Composite order in Kondo-Heisenberg models

A. M. Tsvelik

Phys. Rev. B **94**, 165114
and 205141 (2016).
PNAS **116**, 12729 (2019).

BROOKHAVEN NATIONAL LABORATORY
a passion for discovery
U.S. DEPARTMENT OF ENERGY | Office of Science

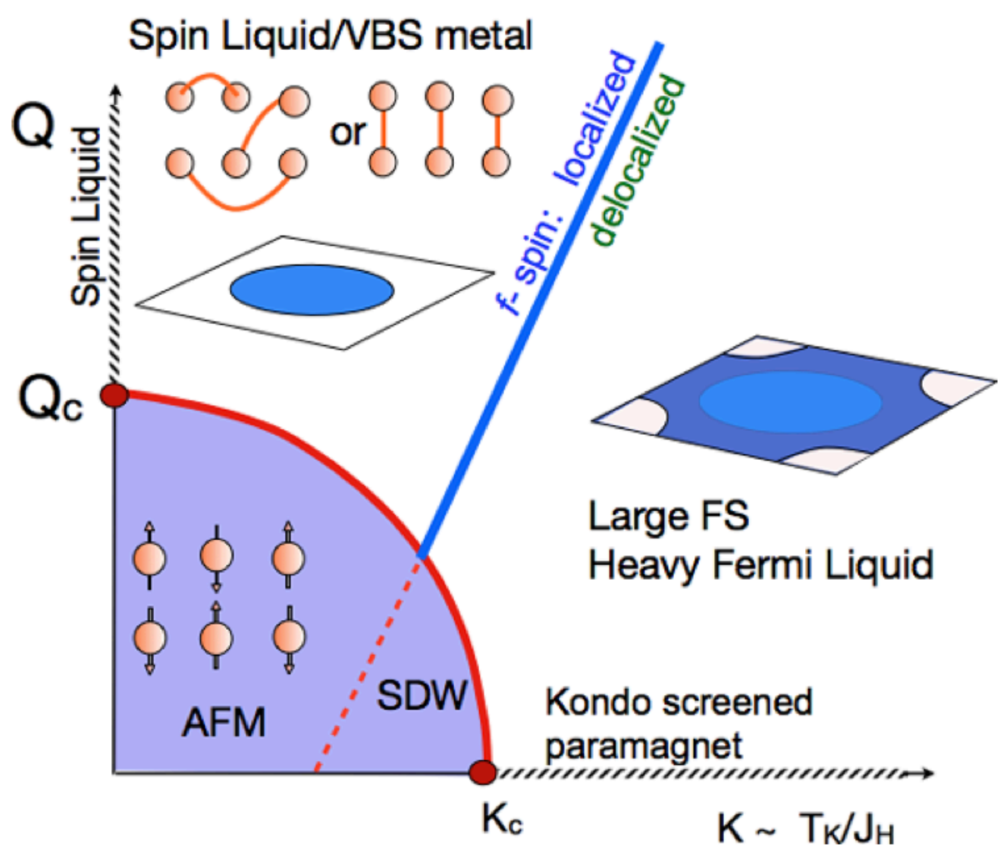
Following the steps:

- Fractionalized order - a great idea!
- Can we have some theoretical support?
- I am going to present a model

(i) which is not divorced from reality,

(ii) the fractionalized order can be rigorously derived.

Kondo lattices: traditional point of view



This picture is taken from a review article by Piers.

The thinking behind it:

the spin-spin interaction *competes* with the Kondo effect.

When it wins the spins and electrons live their separate lives and we have small FS.

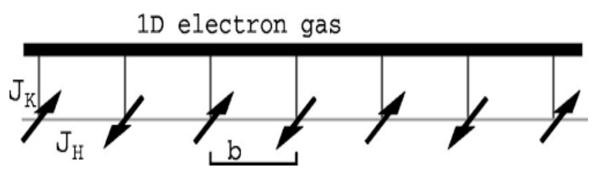
When the Kondo wins the localized electrons are sucked into the conduction band. Large FS.

Alternative Idea: Cooperation

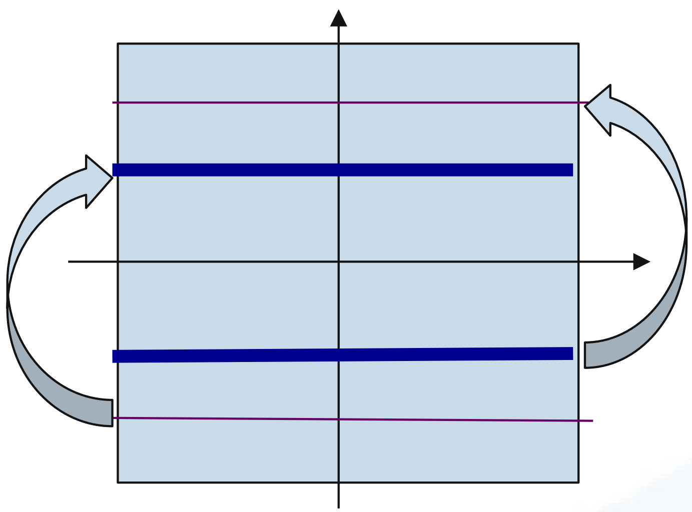
- The Heisenberg exchange and Kondo coupling cooperate to create a *spin liquid*.
- This spin liquid supports *fractionalized order*.
- It also may support *small FS* quasiparticles.

