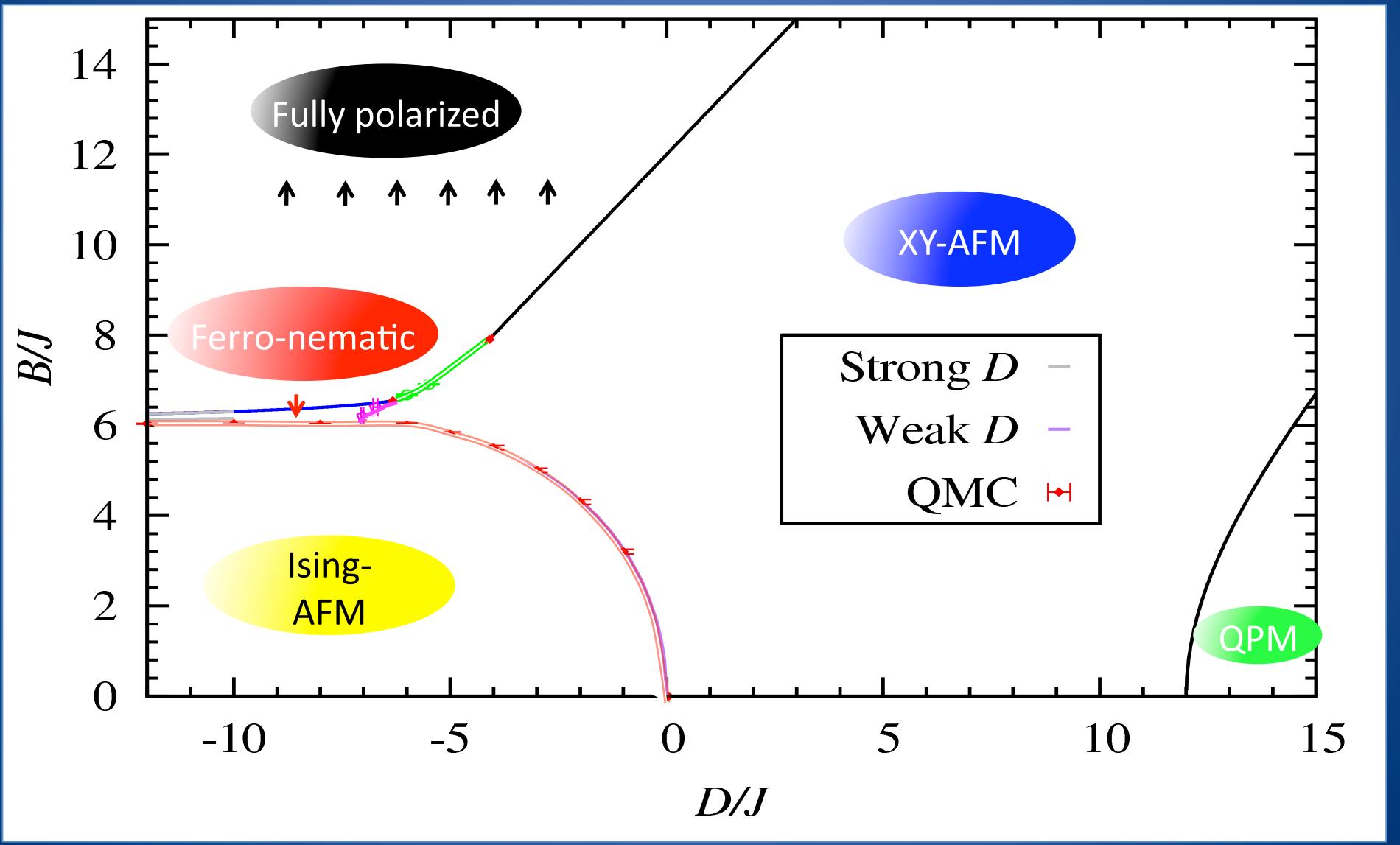
$$H = J \sum_{\langle i,j \rangle} \left(S_i^x S_j^x + S_i^y S_j^y + \Delta S_i^z S_j^z \right) + D \sum_j \left(S_j^z \right)^2 - B \sum_j S_j^z$$

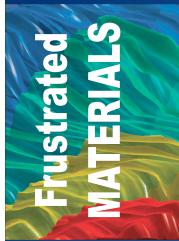
Spin	Particle
Z-component of Magnetization	Density
Magnetic Field	Chemical Potential
Spin Stiffness	Superfluid Density
Longitudinal or Ising-like order	CDW or Solid order
Transverse or XY-like order	Bose-Einstein condensate
$J(S_i^x S_j^x + S_i^y S_j^y)$	$t(b_i^\dagger b_j + b_i^\dagger b_j)$
$\Delta S_i^z S_j^z$	$V(n_i - 1)(n_j - 1)$
$D(S_j^z)^2$	$U(n_j - 1)^2$

Quantum Phase Diagram for $\Delta=1$ and $d=3$



Quantum Phase Diagram for $\Delta=1$ and $d=3$





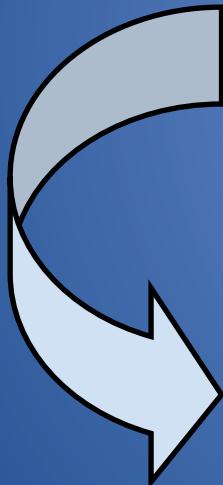
“Spin Supersolid”



$$H = J \sum_{j=1}^{L-1} (S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta S_j^z S_{j+1}^z) + D \sum_{j=1}^L (S_j^z)^2 - B \sum_{j=1}^L S_j^z$$

$$|0_A\rangle = \downarrow \uparrow \downarrow \uparrow \downarrow \uparrow \downarrow \uparrow \quad |0_B\rangle = \uparrow \downarrow \uparrow \downarrow \uparrow \downarrow \uparrow \downarrow$$

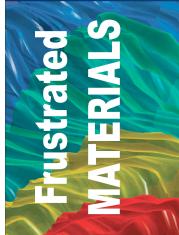
B=0 ground states for $\Delta J \gg D \gg J$



Particle representation:

$$V \gg U \gg t_j$$

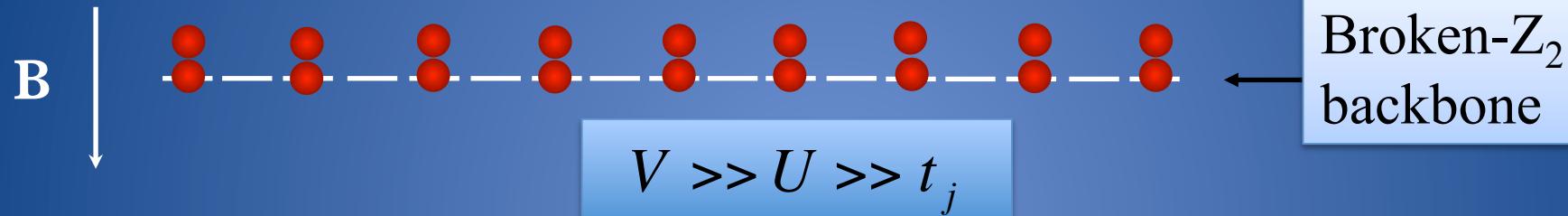
$$|0_A\rangle = \bullet \quad |0_B\rangle = \bullet \bullet \bullet \bullet \bullet \bullet \bullet \bullet \bullet \bullet$$



Single-ion & Exchange Uniaxial Anisotropy



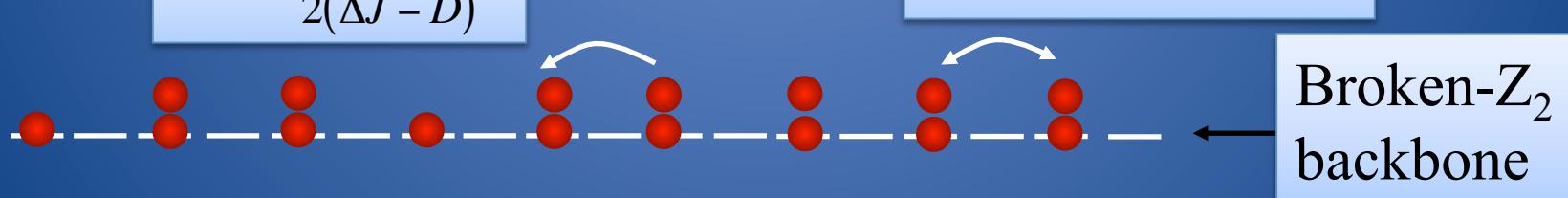
$$H = J \sum_{j=1}^{L-1} \left(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta S_j^z S_{j+1}^z \right) + D \sum_{j=1}^L \left(S_j^z \right)^2 - B \sum_{j=1}^L S_j^z$$



