Instability of 3-band Tomonaga-Luttinger liquids: renormalization group analysis and possible application to K₂Cr₃As₃



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Cr based superconductors under ambient pressure: A₂Cr₃As₃ (A=K,Rb,Cs)



Quasi-1D crystal and electronic structure



Guang-Han Cao's group, Phys. Rev. X 5, 011013 (2015). arXiv:1412.0067



Jiang, Cao, Cao, arXiv:1412.1309 (2014)

Specific heat: deviation from BCS



Large Sommerfeld coefficient

Guang-Han Cao's group, Phys. Rev. X 5, 011013 (2015); Phys. Rev. B 91, 020506(R) (2015); Science China Materials, 58(1) 16-10 (2015).



Magnetic field dependent y(H)

 $\succ \gamma(H) \equiv C_v/T \propto H^{1/2}$ indicates nodes in the gap function



Guang-Han Cao's group, Phys. Rev. B 91, 020506(R) (2015).

Upper critical field H_{c2}



Science China Materials, 58(1) 16-10 (2015). Ames' group, RRB 91, 020507(R) (2015).



Rb₂Cr₃As₃

Angle resolved upper critical field



ZengWei Zhu, Guang-Han Cao et. al., arXiv:1511.06169

Penetration depth: K₂Cr₃As₃



Linear T dependent penetration depth is an evidence for line nodal superconducting gap.

H. Q. Yuan's group in ZJU, PRB 91, 220502(R) (2015).





ISIS facilty, Phys. Rev. B 92, 134505 (2015)

Unconventional superconducting states

Specific heat

- Large Sommerfeld coefficient: band renormalization
- Large specific-heat jump: deviation from BCS scenario

G.H. Cao et al. (2014, 2015)

Upper critical field

• Exceeding Pauli limit: $2H_P$ for H//c; $3.4H_P$ for H//ab

G.H. Cao et al. (2014, 2015), Ames' group (2015)

• Three-fold or six-fold modulation of H_{c2}

Z.W. Zhu et al. (2015)

NMR/NQR

- Absence of Hebel-Slichter coherence peak
- $1/T_1T \propto T^4$? or T^5 (T^5 indicates point nodal gap)

T. Imai et al. (2015); G.q. Zheng et al. (2015)

- Penetration depth
 - $\Delta\lambda \propto T$ (line nodal gap)

H.Q. Yuan et al. (2015)

muSR

• Weak evidence of a spontaneous internal magnetic field above T_c

ISIS facility (2015)

Normal state: NMR / NQR



Normal state: transport, polycrystal



Normal state: smectic metal



 $\rho_c = \rho_0 + AT^{\alpha}, \alpha \approx 3$

Guang-Han Cao's group (unpublished)

Previous theoretical studies

Yi Zhou, Chao Cao, and Fu-Chun Zhang, arXiv:1502.03928

- Effective Hamiltonian in 3D
- Superconducting instability by RPA

Other groups

• Strong coupling approach

Xianxin Wu, Fan Yang, Congcong Le, Heng Fan, Jiangping Hu, arXiv:1503.06707

• Effective Hamiltonian for a single-tube Cr2As3

Hanting Zhong, Xiao-Yong Feng, Hua Chen, Jianhui Dai, arXiv:1503.08965

Extract tight-binding model from DFT



At least three orbitals per unit cell are required to catch the low energy electronic features.

A three-orbital model is sufficient to describe both 1D and 3D features for superconductivity.



Jiang, Cao, Cao, arXiv:1412.1309 (2014)

Three-orbital model

$D_{3h} = D$	$\Theta_3 \times \sigma_h(\bar{6}m2)$		E	$2C_3$	$3C_2$	σ_h	$2S_3$	$3\sigma_v$
$x^2 + y^2, z^2$	$x(x^2 - 3y^2)$	(A'_1)	1	1	1	1	1	1
	$y(3x^2 - y^2)$	$\overline{A'_2}$	1	1	-1	1	1	-1
$(x^2 - y^2, xy)$	$(x,y),(xz^2,yz^2)$	(E')	2	-1	0	2	-1	0
$yz(3x^2 - y^2)$		$\widetilde{A_1''}$	1	1	1	-1	-1	-1
$xz(x^2 - 3y^2)$	z,z^3	A_2''	1	1	-1	-1	-1	1
(xz, yz)	$(z(x^2 - y^2), zxy)$	E''	2	-1	0	-2	1	0

TABLE I: Character table for D_{3h} group.

Selected by the principle of symmetry.

➤ Too many atomic orbitals, more than 10 atomic orbitals per unit cell.

> Three relevant molecular (per Cr_6As_6 cluster) orbitals: A'_1 and E' states.

Neglect spin-orbit coupling at first for simplicity.

Yi Zhou, Chao Cao, and Fu-Chun Zhang, arXiv:1502.03928

Crystal: D_{3h} point group



Superconducting pairing instability

Parameters:

$$U_1 = U'_1 = U, U'_2 = U_2 \text{ and } J' = J$$

The results are similar when 0.5 < J'/J < 2.

All the dominant states are spin-triplet states.

> For small *U*, the pairing arises from 3D γ -band, and has spatial *f*-wave symmetry when *J/U*>1/3.

- Driving force: Hund's coupling
- Line nodes in the gap function

DOS at Fermi level at γ-band is the largest

>For large *U*, a fully gapped *p*-wave state dominates at the quasi-1D α -band.



lssues

• How the superconducting state is related to the smectic metal normal state?

Superconducting instability in a single-tube K₂Cr₃As₃?

