80th birthday of Professor Sergei Matinyan
"Low-Dimensional Physics and Gauge Principles"

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QUANTUM CRITICALITIES IN A SPIN-ORBITAL CHAIN: A FIELD THEORETICAL APPROACH

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AN, G.-W. Chern, N.Perkins, Phys. Rev. B **83***, 205132 (2011)*

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Qiasi-1D Mott insulators: CaV_2O_4, ZnV_2O_4

G.-W.Chern, N.Perkins, Phys.Rev. B 80, 220405(R) (2009)

⇒ **1D toy model**

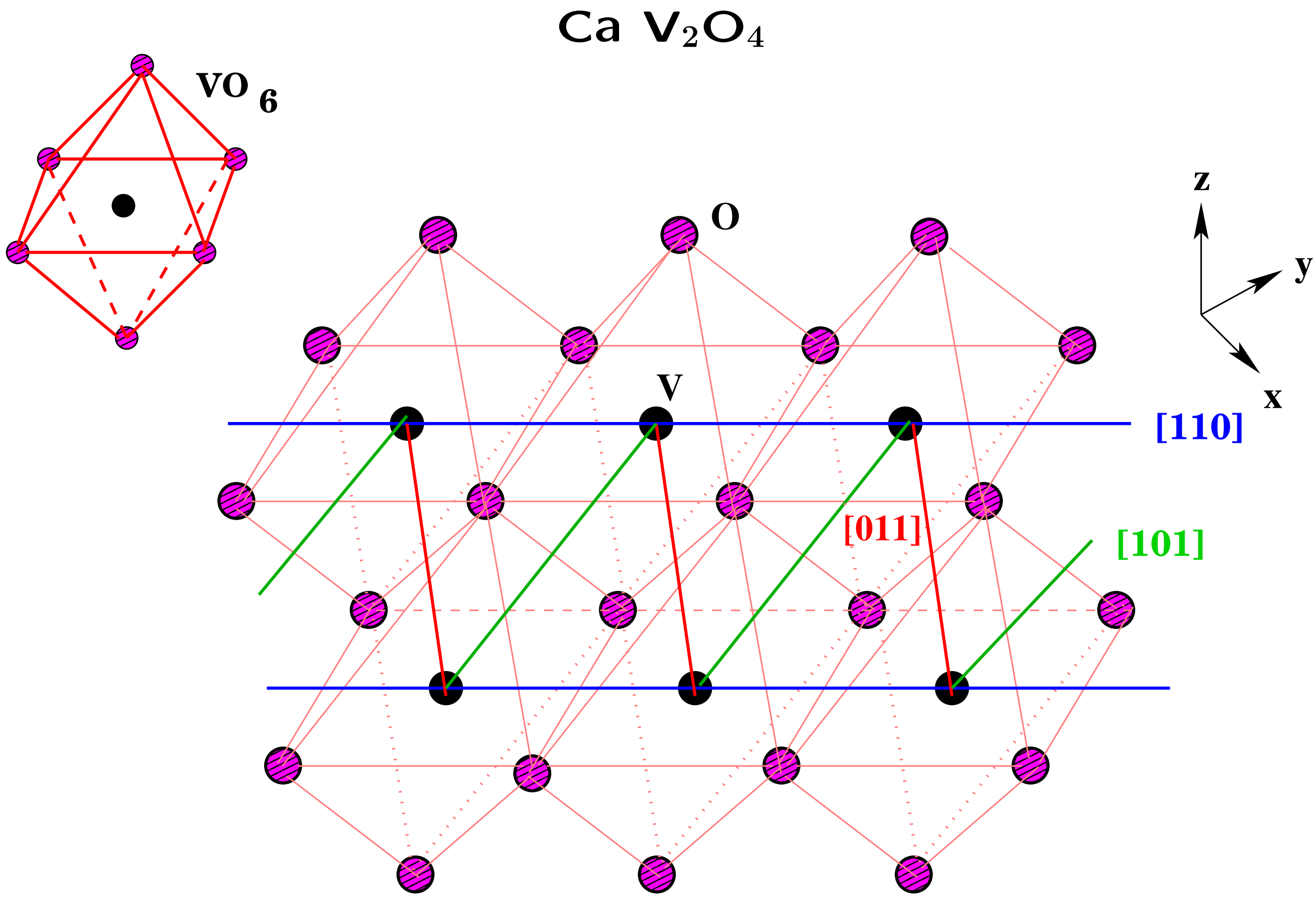
$$H = J\sum_m \mathbf{S}_m \cdot \mathbf{S}_{m+1} + J_\tau \sum_m \tau^z_m \tau^z_{m+1} - \lambda \sum_m \tau^x_m S^z_m$$

– spin/orbit (quantum/classical) interplay caused by SO interaction:

- anisotropy in spin-1 subsystem;
- source of quantum effects in orbital sector – orbital quantum spin liquid, Tomonaga-Luttinger liquid regime

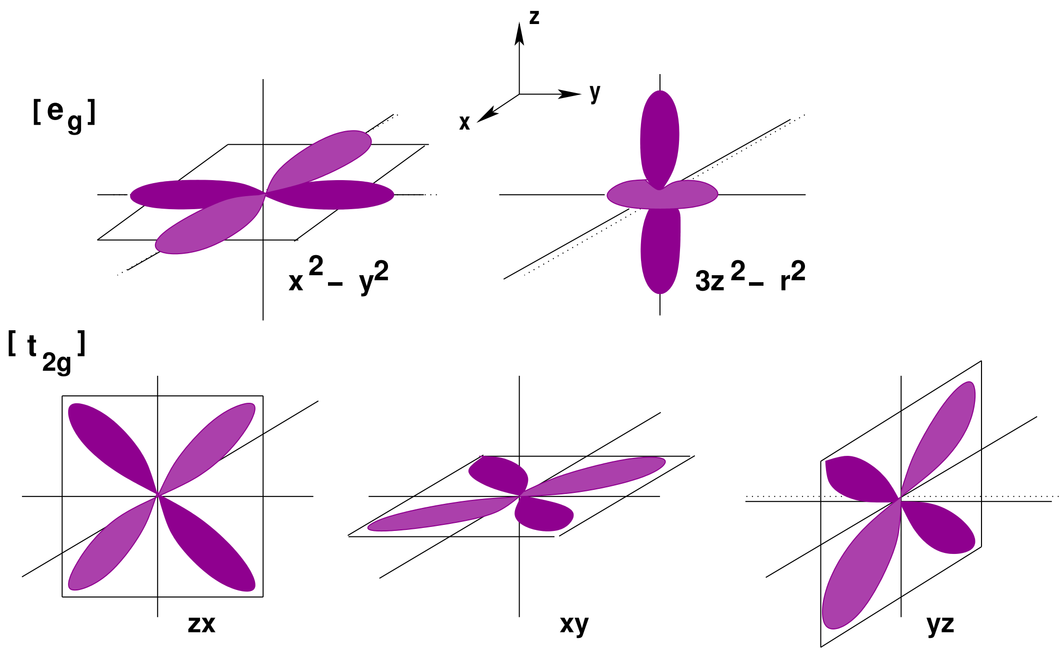
– ground state phase diagram: massive phases and quantum criticalities

