Predicting And Probing Carrier Interactions In Quantum Matter Using Electron Hydrodynamics

Prineha Narang

School on Quantum Materials | July 2022

NARANGLAB

Contact me for Ph.D & Postdoctoral Positions!

Electron Hydrodynamics?

'Hydrodynamics' → effective theory of conserved quantities in an interacting fluid.

'Semi-classical' → electrons are ultimately many-body quantum systems; however, resulting equations are classical.

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Why is it Important?

Fundamental importance → experimental probe for strong condensed matter interactions.

Technological importance → shrinking nano-electronic devices; non-diffusive current densities result in spatially-varying dissipation.

"Electron hydrodynamics is observed when microscopic scattering processes conserve momentum over time- and length-scales that are large compared to those of the experimental probe."

Billiard Dynamics

Ballistic Flow

- Applicable in ‘ultraclean’ metals as T → 0K
  - Electrons scatter against **sample edges** *diffusively*

- Special case of the **Boltzmann Transport Equation**

Billiard Dynamics

Diffusive Flow

- Proposed by Lorentz in 1905.
- Applicable in ‘dirty’ metals.
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Billiard Dynamics

Diffusive Flow

- Proposed by Lorentz in 1905.
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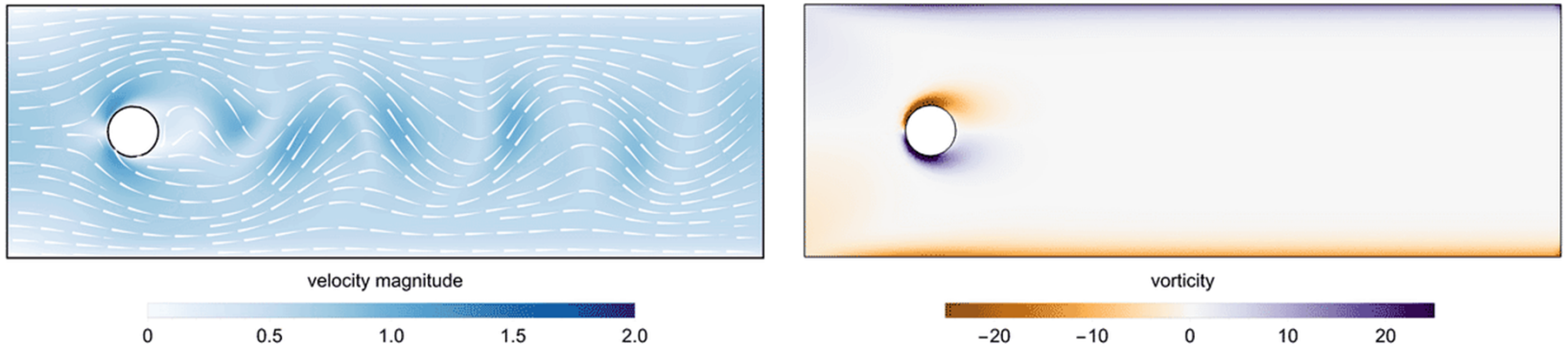
- Special case of the **Boltzmann Transport Equation.**
  - Average distance between collisions → mean free path, l or λ.

Fluid Dynamics

Hydrodynamic Flow



- Applicable in ‘ultraclean’ (semi-)metals with *strong* interactions.
  - Electrons scatter against **each other,** leading to viscous flow.

- Limiting case of the **Boltzmann Transport Equation.**

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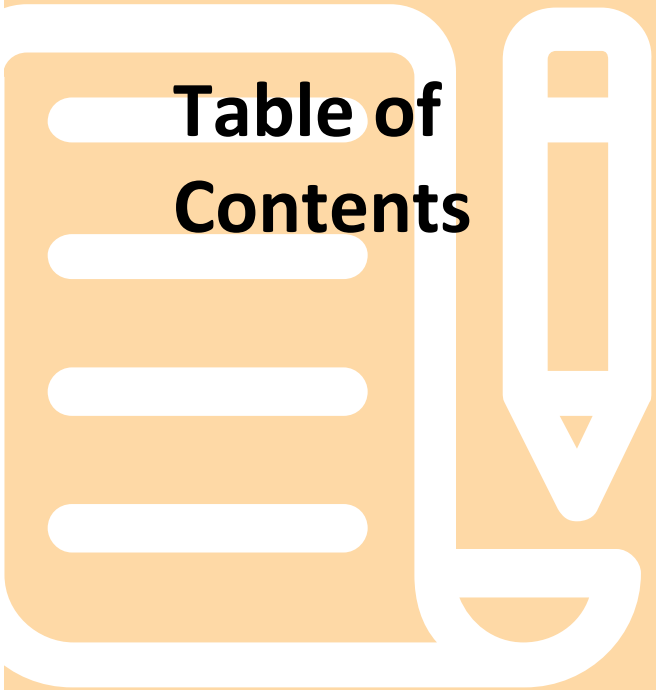