- Spin-orbit coupling will mix spin-singlet and spin-triplet SC pairing through broken inversion symmetry.
- Which component (singlet or triplet) will be more important?
- Why Rb compound exhibit different temperature dependence in 1/T1 from K compound in the normal state?

1D three-band Hubbard model

Hamiltonian



А

Irreducible representations for D_{3h} group $\Rightarrow U = U' + 2J$ We also set J = J'

Scattering processes and "g-ology"

Single-band scattering processes

back scattering



forward scattering (intra-chirality)



Umklapp scattering



forward scattering (inter-chirality)



Three-band scattering processes

	chirality	band				spin		
$g^{(1)}$	$\psi_p^{\dagger}\psi_{\bar{p}}^{\dagger}\psi_p\psi_{\bar{p}}$	g_1	$\psi_m^{\dagger}\psi_{\bar{m}}^{\dagger}\psi_m\psi_{\bar{m}}$	f_1	$\psi_m^{\dagger}\psi_0^{\dagger}\psi_m\psi_0 + h.c.$	$ g_{\parallel} $	$\psi^{\dagger}_{\sigma}\psi^{\dagger}_{\sigma}\psi_{\sigma}\psi_{\sigma}$	
$g^{(2)}$	$\psi_p^{\dagger}\psi_{\bar{p}}^{\dagger}\psi_{\bar{p}}\psi_p$	g_2	$\psi_m^{\dagger}\psi_{\bar{m}}^{\dagger}\psi_{\bar{m}}\psi_m$	f_2	$\psi_m^{\dagger}\psi_0^{\dagger}\psi_0\psi_m + h.c.$	g_{\perp}	$\psi^{\dagger}_{\sigma}\psi^{\dagger}_{\bar{\sigma}}\psi_{\bar{\sigma}}\psi_{\sigma}$	
$g^{(3)}$	$\psi_p^{\dagger}\psi_p^{\dagger}\psi_{\bar{p}}\psi_{\bar{p}}$	g_3	$\psi_m^{\dagger}\psi_m^{\dagger}\psi_{\bar{m}}\psi_{\bar{m}}$	f_3	$\psi_m^{\dagger}\psi_m^{\dagger}\psi_0\psi_0 + h.c.$			
$g^{(4)}$	$\psi_p^{\dagger}\psi_p^{\dagger}\psi_p\psi_p$	g_4	$\psi_m^{\dagger}\psi_m^{\dagger}\psi_m\psi_m$	g	$\psi_0^\dagger \psi_0^\dagger \psi_0 \psi_0$			

Four dominant scattering processes at incommensurate filling





Bosonization for 1D systems

Abelian bosonization

$$\psi_{pm\sigma} = \frac{\eta_{m\sigma}}{\sqrt{2\pi a}} e^{ipk_{Fm}x} e^{-ip\varphi_{pm\sigma}}$$

$$\{\eta_{m\sigma}, \eta_{m'\sigma'}\} = 2\delta_{mm'}\delta_{\sigma\sigma'}$$

Chiral and non-chiral fields

$$\varphi_{pm\sigma} = \phi_{m\sigma} - p\theta_{m\sigma}$$

 $\nabla \phi_{m\sigma} \propto n_{m\sigma} = \psi_{Rm\sigma}^{\dagger} \psi_{Rm\sigma} + \psi_{Lm\sigma}^{\dagger} \psi_{Lm\sigma}$ $\nabla \theta_{m\sigma} \propto j_{m\sigma} = \psi_{Rm\sigma}^{\dagger} \psi_{Rm\sigma} - \psi_{Lm\sigma}^{\dagger} \psi_{Lm\sigma}$

Charge and spin degrees of freedom

$$\phi_{m\sigma} = \frac{1}{\sqrt{2}} \left(\phi_{cm} + \sigma \phi_{sm} \right)$$
$$\theta_{m\sigma} = \frac{1}{\sqrt{2}} \left(\theta_{cm} + \sigma \theta_{sm} \right)$$

Gauge choice for Klein factors

$$\eta_{m\sigma}\eta_{\bar{m}\sigma} = im\sigma$$
$$\eta_{m\sigma}\eta_{\bar{m}\sigma} = i\sigma$$
$$\eta_{m\sigma}\eta_{\bar{m}\sigma} = im$$
$$\eta_{0\sigma}\eta_{m\sigma} = im\sigma$$
$$\eta_{0\sigma}\eta_{0\bar{\sigma}} = i\sigma$$
$$\eta_{0\sigma}\eta_{m\bar{\sigma}} = im$$

Non-interacting bosonic Hamiltonian

$$H_0^B = \frac{1}{2\pi} \int dx \sum_{\substack{\mu = c, s \\ \nu = 0, \pm 1}} v_{\mu\nu} \left[K_{\mu\nu} \left(\nabla \theta_{\mu\nu} \right)^2 + \frac{1}{K_{\mu\nu}} \left(\nabla \phi_{\mu\nu} \right)^2 \right]$$

Luttinger liquid fixed point: gives rise to smectically metallic behaviors in normal state.

