Iowa State University

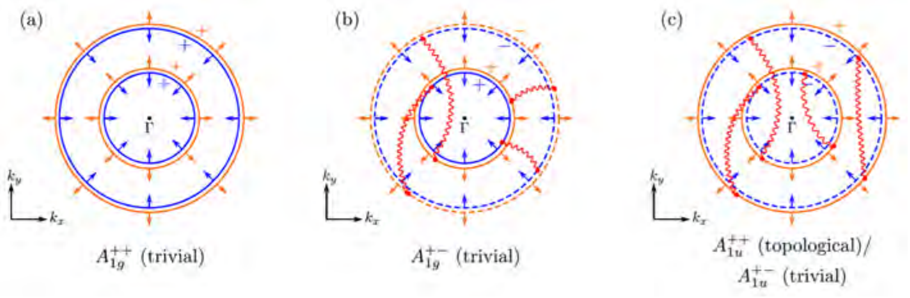
Department of Physics and Astronomy

Electron irradiation effects on superconductivity in $PdTe_2$: An application of a generalized Anderson theorem

Peter P. Orth (Iowa State University & Ames Laboratory)

Collaboration with M. S. Scheurer, Y. Lee, L. Ke, O. Cavani, M. Konczykowski, & groups of P. Canfield and R. Prozorov

Virtual March Meeting, March 18, 2021



References:
- E. I. Timmons *et al.*, PRR **2**, 023140 (2020)
- S. Teknowijoyo *et al.*, PRB **98**, 024508 (2018)

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Collaborators

Theory collaborators:

- M. S. Scheurer (Harvard)
- Y. Lee, L. Ke (Ames Lab)

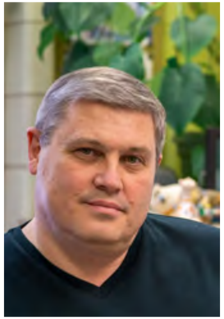
Experimental collaborators:

- O. Cavani, M. Konczykowski (Ecole Polytechnique)
- Groups of P. Canfield (Ames Lab) & R. Prozorov (Ames Lab)

M. S. Scheurer

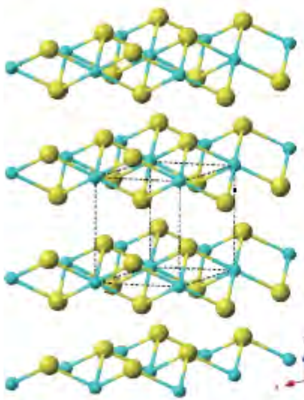
L. Ke

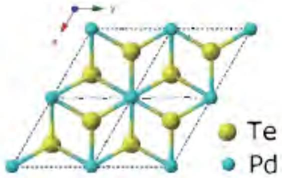
P. Canfield



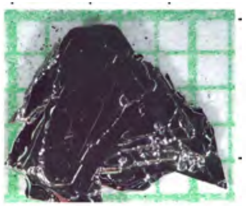
R. Prozorov

$PdTe_2$: crystal and electronic structure





$P\bar{3}m1(164)$



Single crystals

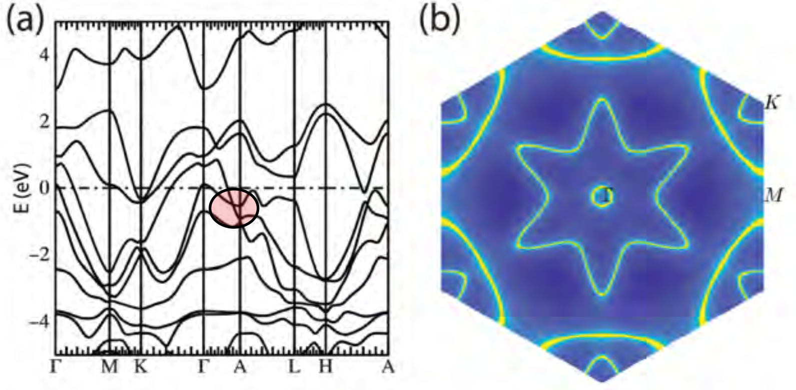
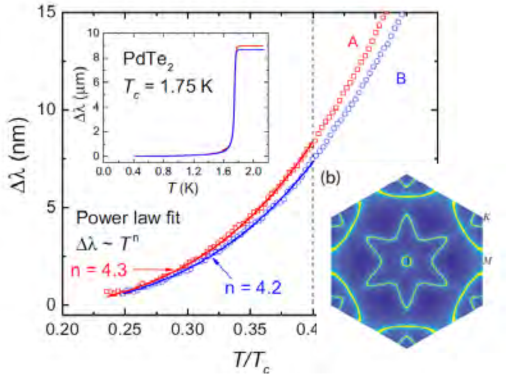


