Dimerized & frustrated spin chains

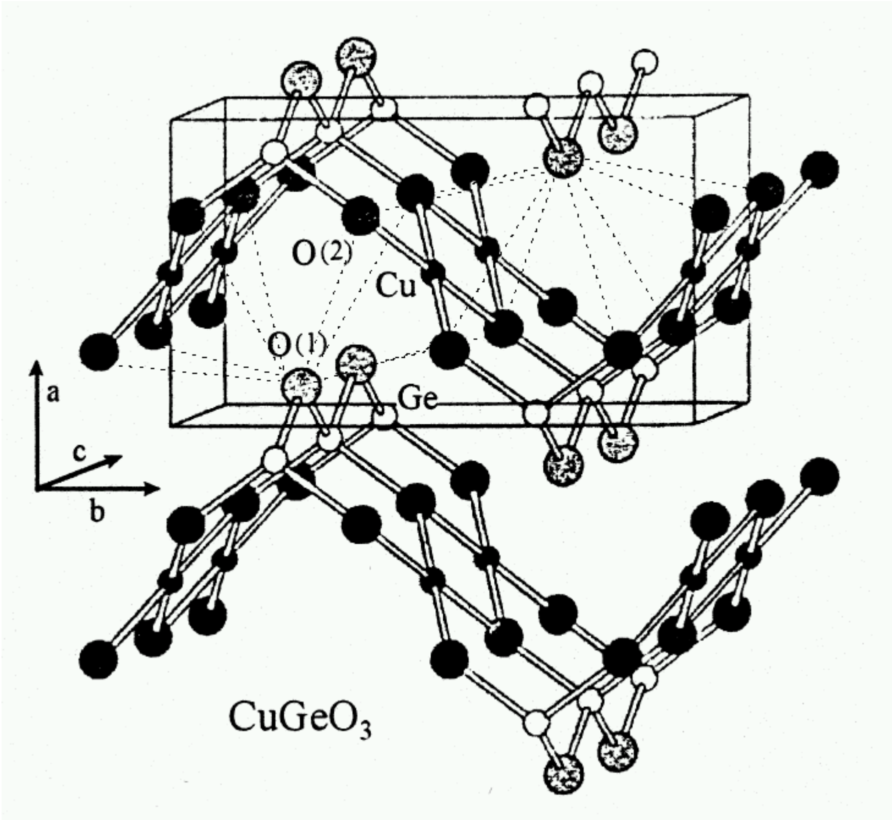
Application to copper-germanate

Outline

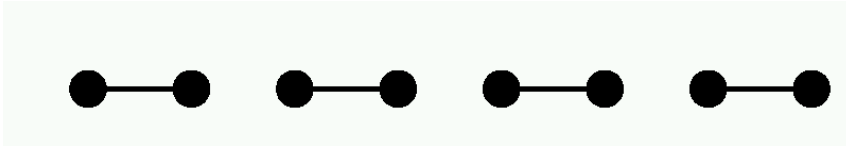
- CuGeO & basic microscopic models
- Excitation spectrum
- Confront theory to experiments
- Doping Spin-Peierls chains

A typical S=1/2 dimerized chain

Structure of $CuGeO_3$



Chains direction (copper atoms)



Schematic dimerized GS

Spin-Peierls: dimerized GS (X-ray) if $T < T_{SP}$

Basics microscopic models

XXZ chain

$$H_{\mathrm{XXZ}} = \frac{J}{2}\sum_i \{(S_i^+ S_j^- + S_i^- S_j^+) + J_z S_i^z S_j^z\}$$

- Bethe Ansatz:
  - Bethe 1931 (SU(2) Heisenberg $J_z = J$)
  - Luther & Peschel 1975

- Bosonization & Renormalization Group

Bosonization (notions)

Field theory in the long wave-length limit:

Bosonic field Φ and conjugate Π

$$S^{+}(x) = \frac{e^{-i\theta(x)}}{\sqrt{2\pi a}}\left(\exp\left(-i\pi x/a\right) + \cos 2\Phi(x)\right)$$

$$S^{z}(x) = -\frac{1}{\pi}\partial_x \Phi(x) + \exp\left(i\pi x/a\right)\frac{\cos 2\Phi(x)}{a\pi}$$

where the angle $\theta = \pi \int \Pi dx$

Sine-Gordon field-theory model

Stiffness & Inverse compressibility

$$H_{\mathsf{SG}} = \int \frac{dx}{2\pi}\left(uK(\pi\Pi)^2 + \frac{u}{K}(\partial_x\Phi)^2\right) + g\int dx \cos 4\Phi$$

Elastic chain

(Luttinger Liquid)

Interaction

where $g = -\frac{2aJ_z}{(2\pi a)^2}$

and $K = 1 - \frac{2J_z}{\pi J} + \ldots$

and $u/aJ = 1 + \frac{2J_z}{\pi J} + \ldots$

Spin-spin correlation functions

$$\langle S^z(x) S^z(0) \rangle \sim (-1)^x \frac{1}{x^{2K}}$$

$$\langle S^+(x) S^-(0) \rangle \sim (-1)^x \frac{1}{x^{1/2K}}$$

- XY model: g=0 & K=1
- Heisenberg: SU(2) symmetric => K=1/2

Renormalization Group
Stability of the Luttinger Liquid

Jose et al., 1977

Treat g in perturbation

change of scale : $l = \ln(L) \to l + dl$

$$\frac{dK}{dl} = -g^2$$

$$\frac{dg}{dl} = (2 - 4K)g + O(g^2)$$

Equals 0 for $K = K^* = \frac{1}{2}$

Equivalent to **Kosterlitz-Thouless** equations
for superfluid transition (2D classical XY model)

Phase diagram of XXZ chain

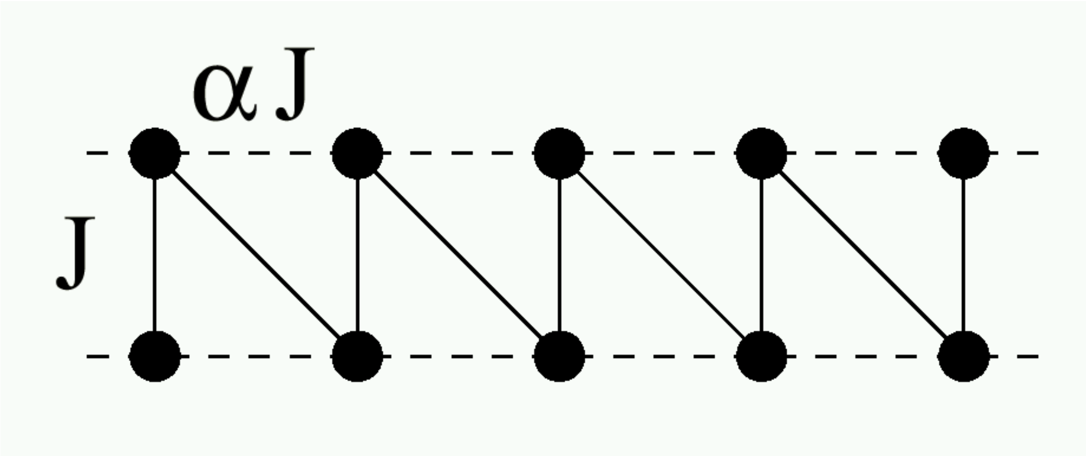
- If $K \geq 1/2$: the Luttinger Liquid is stable
- If $K < 1/2$: g flows to strong coupling
- From Bethe-Ansatz:

$$K = \frac{\pi}{2(\pi - \arccos(J_z/J))}$$

For $|J_z/J| \leq 1$: Luttinger liquid
For $|J_z/J| > 1$: Ising (AF or F) gapped phase

Frustrated (or zig-zag) chain model

$$H_{\mathrm{F}} = J \sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+1} + J_2 \sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+2}$$

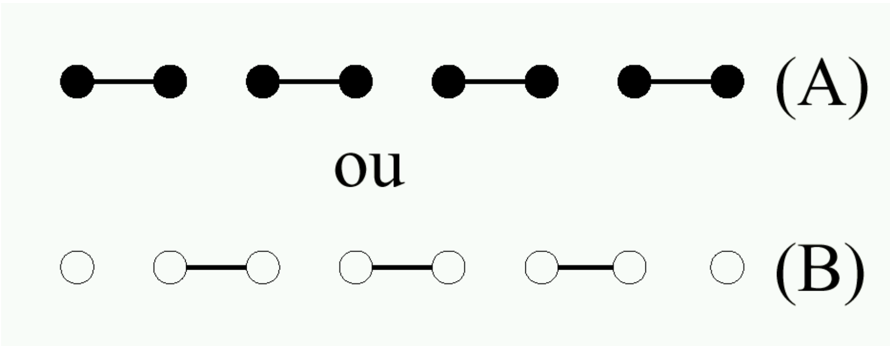


Frustration: $\alpha = J_2/J$

Spontaneous symmetry breaking

Relevant perturbation:

$$H_{\mathrm{pert}} = (\alpha - \alpha_c)\cos(4\Phi)$$



$$2\Phi = \pm\frac{\pi}{2}$$

$\alpha > \alpha_c$:

Dimerized GS

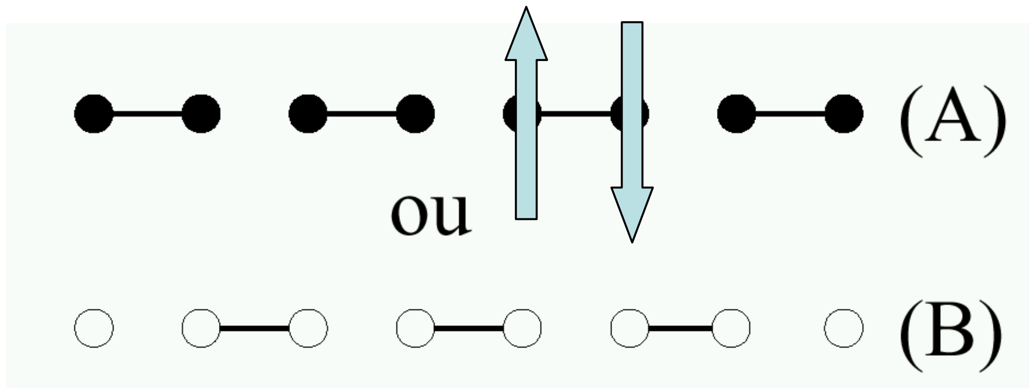
(two-fold degenerate)

Majumdar-Ghosh exact GS

J. Math. Phys. **10**, 1399 (1969)

Special point: $\alpha = J_2/J = 0.5$

Two-fold GS:
(see tutorial 3)



"Valence Bond Crystal" (VBC)

Spin-gap of order ~J/4
& very short spin correlation length

Simple proof

$$H_{MG} = \sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+1} + \frac{1}{2}\mathbf{S}_i \cdot \mathbf{S}_{i+2}$$

Can be re-written as:

$$H_{MG} = \frac{1}{4}\sum_i (\mathbf{S}_i + \mathbf{S}_{i+1} + \mathbf{S}_{i+2})^2 - \frac{3}{4}\sum_i (\mathbf{S}_i)^2$$

⇨ spin-1/2 on each “triangle” (1,i+1,i+2)

⇩

$$E_{MG} = -\frac{1}{2}S(S+1) = -\frac{3}{8}$$

Numerical investigation

DMRG on rings with up to 200 sites

White & Affleck, PRB 54, 9862 (1996)

- "Quantum critical point" at $\alpha_c \simeq 0.2412$

  => Kosterlitz-Thouless transition:

- $\alpha \leq \alpha_c$: "critical" or "quasi-ordered" phase
- $\alpha \geq \alpha_c$: spin-gapped dimerized phase:

$$\Delta^{01} \propto \exp\left(-\mathrm{Cst}/(\alpha - \alpha_c)\right)$$

Spin-Peierls “standard” model

Frustration

$$H_{SP} = \sum_i (1 + (-1)^i \delta) \mathbf{S}_i \cdot \mathbf{S}_{i+1} + \alpha J \sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+2}$$

Fixed dimerization
Assuming a magneto-elastic coupling to a 2D lattice

Effect of the dimerization

$$H_D = J\delta \sum_i (-1)^i \mathbf{S}_i \cdot \mathbf{S}_{i+1}$$

Bosonized form:

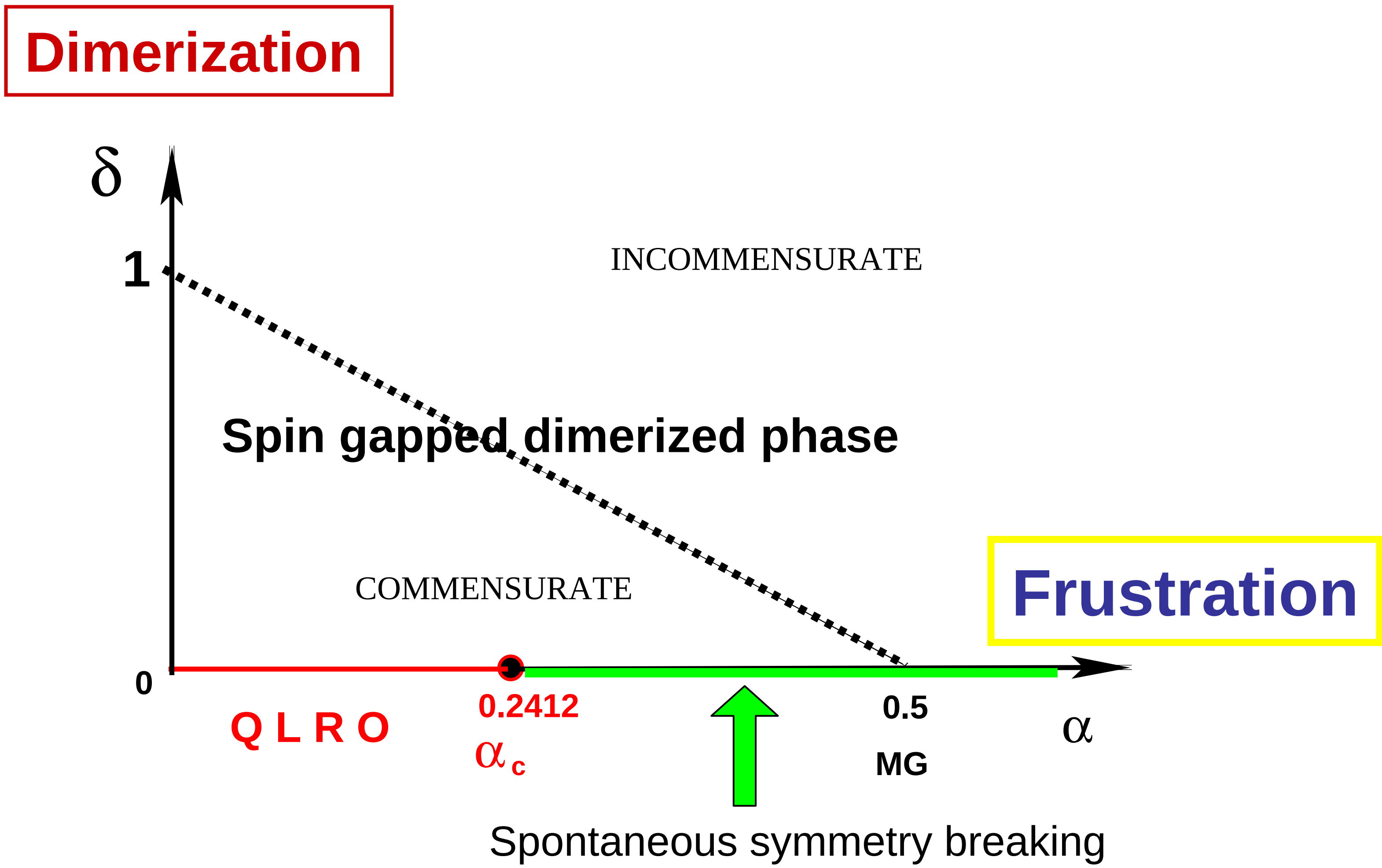
$$H_D = c\delta \int \frac{dx}{2\pi} \sin(2\Phi)$$

$\Rightarrow$ Perturbation always relevant

$\Rightarrow$ Lift degeneracy & select one specific GS:

$$2\Phi = -\pi/2$$

Complete phase diagram



Parameters for copper-germanate

$CuGeO_3$

- Spin-Peierls transition at T=14K
- $J_1 \sim 150K$, $\alpha \sim 0.36$, $\delta \sim 0.014$

Riera & Dobry, PRB **51**, 16098 (1995)
Castilla et al., PRL **75**, 1823 (1995)

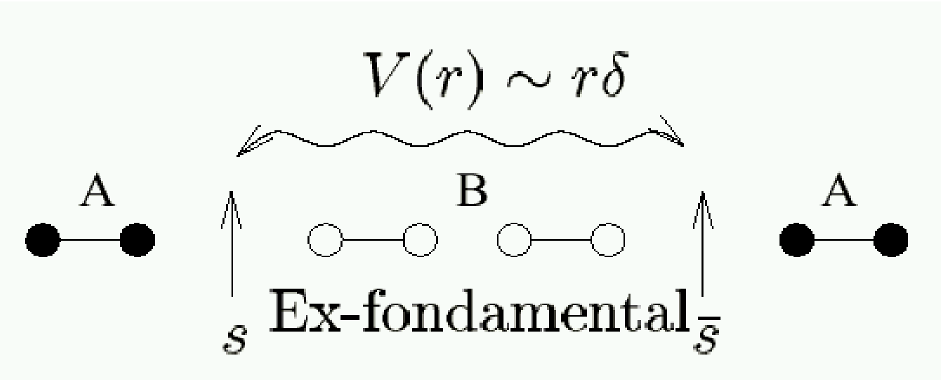
Excitation spectrum

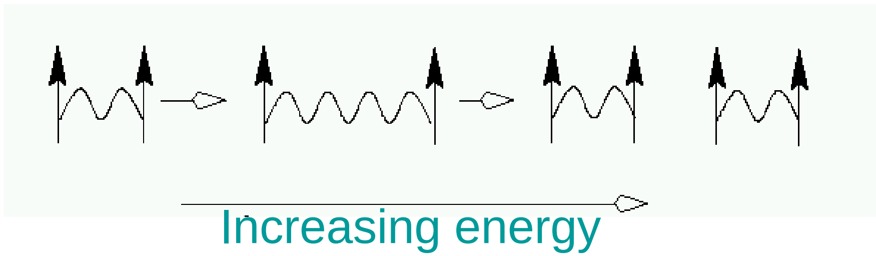
(De)confinement

Confront theory to experiment !