Renormalized Fermi velocities and Luttinger parameters

$$\begin{aligned} v_{c(s)\pm1} &= v_F \left\{ 1 - \frac{\left[\left(+ (-) g_{4\perp}^{(2)} \right) - \left(g_{2\parallel}^{(2)} + (-) g_{2\perp}^{(2)} \right) \right]^2}{(2\pi v_F)^2} \right\}^{1/2} \\ v_{c(s)0} &= v_F \left\{ 1 - \frac{\left[\left(+ (-) g_{4\perp}^{(2)} \right) + 2 \left(g_{2\parallel}^{(2)} + (-) g_{2\perp}^{(2)} \right) \right]^2}{(2\pi v_F)^2} \right\}^{1/2} \\ K_{c(s)\pm1} &= \left\{ \frac{1 - \frac{1}{2\pi v_F} \left[\left(+ (-) g_{4\perp}^{(2)} \right) - \left(g_{2\parallel}^{(2)} + (-) g_{2\perp}^{(2)} \right) \right]}{1 + \frac{1}{2\pi v_F} \left[\left(+ (-) g_{4\perp}^{(2)} \right) - \left(g_{2\parallel}^{(2)} + (-) g_{2\perp}^{(2)} \right) \right]} \right\}^{1/2} \\ K_{c(s)0} &= \left\{ \frac{1 - \frac{1}{2\pi v_F} \left[\left(+ (-) g_{4\perp}^{(2)} \right) + 2 \left(g_{2\parallel}^{(2)} + (-) g_{2\perp}^{(2)} \right) \right]}{1 + \frac{1}{2\pi v_F} \left[\left(+ (-) g_{4\perp}^{(2)} \right) + 2 \left(g_{2\parallel}^{(2)} + (-) g_{2\perp}^{(2)} \right) \right]} \right\}^{1/2} \end{aligned}$$

Interacting bosonic Hamiltonian

$$\begin{split} H_{int}^{B} &= -g_{1\perp}^{(1)} \frac{4}{(2\pi a)^{2}} \int dx \cos\left(\frac{2}{\sqrt{3}} \tilde{\phi}_{s-1} + \frac{4}{\sqrt{6}} \tilde{\phi}_{s0}\right) \cos\left(2\tilde{\theta}_{s+1}\right) \\ &+ g_{2\parallel}^{(1)} \frac{4}{(2\pi a)^{2}} \int dx \cos\left(2\tilde{\phi}_{c+1}\right) \cos\left(2\tilde{\phi}_{s+1}\right) \\ &+ g_{2\perp}^{(1)} \frac{4}{(2\pi a)^{2}} \int dx \cos\left(2\tilde{\phi}_{c+1}\right) \cos\left(\frac{2}{\sqrt{3}} \tilde{\phi}_{s-1} + \frac{4}{\sqrt{6}} \tilde{\phi}_{s0}\right) \\ &+ g_{3\parallel}^{(1)} \frac{4}{(2\pi a)^{2}} \int dx \cos\left(2\tilde{\theta}_{c+1}\right) \cos\left(2\tilde{\theta}_{s+1}\right) \\ &+ g_{3\perp}^{(1)} \frac{4}{(2\pi a)^{2}} \int dx \cos\left(2\tilde{\theta}_{c+1}\right) \cos\left(\frac{2}{\sqrt{3}} \tilde{\phi}_{s-1} + \frac{4}{\sqrt{6}} \tilde{\phi}_{s0}\right) \\ &+ g_{3\perp}^{(1)} \frac{4}{(2\pi a)^{2}} \int dx \cos\left(2\tilde{\theta}_{c+1}\right) \cos\left(\frac{2}{\sqrt{3}} \tilde{\phi}_{s-1} + \frac{4}{\sqrt{6}} \tilde{\phi}_{s0}\right) \\ &- g_{1\perp}^{(2)} \frac{4}{(2\pi a)^{2}} \int dx \cos\left(2\tilde{\phi}_{c+1}\right) \cos\left(2\tilde{\theta}_{s+1}\right) \\ &+ g_{3\perp}^{(2)} \frac{4}{(2\pi a)^{2}} \int dx \cos\left(2\tilde{\phi}_{c+1}\right) \cos\left(2\tilde{\theta}_{s+1}\right) \\ &- f_{1\perp}^{(1)} \frac{8}{(2\pi a)^{2}} \int dx \cos\left(2\tilde{\theta}_{c+1}\right) \cos\left(2\tilde{\theta}_{s-1} + \frac{4}{\sqrt{6}} \tilde{\phi}_{s0}\right) \cos\tilde{\theta}_{s+1} \cos\sqrt{3}\tilde{\theta}_{s-1} + (\cos \rightarrow \sin) \right] \\ &+ f_{3\parallel}^{(1)} \frac{8}{(2\pi a)^{2}} \int dx \left[\cos\tilde{\phi}_{c+1}\cos\sqrt{3}\tilde{\theta}_{c-1}\cos\tilde{\phi}_{s+1}\cos\sqrt{3}\tilde{\theta}_{s-1} + (\cos \rightarrow \sin)\right] \\ &+ f_{3\perp}^{(1)} \frac{8}{(2\pi a)^{2}} \int dx \left[\cos\tilde{\theta}_{c+1}\cos\sqrt{3}\tilde{\theta}_{c-1}\cos\tilde{\phi}_{s+1}\cos\left(-\frac{1}{\sqrt{3}}\tilde{\phi}_{s-1} + \frac{4}{\sqrt{6}}\tilde{\phi}_{s0}\right) + (\cos \rightarrow \sin) \right] \\ &+ f_{3\perp}^{(2)} \frac{8}{(2\pi a)^{2}} \int dx \left[\cos\tilde{\theta}_{c+1}\cos\sqrt{3}\tilde{\theta}_{c-1}\cos\tilde{\phi}_{s+1}\cos\sqrt{3}\tilde{\phi}_{s-1} + (\cos \rightarrow \sin)\right] \\ &+ g_{3\perp}^{(2)} \frac{2}{(2\pi a)^{2}} \int dx \left[\cos\tilde{\theta}_{c+1}\cos\sqrt{3}\tilde{\theta}_{c-1}\cos\tilde{\phi}_{s+1}\cos\sqrt{3}\tilde{\phi}_{s-1} + (\cos \rightarrow \sin)\right] \\ &+ g_{3\perp}^{(2)} \frac{2}{(2\pi a)^{2}} \int dx \left[\cos\tilde{\theta}_{c+1}\cos\sqrt{3}\tilde{\theta}_{c-1}\cos\tilde{\phi}_{s+1}\cos\sqrt{3}\tilde{\phi}_{s-1} + (\cos \rightarrow \sin)\right] \\ &+ g_{3\perp}^{(2)} \frac{2}{(2\pi a)^{2}} \int dx \left[\cos\tilde{\theta}_{c+1}\cos\sqrt{3}\tilde{\theta}_{c-1}\cos\tilde{\phi}_{s+1}\cos\sqrt{3}\tilde{\phi}_{s-1} + (\cos \rightarrow \sin)\right] \\ &+ g_{3\perp}^{(2)} \frac{2}{(2\pi a)^{2}} \int dx \cos\left(-\frac{4}{\sqrt{3}}\tilde{\phi}_{s-1} + \frac{4}{\sqrt{6}}\tilde{\phi}_{s0}\right) \end{aligned}$$