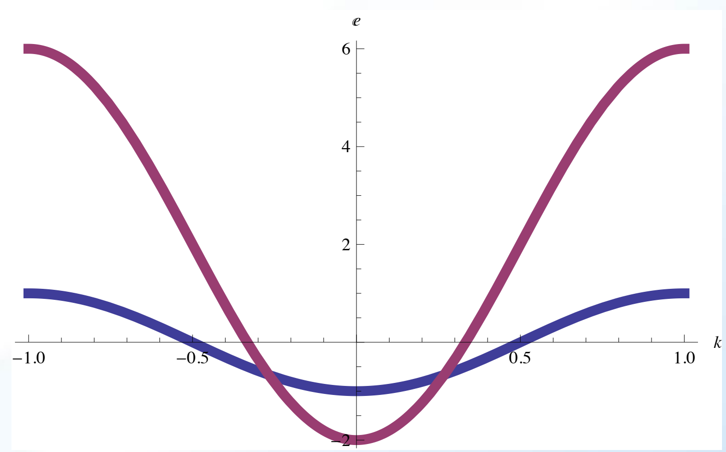
Cartoon explanation

- Starting point: array of uncoupled wires.
- Each wire - 1D electron gas + S=1/2 Heisenberg chain:

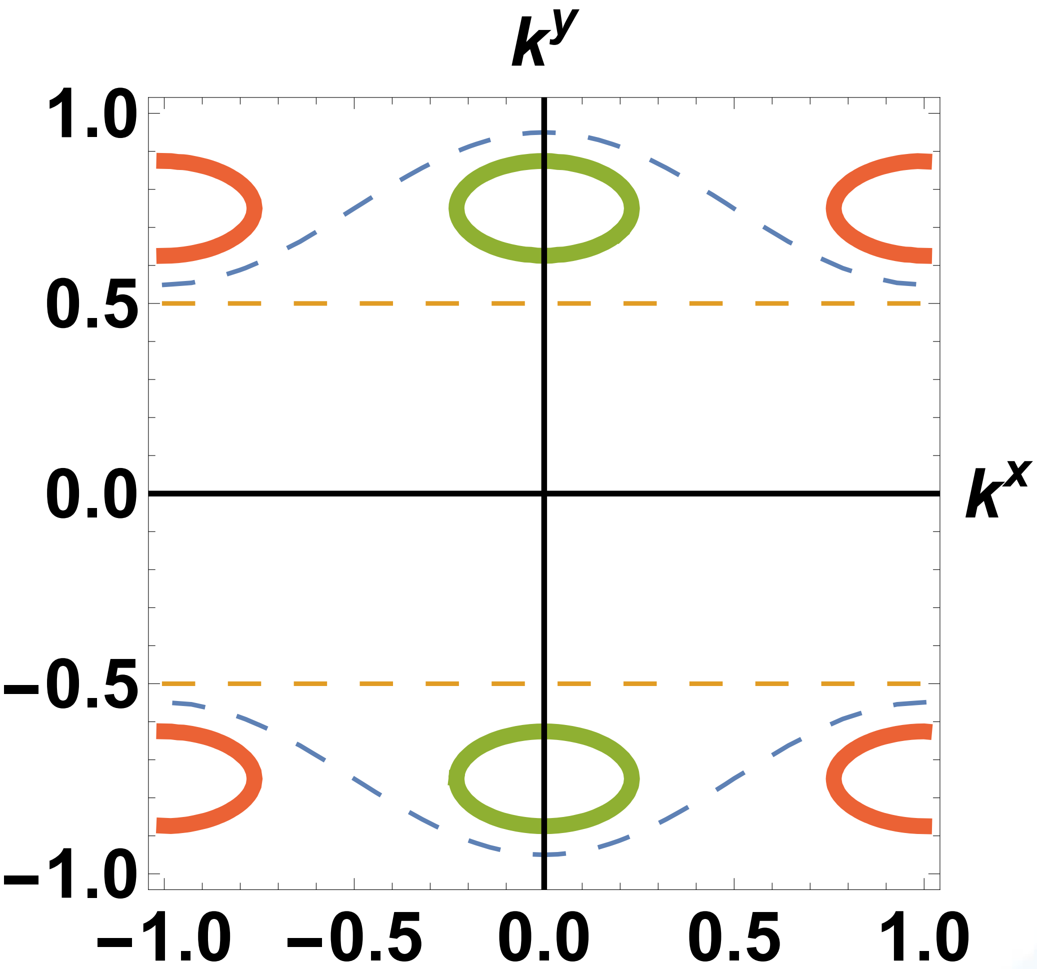


Their FS are flat, the spinons and electrons with opposite chirality hybridize and create   spin gaps.





Adding interchain tunneling



If the warping of the FS is sufficiently large not all FS is gapped.

Pockets of quasiparticles appear:

Compensated metal.

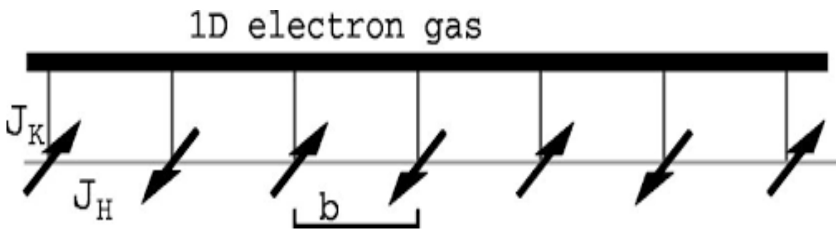
There is more!
The spin liquid has most curious properties.

- It has fractionalized composite order.
- The Luttinger-Oshikawa theorem is fulfilled *on the level of individual chains* via zeroes of the Green's function.
- Hence interchain tunneling cannot change the Luttinger volume. The resulting metallic state in **D>1** where the Fermi surface volume is zero (**compensated metal**).

The first step: Kondo-Heinseberg ladder

Spin S=1/2 chain interacting with 1D electron gas.

$$H = \sum_k \epsilon(k)\psi^+_{k\alpha}\psi_{k\alpha} + \frac{J_K}{2}\sum_{k,q}\psi^+_{k+q,\alpha}\vec{\sigma}_{\alpha\beta}\psi_{k,\beta}\mathbf{S}_q + J_H\sum_n \mathbf{S}_n\mathbf{S}_{n+1}.$$



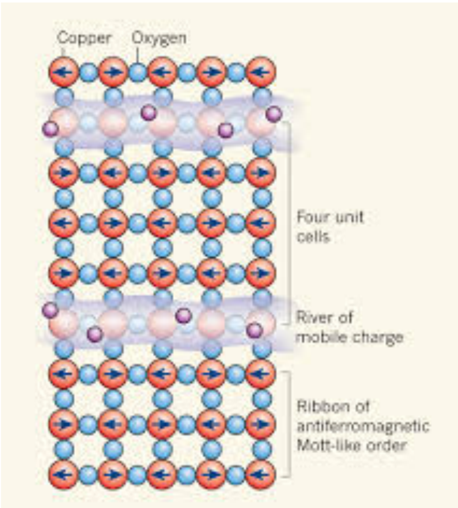
$J_K << J_H$

The electron band is *incommensurate* with the lattice: **k_F not equal $\pi/2$.**

This model has a spin gap and gapless charge excitations.