Model not integrable → limiting cases: $J_\tau \gg J$, $J_\tau \ll J$

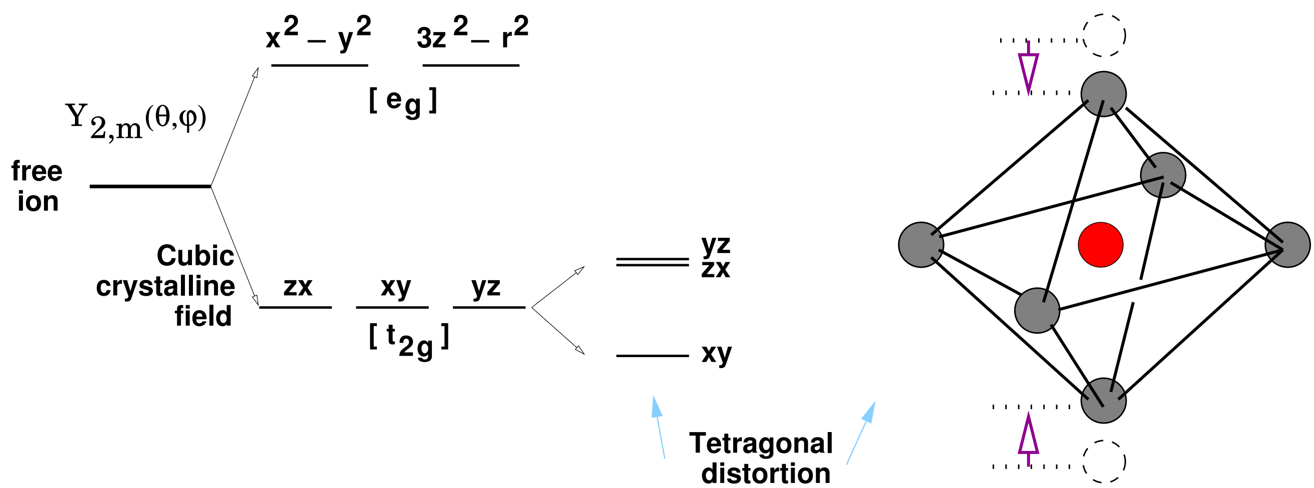


Ca V_2O_4
VO_6
O
V
z
y
x
[110]
[011]
[101]

Isolated VO_6 octahedron



V: $(1s)^2(2s)^2(2p)^6(3s)^2(3p)^6(3d)^2 \quad \longrightarrow \quad (t_{2g})^2(e_g)^0$
Hund's rule $\longrightarrow$ $\mathbf{S = 1}$



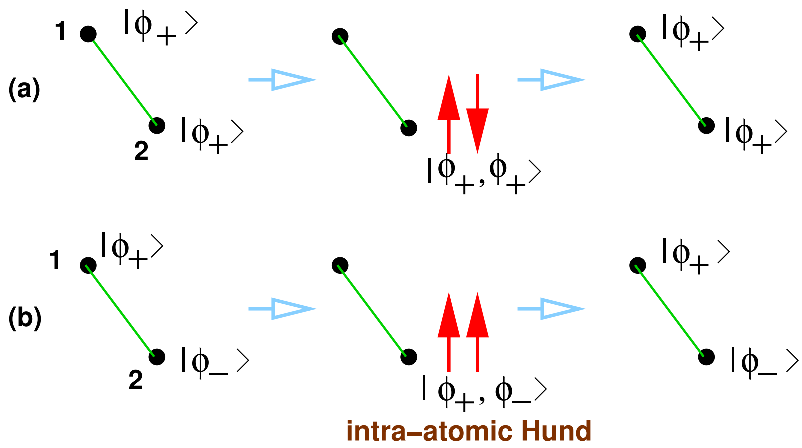
$|xy\rangle$-orbital quenched: AF spin exchange along the chains
Jahn-Teller coupling is weak → orbital **correlations** dominant

Orbital double degeneracy – pseudospin $\frac{1}{2}\boldsymbol{\tau}$

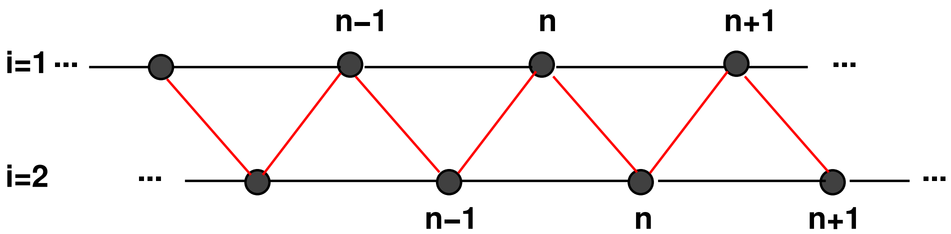
$$\phi_+ \equiv |yz\rangle, \quad \phi_- \equiv \mathrm{i}|zx\rangle, \qquad \tau^z \phi_\pm = \pm\phi_\pm$$