Background

01 Boltzmann Transport Equation Theory

02 Electron Transport Regimes

03 Anisotropic Electron Fluids

Results

04 Spatially-Resolved Transport Framework

05 Observables Sensitivity to Scattering Details

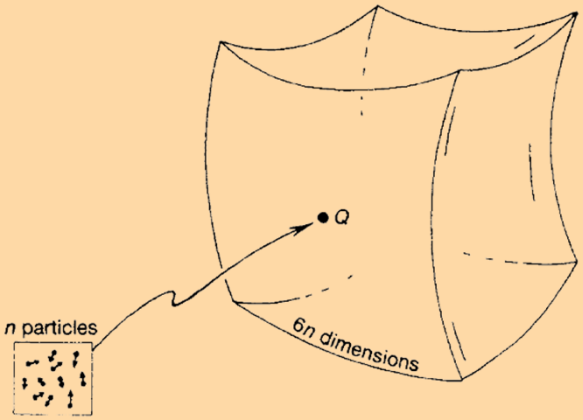
01. Boltzmann Transport Equation Theory

Semi-classical BTE

One-body distribution function:

$$f(\boldsymbol{r}, \boldsymbol{k}, t)\; d^3r\, d^3k$$

# of carriers with positions within d^3r of r and (quasi-)momentum within d^3k of k.



Penrose, R. (1989). The emperor's new mind

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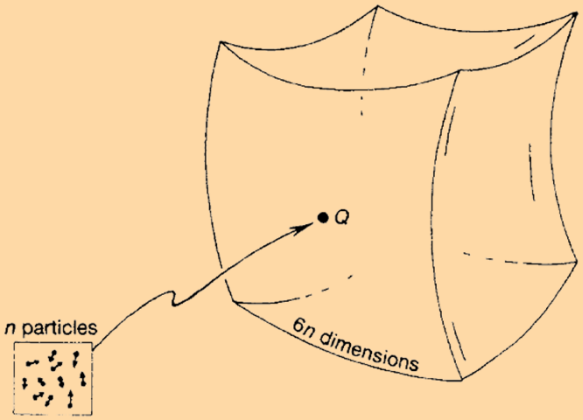

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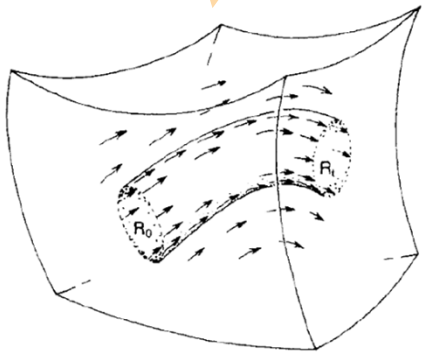

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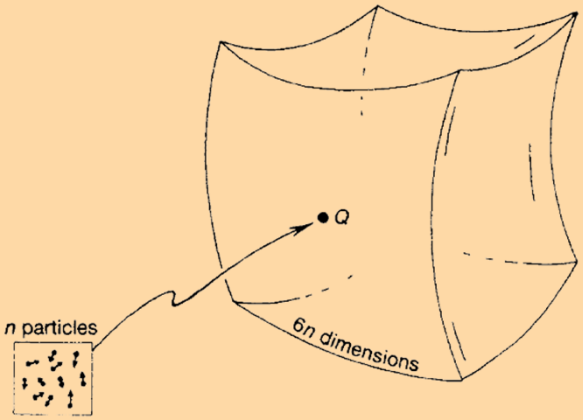

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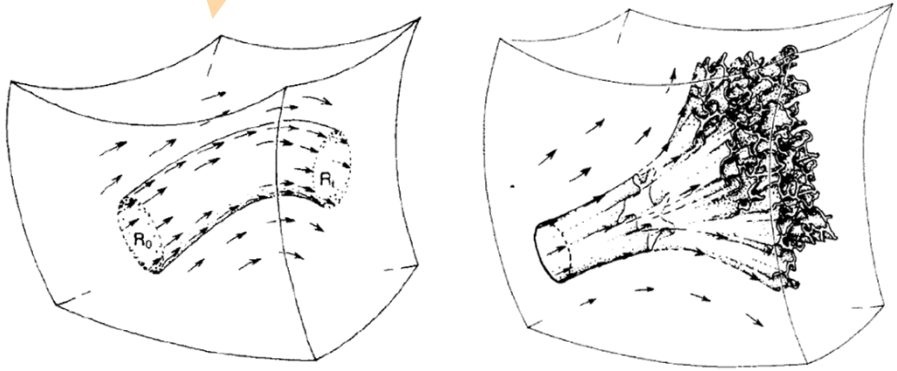

Streaming

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Electron Collisions

In typical conductors,
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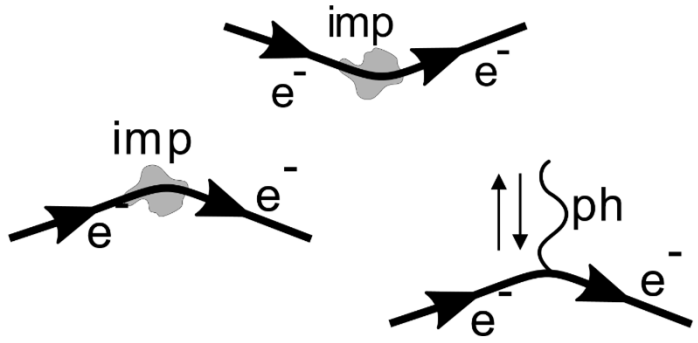
Momentum-Relaxing (τ_{mr})



Electron Collisions

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In the presence of strong electron-electron
interactions, electrons can flow collectively;
akin to molecules in a fluid, conserving
their momentum.