Topological excitations of dimerized chain

Simple qualitative argument:





Soliton-antisoliton S=0 or S=1 pair

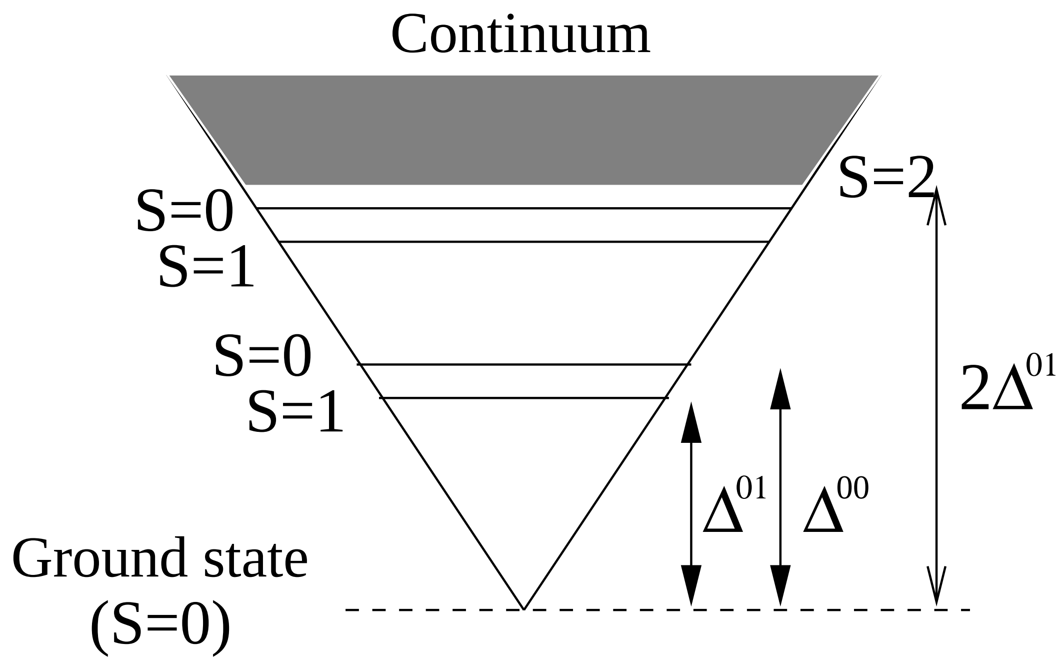
Other terminology: kink & anti-kinks (from bosonisation !)

Low energy spectrum in dimerized chain

Analogy with Schrödinger eq. in linear potential

$s\bar{s}$ bound states

$s\bar{s} - s\bar{s}$ continuum



Spin gap Δ^{01} = smallest energy to create a $s\bar{s}$ pair excitation

Linear potential for soliton-antisoliton

$$-\frac{\partial^2\Phi}{\partial x^2} + c\delta x\Phi = E\Phi$$

Change of scale: x=ay

↓

$$(c\delta)^{2/3}\left(-\frac{\partial^2\Phi}{\partial y^2} + c\delta y\Phi\right) = E\Phi$$

↓

Singlet-triplet gap $\Delta^{01}(\delta) - \Delta^{01}(0) \sim \delta^{2/3}$

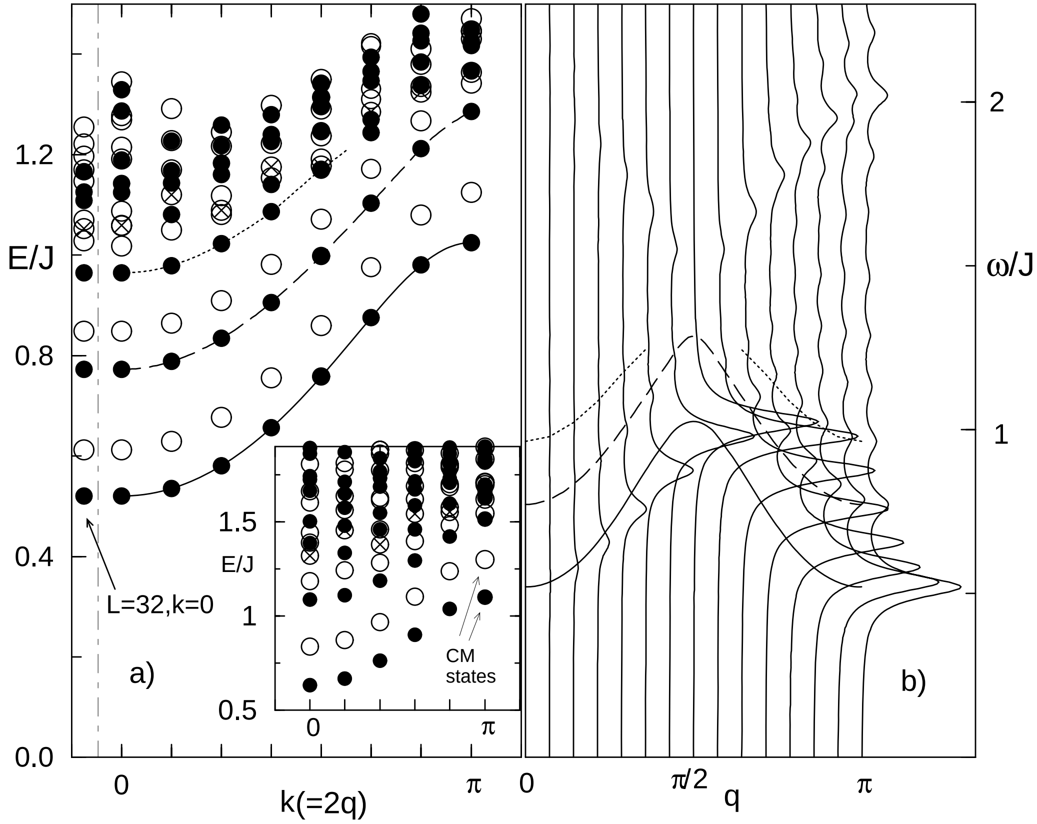
Properties of soliton-antisoliton boundstates

Low energy spectrum (ED of a 28-site ring)

- Mobile $s\bar{s}$ pair
  $\Rightarrow$ finite dispersion

- Associated to peaks in the magnetic Structure Factor:

$$A = S_k^Z$$
$$\Downarrow$$
$$S(k,\omega)$$



Sorensen et al.,PRB **58**, R14701 (1999)

Experiments in copper-germanate

Raman scattering

Loudon-Floury operator

$$A_{\text{Raman}} \sim \sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+1}$$

Inelastic Neutron scattering

$$A_{\text{INS}} = \mathbf{S}_{\mathbf{k}}$$

$$I(\omega) = \langle A(t) A^{\dagger}(0) \rangle_{\omega}$$

Two-magnon scattering
with
selection rules:

$$k = 0 \text{ and } \Delta S = 0$$

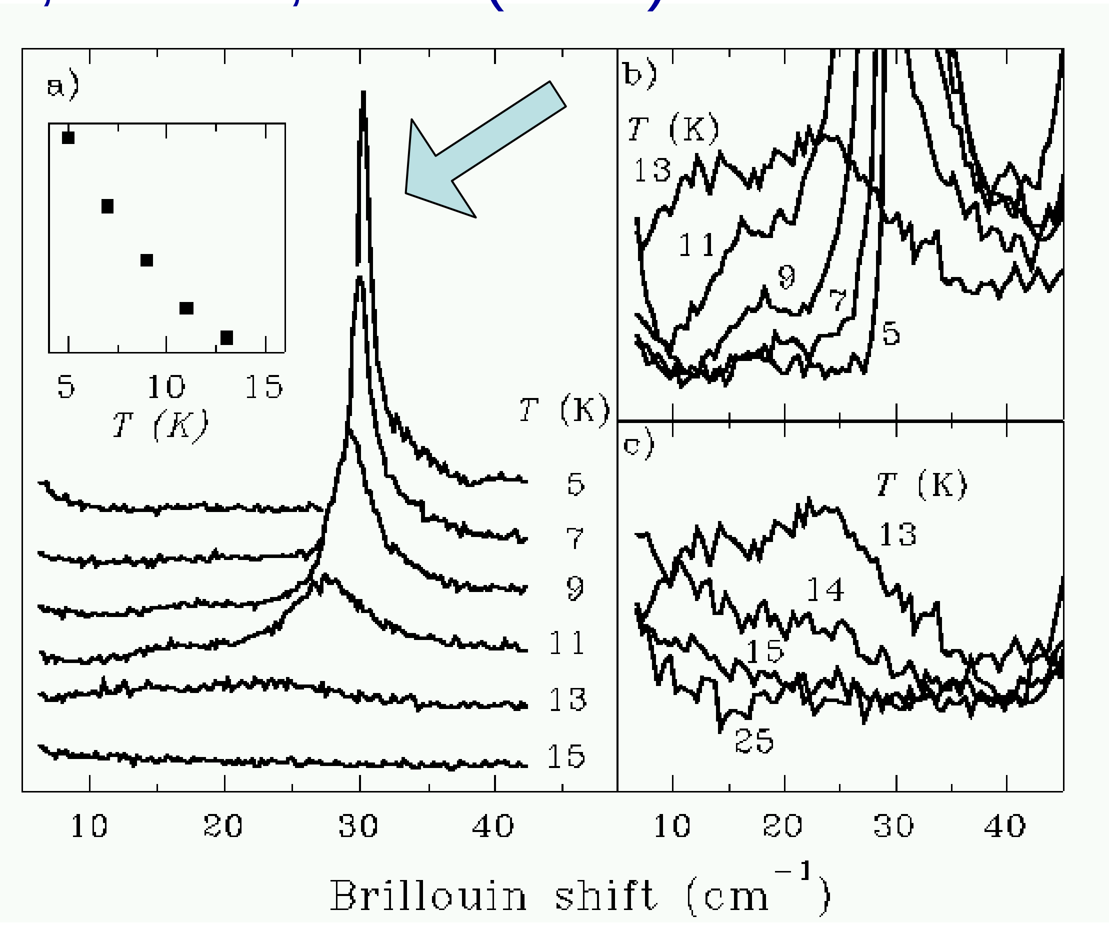
Dynamical spin structure factor

$$\text{All } k\text{'s and } \Delta S = 1$$

Raman scattering

Els et al., PRL **79**, 5138 (1997)

Probe $k = 0$
and $\Delta S = 0$

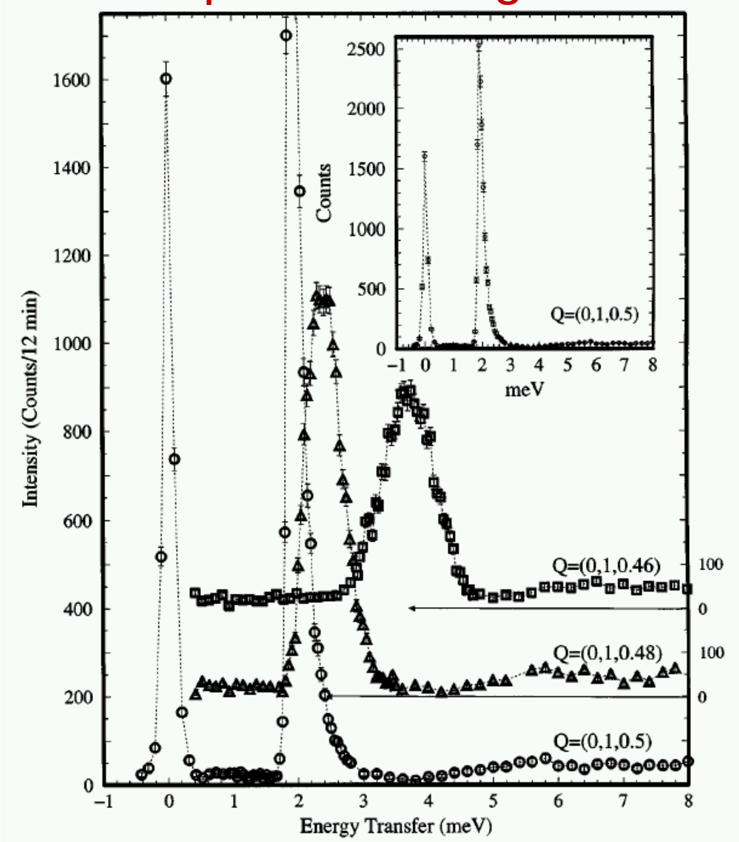


Well defined low energy singlet excitations !

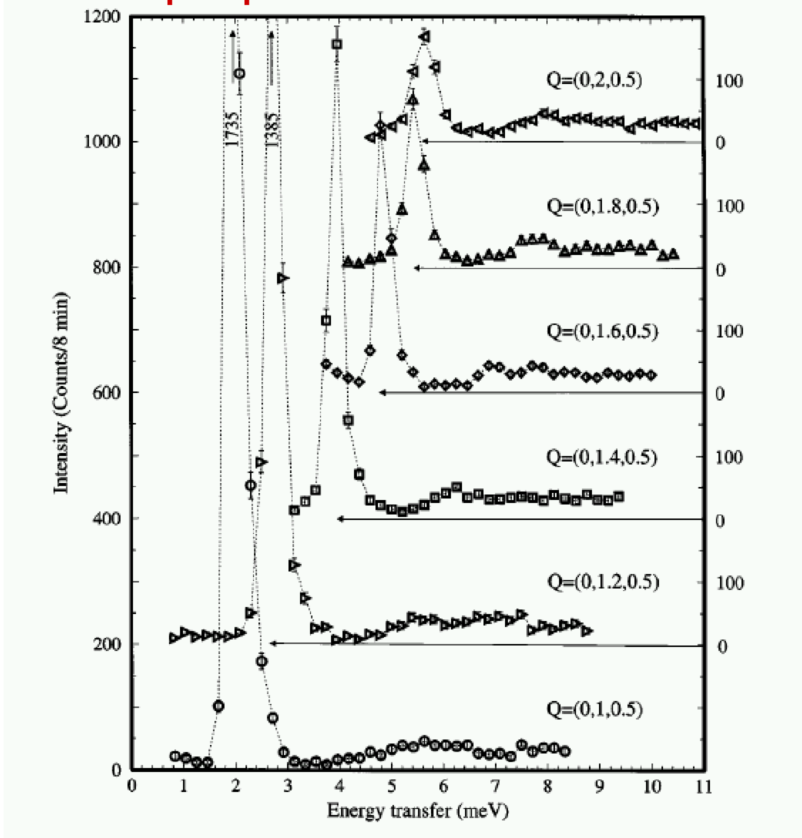
Neutron inelastic scattering

Aïn et al., PRL **78**, 1560 (1997)

Dispersion along chains



& perpendicular to chains



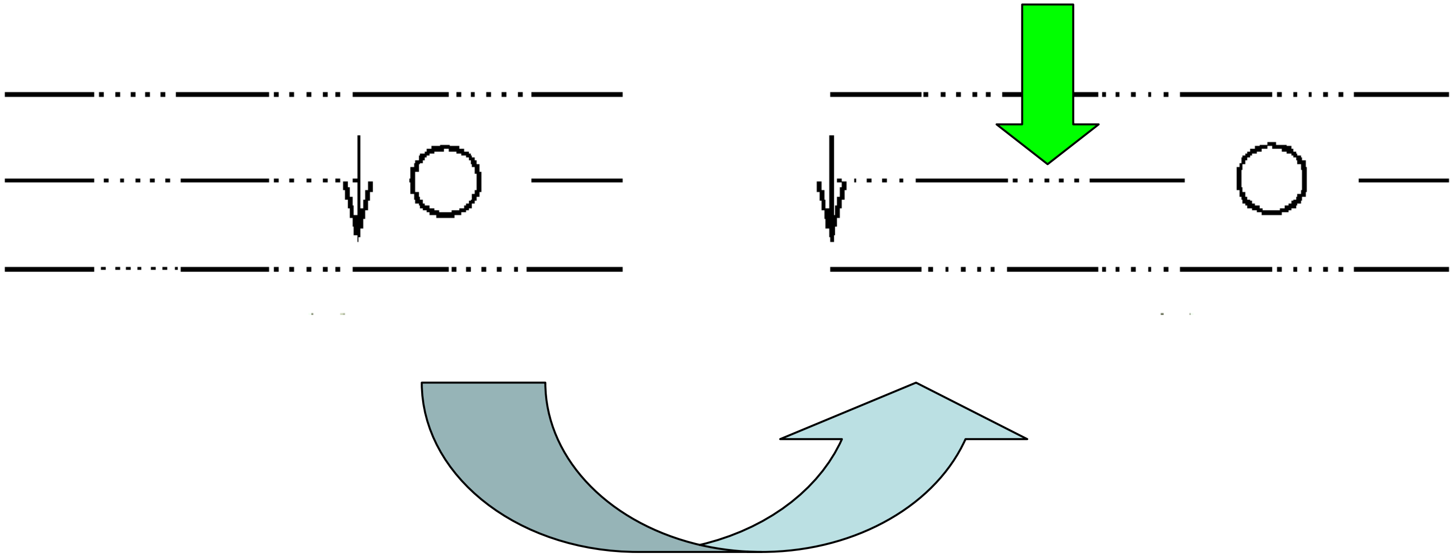
Sharp triplet excitation => soliton-antisoliton pair

Doping Spin-Peierls chains by static non-magnetic impurities

Doping with non-magnetic impurities

$Cu_{1-x}M_xGeO_3$: $Cu^{2+} \rightarrow M^{2+} = Zn^{2+}$ or Mg^{2+}

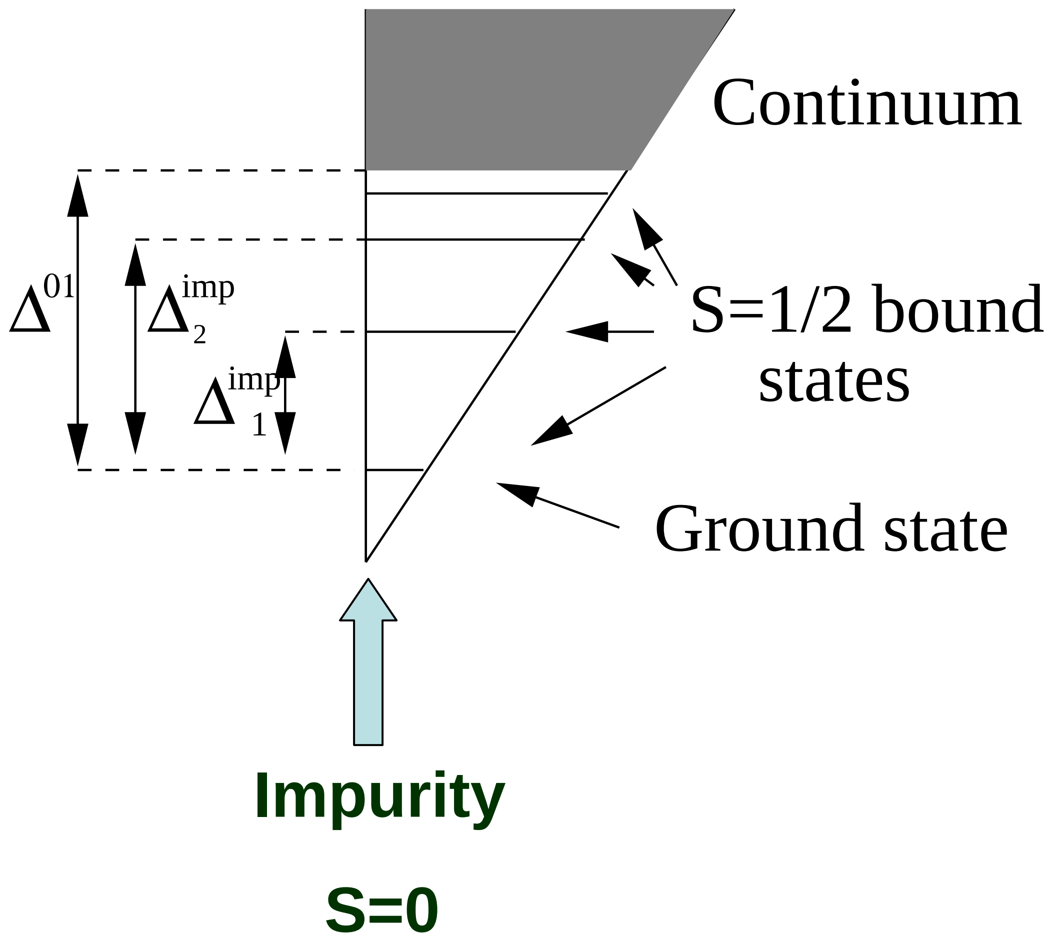
“string” length increases …



Spin down tries to delocalize to gain kinetic energy ….

