



Pair Density Wave in the Presence of a Nested Fermi Surface

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Jin-Tao Jin, Kun Jiang^{*}, Hong Yao[†] and Yi Zhou[‡], PRL, **129**, 167001 (2022).

Outline

1. Pair Density Wave (PDW)

Definition and general properties

PDW in the presence of a nested fermi surface (FS)

2. Experimental observables in kagome SC AV_3Sb_5 (A=K, Rb, Cs)

Normal state

Superconducting state

3. A related phenomenological model

Model Hamiltonian and ground state

Density of states

Quasiparticle interference

4. Summary and outlook

Pair Density Wave

BCS effective Hamiltonian

$$H = \sum_{\mathbf{k}\sigma} \xi_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \frac{1}{N} \sum_{\mathbf{k}\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow} c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow}$$

• Mean-field $\langle c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow} \rangle$

$$H = \sum_{\mathbf{k}\sigma} \xi_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} - \sum_{\mathbf{k}} \left(\Delta_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow} + \Delta^{*}_{\mathbf{k}} c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \right) + \sum_{\mathbf{k}} \Delta_{\mathbf{k}} \left\langle c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow} \right\rangle$$



- Gap function $\Delta_{\mathbf{k}} = -\frac{1}{N} \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \left\langle c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow} \right\rangle$
- > Why zero momentum pairing?

$$\xi_{\mathbf{k}} = \xi_{-\mathbf{k}}$$



Finite momentum pairing?

FFLO state in the presence of extra magnetic field



FF: $\Delta(\mathbf{r}) \propto e^{i\mathbf{Q}\cdot\mathbf{r}}$ LO: $\Delta(\mathbf{r}) \propto \cos(\mathbf{Q}\cdot\mathbf{r} + \phi)$

P. Fulde, R.Ferrell, Phys. Rev. 135, A550-63 (1964).A. Larkin, Y.Ovchinnikov, JETP 20, 762 (1965.)



 κ -(BEDT-TTF)₂Cu(NCS)₂

Nature Physics, **10**(12):928–932, 2014.

Pair density wave (PDW)

 $\Delta_{\mathbf{Q}} = -g \langle c_{\mathbf{k},\uparrow} c_{-\mathbf{k}+\mathbf{Q},\downarrow} \rangle \neq 0 \quad \text{with no extra field}$

- Break translational symmetry
- Amperean pairing in cuprates $|\mathbf{Q}| \simeq 2k_F$

Patrick A. Lee. PRX, 4:031017 (2014).

> Experimental evidences of possible PDW SC

Cuprates Bi₂Sr₂CaCu₂O₈ Science, **364**, 976, (2019) Bi₂Sr₂CuO_{6+ δ} PRX, **11**, 011007 (2021)

Nature **599**, 222–228 (2021)

 CsV_3Sb_5

Gapless fermi surfaces of Bogoliubov quasiparticles



- Descendant orders (secondary orders in PDW state)
- Charge density wave (CDW) order

$$\rho_{\mathbf{P}_i-\mathbf{P}_j} \propto (\Delta_{\mathbf{P}_i} \Delta^*_{\mathbf{P}_j} + \Delta_{-\mathbf{P}_j} \Delta^*_{-\mathbf{P}_i})$$

• Charge-4e SC order (uniform)

$$\Delta_{4e} \propto \Delta_{\mathbf{P}} \Delta_{-\mathbf{P}}$$

• Ising nematic order

$$\epsilon_{x^2-y^2} \propto (|\Delta_{\mathbf{P}_x}|^2 + |\Delta_{-\mathbf{P}_x}|^2 - |\Delta_{\mathbf{P}_y}|^2 - |\Delta_{-\mathbf{P}_y}|^2)$$

Annu. Rev. Condens. Matter Phys. 11, 231 (2020)

Nested fermi surface





Parallel fermi surface



tetragonal lattice

hexagonal lattice

PDW pairing on parallel fermi surface segments



The nesting feature allows full pairing in the region near the FS!

Kagome Materials AV₃Sb₅

Normal state



- **Cs:** Triangular lattice
- V: Kagome lattice
- Sb: Honeycomb lattice







Hexagonal first Brillouin Zone (BZ) Nearly nested fermi surface

PRL, **125**, 247002 (2020)

Superconducting state

S-Wave Superconductivity in Kagome Metal CsV₃Sb₅ Revealed by ^{121/123}Sb NQR and ⁵¹V NMR Measurements

Chin. Phys. Lett. 38, 077402 (2021)



Fig. 3. Temperature dependence of ΔK of ¹²¹Sb with (a) $H \parallel a$, (b) $H \parallel a^*$, and (c) $H \parallel c$, where a and a^* are orthogonal directions in the basal plane. The vertical dashed lines indicate the position of T_c .

Knight shift: spin-singlet pairing



Fig. 4. Temperature dependence of ${}^{121}(1/T_1T)$ (left axis) and ${}^{123}(1/T_1T)$ (right axis). A Hebel–Slichter coherence peak appears just below T_c . The curve and line are guides to the eyes.

Hebel–Slichter coherence peak below T_c : no sign-change of gap • Tunneling diode oscillator: magnetic penetration depth

Nodeless superconductivity in the kagome metal CsV₃Sb₅

Sci. China Phys. Mech. Astron. 64, 107462 (2021)

$$\Delta\lambda(T) \sim T^{-\frac{1}{2}} \exp\left(-\frac{\Delta(0)}{k_{\rm B}T}\right)$$
 • Multiband s-wave

• STM: density of states (DOS)



Multiband Superconductivity with Sign-Preserving Order Parameter in Kagome Superconductor CsV₃Sb₅

PRL 127, 187004 (2021)

• Thermal conductivity: residual DOS in the SC state

Nodal superconductivity and superconducting domes in the topological Kagome metal CsV₃Sb₅

arXiv:2102.08356





Roton pair density wave in a strong-coupling kagome superconductor

Nature **599**, 222–228 (2021)





The AV₃Sb₅ is shown to be a spin-singlet SC hosting s-wave features

A residual thermal transport at T = 0 and "multigap" V-shaped DOS with residual zero-energy contributions conflict with the conventional s-wave nature

A PDW state ordering has been observed in STM measurements



Kagome superconductors AV₃Sb₅ (A=K, Rb, Cs), *National Science Review*, nwac199 (2022)

Phenomenological Model

Model Hamiltonian

$$H = \sum_{\mathbf{k},\sigma} \xi_{\mathbf{k}} c_{\mathbf{k},\sigma}^{\dagger} c_{\mathbf{k},\sigma} + \sum_{\mathbf{k},\alpha} [\Delta_{\mathbf{Q}_{\alpha}}(\mathbf{k}) c_{\mathbf{k},\uparrow}^{\dagger} c_{-\mathbf{k}+\mathbf{Q}_{\alpha},\downarrow}^{\dagger} + \Delta_{-\mathbf{Q}_{\alpha}}(\mathbf{k}) c_{\mathbf{k},\uparrow}^{\dagger} c_{-\mathbf{k}-\mathbf{Q}_{\alpha},\downarrow}^{\dagger} + \mathrm{H.c.}]$$

$$\xi_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu = -2\{\cos(k_x) + \cos\left[\frac{1}{2}k_x + \sqrt{3}/2\right)k_y] + \cos\left[\frac{1}{2}k_x - (\sqrt{3}/2)k_y\right] + 1\}$$

$$\begin{split} \Delta_{\pm \mathbf{Q}_{\alpha}}(\mathbf{k}) &= \Delta_{\pm \mathbf{Q}_{\alpha}} \exp\left[-(|\xi_{\mathbf{k}}| + |\xi_{-\mathbf{k}\pm \mathbf{Q}_{\alpha}}|)/(2\Lambda)\right] \\ & \Lambda : \text{energy cutoff} \\ \Delta_{\pm \mathbf{Q}_{\alpha}} &= \Delta e^{i\theta_{\alpha}} e^{\pm i(\phi_{\alpha}/2)} \\ \end{split}$$

• Real space pairing function

$$\Delta(\mathbf{r}) \propto \sum_{\alpha} e^{i\theta_{\alpha}} \cos\left(\mathbf{Q}_{\alpha} \cdot \mathbf{r} + \frac{\phi_{\alpha}}{2}\right) \quad \begin{array}{l} \phi_{\alpha} \neq 0 : \text{ Inversion symmetry breaking} \\ \theta_{\alpha} \neq 0, \pi : \text{ Time reversal symmetry breaking} \end{array}$$



$$\mathbf{Q}_{\alpha} = \frac{1}{4}\mathbf{G}_{\alpha}$$



$$\begin{split} \hat{C}_{\mathbf{k},\sigma}^{\dagger} = & (c_{\mathbf{k},\sigma}^{\dagger}, c_{\mathbf{k}+\mathbf{Q}_{1},\sigma}^{\dagger}, c_{\mathbf{k}-\mathbf{Q}_{1},\sigma}^{\dagger}, c_{\mathbf{k}+\mathbf{Q}_{2},\sigma}^{\dagger}, c_{\mathbf{k}-\mathbf{Q}_{2},\sigma}^{\dagger}, c_{\mathbf{k}+\mathbf{Q}_{3},\sigma}^{\dagger}, \\ & c_{\mathbf{k}-\mathbf{Q}_{3},\sigma}^{\dagger}, c_{\mathbf{k}+2\mathbf{Q}_{1},\sigma}^{\dagger}, c_{\mathbf{k}+2\mathbf{Q}_{2},\sigma}^{\dagger}, c_{\mathbf{k}+2\mathbf{Q}_{3},\sigma}^{\dagger}, c_{\mathbf{k}+\mathbf{Q}_{1}-\mathbf{Q}_{2},\sigma}^{\dagger}, \\ & c_{\mathbf{k}-\mathbf{Q}_{1}+\mathbf{Q}_{2},\sigma}^{\dagger}, c_{\mathbf{k}+\mathbf{Q}_{2}-\mathbf{Q}_{3},\sigma}^{\dagger}, c_{\mathbf{k}-\mathbf{Q}_{2}+\mathbf{Q}_{3},\sigma}^{\dagger}, \\ & c_{\mathbf{k}+\mathbf{Q}_{3}-\mathbf{Q}_{1},\sigma}^{\dagger}, c_{\mathbf{k}-\mathbf{Q}_{3}+\mathbf{Q}_{1},\sigma}^{\dagger}), \end{split}$$

Diagonalize the 32 by 32 matrix gives rise to the energy spectrum

$$H_{\mathbf{k}} = \sum_{i=1}^{16} E(\mathbf{k})_{i}^{+} \gamma_{\mathbf{k},\uparrow,i}^{\dagger} \gamma_{\mathbf{k},\uparrow,i} + E(\mathbf{k})_{i}^{-} (-\gamma_{-\mathbf{k},\downarrow,i}^{\dagger} \gamma_{-\mathbf{k},\downarrow,i} + 1)$$

- Particle-hole symmetry: $E(\mathbf{k})_i^+ = -E(-\mathbf{k})_i^-$
- 4 by 4 folding of the BZ: $E(\mathbf{k})_i^{\pm} = E(\mathbf{k} \pm \mathbf{Q}_{\alpha})_i^{\pm}$

Ground state

Condensation energy

$$E_{c}[\phi_{\alpha}, \theta_{\alpha}] = (1/N) \sum_{\mathbf{k}} \left[(1/16) \sum_{i=1}^{16} \sum_{s=\pm} \sum_{E(\mathbf{k})_{i}^{s} > 0} E(\mathbf{k})_{i}^{s} - |\xi_{\mathbf{k}}| \right]$$



 $c_{\mathbf{r},\sigma} \mapsto e^{i\theta_1/2}c_{\mathbf{r},\sigma} \quad [\theta_1, \theta_2, \theta_3] \mapsto [0, \theta_2 - \theta_1, \theta_3 - \theta_1]$



$$\phi_{\alpha} = \pm \frac{\pi}{2}$$
$$\theta_2 - \theta_1 = \theta_3 - \theta_2 = \pm \frac{2\pi}{3} \mod \pi$$

Inversion and time reversal symmetry breaking

Nat. Mater. **20**, 1353 (2021) Nature **602**, 245 (2022) Sci. Bull. **66**, 1384 (2021)

Ginzburg Landau free energy

Gorkov Green's function

$$\mathcal{G}^{-1}(i\omega_n, \mathbf{k}) \equiv \mathcal{G}^{-1}_0(i\omega_n, \mathbf{k}) + \Sigma(\mathbf{k}) \qquad \qquad \mathcal{G}^{-1}_0(i\omega_n, \mathbf{k}) = \begin{pmatrix} G^{-1}_0(i\omega_n, \mathbf{k}) & 0\\ 0 & -G^{-1}_0(-i\omega_n, -\mathbf{k}) \end{pmatrix}, \ \Sigma(\mathbf{k}) = \begin{pmatrix} 0 & -\hat{\Delta}(\mathbf{k})\\ -\hat{\Delta}^{\dagger}(\mathbf{k}) & 0 \end{pmatrix}$$

• free energy

$$\mathcal{F}[\Delta_{\pm \mathbf{Q}_{\alpha}}] \equiv -\frac{1}{16\beta} \sum_{n,\mathbf{k}} \operatorname{Tr} \ln \mathcal{G}^{-1}(i\omega_n,\mathbf{k}) = \mathcal{F}^{(0)} - \frac{1}{16\beta} \sum_{n,\mathbf{k}} \operatorname{Tr} \ln (1 + \mathcal{G}_0(i\omega_n,\mathbf{k})\Sigma(\mathbf{k})) = \mathcal{F}^{(0)} + \sum_{j=1}^{\infty} \mathcal{F}^{(2j)}(i\omega_j,\mathbf{k}) = \mathcal{F}^{(0)} + \sum_{j=1}^{\infty} \mathcal{F}^{(2j)}(i\omega_j,\mathbf{k}) = \mathcal{F}^{(0)}(i\omega_j,\mathbf{k}) = \mathcal{F}^{(0)}(i\omega_j,\mathbf$$

$$\mathcal{F}^{(2j)} = \frac{1}{32j\beta} \sum_{n,\mathbf{k}} \operatorname{Tr}\left[\left(\mathcal{G}_0(i\omega_n,\mathbf{k})\Sigma(\mathbf{k}) \right)^{2j} \right] = \frac{1}{16j\beta} \sum_{n,\mathbf{k}} \operatorname{Tr}\left[\left(-G_0(i\omega_n,\mathbf{k})\hat{\Delta}(\mathbf{k})G_0(-i\omega_n,-\mathbf{k})\hat{\Delta}^{\dagger}(\mathbf{k}) \right)^j \right]$$

$$\begin{split} \mathcal{F}^{(4)} = & g_{1}^{(4)} \left(\left| \Delta_{\mathbf{Q}_{1}} \right|^{4} + \left| \Delta_{-\mathbf{Q}_{1}} \right|^{4} + \left| \Delta_{\mathbf{Q}_{2}} \right|^{4} + \left| \Delta_{-\mathbf{Q}_{2}} \right|^{4} + \left| \Delta_{\mathbf{Q}_{3}} \right|^{4} + \left| \Delta_{-\mathbf{Q}_{3}} \right|^{4} \right) \\ & + g_{2}^{(4)} \left(\left| \Delta_{\mathbf{Q}_{1}} \right|^{2} \left| \Delta_{-\mathbf{Q}_{1}} \right|^{2} + \left| \Delta_{\mathbf{Q}_{2}} \right|^{2} \left| \Delta_{-\mathbf{Q}_{2}} \right|^{2} + \left| \Delta_{\mathbf{Q}_{3}} \right|^{2} \left| \Delta_{-\mathbf{Q}_{3}} \right|^{2} \right) \\ & + g_{3}^{(4)} \left(\left| \Delta_{\mathbf{Q}_{1}} \right|^{2} \left| \Delta_{\mathbf{Q}_{2}} \right|^{2} + \left| \Delta_{\mathbf{Q}_{2}} \right|^{2} \left| \Delta_{\mathbf{Q}_{3}} \right|^{2} + \left| \Delta_{\mathbf{Q}_{3}} \right|^{2} + \left| \Delta_{\mathbf{Q}_{3}} \right|^{2} \left| \Delta_{-\mathbf{Q}_{1}} \right|^{2} \left| \Delta_{-\mathbf{Q}_{2}} \right|^{2} + \left| \Delta_{-\mathbf{Q}_{2}} \right|^{2} \left| \Delta_{-\mathbf{Q}_{3}} \right|^{2} + \left| \Delta_{-\mathbf{Q}_{3}} \right|^{2} \left| \Delta_{-\mathbf{Q}_{3}} \right|^{2} \left| \Delta_{-\mathbf{Q}_{3}} \right|^{2} + \left| \Delta_{-\mathbf{Q}_{3}} \right|^{2} \left| \Delta_{-\mathbf{Q}_{3}} \right|^{2} \left| \Delta_{-\mathbf{Q}_{3}} \right|^{2} + \left| \Delta_{-\mathbf{Q}_{3}} \right|^{2} \left| \Delta_{-\mathbf{Q}_{3}} \right|^{2} \left| \Delta_{-\mathbf{Q}_{3}} \right|^{2} \right|^{2} \left| \Delta_{-\mathbf{Q}_{3}} \right|^{2} \left| \Delta_{-\mathbf{$$

