Ordering, Dimerization & Criticality in Some Quantum Spin Systems

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What All This is About:

Low Dimension

Strong Fluctuations

Strong Quantum Fluctuations

e.g., Long Range Order (LRO)

Conventional Classical Effects

Quantum Effects

QCP
Gap (Mass) Generation
No LRO (Order Parameter), No SSB
Hidden/Exotic/Non-Local Order Parameters (??)
No Ginzburg-Landau
Example: FQHE
Topological Order
Counter-Intuitive Example:

Two $\frac{1}{2}$-spins coupled antiferromagnetically ($J$)

Naïve (classical) GS expectation: $E = -\frac{1}{4}J$

QM result for GS: singlet $E = -\frac{3}{4}J$
Outline:

**Part 1: Spin-SAF Transition**
- Motivation-1
- Spin-Pseudospin Model and Approximation
- Phase Diagram
- Dimerized XXX Chain
- BCS Ratio
- More Applications of Spin-SAF Theory to NaV$_2$O$_5$

**Part 2: Gaps & Quantum Criticality in Dimerized Spin Ladders**
- Motivation-2 (Two & Three-Leg Ladders)
- Gaplessness out of Gapped Building Blocks
- Staggering Patterns & Quantum Criticality: Results

Summary & Discussion
Part I: Spin-SAF Transition
Phase Transition in NaV$_2$O$_5$: Experiment

- **1/4-filled ladder compound:**

- **Spin Gap:** $T_c \approx 34K$, $\Delta_{sg} \approx 106K$
  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 - NO
- Charge+Spin - ??
Mapping onto the Spin-Pseudospin Model

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

Spin ↔ Spin
Spin Sector: Heisenberg Chains

Heisenberg Chain:
Gapless State (Luttinger Liquid Universality Class)
No Magnetic LRO

\[ \mathcal{H} = J \sum_n S_n S_{n+1} \]

Dimerized Heisenberg Chain:
Gapped GS
No Magnetic LRO

\[ \mathcal{H} = J \sum_n [1 + (-)^n \delta] S_n S_{n+1} \]
Charge Sector: 2D (nn+nnn) Ising Model

Frustrations!!

\[ H = \frac{1}{2} \sum_{\langle i,j \rangle} J_{i,j} T_i^x T_j^x + \frac{1}{2} \sum_{\langle\langle k,l \rangle\rangle} J_{k,l} T_k^x T_l^x \]

Ground-State Phase Diagram
Charge Sector (Getting Worse):
2D (nn+nnn) Ising Model + Transverse Field

- Transverse (Quantum) Ising Model:

\[ H = \frac{1}{2} \sum_{nn,nnn} J_{kl} T_k^x T_l^x - \Omega \sum_i T_i^z \]

- Special Case: \( J_\square^2 < 4 J_1 J_2 \), \( (J_1, J_2) > 0 \)

2 Phases (PM/SAF) with a Quantum Critical Point (QCP)
Coupled Spin-Pseudospin Model and Approximation

\[ \mathcal{H}_{\text{IMTF}} = -\Omega \sum_k \mathcal{T}_k^z + \frac{1}{2} \sum_{nn, nnn} J_{k,1} \mathcal{T}_k^x \mathcal{T}_1^x \]

\[ \mathcal{H} = \mathcal{H}_{\text{IMTF}} + \sum_{m,n} S_{mn} S_{m,n+1} \left[ J + \lambda \mathcal{T}_{mn} \mathcal{T}_{m,n+1} + \varepsilon \left( \mathcal{T}_{m+1,n+1}^x - \mathcal{T}_{m-1,n}^x \right) \right]. \]

Approximation:

*Ising Sector* -- Mean-Field

*Spin Sector (XX, XXX)* -- Exactly

Creates Dimerization in the SAF phase

Transverse (Quantum) Ising Model Hamiltonian

Coupled Model
Spin-Pseudospin (Coupled) Model: Phase Diagram

- Coupled Model always orders via spin-SAF transition
- QCP is destroyed
- Ordered (spin-SAF) Phase:
  - SAF charge/Ising LRO +
  - Spin Gap/Dimerization
Coupled (XY) Model: Phase Diagram (detailed)

- $\mathcal{H} = -\sum_{m,n} T_{mn}^z + \frac{1}{2} \sum_{m,n} g_{\pi} T_{mn}^x T_{m,n+1}^x + \sum_{m,n} S_{mn} S_{m,n+1} [J + \lambda T_{mn}^z T_{m,n+1}^z + \varepsilon (T_{m+1,n+1}^x - T_{m-1,n}^x)]$