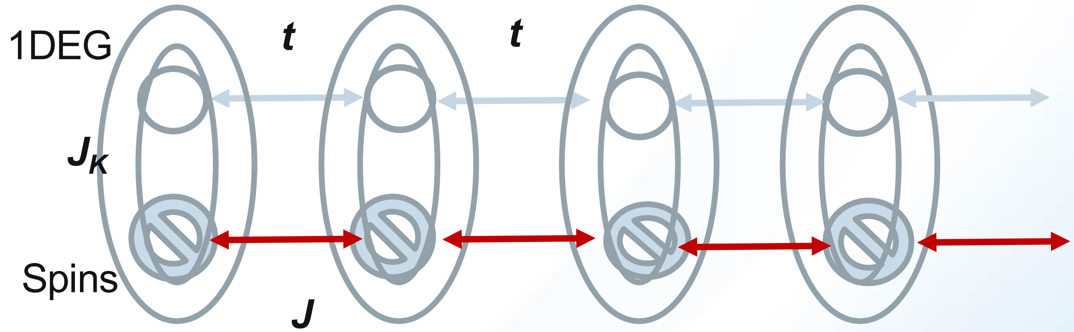
Zachar, Tsvelik, PRB 64, 3103 (2001);
Berg et.al. PRL 105, 146403 (2010).

Next step: make $D > 1$ array of Kondo-Heisenberg ladders



This would be the most realistic arrangement, like in $La_{2-x}Ba_xCuO_4$ (x=1/8).

I will discuss a less realistic model first (Tsvelik,PRB 94, 165114 (2016):



This model allows controllable treatment. It gives us answers to all questions posed in the beginning.

The core model: Kondo-Heisenberg ladder

$$H = \sum_k \epsilon(k)\psi^+_{k\alpha}\psi_{k\alpha} + \frac{J_K}{2}\sum_{k,q}\psi^+_{k+q,\alpha}\vec{\sigma}_{\alpha\beta}\psi_{k,\beta}\mathbf{S}_q + J_H\sum_n \mathbf{S}_n\mathbf{S}_{n+1}.$$

This model constitutes an elementary block for a 2D or 3D model of fractionalized FL.
I'll derive its continuum limit using non-Abelian bosonization.

The 1st step is to linearize the spectrum of 1DEG:

$$\epsilon(k) \approx \pm v_F(k \mp k_F)$$

$$\psi(x) = e^{-ik_F x}R(x) + e^{ik_F x}L(x)$$

Bosonization of 1DEG

$$F_R^a = \frac{1}{2} R^+ \sigma^a R, F_L^a = \frac{1}{2} L^+ \sigma^a L$$

Belong to the $SU_1(2)$ Kac-Moody algebra for spin currents and

$$I_R^z = R_\alpha^+ R_\alpha, \quad I_R^+ = R_\uparrow^+ R_\downarrow^+, \quad I_R^- = R_\downarrow R_\uparrow$$

belong to the $SU_1(2)$ Kac-Moody algebra for charge currents:

$$[j_R^a(x), j_R^b(x')] = i\epsilon^{abc} j_R^c(x)\delta(x-x') + \frac{i}{4\pi}\delta_{ab}\delta'(x-x')$$

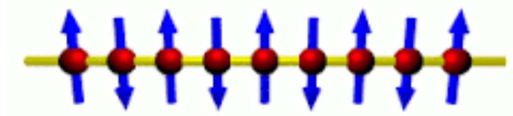
The Hamiltonian density of the 1DEG (free fermions) is

$$\mathcal{H}_{charge} = \frac{2\pi v_F}{3}\Big(: \mathbf{I}_R \mathbf{I}_R : + : \mathbf{I}_L \mathbf{I}_L : \Big)$$

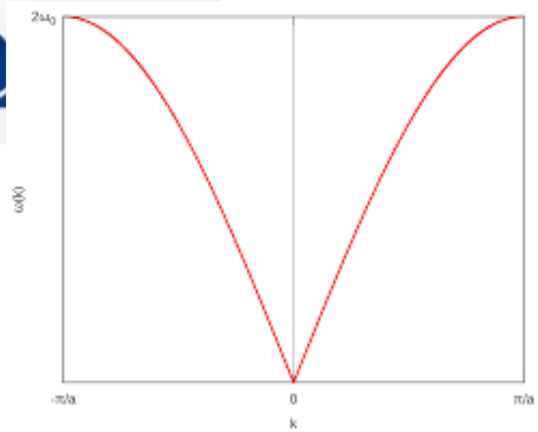
$$\mathcal{H}_s = \frac{2\pi v_F}{3}(: \mathbf{F}_R \mathbf{F}_R : + : \mathbf{F}_L \mathbf{F}_L :),$$

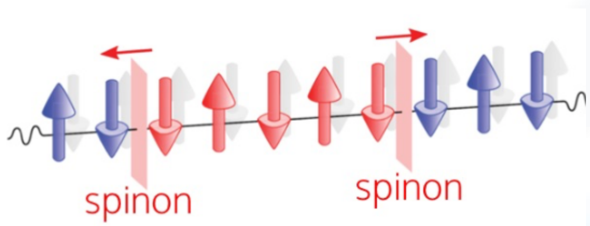
Heisenberg antiferromagnetic S=1/2 chain

At high energies we see individual spins.
But it is not them who is active at low energies.



At energies << J_H we see **collective** excitations - **spinon** waves traveling in opposite directions:





Each spinon carries spin ½,
The spectrum can be split into
Right and **Left** movers.

Bosonization of the S=1/2 Heisenberg chain

$$\mathcal{H}_H = \frac{2\pi v_H}{3}(:\mathbf{j}_L\mathbf{j}_L: + :\mathbf{j}_R\mathbf{j}_R:).$$

$$v_H = \pi J_H/2$$

$$\mathbf{S}_n = [\mathbf{j}_R(x) + \mathbf{j}_L(x)] + (-1)^n \mathbf{N}_s(x) + ..., \quad x = na_0$$

$$\frac{1}{2}\psi^+\vec{\sigma}\psi(x) = \mathbf{F}_R + \mathbf{F}_L + \left[e^{2ik_F x}\mathbf{s} + H.c.\right] + ...,$$

The Hamiltonian is the same as the spin part of the electron gas.