with all possible 13 running coupling constants

Order parameters

Definition

$$O_{ph}^{ij} = \sum_{mm'\sigma\sigma'} \lambda_{mm'}^{i} \sigma_{\sigma\sigma'}^{j} \psi_{Rm\sigma}^{\dagger} \psi_{Lm'\sigma'}$$
$$O_{pp}^{ij} = \sum_{mm'\sigma\sigma'} \lambda_{mm'}^{i} \sigma \sigma_{\sigma\sigma'}^{j} \psi_{Rm\sigma}^{\dagger} \psi_{Lm'\bar{\sigma'}}^{\dagger}$$

- λ^i : Gell-Mann matrices
- σ^{j} : Pauli matrices

Examples for bosonization

SDW

$$O_{ph}^{13} \propto e^{-i2k_F x + i\left(\frac{1}{\sqrt{3}}\tilde{\phi}_{c-1} + \frac{2}{\sqrt{6}}\tilde{\phi}_{c0}\right)} \left[\cos\left(\frac{1}{\sqrt{3}}\tilde{\phi}_{s-1} + \frac{2}{\sqrt{6}}\tilde{\phi}_{s0}\right)\sin\tilde{\theta}_{c+1}\cos\tilde{\theta}_{s+1} + i\left(\cos\leftrightarrow\sin\right)\right]$$

Spin-triplet superconducting state

$$O_{pp}^{23} \propto e^{i\left(\frac{1}{\sqrt{3}}\tilde{\theta}_{c-1} + \frac{2}{\sqrt{6}}\tilde{\theta}_{c0}\right)} \left[\cos\left(\frac{1}{\sqrt{3}}\tilde{\phi}_{s-1} + \frac{2}{\sqrt{6}}\tilde{\phi}_{s0}\right)\cos\tilde{\phi}_{c+1}\cos\tilde{\theta}_{s+1} - i\left(\cos\leftrightarrow\sin\right)\right]$$

Renormalization group

Operator product expansion (OPE)

$$\frac{dg_k}{dl} = (d - \Delta_k) g_k - \sum_{ij} C_{ij}^k g_i g_j$$

tree level one-loop

Renormalized coupling constants

$$y_i = \frac{g_i}{\pi v_F}$$
$$x_i = \frac{f_i}{\pi v_F}$$

Tree-level RG equations

$$\begin{split} \frac{dg_{1\perp}^{(1)}}{dl} &= \left[2 - \left(\frac{1}{3}K_{s-1} + \frac{2}{3}K_{s0} + K_{s+1}^{-1}\right)\right]g_{1\perp}^{(1)} \\ \frac{dg_{2\parallel}^{(1)}}{dl} &= \left[2 - \left(K_{c+1} + K_{s+1}\right)\right]g_{2\parallel}^{(1)} \\ \frac{dg_{2\perp}^{(1)}}{dl} &= \left[2 - \left(K_{c+1} + \frac{1}{3}K_{s-1} + \frac{2}{3}K_{s0}\right)\right]g_{2\perp}^{(1)} \\ \frac{dg_{3\parallel}^{(1)}}{dl} &= \left[2 - \left(K_{c+1}^{-1} + K_{s+1}^{-1}\right)\right]g_{3\parallel}^{(1)} \\ \frac{dg_{3\perp}^{(1)}}{dl} &= \left[2 - \left(K_{c+1}^{-1} + \frac{1}{3}K_{s-1} + \frac{2}{3}K_{s0}\right)\right]g_{4\perp}^{(1)} \\ \frac{dg_{4\perp}^{(1)}}{dl} &= \left[2 - \left(K_{c+1} + \frac{1}{3}K_{s-1} + \frac{2}{3}K_{s0}\right)\right]g_{4\perp}^{(1)} \\ \frac{dg_{4\perp}^{(2)}}{dl} &= \left[2 - \left(K_{c+1} + K_{s+1}^{-1}\right)\right]g_{1\perp}^{(2)} \\ \frac{dg_{3\perp}^{(2)}}{dl} &= \left[2 - \left(K_{c+1} + K_{s+1}^{-1}\right)\right]g_{3\perp}^{(2)} \\ \frac{df_{3\perp}^{(1)}}{dl} &= \left[2 - \left(K_{c+1} + K_{s+1}\right)\right]g_{3\perp}^{(2)} \\ \frac{df_{3\perp}^{(1)}}{dl} &= \left[2 - \left(\frac{1}{4}K_{s+1} + \frac{1}{12}K_{s-1} + \frac{2}{3}K_{s0} + \frac{1}{4}K_{s+1}^{-1} + \frac{3}{4}K_{s-1}^{-1}\right)\right]f_{1\perp}^{(1)} \\ \frac{df_{3\parallel}^{(1)}}{dl} &= \left[2 - \left(\frac{1}{4}K_{c+1}^{-1} + \frac{3}{4}K_{c-1}^{-1} + \frac{1}{4}K_{s+1}^{-1} + \frac{3}{4}K_{s-1}^{-1}\right)\right]f_{3\parallel}^{(1)} \\ \frac{df_{3\perp}^{(2)}}{dl} &= \left[2 - \left(\frac{1}{4}K_{c+1}^{-1} + \frac{3}{4}K_{c-1}^{-1} + \frac{1}{4}K_{s+1} + \frac{3}{12}K_{s-1} + \frac{2}{3}K_{s0}\right)\right]f_{3\perp}^{(1)} \\ \frac{df_{3\perp}^{(2)}}{dl} &= \left[2 - \left(\frac{1}{4}K_{c+1}^{-1} + \frac{3}{4}K_{c-1}^{-1} + \frac{1}{4}K_{s+1} + \frac{3}{4}K_{s-1}\right)\right]f_{3\perp}^{(2)} \\ \frac{dg_{3\perp}^{(1)}}{dl} &= \left[2 - \left(\frac{1}{4}K_{c+1}^{-1} + \frac{3}{4}K_{c-1}^{-1} + \frac{1}{4}K_{s+1} + \frac{3}{4}K_{s-1}\right)\right]f_{3\perp}^{(2)} \end{aligned}$$