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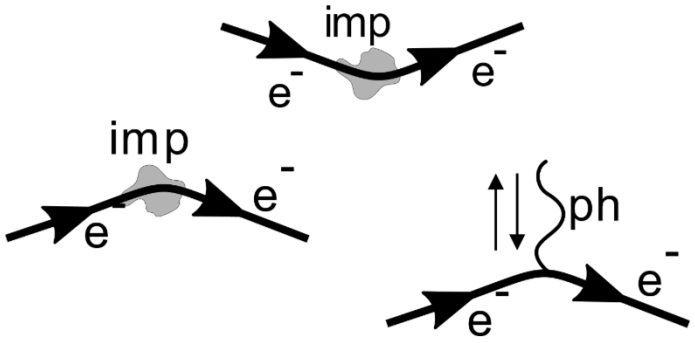
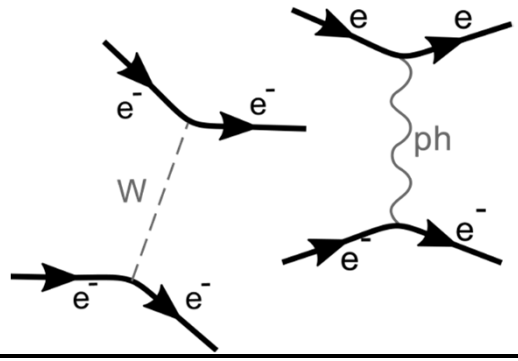


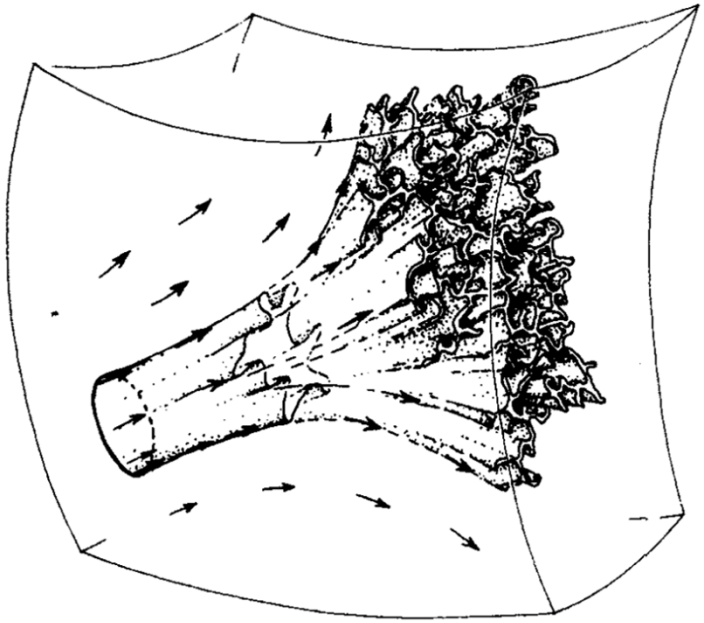
Momentum-Conserving (τ_{mc})



Collisional Invariants

- Streaming operator conserves average values of operators
- Changes from collision operator

$$\frac{dA}{dt} = \int \frac{d^3k}{(2\pi)^3}\, d^3r\; A(\boldsymbol{r}, \boldsymbol{k}) \left(\frac{\partial f}{\partial t}\right)_{\text{coll}}$$



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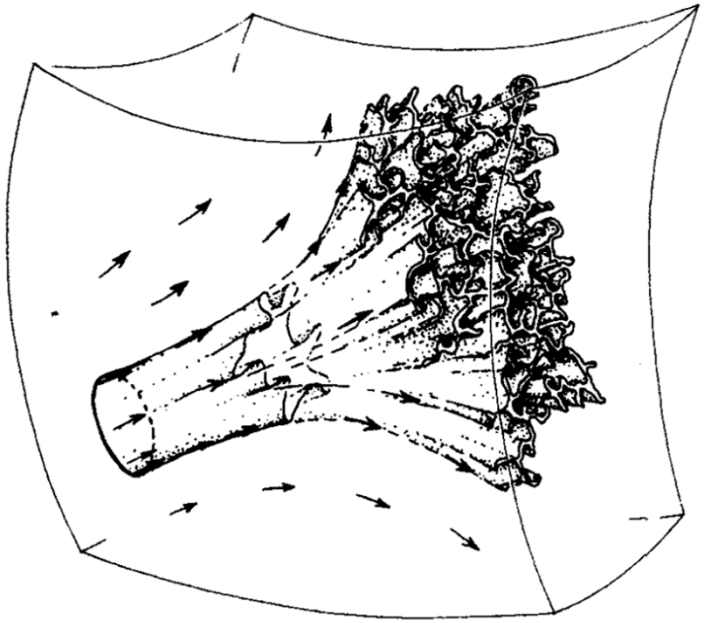
  - Total energy
  - Total momentum ?