Excitation spectrum next to impurity

- Spin-1/2 soliton liberated
- Equivalent to open chain: linear potential for x>0
- S=1/2 moment localized in some vicinity



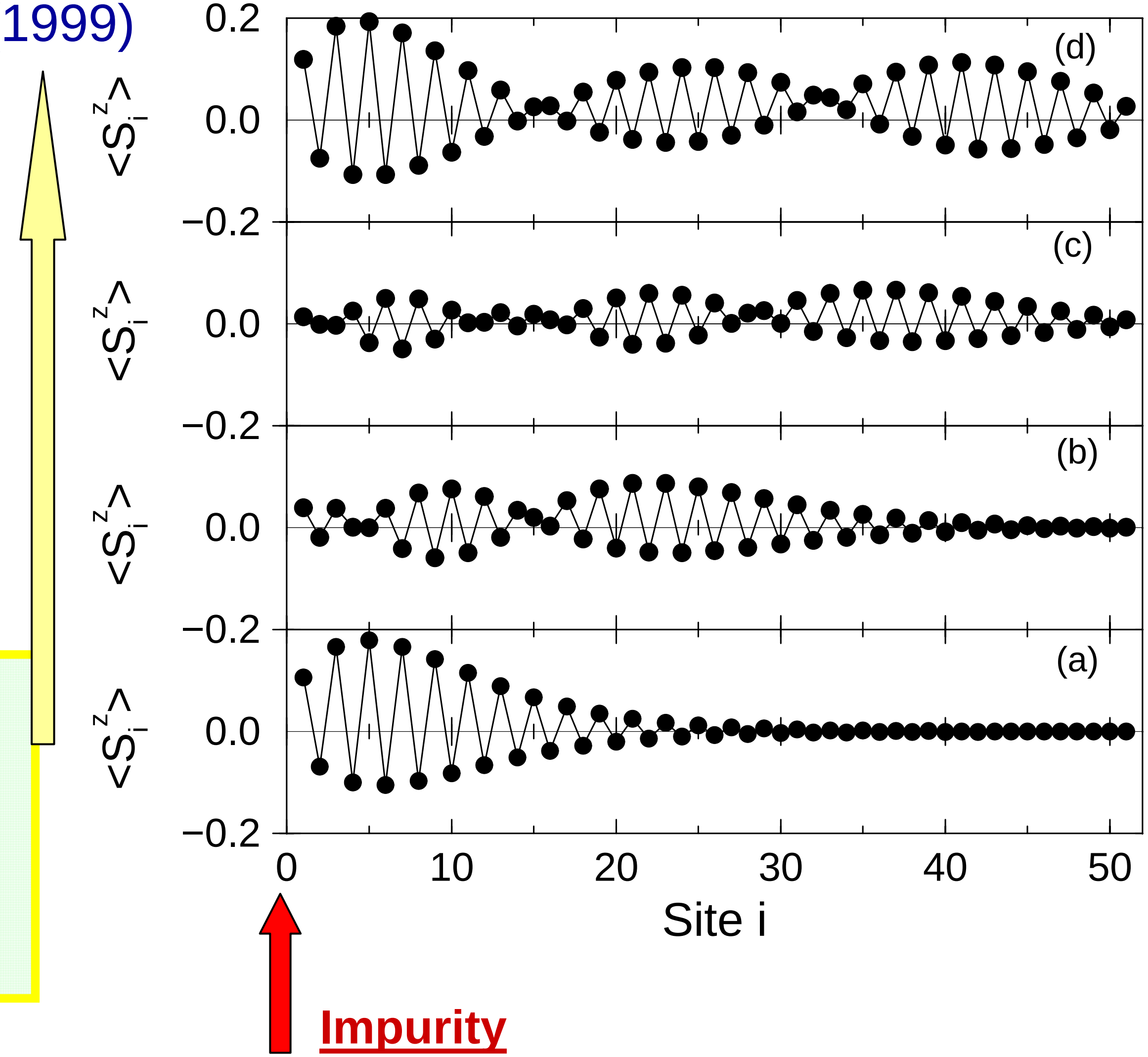
Edge state wavefunctions

DMRG computation

Augier et al., PRB **60**, 1075 (1999)

Increasing energy

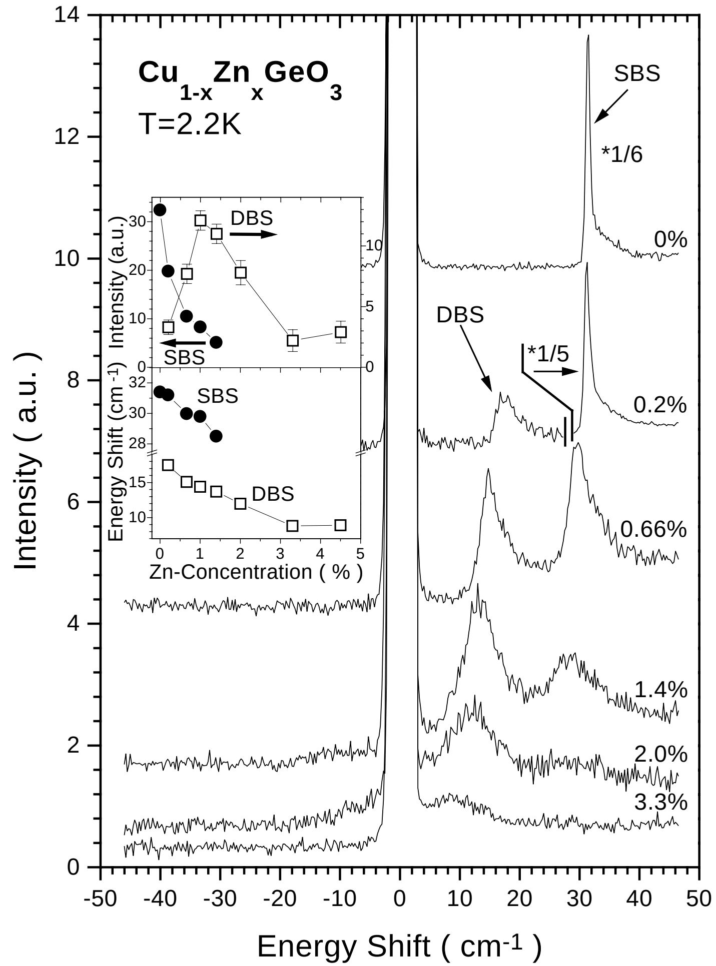
S=1/2 spinon states bound to the edge with increasing No of nodes.