Local spin-orbit coupling $\lambda \mathbf{L}\cdot\mathbf{S}$ projected to subspace $\{\phi_\pm\}$:

$$\langle L^x\rangle_{\{\phi_\pm\}} = \langle L^y\rangle_{\{\phi_\pm\}} = 0$$
$$L^z = -\mathrm{i}\,(x\partial_y - y\partial_x)\,, \quad L^z\phi_\pm = \phi_\mp$$
$$(L^z)_{\{\phi_\pm\}} = \tau^x, \quad \lambda\mathbf{L}\cdot\mathbf{S}\Big|_{\{\phi_\pm\}} = \lambda\tau^x S^z$$

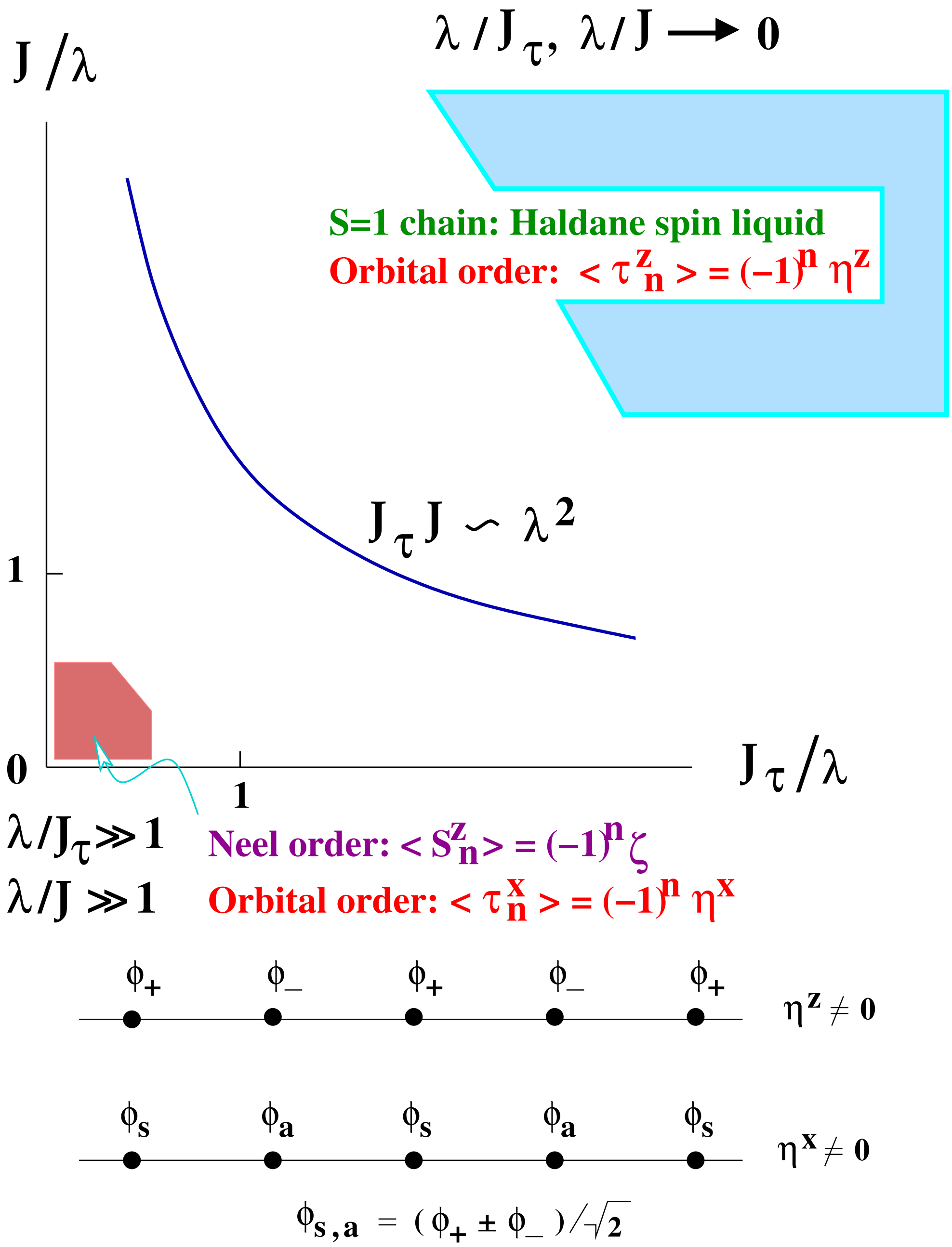


AF Ising-like orbital correlations along zigzag bonds – spin-orbital ladder



(Over)simplified, single-chain version:

$$H = J\sum_m \mathbf{S}_m\cdot\mathbf{S}_{m+1} + J_\tau\sum_m \tau^z_m\tau^z_{m+1} - \lambda\sum_m \tau^x_m S^z_m$$



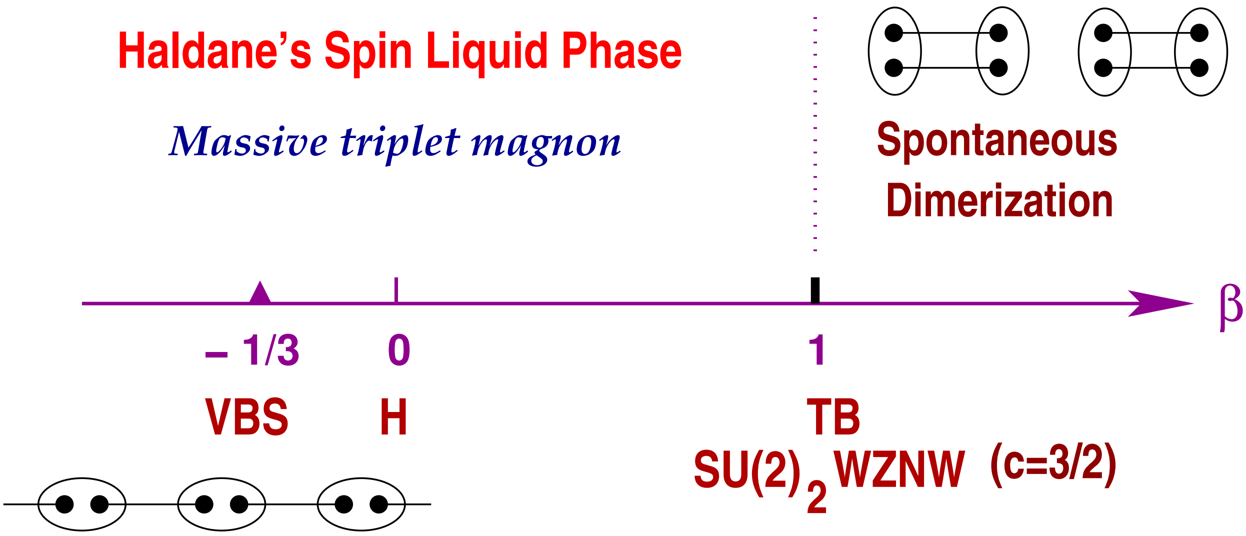
To be explained:

– reorientation transition in orbital sector: $\eta^z \rightarrow \eta^x$
– Neel ordering of S=1 chain

Important: Due to SO coupling orbital degrees of freedom become **quantum**

Antiferromagnetic spin-1 chain

$$H_S = J \sum_n \left[\mathbf{S}_n \cdot \mathbf{S}_{n+1} - \beta \left(\mathbf{S}_n \cdot \mathbf{S}_{n+1} \right)^2 \right] \qquad (S = 1)$$



$$\Im m \; \chi_{\rm SS}(q,\omega) \sim \frac{\Delta_S}{|\omega|} \delta \left(\omega - \sqrt{(q-\pi)^2 v_S^2 + \Delta_S^2} \right)$$

Zamolodchikov and Fateev (1986):

$SU(2)_2$ WZNW $\rightarrow$ **O(3) theory of massless Majorana fermions**

$\equiv$ **3 copies of 2D critical Ising models**

Tsvelik (1990): S=1 chain, $|\beta - 1| \ll 1$ - triplet of **massive** Majoranas

Shelton, A.N., and Tsvelik (1996): closely related theory of S=1/2 spin ladder

O(3) Majorana field theory

$$\mathcal{H}_\mathrm{M} = \sum_{a=1,2,3} \left[\frac{\mathrm{i}}{2} (\xi_L^a \partial_x \xi_L^a - \xi_R^a \partial_x \xi_R^a) - \mathrm{i} m \xi_R^a \xi_L^a \right] + \frac{1}{2} g \sum_a (\xi_R^a \xi_L^a)^2 , \quad (g < 0)$$

Massive Majorana fermion $\leftrightarrow$ 2D Ising model close to criticality

$$\xi^a \leftrightarrow (\sigma_a, \mu_a), \qquad m \sim 1 - \beta \sim (T - T_c)/T_c$$

$$\mathbf{S}(x) = \mathbf{I}_R(x) + \mathbf{I}_L(x) + (-1)^{x/a_0} \mathbf{N}(x), \qquad \mathbf{N}(x) \sim (\sigma_1 \mu_2 \mu_3,\ \mu_1 \sigma_2 \mu_3,\ \mu_1 \mu_2 \sigma_3)$$

$$\mathbf{I}_\nu(x) = -\frac{i}{2} \boldsymbol{\xi}_\nu(x) \times \boldsymbol{\xi}_\nu(x) \quad (\nu = R, L), \qquad \epsilon(x) = (-1)^n \mathbf{S}_n \cdot \mathbf{S}_{n+1} \sim \sigma_1 \sigma_2 \sigma_3$$

Spin liquid phase: $\beta < 1$, $m > 0 \to T > T_c$: $\quad \langle \sigma_a \rangle = 0, \quad \langle \mu_a \rangle \neq 0$

$\langle \mathbf{N} \rangle = \langle \epsilon \rangle = 0 :$ unbroken $SO(3)$ and parity

Dynamical spin correlations Wu,McCoy *et al* (1976)

$$\mathbf{r} = (v_s \tau, x), \quad \xi_S \sim v_s/m \qquad \langle \mu(\mathbf{r}) \mu(\mathbf{0}) \rangle \sim (a/\xi_S)^{1/4} \left[1 + O(e^{-2r/\xi_S}) \right]$$

$$\langle \sigma(\mathbf{r}) \sigma(\mathbf{0}) \rangle \sim (a/\xi_S)^{1/4} \sqrt{\xi_S/r}\ e^{-r/\xi_S}$$

$$\langle \mathbf{N}(\mathbf{r}) \mathbf{N}(\mathbf{0}) \rangle \sim (a/\xi_S)^{3/4} \sqrt{\xi_S/r}\ e^{-r/\xi_S}$$

Majorana theory:

– *is* quantitatively *correct at* $|\beta - 1| \ll 1$*;*
– *has status of a* phenomenological *theory at any* β*.*

$J_{\tau} \gg \Delta_S, \lambda$

Pseudospins "fast", spins "slow": integrate pseudospins out

$$\delta^{(2)} S_S = -\frac{1}{2}\lambda^2 \sum_{nm} \int \mathrm{d}\tau_1 \int \mathrm{d}\tau_2 \, \langle \tau_n^x(\tau_1)\tau_m^x(\tau_2)\rangle_{\text{orb}} \, S_n^z(\tau_1) S_m^z(\tau_2)$$

$$\langle \tau_n^x(\tau_1)\tau_m^x(\tau_2)\rangle_{\text{orb}} = \delta_{nm} \exp\left(-4J_\tau|\tau_1 - \tau_2|\right), \quad |\tau_1 - \tau_2| \ll 1/\Delta_S$$

Generation of **easy-axis** single-ion anisotropy:

$$H_S \to H_S + H_{\text{anis}}, \quad H_{\text{anis}} = -\frac{\lambda^2}{4J_\tau} \sum_n (S_n^z)^2$$

