Superconductivity from piezoelectric interactions in Weyl semimetals

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Low-dimensional emergent phenomena in correlated systems and topological quantum matter
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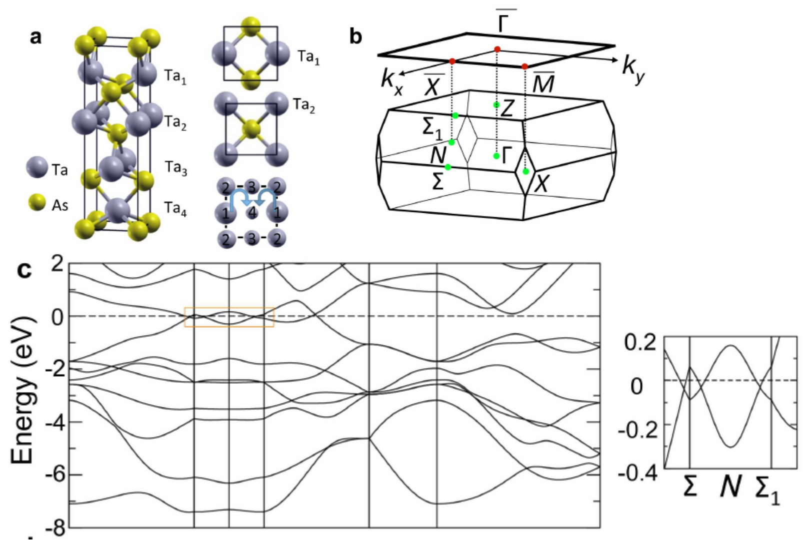
Outline

Introduction

TaAs

Xu et al. Science 349 (2015) 613; Lv et al. PRX 5 (2015) 031013 ; Nat. Phys. 11 (2015) 724



Huang et al. Nat. Commun. 6:7373 (2015) , Weng et al. PRX 5 011029 (2015)

Weyl semimetals

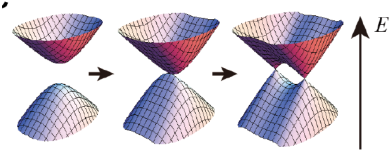
An *undoped* Weyl semimetal around each Weyl point:

$$H_0 = \sum_{\mathbf{p}} \psi^\dagger(\mathbf{p}) \left[v_\perp \left(p_1\sigma_1 + p_2\sigma_2 \right) + v_3 p_3 \sigma_3 \right] \psi(\mathbf{p}) \qquad \psi = (\psi_\uparrow, \psi_\downarrow)^t$$

- momentum $\mathbf{p}$ measured with respect to the *Weyl node* at $\pm\mathbf{b}$
- gapless dispersion relation

$$E(\mathbf{p}) = \pm\sqrt{v_\perp^2 \mathbf{p}_\perp^2 + v_3^2 p_3^2}$$

- no inversion symmetry
- gap closing between trivial insulator and topological insulator phases



- even number $2N$ of Weyl nodes
- robust. Destroyed only by:
  - scattering among nodes
  - violate charge conservation (superconductivity)

Murakami et al. Sci. Adv. 3 (2017) 1602680; Hosur & Qi, C. R. Physique 14, 857 (2013)

Lattice deformations

- Lattice displacement $\mathbf{R}_{atom} \to \mathbf{R}_{atom} + \mathbf{u}_{atom}$
- Continuum limit $\mathbf{u} = \mathbf{u}(\mathbf{r})$
- Euclidean action

$$S_{\mathrm{ph}} = \int d^4x \left(\frac{\rho_0}{2} (\partial_\tau \mathbf{u})^2 + \frac{1}{2} \sum_{ijkl} C_{ijkl} u_{ij} u_{kl} \right)$$

- linearized strain tensor

$$u_{jk} = \frac{1}{2} (\partial_j u_k + \partial_k u_j)$$

- stiffness tensor C_{ijkl}

$$C_{ijkl} \to \lambda \delta_{ij} \delta_{kl} + \mu \left(\delta_{il} \delta_{jk} + \delta_{ik} \delta_{jl} \right)$$