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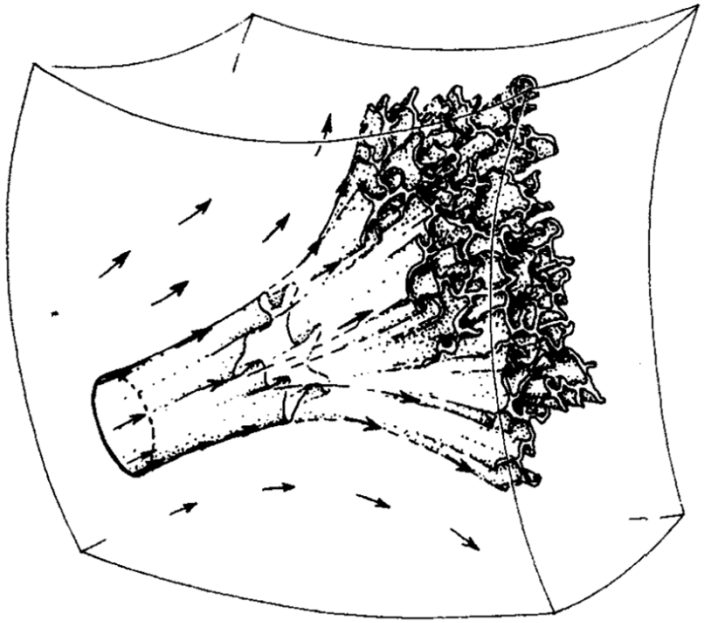
→ Hydrodynamic theories



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Collision Integral Approximations

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$$\left(\frac{\partial f}{\partial t}\right)_{\text{coll}} = \frac{f_0 - f}{\tau}$$

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$$\left(\frac{\partial f}{\partial t}\right)_{\text{coll}} = \frac{1}{\tau_{\text{mr}}}\left(-f + \int \frac{d\hat{\boldsymbol{v}}}{4\pi} f\right)$$
$$\equiv \frac{1}{\tau_{\text{mr}}}\left(\mathbb{P}_n - 1\right) f$$

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H. Lorentz (1905), Arch. Neerl. **10**, 336

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De Jong, Molenkamp (1995), **Phys. Rev. B.** 51, 13389

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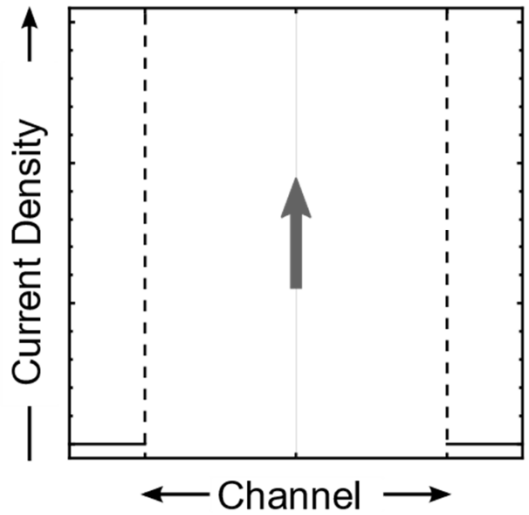
- Models parametrized using:
  - Momentum-relaxing lifetime, τ_{mr}
  - Momentum-conserving lifetime, τ_{mc}

02. Electron Transport Regimes

[VHV21] Vool*, Hamo*, Varnavides*, Wang*, et al. (2021), **Nat Phys** 1745-2481
[WV21] Wang*, Varnavides*, et al., (2021), **ArXiv:** 2109.00550 **Phys Rev Materials**
[VW22] Varnavides*, Wang*, et al. (2022), **Phys Rev Materials** 6, 045002

See also work by S. Ilani, E. Zheldov, D. Bonn, more!

