# On the Unifying Properties of the Spin-SAF and Other Peierls-type Phase Transitions

**Gennady Y. Chitov**

*Laurentian University*
*Sudbury, Canada*

## *Collaborators:*

***Claudius Gros, Frankfurt, Germany***
***Jesse Leeson, former LU student***

## *Supported by:*

NSERC
CRSNG

Laurentian University
Université Laurentienne

# Outline:

- *Motivation*
- *Spin-Pseudospin Model and Spin-SAF Transition*
- *XXX Chain – Interacting Fermions – sine-Gordon Model – “New” BCS Ratio*
- *BCS Ratio – experimental*
- *Conclusions*

## 1. Spin-Peierls Transition

3D Phonons + Heisenberg chains →
Frozen Lattice Distortions →
Dimerization → Spin Gap

Examples: various organic compounds,
non-organic: CuGeO3, TiPO4, TiOBr,TiOCl

## 2. Spin-SAF Transition

( SAF = Super-Anti-Ferro-electric [magnetic] )

2D Charge modes + Heisenberg chains →
SAF Charge Long Range Order →
Dimerization → Spin Gap

Examples: NaV2O5, Zn(pyz)V4O10

## 3. Peierls-like Transitions

Charge / Orbital degrees of freedom + Heisenberg chains →
Charge /Orbital Long Range Order → Spin Gap

Examples: transition metal oxides, spinels

# References:

[1] See, e.g., J.-P. Pouget, Eur. Phys. J. B **20**, 321 (2001); *Erratum: ibid*, **24**, 415 (2001).

[2] M.C. Cross and D.S. Fisher, Phys. Rev. B **19**, 402 (1979).

[3] K.I. Kugel and D.I. Khomskii, Usp. Fiz. Nauk **136**, 621 (1982); [Sov. Phys. Usp. **25**(4), 231 (1982)].

[4] A. M. Oles, Acta Phys. Polon. A **118**, 212 (2010).

[5] D.I. Khomskii and T. Mizokawa, Phys. Rev. Lett. **94**, 156402 (2005).

[6] M.V. Mostovoy and D.I. Khomskii, Solid St. Comm. **113**, 159 (1999); M.V. Mostovoy, D.I. Khomskii, and J. Knoester, Phys. Rev. B **65**, 064412 (2002).

[7] G.Y. Chitov and C. Gros, Phys. Rev. B **69**, 104423 (2004).

[8] G.Y. Chitov and C. Gros, J. Phys.: Condens. Matter **16**, L415 (2004).

[9] C. Gros and G.Y. Chitov, Europhys. Lett. **69**, 447 (2005).

[10] G.Y. Chitov and C. Gros, Low Temperature Physics **31**, 722 (2005) [Fizika Nizkikh Temperatur **31**, 952 (2005)].

[11] B. Yan, M.M. Olmstead, and P.A. Maggard, J. Am. Chem. Soc. **129**, 12646 (2007).

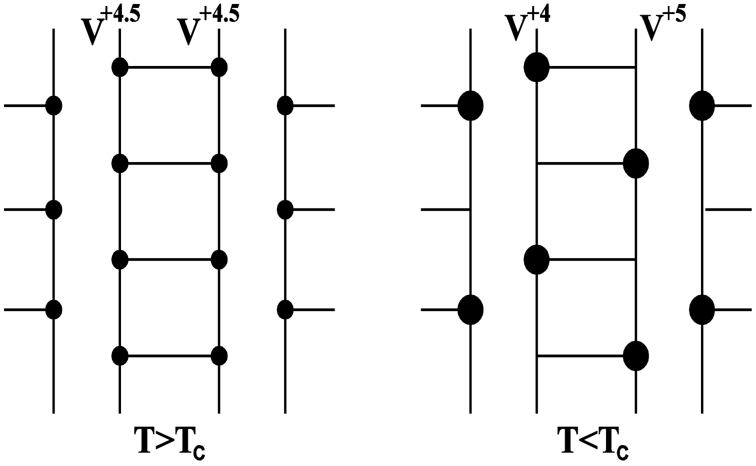
# Phase Transition in $NaV_2O_5$: Experiment

- 1/4-filled ladder compound:
  Smolinski, et al, 1998

- Spin Gap: $T_c \approx 34K, \ \Delta_{sg} \approx 106\,K$
  Isobe & Ueda, 1996

- 2D charge order:
  van Smaalen, et al, 2002
  Grenier, et al, 2002
  Chitov & Gros, 2004 (SAF)