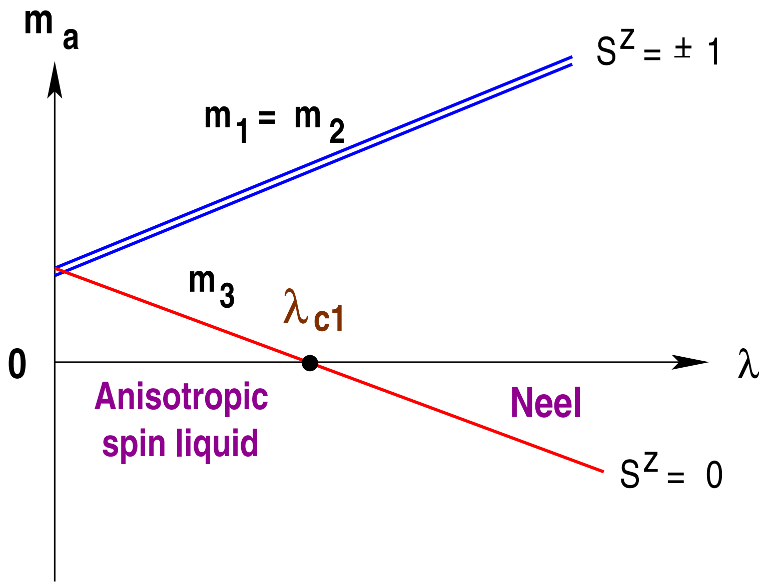
Continuum limit:

$$H_M = \sum_{a=1,2,3} \left[\frac{\mathrm{i}}{2}\left(\xi_L^a \partial_x \xi_L^a - \xi_R^a \partial_x \xi_R^a\right) - \mathrm{i} m_a \, \xi_R^a \xi_L^a\right] + \frac{1}{2}\sum_{a \neq b} g_{ab} \sum_a \left(\xi_R^a \xi_L^a\right)\left(\xi_R^b \xi_L^b\right)$$

$$m_1 = m_2 = m + \frac{\pi C \lambda^2}{4J_\tau}, \quad m_3 = m - \frac{\pi C \lambda^2}{4J_\tau}$$

$$g_{13} = g_{23} \neq g_{12}$$

Ising transition in spin sector



$$\lambda_{c1} \sim \sqrt{J_\tau m}$$

$\lambda < \lambda_{c1}$:

$$\Im m\ \chi^{xx}(q,\omega) = \Im m\ \chi^{yy}(q,\omega) \sim \frac{m_1}{|\omega|}\delta\left(\omega - \sqrt{(q-\pi)^2 v^2 + m_1^2}\right)$$

$$\Im m\ \chi^{zz}(q,\omega) \sim \frac{m_3}{|\omega|}\delta\left(\omega - \sqrt{(q-\pi)^2 v^2 + m_3^2}\right)$$

$\lambda > \lambda_{c1}$: $\mathbf{N}(x) \sim (\sigma_1\mu_2\mu_3,\ \mu_1\sigma_2\mu_3,\ \mu_1\mu_2\sigma_3)$

$m_1 = m_2 > 0,\ m_3 < 0 \ \rightarrow\ \langle\sigma_3\rangle \neq 0$: $\langle N_3 \rangle = \zeta(\lambda) \neq 0$ **(Neel phase)**

$$0 < \lambda - \lambda_{c1} \ll \lambda_{c1}: \quad \zeta(\lambda) \sim \left(\frac{\lambda - \lambda_{c1}}{\lambda_{c1}}\right)^{1/8}$$

Pairs of massive topological kinks – broad continuum of **incoherent** transverse spin fluctuations:

$$\Im m\ \chi^{xx}(q,\omega) \sim \frac{1}{\sqrt{m_1|m_3|}}\frac{\theta(\omega^2 - (q-\pi)^2 v^2 - (m_1 + |m_3|)^2)}{\sqrt{\omega^2 - (q-\pi)^2 v^2 - (m_1 + |m_3|)^2}}$$

Neel phase in spin sector: Ising transition in orbital sector

$\boldsymbol{\lambda > \lambda_{c1}}$: orbital sector acquires **quantum dynamics:** – Neel ordering of spins generates **transverse** orbital "magnetic" field:

$$H_{\text{so}} \to -h\sum_n (-1)^n \tau_n^x + H_{\text{so}}^{\text{fluc}}, \qquad h = \lambda\langle N_3\rangle \equiv \lambda\zeta(\lambda)$$

Quantum Ising model in orbital sector:

$$H_{\tau;\text{eff}} = J_\tau \sum_n \tau_n^z \tau_{n+1}^z - h\sum_n (-1)^n \tau_n^x$$

$0 < \lambda - \lambda_{c1} \ll \lambda_{c1}$

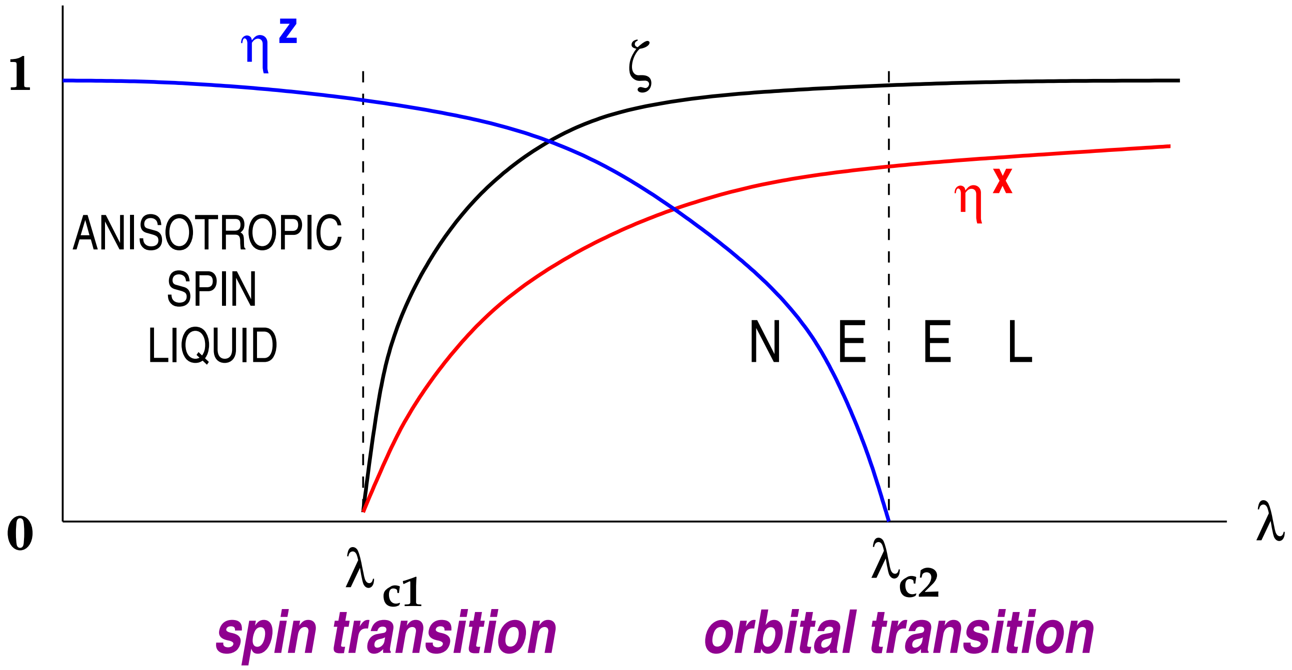
$$\eta^x \equiv (-1)^n \langle \tau_n^x \rangle \sim \left(\frac{h}{J_\tau}\right) \sim \sqrt{\frac{\Delta_S}{J_\tau}} \left(\frac{\lambda - \lambda_{c1}}{\lambda_{c1}}\right)^{1/8}$$

