Superconductivity from piezoelectric interactions in Weyl semimetals

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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:

\[ H_0 = \sum_p \psi^\dagger(p) \left[ \nu_\perp (p_1 \sigma_1 + p_2 \sigma_2) + \nu_3 p_3 \sigma_3 \right] \psi(p) \]

\[ \psi = (\psi_\uparrow, \psi_\downarrow)^t \]

- momentum \( p \) measured with respect to the Weyl node at \( \pm b \)
- gapless dispersion relation

\[ E(p) = \pm \sqrt{\nu_\perp^2 p_\perp^2 + \nu_3^2 p_3^2} \]

- 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 $\mathbf{R}_{\text{atom}} \rightarrow \mathbf{R}_{\text{atom}} + \mathbf{u}_{\text{atom}}$
- Continuum limit $\mathbf{u} = \mathbf{u}(\mathbf{r})$
- Euclidean action

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

- Linearized strain tensor

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

- Stiffness tensor $C_{ijkl}$

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

Landau & Lifshitz, Theory of Elasticity (1970)
Phonons

- Phonons = quantized excitation of the displacement
  \[ u(r) = \sum_{J=1}^{3} \sum_{q} \frac{\epsilon^J(q) e^{i \mathbf{q} \cdot \mathbf{r}}}{\sqrt{2 \rho_0 \Omega_J(q)}} \left( a_J(q) + a_J^\dagger(-q) \right) \]

- In this work: acoustic phonons \[ \Omega_J(q) = c_J(\hat{q}) |q| \]

- Polarization vectors \( \epsilon^J(\hat{q}) \)

- Sound velocities \( c_J(\hat{q}) \rightarrow c_t, c_l \sim c_{ph} \)

- Low temperature \( k_B T \ll c_{ph} |b| \)
Piezoelectric interaction
Phonons in a piezoelectric material

- Weyl SM can be obtained from noncentrosymmetric materials.
  - Liu & Vanderbilt, PRB90 (2014) 155316

- TaAs, NbAs, NbP, TaP → $C_{4v}$
  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, $\varepsilon_{ij}$ = permittivity tensor

- No free charges:

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

- The electric field is (mainly) longitudinal:

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

Solve for $E$

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

and define a potential

$$\Phi(q) = \frac{-ie_{jmn} q_j u_{mn}(q)}{q_r \varepsilon_{rs} q_s}$$

such that

$$\mathbf{E} = -\nabla \Phi$$
The piezoelectric interaction Hamiltonian

- $\varepsilon_{ij} = \varepsilon \delta_{ij}$
- Scalar potential $\Phi$ couples to the electronic charge density $\rho_e$
- Piezoelectric e-p interaction Hamiltonian

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

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

$$\psi^\dagger_{\pm} \sigma_0 \psi_{\pm} \sum_j u_{jj} \quad \psi^\dagger_{\pm} \sigma_0 \psi_{\pm} u_{33} \quad \psi^\dagger_{\pm} \sigma_3 \psi_{\pm} \sum_j u_{jj}$$

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

...
Interactions

- electron-phonon interaction

- electron-electron interaction

- "Piezoelectric stiffening"

\[
S_{\text{int}} = \int \frac{d^4 q}{(2\pi)^4} \left( \frac{e^2}{2\varepsilon |q|^2} \rho_e(q) \rho_e(-q) + \frac{e}{\varepsilon} \sum_{ijk} e_{ijk} \frac{q_i q_j}{|q|^2} u_k(q) \rho_e(-q) \right. \\
+ \left. \frac{1}{2\varepsilon} \sum_{ijk} \sum_{lmn} e_{ijk} e_{lmn} \frac{q_i q_j q_l q_m}{|q|^4} u_k(q) u_n(-q) \right)
\]

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

The interaction is carried by the auxiliary boson $\varphi$

$$
S = S_{\text{ph}} + \int d^4x \left[ \psi^* \partial_\tau \psi - i v \psi^* (\nabla \cdot \sigma) \psi \\
+ \frac{1}{2} (\nabla \varphi)^2 + i g_e \psi^* \psi \varphi + i g_{ph} \sum_{jkl} e_{jkl} \partial_j \varphi u_{kl} \right]
$$

Integrating out $\varphi$, we obtain

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

$$
\Rightarrow \quad g_e = \frac{e}{\sqrt{\varepsilon}}, \quad g_{ph} = \frac{1}{\sqrt{\varepsilon}}
$$
Effective e-e interaction

