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Theory of giant phonon magnetic moment in Dirac semimetals

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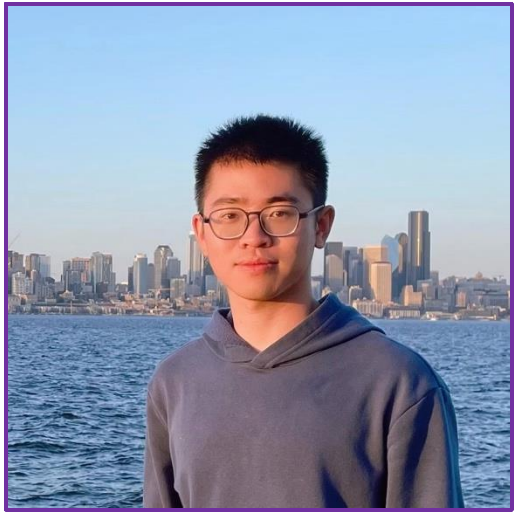
@ Chiral Phonons Workshop

Outline

- Introduction to phonon magnetic moment
- Gauge theory of Giant phonon magnetic moment in Dirac semimetal
- Giant phonon magnetic moment due to curved space in Dirac semimetal
- Summary

W. Q. Chen, X. W. Zhang, Y. Su, T. Cao, D. Xiao* and **SZL***, PRB 111, 035126 (2025)
W. Q. Chen, X. W. Zhang, T. Cao, **SZL* and** D. Xiao*, arXiv:2505.09732 (2025)


Wenqin Chen (LANL student intern, U. Washington)

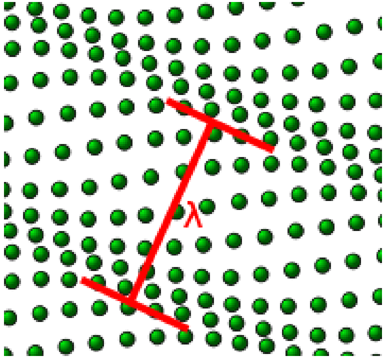

Xiaowei Zhang (U. Washington)


Ying Su (LANL➔ UESTC)


Ting Cao (U. Washington)

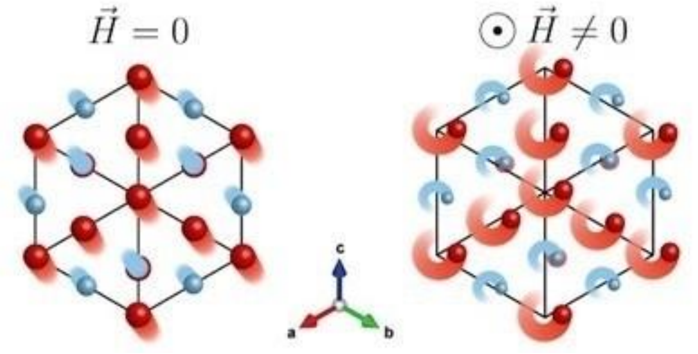

Di Xiao (U. Washington)

What about phonon magnetic moment?



Phonon: collective motion of ions

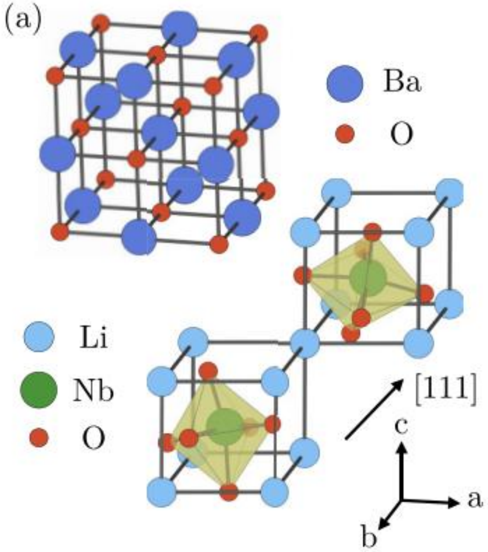
But ions are way heavier



Expectation:

$$\mu_{ph} = \frac{e\hbar}{2M} \sim \frac{1}{2000}\mu_B$$

Phonon magnetic moment in ionic crystals



Juraschek and Spaldin, Phys. Rev. Materials 3, 064405 (2019)

DFT results

In unit of nuclear magneton, $\mu_N \approx \frac{1}{2000}\mu_B$

Compound	ν_0	Z	d/d_0	N	μ_{ph}	M	$\Delta\Omega/\Omega_0$
Rocksalt structure[a]							
BaO	3.0	0.7	9	6	0.15	1.0	0.0002
CsF	3.6	0.3	3	1	0.06	0.1	0.00008
CsH	11.9	1.1	25	15	1.12	16.8	0.0005
LiI	4.8	0.5	7	3	0.18	0.5	0.0002
MgO	11.7	0.6	4	5	0.04	0.2	0.00002
PbO[b]	7.7	1.2	7	16	0.13	2.1	0.00008
PbS	2.2	0.8	8	8	0.12	1.0	0.0003
PbSe	1.6	0.6	4	5	0.04	0.2	0.0001
PbTe	1.4	0.7	3	5	0.02	0.1	0.00006
SnTe	1.0	1.0	5	13	0.004	0.1	0.00002

Compound	ν_0	Z	d/d_0	N	μ_{ph}	M	$\Delta\Omega/\Omega_0$
Wurtzite structure[c]							
BN	31.8	1.1	4	13	0.05	0.7	6×10^{-6}
AlN	20.0	1.2	5	16	0.11	1.7	0.00002
GaN	17.1	1.1	6	15	0.17	2.5	0.00005
InN	14.7	1.2	6	16	0.2	3.2	0.00006
BeO	21.9	1.1	7	13	0.1	1.3	0.00002
CuH	31.0	0.7	12	6	0.49	2.7	0.00008
SiC	23.7	1.3	6	20	0.15	2.9	0.00003
Zinc-blende structure[d]							
BeS	17.3	0.6	5	4	0.13	0.5	0.00004
BeSe	15.3	0.5	5	3	0.15	0.5	0.00005
BeTe	14.1	0.4	4	2	0.14	0.3	0.00005
GaAs	7.9	0.4	1	2	0.002	0.004	1×10^{-6}

Compound	ν_0	Z	d/d_0	N	μ_{ph}	M	$\Delta\Omega/\Omega_0$
$BaHfO_3$[a]	15.7	0.8	5	8	0.04	0.3	0.00001
	5.9	1.1	7	14	0.12	1.7	0.0001
$BaZrO_3$[a]	15.0	0.9	6	10	0.04	0.4	0.00001
	5.8	1.0	5	12	0.04	0.4	0.00003
	3.1	0.7	5	6	0.07	0.4	0.0001
$KTaO_3$[a]	15.8	1.0	6	12	0.003	0.04	9×10^{-7}
	2.3	1.4	14	24	0.12	3.0	0.0003
$BiAlO_3$[b]	18.5	0.6	2	4	0.08	0.3	0.00002
	12.8	0.1	–	–	0.14	–	0.00005
	11.5	1.4	6	22	0.05	1.1	0.00002
	3.9	1.1	6	14	0.05	0.7	0.00006
$CsPbF_3$[b]	9.1	0.04	–	–	0.001		3×10^{-7}
	4.9	0.6	3	4	0.04	0.2	0.00004
	1.5	0.02	–	–	0.04	–	0.0001
$LiNbO_3$[b]	17.0	1.6	6	32	0.04	1.4	0.00001
	10.6	0.8	7	7	0.13	0.9	0.00006
	4.3	1.0	6	12	0.1	1.2	0.0001

