Interplay between electronic topology and phonons in Dirac materials

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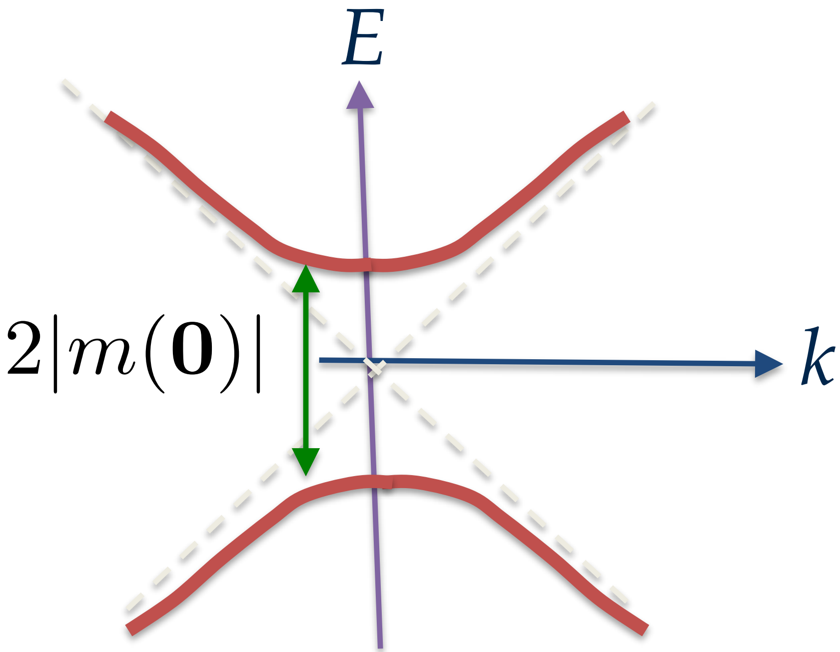
Prelude: Dirac materials

A recent review:

Ando, JPSJ **82**, 102001 (2013).

3D (massive) Dirac fermions in crystals

$$\boxed{h(\mathbf{k}) = v\mathbf{k}\cdot\boldsymbol{\sigma}\tau^x + m(\mathbf{k})\,\tau^z}$$



$\boldsymbol{\sigma}$ = spin

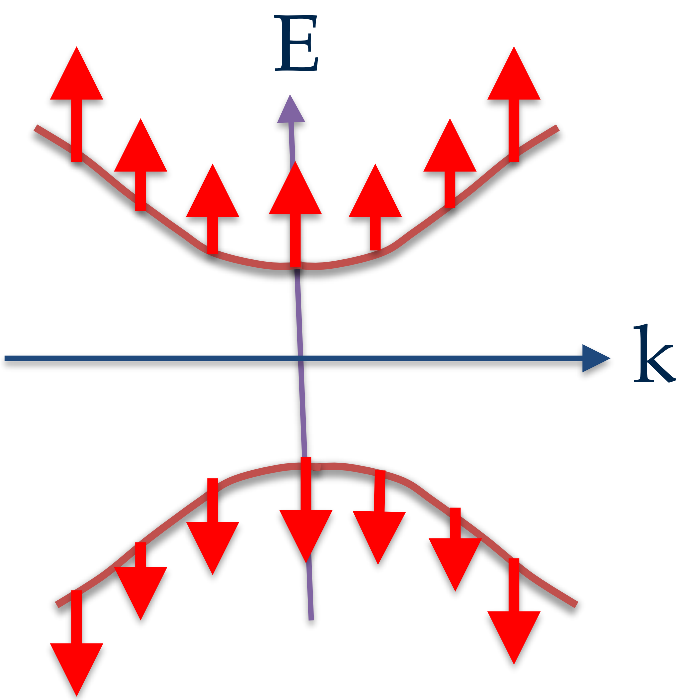
$\boldsymbol{\tau}$ = orbital (parity)

Time-reversal and inversion symmetry

$$m(\mathbf{k}) = m + tk^2$$

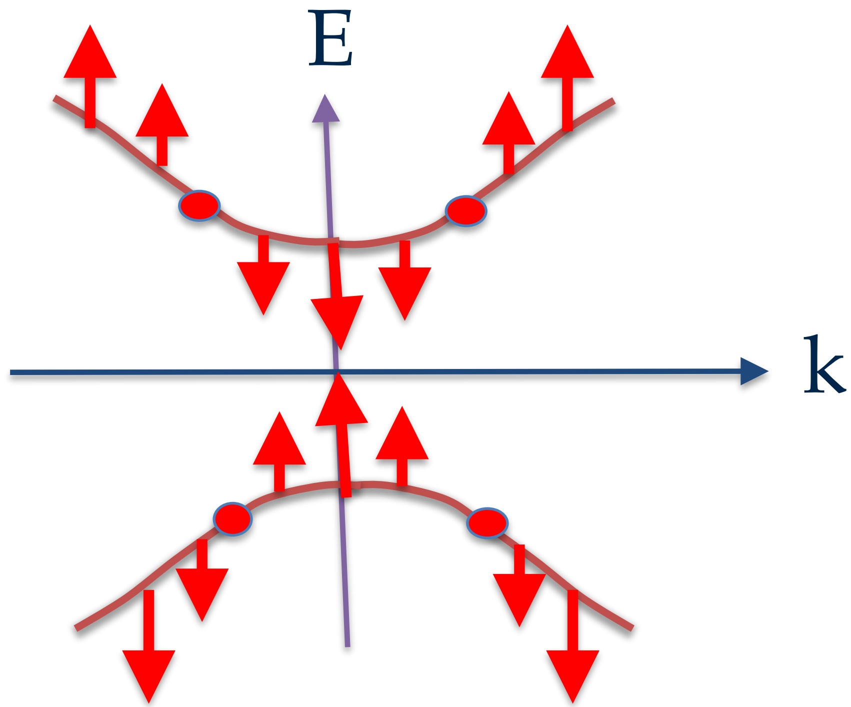
$\langle \tau^z \rangle$ in k-space

Trivial insulator



$$mt > 0$$

Topological insulator



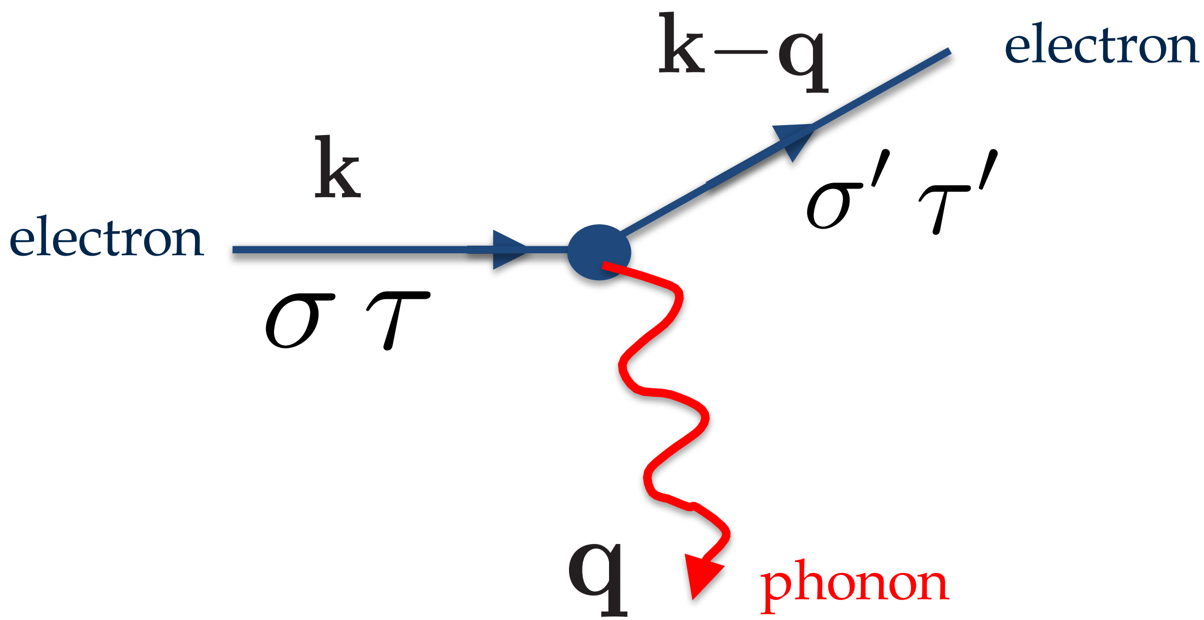
$$mt < 0$$

Part I:
Effect of phonons on band topology

I. Garate, PRL **110**, 046402 (2013).

K. Saha and I. Garate, PRB **89**, 205103 (2014).

Electron-phonon interaction



Electron-phonon interaction

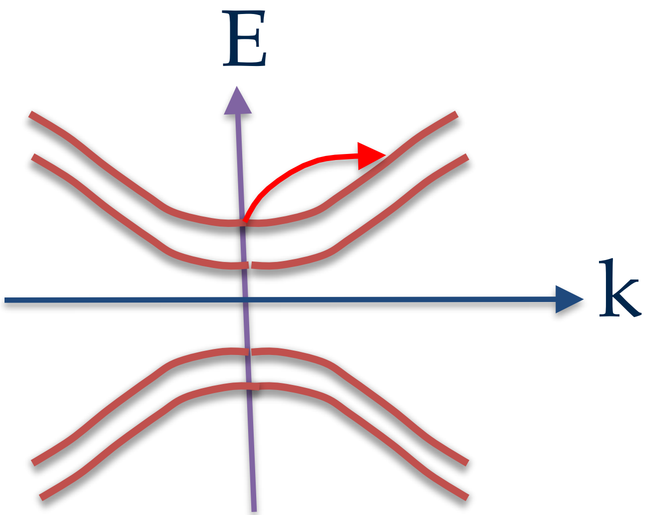
Long wavelength + local-in-space

Electron-phonon coupling	Phonon parity
$\mathbf{1}_2 \otimes \mathbf{1}_2$	Even

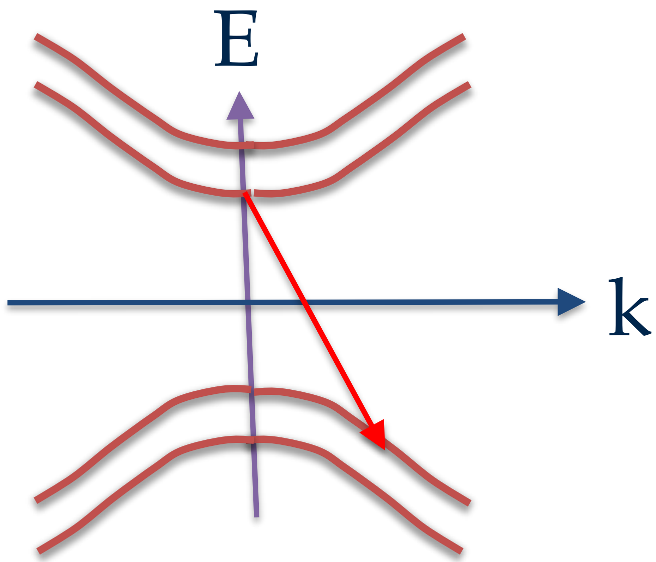
Effect of phonons on energy gap

$$\Delta E_{\mathbf{0}n} = \sum_{n'\mathbf{q}} g_{\mathbf{q}}^2 \frac{|\langle n\mathbf{0}|n'\mathbf{q}\rangle|^2}{E_{\mathbf{0}n} - E_{\mathbf{q}n'}}$$ = intraband + interband

Intraband transitions



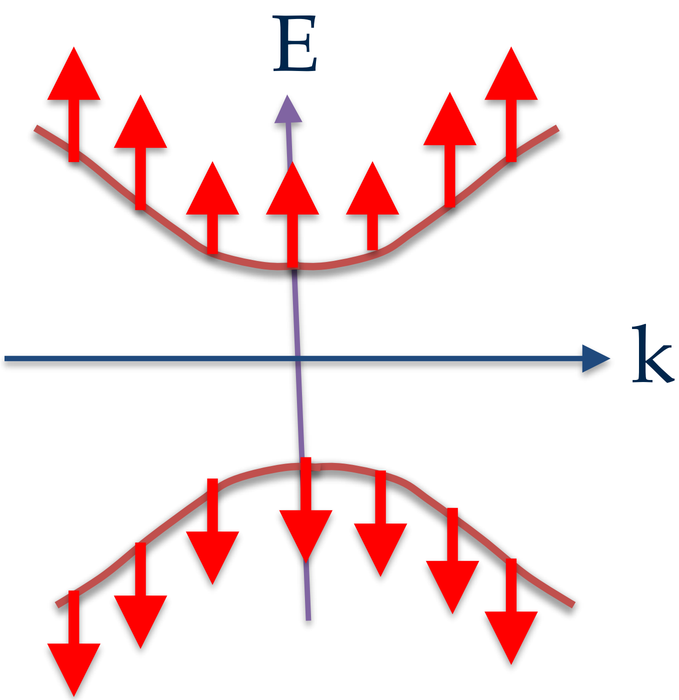
Interband transitions



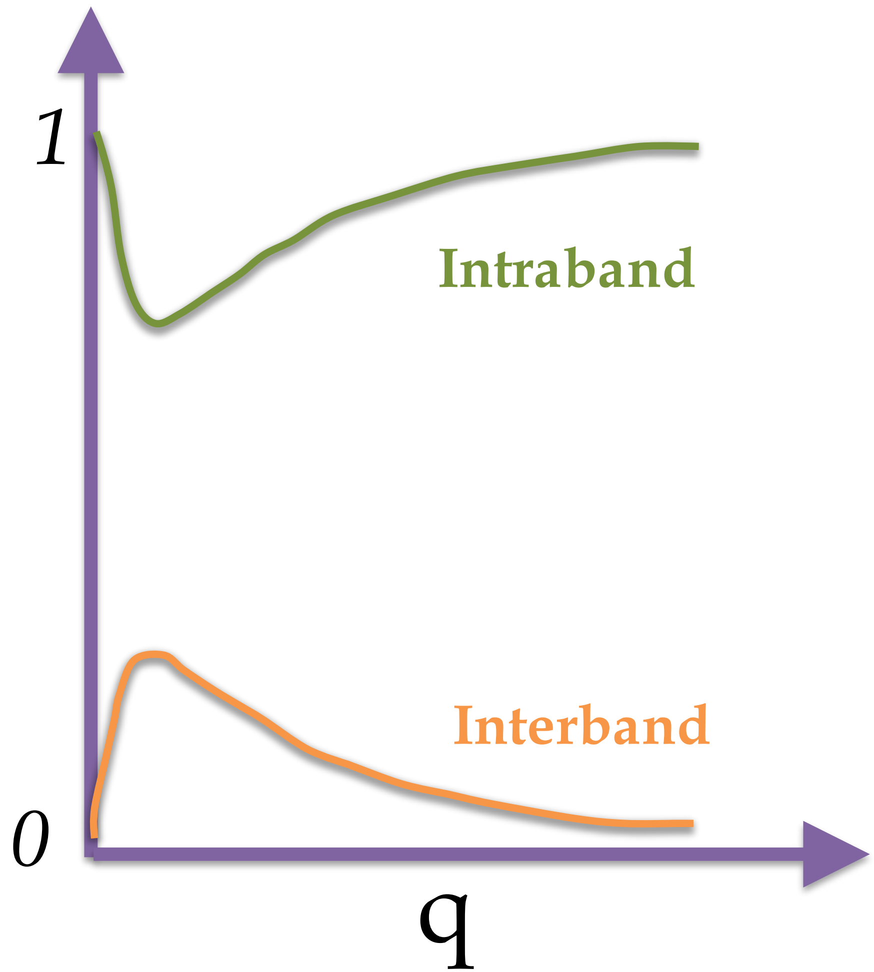
Electron-phonon matrix elements

$$\boxed{|\langle \mathbf{0}n|\mathbf{q}n'\rangle|^2}$$

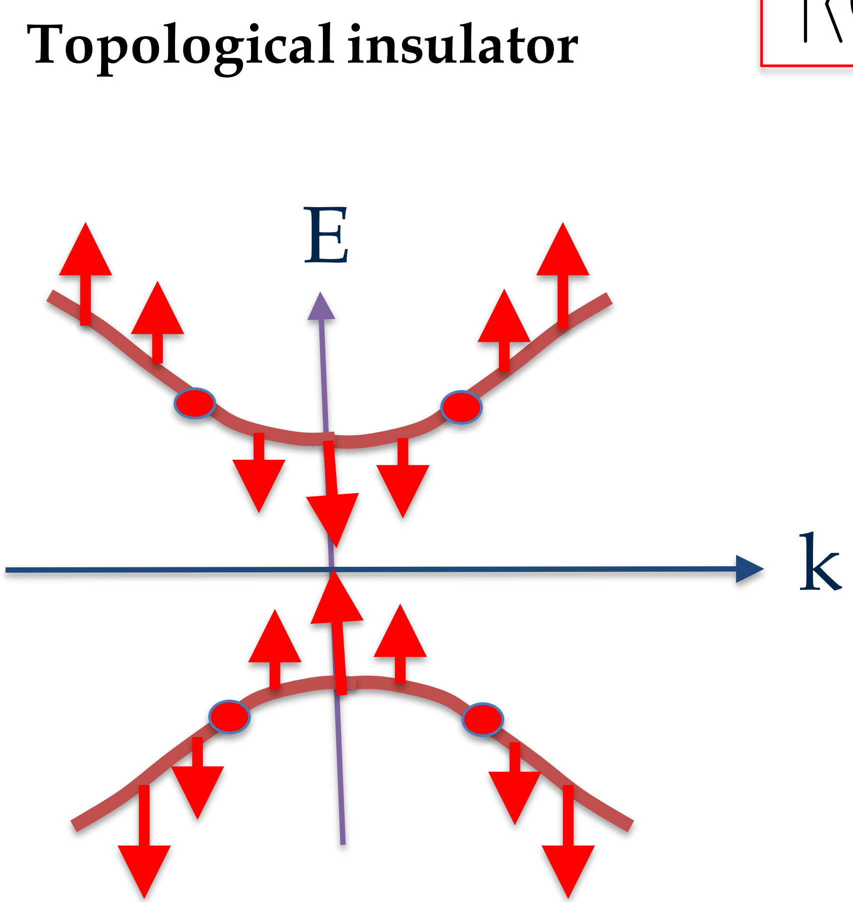
Trivial insulator



Arrows = orbital pseudospin

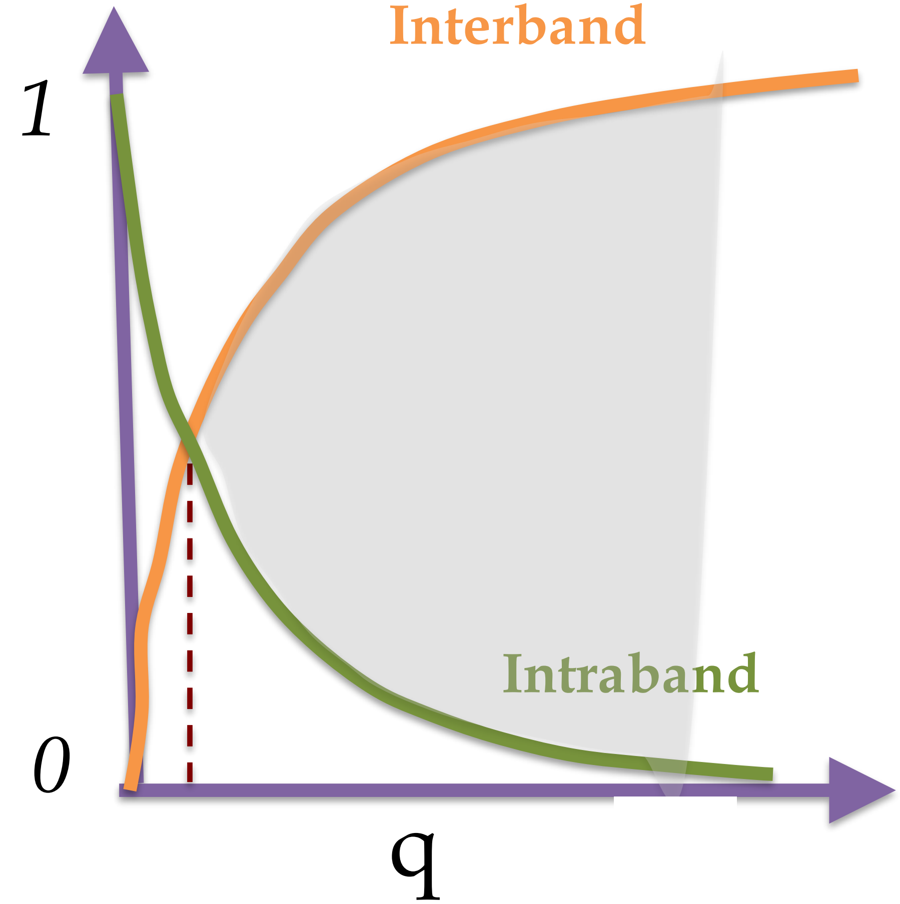


Electron-phonon matrix elements

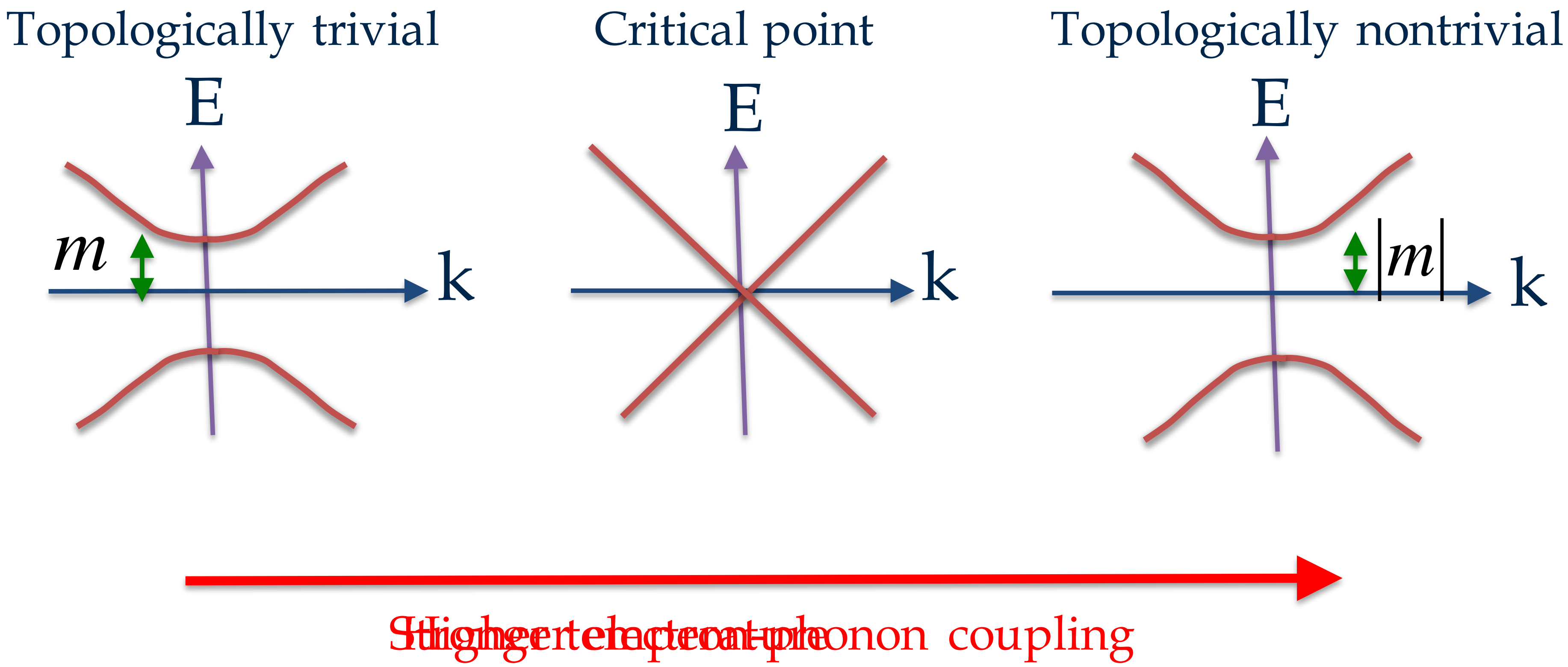


Arrows = orbital pseudospin

$$|\langle \mathbf{0}n|\mathbf{q}n'\rangle|^2$$



Phonon-induced topological insulation



Thermal topological transition (crossover).

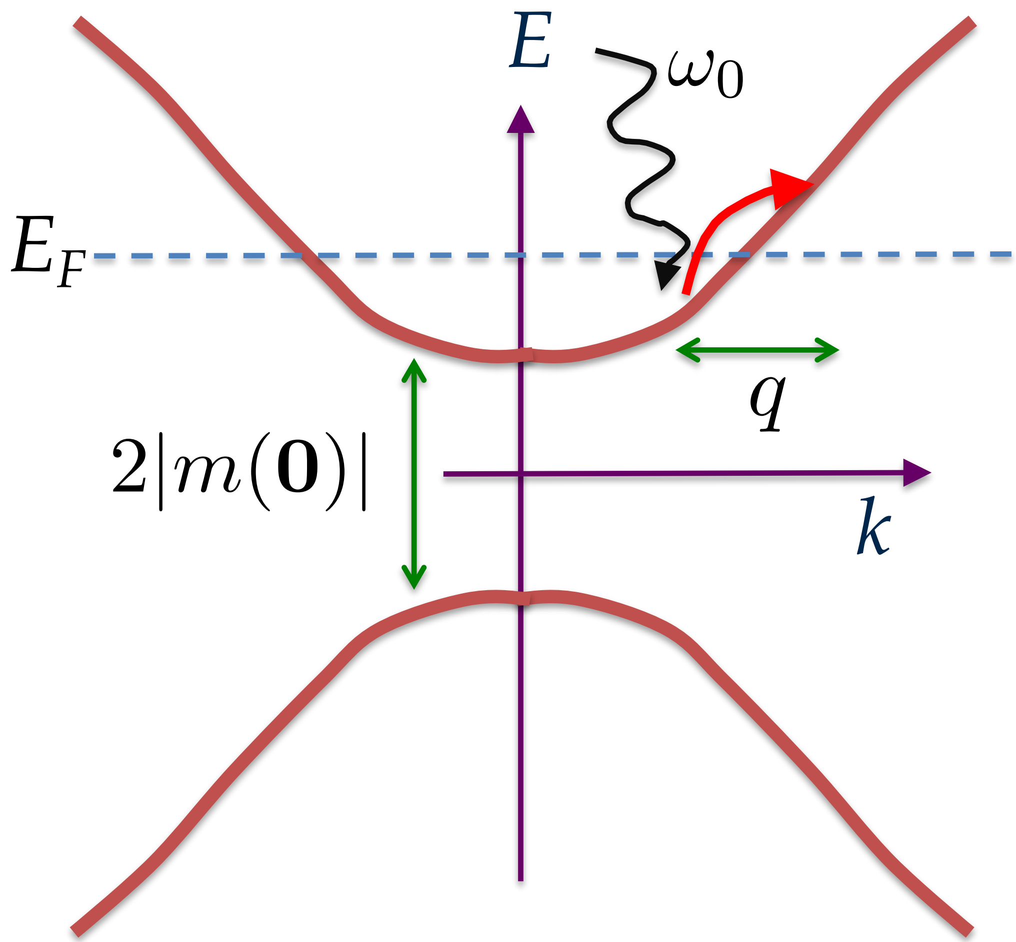
Part II:
Back action of band topology on phonons

K. Saha, K. Légaré and I. Garate

arXiv: 1506.02621

Phonon linewidth

Case I: Phonon frequency < Bandgap



Small (but nonzero) q

Fermi-surface average

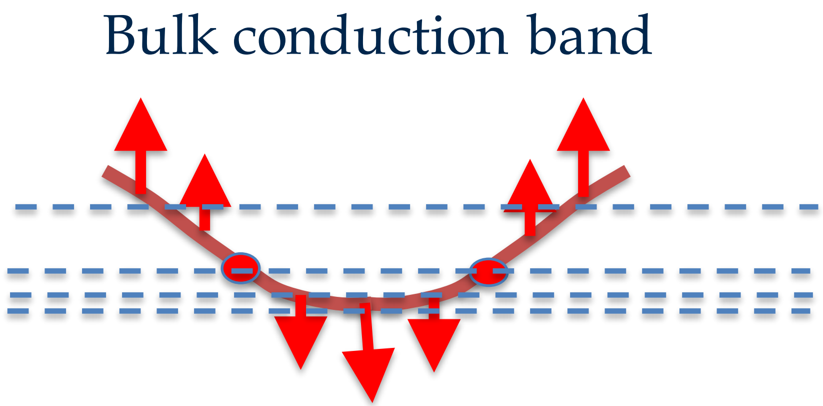
$$\boxed{\gamma_\lambda = g_\lambda D(\epsilon_F)\overline{|\langle h_{\rm ep}\rangle|^2}}$$

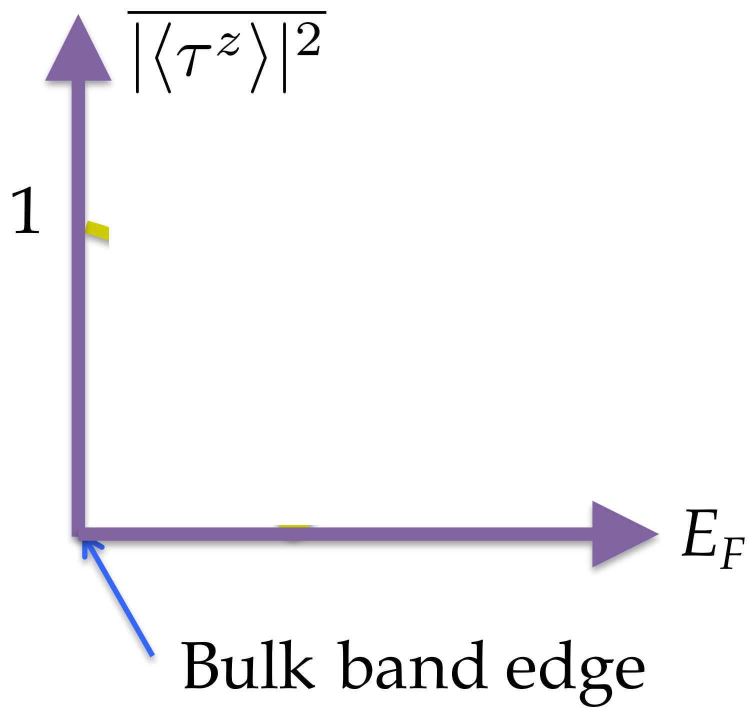
Electronic DOS at Fermi level

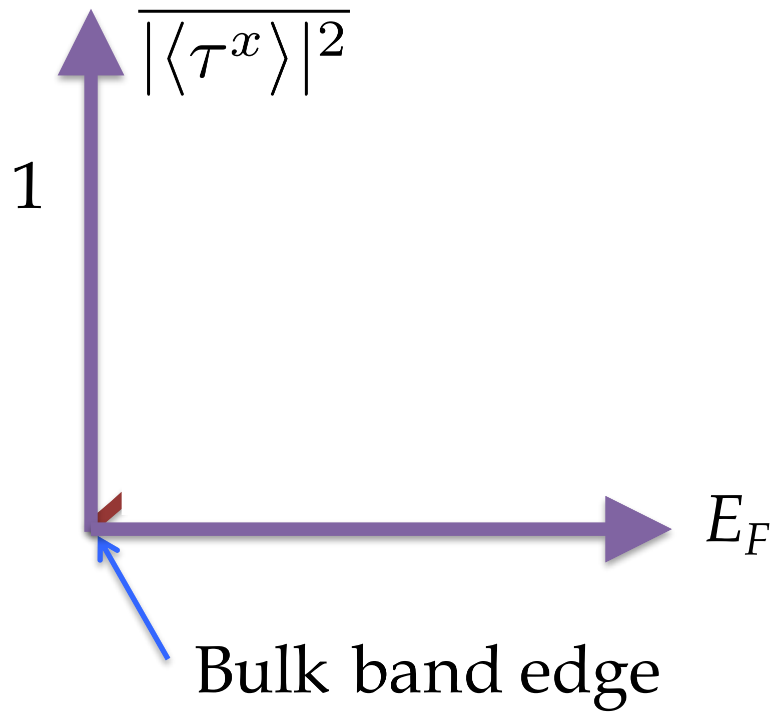
Electron-phonon coupling

Raman-active phonon	IR-active phonon
$h^z_{\rm ep} \propto \mathbf{1}_2 \otimes \tau^z$	$h^x_{\rm ep} \propto \mathbf{1}_2 \otimes \tau^x$
$\gamma_z = g_z D(\epsilon_F)\overline{|\langle \tau^z\rangle|^2}$	$\gamma_x = g_z D(\epsilon_F)\overline{|\langle \tau^x\rangle|^2}$

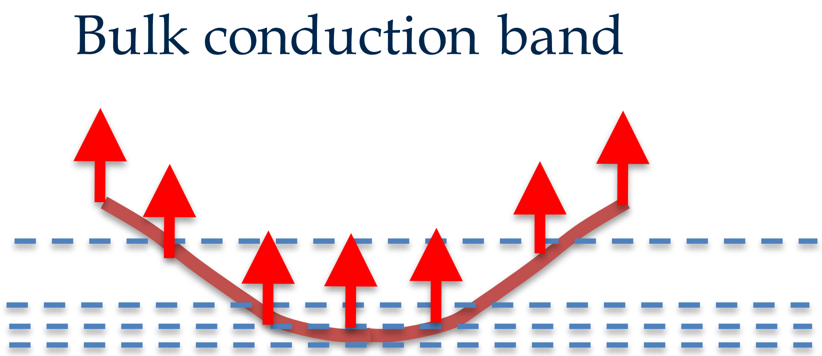
Matrix elements (I): topological phase

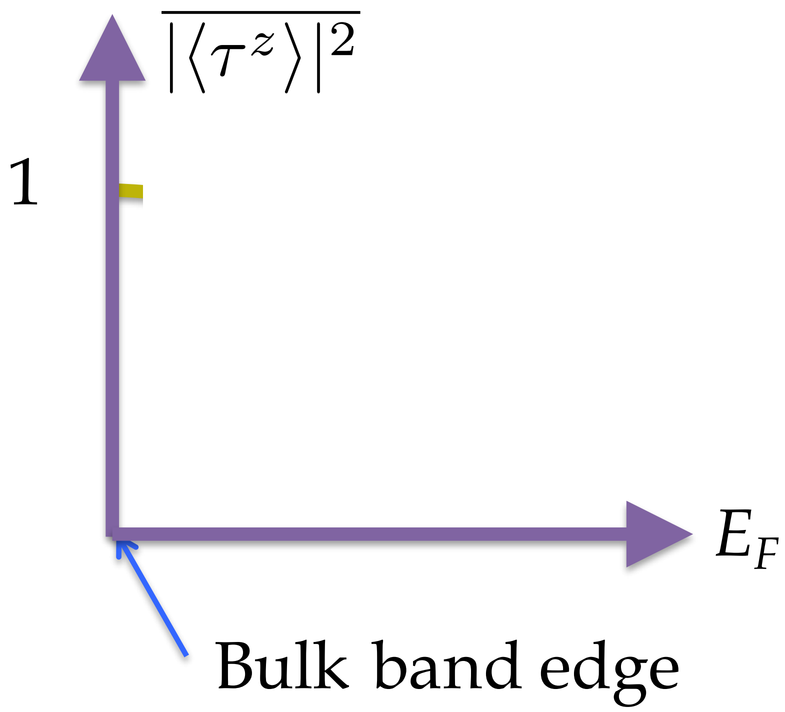


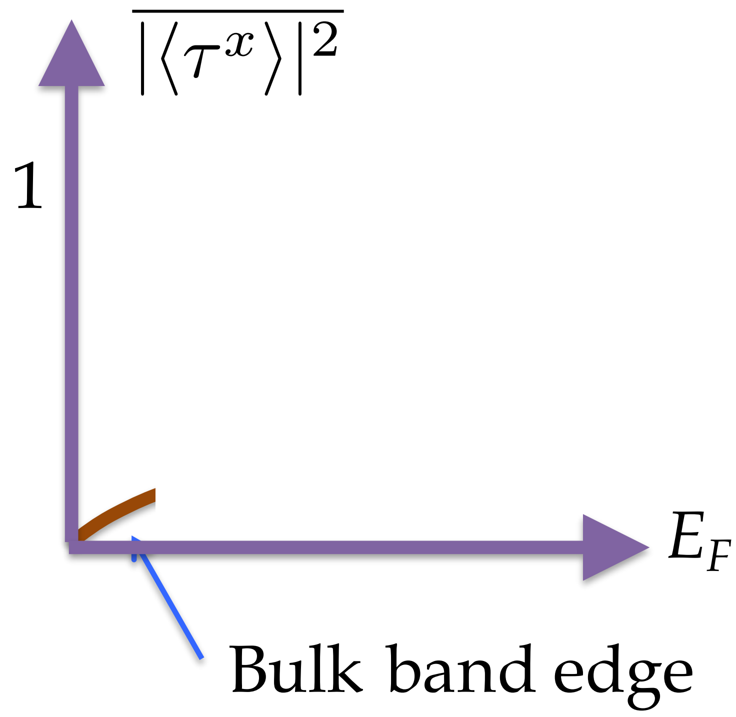


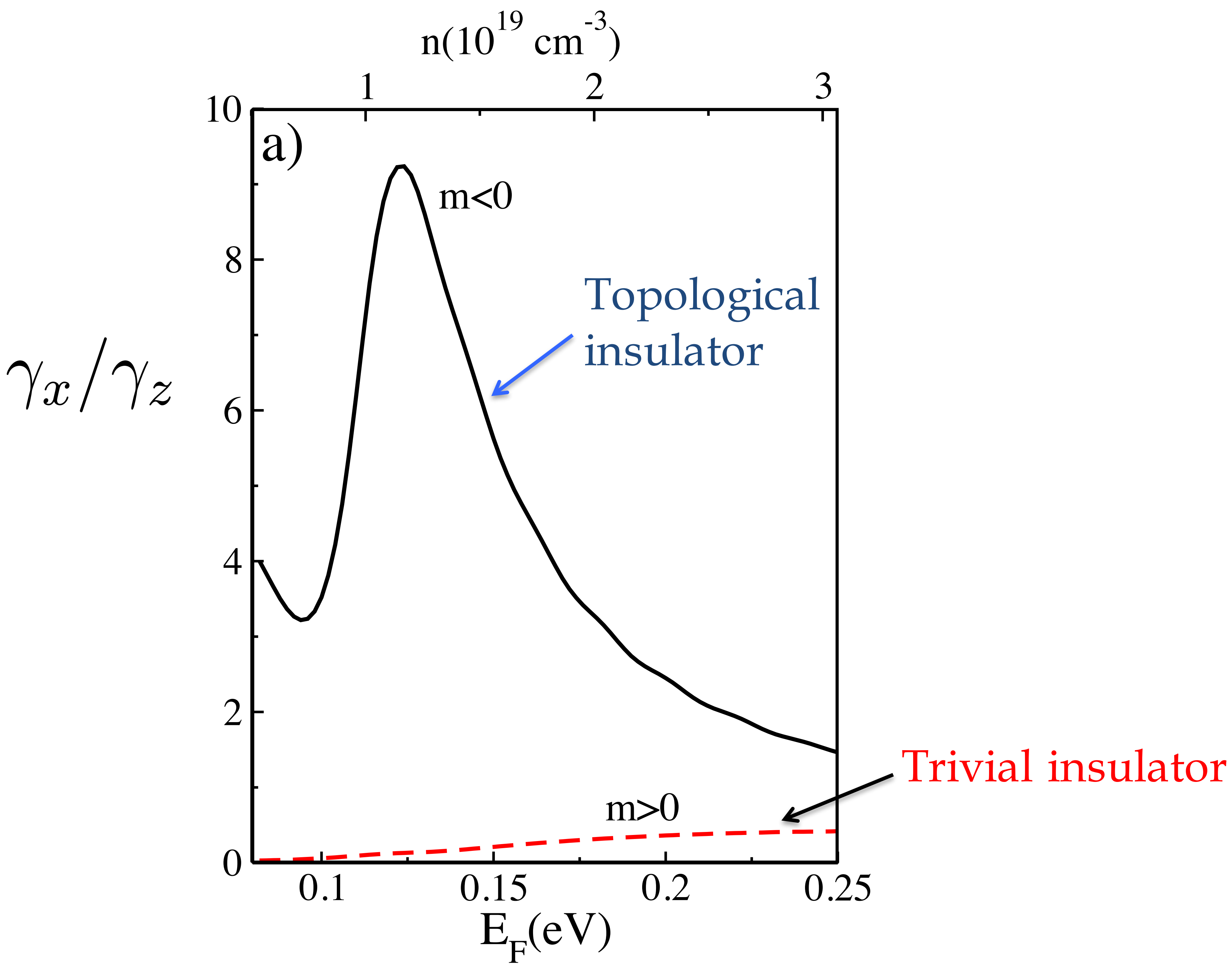


Matrix elements (II): trivial phase

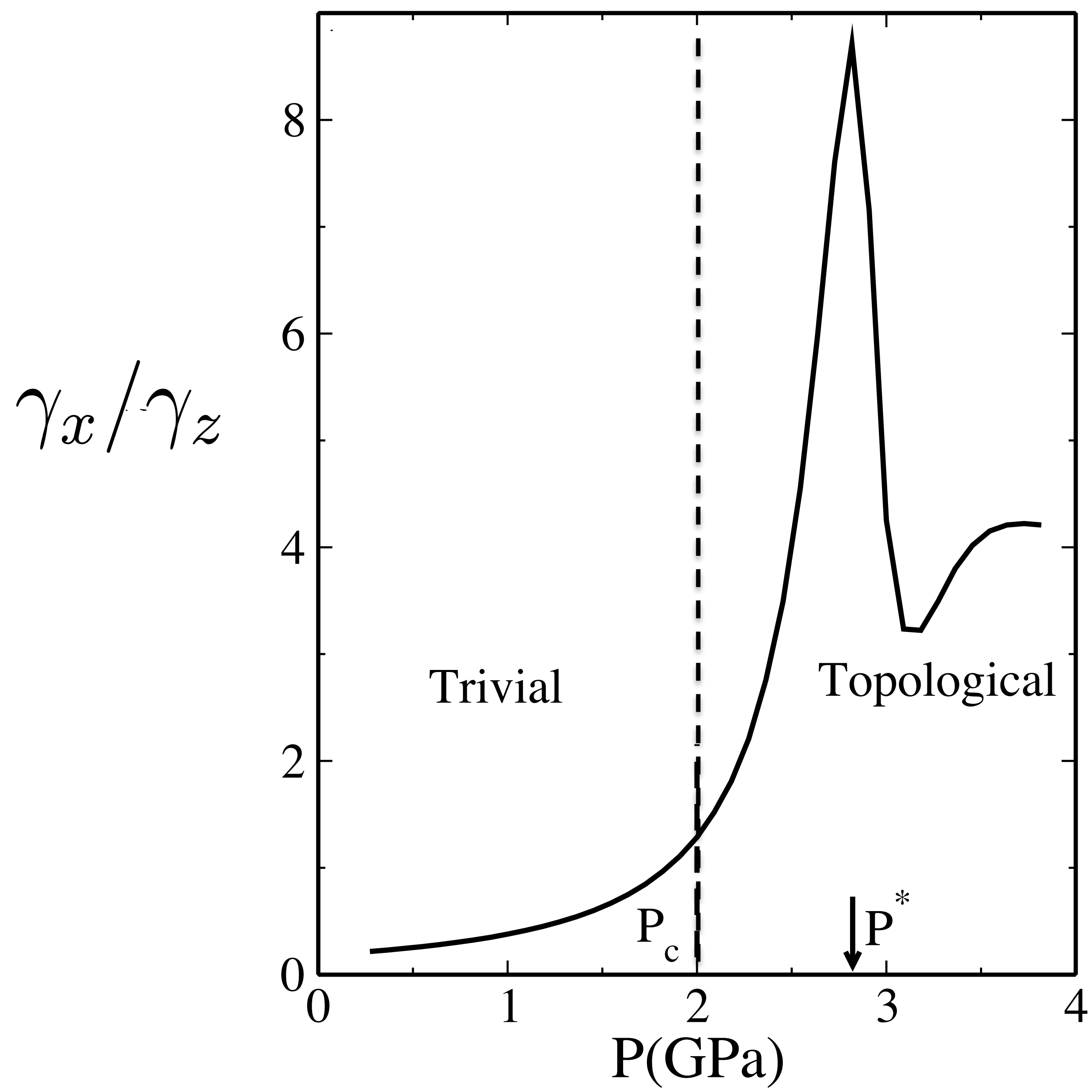








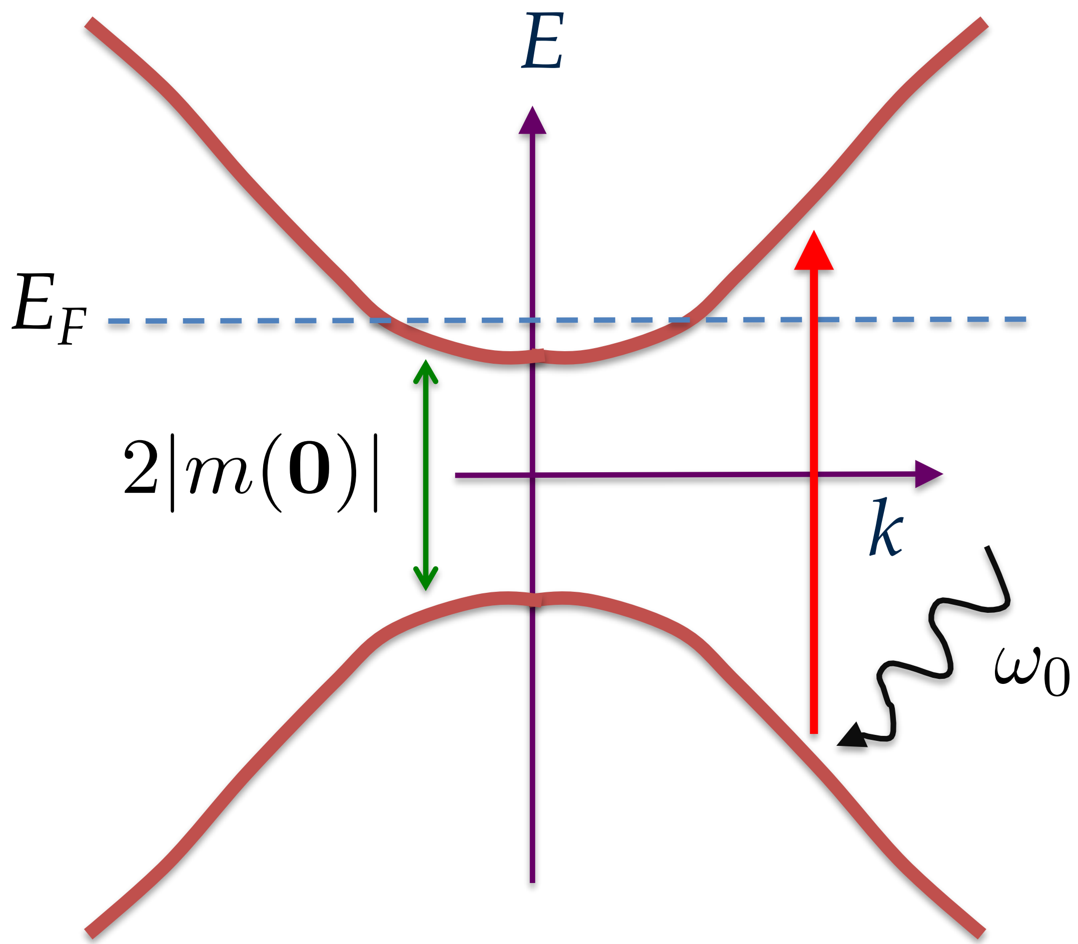
n(10^19 cm^-3)
1
2
3
10
8
6
4
2
0
a)
m<0
Topological insulator
Trivial insulator
m>0
γ_x/γ_z
0.1
0.15
0.2
0.25
E_F(eV)



γ_x/γ_z
8
6
4
2
0
0
1
2
3
4
P(GPa)
Trivial
Topological
P_c
P^*

Phonon linewidth

Case II: Phonon frequency > Bandgap



q=0 linewidth:

$$\boxed{\gamma_\lambda = g_\lambda D_{\text{joint}}(\omega_0)\overline{|\langle \text{c}|h_{\text{ep}}|\text{v}\rangle|^2}}$$

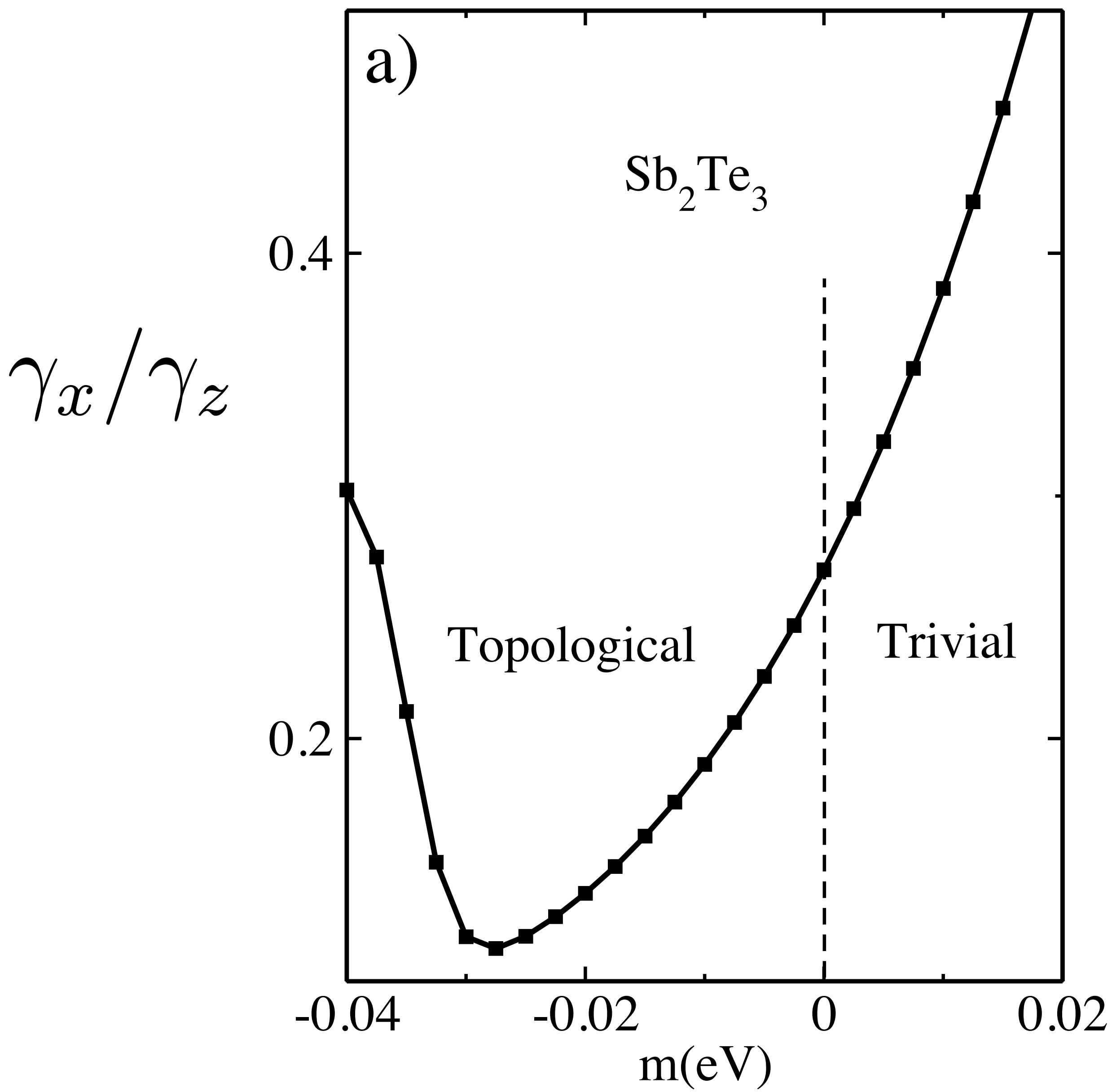
Joint DOS

Interband matrix element

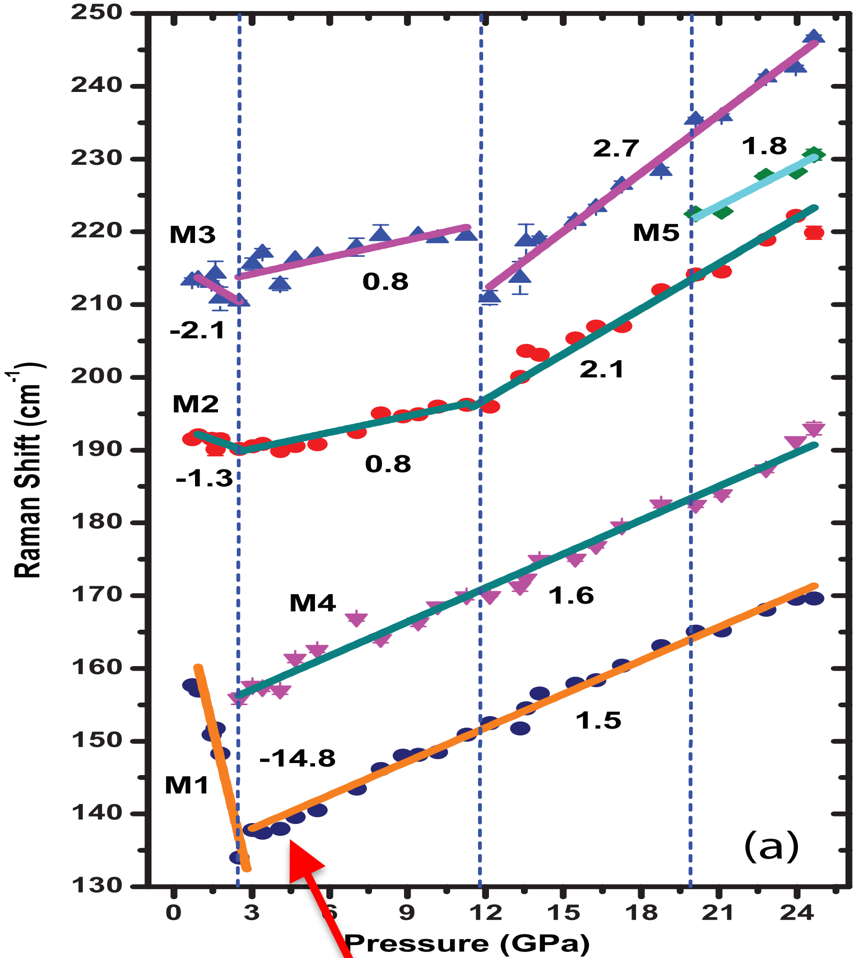
A property of interband matrix elements:

$$|\langle \text{v}\mathbf{k}|\tau^z|\text{c}\mathbf{k}\rangle|^2 = |\langle \text{c}\mathbf{k}|\tau^x|\text{c}\mathbf{k}\rangle|^2$$

Theoretical prediction



Experiments?



Phonon anomaly

A. Bera *et al.*, PRL **110**, 107401 (2013).

- Linewidths are hard to measure
- Anharmonic contribution

Summary and Conclusions

Phonons can change the electronic band topology

Phonons can inherit unique signatures of the electronic band topology

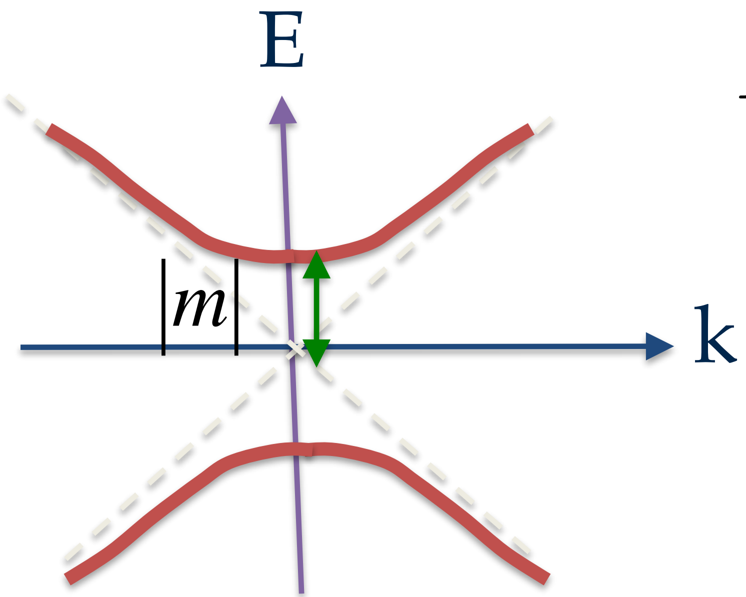
Interesting interplay between phonons and electronic band topology

Dirac fermions (spin ½)

$$\boxed{\mathcal{H} = v\mathbf{k}\cdot\boldsymbol{\sigma}\tau^x + m\,\tau^z}$$

Dirac velocity

Dirac mass



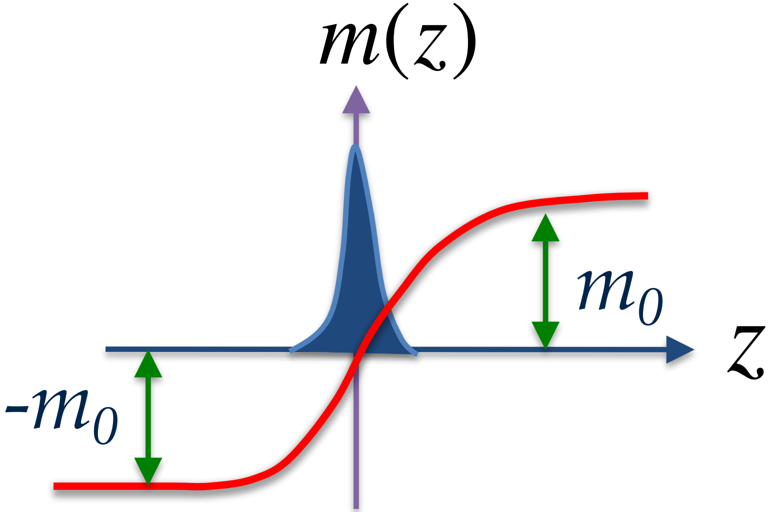
$$E_{\mathbf{k}} = \pm\sqrt{v^2k^2 + m^2}$$

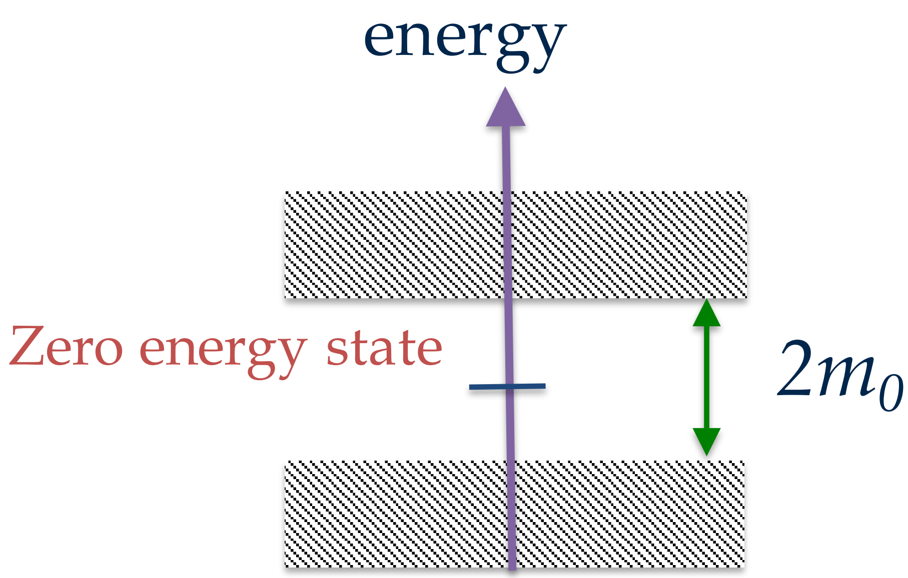
Jackiw-Rebbi zero mode

[PRD **13**, 3398 (1976)]

Dirac fermions in 1D

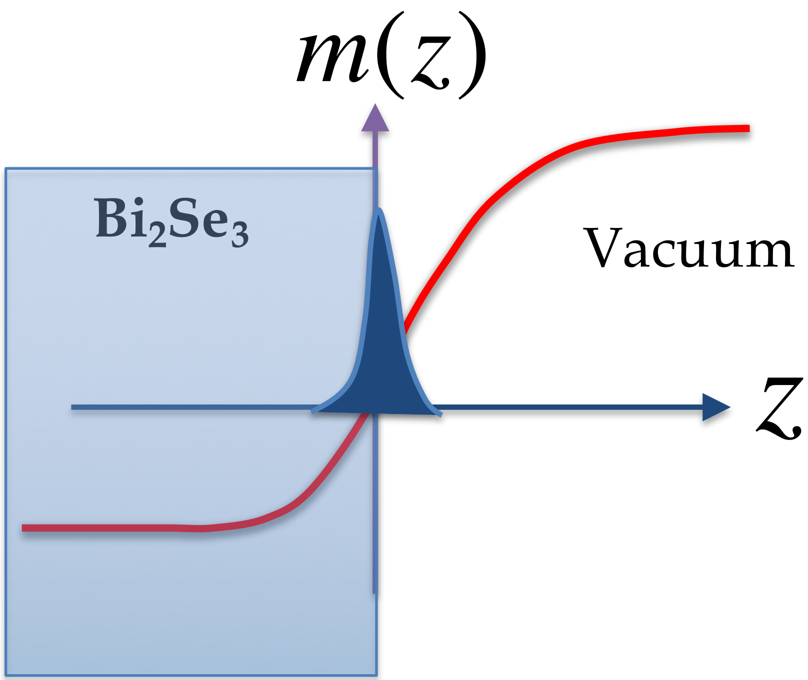
"Domain wall":



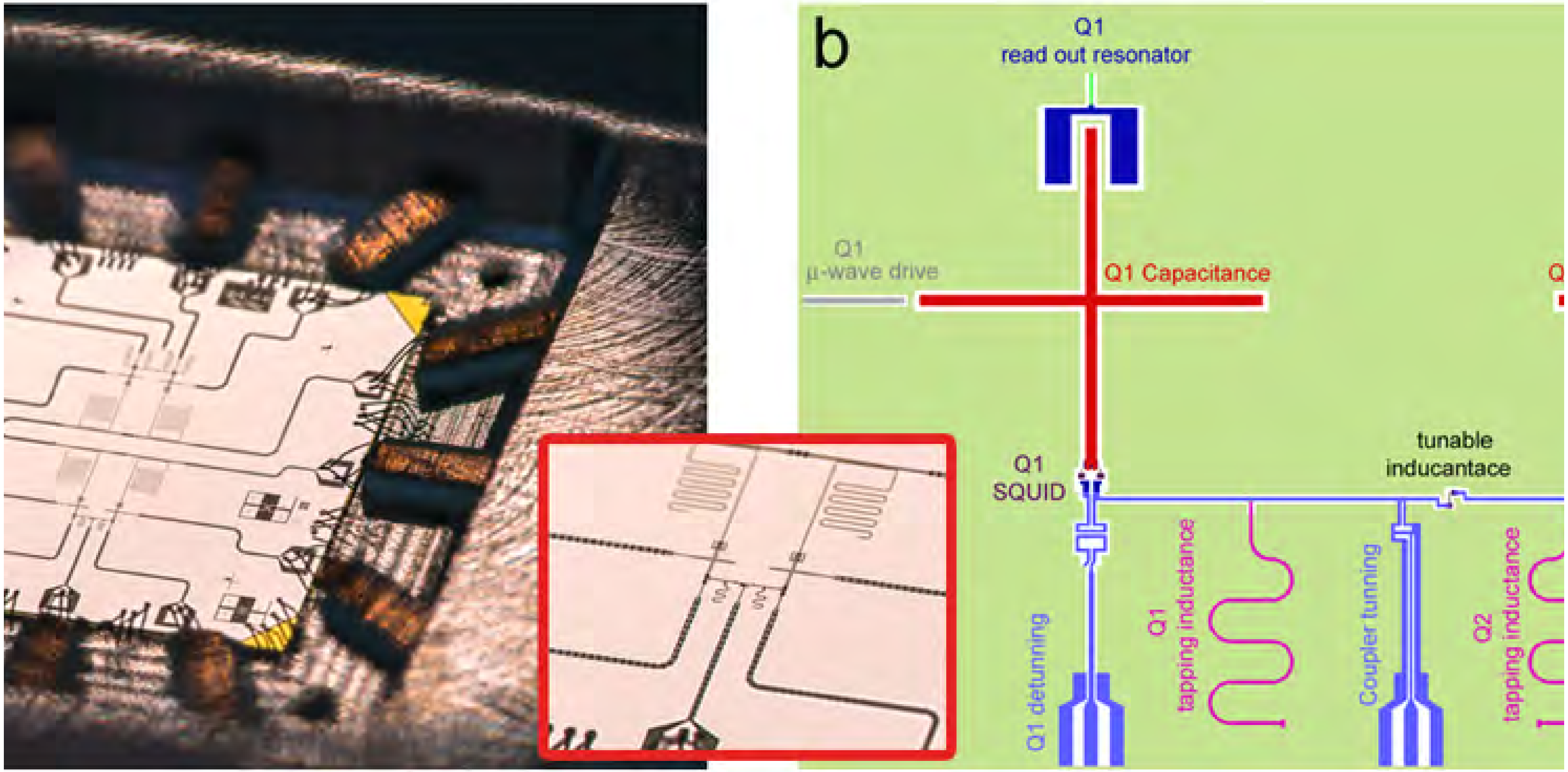


Insensitive to details of the Hamiltonian

Topological insulators



Topological phases in superconducting circuits

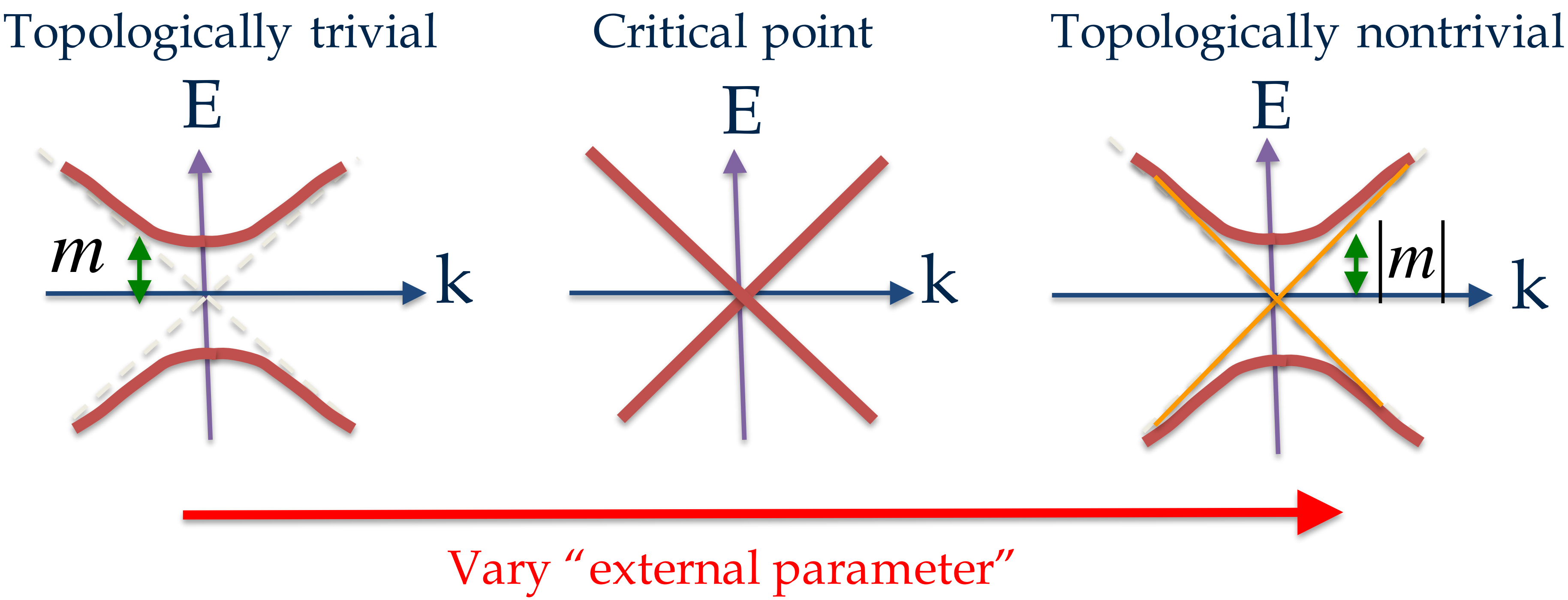


Roushan et al., Nature (2014)

Examples of topological Dirac materials

CdTe/HgTe/CdTe	$TlBiSe_2$	Ag_2Te
AlSb/InAs/GaSb/AlSb	$TlBiTe_2$	SmB_6
$Bi_{1-x}Sb_x$	$TlBi(S,Se)_2$	$Bi_{14}Rh_3I_9$
Sb	$PbBi_2Te_4$	RBiPt (R = Lu, Dy, Gd)
Bi_2Se_3	$PbSb_2Te_4$	$Nd_2(Ir_{1-x}Rh_x)_2O_7$
Bi_2Te_3	$GeBi_2Te_4$	
Sb_2Te_3	$PbBi_4Te_7$	
Bi_2Te_2Se	$GeBi_{4-x}Sb_xTe_7$	
$(Bi,Sb)_2Te_3$	$(PbSe)_5(Bi_2Se_3)_6$	
$Bi_{2-x}Sb_xTe_{3-y}Se_y$	$(Bi_2)(Bi_2Se_{2.6}S_{0.4})$	
$Bi_2Te_{1.6}S_{1.4}$	$(Bi_2)(Bi_2Te_3)_2$	
$Bi_{1.1}Sb_{0.9}Te_2S$	SnTe	
Sb_2Te_2Se	$Pb_{1-x}Sn_xTe$	
$Bi_2(Te,Se)_2(Se,S)$	$Pb_{0.77}Sn_{0.23}Se$	
	Bi bilayer	

Topological quantum phase transition



"External parameter": doping, pressure...

(Experiment: Xu *et al.*, Science **332**, 560 (2011))

Can there be a thermal topological transition?

Electron-phonon interaction

We focus on two types:

1) Parity-even phonon (Raman active)

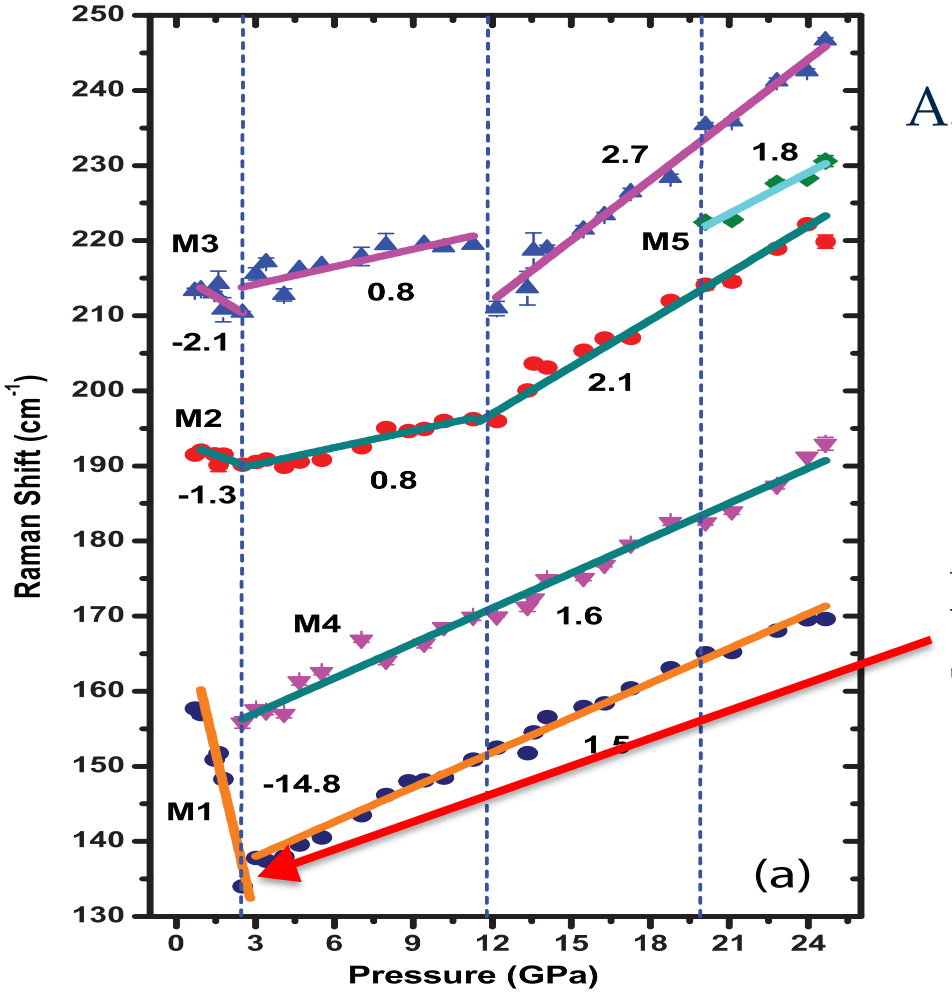
$$h_{\mathrm{ep}} \propto \mathbf{1}_2 \otimes \tau^z$$

2) Parity-odd phonon (infrared active)

$$h_{\mathrm{ep}} \propto \mathbf{1}_2 \otimes \tau^x$$

Influence of band topology on phonons

Experiment in Sb_2Se_3



A. Bera *et al.*, PRL **110**, 107401 (2013).

Phonon anomaly

Topological phase transition?

Electron-phonon interaction

Long wavelength + local-in-space

Electron-phonon coupling	Phonon parity
$h^{0}_{\text{ep}}(\mathbf{r}) = u_0(\mathbf{r})\ \mathbf{1}_2 \otimes \mathbf{1}_2$	Even
$h^{z}_{\text{ep}}(\mathbf{r}) = u_z(\mathbf{r})\ \mathbf{1}_2 \otimes \tau^z$	Even
$h^{x}_{\text{ep}}(\mathbf{r}) = u_x(\mathbf{r})\ \mathbf{1}_2 \otimes \tau^x$	Odd
$h^{iy}_{\text{ep}}(\mathbf{r}) = u_{iy}(\mathbf{r})\ \sigma^i \otimes \tau^y$	Odd

Theoretical issue

Thus far we have assumed that a parity-even phonon mode can couple to electrons purely through

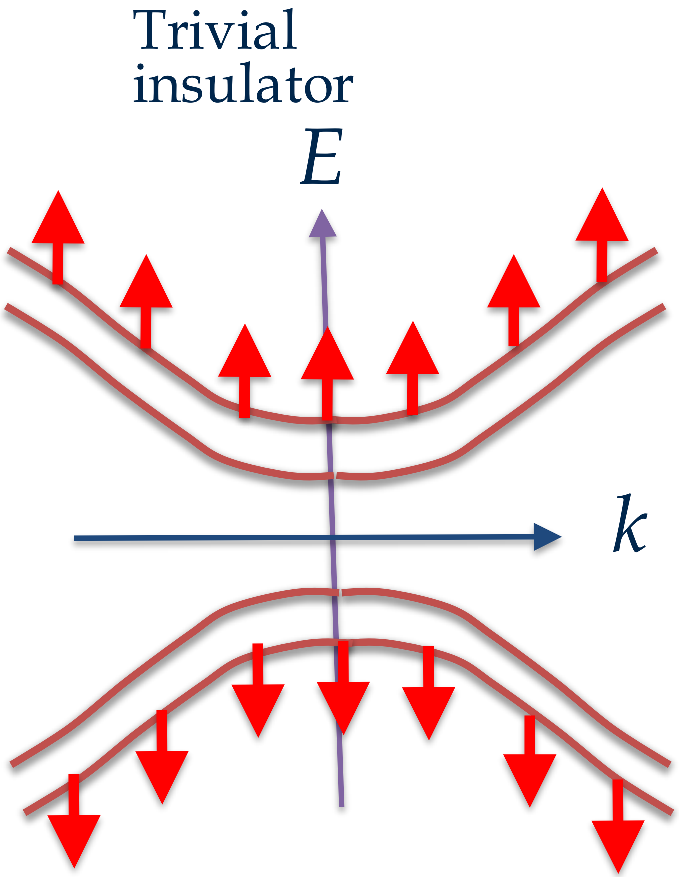
$$h_{\rm ep} \propto \mathbf{1}_2 \otimes \tau^z$$

In general, it could also couple to electrons via

$$h_{\rm ep} \propto \mathbf{1}_2 \otimes \mathbf{1}_2$$

The latter is not sensitive to band topology and therefore can mask the effect of the former.

Dirac insulator with small energy gap



Intraband transitions dominate
→ phonons decrease bandgap