Formation of the spin liquid

- Since 1DEG and Heisenberg chain are incommensurate, the staggered components of the magnetizations do not couple.

$$\frac{1}{2}\psi^{+}\vec{\sigma}\psi(x)\vec{S} \rightarrow (\mathbf{F}_R + \mathbf{F}_L)(\mathbf{j}_L + \mathbf{j}_R)$$

The *strictly marginal* interaction of currents of *same chirality* can be neglected.

$$\mathcal{H}_{eff} = \mathcal{H}_{charge} + \mathcal{H}_s^{(Rl)} + \mathcal{H}_s^{(Lr)},$$

$$\mathrm{H}_s^{(Rl)} = \frac{2\pi v_F}{3} : \mathbf{F}_R\mathbf{F}_R : + \frac{2\pi v_H}{3} : \mathbf{j}_L\mathbf{j}_L : + J_K\mathbf{F}_R\mathbf{j}_L,$$

$$\mathrm{H}_s^{(Lr)} = \frac{2\pi v_F}{3} : \mathbf{F}_L\mathbf{F}_L : + \frac{2\pi v_H}{3} : \mathbf{j}_R\mathbf{j}_R : + J_K\mathbf{F}_L\mathbf{j}_R,$$

These models are exactly solvable (N. Andrei, 1980).

Spin gap formation in a single KH ladder.

- When *k_F not equal to $\pi/2$*, spinons from 1DEG pair with spinons of opposite chirality from spin chain. The result is *TWO branches* of gapped spinons.

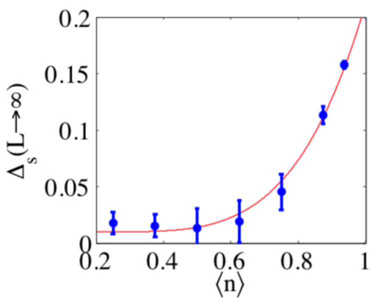
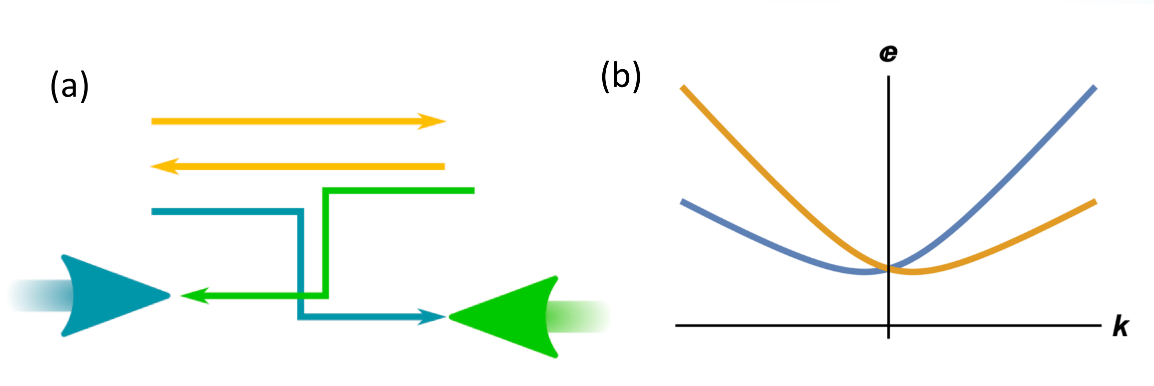


FIG. 1: (Color online.) The spin gap vs. the electron concentration in the 1DEG. $J_H = J_K = 2t$. The error bars are a result of the extrapolation to the thermodynamic limit. (Relative to the extrapolation error, the DMRG truncation error is negligible.)

Berg et.al. PRL 105, 146403 (2010)



$$E(k)_\pm = \pm k(v_H - v_F)/2 + \sqrt{k^2(v_F + v_H)^2/4 + \Delta^2},$$

$$\Delta = C\sqrt{J_K J_H}\exp[-\pi(v_F + v_H)/J_K],$$

Exact solution, N. Andrei, 1980

Order parameters of KH ladder

$$\mathcal{O}_{cdw} = \psi^+(x)\Big[(\mathbf{S}_x\mathbf{S}_{x+a_0})\hat{I} + i(\vec{\sigma}\mathbf{S}_x)\Big]\psi(x)e^{i(\pi/a_0+2k_F)x}$$

$$\mathcal{O}_{sc} = i(-1)^{x/a_0}\psi(x)\sigma^y\Big[(\mathbf{S}_x\mathbf{S}_{x+a_0})\hat{I} + i(\vec{\sigma}\mathbf{S}_x)\Big]\psi(x)$$

$$\Delta_{OSC} = \dot{\psi}(\tau,x)\sigma^y\psi(\tau,x)(-1)^{x/a_0}, \quad \Delta_{OCDW} = \dot{\psi}^+(\tau,x)\psi(\tau,x)\mathrm{e}^{\mathrm{i}(2k_F+\pi/a_0)x}$$

$$\hat{\mathcal{O}} = \begin{pmatrix} \mathcal{O}_{cdw} & \mathcal{O}^+_{sc} \\ -\mathcal{O}_{sc} & \mathcal{O}^+_{cdw} \end{pmatrix} = A\hat{g},$$

A is a numerical amplitude and g is an SU(2) matrix.

- The wave vector of the Friedel oscillations $2k_F + \pi/a_0$ includes ALL electrons (Oshikawa theorem).