Compound	ν_0	Z	d/d_0	N	μ_{ph}	M	$\Delta\Omega/\Omega_0$
$LiTaO_3$[b]	17.4	1.5	5	25	0.04	1.0	0.00001
	10.9	0.9	8	10	0.13	1.3	0.00006
	4.2	1.0	4	11	0.07	0.8	0.00008
$BaTiO_3$[c]	14.1	0.8	3	8	0.03	0.3	0.00001
	8.9	0.01	–	–	0.14	–	0.00007
	6.5	2.2	9	58	0.02	1.0	0.00001
$KNbO_3$[c]	15.2	1.7	7	35	0.01	0.5	5×10^{-6}
	8.1	0.02	–	–	0.18	–	0.0001
	6.0	2.2	10	55	0.13	7.0	0.0001
$PbTiO_3$[d]	14.9	0.8	6	8	0.09	0.7	0.00003
	8.1	0.1	1	0.2	0.19	0.05	0.0001
	2.6	0.8	7	7	0.08	0.6	0.0001
$SrTiO_3$[e]	15.7	1.1	4	15	0.03	0.4	9×10^{-6}
	7.3	0.04	–	–	0.18	–	0.0001
	1.7	2.5	21	74	0.1	7.2	0.0003

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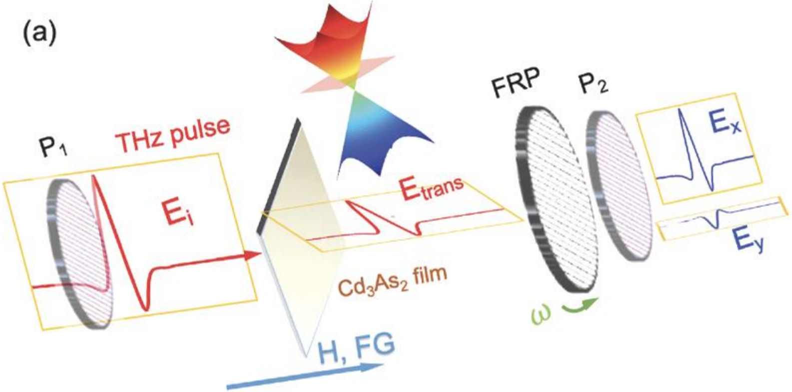
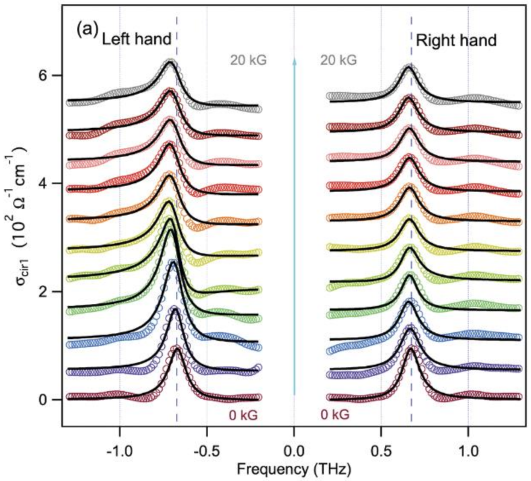
However, giant phonon magnetic observed by experiment

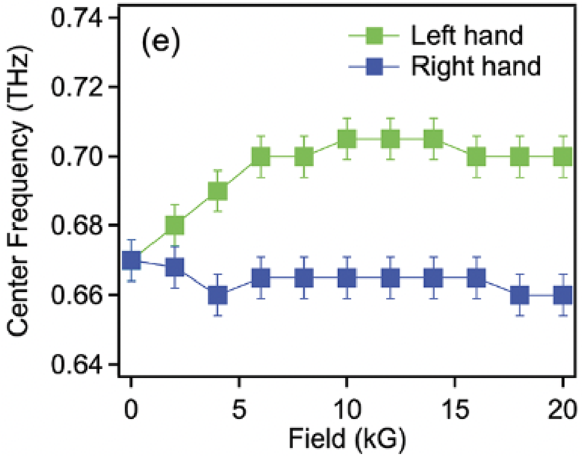
time-domain magnetoterahertz spectrometer.



Cheng et al., Nano Lett. 20, 5991 (2020)

Cd_3As_2 Dirac semimetal



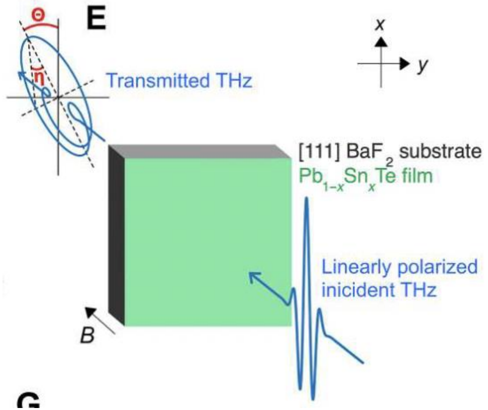


Phonon moment

$\mu_{ph} \approx 2.7\mu_B$

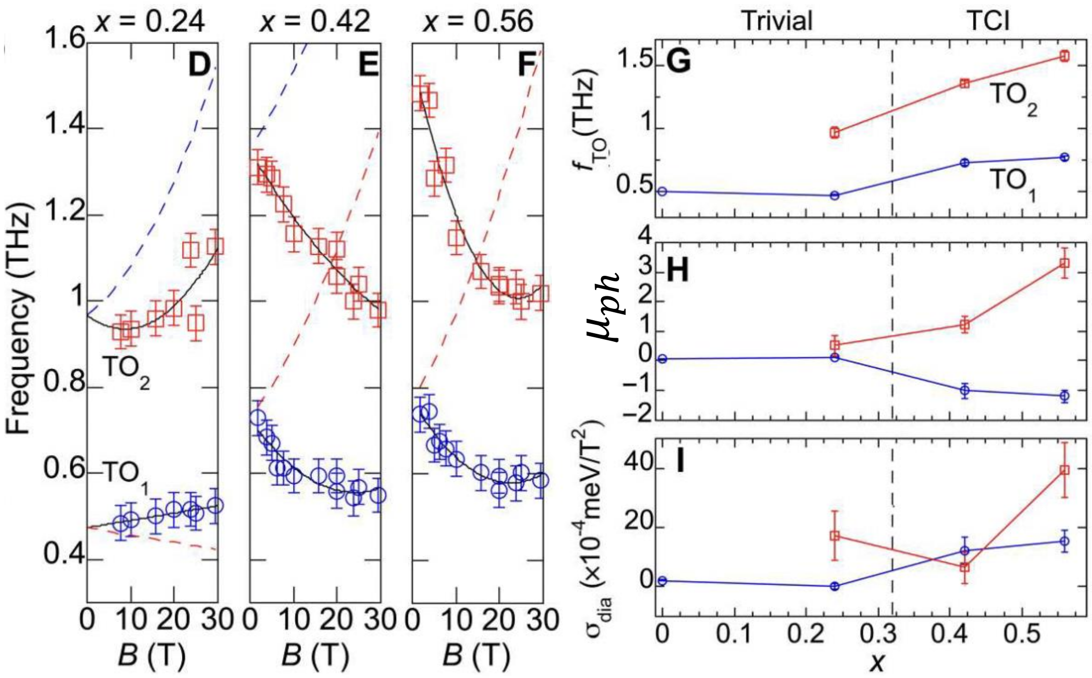
However, giant phonon magnetic observed by experiment

Polarization-dependent terahertz magnetospectroscopy measurements



$Pb_{1-x}Sn_xTe$: Topological crystalline insulator when x>0.32

Hernandez et al., Science Advances (2023)



Phonon moment: $\mu_{ph} \approx -1.2 \pm\ 0.2\mu_B$ for TO_1

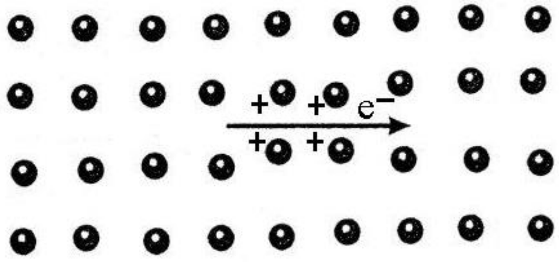
$\mu_{ph} \approx 3.3 \pm\ 0.5\mu_B$ for TO_2

- Phonon magnetic moment ~ μ_B
- Must be due to electrons
- Question: how does the electron-phonon coupling give rise to the large phonon magnetic moment?

Adiabatic theory

Y. F. Ren, Q. Niu et al., Phys. Rev. Lett. 127, 186403 (2021)

Slow ions and fast electrons



- In insulators, electrons follow the motion of ions adiabatically
- Same idea as Thouless pump
- Extend the dimensionality of the system by treating ion coordinate as synthetic dimensions

Electron wave function $\psi(k_x, k_y, u_x, u_y)$

$$M_z = \frac{e}{2m_I} L_I \int \frac{dk}{(2\pi)^2} \Omega_{k_\alpha k_\beta u_x u_y} \qquad L_I = (m_I/T) \int_0^T (\boldsymbol{u} \times \dot{\boldsymbol{u}})_z dt$$

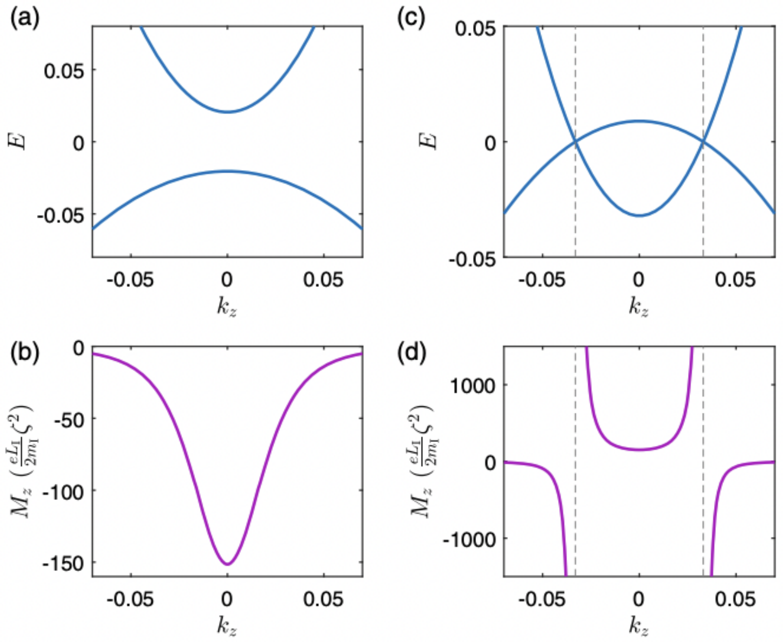
Second Chern form in 4 synthetic dimensions

However

Y. F. Ren, Q. Niu et al., Phys. Rev. Lett. 127, 186403 (2021)

An effective model for Cd_3As_2

- (a), (b) before band inversion➔ semiconductor and the adiabatic theory works. Estimated $\mu_{ph}{\sim}1\ -10\ \mu_B$
- (c) and (d) after band inversion ➔ Dirac semimetal and adiabatic theory breaks.



Doomed to fail for Dirac semimetal because of the breakdown of adiabaticity

Need a new theory framework for Dirac semimetals!

Our theories

In Dirac semimetal, depending on symmetries

- Phonon is an emergent gauge field for electrons (gauge theory perspective)

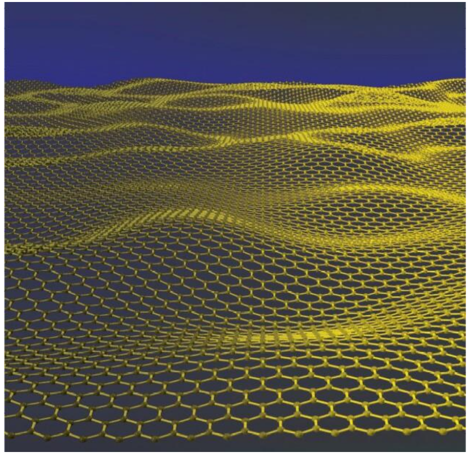
- Phonon creates curved space for electrons (general relativity perspective)

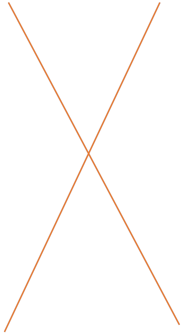
Multiscale approach:

DFT (materials) ➔ tight binding (model validation)➔ QFT + symmetry (physical picture)

Response of Dirac node to phonon

With strain

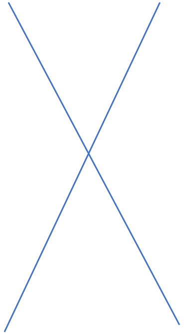




Shift node position

Strain as a gauge field

$$\mathbf{k} \rightarrow \mathbf{k} - \mathbf{a}$$



Renormalize Dirac velocity

Strain as a curved space

$$v_{\mathrm{i}} \rightarrow g^{ij} v_j$$

When phonon is a gauge field

The minimal coupling between momentum and phonon field as a gauge field should be compatible with the little group at the Dirac node.

The little group at $+K$ for graphene: $C_{3z} \otimes IT$

$$\mathcal{H}_+ = v((k_x - a_x)\sigma_x + (k_y - a_y)\sigma_y)$$

Emergent gauge field due to strain (acoustic phonon):

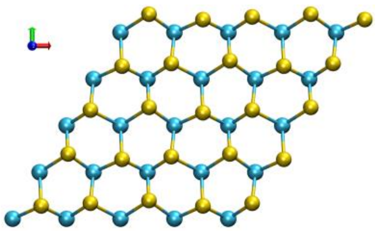
$a_x \propto u_{11} - u_{22}$ and $a_y \propto -2u_{12}$

Vozmediano et al, Physics Reports 496, 109 (2010)

$\mathbf{k}$ and $\mathbf{a}$ transform in the same way under C_{3z} and IT

Under C_{3z}, $\mathbf{k}$ has angular momentum 1 and $\mathbf{a}$ has momentum -2. but 1=-2 for C_{3z} symmetry.

Optical phonon



Emergent gauge field due to strain (optical phonon):

$$a_x \propto u_y \text{ and } a_y \propto -u_x$$

$\mathbf{u} = \mathbf{R}_B - \mathbf{R}_A$ is even under inversion, because the inversion swaps B and A sublattice

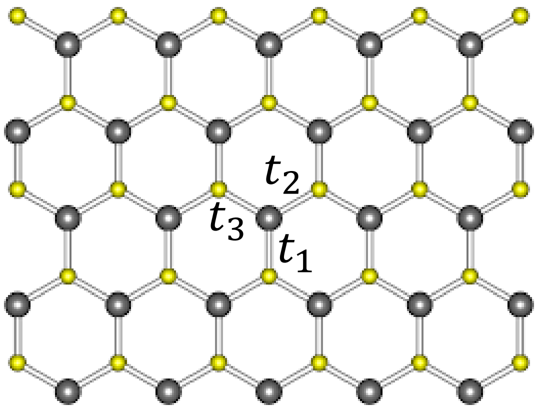
$\mathbf{k}$ and $\mathbf{a}$ transform in the same way under C_{3z} and IT

The result at –K valley is obtained by I or T of the K valley

$$\mathcal{H}_- = v(-(k_x + a_x)\sigma_x + (k_y + a_y)\sigma_y)$$

The emergent gauge field is opposite for the opposite valley, because phonon does not break TRS.

Tight binding model



Hamiltonian for distorted lattice

$$\mathcal{H}_+ = v((k_x - a_x)\sigma_x + (k_y - a_y)\sigma_y)$$

$$v_F e a_x = -\frac{1}{2}\delta t_1 + \delta t_2 - \frac{1}{2}\delta t_3,$$

$$v_F e a_y = \frac{\sqrt{3}}{2}(\delta t_1 - \delta t_3)$$

Koster-Slater hopping integral

$$\delta t_1 = \beta t(\kappa_{\rm ac}\partial_y u_y + \kappa_{\rm op}\partial_y v_y - 2\kappa_{\rm op}\frac{v_y}{a})$$

$$\delta t_2 = \beta t[\kappa_{\rm ac}(\frac{3}{4}\partial_x u_x - \frac{\sqrt{3}}{4}\partial_y u_x - \frac{\sqrt{3}}{4}\partial_x u_y + \frac{1}{4}\partial_y u_y) + \kappa_{\rm op}(\frac{3}{4}\partial_x v_x - \frac{\sqrt{3}}{4}\partial_y v_x - \frac{\sqrt{3}}{4}\partial_x v_y + \frac{1}{4}\partial_y v_y) + \kappa_{\rm op}(-\sqrt{3}\frac{v_x}{a} + \frac{v_y}{a})]$$

$$\delta t_3 = \beta t[\kappa_{\rm ac}(\frac{3}{4}\partial_x u_x + \frac{\sqrt{3}}{4}\partial_y u_x + \frac{\sqrt{3}}{4}\partial_x u_y + \frac{1}{4}\partial_y u_y) + \kappa_{\rm op}(\frac{3}{4}\partial_x v_x + \frac{\sqrt{3}}{4}\partial_y v_x + \frac{\sqrt{3}}{4}\partial_x v_y + \frac{1}{4}\partial_y v_y) + \kappa_{\rm op}(\sqrt{3}\frac{v_x}{a} + \frac{v_y}{a})]$$

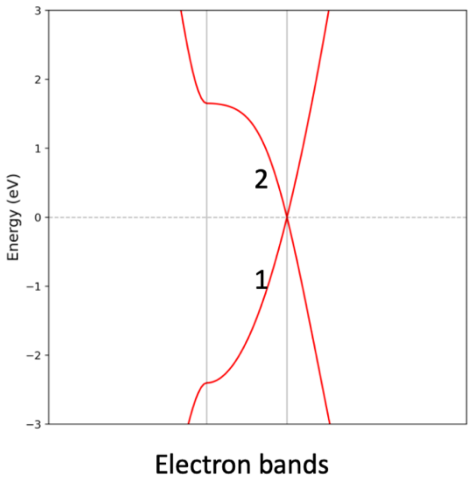
DFT for graphene

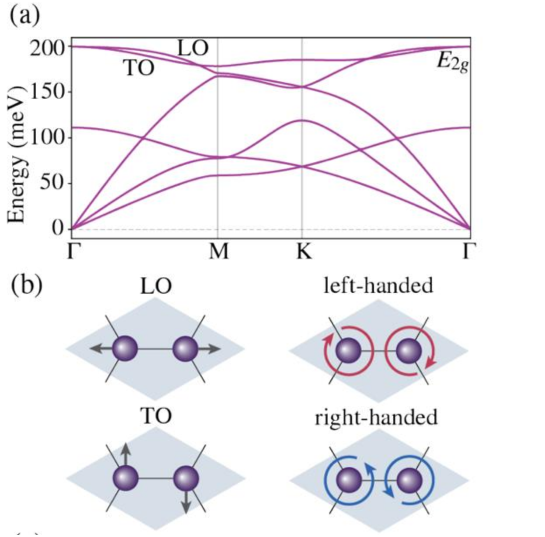
- Zone-center phonon modes

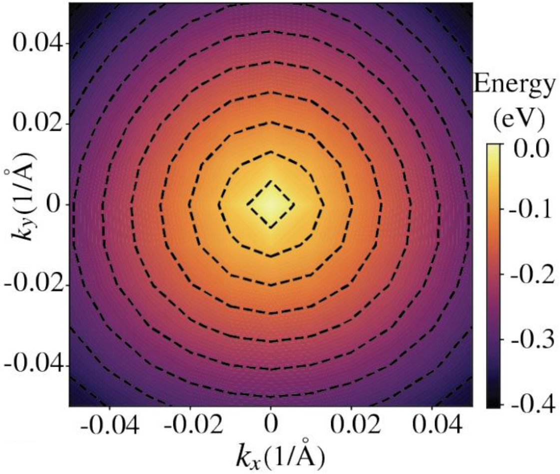
  A_{2u}: ZA, E_{1u}: LA, TA

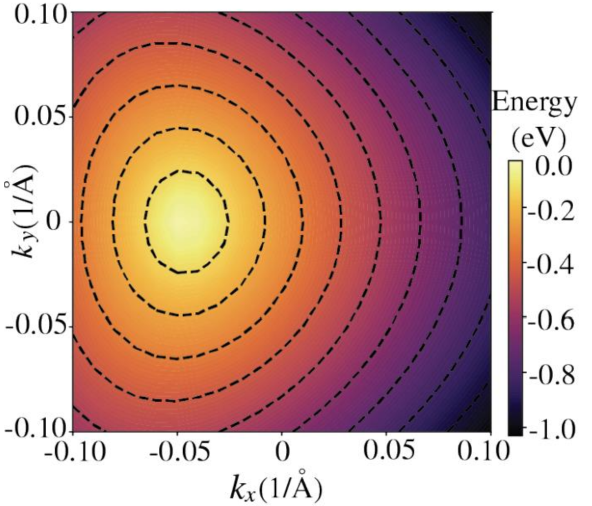
  B_{2g}: ZO, $\mathbf{E_{2g}}$**: LO, TO** (48.19 THz)

- Electron band structure (energy contours) after displacing the atoms according to E_{2g} optical modes
- Shift of Dirac node ➔ emergent gauge field due to optical phonon
- Estimate the e-ph coupling
- Also deformation of the Dirac cone









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Hall conductivity

A: physical EM gauge
a: emergent gauge due to strain

$$\mathcal{H}_{\boldsymbol{\tau}}(\mathbf{k}, \mathbf{A}, \boldsymbol{a}) = \sum_j v\left(k_j - A_j - \tau a_j\right)\sigma_j - \mu_F$$

Hall conductivity σ_{xy} when apply a magnetic field to doped Dirac system

Chern-Simons action $S_{CS}[\boldsymbol{A}] = \frac{\sigma_{xy}}{2} \int d^3x\, \epsilon^{\mu\nu\rho} A_\mu \partial_\nu A_\rho$

Because the action is second order in A, the opposite sign of a for the opposite valley cancels out

Chern-Simons action $S_{CS}[\boldsymbol{a}] = \frac{\sigma_{xy}}{2} \int d^3x\, \epsilon^{\mu\nu\rho} a_\mu \partial_\nu a_\rho$

For time-reversal symmetric Dirac insulator: Su, Balatsky and **SZL**, PRL 134, 026304 (2025)

Phonon Hall viscosity

$a_x \propto u_y$ and $a_y \propto -u_x$

$Q = 0$ Phonon Hall viscosity (non-dissipative)

$$\mathcal{L}_\eta = \eta(u_y \dot{u}_x - u_x \dot{u}_y) \qquad \eta \propto \sigma_{xy}$$

Total phonon Lagrangian

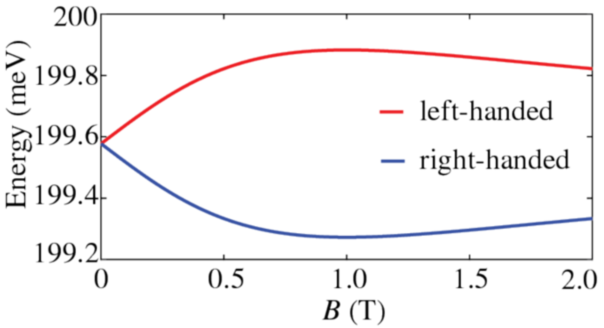
$$\mathcal{L}_{ph} = \eta\left(u_y \dot{u}_x - u_x \dot{u}_y\right) + \frac{\rho}{2}[\dot{u}_x^2 + \dot{u}_y^2 - \omega_0^2(u_x^2 + u_y^2)]$$

Splitting of the left-hand and right-hand phonon

$$\omega_- = \frac{\sqrt{\eta^2 + \rho^2\omega_0^2} - \eta}{\rho}$$

$$\omega_+ = \frac{\sqrt{\eta^2 + \rho^2\omega_0^2} + \eta}{\rho}$$

Existing experiment



Drude formula $\sigma_{xy} = -\sigma_0 \frac{\omega_c \tau}{1 + \omega_c^2 \tau^2}$

At doping level $n = 3.5 \times 10^{11} \mathrm{cm}^{-2}$, phonon magnetic moment is about $1 \sim 10\ \mu_B$

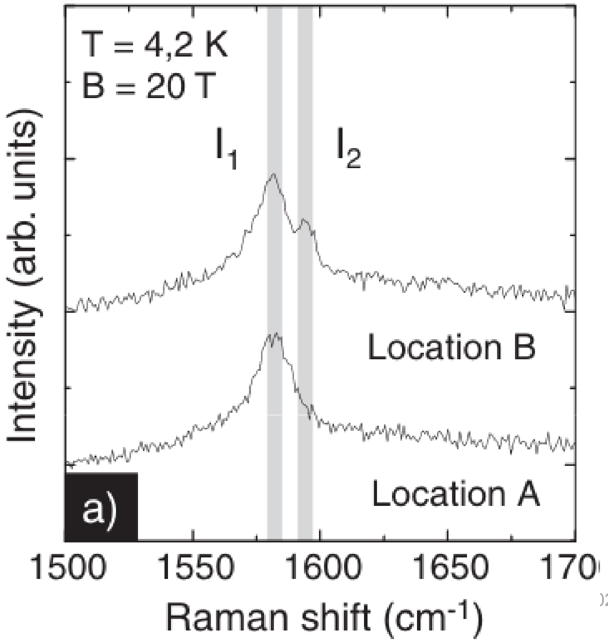
Magneto-Raman Scattering of Graphene on Graphite: Electronic and Phonon Excitations

C. Faugeras, M. Amado, P. Kossacki, M. Orlita, M. Kühne, A. A. L. Nicolet, Yu. I. Latyshev, and M. Potemski
Phys. Rev. Lett. **107**, 036807 – Published 14 July 2011

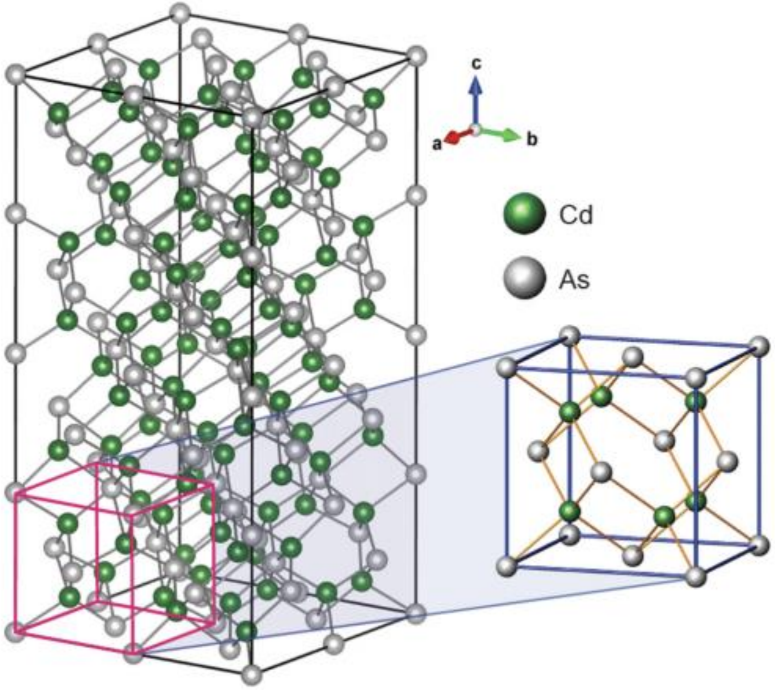
- Not designed to measure phonon magnetic moment

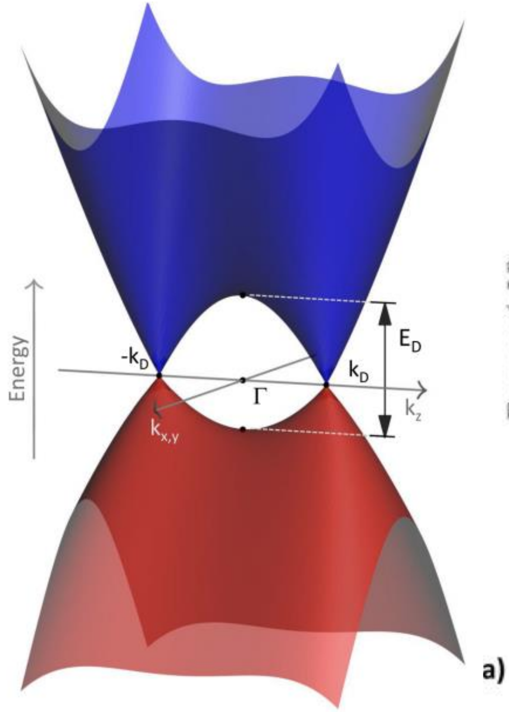
- Splitting of E_{2g} optical modes under magnetic field.

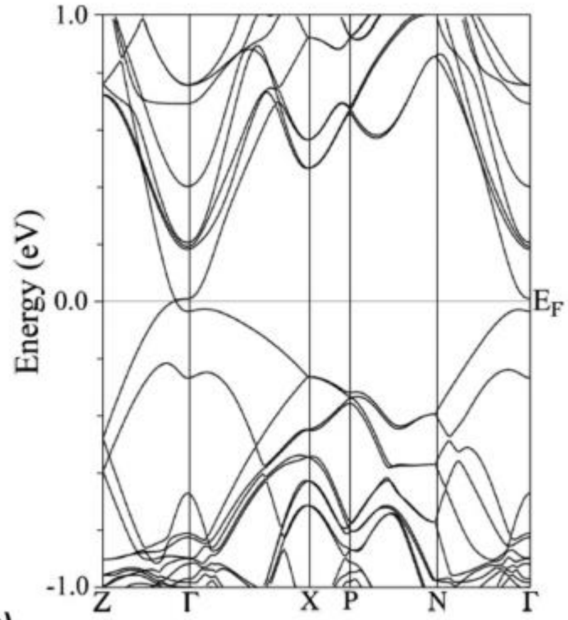
  Assume a linear splitting, an estimate of $m_{ph} \approx 2\ \mu_B$



3D Dirac Semimetal Cd_3As_2





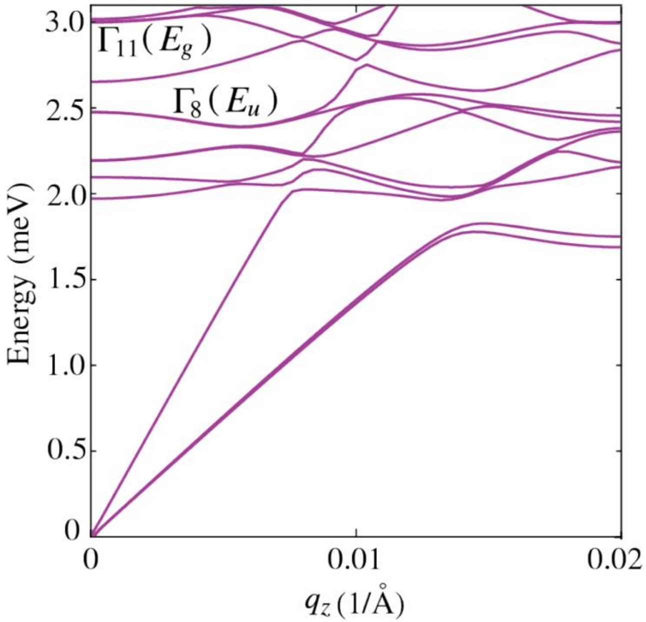


Crassee et al., Phys. Rev. Materials 2, 120302 (2018)

Phonon mode is Cd_3As_2

- DFT results of doubly degenerate zone-center optical phonon modes in THz frequency regime:

1. mode-[6,7] 0.53 THz E_g
2. mode-[8,9] 0.59 THz E_u IR-active
3. mode-[11, 12] 0.73 THz E_g
4. mode-[15, 16] 0.80 THz E_g
5. mode-[18, 19] 0.91 THz E_g
6. mode-[20, 21] 0.96 THz E_u IR-active



E_u (x, y)

E_g (zx, zy)

E_u is odd under spatial inversion

E_g is even under spatial inversion

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Compatibility check for gauge field description

The minimal coupling between momentum and strain field as a gauge field should be compatible with the little group at the Dirac node.

The little group at $\tau = \pm$ valley: $C_{4z} \otimes IT$

$$\mathcal{H}_{\boldsymbol{\tau}}(\mathbf{k}, \mathbf{A}, \boldsymbol{a}) = \sum_j v_{\tau,j} \Gamma_j \left(k_j - A_j - \tau a_j\right) - \mu_F$$

- E_g phonon mode: (zx, zy), $a_x \propto u_{zx}, a_y \propto u_{zy}, a_z \propto u_{zz}$ ✓

Tight-binding model: Cortijo e al., PRL 115, 177202 (2015)
Pikulin et al., PRX 6, 041021 (2016)

- E_u phonon mode: (x, y), incompatible with IT because E_u is odd under spatial inversion ✗

Tight binding model for Cd_3As_2

Pikulin et al., PRX 6, 041021 (2016)

Relevant spin-orbit coupled states $|P_{\frac{3}{2}}, \frac{3}{2}\rangle$, $|S_{\frac{1}{2}}, \frac{1}{2}\rangle$, $|S_{\frac{1}{2}}, -\frac{1}{2}\rangle$, and $|P_{\frac{3}{2}}, -\frac{3}{2}\rangle$

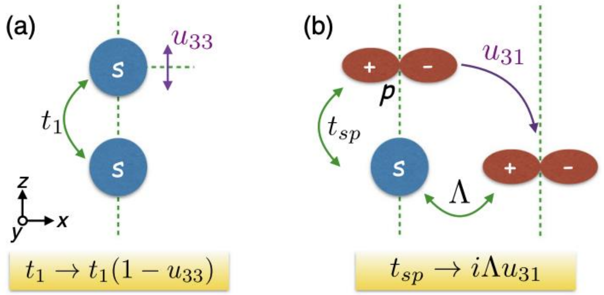
$$H^{\text{latt}} = \epsilon_{\boldsymbol{k}} + \begin{pmatrix} h^{\text{latt}} & 0 \\ 0 & -h^{\text{latt}} \end{pmatrix},$$

$$h^{\text{latt}}(\boldsymbol{k}) = m_{\boldsymbol{k}}\tau^z + \Lambda(\tau^x \sin ak_x + \tau^y \sin ak_y).$$

$$m_{\boldsymbol{k}} = t_0 + t_1 \cos ak_z + t_2(\cos ak_x + \cos ak_y)$$

Modified hopping due to strain

$$t_1\tau^z \to t_1(1 - u_{33})\tau^z + i\Lambda \sum_{j\neq 3} u_{3j}\tau^j,$$



Additional term in the Hamiltonian due to strain

$$\delta h^{\text{latt}}(\boldsymbol{k}) = -t_1 u_{33}\tau^z \cos ak_z + \Lambda(u_{13}\tau^x - u_{23}\tau^y) \sin ak_z.$$

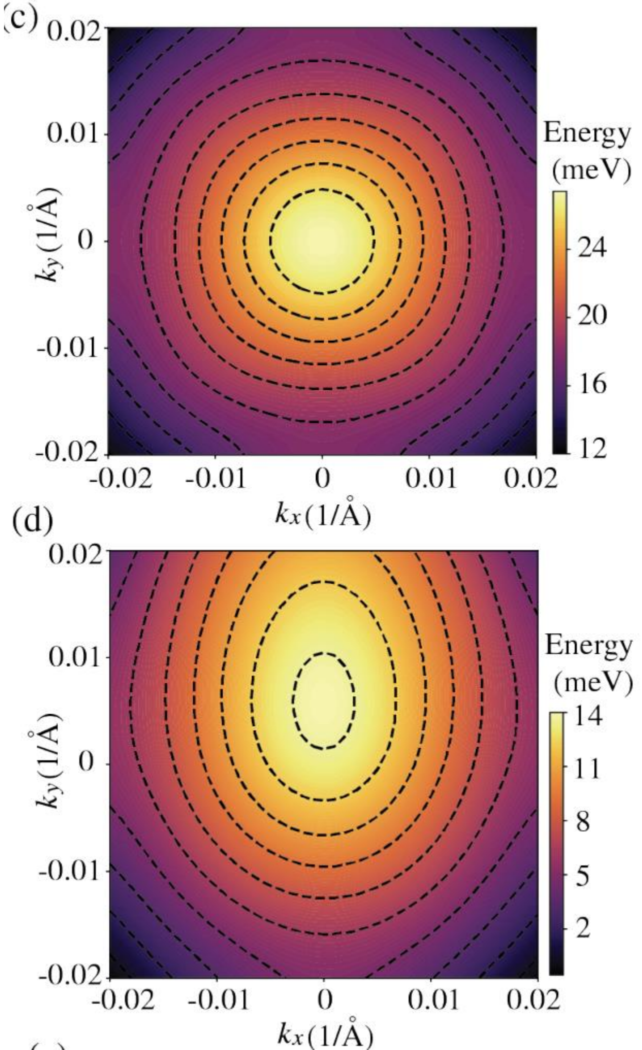
Therefore $a_x \propto u_{zx}$, $a_y \propto u_{zy}$, $a_z \propto u_{zz}$

DFT results for Cd_3As_2

- E_g **phonon mode:** (zx, zy)
- Significant displacement of Dirac point in k-space

  Gauge field description

- Change of shape is also significant
- Expected large phonon magnetic moment. Theory estimate $m_{ph} \approx 1\ \mu_B$.



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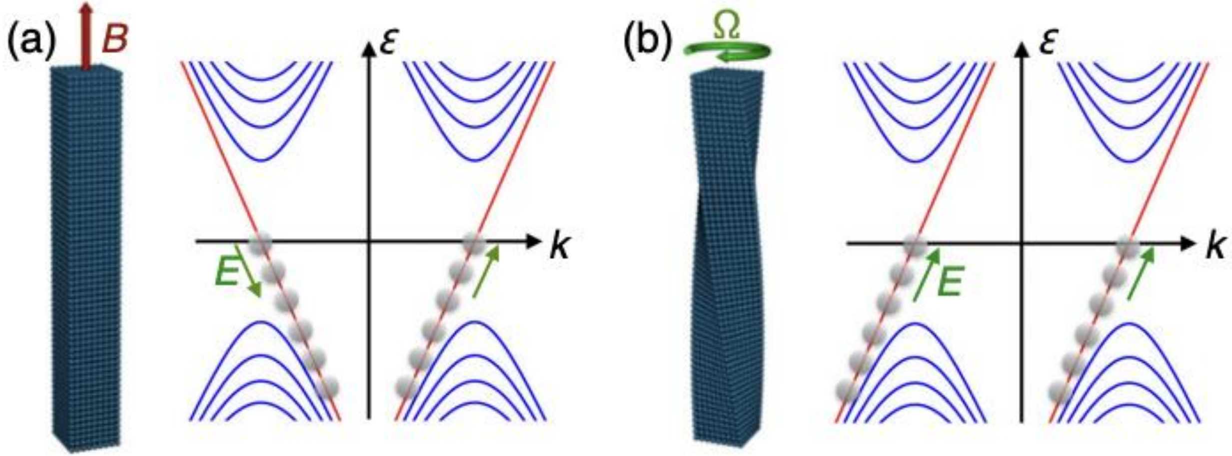
E_g phonon mode: (zx, zy)

$$\mathcal{H}_{\boldsymbol{\tau}}(\mathbf{k}, \mathbf{A}, \boldsymbol{a}) = \sum_j v_{\tau,j}\Gamma_j\left(k_j - A_j - \tau a_j\right) - \mu_F$$

- Same as graphene, phonon Hall viscosity term is induced in the presence of magnetic field ➔ large phonon magnetic moment
- Other consequences, e.g. chiral anomaly due to strain (acoustic phonon)



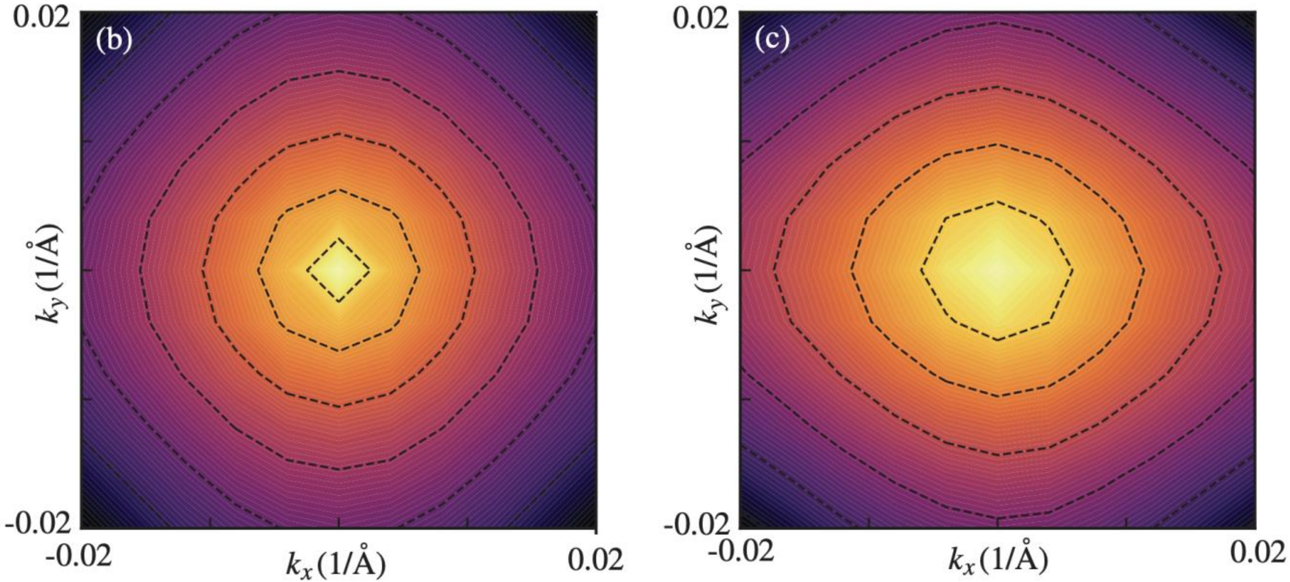
Pikulin et al., PRX 6, 041021 (2016)

DFT results for Cd_3As_2

- $\boldsymbol{E_u}$ **phonon mode:** $(\boldsymbol{x}, \boldsymbol{y})$
- No displacement of Dirac point in k-space

Not a gauge field

- Change of shape



No gauge description when the Dirac node is at the time reversal invariant point

eg. $HfTe_5$, $ZrTe_5$, $Pb_{1-x}Sn_xTe$

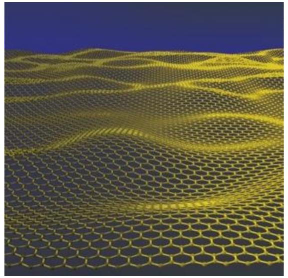
$$\mathbf{k} \to \mathbf{k} - \mathbf{a} \quad \times$$

Need a new theory framework: curved space due to phonon

Observation: Distance between ions after strain deformation, $x'_i \to x_i + u_i(x)$

$$dl^2 = \frac{\partial x'_k}{\partial x_i}\frac{\partial x'_k}{\partial x_j} dx_i dx_j = \left(\delta_{ij} + \partial_i u_j + \partial_j u_i + \partial_i u_k \partial_j u_k\right) dx_i dx_j = g_{ij} dx_i dx_j \, .$$

Dirac fermions coupling to geometric perturbations



- Phonon induces curved space for the Dirac fermion, which can be described by the frame fields $\boldsymbol{e}^a$ (Emergent gravity)

- 2D massive Dirac fermions

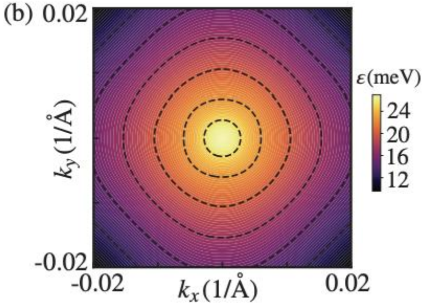
$$S = \int d^3x \det(\boldsymbol{e})\bar{\psi}(p_\mu e^\mu_a \gamma^a - m)\psi$$

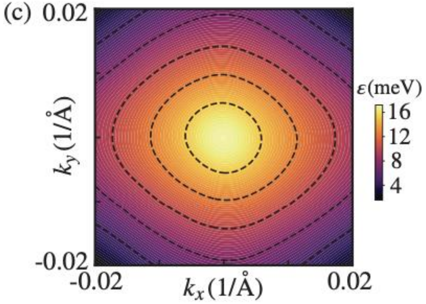
$$a = 0,1,2, \quad \gamma^a = (\sigma^z, i\sigma^y, -i\sigma^x)$$

- The energy dispersion

$$E_\pm = \pm\sqrt{p_1^2 + p_2^2 + m^2}$$

with $p_a = e^\mu_a p_\mu$. Anisotropic dispersion can be described by a nontrivial





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Quantum Hall viscosity

Hughes, Leigh, and Fradkin, Phys. Rev. Lett. 107, 075502 (2011)

- Integrate out Dirac fermions to get an effective Chern-Simons action for e_μ^a

$$S_{\text{eff}}[e_\mu^a] = \frac{\eta_H}{2}\int d^3x\, \epsilon^{\mu\nu\rho} e_\mu^a \partial_\nu e_\rho^b \eta_{ab} \qquad \eta_{ab} = \text{diag}[1,-1,-1]$$

- For the state in which the lowest ν Landau levels are filled under magnetic field

$$\eta_H = \frac{\hbar}{8\pi l_B^2}\nu$$

l_B is the magnetic length

- Hall conductivity

$$\sigma_{xy} = \frac{e^2}{h}\nu$$

- Again η_H is proportional to σ_{xy}

$$\eta_H = \frac{\hbar^2}{4e^2 l_B^2}\sigma_{xy}$$

Modeling phonons as vierbein fields

- Anisotropic dispersion of Dirac fermion due to the E_u circularly polarized phonons

$$E_\pm = \pm\sqrt{(e_1^x p_x)^2 + \left(e_2^y p_y\right)^2 + m^2}$$

We know

$$e_1^x = \lambda u_x, \qquad e_2^y = \lambda u_y$$

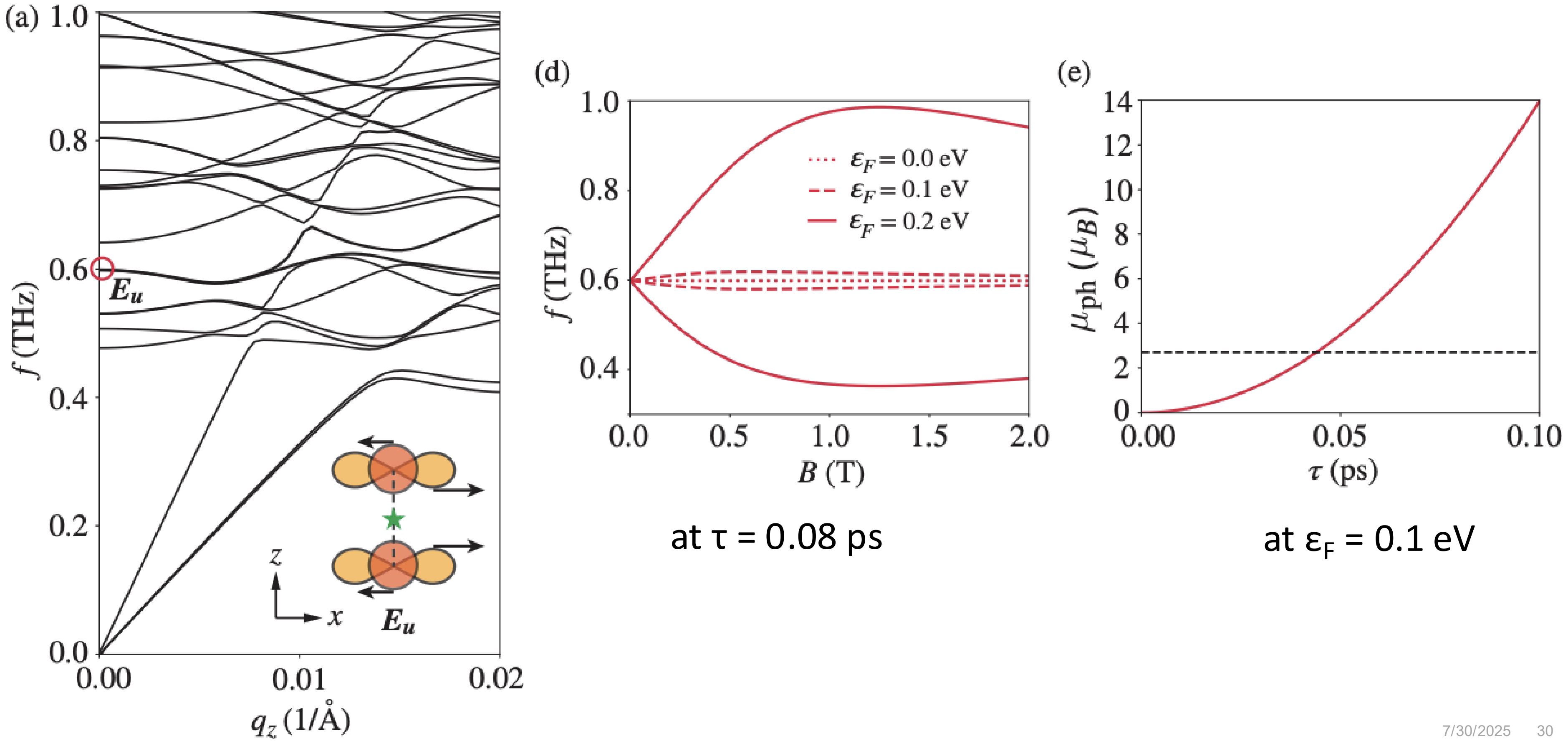
- Phonon Hall viscosity term

$$\mathcal{L}_\eta = \frac{\eta_H}{2}\lambda^2(u_x \dot{u}_y - u_y \dot{u}_x)$$

- Orbital phonon magnetic moment

$$m_{\mathrm{ph}} \equiv \frac{\hbar(\omega_+ - \omega_-)}{2B} = \frac{\hbar}{B\rho_I}\eta_H \lambda^2$$

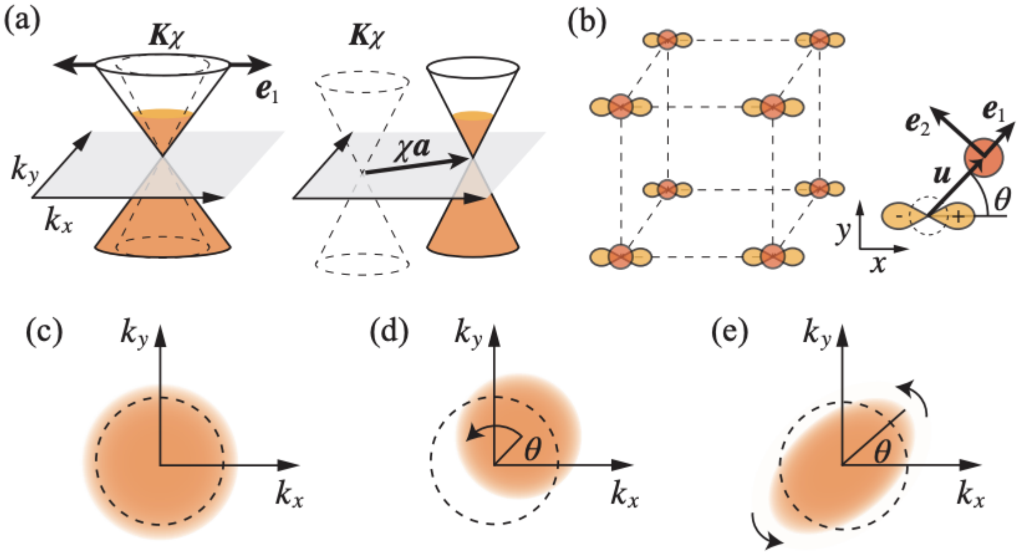
First-principle results of the E_u phonon mode in Cd_3As_2



at τ = 0.08 ps

at ε_F = 0.1 eV

Gauge vs gravitational fields



Phonon/Dirac deformation	$l = 0$ (Frame)	$l = 1$ (Gauge)	$l = 2$ (Frame)
Inversion-even	✓	✓	✓
Inversion-odd	✓	×	✓
μ_{ph}	0	σ_{xy}	η_H

Summary

- Giant phonon orbital magnetic moment in doped Dirac semimetal
  - E_g phonon acts as an emergent gauge field, $\mu_{ph} \propto \sigma_{xy}$ (electrical Hall conductivity)
  - E_u phonon acts as a frame field, $\mu_{ph} \propto \eta_H$ (electrical Hall viscosity)
- Probe electrical Hall viscosity by phonon
- Expect large phonon thermal Hall conductivity
- Baby Standard Model in Dirac semimetals with phonon fields

Chen et al., PRB 111, 035126 (2025)
Chen et al., arXiv:2505.09732 (2025)

To see a World in a Grain of Sand by William Blake