Transport Regime Limits



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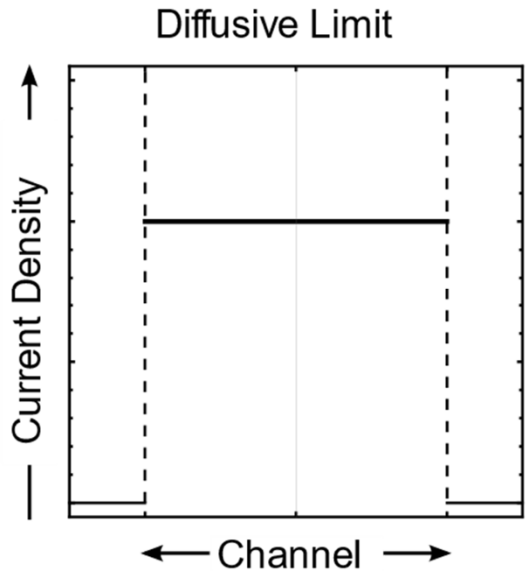

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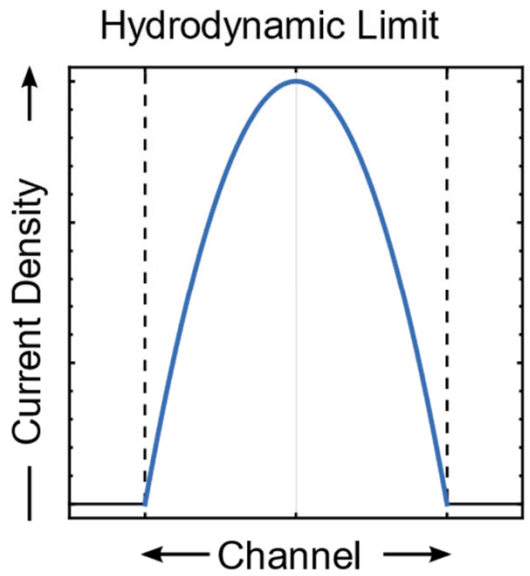
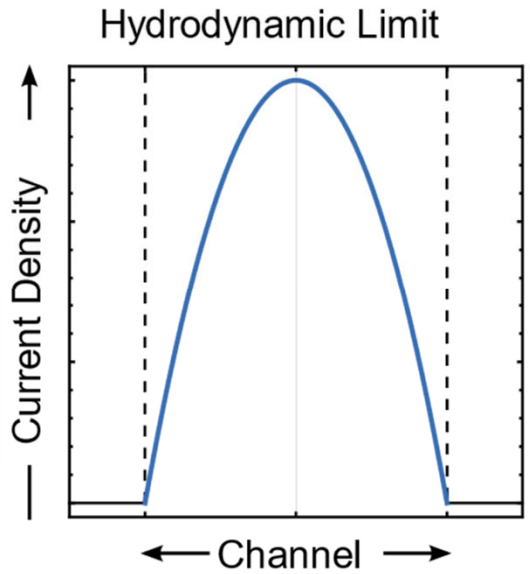


Transport Regime Limits

- **Normalized physical parameters**
  - Momentum-relaxing mean free path (l_{MR}/W)
  - Momentum-conserving mean free path (l_{MC}/W)



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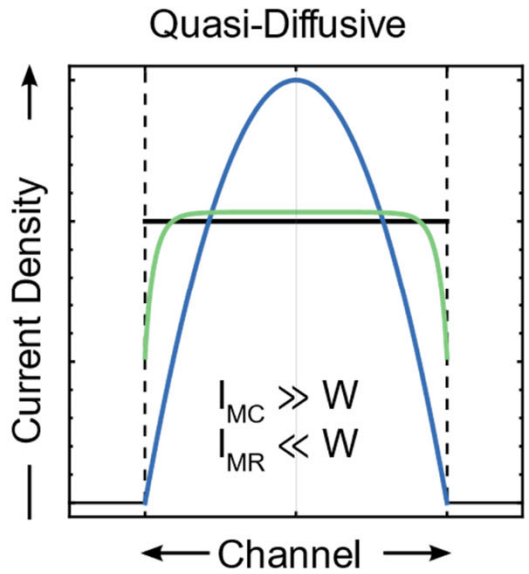

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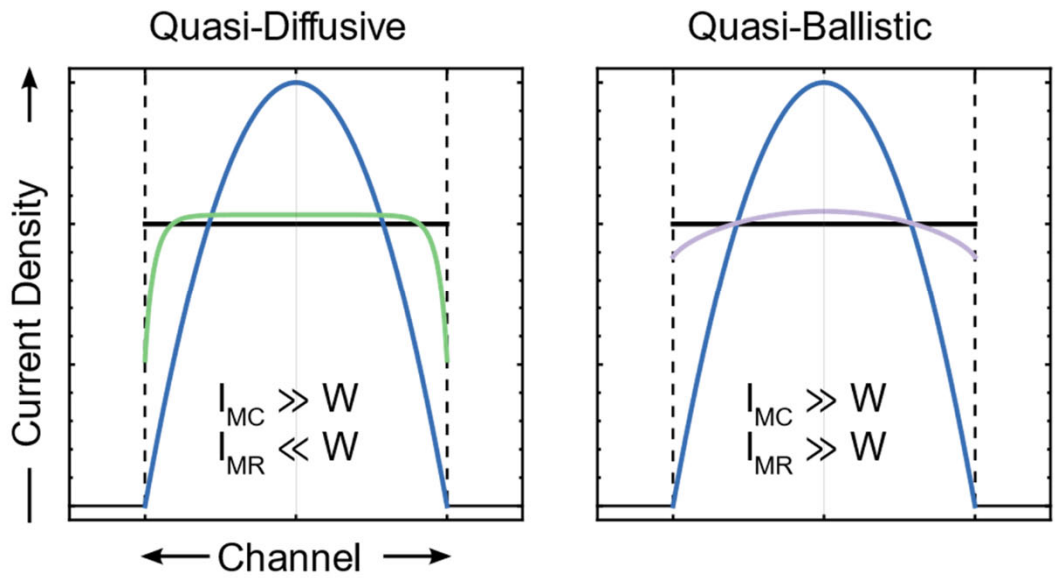