Renormalize coupling constants

$$y_i = \frac{g_i}{\pi v_F}$$
$$x_i = \frac{f_i}{\pi v_F}$$

Expanding Luttinger paramters

$$K_{\mu\nu} = 1 - y_{\mu\nu}$$

with

$$y_{c\pm 1} = \frac{1}{2} \left[\left(y_{4\perp}^{(2)} \right) - \left(y_{2\parallel}^{(2)} + y_{2\perp}^{(2)} \right) \right]$$
$$y_{c0} = \frac{1}{2} \left[\left(y_{4\perp}^{(2)} \right) + 2 \left(y_{2\parallel}^{(2)} + y_{2\perp}^{(2)} \right) \right]$$
$$y_{s\pm 1} = \frac{1}{2} \left[\left(-y_{4\perp}^{(2)} \right) - \left(y_{2\parallel}^{(2)} - y_{2\perp}^{(2)} \right) \right]$$
$$y_{s0} = \frac{1}{2} \left[\left(-y_{4\perp}^{(2)} \right) + 2 \left(y_{2\parallel}^{(2)} - y_{2\perp}^{(2)} \right) \right]$$

Tree-level RG equations

$$\begin{split} \frac{dy_{1\perp}^{(1)}}{dl} &= \left(y_{2\parallel}^{(2)} - y_{2\perp}^{(2)}\right) y_{1\perp}^{(1)}, \\ \frac{dy_{2\parallel}^{(1)}}{dl} &= -y_{2\parallel}^{(2)} y_{2\parallel}^{(1)}, \\ \frac{dy_{3\parallel}^{(1)}}{dl} &= -y_{2\perp}^{(2)} y_{2\perp}^{(1)}, \\ \frac{dy_{3\parallel}^{(1)}}{dl} &= y_{2\parallel}^{(2)} y_{3\parallel}^{(1)}, \\ \frac{dy_{4\perp}^{(1)}}{dl} &= \left(-y_{4\perp}^{(2)} + y_{2\parallel}^{(2)}\right) y_{3\perp}^{(1)}, \\ \frac{dy_{4\perp}^{(1)}}{dl} &= -y_{2\perp}^{(2)} y_{4\perp}^{(1)}, \\ \frac{dy_{3\perp}^{(2)}}{dl} &= \left(-y_{4\perp}^{(2)} - y_{2\perp}^{(2)}\right) y_{1\perp}^{(2)}, \\ \frac{dy_{3\perp}^{(2)}}{dl} &= \left(-y_{4\perp}^{(2)} + y_{2\perp}^{(2)}\right) y_{3\perp}^{(2)}, \\ \frac{dx_{3\parallel}^{(1)}}{dl} &= \left(y_{2\parallel}^{(2)} - y_{2\perp}^{(2)}\right) x_{1\perp}^{(1)}, \\ \frac{dx_{3\parallel}^{(1)}}{dl} &= y_{2\parallel}^{(2)} x_{3\parallel}^{(1)}, \\ \frac{dx_{3\perp}^{(1)}}{dl} &= \left(-y_{4\perp}^{(2)} + y_{2\parallel}^{(2)}\right) x_{3\perp}^{(1)}, \\ \frac{dx_{3\perp}^{(2)}}{dl} &= \left(-y_{4\perp}^{(2)} + y_{2\parallel}^{(2)}\right) x_{3\perp}^{(1)}, \\ \frac{dx_{3\perp}^{(2)}}{dl} &= \left(-y_{4\perp}^{(2)} + y_{2\parallel}^{(2)}\right) x_{3\perp}^{(2)}, \\ \frac{dy_{\perp}^{(1)}}{dl} &= -y_{4\perp}^{(2)} y_{\perp}^{(1)}. \end{split}$$

Relevant coupling constants

$$\begin{array}{lll} J < U/3 & x_{3\parallel}^{(1)}, \ y_{3\parallel}^{(1)} \ \mbox{and} \ y_{1\perp}^{(2)} \\ \\ J > U/3 & y_{2\parallel}^{(1)} \ \mbox{and} \ y_{1\perp}^{(2)} \end{array}$$