Orbital quantum Ising transition:

$$h = J_\tau : \quad \zeta \sim 1 \quad \to \quad \lambda_{c2} \sim J_\tau$$

$$\frac{\lambda_{c2}}{\lambda_{c1}} \sim \left(\frac{J_\tau}{\Delta_S}\right)^{1/2} \gg 1$$

Ground state phase diagram at $J_\tau \gg \Delta_S$



$$(-1)^n \langle \tau^z_n \rangle = \eta^z \qquad (-1)^n \langle \tau^x_n \rangle = \eta^x \qquad (-1)^n \langle S^z_n \rangle = \zeta$$

$$\lambda_{c1} \sim \sqrt{J_\tau \Delta_S} \qquad \lambda_{c2} \sim J_\tau$$

– orbital η^x ordering induced by Neel spin alignment

(agreement with numerical data by *Chern et al*)

$J_{\boldsymbol{\tau}} \ll \Delta_{\rm S}$

Spins "fast", pseudospins "slow": integrate spins out

$$\delta^{(2)} S_\tau = -\frac{1}{6}\lambda^2 \sum_{nm} \int \mathrm{d}\tau_1 \int \mathrm{d}\tau_2 \ \langle \mathbf{S}_n(\tau_1)\cdot \mathbf{S}_m(\tau_2)\rangle_S \ \tau_n^x(\tau_1)\tau_m^x(\tau_2)$$

$$\langle \mathbf{S}_l(\tau)\mathbf{S}_0(0)\rangle \simeq (-1)^l f(r/\xi_S), \quad r = \sqrt{v_s^2\tau^2 + x^2}$$
$$f(x) \sim x^{-1/2} e^{-x}$$

Generated xx-exchange in orbital sector

$$\Delta H_\tau = \sum_n \sum_{m\geq 1} (-1)^{m+1} J'_\tau(m) \tau_n^x \tau_{n+m}^x, \quad J'_\tau(m) \sim (\lambda^2/\Delta_S) e^{-m a_0/\xi_S}$$

$\xi_S =$ few a_0 $\rightarrow$ $m=1$ – leading term, $m = 2, 3, \ldots$ – perturbation

$\pi/2$ pseudospin rotation: $\tau_n^z \rightarrow \tau_n^y$, $\tau_n^y \rightarrow -\tau_n^z$

$$H_\tau^{[\mathrm{eff}]} = \sum_n \left[J_x \tau_n^x \tau_{n+1}^x + J_y \tau_n^y \tau_{n+1}^y \right] + H'_\tau$$
$$H'_\tau = -J'_\tau(2) \sum_n \tau_n^x \tau_{n+2}^x + \cdots$$

$$J_y = J_\tau, \quad J_x = J'_\tau(1) \sim \lambda^2/\Delta_S, \quad J'_\tau(2) < J'_\tau(1)$$

Gaussian transition in orbital sector

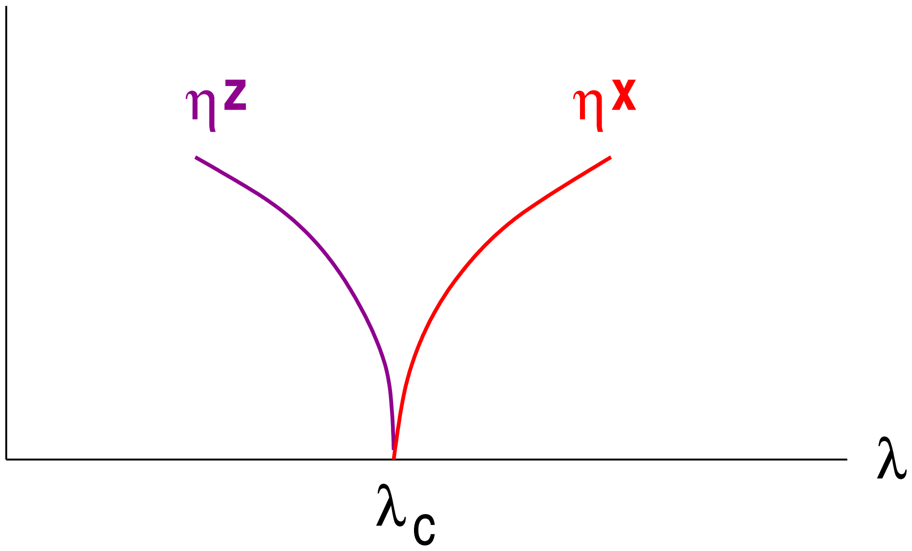
$H'_\tau = 0 \rightarrow$ **(pseudo)spin-1/2 XY chain**.