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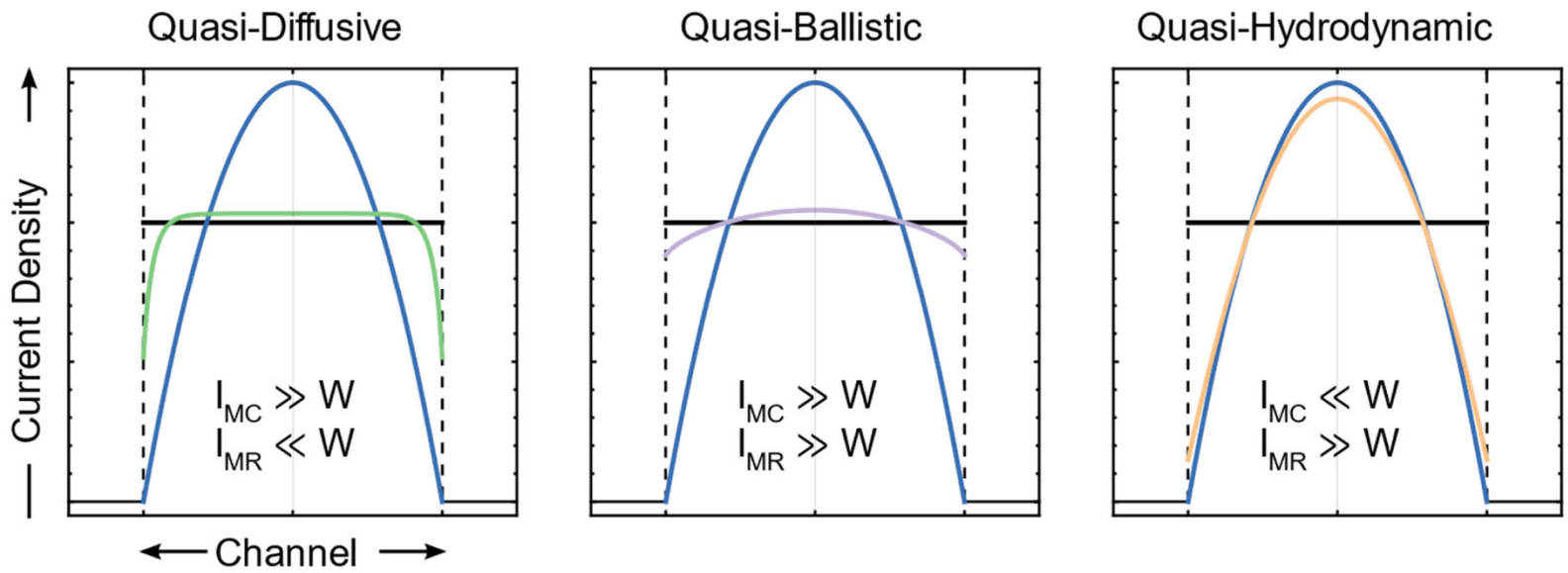

Transport Regime Diagram

- More generally, current density profiles exist on a spectrum.
- We solve Callaway's hydro model

$$\left(\frac{\partial f}{\partial t}\right)_{\text{coll}} \equiv \frac{1}{\tau_{\text{mr}}}\left(\mathbb{P}_n - 1\right) f + \frac{1}{\tau_{\text{mc}}}\left(\mathbb{P}_m - 1\right) f$$

  - on a grid of (l_{MC}/W, l_{MR}/W) pairs.
- Scalar observable → curvature (in middle of channel).