Fixed points (hypersurface)

$$J < U/3 \qquad y_{3\parallel}^{(1)} = y_{3\parallel}^{(1)*}$$
$$y_{1\perp}^{(2)} = y_{1\perp}^{(2)*}$$
$$x_{3\parallel}^{(1)} = x_{3\parallel}^{(1)*}$$
$$J > U/3 \qquad y_{1\perp}^{(1)} = y_{1\perp}^{(1)*}$$

$$\begin{array}{l} y_{2\parallel}^{(1)} = y_{2\parallel}^{(1)*} \\ y_{1\perp}^{(2)} = y_{1\perp}^{(2)*} \end{array}$$

Insufficient to determine the ground state.
One-loop correction will change these results.

One-loop RG equations (spin rotational symmetry has been applied for simplicity)

$$\begin{split} \frac{dy_{1\perp}^{(1)}}{dl} &= -\left(y_{1\perp}^{(1)}\right)^2 - y_{2\perp}^{(1)}y_{1\perp}^{(2)} + y_{3\parallel}^{(1)}y_{3\perp}^{(1)}, \\ \frac{dy_{2\parallel}^{(1)}}{dl} &= \frac{1}{2}y_{1\perp}^{(1)}y_{2\parallel}^{(1)} - y_{2\perp}^{(1)}y_{4\perp}^{(1)}, \\ \frac{dy_{2\perp}^{(1)}}{dl} &= -\frac{1}{2}y_{1\perp}^{(1)}y_{2\perp}^{(1)} - y_{1\perp}^{(1)}y_{1\perp}^{(2)} - y_{2\parallel}^{(1)}y_{4\perp}^{(1)}, \\ \frac{dy_{3\parallel}^{(1)}}{dl} &= -\frac{1}{2}y_{1\perp}^{(1)}y_{3\parallel}^{(1)} + y_{1\perp}^{(1)}y_{3\perp}^{(1)}, \\ \frac{dy_{3\perp}^{(1)}}{dl} &= -\left(y_{4\perp}^{(1)} + \frac{1}{2}y_{1\perp}^{(1)}\right)y_{3\perp}^{(1)} + y_{1\perp}^{(1)}y_{3\parallel}^{(1)} - y_{4\perp}^{(1)}y_{3\perp}^{(2)}, \\ \frac{dy_{4\perp}^{(1)}}{dl} &= \frac{1}{2}y_{1\perp}^{(1)}y_{4\perp}^{(1)} - y_{2\parallel}^{(1)}y_{2\perp}^{(1)} - y_{3\perp}^{(1)}y_{3\perp}^{(2)}, \\ \frac{dy_{3\perp}^{(2)}}{dl} &= \left(-y_{4\perp}^{(1)} - \frac{1}{2}y_{1\perp}^{(1)}\right)y_{1\perp}^{(2)} - y_{1\perp}^{(1)}y_{2\perp}^{(1)}, \\ \frac{dy_{3\perp}^{(2)}}{dl} &= \left(-y_{4\perp}^{(1)} + \frac{1}{2}y_{1\perp}^{(1)}\right)y_{3\perp}^{(2)} - y_{3\perp}^{(1)}y_{4\perp}^{(1)}, \\ \frac{dx_{3\perp}^{(1)}}{dl} &= -\left(x_{1\perp}^{(1)}\right)^2 + x_{3\parallel}^{(1)}x_{3\perp}^{(1)}, \\ \frac{dx_{3\perp}^{(1)}}{dl} &= -\left(y_{\perp}^{(1)} + \frac{1}{2}x_{1\perp}^{(1)}\right)x_{3\perp}^{(1)} + x_{1\perp}^{(1)}x_{3\parallel}^{(1)}, \\ \frac{dx_{3\perp}^{(1)}}{dl} &= -\left(y_{\perp}^{(1)} + \frac{1}{2}x_{1\perp}^{(1)}\right)x_{3\perp}^{(2)}, \\ \frac{dx_{3\perp}^{(2)}}{dl} &= \left(-y_{\perp}^{(1)} + \frac{1}{2}x_{1\perp}^{(1)}\right)x_{3\perp}^{(2)}, \\ \frac{dx_{3\perp}^{(2)}}{dl} &= \left(-y_{\perp}^{(1)} + \frac{1}{2}x_{1\perp}^{(1)}\right)x_{3\perp}^{(2)}, \end{split}$$



Relevant scaling field and corresponding ground states

J < U/3

Scaling field	$x_{1\perp}^{(1)} + x_{3\perp}^{(1)}$	$y_{1\perp}^{(1)} + y_{3\perp}^{(1)}$	$y_{1\perp}^{(1)} - y_{2\perp}^{(1)}$
Instability	SDW	SDW	SSC
Order parameter	O_{ph}^{43}, O_{ph}^{63}	O_{ph}^{13}	O_{pp}^{20}
Saddle point	$\frac{1}{2}\tilde{\phi}_{s+1} - \frac{1}{\sqrt{12}}\tilde{\phi}_{s-1} + \frac{2}{\sqrt{6}}\tilde{\phi}_{s0} = 0\left(\frac{\pi}{2}\right) \\ \frac{1}{2}\tilde{\theta}_{c+1} + \frac{3}{\sqrt{12}}\tilde{\theta}_{c-1} = \frac{\pi}{2}\left(0\right) \\ \frac{1}{2}\tilde{\theta}_{s+1} + \frac{3}{\sqrt{12}}\tilde{\theta}_{s-1} = 0\left(\frac{\pi}{2}\right)$	$\frac{1}{\sqrt{3}}\tilde{\phi}_{s-1} + \frac{2}{\sqrt{6}}\tilde{\phi}_{s0} = 0\left(\frac{\pi}{2}\right)$ $\tilde{\theta}_{c+1} = \frac{\pi}{2}\left(0\right)$ $\tilde{\theta}_{s+1} = 0\left(\frac{\pi}{2}\right)$	$\frac{1}{\sqrt{3}}\tilde{\phi}_{s-1} + \frac{2}{\sqrt{6}}\tilde{\phi}_{s0} = 0\left(\frac{\pi}{2}\right)$ $\tilde{\phi}_{c+1} = \frac{\pi}{2}\left(0\right)$ $\tilde{\theta}_{s+1} = \frac{\pi}{2}\left(0\right)$