Jordan-Wigner: mapping onto spinless fermions (*Lieb, Schultz, Mattis*)

$$H_{\mathsf{XY}} = (J_x+J_y)\sum_n \left(a_n^\dagger a_{n+1} + h.c.\right) + (J_x-J_y)\sum_n \left(a_n^\dagger a_{n+1}^\dagger + h.c.\right).$$

$J_x = J_y \quad \rightarrow \quad \lambda = \lambda_c \sim \sqrt{J_\tau \Delta_S}$: **quantum XX criticality**
− free massless fermions

Pseudospin reorientation transition



$$\begin{aligned} \boldsymbol{\lambda}<\boldsymbol{\lambda_c}: &\quad \eta^z \neq 0, \quad \eta^x = 0 \\ \boldsymbol{\lambda}>\boldsymbol{\lambda_c}: &\quad \eta^z = 0, \quad \eta^x \neq 0 \end{aligned} \tag{1}$$

Adding n.n.n. perturbation H'_τ:
XY chain $\rightarrow$ XYZ chain (weak ferro zz-coupling)

Weak XY anisotropy, $|\lambda - \lambda_c| \ll \lambda_c$: **bosonization, quantum sine-Gordon model**:

$$\mathcal{H} = \frac{u}{2}\left[K\Pi^2 + \frac{1}{K}(\partial_x\Phi)^2\right] - \frac{2\gamma}{\pi\alpha}\cos\sqrt{4\pi}\Theta, \qquad \partial_x\Theta = \Pi$$
$$\gamma \sim J_\tau\left(\frac{\lambda - \lambda_c}{\lambda_c}\right), \qquad K = 1 + 2g + O(g^2), \quad g = J'_\tau(2)/\pi v \ll 1$$

$\lambda = \lambda_c$: **Gaussian criticality: orbital Luttinger liquid**

$|\lambda - \lambda_c| \ll \lambda_c$: mass gap

$$M_{\text{orb}} \sim \left|\frac{\lambda - \lambda_c}{\lambda_c}\right|^{\frac{K}{2K-1}}$$

Massive phases:

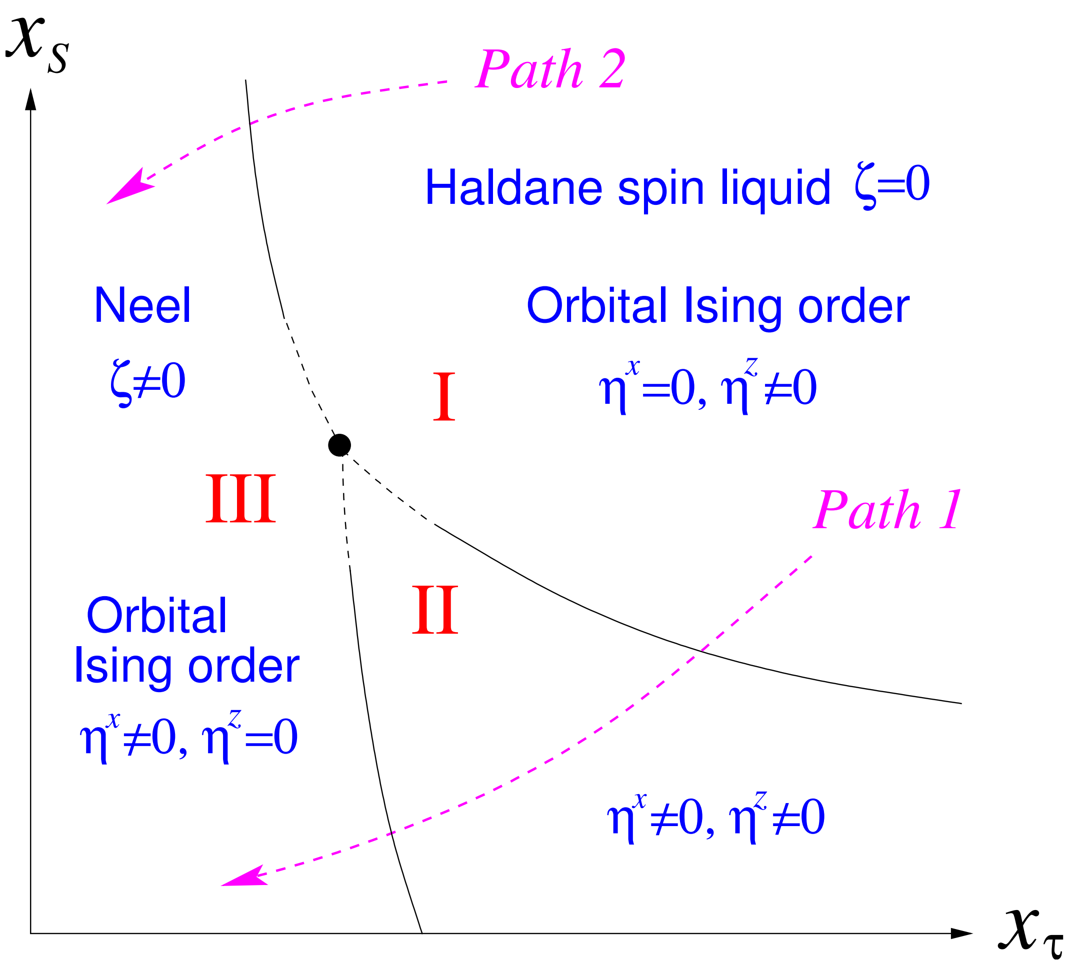
$$\eta^x \sim \cos\sqrt{\pi}\Theta, \qquad \eta^z_n \sim \sin\sqrt{\pi}\Theta \qquad (d = 1/4K)$$

$$\eta^z(\lambda) \sim (\lambda_c - \lambda)^{\frac{1}{4(2K-1)}}, \qquad \lambda < \lambda_c$$
$$\eta^x(\lambda) \sim (\lambda - \lambda_c)^{\frac{1}{4(2K-1)}}, \qquad \lambda > \lambda_c$$

η^x orbital ordering generates staggered magnetic field:

$$H_{\text{SO}} \rightarrow -h_S\sum_n(-1)^n S^z_n, \qquad h_S \sim \lambda\eta^x$$
$$\zeta = (-1)^n\langle S^z_n\rangle \sim h_S/\Delta_S \sim (\lambda/\Delta_S)(\lambda - \lambda_c)^{\frac{1}{4(2K-1)}}$$

– Neel spin alignment **induced** by orbital order



x_s
Path 2
Haldane spin liquid ζ=0
Neel
ζ≠0
Orbital Ising order
η^x=0, η^z≠0
I
III
Path 1
II
Orbital
Ising order
η^x≠0, η^z=0
η^x≠0, η^z≠0
x_τ

How to observe strong quantum orbital fluctuations?