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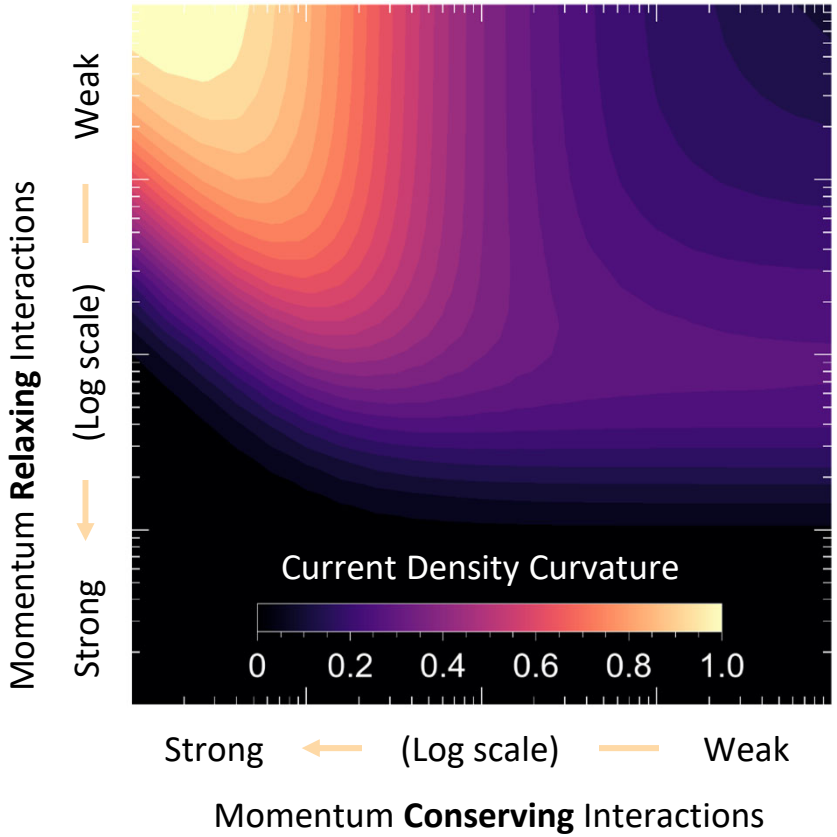

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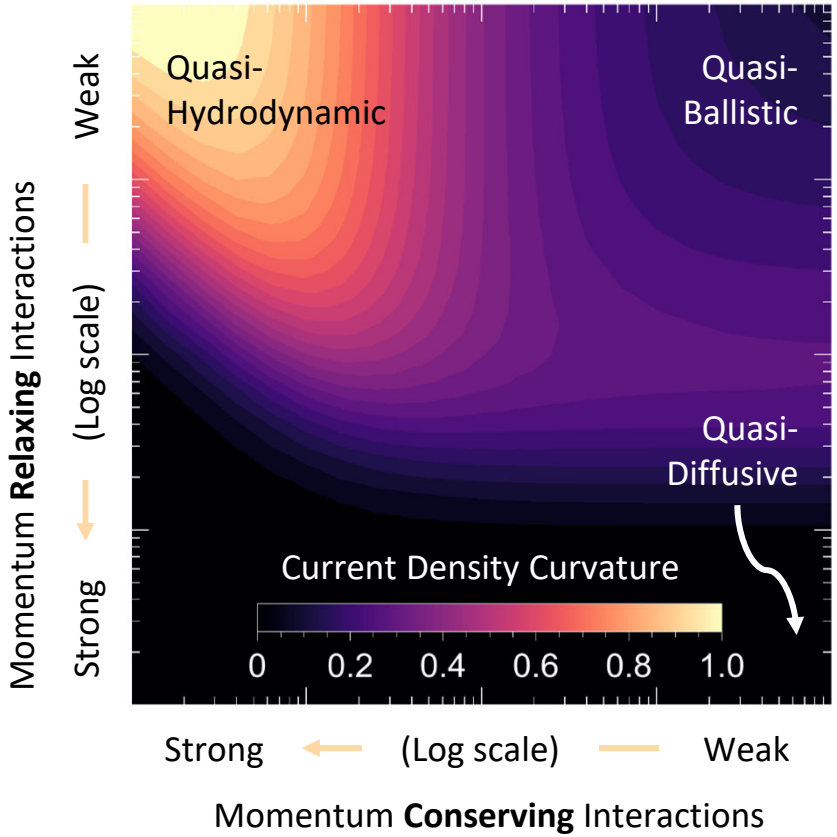
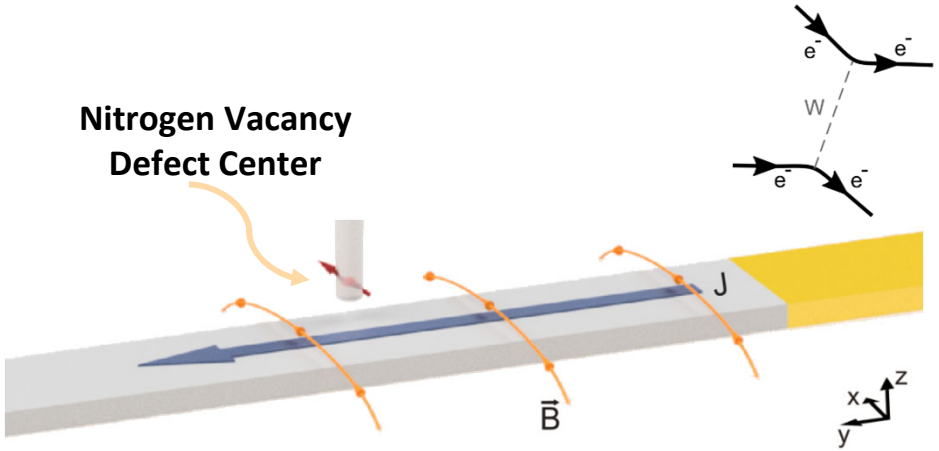