J > U / 3

Scaling field	$y_{2\perp}^{(1)} + y_{4\perp}^{(1)}$	$y_{1\perp}^{(1)} - y_{2\perp}^{(1)}$
Instability	SDW	TSC
Order parameter	$O_{ph}^{03} + rac{\sqrt{3}}{2} O_{ph}^{83}$	O_{pp}^{23}
Saddle point	$ \frac{1}{\sqrt{3}}\tilde{\phi}_{s-1} + \frac{2}{\sqrt{6}}\tilde{\phi}_{s0} = 0\left(\frac{\pi}{2}\right) $ $ \tilde{\phi}_{c+1} = \frac{\pi}{2}\left(0\right) $ $ \tilde{\phi}_{s+1} = \frac{\pi}{2}\left(0\right) $	$ \frac{1}{\sqrt{3}}\tilde{\phi}_{s-1} + \frac{2}{\sqrt{6}}\tilde{\phi}_{s0} = 0\left(\frac{\pi}{2}\right) $ $ \tilde{\phi}_{c+1} = 0\left(\frac{\pi}{2}\right) $ $ \tilde{\theta}_{s+1} = 0\left(\frac{\pi}{2}\right) $

Phase diagram

• Determined by initial coupling constants, say, the microscopic model.



U = U' + 2J

Normal state: TLL fixed point

NMR: Spin-lattice relaxation rate

$$\frac{1}{T_1} = A_f^2 T \sum_q \frac{Im\chi\left(q,\omega\right)}{\omega}$$

Three-band model

$$\frac{1}{T_{1}} \propto A_{1}T
+ A_{2}T^{\frac{1}{2}\left[\left(K_{c+1} + \frac{1}{3}K_{c-1} + \frac{2}{3}K_{c0}\right) + \left(K_{s+1} + \frac{1}{3}K_{s-1} + \frac{2}{3}K_{s0}\right)\right] - 1}
+ A_{3}T^{\frac{1}{2}\left[\left(\frac{4}{3}K_{c-1} + \frac{2}{3}K_{c0}\right) + \left(\frac{4}{3}K_{s-1} + \frac{2}{3}K_{s0}\right)\right] - 1}.$$
(C3)

Spin-rotational symmetric system

$$\frac{1}{T_1} \propto A \ T + B \ T^{1 - \frac{U}{2\pi v_F}}$$

U>0 and U<0 will result in different low temperature behaviors !

Possible superconducting ground states

0<J<U/3



spin-singlet, odd parity, orbital antisymmetric

U/3<J<U/2



spin-triplet, even parity, orbital antisymmetric

Discussion: Lifted degeneracy

• The two-fold degenerate of *E*' bands will be lifted by *inter-chain coupling*.