Density of states

$$\Delta = 0.02, \Lambda = 0.1, \phi_{\alpha} = \frac{\pi}{2}, \theta_1 = 0, \theta_2 = \frac{2\pi}{3}, \theta_3 = -\frac{2\pi}{3}$$

 $\succ E(\mathbf{k})_1^+$ (particle) and $E(\mathbf{k})_1^-$ (hole) Bogoliubov fermi surface



CDW order

$$\rho(\mathbf{q}) = \frac{2}{N} \sum_{\mathbf{k}} \langle c_{\mathbf{k},\uparrow}^{\dagger} c_{\mathbf{k}+\mathbf{q},\uparrow} \rangle$$

Local DOS

$$\rho(\mathbf{q},\omega) = -\frac{2}{N} \sum_{\mathbf{k}} \sum_{j} \left[u(\mathbf{k})_{1j} u^* (\mathbf{k} + \mathbf{q})_{1j} \frac{\partial n_F \left(\omega - E(\mathbf{k})_j^+ \right)}{\partial \omega} + v(\mathbf{k})_{1j} v^* (\mathbf{k} + \mathbf{q})_{1j} \frac{\partial n_F \left(\omega - E(\mathbf{k})_j^- \right)}{\partial \omega} \right] \bar{\delta}_{\mathbf{k},\mathbf{k}+\mathbf{q}}$$

$$\begin{split} \rho_A(\omega) &= |\rho(\mathbf{q} = \mathbf{0}, \omega)|, \\ \rho_B(\omega) &= |\rho(\mathbf{q} = \pm \mathbf{Q}_1, \omega)| = |\rho(\mathbf{q} = \pm \mathbf{Q}_2, \omega)| = |\rho(\mathbf{q} = \pm \mathbf{Q}_3, \omega)|, \\ \rho_C(\omega) &= |\rho(\mathbf{q} = \pm 2\mathbf{Q}_1, \omega)| = |\rho(\mathbf{q} = \pm 2\mathbf{Q}_2, \omega)| = |\rho(\mathbf{q} = \pm 2\mathbf{Q}_3, \omega)|, \\ \rho_D(\omega) &= |\rho(\mathbf{q} = \pm (\mathbf{Q}_1 - \mathbf{Q}_2), \omega)| = |\rho(\mathbf{q} = \pm (\mathbf{Q}_2 - \mathbf{Q}_3), \omega)| = |\rho(\mathbf{q} = \pm (\mathbf{Q}_3 - \mathbf{Q}_1), \omega)| \end{split}$$

Nature **599**, 222–228 (2021) Phys. Rev. X **11**, 031026 (2021)





Quasiparticle interference (QPI)

In the presence of elastic scatterings, the LDOS will be modulated

$$\begin{split} \delta\rho(\mathbf{q},\omega) \\ &\equiv \rho_s(\mathbf{q},\omega) - \rho(\mathbf{q},\omega) \\ &= -\frac{1}{16\pi N} \sum_{\mathbf{k}} \mathrm{Im} \tilde{\mathrm{Tr}}[\hat{\mathcal{G}}(\mathbf{k}+\mathbf{q},\omega+i\delta)\hat{T}(\omega)\hat{\mathcal{G}}(\mathbf{k},\omega+i\delta)] \end{split}$$

• Scattering matrix

$$\hat{T}(\omega) = \left[(V_s \hat{\tau}_3)^{-1} - (1/N) \sum_{\mathbf{k}} \hat{\mathcal{G}}(\mathbf{k}, \omega + i\delta) \right]^{-1}$$

Electron spectrum function

 $A(\mathbf{k},\omega) = -(1/\pi) \mathrm{Im}[\hat{\mathcal{G}}(\mathbf{k},\omega+i\delta)]_{11}$

PRB 67, 020511(R) (2003)



 $\omega = 0.01 < \Delta$

Summary & Outlook

Summary

- A phenomenological model related to PDW in AV₃Sb₅
- Inversion and time-reversal symmetry breaking ground state
- Bogoliubov fermi surfaces and V-shaped multi-gap DOS
- Local DOS and CDW
- Quasiparticle interference

• Microscopic models and pairing mechanics of PDW in kagome materials

• Other descendant orders such as charge-4e SC order

• Similar models on other lattices with nested fermi surfaces

Thanks for your attention!