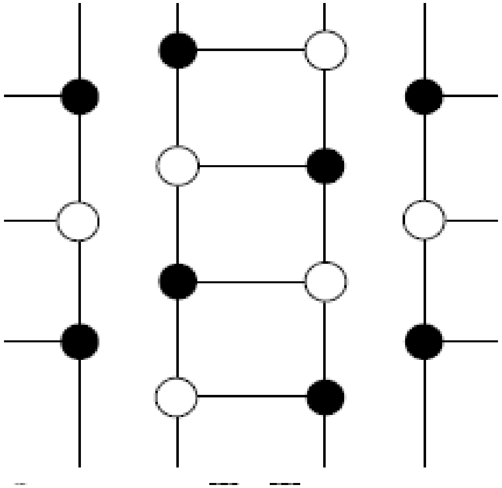
- Phase transition:
  Thermal, close to 2D Ising universality class
  Ravy, et al, 1999
  Gaulin, et al, 2000
  Fagot-Revurat, et al, 2000

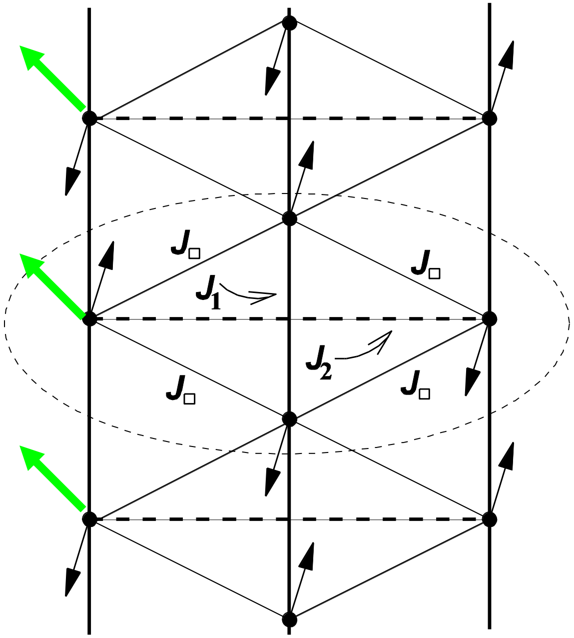


**Mechanism:**

spin-Peierls - like
Charge+Spin

# Mapping onto the Spin-Pseudospin Model

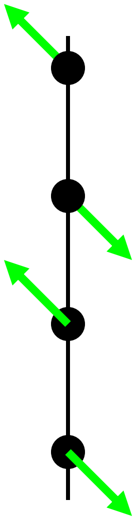




Left/Right (Charge) ⟺ Pseudospin (Ising) Up/Down

**Spin** ⟺ **Spin**

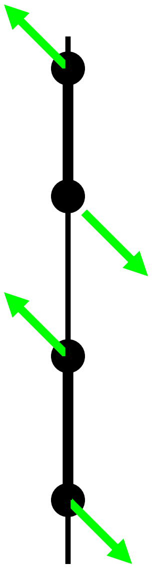
# Spin Sector: Heisenberg Chains



$$\mathcal{H} = J \sum_n \mathbf{S}_n \mathbf{S}_{n+1}$$

Heisenberg Chain:

- Gapless State (Luttinger Liquid Universality Class)
- No Magnetic LRO

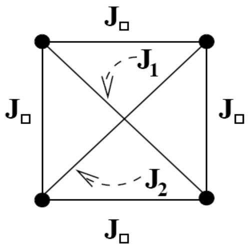


$$\mathcal{H} = J \sum_n [1 + (-)^n \delta] \mathbf{S}_n \mathbf{S}_{n+1}$$

Dimerized Heisenberg Chain:

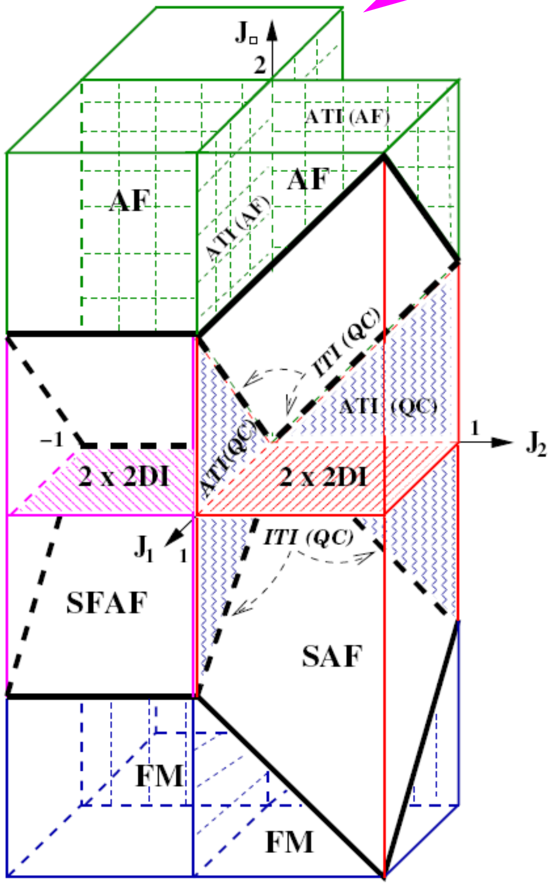
- Gapped GS
- No Magnetic LRO

# Charge Sector: 2D (nn+nnn) Ising Model

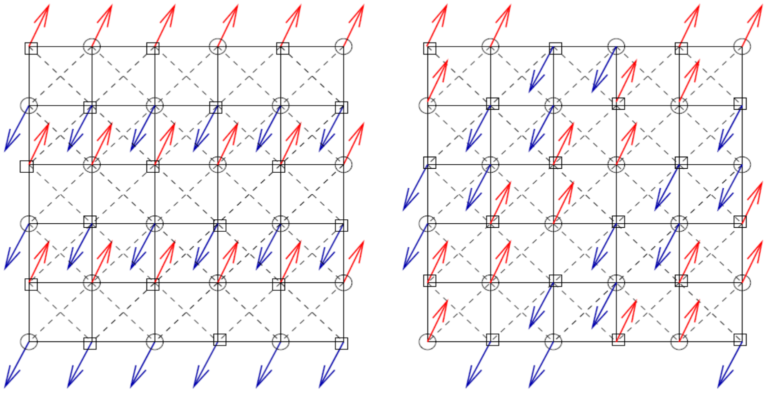


$$H = \frac{1}{2}\sum_{\langle \mathbf{i},\mathbf{j}\rangle} J_{\Box}\, \mathcal{T}^{x}_{\mathbf{i}} \mathcal{T}^{x}_{\mathbf{j}} + \frac{1}{2}\sum_{\langle\langle \mathbf{k},\mathbf{l}\rangle\rangle} J_{\mathbf{kl}}\, \mathcal{T}^{x}_{\mathbf{k}} \mathcal{T}^{x}_{\mathbf{l}}$$

Ground-State Phase Diagram



Frustrations!!



SAF

SFAF

Super-AntiFerromagnetic

4x4

# Spin-SAF (Coupled Ising-XXX) Model:

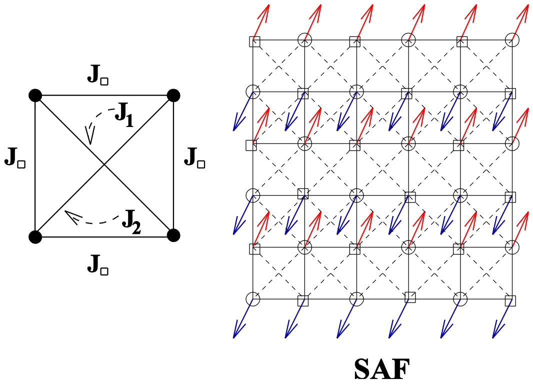
$$H_{\mathrm{IMTF}} = \frac{1}{2} \sum_{nn,nnn} J_{\sharp} T_{\mathrm{k}}^{x} T_{\mathrm{l}}^{z} - \Omega \sum_{\mathrm{k}} T_{\mathrm{k}}^{z}$$

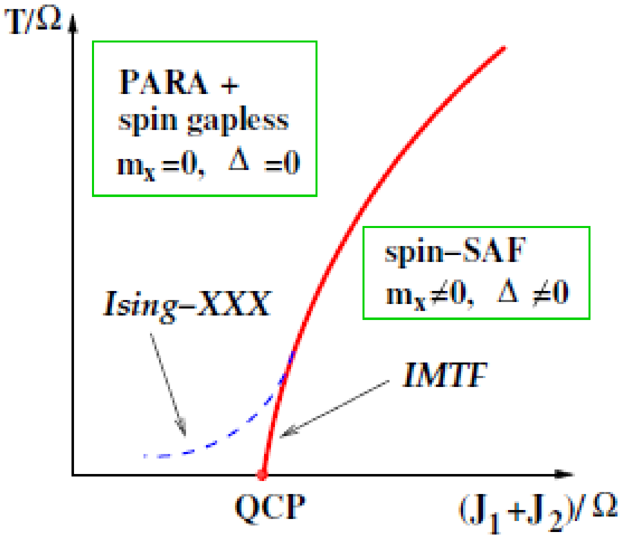
$$H_S = J \sum_{m,n} \mathbf{S}_{mn} \mathbf{S}_{m,n+1}$$

$$H_{ST} = \frac{1}{2} \varepsilon \sum_{m,n} \mathbf{S}_{mn} \mathbf{S}_{m,n+1} \left( T_{m+1,n+1}^{x} - T_{m-1,n}^{x} \right)$$

$$\boxed{H = H_{\mathrm{IMTF}} + H_S + H_{ST}}$$

$$\boxed{H_{\mathrm{XXX}} = \sum_{n} J(1 + (-1)^n \delta) \mathbf{S}_n \mathbf{S}_{n+1}}$$





Phase diagram of the coupled Ising-XXX model.

## 1. Spin-Peierls Transition

3D Phonons + Heisenberg chains →
Frozen Lattice Distortions →
Dimerization → Spin Gap

Examples: various organic compounds,
non-organic: $CuGeO_3$, $TiPO_4$, TiOBr, TiOCl

## 2. Spin-SAF Transition

( SAF = Super-Anti-Ferro-electric [magnetic] )

2D Charge modes + Heisenberg chains →
SAF Charge Long Range Order →
Dimerization → Spin Gap

Examples: $NaV_2O_5$, $Zn(pyz)V_4O_{10}$

## 3. Peierls-like Transitions

Charge / Orbital degrees of freedom + Heisenberg chains →
Charge /Orbital Long Range Order → Spin Gap

Examples: transition metal oxides, spinels

# All Peierls-type Phase Transitions:

**Hamiltonian: lattice, charge, etc coupled to spin chains**

**LRO**

**Spin Sector:**
**Dimerized XXX Chains**
**Spin Gap**

$$\mathcal{H}_{\mathrm{XXX}} = J\sum_{n}[1+(-)^{n}\delta]\mathbf{S}_{n}\mathbf{S}_{n+1}$$