FIG. 7. (a) Band structure of $PdTe_2$. The horizontal dot-dashed line indicates the Fermi level. (b) Fermi surface contour in $PdTe_2$ for the $k_z = 0$ (Γ-M-K) plane.

- Centrosymmetric material, D_{3h} point group symmetry
- Type-II Dirac semimetal: nodal point 0.5 eV below E_F
- Significant spin-orbit coupling strength
- Fermi surface: 2 hole pockets around G and 2 electron pockets around K

[1] H.-J. Noh et al., (2017).
[2] F. Fei et al., (2017).
[3] E. I. Timmons et al., (2020).
[4] S. Teknowijoyo et al. (2018).
[5] deVisser et al. (2018).

Superconductivity in $PdTe_2$



Singlet SC pairing gap (g IRs)

$$\Delta_k = \Delta_0(\boldsymbol{k}) i\sigma_2$$

Triplet SC pairing gap (u IRs)

$$\Delta_k = \sum (\boldsymbol{d}_k)_j \sigma_j i\sigma_2$$

D_{3h}

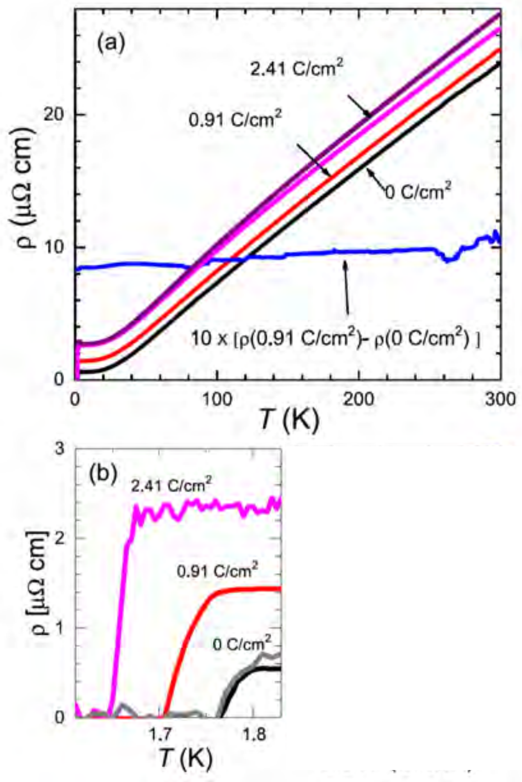
IR	Pairing	d_n	TRS	Order parameter $\Delta i\sigma_y$	Minimal number of nodes per FS	Topology
A_{1g}	s wave	1	y	$a + b(X^2 + Y^2) + cZ^2$	0	trivial
A_{2g}	g wave	1	y	$XZ(X^2 - 3Y^2)$	4 nodal lines	
E_g	$e_{g(1,0)}$ wave	2	y	$a(X^2 - Y^2) + bYZ$	2 nodal lines	
E_g	$e_{g(0,1)}$ wave	2	y	$aXY + bXZ$	2 nodal lines	
E_g	$e_{g(1,i)}$ wave	2	n	$a(X + iY)^2 + bZ(Y + iX)$	2 nodal points	
A_{1u}	p wave	1	y	$a(X\sigma_x + Y\sigma_y) + bZ\sigma_z$	0	trivial/top.
A_{2u}	p wave	1	y	$a(Y\sigma_x - X\sigma_y) + bX(X^2 - 3Y^2)\sigma_z$	2 nodal points	
E_u	$e_{u(1,0)}$ wave	2	y	$aX(X^2 - 3Y^2)\sigma_x + bZ\sigma_y + cY\sigma_z$	0	trivial/top.
E_u	$e_{u(0,1)}$ wave	2	y	$aZ\sigma_x + bX(X^2 - 3Y^2)\sigma_y + cX\sigma_z$	2 nodal points	
E_u	$e_{u(1,i)}$ wave	2	n	$[aZ + ibX(X^2 - 3Y^2)](\sigma_x + i\sigma_y) + c(X + iY)\sigma_z$	2 nodal points [44]	