Spin Sector = Free Spinless Fermions

$T_c \approx \begin{cases} \frac{g}{4}, & g \gg g_\lambda \\ \frac{\hbar j}{2} \exp \left[ -\frac{\pi j}{4\varepsilon^2} (g_\lambda - g) \right], & \text{BCS regime} \end{cases}$

BCS ratio

$\frac{\Delta_{SG}^\circ}{T_c} = \frac{\pi}{e^\gamma} \approx 1.76$, BCS regime
Coupled Model: XXX (Heisenberg) Spin Sector

\[ \mathcal{H} = \mathcal{H}_{\text{IMTF}} + \sum_{m,n} S_{mn} S_{m,n+1} \left[ J + \varepsilon \left( T_{m+1,n+1}^x - T_{m-1,n}^x \right) \right] \]

Spin Sector \hspace{1cm} \rightarrow \hspace{1cm} \text{Dimerized XXX Chains}

\[ \mathcal{H}_{\text{XXX}} = J \sum_n \left[ 1 + (-1)^n \delta \right] S_n S_{n+1} \]

Interacting Spinless Fermions \hspace{1cm} \rightarrow \hspace{1cm} \text{Bosonization}
Dimerized XXX Heisenberg Chain

\[ \mathcal{H}_{XXX} = J \sum_n [1 + (-)^n \delta] S_n S_{n+1} \]

\[ H = \int \frac{dx}{2\pi} \left[ uK(\pi \Pi)^2 + \frac{u}{K}(\partial_x \phi)^2 \right] - \frac{2g_1}{(2\pi a)^2} \cos \sqrt{2}\phi 
- \frac{2g_2}{(2\pi a)^2} \int dx \cos \sqrt{8}\phi. \]  

(Orignac, 2004)

Sine-Gordon

Marginal Term

Log-corrections

\[ g_1 = 6J \left( \frac{\pi}{2} \right)^{1/4} \delta a. \]
Dimerized XXX Heisenberg Chain (Continued)

\[ f_s \approx -J t_0 - \alpha J \frac{\delta^{4/3}}{\ln \frac{\delta_0}{\delta}}, \quad T = 0 \]

\[ \Delta_{SG} = \sqrt{\alpha S J} \frac{\delta^{2/3}}{\ln^{1/2} \frac{\delta_S}{\delta}}, \quad T = 0 \]

\[ \eta_n \propto \frac{\partial f_s}{\partial \delta} \]

\[ \eta_n \approx \frac{4\alpha}{3} \frac{1}{\delta^{2/3} \ln \frac{\delta_0}{\delta}}, \quad T = 0 \]

\[ \eta_n \approx \frac{a_0 J}{T} \frac{1}{\ln^{3/2} \frac{C J}{T}}, \quad \delta = 0 \]

Dimerization Susceptibility

\[ \eta_n \approx \frac{a_0 J}{T} \frac{1}{\ln^{3/2} \left( \frac{C J}{T} \right)}, \quad \delta = 0 \]

Klumper et al, 2000, DMRG

Cros & Fisher, 1979
No log

\textit{NB: NaV2O5: Tc/J = 0.06}
\[ \Delta_{SG} = \sqrt{\alpha S J} \frac{\delta^{2/3}}{\ln^{1/2} \frac{\delta_S}{\delta}}, \quad T = 0 \]

Papenbrock et al, 2003, DMRG
Spin Gap vs $T_c$ : BCS Ratio

XY Dimerized Chain (Free Fermions):

$$\frac{\Delta_{SG}^\circ}{T_c} = \frac{\pi}{\text{e}^\gamma} \approx 1.76, \text{ spin-Peierls, spin-SAF}$$

XXX Dimerized Chain: Neglected Marginal (log) Terms
Orignac & Chitra, 2004, spin-Peierls Theory

$$\frac{\Delta(T = 0)}{T_{SP}} \approx 2.47 \text{ spin-Peierls, spin-SAF}$$

XXX Dimerized Chain: Marginal (log) Terms Included

$$\frac{\Delta_{SG}^\circ}{T_c} \approx 2.44 \text{ spin-SAF spin-Peierls (?)}$$

BCS Ratio -- Experiments:

spin-Peierls: (Organics, $CuGeO_3$) $\sim 2 - 4$ (Pouget, 2001)
spin-SAF: (Na$V_2$O$_5$) $\sim 3.1$
Spin-SAF Theory: Further Application to NaV$_2$O$_5$

- Parameters:

\[ g_\lambda = 4t_a, \quad t_a = 0.35 \text{ eV}, \quad \varepsilon \approx 0.4J_1 = 19.3 \text{ meV} \quad \text{(Gros & Chitov, 2005)} \]
\[ T_c = 34 \text{ K} = 2.93 \text{ meV} \]

\[ g_\lambda - g \approx 0.132 \text{ eV}, \quad \text{or} \quad g/g_\lambda \approx 0.91 \]