**Appears simultaneously with LRO**

# BCS Ratio:

$$\boxed{\frac{\Delta^{\circ}_{\mathrm{SG}}}{T_c}} \qquad (k_B = 1)$$

**Unifying (?) Universal (?) Parameter**

# BCS Ratio: Conventional Superconductors

$$\frac{\Delta\,(0)}{k_B T_c} = 1{,}76.$$

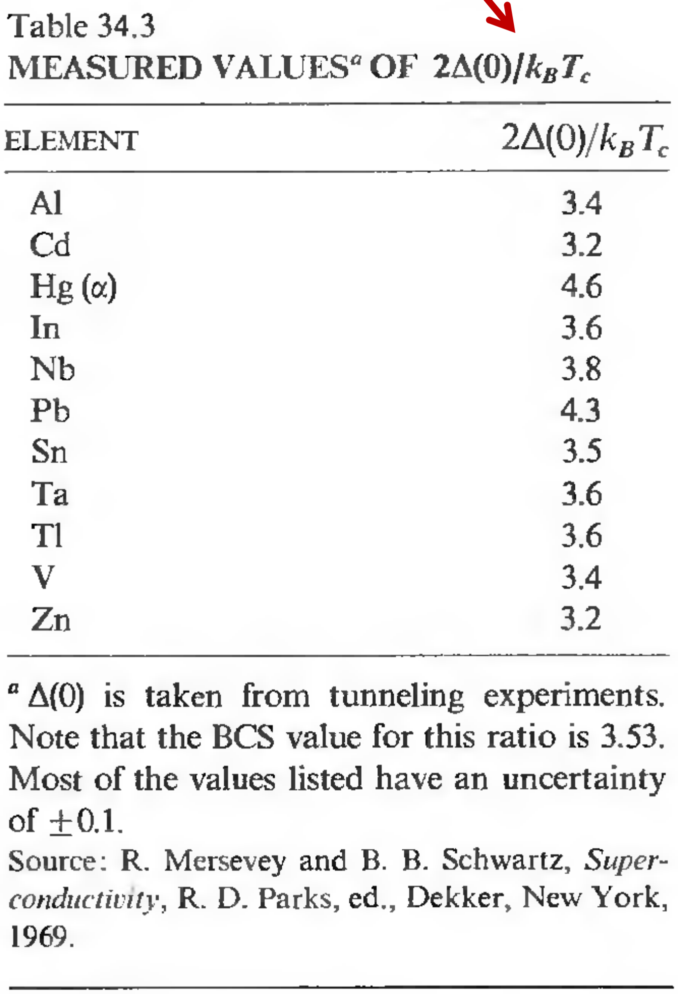


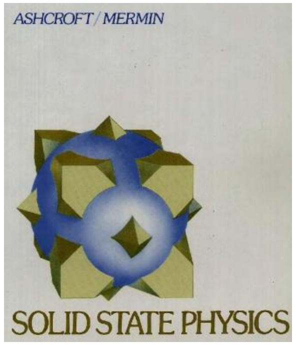
Table 34.3

MEASURED VALUES[a] OF $2\Delta(0)/k_B T_c$

| ELEMENT | $2\Delta(0)/k_B T_c$ |
|---|---|
| Al | 3.4 |
| Cd | 3.2 |
| Hg ($\alpha$) | 4.6 |
| In | 3.6 |
| Nb | 3.8 |
| Pb | 4.3 |
| Sn | 3.5 |
| Ta | 3.6 |
| Tl | 3.6 |
| V | 3.4 |
| Zn | 3.2 |

[a] $\Delta(0)$ is taken from tunneling experiments. Note that the BCS value for this ratio is 3.53. Most of the values listed have an uncertainty of ±0.1.

Source: R. Mersevey and B. B. Schwartz, *Superconductivity*, R. D. Parks, ed., Dekker, New York, 1969.



# Coupled Model: XXX (Heisenberg) Spin Sector

$$\mathcal{H} = \mathcal{H}_{\rm IMTF} + \sum_{m,n} \mathbf{S}_{mn}\mathbf{S}_{m,n+1}\left[J + \varepsilon\left(\mathcal{T}^x_{m+1,n+1} - \mathcal{T}^x_{m-1,n}\right)\right]$$

**Spin Sector** → **Dimerized XXX Chains**

$$\boxed{\mathcal{H}_{\rm XXX} = J\sum_n [1+(-)^n\delta]\mathbf{S}_n\mathbf{S}_{n+1}}$$