The operators can be factorized:

$$z_\sigma = (2\pi a_0)^{-1/4} \exp[i\sigma\sqrt{2\pi}\varphi], \quad \bar{z}_\sigma = (2\pi a_0)^{-1/4} \exp[-i\sigma\sqrt{2\pi}\bar{\varphi}], \quad \sigma = \pm 1.$$

$$\mathrm{z}_\sigma = z^+_{-\sigma}.$$

For instance, the WZNW matrix field for the Heisenberg model and the 1DEG fermior

$$\hat{G}(x) = (-1)^n \Big[A(\mathbf{S}_n \mathbf{S}_{n+1}) + iB(\boldsymbol{\sigma}\mathbf{S}_n) \Big], \quad x = a_0 n,$$

can be written as $$G_{\sigma\sigma'} = \frac{1}{\sqrt{2}} e^{i\pi(1-\sigma\sigma')/4} z^H_\sigma [\bar{z}^H{}_{\sigma'}]^+.$$

$$R_\sigma = \xi_\sigma \Big(z^c_- z^s_\sigma \Big), \quad L_\sigma = \xi_\sigma \Big(\bar{z}^c_- \bar{z}^s_\sigma \Big)$$

From z-quanta of various WZNW one can construct **nonlocal OPs** of the spin liqu

$$\langle \mathcal{O}_{rL} \rangle = \sum_\sigma \langle z^s_\sigma [\bar{z}^H{}_\sigma]^+ \rangle, \quad \langle \mathcal{O}_{lR} \rangle = \sum_\sigma \langle [\bar{z}^s_\sigma]^+ z^H_\sigma \rangle$$

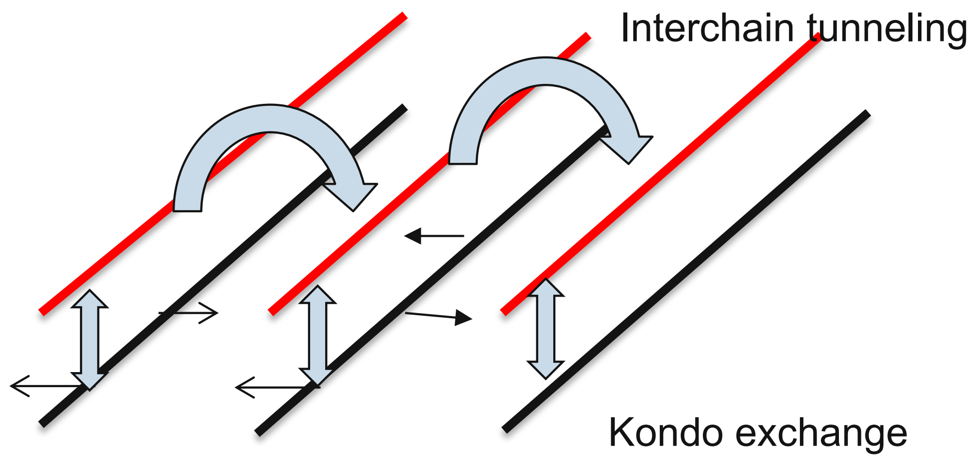
Robustness against local perturbations

- All local primary fields both for 1DEG and Heisenberg chains can be factorized.

- Chiral parts of spin operators pair with parts with opposite chirality from 1DEG. Therefore the perturbations cannot acquire a vacuum average and thus lift the ground state degeneracy.

Beyond 1D: coupled layers: red – electrons, black - spins

Electrons tunnel between the chains. This tunneling will also generate an exchange between the Heisenberg chains.



$$H_{tunn} = t\sum_y \int dx(\psi_y^+(x)\psi_{y+1}(x) + H.c.),$$

$$H_{ex} = \sum_y \tilde{J}\int dx \mathbf{N}_y(x)\mathbf{N}_{y+1}(x), \qquad \tilde{J}_{ferro} \sim -J_K^2 t^2/W^3$$

Collective excitations

- If the interchain tunneling is smaller than the spin gap, the only gapless excitations are collective ones.
- The system undergoes an ordering transition at some T, above it it is a Bose metal.

Ginzburg-Landau functional

- Since OPs contain localized spins, to arrange the Josephson coupling *one needs spin exchange* besides the tunneling:

$$S = \sum_y \Big[W[g_y] - \mathcal{J} \int_0^{1/T} d\tau \int dx \mathrm{Tr}(\sigma^z g_y \sigma^z g^+_{y+1} + H.c.) \Big]$$

$$\mathcal{J} \sim \tilde{J}(t/\Delta)^2$$

To get the Fermi pockets one needs **t ~Δ**, but since the exchar
is an independent
parameter, the transition temperature
may be **<<** than the Fermi energy of QPs.

Few facts about WZNW models

The action of the $SU_1(2)$ WZNW model can be written in terms of SU(2) matrix field:

$$W[g] = \frac{1}{16\pi}\int d\tau dx \mathrm{Tr}(\partial_\mu g^+ \partial_\mu g) - \frac{i}{24\pi}\int_0^\infty d\xi \int d\tau dx \epsilon^{\alpha\beta\gamma}\mathrm{Tr}(g^+\partial_\alpha g g^+ \partial_\beta g g^+ \partial_\gamma g).$$

However, it can also be written in terms of the free bosonic field:

$$\mathcal{H}_{charge} = \frac{v_F}{2}\Big[(\partial_x\Theta_c)^2 + (\partial_x\Phi_c)^2\Big]$$

$$[\Phi_c(x), \partial_x\Theta_c(x')] = i\delta(x - x')$$

Then important objects are holomorphic (dependent on $z = \tau - ix/v_F$) and antiholomorphic fields:

$$\varphi = (\Phi + \Theta)/2, \quad \bar{\varphi} = (\Phi - \Theta)/2.$$

Ginzburg-Landau theory – similar to He^3 -A

- The order parameter is SU(2) matrix and can be parametrized by three angles or by angle ϕ and a unit vector

$$g = \exp\left(\frac{\mathrm{i}}{2}\sigma^z\phi\right)\exp\left(\frac{\mathrm{i}}{2}\sigma^x\theta\right)\exp\left(\frac{\mathrm{i}}{2}\sigma^z\psi\right).$$

$$F = \frac{1}{2}\int \mathrm{d}V\left(\omega^3_\mu\rho^{\|}_{\mu\nu}\omega^3_\nu + \partial_\mu \mathbf{n}\rho^{\perp}_{\mu\nu}\partial_\nu \mathbf{n}\right),$$

$$\omega^3_\mu = \partial_\mu\phi - \cos\theta\partial_\mu\psi, \quad \mathbf{n} = (\cos\theta, \sin\theta\cos\psi, \sin\theta\sin\psi).$$

$$\partial_\mu\phi \rightarrow \partial_\mu\phi - (2e/c)A_\mu, \quad \partial_\mu\psi \rightarrow \partial_\mu\psi + (2e/c)A_\mu.$$

Magnetic field will not destroy the OP, it will just rotate it from SC to CDW.
At $H > H_{c1}$ the flux is equal to the *topological charge* of **n**-field.