- Pseudospin (charge) excitations (theory):

\[ E_0/q_{SAF} = 2t_a \sqrt{1 \pm g/g_\lambda} \]

\[ E_0 \approx 0.97 \text{ eV} \approx 7800 \text{ cm}^{-1} \]

\[ E_{q_{SAF}} \approx 0.21 \text{ eV} \approx 1700 \text{ cm}^{-1} \]

\[ 2E_{q_{SAF}} \approx 3400 \text{ cm}^{-1} \quad \text{broad peak near 4000 cm}^{-1} \]
\[ \quad \text{2-particle (pseudospin) excitations with} \quad q_{SAF} \]

Stacking Charge Order in NaV$_2$O$_5$

- Charge order in NaV$_2$O$_5$ (X-ray): from Grenier, et al

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- Ground states in the nn and nnn axial Ising model

- Devil’s staircase in NaV$_2$O$_5$: from Ohwata, et al PRL’01
Part 2: Gaps & Quantum Criticality in Dimerized Spin Ladders
n-Leg Spin-1/2 Ladders (No Dimerization)

See, e.g., T. Giamarchi, *Quantum Physics in One Dimension*, 2004

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FIG. 6.17. (a) In an even leg antiferromagnetic ladder, the spins on a rung are locked into a singlet state. The ground state is essentially a collection of singlets. (b) For an odd leg antiferromagnetic ladder, one of the spins on the rung remains free. The system is thus essentially equivalent to a spin 1/2 system.
Two- & Three-Leg Ladders: Experiments

Figure 6. Schematic representation of (a) the Cu$_2$O$_3$ sheets of SrCu$_2$O$_3$ (from Azuma et al. 1994). The three-leg ladder Sr$_2$Cu$_3$O$_5$ is also shown in (b). The filled circles are Cu$^{2+}$ ions, and O$^{2-}$ ions are located at the corners of the squares drawn with solid lines.

Figure 7. The temperature dependence of the magnetic susceptibility of SrCu$_2$O$_3$ (from Azuma et al. 1994). Details can be found in the text.

Figure 8. As figure 7 but for the three-leg compound Sr$_2$Cu$_3$O$_5$ (from Azuma et al. 1994). In this case a large susceptibility is observed even at low temperatures, indicative of the absence of a spin gap, in agreement with theoretical expectations.
Dimerized 2-leg Ladders:

\[ H_{2L} = \sum_{\alpha=1,2} \sum_{n=1}^{N} J_\alpha(n) S_\alpha(n) \cdot S_\alpha(n+1) + J_\perp \sum_{n=1}^{N} S_1(n) \cdot S_2(n). \]

\[ J_\alpha(n) = J[1 + (-1)^{n+\alpha}\delta]. \]

Conjecture:
Martin-Delgado, Shankar, Sierra, PRL 1996

- Line of Quantum Criticality = No Gap (Mass)
- QCP & No (Apparent) Symmetry Change or SSB
- Non-Local String Order Parameter (?)
- Topological Order Parameter (?)

NB: 3-Leg Ladders, Similar Properties, omitted for brevity
Dimerization Patterns: (Chitov, et al, PRB 08)

FIG. 1: Dimerized two-leg ladder. Bold/thin/dashed lines represent the stronger/weaker chain coupling $J(1 \pm \delta)$ and rung coupling $J_\perp$, respectively. Dimerization patterns: (a) - staggered; (b) - columnar.

FIG. 2: Completely dimerized ladder, $\delta = 1$. (a): Alternated staggering reduces the model (1) to a snake-like dimerized Heisenberg chain of $2N$ spins; (b): Columnar order degenerates into a set of $N/2$ decoupled plaquettes.

Hints: 3-leg Spin-Peierls Ladder, Azzouz, Shahin, Chitov, PRB 07
Results:

Methods: Jordan-Wigner Transformation (Bond) Mean-Field Theory; Azzouz, PRB 93

Conclusions:
• Stable State is always Gapped
• Special Mechanism Needed to bring the ladder into QC staggered phase
Summary & Conclusions

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

2. Novelty: Destruction of the QCP

3. Quantitative Applicability of the Spin-Saf theory for NaV2O5
   Numerical parameters of the effective Hamiltonian
   Peaks in the optical conductivity, absence of the soft mode

4. BCS ratio is calculated.
   Similarities between spin-SAF and spin-Peierls are emphasized.

5. Quantum Criticality in Dimerized 2- and 3-leg ladders is Analyzed
   (a) Stable State is always Gapped
   (b) Special Mechanism Needed to bring ladder into QC staggered phase
References: