Geometric Frustration and Dimensional Reduction at a Quantum Critical Point

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S. Sebastian, N. Harrison, C.D.Batista, L. Balicas, M. Jaime, P. A. Sharma, N. Kawashima and I. Fisher,
Nature 44, 617 (2006) .

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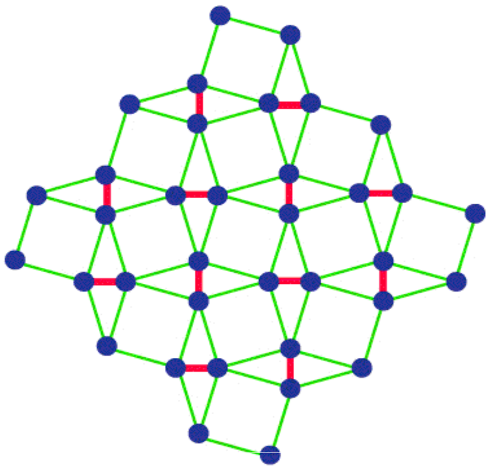
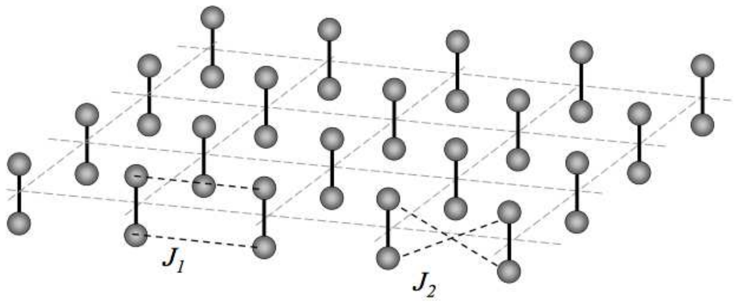
Spin Dimer Frustrated Systems





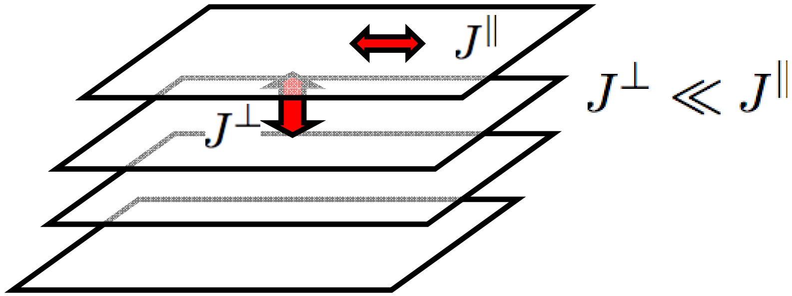
$BaCuSi_2O_6$ **$SrCu_2(BO_3)_2$** **To be Discovered**

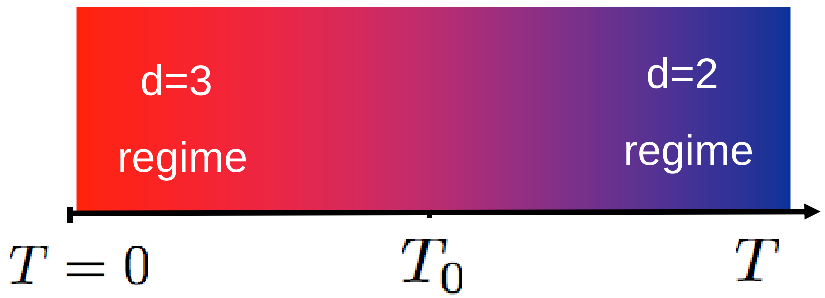
Bose Einstein Condensate	Crystals	Supersolid