Low energy effective model $0 \leq |M_z| \leq L/2$

$$\tilde{t} = -\frac{J^2}{2(\Delta J - D)}$$

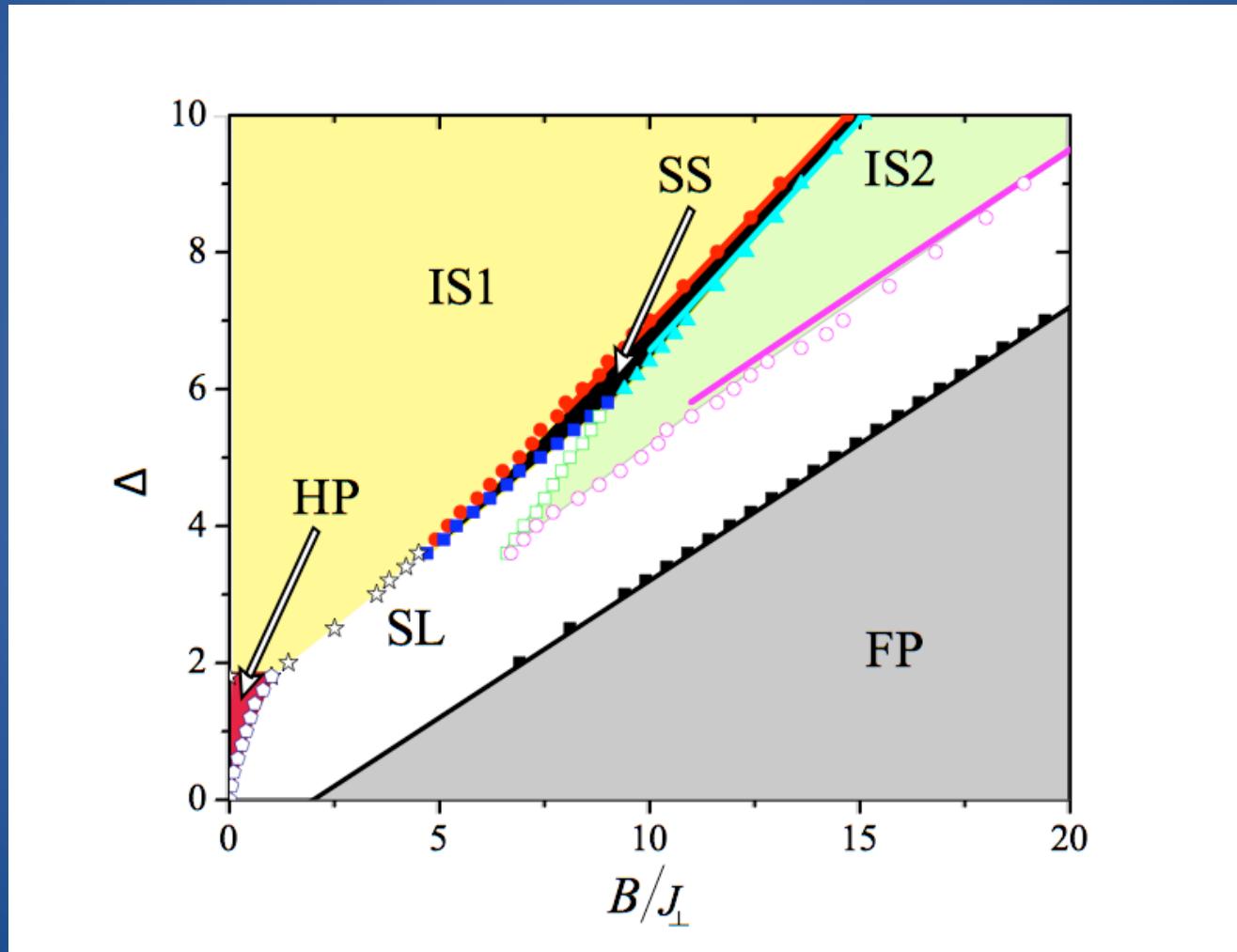
$$\tilde{V} = -\frac{J}{\Delta} - 2\tilde{t} - \frac{2J^2}{3\Delta J - 2D}$$



$$\tilde{\mu} = \frac{J}{\Delta} - 2\tilde{t} - \frac{4J^2}{3\Delta J - 2D} + B + D - 2\Delta J$$



“Spin Supersolid”



Conclusions

- Treating spin systems as gases of bosons can be very advantageous in the proximity of field induced quantum critical points.*
- Although field induced QCPs are very simple, unusual phenomena such as dimensional reduction can occur in presence of frustration .*
- Extensions of spin-wave theory to SU(N) provide a natural way of studying quantum magnets with strong anisotropy.*
- Unusual field induced states such as nematic order or spin-supersolids emerge in presence of strong single-ion anisotropy.*
- Future Directions: Disorder (Bose Glass to BEC transition, $dv < 2$), thermal transport and dynamical properties near the BEC-QCP*

NMR: E. Orignac, R. Citro, T. Giamarchi, PRB 75, 140403 (2007).

Disorder: Rong Yu, Cornelius F. Miclea, Franziska Weickert, Roman Movshovich, 2 Armando Paduan-Filho, Vivien S. Zapf and Tommaso Roscilde, **arXiv:1204.5409**