Quasipartices

When the interchain tunneling is sufficiently strong, pockets of quasiparticles appear:

$$G(\omega, \mathbf{k}) = [G_{1D}^{-1}(\omega, k_x) - t(\mathbf{k})]^{-1},$$

When

$$|t(k_y)| > 3.33\Delta(v_F/v_H)^{1/2}$$

the RPA Green's function has poles.

The Green's functions

- The *single particle Green's function* is calculated from the symmetry considerations using a minimal information from the exact solution (Essler, Tsvelik, 2001):

$$G(\omega, k \pm k_F) = G_{RR,LL}(\omega, k), \quad G_{RR}(\omega, k) = G_{LL}(\omega, -k)$$

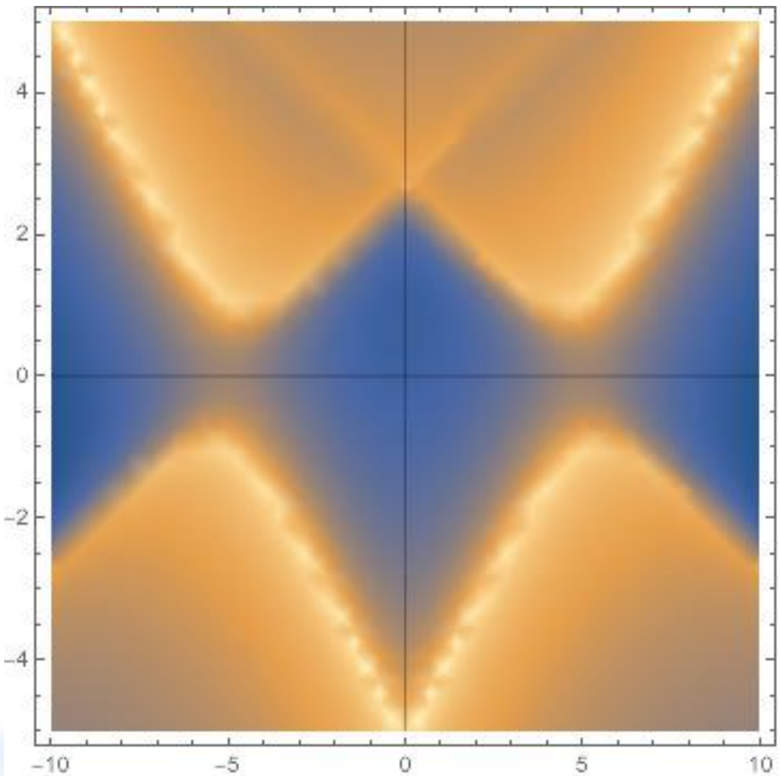
$$\mathrm{G}_{RR}(\omega, k) = \frac{Z_0}{\omega - v_F k}\left[\frac{\Delta}{\sqrt{-(\omega - v_F k)(\omega + v_H k) + \Delta^2}} - 1\right] + \ldots,$$

The Luttinger theorem is fulfilled through zeroes:

$$G(0, \pm k_F) = 0$$

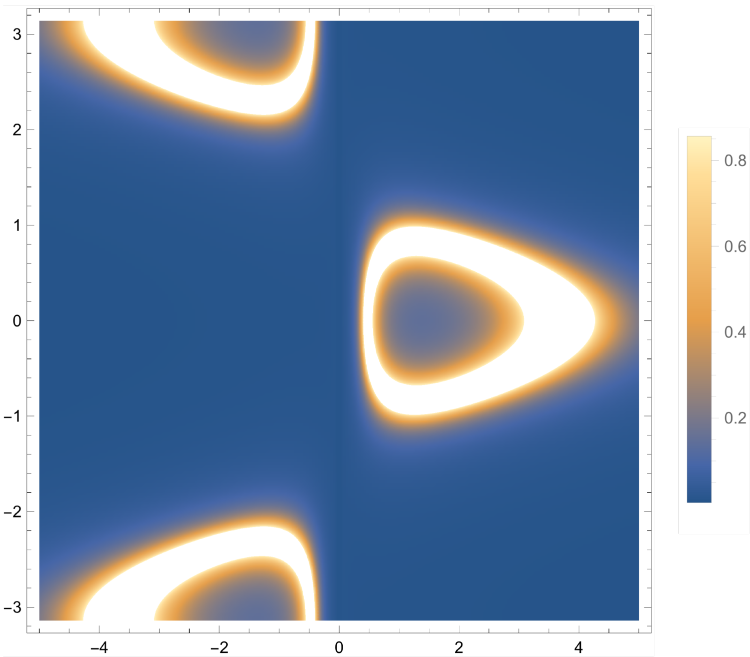
The *single particle Green's function* for a single chain calculated from the exact solution (Essler, Tsvelik, 2001):

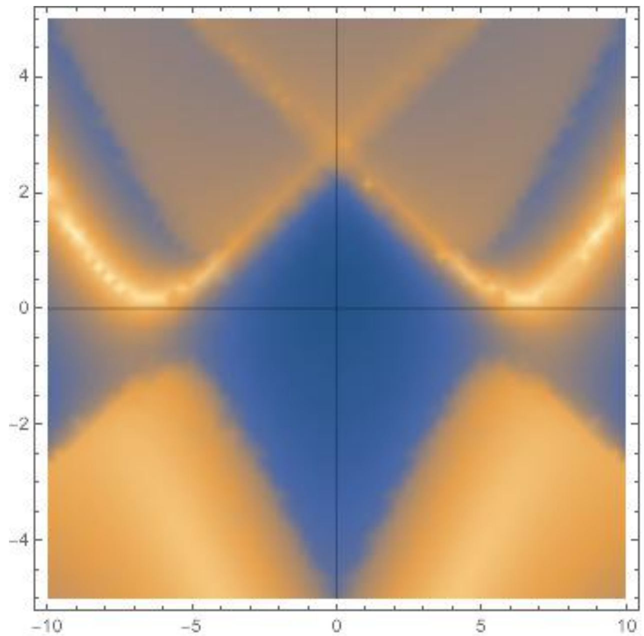
$$G(\omega, k \pm k_F) = G_{RR,LL}(\omega, k), \quad G_{RR}(\omega, k) = G_{LL}(\omega, -k)$$



$$\mathrm{G}_{RR}(\omega, k) = \frac{Z_0}{\omega - v_F k}\left[\frac{\Delta}{\sqrt{-(\omega - v_F k)(\omega + v_H k) + \Delta^2}} - 1\right] + ...,$$

When interchain tunneling is allowed, spinons and holons recombine into quasiparticles which propagate in D>1. The q.-p. dispersion is in the gap.