S. Sebastian, N. Harrison S, C. D. Batista, L. Balicas, M. Jaime, N. Kawashima, I. Fisher, Nature **441**, 617 (2006).

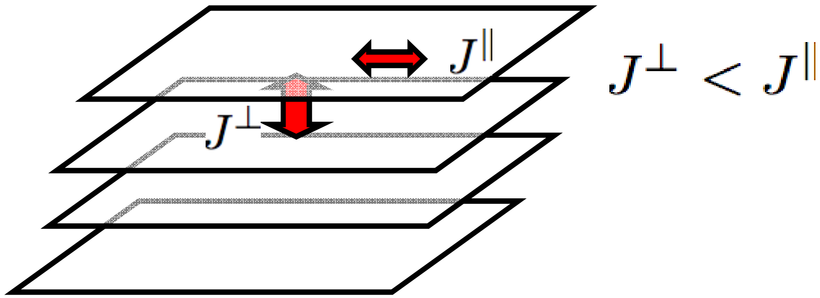
Dimensional Reduction

Usual situation for anisotropic systems

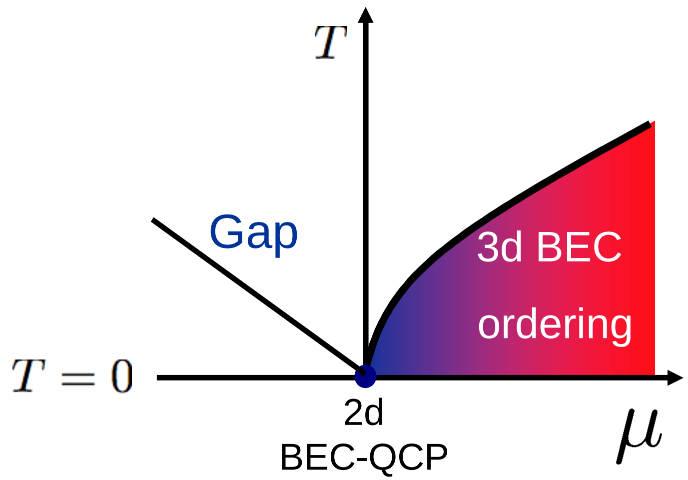




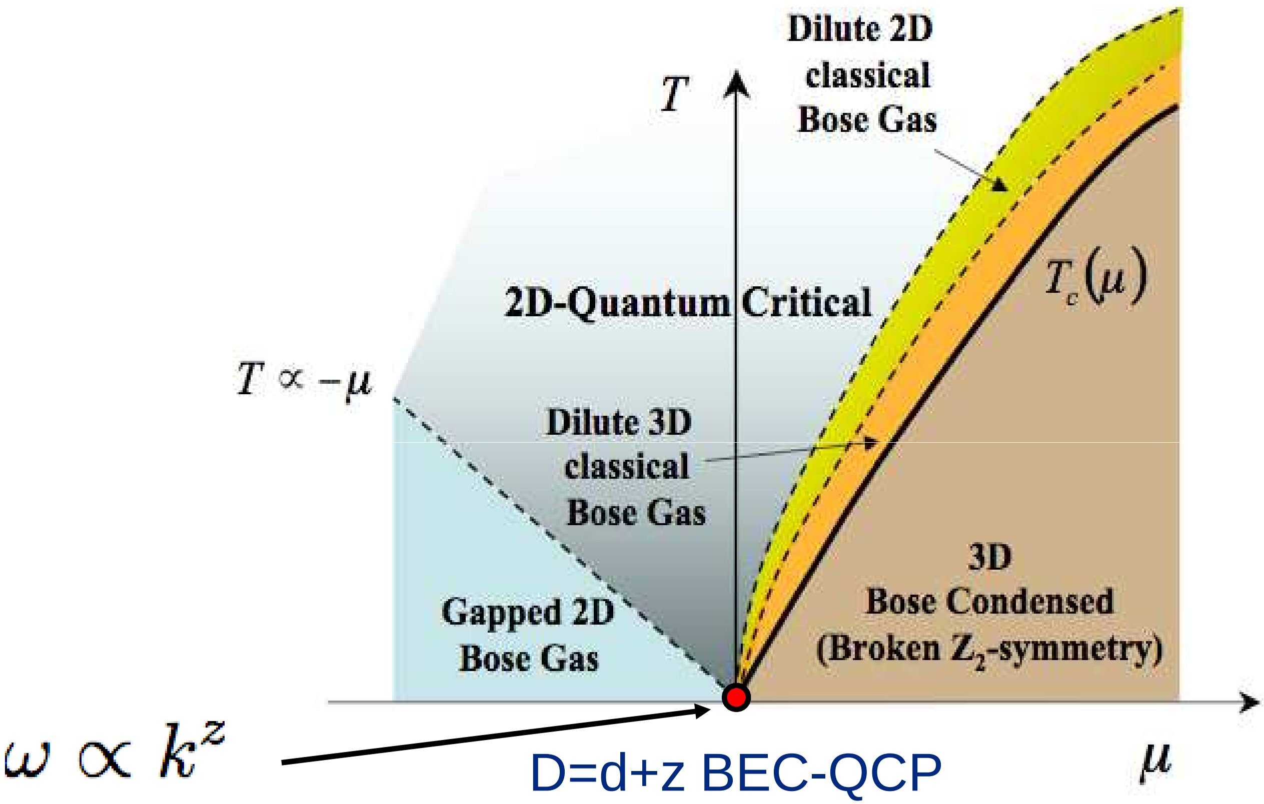
Case of Interest



The inter-layer interaction is geometrically frustrated

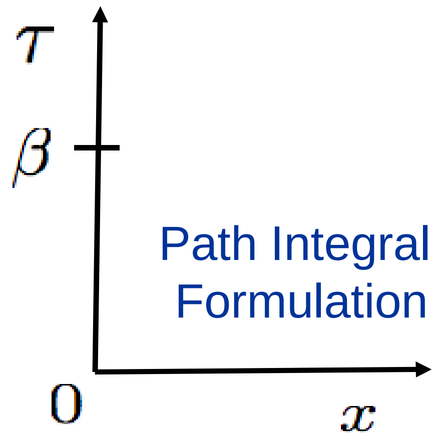


RG Phase Diagram



D=d+z BEC-QCP

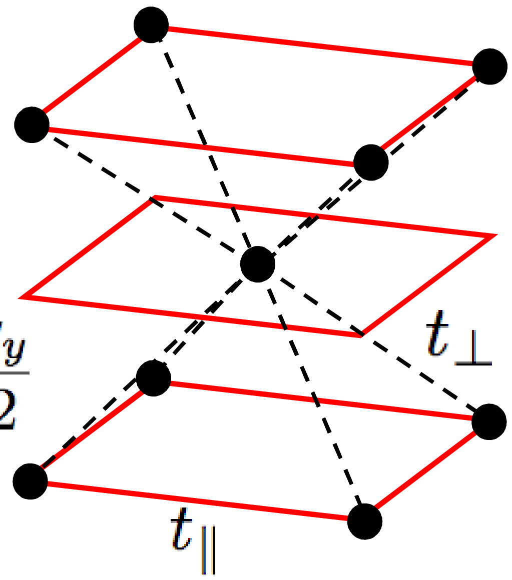
z=2 and d=2



Path Integral Formulation

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

Gas of interacting bosons on a BCT lattice



Bct lattice

$$H = \sum_{\mathbf{k}} (\epsilon_{\mathbf{k}} - \mu) a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + u_0 \sum_{\mathbf{x}} n_{\mathbf{x}} n_{\mathbf{x}}$$

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

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

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

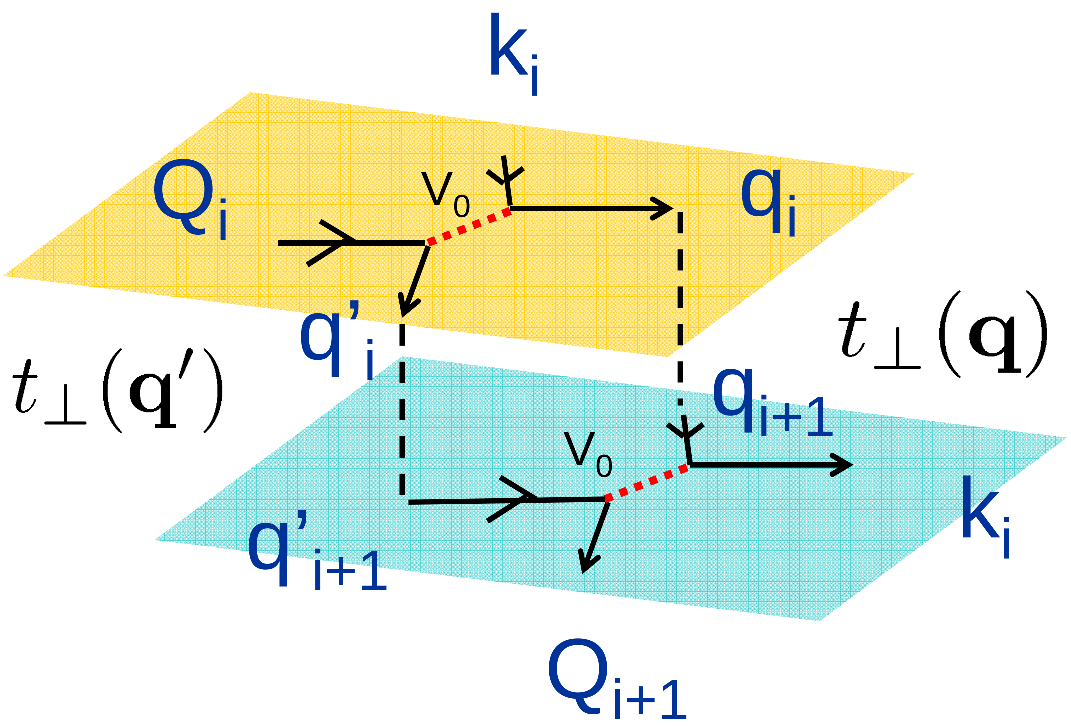
In the long wave-length limit we get:

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

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

Gas of interacting bosons on a bcc lattice

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:



Gas of interacting bosons on a bcc lattice

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$$H = \sum_{\mathbf{k}_{\|},i} [(t_{\|} k_{\|}^2 - \mu)\delta_{i,j} + t_{\perp} k_x k_y \delta_{|i-j|,1}] a^{\dagger}_{k_{\|} i} a_{k_{\|} j} + u_0 \sum_{\mathbf{x}_{\|},i} n_{\mathbf{x}_{\|}} n_{\mathbf{x}_{\|}}$$

$$H^{(0)} = \sum_{k_{\|},q_{\|},p_{\|}} v_0(k_{\|} + q_{\|})(a^{\dagger}_{k_{\|}+p_{\|} i} a^{\dagger}_{q_{\|}-p_{\|} i} a_{k_{\|} i} a_{q_{\|} i} + \mathrm{H.c.})$$

$$H^{(1)} = \sum_{k_{\|},q_{\|},p_{\|}} v_1(k_{\|}, q_{\|}, p_{\|})(a^{\dagger}_{k_{\|}+p_{\|} i+1} a^{\dagger}_{q_{\|}-p_{\|} i+1} a_{k_{\|} i} a_{q_{\|} i} + \mathrm{H.c.})$$

$$H^{(2)} = \sum_{k_{\|},q_{\|},p_{\|}} v_2(k_{\|}, q_{\|}, p_{\|})(a^{\dagger}_{k_{\|}+p_{\|} i+2} a^{\dagger}_{q_{\|}-p_{\|} i+2} a_{k_{\|} i} a_{q_{\|} i} + \mathrm{H.c.})$$