- Superconducting (SC) transition T_c = 1.75 K [1], weak-coupling BCS & type-I SC [2, 3]
- Penetration depth measurements yield a fully gapped SC state [2, 3]
- Only 3 out of 10 possible pairing states have no symmetry enforced nodes
  - A_{1g}: topologically trivial s-wave state. Could be A_{1g}^{++} or A_{1g}^{+-}.
  - A_{1u}: odd-parity p-wave state. Balian-Werthamer state on each FS.
  - $e_{u(1,0)}$: anisotropic odd-parity state that transforms like k_x.

Whether trivial or non-trivial depends on microscopics. Fu-Berg criterion [4] not applicable as total # of enclosed TR momenta is even.

[1] Guggenheim et al. (1961); Hull (1965).
[2] S. Teknowijoyo et al. (2018);
[3] deVisser et al. (2017, 2018, 2020)
[4] Fu, Berg (2010).

Electron irradiation effects on superconductivity and transport

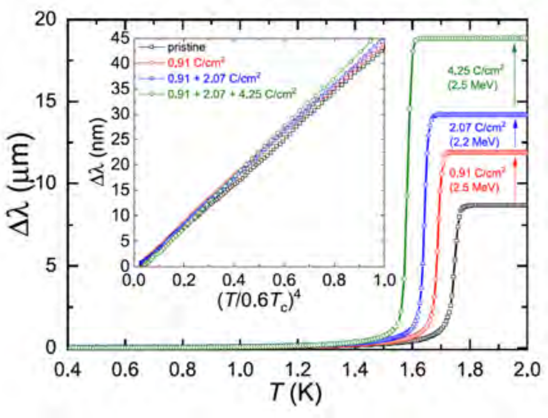


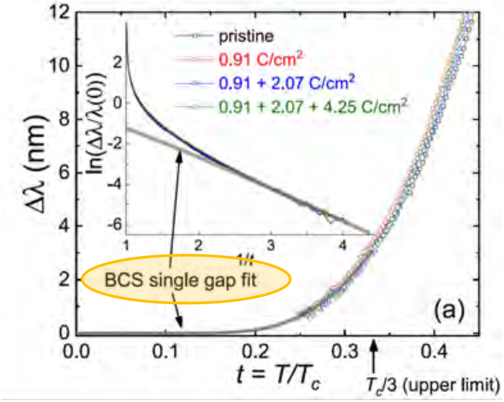
Dose (C/cm^2)	n_e (m^{-3})	n_h (m^{-3})	μ_e (m^2/V s)	μ_h (m^2/V s)	τ_e^{-1} (meV)	τ_h^{-1} (meV)	ℓ_e (nm)	ℓ_h (nm)
0	$4.2(1) \times 10^{27}$	$2.2(1) \times 10^{27}$	0.10(1)	0.28(1)	70(2)	26(2)	344(5)	725(5)
1.33	$4.2(1) \times 10^{27}$	$2.2(1) \times 10^{27}$	0.05(1)	0.14(1)	140(2)	53(2)	172(5)	363(5)