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

with

\[
\gamma(\hat{\mathbf{q}}) = \sum_{J=1}^{3} \gamma_J(\hat{\mathbf{q}}) \quad \gamma_J(\hat{\mathbf{q}}) = \frac{1}{c_J^2(\hat{\mathbf{q}})|\mathbf{q}|^4} \left| \sum_{ijk} e_{ijk} q_i q_j \epsilon^J_{k}(\hat{\mathbf{q}}) \right|^2
\]

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

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

\[
\gamma_2(\theta) = 0, \quad A = \frac{e_{113}}{e_{333}}, \quad B = \frac{e_{311}}{e_{333}}
\]

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

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

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

\[ \alpha_{\text{eff}} = \frac{g_e^2 (1 - \tilde{\gamma})}{4\pi v} \]

RG:

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

Trockmorton et al. PRB 92, 115101 (2015)

\[ \tilde{\gamma} < 1 \text{ WS} \]

\[ \tilde{\gamma} > 1 \text{ unstable} \rightarrow \text{intrinsic superconductor} (\]
Renormalization group
RG beyond the static approximation

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

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

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

\[ C_0 = \frac{1}{15\pi} \left(10A^2 + 4AB + 4A + 2B^2 + 3\right) \quad \bar{C} = \frac{1}{105\pi} \left(42A^2 + 4AB + 4A + 2B^2 - 9\right) \]
RG flow equations

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

\[ \frac{dg_e}{d\ell} = -\frac{N g_e^3}{12\pi^2 \nu}, \]

\[ \frac{dg_{ph}}{d\ell} = -\frac{N g_e^2 g_{ph}}{12\pi^2 \nu}. \]

▶ generally \( \frac{c_{ph}}{\nu} \ll 1 \)

▶ \( \nu \) increases for TaAs (\( \bar{\gamma} = 0.20 \))

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

▶ critical value \( \bar{\gamma} > \frac{2w_{-\gamma}}{3\pi(C_0+\bar{C})} \frac{\nu}{c_{ph}} \)

▶ renormalized velocity \( \nu \to 0 \) when \( \bar{\gamma} \approx 43 \)
Mean field
Mean field

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

$$H_{\text{eff}} = \sum_{h=1}^{2} \sum_{p} \psi_h^\dagger(p) (\nu p \cdot \sigma) \psi_h(p) + \frac{1}{V} \sum_{k,p,q} V_{\text{tot}}(q) \psi_1^\dagger(p+q) \psi_1(p) \psi_2^\dagger(k-q) \psi_2(k)$$

- Spin-matrix order parameter:

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

- Gap function

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

- BdG Hamiltonian

$$H_{BdG} = \sum_{p} \psi_1^\dagger(p) \left( \begin{array}{cc} \nu \sigma \cdot p & \Delta(p) \\ \Delta^\dagger(p) & -\nu \sigma \cdot p \end{array} \right) \psi(p)$$

- Four-component Nambu spinors

$$\psi(p) = \left( \begin{array}{c} \psi_1(p) \\ i\sigma_2 \psi_2(-p) \end{array} \right)$$
Singlet pairing: gap equation

- Write \( \Delta(p) = \Delta_0(p) \sigma_0 \).
- Diagonalize the Hamiltonian
  \[
  \tilde{H} = E_s(k) \tau_3 \sigma_3 \quad \quad E_s(p) = \sqrt{v^2 p^2 + \Delta_0^2(p)}
  \]
- The order parameter is
  \[
  \Xi_0(k) = -\frac{1}{2} \sum_{\sigma \sigma'} (-i \sigma_2)_{\sigma \sigma'} \langle \psi_{2\sigma'}(-k) \psi_{1\sigma}(k) \rangle = \frac{\Delta_0(k)}{2E_s(k)}
  \]
- Assume \( \Delta_0(p) \approx \Delta_0 \). Solve the gap equation
  \[
  \Delta_0 = 2 vb e^{-\frac{\pi}{|\alpha_{\text{eff}}|}} \quad \quad \alpha_{\text{eff}} < 0 \ (\tilde{\gamma} > 1)
  \]
- 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...

$$\Delta(k) = \Delta_0(k)\sigma_0 + a(k) \cdot \sigma$$

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

- Ansatz for $a(k)$
- diagonalize

$$E^2_t(k) = v^2 k^2 + a^2_\perp k^2 + a^2_\parallel k^3 + a^2_\parallel \pm 2|k_\perp| \sqrt{(v^2 + a^2_\perp)a^2_\parallel + v^2 k^2_3 (a_\perp - a_\parallel)^2}$$

- the spectrum has a nodal line in the $xy$ plane

$$|k_\perp| = \frac{|a_2|}{\sqrt{v^2 + a^2_\perp}}, \quad k_3 = 0$$

- gap equations have a solution only if

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