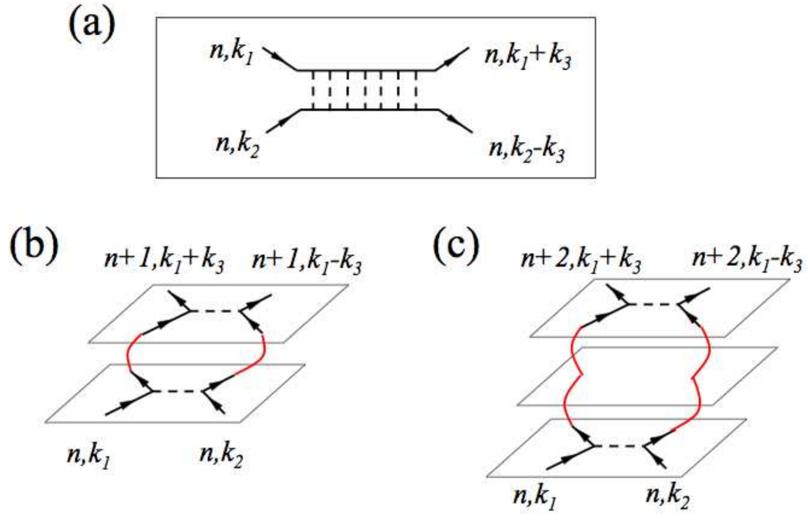
Gas of interacting bosons on a bcc lattice

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

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

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

$$\frac{1}{v_0} = \frac{1}{2}\int_{k_0}^{\pi} \frac{d^2 k_{||}}{4\pi^2}\frac{1}{\epsilon_{\mathbf{k}_{||}}} \propto \frac{\ln \frac{t_{||}}{\mu}}{t_{||}}.$$



$$\begin{aligned} v_1 &= -\frac{v_0^2 t_\perp^2}{8\pi t_{||}^3}\ln\frac{\pi}{k_0}, \\ v_2 &= -\frac{9 v_0^2 t_\perp^4}{128\pi t_{||}^5}\ln\frac{\pi}{k_0}. \end{aligned}$$

Mean-Filed Decoupling and Z_2 symmetry

A mean field decoupling of the effective interactions $H^{(1)}$ and $H^{(2)}$ leads to an effective inter-layer hopping along the z-axis whose amplitude is proportional to the density of bosons:

$$\begin{aligned} n_i n_i &\simeq 2\rho n_i - \rho^2, \\ a_i^\dagger a_i^\dagger a_j a_j &\simeq a_i^\dagger a_j \langle a_i^\dagger a_j \rangle + a_i^\dagger a_j \langle a_i^\dagger a_j \rangle - \langle a_i^\dagger a_j \rangle^2, \end{aligned}$$

$$\boxed{E_{\mathbf{k}}^* = E_{\mathbf{k}} + 2v_1\kappa_1 \cos k_z + 2v_2\kappa_2 \cos 2k_z,} \qquad \boxed{\mu^* = \mu - v_0\rho}$$

$$\kappa_j = \int \frac{d^2k_{\|}}{4\pi^2} \left\langle a_{\mathbf{k}_{\|},i}^\dagger a_{\mathbf{k}_{\|},i+j} \right\rangle$$

$$\left\langle a_{\mathbf{k}_{\|},i}^\dagger a_{\mathbf{k}_{\|},i+j} \right\rangle = \int_{-\pi}^{\pi} \frac{dk_z}{2\pi} \frac{\cos(jk_z)}{e^{\beta\left(E_{\mathbf{k}}^* - \mu^*\right)} - 1}$$

$$\kappa_1 = 0$$

Due to the Z2 symmetry!

Mean-Filed and Phase Boundary

The system undergoes a Bose-Einstein condensation when the effective chemical potential, μ^* becomes equal to zero:

$$\boxed{\mu_c = \quad u_0\rho \simeq -\frac{8\pi t_{\|}\rho}{\ln \rho d^2}} \quad \Rightarrow \quad \kappa_2 \simeq \frac{T t_{\perp}^2 \ln \frac{2T}{t_{\|} k_0^2}}{4\pi t_{\|}^3}$$

$$\boxed{E^*_{\mathbf{k}} = E_{\mathbf{k}} + 2v_2\kappa_2 \cos 2k_z,}$$

$$x_0 = \frac{t_{\|}k_0^2}{T} \simeq -\frac{\rho}{T}\frac{8\pi t_{\|}}{\ln \rho d^2}$$

$$\rho = \frac{1}{(2\pi)^2}\int_{-\pi}^{\pi} dk_z \int_{k_0}^{\infty} \frac{k_{\|}dk_{\|}}{e^{\beta E^*_{\mathbf{k}}} - 1}$$

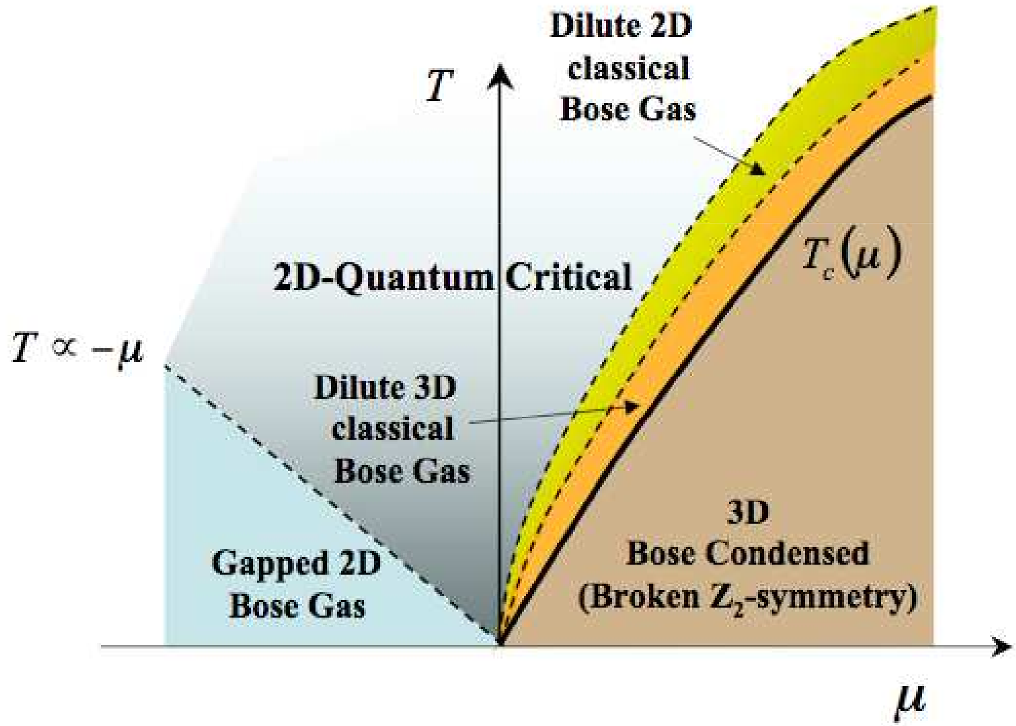
$$\frac{\rho}{T} = \frac{1}{(2\pi)^2}\frac{1}{t_{\|}}\int_0^{\pi} dk_z \int_{x_0}^{\infty} \frac{dx}{e^{x+2v_2\frac{\kappa_2}{T}\cos 2k_z} - 1}$$

$$\boxed{T_c \quad \propto \quad t_{\|}\frac{\rho}{\ln\ln \rho^{-1}},} \qquad \boxed{\mu \quad \propto \quad \frac{T_c}{\ln t_{\|}/T_c},} \qquad \boxed{\rho(\mu = 0, T) \propto T \ln\ln \frac{t_{\|}}{T}}$$

C. D. Batista, J. Schmalian, N. Kawashima, P. Sengupta, S. Sebastian, N. Harrison, M. Jaime, I. Fisher, Phys. Rev. Lett. **98**, 257201 (2007).↑

RG Phase Diagram

Exactly the same results are obtained with a RG approach providing a justification for our heuristic cut-off k_0.



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

Chinese Terracotta Warriors (479-221 BC)

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

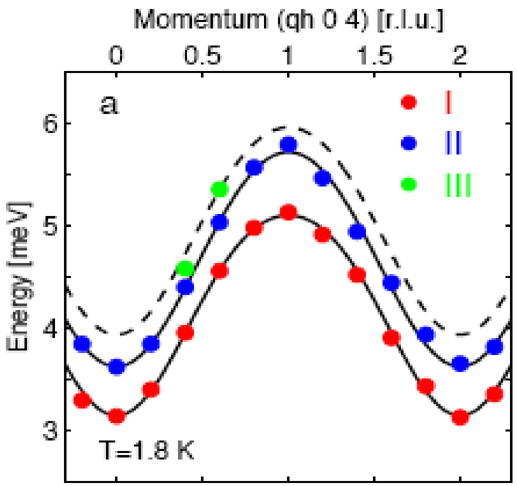
Heinz Berke
Angew. Chem. Int. Ed. **41**, 2483 (2002)

Heisenberg Hamiltonian for $BaCuSi_2O_6$

$$
\begin{aligned}
\mathcal{H} &= J_1 \sum_{\mathbf{i}\in A} \mathbf{S}_{\mathbf{i}1}\cdot\mathbf{S}_{\mathbf{i}2} + J_2 \sum_{\mathbf{i}\in B} \mathbf{S}_{\mathbf{i}1}\cdot\mathbf{S}_{\mathbf{i}2} + J' \sum_{\mathbf{i},j,\nu} \mathbf{S}_{\mathbf{i}j}\cdot\mathbf{S}_{\mathbf{i}+\mathbf{e}_\nu j} \\
&+ J_f \sum_{\mathbf{i},\eta} \mathbf{S}_{\mathbf{i}2}\cdot\mathbf{S}_{\mathbf{i}+\mathbf{e}_\eta 1} - g\mu_B H \sum_{\mathbf{i},j} S^z_{\mathbf{i},j}
\end{aligned}
$$

$$
\begin{aligned}
J_1 &= 4.27\text{meV} \\
J_2 &= 4.72\text{meV} \\
J' &= 0.5\text{meV}
\end{aligned}
$$

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

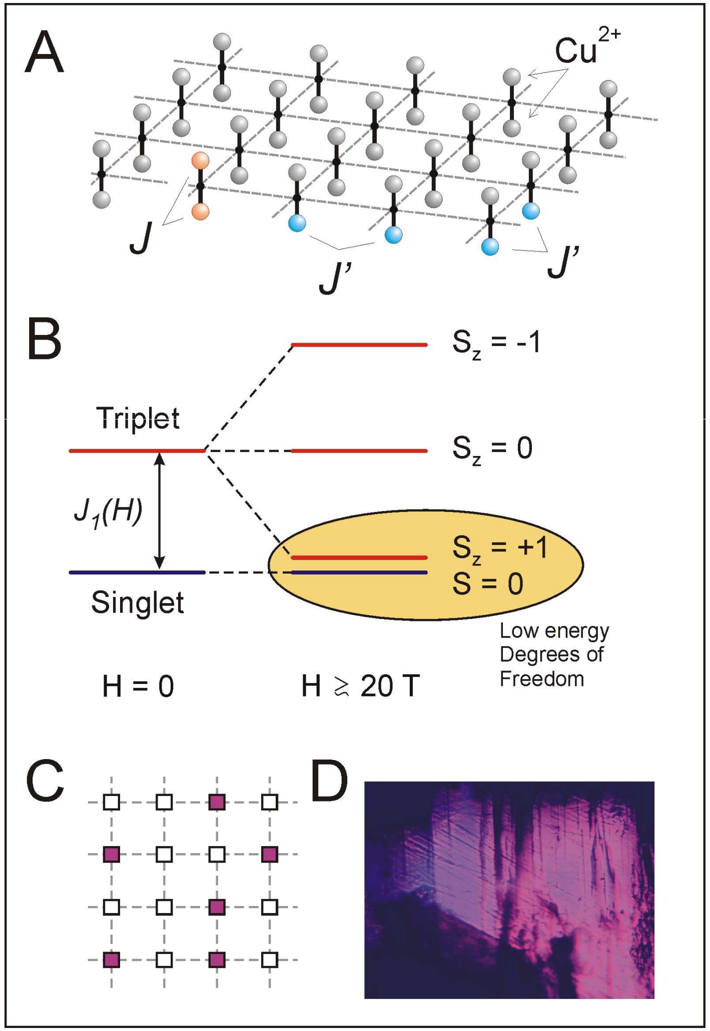


A →

B →

A →

Low Energy Hamiltonian for $BaCuSi_2O_6$



Hard-core Boson Representation of
Effective Low Energy Hamiltonian

$S^z = 1$ triplet $\rightarrow$

$S = 0$ singlet $\rightarrow$

$$m_z = \langle s^z \rangle = \rho$$

$$\mathcal{H}_{\text{eff}} = \mathcal{H}_0 + \mathcal{V}$$

$$\mathcal{H}_0 = \frac{J'}{2}\sum_{\mathbf{i},\nu}(b_{\mathbf{i}}^{\dagger}b_{\mathbf{i}+\mathbf{e}_\nu} + b_{\mathbf{i}+\mathbf{e}_\nu}^{\dagger}b_{\mathbf{i}} + n_{\mathbf{i}}n_{\mathbf{i}+\mathbf{e}_\nu}) - \sum_{\mathbf{i}\in\mathbf{A}}\mu_1 n_{\mathbf{i}} - \sum_{\mathbf{i}\in\mathbf{B}}\mu_2 n_{\mathbf{i}}$$

$$\mathcal{V} = \frac{J_f}{4}\sum_{\mathbf{i},\nu}(b_{\mathbf{i}}^{\dagger}b_{\mathbf{i}+\mathbf{e}_\nu} + b_{\mathbf{i}+\mathbf{e}_\nu}^{\dagger}b_{\mathbf{i}} + n_{\mathbf{i}}n_{\mathbf{i}+\mathbf{e}_\nu})$$