In Random Phase approximation we have

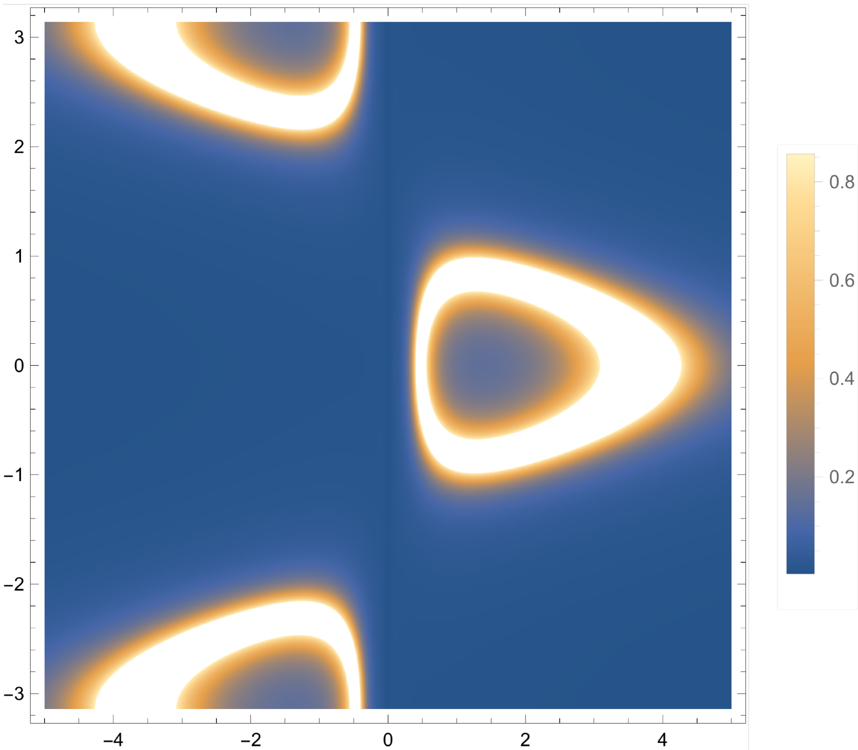
$$G(\omega, \mathbf{k}) = [G_{1D}^{-1}(\omega, k_x) - t(\mathbf{k})]^{-1},$$

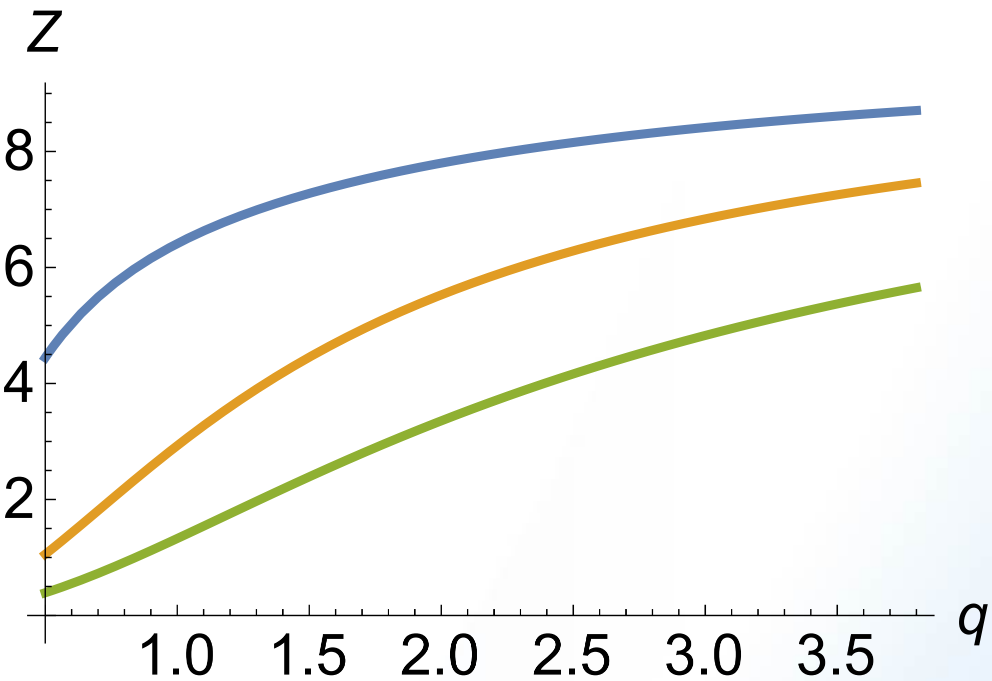
There are quasiparticle poles when

$$|t(k_y)| > 3.33\Delta(v_F/v_H)^{1/2}$$

The plot of the quasiparticle weight near $k_x = k_F$ for $t_0 (v_H/v_F)^{1/2}/\Delta = 5$ and $v_F/v_H = 0.1$. The vertical axis is $k_y b$, the horizontal is $q = (k_x - k_F)(v_H v_F)^{1/2}/\Delta$.

That is how small Fermi surface is formed!
The fractionized particles still exist at finite energies.





The plot of the quasiparticle weight near *$k_x = k_F$* for $t_0 (v_H / v_F)^{1/2} / \Delta = 5$ and $v_F / v_H = 0.1$. The vertical axis is $k_y b$, the horizontal is $q = (k_x - k_F)(v_H v_F)^{1/2} / \Delta$.

The *quasiparticle residue* *Z* as a function o $q = k_x (v_H v_F)^{1/2} / \Delta$ for (from top to bottom) $v_F / v_H = 3, 1, 0.1$.