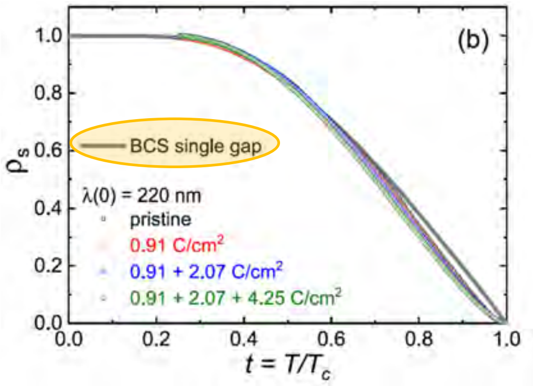
- Electron irradiation (2.5 MeV) creates point-like defects
- Resistivity curves shift up following Matthiessen rule
- Carrier densities unchanged
- Mobilities reduced by about a factor of two for 1.33 C/cm^2 dose
- Superconducting T_c decreases under irradiation

[1] Timmons *et al.*, PRR (2020).

London penetration depth under irradiation







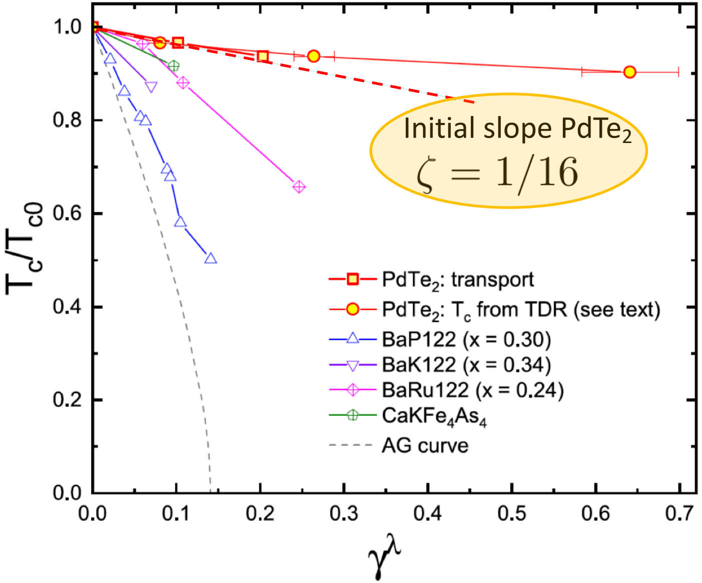
- SC state can still be described by a **single isotropic** and **full gap** energy scale
  - Sets stringent limits on degree of anisotropy required to explain T_c reduction of A_{1g}^{++} state

[1] Timmons *et al.*, PRR (2020).

T_c suppression under irradiation

Anderson (1959), Abrikosov, Gorkov (1959), Hohenberg (1964), Golubov, Mazin (1997)

	BaRu122(x = 0.24)	CaK1144	BaK122 (x = 0.34)	BaP122 (x = 0.30)	PdTe2
L(0) (nm)	200	210	280	300	220
Tc (K)	22	35.3	37.5	31.7	1.76



- Slow suppression of T_c with increased scattering
- Initial slope ζ of T_c suppression $\delta T_c/T_{c,0}$
  - describes fitness of SC order with respect to non-magnetic disorder
  - Measures how many scattering events are pair breaking
  - Yields information about pairing state
  - Anderson theorem (isotropic s-wave): $\delta T_c/T_{c,0} = 0$
  - Abrikosov-Gorkov law (magnetic disorder for isotropic s-wave): $\delta T_c/T_{c,0} = -\frac{\pi^2}{2}\gamma^\lambda$

Dimensionless scattering parameter: $\gamma^\lambda = \frac{\hbar}{2\pi k_B \mu_0} \frac{\Delta\rho_0}{\lambda_0^2 T_{c,0}}$

[1] Timmons *et al.*, PRR (2020).