↕

**Interacting Spinless Fermions**

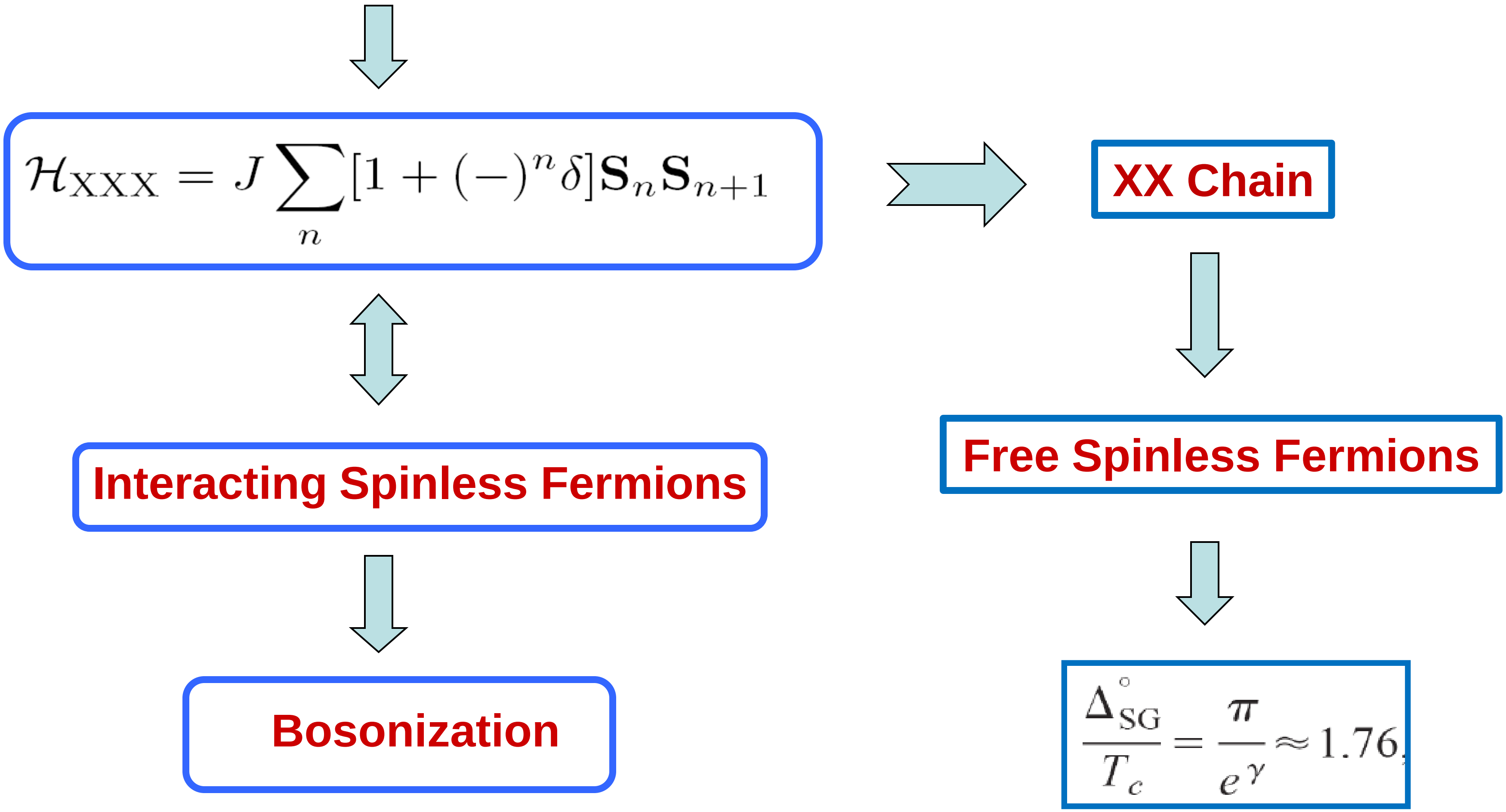
↓

**Bosonization**

# Coupled Model: Heisenberg Spin Sector

$$\mathcal{H} = \mathcal{H}_{\mathrm{IMTF}} + \sum_{m,n} \mathbf{S}_{mn}\mathbf{S}_{m,n+1}\left[J + \varepsilon\left(\mathcal{T}^{x}_{m+1,n+1} - \mathcal{T}^{x}_{m-1,n}\right)\right]$$

## Spin Sector: Dimerized XXX Chains



$$\mathcal{H}_{\mathrm{XXX}} = J\sum_{n}[1 + (-)^{n}\delta]\mathbf{S}_{n}\mathbf{S}_{n+1}$$

**Interacting Spinless Fermions**

**Bosonization**

**XX Chain**

**Free Spinless Fermions**

$$\frac{\Delta^{\circ}_{\mathrm{SG}}}{T_c} = \frac{\pi}{e^{\gamma}} \approx 1.76,$$

# Dimerized XXX Heisenberg Chain

$$\boxed{\mathcal{H}_{\mathrm{XXX}} = J \sum_n [1 + (-)^n \delta] \mathbf{S}_n \mathbf{S}_{n+1}}$$

$\Downarrow$

**Sine-Gordon**

(Orignac, 2004)

$$H = \boxed{\int \frac{dx}{2\pi} \left[ uK(\pi \Pi)^2 + \frac{u}{K} (\partial_x \phi)^2 \right] - \frac{2g_1}{(2\pi a)^2} \cos \sqrt{2}\phi}$$

$$\boxed{- \frac{2g_2}{(2\pi a)^2} \int dx \cos \sqrt{8}\phi.} \qquad (14)$$

$\Uparrow$

**Marginal Term**

$\Downarrow$

**Log-corrections**

# Dimerized XXX Heisenberg Chain

$$\mathcal{H}_{\rm XXX} = J\sum_n [1+(-)^n\delta]\mathbf{S}_n\mathbf{S}_{n+1}$$

**Sine-Gordon**

$$v^{-1}H_{\rm sG} = \frac{1}{2}\int dx\,(\Pi^2+(\partial_x\phi)^2) + 2\mu\int dx\,\cos\sqrt{2\pi}\phi\ ,$$