$\Delta_S \gg J_\tau$: due to SO coupling, staggered magnetization $\mathbf{N}(x)$ acquires a nonzero spectral weight at $|\omega| \ll \Delta_S$

$$S_{SO} \simeq \frac{\lambda a_0}{v_S} \int \mathrm{d}^2\mathbf{r}\ N^z(\mathbf{r})\ n^x(\mathbf{r})$$
$$N^z \to (-1)^n S^z_n, \quad n^x \to (-1)^n \tau^x_n, \quad \mathbf{r} = (v_S \tau, x)$$

$$N^z_P(\mathbf{r}) = \langle e^{-S_{SO}} N^z(\mathbf{r}) \rangle$$
$$= N^z_0(\mathbf{r}) - \frac{\lambda a_0}{v_S} \int \mathrm{d}^2\mathbf{r}_1 \langle N^z_0(\mathbf{r}) N^z_0(\mathbf{r}_1) \rangle_S\ n^x(\mathbf{r}_1) + O(\lambda^2)$$

Low-energy projection $\mathbf{N}_P(x)$ – hybridization effect:

$$N^z_P(\mathbf{r}) \sim \frac{\lambda}{\Delta_S} \left(\frac{\xi_S}{a_0} \right)^{1/4} n^x(\mathbf{r})$$

Measuring **orbital quantum fluctuations** in magnetic neutron scattering and NMR experiments.

Orbital Luttinger-liquid regime:

- $\Im m\chi(q,\omega) \sim (\lambda/\Delta_s)^2[\omega^2 - v^2(q-\pi)]^{\frac{1}{4K}-1}$

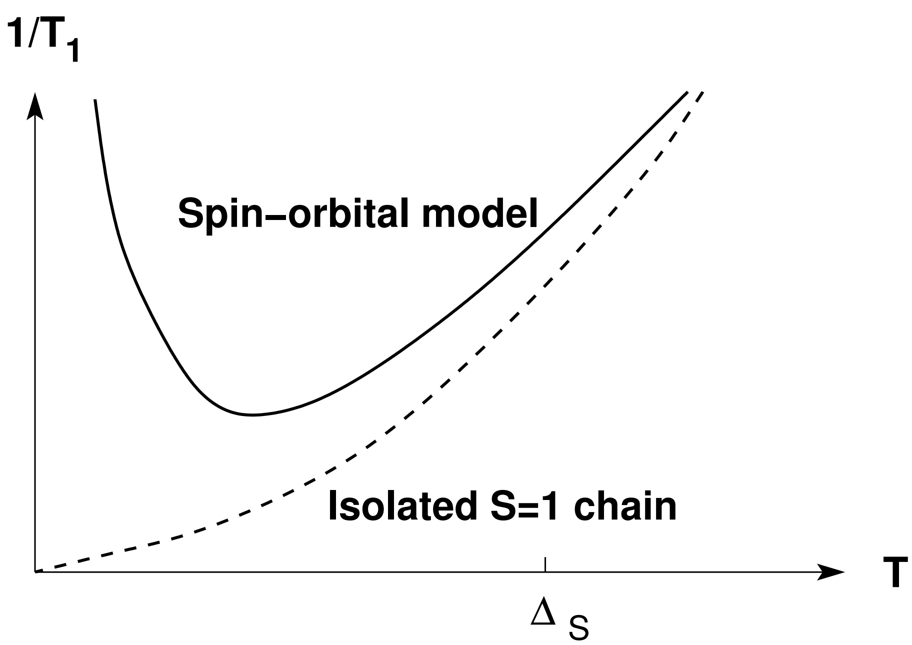
Schulz & Bourbonnais, 1983

- Isolated S = 1 chain :

$$\frac{1}{T_1} \sim A^2 \exp(-2\Delta_s/T) \qquad \textit{Affleck \& Sagi, 1995}$$

Present model :

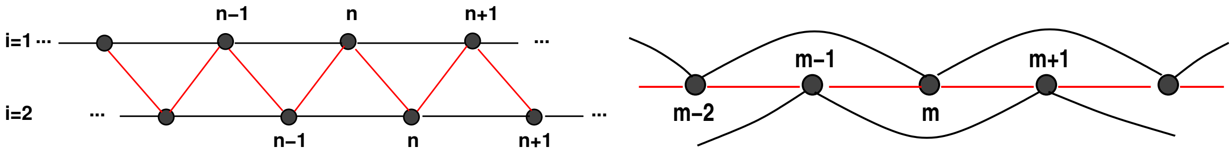
$$\frac{1}{T_1} \sim A^2 \left(\frac{\lambda}{\Delta_S}\right)^2 T^{\frac{1}{2K}-1}, \qquad \frac{1}{2K} - 1 < 0 \text{ (!)}$$



Open questions

- Strong spin-orbital hybridization regime so far unaccessible (no small parameter).
- Generalization to zigzag geometry: new models.
- Quasi-1D effects.

Zigzag ladder: self-dual orbital model



$$x \leftrightarrow z: \qquad H = \sum_{m=1}^{N} \left(J_x \sigma_m^x \sigma_{m+1}^x + J_z \sigma_m^z \sigma_{m+2}^z \right)$$

Duality property

$$\sigma_m^z \sigma_{m+1}^z = \mu_m^x, \qquad \sigma_m^x = \mu_m^z \mu_{m+1}^z$$

$$H = \sum_m \left(J_z \mu_m^x \mu_{m+1}^x + J_x \mu_m^z \mu_{m+2}^z \right)$$

$$H[\{\sigma\};\gamma] = \frac{1}{\gamma} H\left[\{\mu\};\frac{1}{\gamma}\right], \qquad \gamma = J_z/J_x$$

Self-duality point: $\gamma_c = \pm 1$ **?**