Interacting bosonic Hamiltonian when $k_{F-1} \neq k_{F1}$

$$\begin{split} H^B_{int} &= -g_{11}^{(1)} \frac{4}{(2\pi a)^2} \int dx \cos\left(\frac{2}{\sqrt{3}} \tilde{\phi}_{s-1} + \frac{4}{\sqrt{6}} \tilde{\phi}_{s0}\right) \cos\left(2\tilde{\theta}_{s+1}\right) \\ &+ g_{21}^{(1)} \frac{4}{(2\pi a)^2} \int dx \cos\left(2\Delta k_F x + 2\tilde{\phi}_{c+1}\right) \cos\left(\frac{2}{\sqrt{3}} \tilde{\phi}_{s-1} + \frac{4}{\sqrt{6}} \tilde{\phi}_{s0}\right) \\ &+ g_{31}^{(1)} \frac{4}{(2\pi a)^2} \int dx \cos\left(2\Delta k_F x + 2\tilde{\phi}_{c+1}\right) \cos\left(\frac{2}{\sqrt{3}} \tilde{\phi}_{s-1} + \frac{4}{\sqrt{6}} \tilde{\phi}_{s0}\right) \\ &+ g_{31}^{(1)} \frac{4}{(2\pi a)^2} \int dx \cos\left(2\tilde{\theta}_{c+1}\right) \cos\left(\frac{2}{\sqrt{3}} \tilde{\phi}_{s-1} + \frac{4}{\sqrt{6}} \tilde{\phi}_{s0}\right) \\ &+ g_{31}^{(1)} \frac{4}{(2\pi a)^2} \int dx \cos\left(2\tilde{\theta}_{c+1}\right) \cos\left(\frac{2}{\sqrt{3}} \tilde{\phi}_{s-1} + \frac{4}{\sqrt{6}} \tilde{\phi}_{s0}\right) \\ &+ g_{31}^{(1)} \frac{4}{(2\pi a)^2} \int dx \cos\left(2\tilde{\theta}_{c+1}\right) \cos\left(\frac{2}{\sqrt{3}} \tilde{\phi}_{s-1} + \frac{4}{\sqrt{6}} \tilde{\phi}_{s0}\right) \\ &+ g_{41}^{(1)} \frac{4}{(2\pi a)^2} \int dx \cos\left(2\tilde{\theta}_{c+1}\right) \cos\left(\frac{2}{\sqrt{3}} \tilde{\phi}_{s-1} + \frac{4}{\sqrt{6}} \tilde{\phi}_{s0}\right) \\ &+ g_{41}^{(1)} \frac{4}{(2\pi a)^2} \int dx \cos\left(2\tilde{\theta}_{c+1}\right) \cos\left(2\tilde{\theta}_{s+1}\right) \\ &- g_{41}^{(2)} \frac{4}{(2\pi a)^2} \int dx \cos\left(2\tilde{\theta}_{c+1}\right) \cos\left(2\tilde{\theta}_{s+1}\right) \\ &- g_{41}^{(2)} \frac{4}{(2\pi a)^2} \int dx \cos\left(2\tilde{\theta}_{c+1}\right) \cos\left(2\tilde{\theta}_{s-1}\right) \\ &- f_{11}^{(1)} \frac{8}{(2\pi a)^2} \int dx \left[\cos\tilde{\phi}_{s+1}\cos\left(-\frac{1}{\sqrt{3}} \tilde{\phi}_{s-1} + \frac{4}{\sqrt{6}} \tilde{\phi}_{s0}\right) \cos\tilde{\theta}_{s+1}\cos\sqrt{3}\tilde{\theta}_{s-1} + (\cos \rightarrow \sin)\right] \\ &+ f_{41}^{(1)} \frac{8}{(2\pi a)^2} \int dx \left[\cos\tilde{\theta}_{c+1}\cos\sqrt{3}\tilde{\theta}_{c-1}\cos\tilde{\phi}_{s+1}\cos\sqrt{3}\tilde{\theta}_{s-1} + (\cos \rightarrow \sin)\right] \\ &+ f_{31}^{(2)} \frac{8}{(2\pi a)^2} \int dx \left[\cos\tilde{\theta}_{c+1}\cos\sqrt{3}\tilde{\theta}_{c-1}\cos\tilde{\phi}_{s+1}\cos\sqrt{3}\tilde{\theta}_{s-1} + (\cos \rightarrow \sin)\right] \\ &+ f_{31}^{(2)} \frac{8}{(2\pi a)^2} \int dx \left[\cos\tilde{\theta}_{c+1}\cos\sqrt{3}\tilde{\theta}_{c-1}\cos\tilde{\phi}_{s+1}\cos\sqrt{3}\tilde{\theta}_{s-1} + (\cos \rightarrow \sin)\right] \\ &+ f_{31}^{(2)} \frac{8}{(2\pi a)^2} \int dx \left[\cos\tilde{\theta}_{c+1}\cos\sqrt{3}\tilde{\theta}_{c-1}\cos\tilde{\phi}_{s+1}\cos\sqrt{3}\tilde{\theta}_{s-1} + (\cos \rightarrow \sin)\right] \\ &+ f_{31}^{(2)} \frac{8}{(2\pi a)^2} \int dx \left[\cos\tilde{\theta}_{c+1}\cos\sqrt{3}\tilde{\theta}_{c-1}\cos\tilde{\phi}_{s+1}\cos\sqrt{3}\tilde{\theta}_{s-1} + (\cos \rightarrow \sin)\right] \\ &+ f_{31}^{(2)} \frac{8}{(2\pi a)^2} \int dx \left[\cos\tilde{\theta}_{c+1}\cos\sqrt{3}\tilde{\theta}_{c-1}\cos\tilde{\phi}_{s+1}\cos\sqrt{3}\tilde{\theta}_{s-1} + (\cos \rightarrow \sin)\right] \\ &+ f_{31}^{(2)} \frac{2}{(2\pi a)^2} \int dx \left[\cos\tilde{\theta}_{c+1}\cos\sqrt{3}\tilde{\theta}_{c-1}\cos\tilde{\phi}_{s+1}\cos\sqrt{3}\tilde{\theta}_{s-1} + (\cos \rightarrow \sin)\right] \\ &+ f_{31}^{(2)} \frac{2}{(2\pi a)^2}} \int dx \cos\left(-\frac{4}{\sqrt{3}}\tilde{\phi}_{s-1} + \frac{4}{\sqrt{6}}\tilde{\phi}_{s0}\right), \end{aligned}$$

Consequences of lifted degeneracy

- SSC be suppressed, SDW have chance to dominate for J<U/3
- Interband pairing will be modulated by a phase factor
 - Possible FFLO state?
 - Unstable when the degeneracy lift becomes significant.

Phase diagrams





Take home message

One-loop RG analysis to 1D three-band Hubbard model

- Assumption 1: Two of the three bands are (nearly) degenerate
- Assumption 2: Incommensurate electron filling

Results:

- 0<J<U/3, spin-singlet SC (degenerate bands) or spin density wave (non-degenerate bands)
- U/3<J<U/2, spin-triplet SC (nearly degenerate bands)</p>
- ➤ J>U/2 (unphysical region), SDW
- > Possible application to superconductor $K_2Cr_3As_3$
 - Take Luttinger liquid normal state as the starting point
 - Inter-chain coupling will lift band degeneracy and SDW will dominate over SSC when J/U <1/3; while TSC will always dominate over SDW when J/U >1/3.
 - Inter-chain coupling will determine the spatially pairing symmetry



がすうさよ。 ZheJiang University

Thank you !

WITE HALL

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