$$\mu_1 = -J_1 + g\mu_B H \qquad \mu_2 = -J_2 + g\mu_B H$$

M. Jaime, et. Al., Phys. Rev. Lett **93**, 087203 (2004).

Phase Diagram

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

Broken U(1)xZ_2

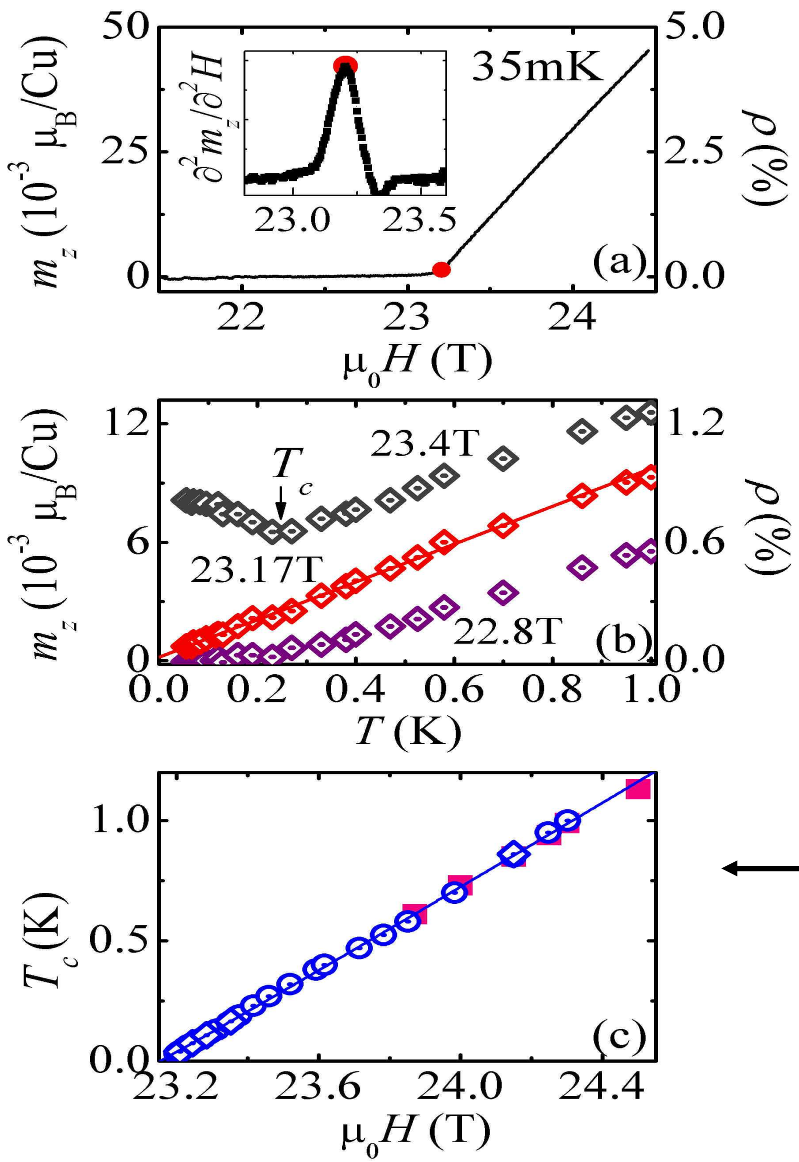
BEC-QPT

Driven by
amplitude
fluctuations

D=d+z
z=2
↑

S. Sebastian, N. Harrison, C. D. Batista, L. Balicas, M. Jaime, N. Kawashima, I. Fisher, Nature **441**, 617 (2006).

Measured Critical exponents for the QCP



$$d \geq 2$$

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

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

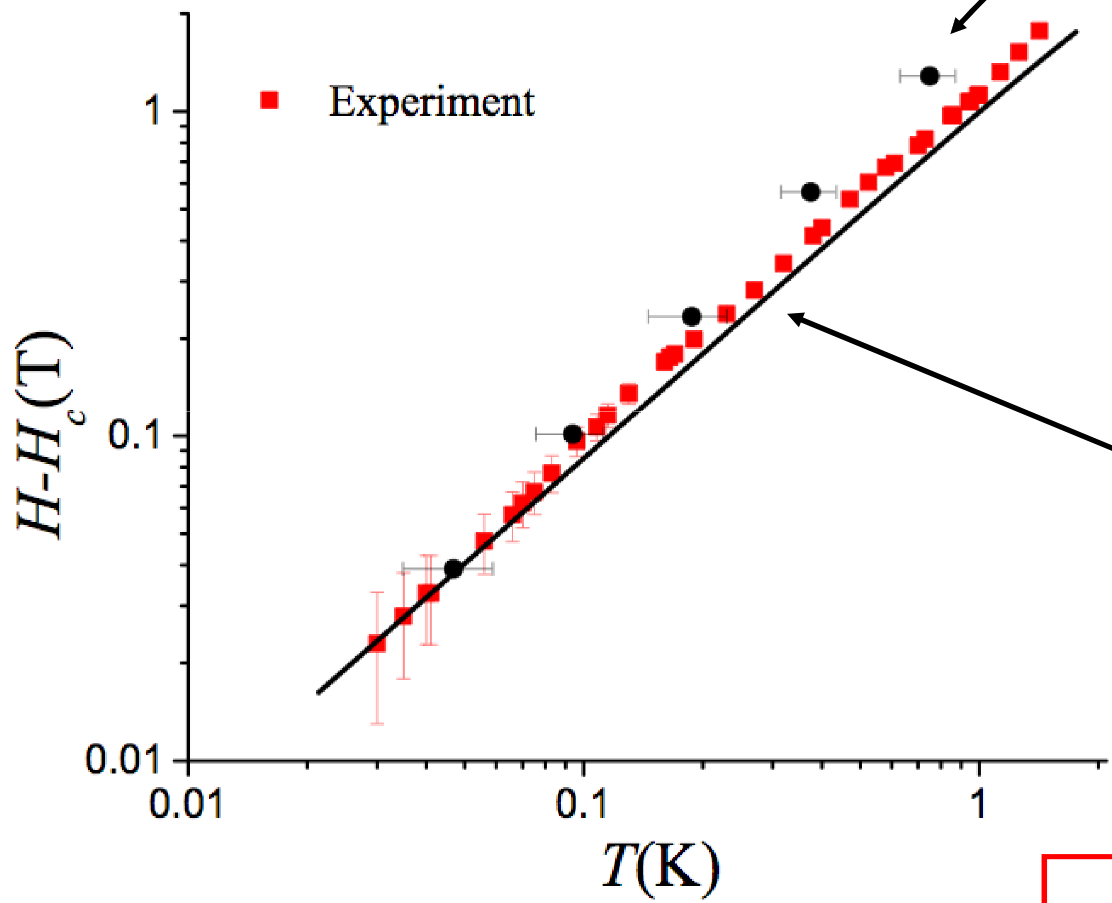
$$T_c \quad \propto \quad (H - H_c)^{2/d}$$

S. Sebastian, N. Harrison, C. D. Batista, L. Balicas, M. Jaime, N. Kawashima, I. Fisher, Nature **441**, 617 (2006).

Linear T_c vs. H-H_c behavior was confirmed by NMR studies:

S. Kramer, R. Stern, M. Horvatic, C. Berthier, T. Kimura and I. R. Fisher, Phys. Rev. B 76, 100406R (2007).

Comparison between experiment and theory



MC simulation for a d=2 gas of hard core bosons hopping:

$$t_{\|} = \frac{J'}{2} = 3\mathrm{K}$$

$$\mu_c = \frac{2u_0 T}{\pi t_{\|}} \ln \frac{2t_{\|}\xi_\mu}{u_0}$$

N. Prokof'ev and B. Sustinov, PRA 66, 043608 (2002).

No free parameters!

C. D. Batista, J. Schmalian, N. Kawashima, P. Sengupta, S. Sebastian, N. Harrison, M. Jaime, I. Fisher, Phys. Rev. Lett. **98**, 257201 (2007).