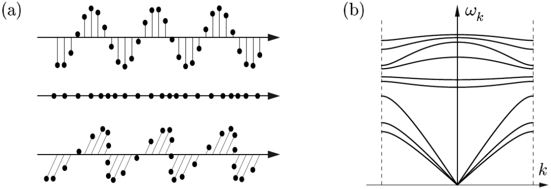
Landau & Lifshitz, Theory of Elasticity (1970)

Phonons

- Phonons = quantized excitation of the displacement

$$\mathbf{u}(\mathbf{r}) = \sum_{J=1}^{3} \sum_{\mathbf{q}} \frac{\epsilon^J(\mathbf{q}) e^{i\mathbf{q}\cdot\mathbf{r}}}{\sqrt{2\rho_0 \Omega_J(\mathbf{q})}} \left(a_J(\mathbf{q}) + a_J^\dagger(-\mathbf{q}) \right)$$

- In this work: *acoustic* phonons $\Omega_J(\mathbf{q}) = c_J(\hat{\mathbf{q}})\,|\mathbf{q}|$
- Polarization vectors $\epsilon^J(\hat{\mathbf{q}})$



- Sound velocities $c_J(\hat{\mathbf{q}}) \;\to\; c_t, c_l \;\sim\; c_{ph}$
- low temperature $k_B T \ll c_{ph}|\mathbf{b}|$

Piezoelectric interaction

Phonons in a piezoelectric material

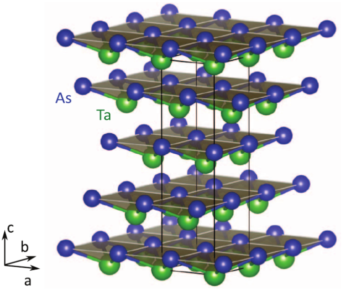
- Weyl SM can be obtained from noncentrosymmetric materials.

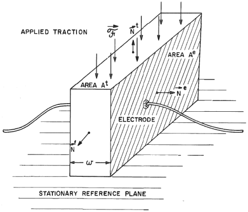
  Liu & Vanderbilt, PRB90 (2014) 155316

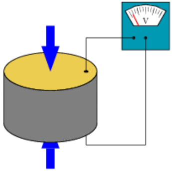
- TaAs, NbAs, NbP, TaP $\rightarrow C_{4v}$ polar symmetry class $4mm$

  Huang et al., Nature Comm. 6:7373 (2015)

- Piezoelectric materials







Nelson, *Electric, optic, acoustic interactions in dielectrics*, (1979)

The piezoelectric e-p interaction

Mahan, *Polarons in heavily doped superconductors* (1972)

Strain induces $\mathbf{D} \neq 0$:

$$D_i = e_{ijk} u_{jk} + \varepsilon_{ij} E_j$$

$e_{ijk} = \frac{\partial D_i}{\partial u_{jk}}$ = piezoelectric tensor, ε_{ij} = permittivity tensor

- No free charges:

$$\nabla \cdot \mathbf{D} = 0 \quad \Rightarrow \quad q_j D_j = 0 = q_j e_{jmn} u_{mn}(\mathbf{q}) + q_j \varepsilon_{jn} E_n(\mathbf{q})$$

- The electric field is (mainly) longitudinal:

$$E_n(\mathbf{q}) = \frac{q_n E(\mathbf{q})}{q}$$

Solve for E

$$E(\mathbf{q}) = -\frac{q q_j e_{jmn} u_{mn}(\mathbf{q})}{q_r \varepsilon_{rs} q_s}$$

and define a potential

$$\Phi(\mathbf{q}) = \frac{-i e_{jmn} q_j u_{mn}(\mathbf{q})}{q_r \varepsilon_{rs} q_s} \qquad \text{such that} \qquad \mathbf{E} = -\nabla \Phi$$

The piezoelectric interaction Hamiltonian

- $\varepsilon_{ij} = \varepsilon\delta_{ij}$
- Scalar potential Φ couples to the electronic charge density ρ_e
- piezoelectric e-p interaction Hamiltonian

$$H_{\rm pz} = \frac{e}{\varepsilon V}\sum_{ijk}\sum_{\mathbf{q}\neq 0} e_{ijk}\frac{q_i q_j}{\mathbf{q}^2}u_k(\mathbf{q})\rho_e(-\mathbf{q}).$$

Ziman, Electrons and phonons (1990); Vogl, PRB 13 (1976) 694

- long-range
- marginal in (3+1)D
- all other allowed e-p interaction are irrelevant

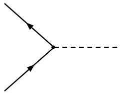
$$\psi_\pm^\dagger\sigma_0\psi_\pm\sum_j u_{jj} \qquad \psi_\pm^\dagger\sigma_0\psi_\pm u_{33} \qquad \psi_\pm^\dagger\sigma_3\psi_\pm\sum_j u_{jj}$$

$$\pm\sum_{j=1,2}\psi_\pm^\dagger\sigma_j\psi_\pm u_{j3} \qquad \psi_\pm^\dagger\sigma_0\psi_\pm\omega_3 \qquad \omega_j = \frac{1}{2}\varepsilon_{jkl}\partial_k u_l$$

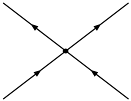
$$\ldots$$

Interactions

- electron-phonon interaction



- electron-electron interaction



- "Piezoelectric stiffening" 

$$S_{\text{int}} = \int \frac{d^4q}{(2\pi)^4}\left(\frac{e^2}{2\varepsilon|\mathbf{q}|^2}\rho_e(q)\rho_e(-q) + \frac{e}{\varepsilon}\sum_{ijk} e_{ijk}\frac{q_iq_j}{|\mathbf{q}|^2}u_k(q)\rho_e(-q)\right.$$

$$\left. + \frac{1}{2\varepsilon}\sum_{ijk}\sum_{lmn} e_{ijk}e_{lmn}\frac{q_iq_jq_lq_m}{|\mathbf{q}|^4}u_k(q)u_n(-q)\right)$$

Nelson, *Electric, optic, acoustic interactions in dielectrics*, (1979)

Decoupling

The interaction is carried by the auxiliary boson φ

$$S = S_{\mathrm{ph}} + \int d^4x \Big[\psi^* \partial_\tau \psi - iv\psi^* (\nabla \cdot \boldsymbol{\sigma})\psi + \frac{1}{2}(\nabla\varphi)^2 + ig_e \psi^* \psi\, \varphi + ig_{ph} \sum_{jkl} e_{jkl} \partial_j \varphi\, u_{kl} \Big]$$

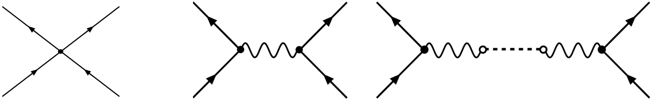
Integrating out φ, we obtain

$$S_{\mathrm{int}} = \int \frac{d^4q}{(2\pi)^4} \left(\frac{g_e^2}{2|\mathbf{q}|^2} \rho_e(q)\rho_e(-q) + g_e g_{ph} \sum_{ijk} e_{ijk} \frac{q_i q_j}{|\mathbf{q}|^2} u_k(q)\rho_e(-q) + + \frac{g_{ph}^2}{2} \sum_{ijk}\sum_{lmn} e_{ijk} e_{lmn} \frac{q_i q_j q_l q_m}{|\mathbf{q}|^4} u_k(q) u_n(-q) \right)$$

$$\Rightarrow \qquad g_e = \frac{e}{\sqrt{\varepsilon}}, \qquad g_{ph} = \frac{1}{\sqrt{\varepsilon}}$$

Effective e-e interaction

e-e interaction



Phonon correction to the Coulomb interaction in the *static* limit

$$V_{\rm tot}(\mathbf{q}) = \frac{g_e^2}{\mathbf{q}^2}\left(1 - \frac{g_{ph}^2}{\rho_0}\gamma(\hat{\mathbf{q}})\right)$$

with

$$\gamma(\hat{\mathbf{q}}) = \sum_{J=1}^{3}\gamma_J(\hat{\mathbf{q}}) \qquad \gamma_J(\hat{\mathbf{q}}) = \frac{1}{c_J^2(\hat{\mathbf{q}})|\mathbf{q}|^4}\left|\sum_{ijk} e_{ijk}q_i q_j \epsilon_k^J(\hat{\mathbf{q}})\right|^2$$

For the $4mm$ crystal class $e_{131}, e_{311}, e_{333} \neq 0$

$$\gamma_1(\theta) = \frac{e_{333}^2}{c_{ph}^2}\cos^2\theta\left[1 + (2A + B - 1)\sin^2\theta\right]^2,$$

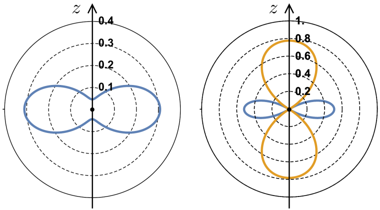
$$\gamma_2(\theta) = 0, \qquad A = \frac{e_{113}}{e_{333}}, \qquad B = \frac{e_{311}}{e_{333}}$$

$$\gamma_3(\theta) = \frac{e_{333}^2}{c_{ph}^2}\sin^2\theta\left[(B-1)\cos^2\theta + A\cos(2\theta)\right]^2$$

TaAs and beyond

left: $e_{333} = -1.89 C/m^2$
$\bar{\gamma} \simeq 0.20$

Buckeridge et al., PRB 93 (2016) 125205



Simplification: angular-averaged total interaction potential

$$\bar{V}_{\mathrm{tot}}(\mathbf{q}) = \frac{g_e^2(1-\bar{\gamma})}{\mathbf{q}^2}$$

with

$$\bar{\gamma} = \frac{g_{ph}^2}{2\rho_0}\int_0^\pi d\theta \sin(\theta)\gamma(\theta) = \frac{w_\gamma}{\rho_0}\left(\frac{g_{ph} e_{333}}{c_{ph}}\right)^2$$

$$w_\gamma = \frac{1}{15}\left[10A^2 + 4A(B+1) + 2B^2 + 3\right]$$

- $\bar{\gamma} > 1$ attractive effective e-e interaction
- $\bar{\gamma} < 1$ repulsive effective e-e interaction (TaAs)

Instability of the WS

Piezoelectric interaction within the static approximation: dimensionless coupling

$$\alpha_{eff} = \frac{g_e^2 (1 - \bar{\gamma})}{4\pi v}$$

RG:

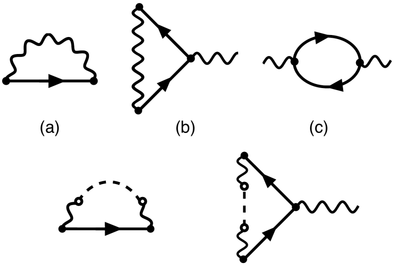
$$\frac{d\alpha_{\text{eff}}}{d\ell} = -\frac{4\alpha_{\text{eff}}^2}{3\pi}$$

Trockmorton et al. PRB 92, 115101 (2015)

- $\bar{\gamma} < 1$ WS
- $\bar{\gamma} > 1$ unstable $\rightarrow$ intrinsic superconductor (

Renormalization group

RG beyond the static approximation



(a) (b) (c) (d) (e)

$$\frac{dv}{d\ell} = \frac{g_e^2}{6\pi^2}\left[1 - \frac{3\pi\left(C_0 + \bar{C}\right)}{2}\frac{c_{ph}}{v}\frac{g_{ph}^2 e_{333}^2}{\rho_0 c_{ph}^2}\right],$$

$$\frac{dg_e}{d\ell} = -\frac{N g_e^3}{12\pi^2 v},$$

$$\frac{dg_{ph}}{d\ell} = -\frac{N g_e^2 g_{ph}}{12\pi^2 v}.$$

$$C_0 = \frac{1}{15\pi}\left(10A^2 + 4AB + 4A + 2B^2 + 3\right) \qquad \bar{C} = \frac{1}{105\pi}\left(42A^2 + 4AB + 4A + 2B^2 - 9\right)$$

RG flow equations

$$\frac{dv}{d\ell} = \frac{g_e^2}{6\pi^2}\left[1 - \frac{3\pi(C_0 + \bar{C})}{2}\frac{c_{ph}}{v}\frac{g_{ph}^2 e_{333}^2}{\rho_0 c_{ph}^2}\right],$$

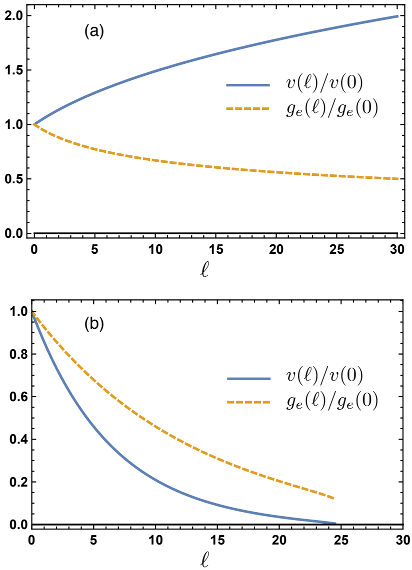
$$\frac{dg_e}{d\ell} = -\frac{N g_e^3}{12\pi^2 v},$$

$$\frac{dg_{ph}}{d\ell} = -\frac{N g_e^2 g_{ph}}{12\pi^2 v}.$$

- generally $\frac{c_{ph}}{v} << 1$
- v increases for TaAs ($\bar{\gamma} = 0.20$)

J. Buckeridge et al. PRB 93, 125205 (2016)

- critical value $\bar{\gamma} > \frac{2w_\gamma}{3\pi(C_0+\bar{C})}\frac{v}{c_{ph}}$
- renormalized velocity $v \to 0$ when $\bar{\gamma} \simeq 43$



Mean field

Mean field

- Two Weyl nodes $h = 1, 2$
- Static approximation

$$H_{\rm eff} = \sum_{h=1}^{2} \sum_{\mathbf{p}} \psi_h^\dagger(\mathbf{p}) \left(v\mathbf{p} \cdot \boldsymbol{\sigma} \right) \psi_h(\mathbf{p}) + \frac{1}{V} \sum_{\mathbf{k},\mathbf{p},\mathbf{q}} V_{\rm tot}(\mathbf{q}) \psi_1^\dagger(\mathbf{p}+\mathbf{q}) \psi_1(\mathbf{p}) \psi_2^\dagger(\mathbf{k}-\mathbf{q}) \psi_2(\mathbf{k})$$

- spin-matrix order parameter:

$$\langle \psi_{1\sigma}(\mathbf{k}) \psi_{2\sigma'}(-\mathbf{k}+\mathbf{q}) \rangle = \delta_{\mathbf{q},0} \left[\boldsymbol{\Xi}(\mathbf{k}) i\sigma_2 \right]_{\sigma\sigma'}$$

- Gap function

$$\boldsymbol{\Delta}(\mathbf{p}) = -\frac{1}{V} \sum_{\mathbf{k}} V_{\rm tot}(\mathbf{p}-\mathbf{k}) \boldsymbol{\Xi}(\mathbf{k})$$

- BdG Hamiltonian

$$H_{BdG} = \sum_{\mathbf{p}} \Psi^\dagger(\mathbf{p}) \begin{pmatrix} v\boldsymbol{\sigma} \cdot \mathbf{p} & \boldsymbol{\Delta}(\mathbf{p}) \\ \boldsymbol{\Delta}^\dagger(\mathbf{p}) & -v\boldsymbol{\sigma} \cdot \mathbf{p} \end{pmatrix} \Psi(\mathbf{p})$$

- Four-component Nambu spinors $\Psi(\mathbf{p}) = \begin{pmatrix} \psi_1(\mathbf{p}) \\ i\sigma_2 \psi_2^\dagger(-\mathbf{p}) \end{pmatrix}$

Singlet pairing: gap equation

- write $\boldsymbol{\Delta}(\mathbf{p}) = \Delta_0(\mathbf{p})\sigma_0$.
- Diagonalize the Hamiltonian

$$\tilde{H} = E_s\left(\mathbf{k}\right)\tau_3\sigma_3 \qquad\qquad E_s(\mathbf{p}) = \sqrt{v^2\mathbf{p}^2 + \Delta_0^2(\mathbf{p})}$$

- The order parameter is

$$\Xi_0\left(\mathbf{k}\right) = -\frac{1}{2}\sum_{\sigma\sigma'}\left(-i\sigma_2\right)_{\sigma\sigma'}\left\langle\psi_{2\sigma'}\left(-\mathbf{k}\right)\psi_{1\sigma}\left(\mathbf{k}\right)\right\rangle = \frac{\Delta_0\left(\mathbf{k}\right)}{2E_s\left(\mathbf{k}\right)}$$

- assume $\Delta_0\left(\mathbf{p}\right) \approx \Delta_0$. Solve the gap equation

$$\Delta_0 = 2vb\, e^{-\frac{\pi}{|\alpha_{eff}|}} \qquad\qquad \alpha_{eff} < 0 \quad (\bar{\gamma} > 1)$$

- topologically trivial superconductor, *s*-wave singlet pairing
- cfr. BCS gap

$$\Delta \sim e^{-1/\nu_F|\lambda|}$$

$\rightarrow$ intrinsic SC impossible if $\nu_F = 0$

Nodal-line triplet pairing

Q: can we have superconductivity at $\bar{\gamma} < 1$?

- maybe with a more general order parameter...

$$\boldsymbol{\Delta}(\mathbf{k}) = \Delta_0(\mathbf{k})\sigma_0 + \mathbf{a}(\mathbf{k}) \cdot \boldsymbol{\sigma}$$

for $\Delta_0 = 0$ we call this a triplet pairing.

- Ansatz for $\mathbf{a}(\mathbf{k})$
- diagonalize

$$E_t^2(\mathbf{k}) = v^2\mathbf{k}^2 + a_\perp^2\mathbf{k}_\perp^2 + a_\parallel^2 k_3^2 + a_2^2 \pm 2|\mathbf{k}_\perp|\sqrt{(v^2 + a_\perp^2)a_2^2 + v^2 k_3^2(a_\perp - a_\parallel)^2}$$

- the spectrum has a nodal line in the xy plane

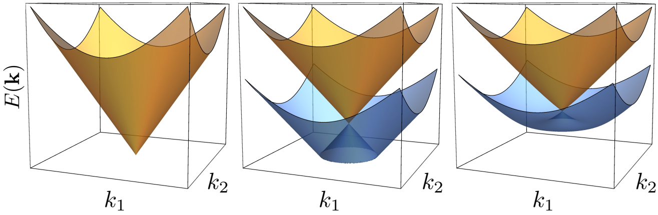
$$|\mathbf{k}_\perp| = \frac{|a_2|}{\sqrt{v^2 + a_\perp^2}}, \quad k_3 = 0$$

- gap equations have a solution only if

$$\bar{\gamma}' = \frac{175 w_\gamma}{126A^2 + 44AB + 44A + 22B^2 + 27} < \bar{\gamma} < 1$$

Superconducting phases

- $\bar{\gamma} < \bar{\gamma}'$: no superconductivity (TaAs $\bar{\gamma} = 0.2 < \bar{\gamma}' = 0.91$)
- $\bar{\gamma}' < \bar{\gamma} < 1$: gapless triplet superconductor
- $\bar{\gamma} > 1$: gapped superconductor with singlet pairing



(a) (b) (c)

Summary

- Piezoelectric interaction in Weyl semimetals can generate different superconducting phases
- Non-vanishing gap with vanishing density of state
- For TaAs, the coupling constant is too small
- Engineer materials with smaller v/c_{ph} ratio?
- Effects of disorder

R. Pereira, F.B., A. De Martino, R. Egger, arXiv:1904.06433