Generalized Anderson theorem

Mean-field SC Hamiltonian with (non-)magnetic disorder

$$H_0 + \Delta H = \frac{1}{2} \sum_{k,k'} \Phi^\dagger_{k\alpha} (\hat{h}^{\text{BdG}})_{k\alpha,k'\alpha'} \Phi_{k'\alpha'}.$$

Nambu spinor

$$\Phi_{k\alpha} = (c_{k\alpha}, T_{\alpha\beta} c^\dagger_{-k\beta})^T$$

BdG Hamiltonian

$$\hat{h}^{\text{BdG}}_n = \begin{pmatrix} \hat{h} & 0 \\ 0 & -\hat{h} \end{pmatrix},$$

Normal state Bloch Hamiltonian $\hat{h}_{k\alpha,k'\alpha'} = \delta_{k,k'} (\hat{h}_k)_{\alpha\alpha'}$

$$\hat{h}^{\text{BdG}}_\Delta = \begin{pmatrix} 0 & \hat{\mathcal{D}} \\ \hat{\mathcal{D}}^\dagger & 0 \end{pmatrix},$$

SC pairing function $(\hat{\mathcal{D}})_{k\alpha,k'\alpha'} = \delta_{k,k'} (\Delta_k T^\dagger)_{\alpha\alpha'}$

$$\hat{h}^{\text{BdG}}_W = \begin{pmatrix} \hat{W}^+ + \hat{W}^- & 0 \\ 0 & -\hat{W}^+ + \hat{W}^- \end{pmatrix},$$

Disorder:

- t_W = +: non-magnetic
- t_W = - : magnetic

Scheurer, Ph.D. thesis (2016); Timmons et al (2020).

Generalized Anderson theorem

Mean-field SC Hamiltonian with (non-)magnetic disorder

$$H_0 + \Delta H = \frac{1}{2}\sum_{k,k'} \Phi^\dagger_{k\alpha} (\hat{h}^{\mathrm{BdG}})_{k\alpha,k'\alpha'} \Phi_{k'\alpha'}.$$

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$$\hat{h}^{\mathrm{BdG}}_n = \begin{pmatrix} \hat{h} & 0 \\ 0 & -\hat{h} \end{pmatrix},$$

Normal state Bloch Hamiltonian $\hat{h}_{k\alpha,k'\alpha'} = \delta_{k,k'} (h_k)_{\alpha\alpha'}$

$$\hat{h}^{\mathrm{BdG}}_\Delta = \begin{pmatrix} 0 & \hat{\mathcal{D}} \\ \hat{\mathcal{D}}^\dagger & 0 \end{pmatrix},$$

SC pairing function $(\hat{\mathcal{D}})_{k\alpha,k'\alpha'} = \delta_{k,k'} (\Delta_k T^\dagger)_{\alpha\alpha'}$

$$\hat{h}^{\mathrm{BdG}}_W = \begin{pmatrix} \hat{W}^+ + \hat{W}^- & 0 \\ 0 & -\hat{W}^+ + \hat{W}^- \end{pmatrix},$$

Disorder:

- t_W = +: non-magnetic
- t_W = - : magnetic

Gap unaffected by disorder if

$$[\hat{h}^{\mathrm{BdG}}_n + \hat{h}^{\mathrm{BdG}}_W, \hat{h}^{\mathrm{BdG}}_\Delta]_+ = 0,$$

Generalized Anderson theorem

$$[\hat{h}, \hat{\mathcal{D}}]_- = 0 \text{ and } [\hat{W}, \hat{\mathcal{D}}]_{-t_W} = 0$$

Naturally holds in normal state eigenbasis

$$(\epsilon_{\boldsymbol{k}n} - \epsilon_{\boldsymbol{k}n'})\langle\phi_{\boldsymbol{k}n}|\Delta_{\boldsymbol{k}} T^\dagger|\phi_{\boldsymbol{k}n'}\rangle = 0$$

Normal state eigenbasis

$$h_{\boldsymbol{k}}|\phi_{\boldsymbol{k}n}\rangle = \sigma_0 \epsilon_{\boldsymbol{k}n}|\phi_{\boldsymbol{k}n}\rangle$$

Requires gap to be identical at points connected by disorder

$$[\Delta_s(\boldsymbol{k}) - t_W \Delta_{s'}(\boldsymbol{k}')]\langle\phi^s_{\boldsymbol{k}}|W|\phi^{s'}_{\boldsymbol{k}'}\rangle$$

Pair breaking scattering & disorder sensitivity

Pair breaking scattering between points where gap is not identical

$$C_{ks,k's'} := [\Delta_s(k) - t_W \Delta_{s'}(k')] \langle \phi_k^s | W | \phi_{k'}^{s'} \rangle$$

- t_W = +: non-magnetic disorder
- t_W = - : magnetic disorder

> SC disorder sensitivity parameter

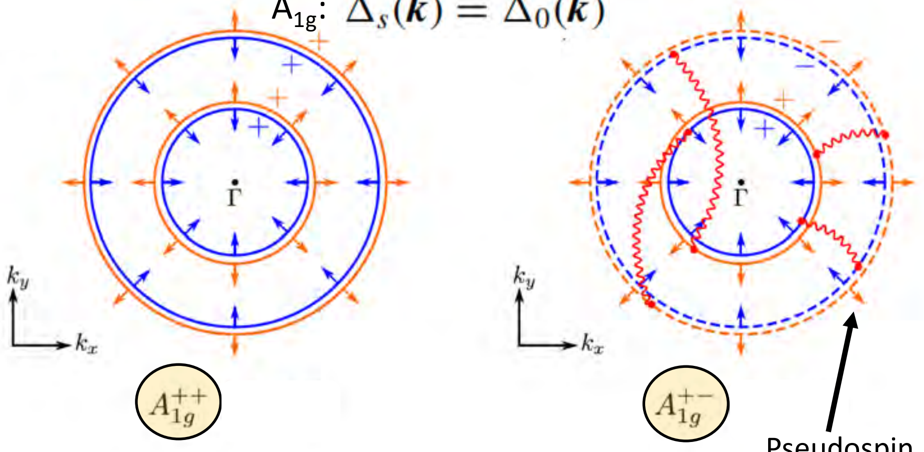
$$\zeta = \frac{\sum_{k,k'}^{FS} \sum_{s,s'} |C_{ks,k's'}|^2}{2\,\mathrm{tr}[W^\dagger W] \sum_k^{FS} \sum_s |\Delta_s(k)|^2}.$$

FS average of violation of generalized Anderson theorem

> Slope of Tc suppression determined by ζ

$$\delta T_c / T_{c,0} \sim -\frac{\pi}{4 T_{c,0}} \tau^{-1} \zeta$$

A$_{1g}$: $\Delta_s(k) = \Delta_0(k)$



SC order parameter

$$\langle \phi_k^{s'} | \Delta_k (i\sigma_2)^\dagger | \phi_k^s \rangle = \delta_{s,s'} \Delta_s(k)$$

A$_{1g}$: $\Delta_s(k) = \Delta_0(k)$

Normal state eigenbasis

$$h_k |\phi_{kn}\rangle = \sigma_0 \epsilon_{kn} |\phi_{kn}\rangle$$

Disorder sensitivity parameter

Abrikosov, Gorkov (1959), Hohenberg (1964), Golubov, Mazin (1997), Cavanagh, Brydon (2020), Michaeli, Fu (2012), Scheurer (2016); Timmons *et al.* (2020).