Stability of the RPA solution

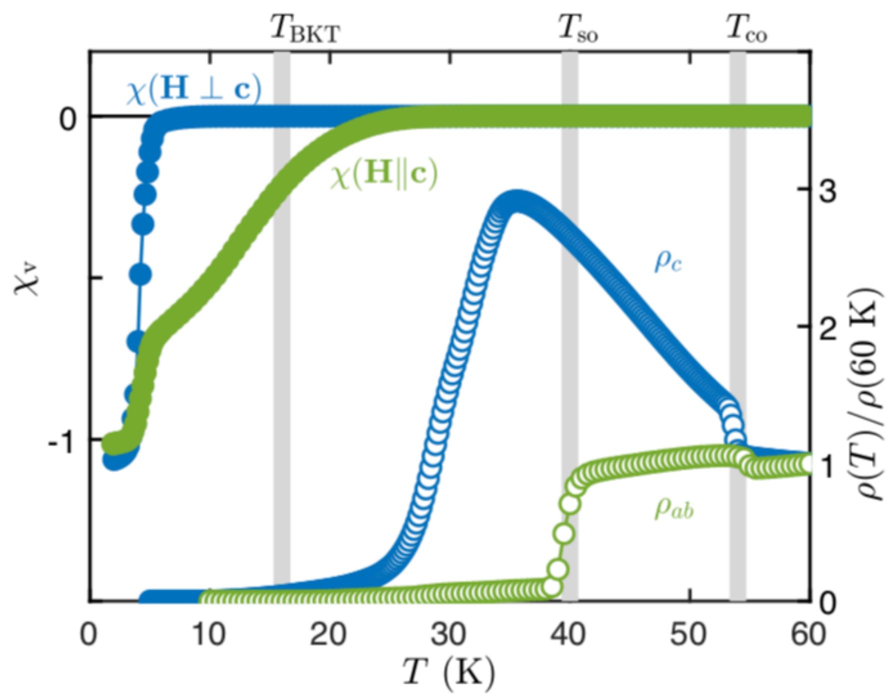
- The quasiparticle FS can be destroyed by two processes.
- **A.)** There is interaction between the gapless collective modes which leads to 3D order.
- - The coupling between the OPs from different chains is an independent parameter: **$T_c << E_F$** .
- **B.)** The QPs can couple to the collective modes:
- **- not possible,** the OPs wave vectors do not connect particle and hole FSs.

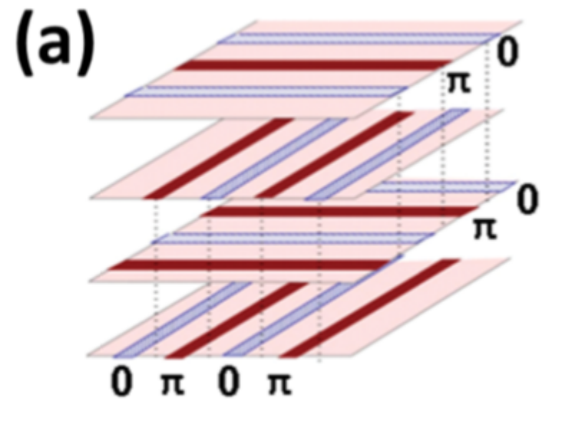
Is the ground state topological?

- Forget for a moment that the charge modes interact.
- Then the GS of spin sector of each chain is 4-times degenerate. Hence the GS of the array is 4^N – degenerate.
- This degeneracy cannot be probed by any local operator.
- In reality this picture holds only approximately, since the charge sector orders at some T.

Are there any material realizations?

Pair Density Wave in $La_{2-x}\ Ba_x\ CuO_2$ with x=1/8.





- Q.Li et.al. PRL 99, 067001 (2007)

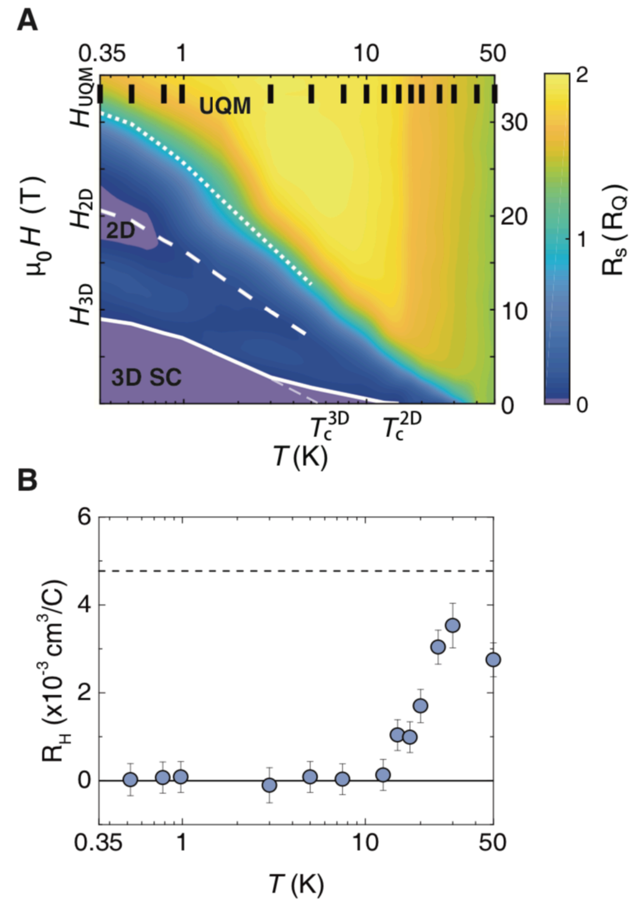
Are there any material realizations? Continued

- Stripe ordered

$La_{2-x}Ba_xCuO_2$ with x=1/8.

- Phase diagram in magnetic field

- T-dependence of the Hall coefficient.



Y. Li et.al. Sci. Adv. 5, eaav7686 (2019);

Tsvelik, PNAS 116, 12729 (2019)

The problem

- May we have a metallic state in **D>1** where the Fermi surface volume is not related to the electron density, as it appears to be in the pseudogap phase of the cuprates?
- Senthil, Sachdev and Vojta (2005): *yes*, but the GS must have a nontrivial topology and fractionalized excitations.
- Their approach: gauge theories. Alas, too many uncontrollable steps.
- My approach: consider a *quasi-1D* model, treat the strongest interactions nonperturbatively in 1D and the rest of them approximately in controlled steps.

Conclusions

- One may have a metallic state where the FS volume is not related to the electron density (in the given case $\mathbf{V_{FS} = 0}$).
- The Luttinger theorem is fulfilled due to the *zeroes* of G(0,k).
- For the KH model it is shown that this state is topologically nontrivial, as was suggested by Senthil *et.al* (2005).