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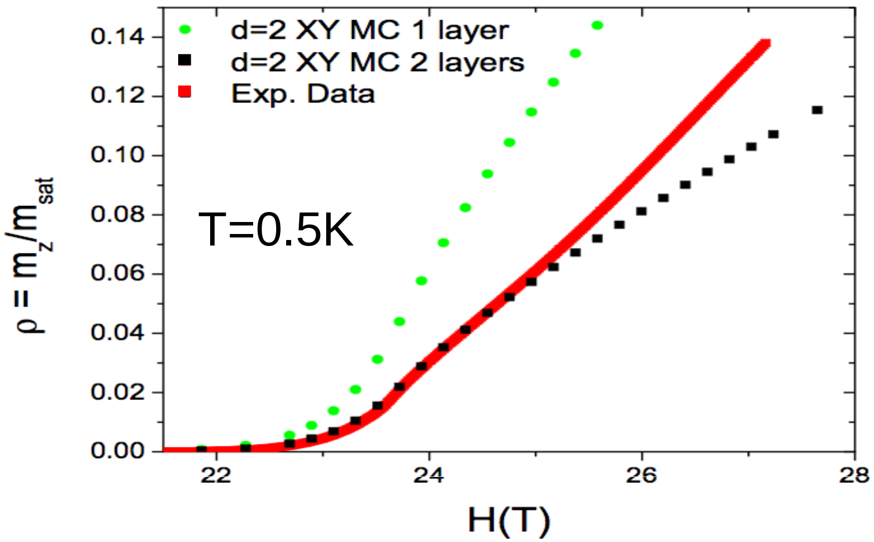
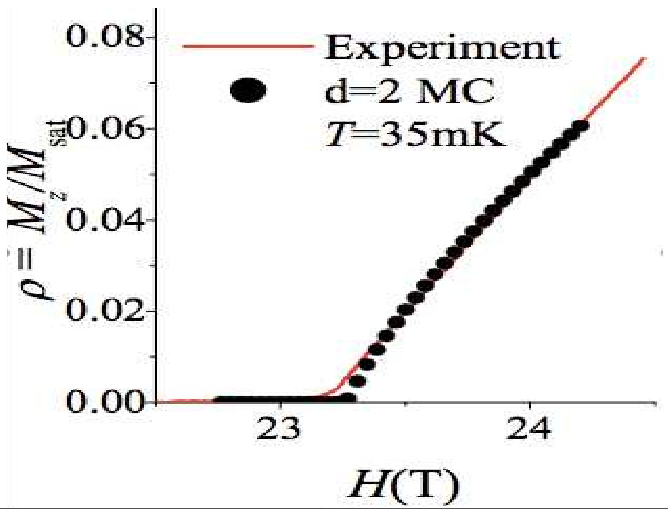




- MC simulation for a d=2 gas of hard core bosons hopping:

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

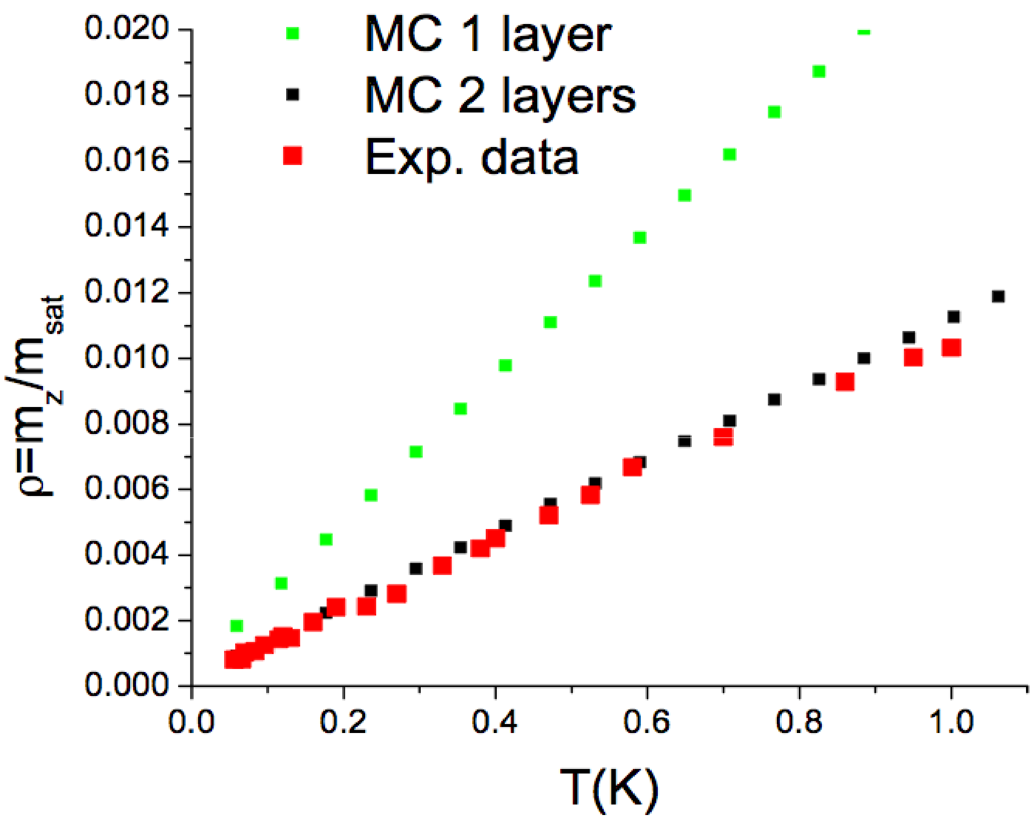
If we assume that there are two non-equivalent layers the agreement is very good as long as:

$$H - H_c \ll \frac{J_1 - J_2}{g\mu_B} = 3.57\text{T}$$

No free parameters!

C. D. Batista, J. Schmalian, N. Kawashima, P. Sengupta, S. Sebastian, N. Harrison, M. Jaime, I. Fisher, Phys. Rev. Lett. **98**, 257201 (2007).

Comparison between experiment and theory



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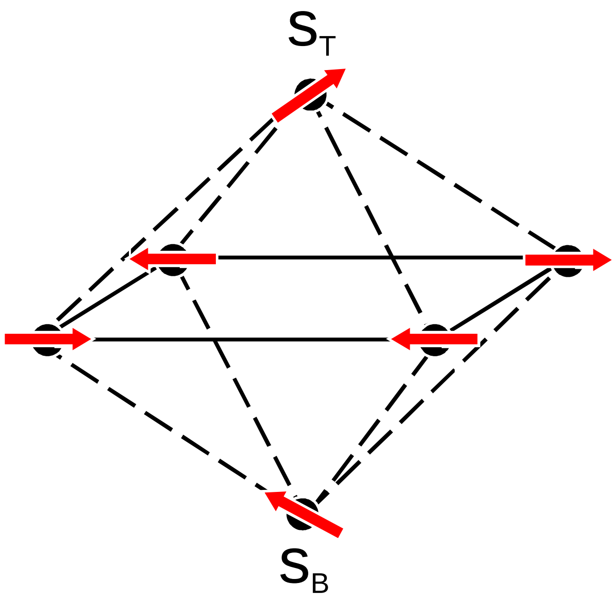
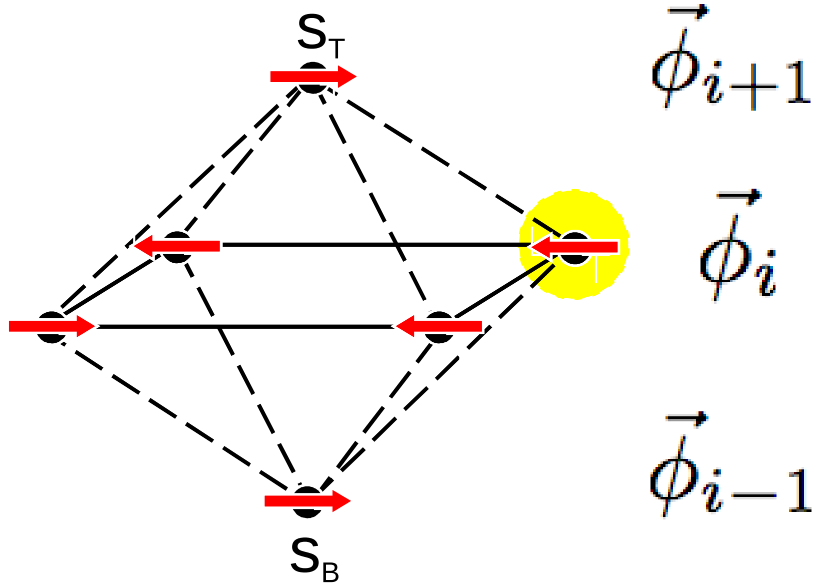
Order From Disorder

Classical system at T=0



S_T and S_B are decoupled

Quantum system at T=0



S_T and S_B are FM coupled

$$\cancel{g_0 \vec{\phi}_{i+1} \cdot \vec{\phi}_i}$$

$$g_1 (\vec{\phi}_{i+1} \cdot \vec{\phi}_i)^2$$

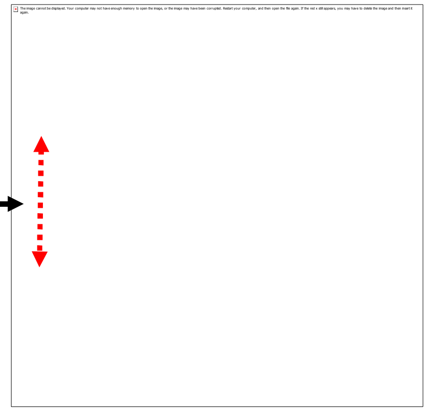
$$g_2 (\vec{\phi}_{i+2} \cdot \vec{\phi}_i) \quad \text{with} \quad g_2 \propto \vec{\phi}_i \cdot \vec{\phi}_i$$

Asymptotic behavior of $BaCuSi_2O_5$ at T<<30mK

- Dipolar interactions of order 10 mK [S. Sebastian et al, PRB 74, 180401 (2006)] break the U(1) symmetry explicitly! Therefore, we expect a crossover from the BEC-QCP to an Ising-like transition D=3+1 below 10mK.

-Longer range non-frustrated interactions will produce a crossover to a 3d BEC-QCP at low enough T in any real system.

Longer range non-frustrated coupling



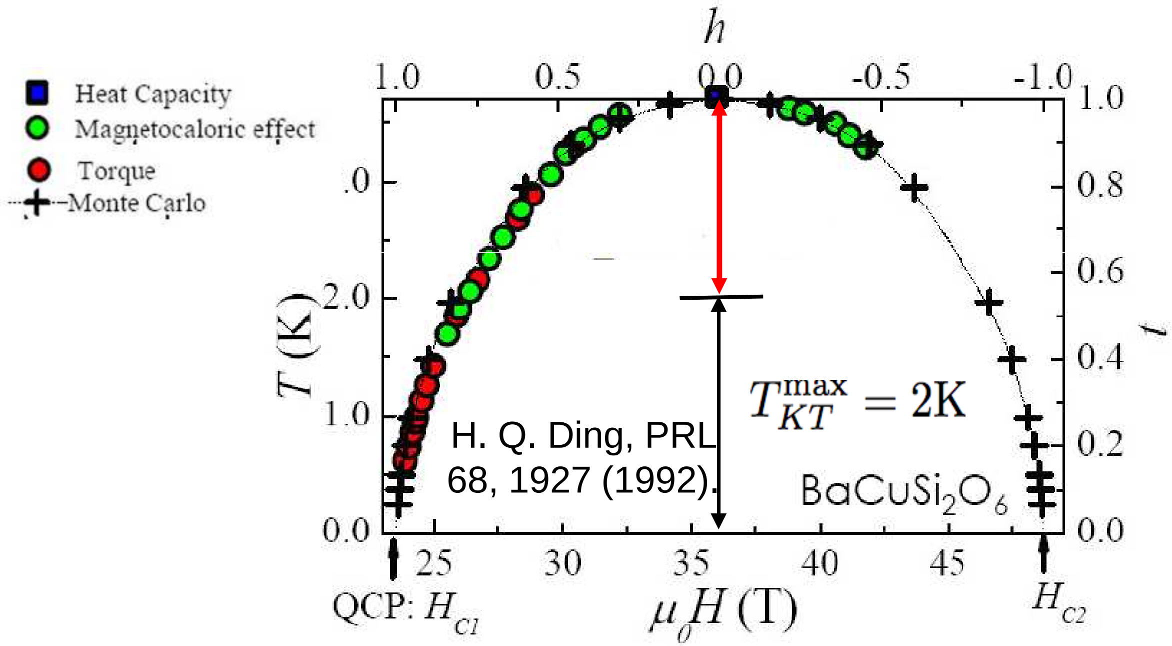
-As it was pointed out recently by O. Rösch and M. Vojta, [PRB 76, 780401R (2007)], the inclusion of the high-energy triplets (Sz=-1,0) leads to a residual inter-layer coupling of order:

$$\boxed{J_f^4/J^3 < 1\mathrm{mK}}$$

Given the magnitude of the dipolar interactions, this observation is only of academic interest!

Modulation of the intra-dimer interaction

-If we assume an alternative scenario for dimensional reduction in which the only mechanism for dimensional reduction is the observed modulation in the intra-dimer interaction:



$T_c^{\mathrm{max}} = 3.7\mathrm{K}$

The non-frustrated coupling that is required for getting this value is:

$$\boxed{J'' = J'/6 \simeq 1\mathrm{K}}$$

[M. Jaime et al, PRL 93, 087203 (2004)]

