Renormalization group study of a quarter filled ladder

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Quarter filled ladder:

Model for the Charge ordering transition T=35 K in NaV_2O_5 (Mostovoy & Khomskii 2000).

Charge ordering transition in $(TMTTF)_2X$

Many coupled chains at quarter filling

Oversimplified model of stripe formation

Hamiltonian

$$H = -t \sum_{i,p,\sigma} (c^\dagger_{i+1,p,\sigma} c_{i,p,\sigma} + c^\dagger_{i,p,\sigma} c_{i+1,p,\sigma}) - t_\perp \sum_{i,\sigma} (c^\dagger_{i,2,\sigma} c_{i,1,\sigma} + \mathrm{H.c.})$$
$$+U \sum_{i,p} n_{i,p,\uparrow} n_{i,p,\downarrow} + V_{\|} \sum_{i,p} n_{i,p} n_{i+1,p} + V_\perp \sum_i n_{i,1} n_{i,2}$$

Strong repulsion, $U, V_{\|} \sim t \gg t_\perp$ $t_\perp$ irrelevant

But an exchange interaction $J \sim t_\perp^2/U$ is generated.

$$H_{\mathrm{exch.}} = J_\perp \sum_i \vec{S}_{i,1} \cdot \vec{S}_{i,2}$$

Phase Hamiltonian (I)

Charge sector:

$$H_+ = \int \frac{dx}{2\pi}\left[u_{\rho+}K_{\rho+}(\pi\Pi_{\rho+})^2 + \frac{u_{\rho+}}{K_{\rho+}}(\partial_x\phi_{\rho+})^2\right] + \frac{2V_\perp}{(2\pi a)^2}\int dx \cos 4\phi_{\rho+}$$

$[\phi_{\rho+}(x), \Pi_{\rho+}(x')] = i\delta(x-x')$: sine Gordon Hamiltonian

$\Rightarrow$ Insulating state when $K_{\rho+} < 1/2$.

Non-interacting: $K_\rho = 1$, Repulsion $K_\rho < 1$

Note: Intrachain Umklapp relevant for $K_\rho < 1/4$

For $U \neq 0, V_{||} = 0$, $K_\rho \geq 1/2$,

$\Rightarrow V_{||}$ is necessary to obtain the insulator.

Phase Hamiltonian (II)
spin-charge separation
Spin excitations and "orbital" modes

$$
\begin{aligned}
H &= \int \frac{dx}{2\pi} \sum_{\nu \in \{\rho-,\sigma+,\sigma-\}} \left[u_\nu K_\nu (\pi \Pi_\nu)^2 + \frac{u_\nu}{K_\nu} (\partial_x \phi_\nu)^2 \right] \\
&+ \frac{2g_1}{(2\pi a)^2} \int dx \cos 2\phi_{\sigma+} \cos 2\phi_{\sigma-} + \frac{2g_2}{(2\pi a)^2} \int dx \cos 2\phi_{\sigma+} \cos 2\theta_{\sigma-} \\
&+ \frac{2g_3}{(2\pi a)^2} \int dx \cos 4\phi_{\rho-} + \frac{2g_4}{(2\pi a)^2} \int dx \cos 2\phi_{\rho-} \cos 2\phi_{\sigma+} \\
&+ \frac{2g_5}{(2\pi a)^2} \int dx \cos 2\phi_{\rho-} \cos 2\phi_{\sigma-} + \frac{2g_6}{(2\pi a)^2} \int dx \cos 2\phi_{\rho-} \cos 2\theta_{\sigma-},
\end{aligned}
$$

$$\theta_\nu(x) = \int dx' \pi \Pi_\nu(x') \Rightarrow [\theta_{\sigma-}(x), \phi_{\sigma-}(x')] \neq 0$$

$\theta_{\sigma-}$ and $\phi_{\sigma-}$ cannot order simultaneously.

Phase Hamiltonian (III)

$$
\begin{aligned}
K_{\sigma+} &= \left(1 + \frac{J_\perp a}{2\pi v_F}\right)^{-1/2}, \\
K_{\sigma-} &= \left(1 - \frac{J_\perp a}{2\pi v_F}\right)^{-1/2}, \\
g_1 &= 0 \; g_2 = J_\perp a, \\
g_3 &= 2C^2 V_\perp a, \\
g_4 &= (2V_\perp - \frac{J_\perp}{2})a, \\
g_5 &= (2V_\perp + \frac{J_\perp}{2})a, \\
g_6 &= J_\perp a
\end{aligned}
$$

Order Parameters (I)

$$O_{CDW(\pi,q_y)}(n) = (-)^n (n_{n,1} + \cos(q_y) n_{n,2})$$

$$O_{BOW(\pi,q_y)}(n) = (-)^n \sum_\sigma (c^\dagger_{n+1,1,\sigma} c^\dagger_{n+1,1,\sigma} + \cos(q_y) c^\dagger_{n+1,2,\sigma} c^\dagger_{n+1,2,\sigma})$$

$$O_{CDW(\frac{\pi}{2},q_y)}(n) = e^{-i\frac{\pi}{2}n} (e^{iq_y/2} n_{n,1} + e^{-iq_y/2} n_{n,2})$$

CDW = Charge Density Wave (on the sites)

BOW = Bond Order Wave (on the links, *à la Peierls*)

In terms of phase variables:

Order Parameters (II)

$$
\begin{aligned}
O_{CDW(\pi,0)} &\sim \frac{1}{2\pi\alpha}\cos 2\phi_{\rho+}\cos 2\phi_{\rho-} \\
O_{CDW(\pi,\pi)} &\sim \frac{1}{2\pi\alpha}\sin 2\phi_{\rho+}\sin 2\phi_{\rho-} \\
O_{BOW(\pi,0)} &\sim \frac{1}{2\pi\alpha}\sin 2\phi_{\rho+}\cos 2\phi_{\rho-} \\
O_{BOW(\pi,\pi)} &\sim \frac{1}{2\pi\alpha}\cos 2\phi_{\rho+}\sin 2\phi_{\rho-} \\
O_{CDW(\frac{\pi}{2},0)} &\sim \frac{1}{2\pi\alpha}e^{i\phi_{\rho+}}\cos\phi_{\rho-} \\
O_{CDW(\frac{\pi}{2},\frac{\pi}{2})} &\sim \frac{1}{2\pi\alpha}e^{i\phi_{\rho+}}\cos(\phi_{\rho-}-\frac{\pi}{4}) \\
O_{CDW(\frac{\pi}{2},\pi)} &\sim \frac{1}{2\pi\alpha}e^{i\phi_{\rho+}}\sin\phi_{\rho-} \\
O_{CDW(\frac{\pi}{2},-\frac{\pi}{2})} &\sim \frac{1}{2\pi\alpha}e^{i\phi_{\rho+}}\cos(\phi_{\rho-}+\frac{\pi}{4})
\end{aligned}
$$

RG Equations

$$\frac{d}{dl}\left(\frac{1}{K_{\rho-}}\right) = y_3^2 + \frac{1}{8}(y_4^2 + y_5^2 + y_6^2),$$

$$\frac{dy_{\sigma-}}{dl} = \frac{1}{4}(y_6^2 + y_2^2 - y_1^2 - y_5^2);\ \frac{dy_{\sigma+}}{dl} = -\frac{1}{4}(y_1^2 + y_2^2 + y_4^2),$$

$$\frac{dy_1}{dl} = -\frac{1}{2}\left[(y_{\sigma+} + y_{\sigma-})y_1 + y_4 y_5\right],$$

$$\frac{dy_2}{dl} = -\frac{1}{2}\left[(y_{\sigma+} - y_{\sigma-})y_2 + y_4 y_6\right],$$

$$\frac{dy_3}{dl} = (2 - 4K_{\rho-})y_3 - \frac{1}{8}(y_4^2 + y_5^2 + y_6^2),$$

$$\frac{dy_4}{dl} = (1 - K_{\rho-})y_4 - \frac{1}{2}(y_{\sigma+}y_4 + y_1 y_5 + y_2 y_6 + y_3 y_4),$$

$$\frac{dy_5}{dl} = (1 - K_{\rho-})y_5 - \frac{1}{2}(y_{\sigma-}y_5 + y_3 y_5 + y_1 y_4),$$

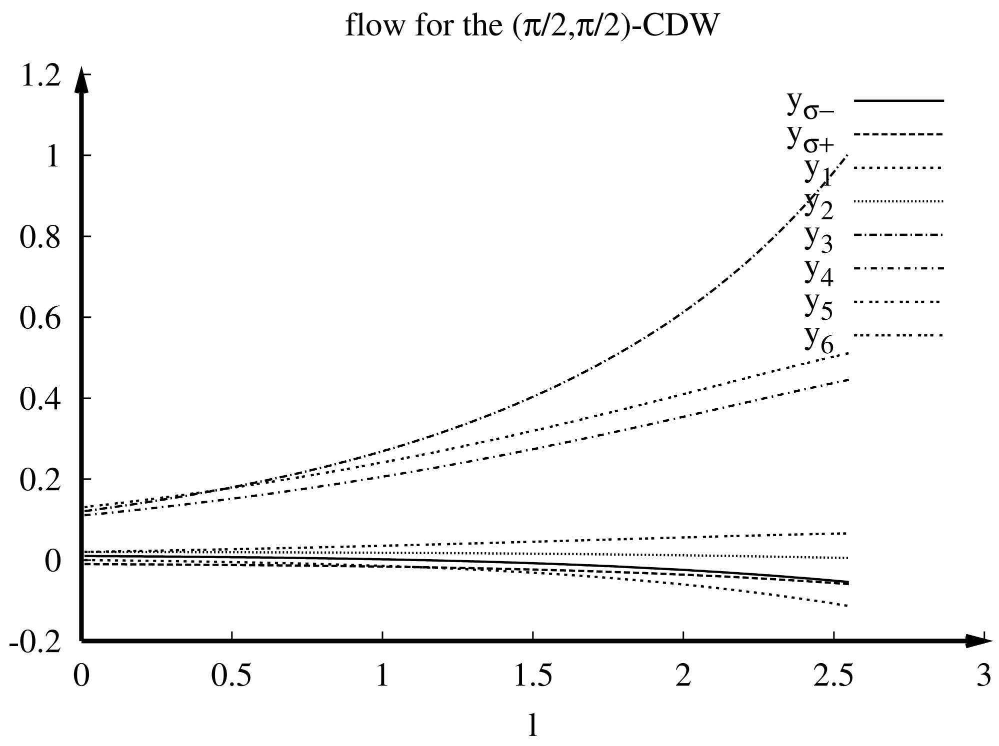
$$\frac{dy_6}{dl} = (1 - K_{\rho-})y_6 + \frac{1}{2}(y_{\sigma-}y_6 - y_3 y_6 - y_2 y_4).$$

Where we have:
$y_i = \frac{g_i}{\pi v_F}$ and $K_{\sigma\pm} = 1 + \frac{y_{\sigma\pm}}{2}$.
SU(2) symmetry $\Rightarrow$

$$y_{\sigma+}(l) + y_{\sigma-}(l) = y_1(l),$$
$$y_{\sigma-}(l) - y_{\sigma+}(l) = y_2(l),$$
$$y_5(l) - y_4(l) = y_6(l).$$

Fixed points:

- $y_3 \to +\infty$: $\langle \phi_{\rho-} \rangle = \frac{\pi}{4}$
  - $y_1 \to -\infty$: $\langle \phi_{\sigma-} \rangle = \langle \phi_{\sigma+} \rangle = 0$
  - $y_2 \to +\infty$: $\langle \theta_{\sigma-} \rangle = \frac{\pi}{2}$; $\langle \phi_{\sigma+} \rangle = 0$
- y_4, y_5 or $y_6 \to \infty$: $\langle \phi_{\rho-} \rangle = \frac{\pi}{2}$; $\langle \phi_{\sigma+} \rangle = 0$
  - $y_5 \to +\infty$: $\langle \phi_{\sigma-} \rangle = 0$
  - $y_6 \to +\infty$: $\langle \theta_{\sigma-} \rangle = 0$


flow for the (π/2,π/2)-CDW
1.2
1
0.8
0.6
0.4
0.2
0
-0.2
0
0.5
1
1.5
2
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3
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yσ−
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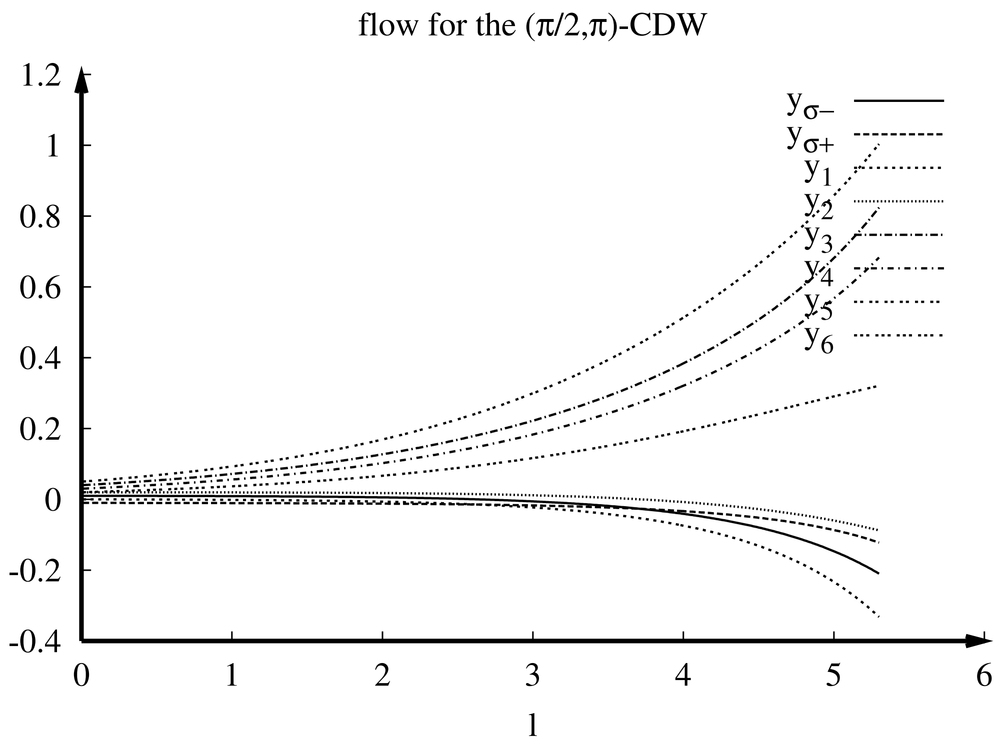
y1
y2
y3
y4
y5
y6


flow for the (π/2,π)-CDW
1.2
1
0.8
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-0.2
-0.4
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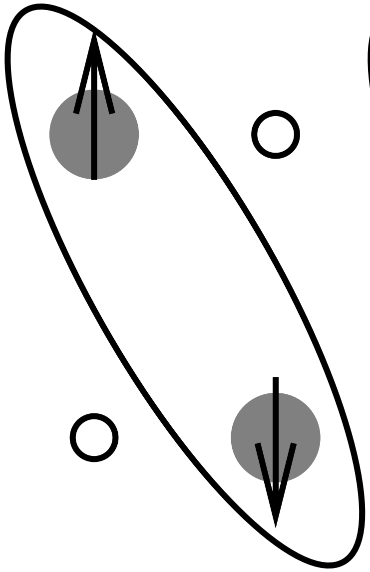
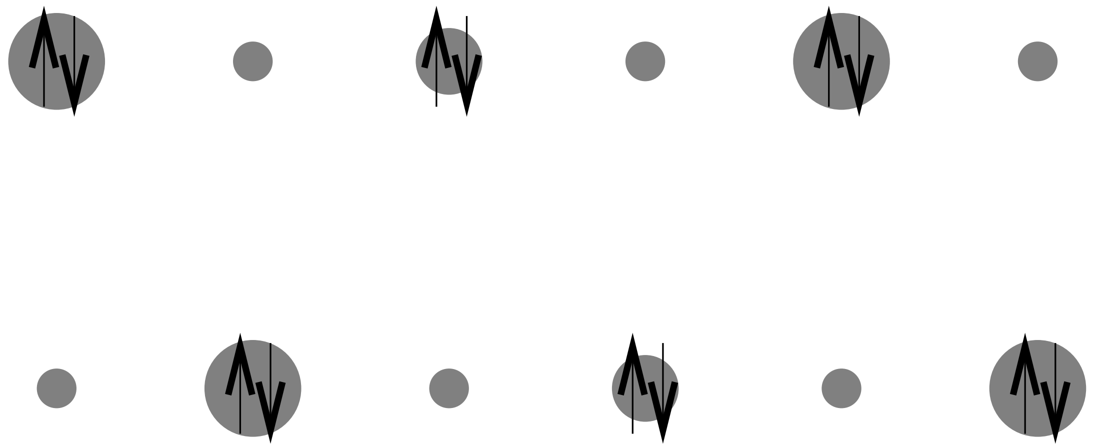
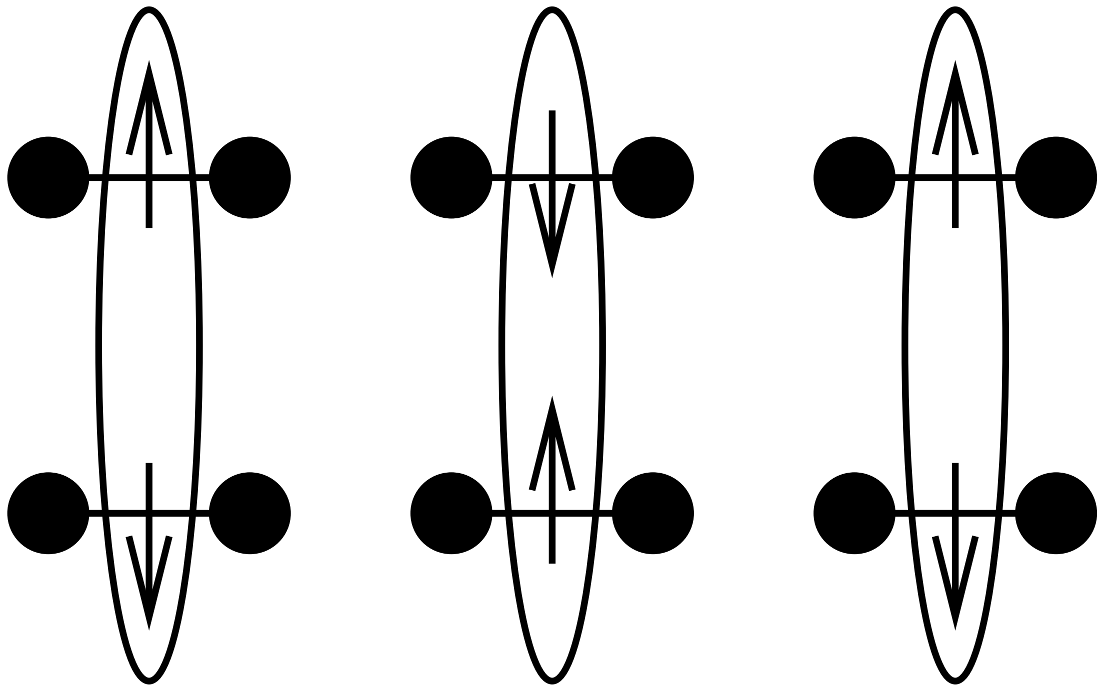
yσ−
yσ+
y1
y2
y3
y4
y5
y6



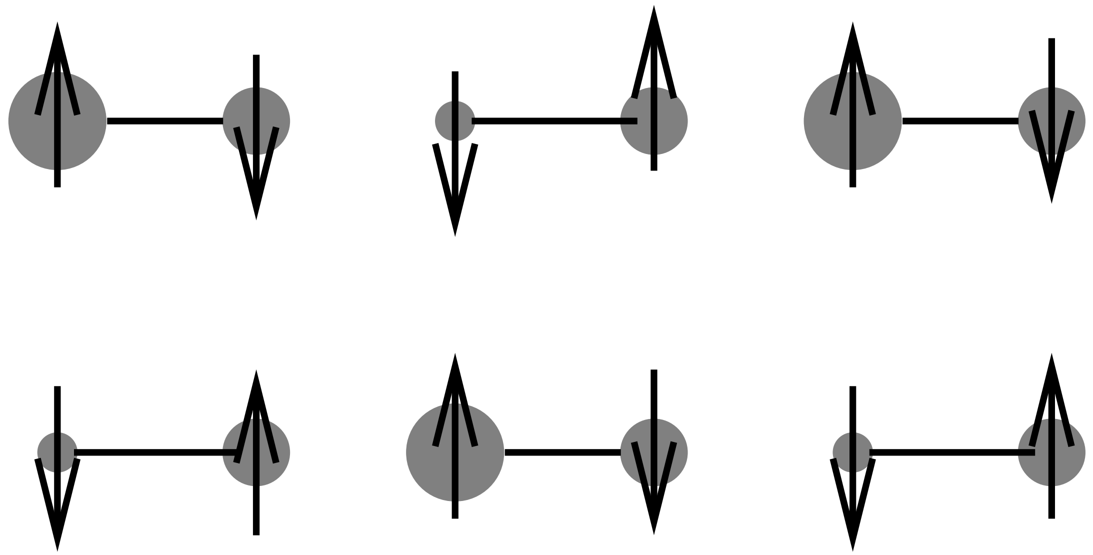
(π, π)-CDW or zig-zag charge order. This phase corresponds to $\langle \phi_{\rho -} \rangle = \frac{\pi}{4}$, $\langle \phi_{\sigma +} \rangle = 0$, $\langle \theta_{\sigma -} \rangle = \frac{\pi}{2}$. A spin gap is formed by interchain exchange $J_\perp$. The orbital modes decouple from the spin modes. The effective theory describing the spin modes is also the theory that describes the zig-zag spin-ladder [Allen et al. Phys. Rev. B **61** 8871 (2000)] in agreement with strong coupling theory [Vojta et al. Phys. Rev. B **63** 045105 (2001)]. This phase obtains for strong repulsion $1/4 < K_\rho < 1/3$.



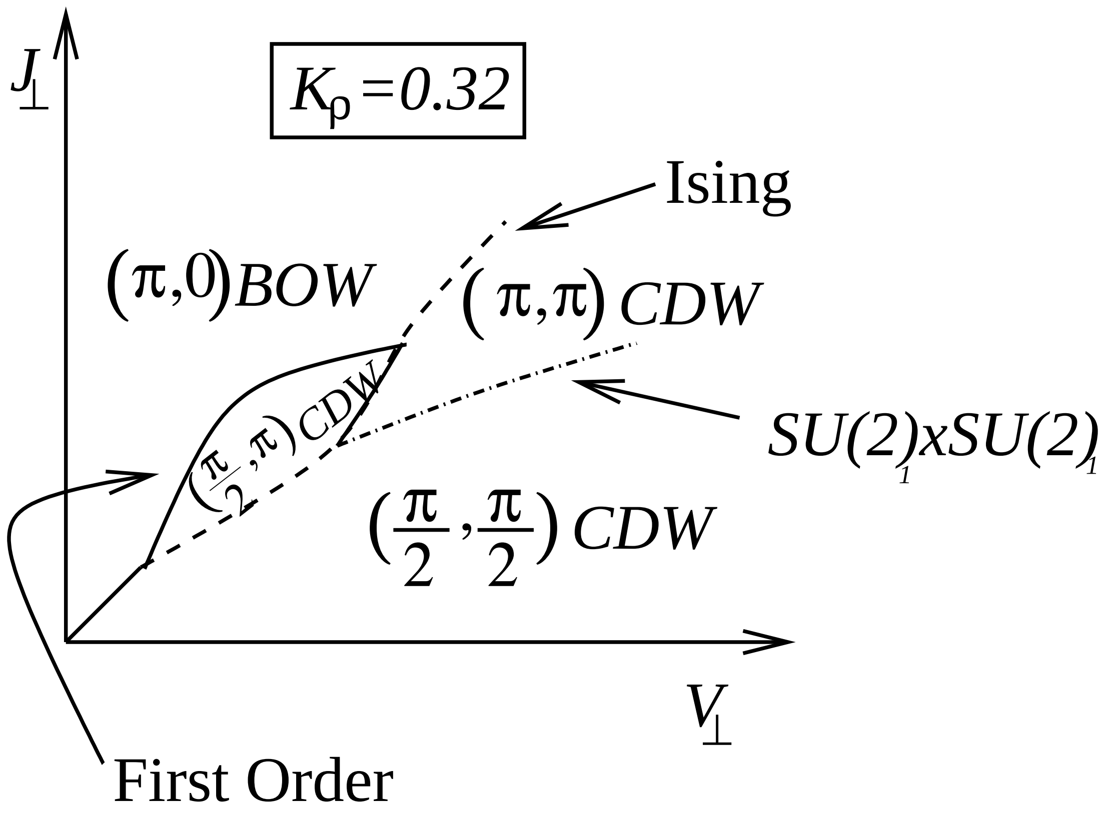
$(\frac{\pi}{2}, \frac{\pi}{2}) + (\pi, \pi)$-CDW. This phase corresponds to $\langle \phi_{\rho-} \rangle = \frac{\pi}{4}$, $\langle \phi_{\sigma+} \rangle = 0$, $\langle \phi_{\sigma-} \rangle = 0$. Each chain forms its own CDW, and the phases of CDWs are locked together by interchain repulsion $V_\perp$. The coupling of $4k_F$ components of the density is dominant. "Orbital" modes decouple from spin modes. This phase corresponds to strong repulsion $1/4 < K_\rho < 1/3$.



$(\pi, 0)$-BOW. This phase corresponds to $\langle \phi_{\rho-} \rangle = \frac{\pi}{2}$, $\langle \phi_{\sigma+} \rangle = 0$ $\langle \theta_{\sigma-} \rangle = 0$. Interchain spin singlets are formed by $J_\perp$ and are localized on the **links** by intrachain repulsion $V_\parallel$. This phase is obtained for intermediate repulsion $1/3 < K_\rho < 1/2$. Orbital modes remain coupled to spin modes.



$(\frac{\pi}{2}, \pi)$-CDW. This phase corresponds to $\langle \phi_{\rho-} \rangle = \frac{\pi}{2}$, $\langle \phi_{\sigma+} \rangle = 0$, $\langle \phi_{\sigma-} \rangle = 0$. Spin singlets are formed inside the chains. Each chain has its own CDW, and the phases of the CDW are locked together by interchain repulsion. The CDWs are coupled by the $2k_F = \frac{\pi}{2}$ component of the charge density, in contrast to the $(\frac{\pi}{2}, \frac{\pi}{2})$-CDW. This phase is obtained for intermediate repulsion $1/3 < K_\rho < 1/2$. Orbital modes remain coupled to spin modes.


$J_\perp$
$K_\rho=0.32$
Ising
$(\pi,0)BOW$
$(\pi,\pi)\ CDW$
$(\frac{\pi}{2},\pi)CDW$
$SU(2)_1xSU(2)_1$
$(\frac{\pi}{2},\frac{\pi}{2})\ CDW$
$V_\perp$
First Order

Topology of the phase diagram resulting from the competition $J_\perp/V$.
Different regimes depending on the strength of repulsion $U, V_{||}$

Open Problems:

Weaker repulsion: role of interchain hopping $t_\perp$
1/4 filled zig-zag ladders: $PrBa_2Cu_4O_8$ (Amasaki, Shibata, Ohta 2000)
Systems with more than 2 chains