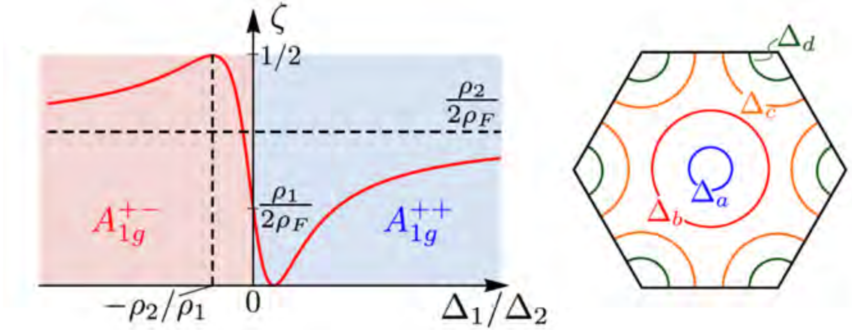
- SC disorder sensitivity parameter

$$\zeta = \frac{\sum_{k,k'}^{\mathrm{FS}} \sum_{s,s'} |C_{ks,k's'}|^2}{2\,\mathrm{tr}[W^\dagger W] \sum_{k}^{\mathrm{FS}} \sum_{s} |\Delta_s(\boldsymbol{k})|^2}.$$

- Slope of Tc suppression determined by ζ

$$\delta T_c / T_{c,0} \sim -\frac{\pi}{4T_{c,0}} \tau^{-1} \zeta$$

Isotropic multi-band SC



Density of states of pocket n

$$\zeta = \frac{1}{2}\left[1 - \frac{\left(\sum_n \rho_n \Delta_n\right)^2}{\left(\sum_n \rho_n \Delta_n^2\right) \sum_n \rho_n}\right].$$

Timmons *et al.*, PRR (2020).

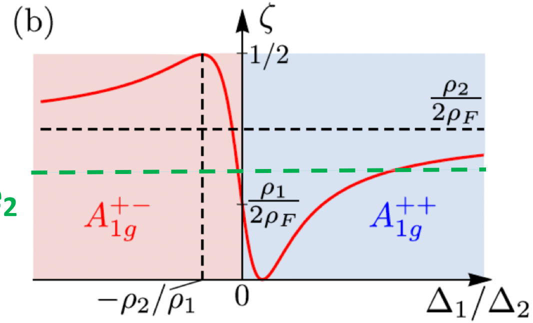
Gap anisotropies in $PdTe_2$ required for observed T_c suppression

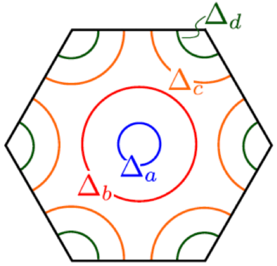
$\nu = \sum_{n\in C_1} \rho_n / (\sum_n \rho_n - \sum_{n\in C_1} \rho_n)$

C_1	ν	$(\Delta_1/\Delta_2)_1$	$(\Delta_1/\Delta_2)_2$
$\{a\}$	7.5×10^{-3}	5.6	−3.3
$\{b\}$	0.40	2.1	0.32
$\{c\}$	2.1	2.8	0.48
$\{d\}$	0.034	3.3	−0.98
$\{a, b\}$	0.41	2.1	0.33
$\{a, c\}$	2.1	2.8	0.48
$\{a, d\}$	0.042	3.1	−0.78
$\{c, d\}$	2.4	3.0	0.47

Experimental value for $PdTe_2$

$\zeta = 1/16$





> A_{1g}^{++} requires $\Delta_1/\Delta_2 = 2.1$

Substantial anisotropy necessary for A_{1g}^{++} state to be consistent with T_c suppression

> A_{1g}^{+-} can be isotropic $\Delta_1/\Delta_2 = -0.98$

Unconventional isotropic A_{1g}^{+-} state is most likely candidate.

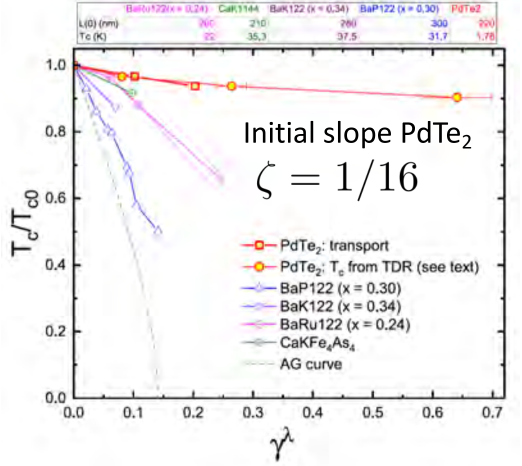
$$\Delta_a = \Delta_b = \Delta_c = \Delta_2, \Delta_d = \Delta_1.$$

Sign change between three inner and small outer most pocket at K point.