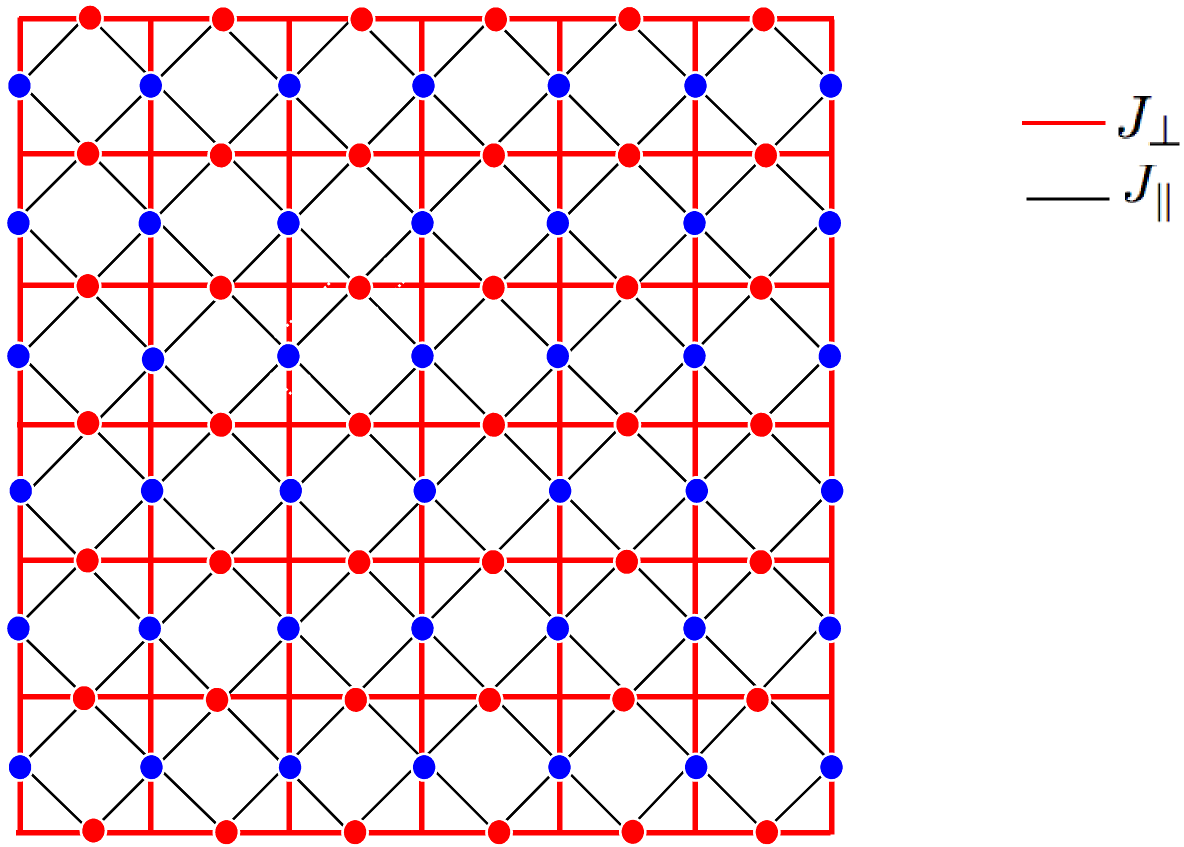
The expected dispersion along the z-axis in the presence of a modulation J_1-J_2=5.5K is:

$$\boxed{\frac{J''^2}{J_1 - J_2} = 180\mathrm{mK} \gg 30\mathrm{mK}}$$

Conclusions

- Geometric frustration can change the universality class of a QCP.
- Hyper-planes coupled by frustrating interactions in a d-dimensional space have a BEC QCP of dimension d-1 for $d \geq 3$.
- Dimensional reduction to d=1 occurs for crossed chains coupled by frustrated interactions.
- This theory explains the measured exponents on $BaCuSi_2O_4$. There are only two non-equivalent layers!
- Predictions: $C_v \propto T$ at the QCP and log dependence for the NMR relaxation time $1/T_1$.
- The same dimensional reduction should be observed in other antiferromagnets on bcc lattices at the field induced QCP's.

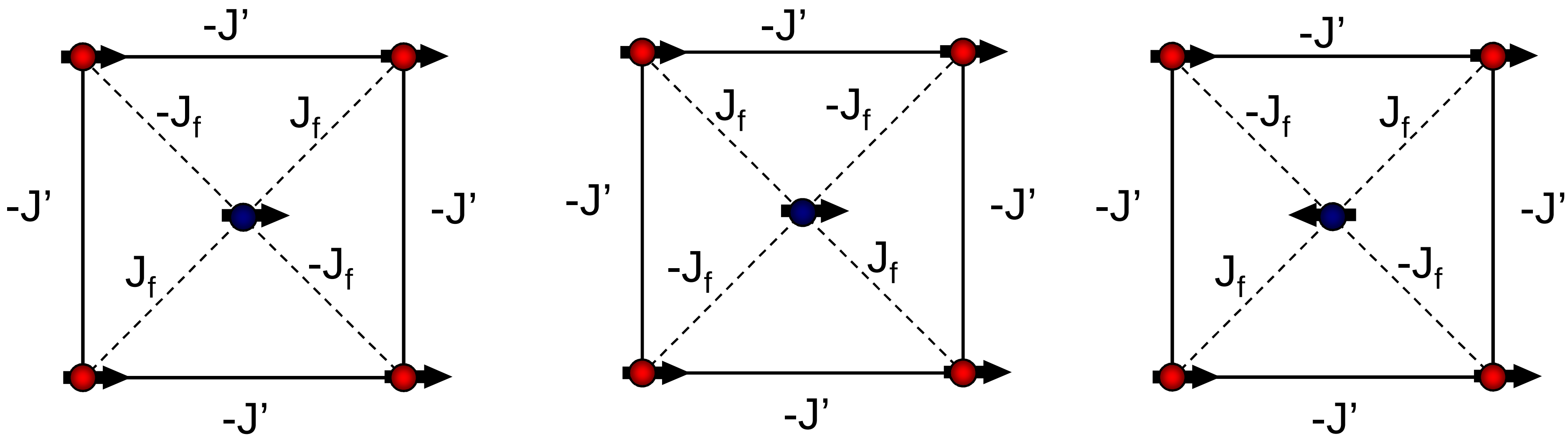
Crossed Chains

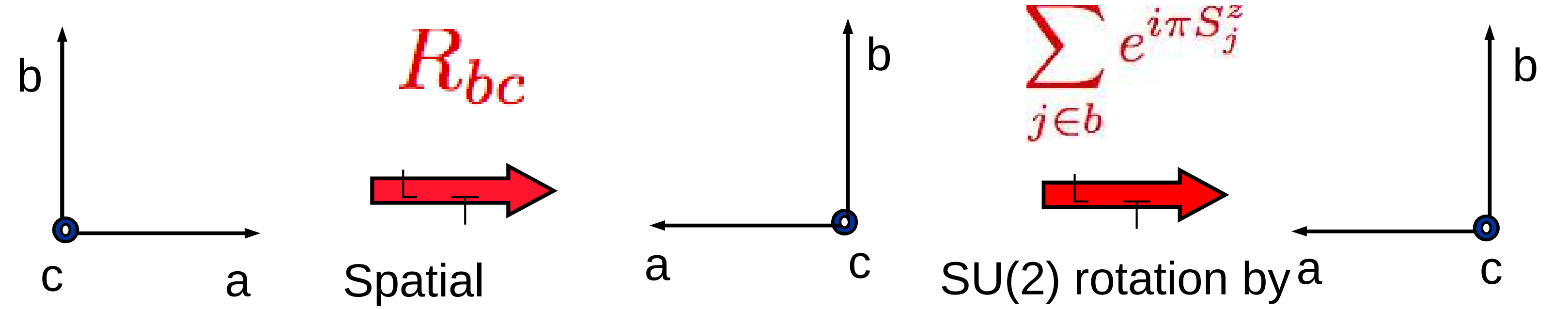


Outline

- Motivation.
- Emergent symmetries in classical frustrated systems.
- Order from Disorder.
- BEC quantum phase transition on a BCT lattice.
- Dimensional reduction at the BEC quantum critical point.
- Experimental realization: the spin-dimer compound $BaCuSi_2O_6$.
- Comparison between experiment and theory.
- Conclusions.

Z_2-Symmetry





Spatial reflection in the bc-plane.

SU(2) rotation by π around the z-axis for the blue sublattice.

$$T = R_{bc} \sum_{j \in b} e^{i\pi S_j^z} \qquad g_0 \vec{\phi}_{i+1} \cdot \vec{\phi}_i \rightarrow -g_0 \vec{\phi}_{i+1} \cdot \vec{\phi}_i$$

Body Centered Tetragonal Lattice