$v = \frac{\pi}{2}J$

$\mu = \frac{A_\epsilon}{\pi}\delta$

$A_\epsilon = \frac{3}{\pi^2}\left(\frac{\pi}{2}\right)^{\frac{1}{4}}$

**???**

**Orignac, 2004**

**Exact amplitude: Lukyanov, 2010-, unpublished**

# Dimerized XXX Heisenberg Chain = Sine-Gordon

*(G.Y.C., arXiv:1111.1201)*

$$f_s(T,\delta) = -Jt_\circ - \frac{1}{3}\frac{T^2}{J} - \frac{1}{2}\frac{J^2 a_\circ}{T}\delta^2$$

$$a_\circ \equiv \frac{1}{4}\left(\frac{\Gamma(1/4)}{\Gamma(3/4)}\right)^2 A_\epsilon^2 \equiv \vartheta_1 A_\epsilon^2$$

$$T_c = \vartheta_1 A_\epsilon^2 \frac{\varepsilon^2}{\mathcal{J}_c - \mathcal{J}}$$

$$f_s(0,\Delta_\circ) = -Jt_\circ - \frac{1}{2\pi\sqrt{3}}\frac{\Delta_\circ^2}{J}$$

*Al. Zamolodchikov, 1995*

$$\Delta_\circ = J\sqrt{\pi}\left(\frac{\Gamma(3/4)}{\Gamma(1/4)}\right)^{2/3}\frac{\Gamma(1/6)}{\Gamma(2/3)}A_\epsilon^{2/3}\delta^{2/3}$$

$$\Delta_\circ = \vartheta_2 A_\epsilon^2 \frac{\varepsilon^2}{\mathcal{J}_c - \mathcal{J}} \ , \quad T = 0$$

**BCS Ratio:**

$$\frac{\Delta_\circ}{T_c} = \frac{\vartheta_2}{\vartheta_1} = 6\sqrt{3}\frac{\left(\Gamma(1/3)\right)^9}{\left(\Gamma(1/4)\right)^8} = 2.47\ldots$$

*Orignac & Chitra, 2004*

# BCS Ratios:

| | Type | Tc (K) | $\Delta / k_B (K)$ | BCS ratio | Ref. |
|---|---|---|---|---|---|
| **MEM(TCNQ)2 and more organics** | **SP** | **18** | **30** | **1.67** | **Pouget, 01** |
| **CuGeO3** | **SP** | **14.3** | **24-30** | **1.7-2.0** | **Lemmens, et al, 03** |
| **(TMTTF)2AsF6** | **SP** | **13** | **35** | **2.69** | **Dressel, et al, 11** |
| **(TMTTF)2PF6** | **SP** | **19** | **47** | **2.47** | **Dressel, et al, 11** |
| **NaV2O5** | **Spin-SAF** | **34** | **106** | **3.1** | **Lemmens, et al, 03** |
| **Zn(pyz)V4O10** | **Spin-SAF** | **22** | **?** | **?** | **Yan, et al, 07** |
| **TiOCl** | **SP** | **92** | **430-440** | **4.7-4.8** | **Clancy, et al, 11** |
| **TiOBr** | **SP** | **48** | **250** | **5.2** | **Clancy, et al, 11** |

$\Delta / T_c \approx 1.76$

$\Delta / T_c \approx 2.47$

**???**

# Summary & Discussion

1. Theory of spin-SAF transition is reviewed.
   Spin-SAF phase = simultaneous Super-Anti-Ferroelectric (SAF)
   charge order + spin gap.

2. New interacting BCS ratio is calculated.
   Similarities between spin-SAF, spin-Peierls and Peierls-like transitions
   are emphasized.

3. Further progress:
   (i) BCS-ratio – accounting for the marginal terms
   (ii) Ising (pseudospin / charge) sector beyond mean-field (??)
   Fate of QCP?
   (iii) nn+nnn Ising model (some work in progress, more warranted)

# THE END

# THANK YOU!