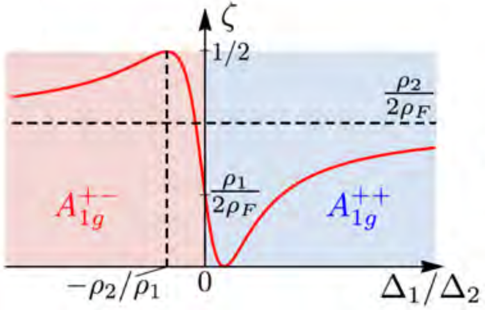
Timmons *et al.*, PRR (2020).

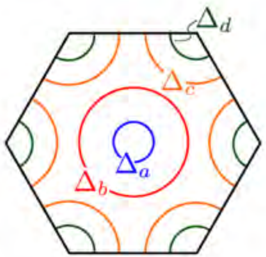
Summary

- Penetration depth λ ▻ single isotropic full SC gap
- Slow but finite T_c suppression under electron irradiation ▻ $\zeta = \dfrac{1}{16}$
- Minimal required anisotropy for s^{++} state: $\Delta_1/\Delta_2 \approx 2.1$
- Minimal required anisotropy for s^{+-} state: $\Delta_1/\Delta_2 \approx -0.98$



Unconventional A_{1g}^{+-} state more likely than A_{1g}^{++} due to weak observed anisotropy.





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Thank you for your attention!

Disorder sensitivity parameter

Abrikosov, Gorkov (1959), Hohenberg (1964), Golubov, Mazin (1997), Cavanagh, Brydon (2020), Michaeli, Fu (2012), Scheurer (2016); Timmons *et al.* (2020).

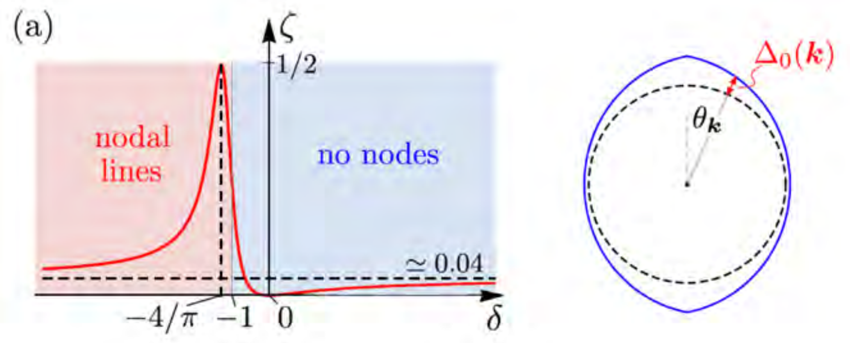
- SC disorder sensitivity parameter

$$\zeta = \frac{\sum_{k,k'}^{\mathrm{FS}} \sum_{s,s'} |C_{ks,k's'}|^2}{2\,\mathrm{tr}[W^\dagger W] \sum_{k}^{\mathrm{FS}} \sum_{s} |\Delta_s(\boldsymbol{k})|^2}.$$

- Slope of Tc suppression determined by ζ

$$\delta T_c / T_{c,0} \sim -\frac{\pi}{4T_{c,0}} \tau^{-1} \zeta$$

Anisotropic s-wave



$$\Delta_0(\boldsymbol{k}) = \Delta_0[1 + \delta \sin(\theta_{\boldsymbol{k}})]$$

$$\Rightarrow \zeta = \frac{(32 - 3\pi^2)\delta^2}{16(6 + 3\pi\delta + 4\delta^2)}.$$

Timmons *et al.*, PRR (2020).