Raman scattering – doped system

Els et al., EPL **43**, 463 (1998)

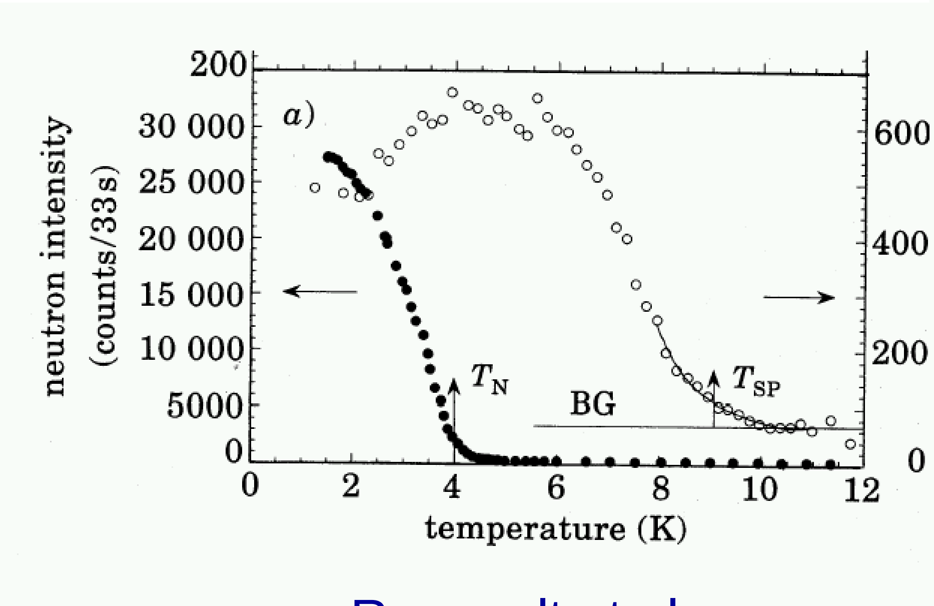
New low-energy excitation within the spin gap



Raman probes $\Delta S = 0$ transitions between **bound** spinons: $S = \frac{1}{2}\, |\Psi_0\rangle \Rightarrow S = \frac{1}{2}\, |\Psi_1\rangle$

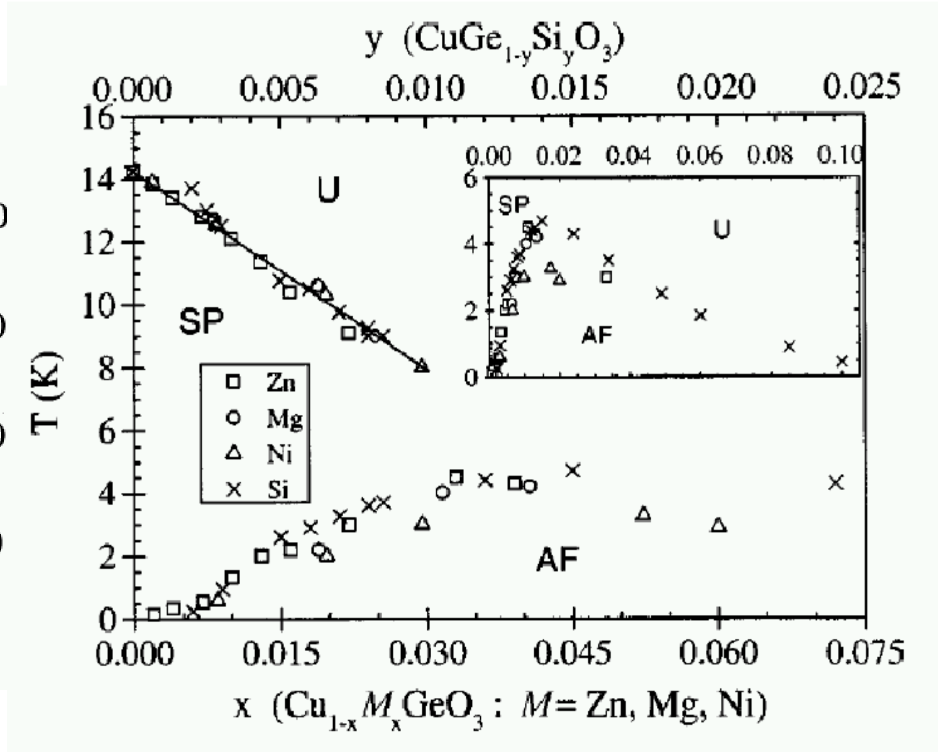
Coexistence between SP & AF

Neutron scattering



Regnault et al.,
Europhys. Lett **32**, 579 (1995)

(x,T) phase diagram



Grenier et al., PRB **58**, 8202 (1998)

Anisotropic spin-lattice model

Dobry et al., PRB **60**, 4065 (1999)

$$H_{\text{mag}} = J \sum_{i,a} \{ (1 + \delta_{i,a}) \mathbf{S}_{i,a} \cdot \mathbf{S}_{i+1,a} + J_{\perp} \mathbf{S}_{i,a} \cdot \mathbf{S}_{i,a+1} \}$$

Spontaneous dimerization: $\delta_{i,a} \propto (-1)^i$

Leads to effective coupling between impurities

Lattice rigidity

$$H_{\text{el}} = \sum_{i,a} \{ \tfrac{1}{2} K_{\|} \delta_{i,a}^2 + K_{\perp} \delta_{i,a} \delta_{i,a+1} \}$$

1) **Inforces in- or out-of-phase dimerization between chains**
2) **Leads to confinement of S=1/2 spinons next to impurities**

Effective magnetic interaction between induced spins ½

- Doping with non-magnetic impurities induces localized spins ½
- At low T => only localized spins degrees of freedom relevant (because of spin gap)
- **Effective model**:

$$J^{\text{eff}}(\mathbf{r}) \propto (-1)^{r_{\parallel}+r_{\perp}+1} \exp\left(-\frac{r_{\parallel}}{\xi_{\parallel}} - \frac{r_{\perp}}{\xi_{\perp}}\right)$$

F & AF couplings alternate
⇒ Not frustrated => SSE QMC
⇒ Staggered mag. scales like x

Extend to a few lattice spacings

Cf. Laflorencie's PhD, Toulouse, 2004

Summary / conclusions

- **Rich physical behaviors** in dimerized chains: spin gap, solitons, confinement of solitons, …
- Unique opportunity to confront **theory** & **experiments** (e.g. CuGeO3) in details
- **Doping** SP system provides a new PROBE of local physics + offers new phenomena (like co-existence etc…)