Recent Experimental Observations

- Direct (Coulomb) interactions:
  - Yes, in low carrier-density materials
    - graphene (Nature, 576; Nature, 583)
    - GaAs (Phys. Rev. B 51, 13389)
  - Nitrogen-vacancy center magnetometry
    - Measures induced magnetic field



Ku, Yacoby, et al., (2020), **Nature** 583, 537-541

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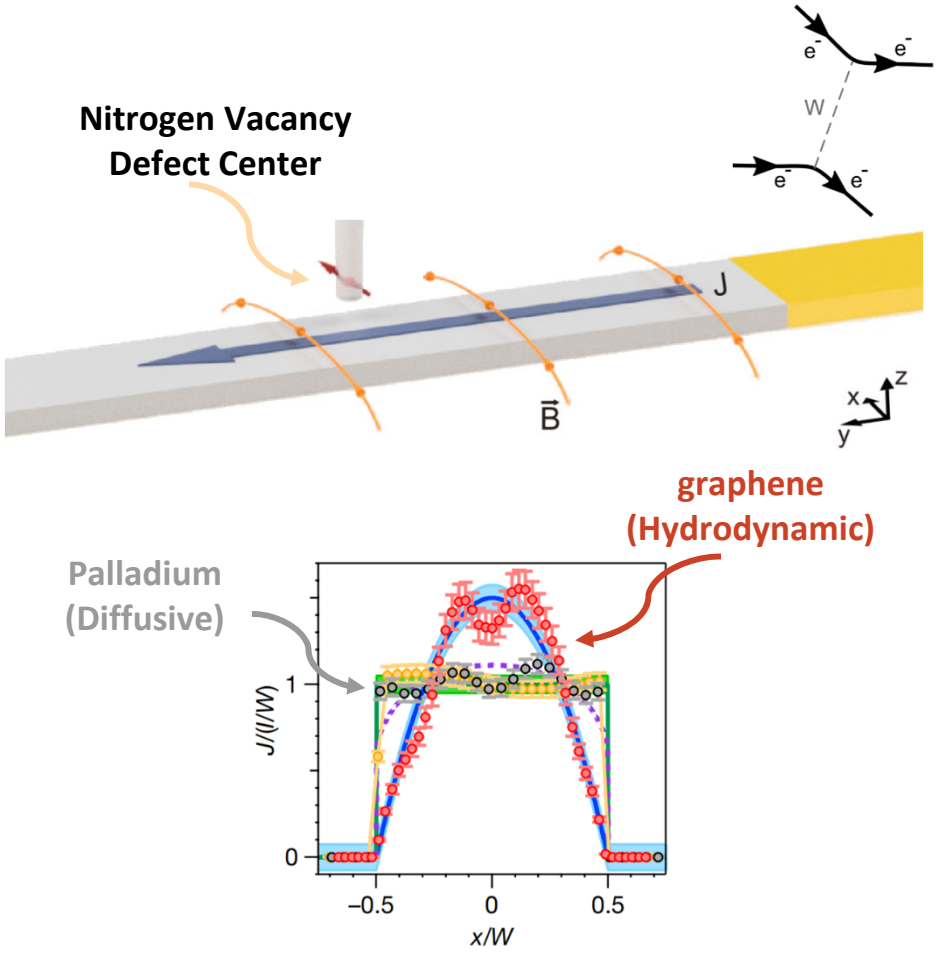

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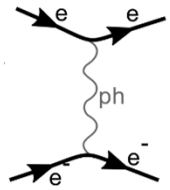

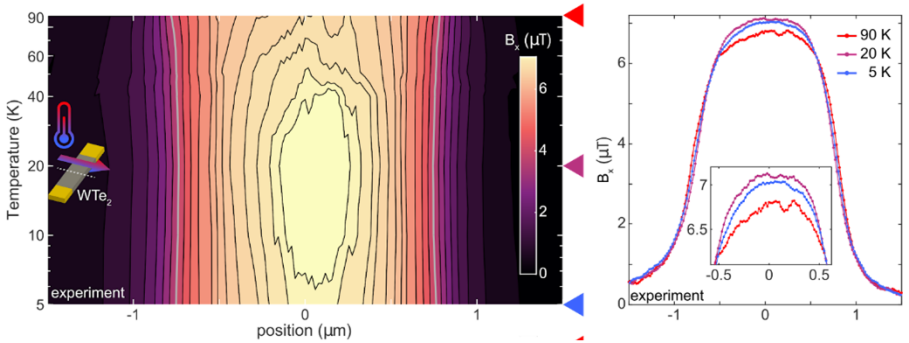

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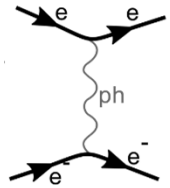

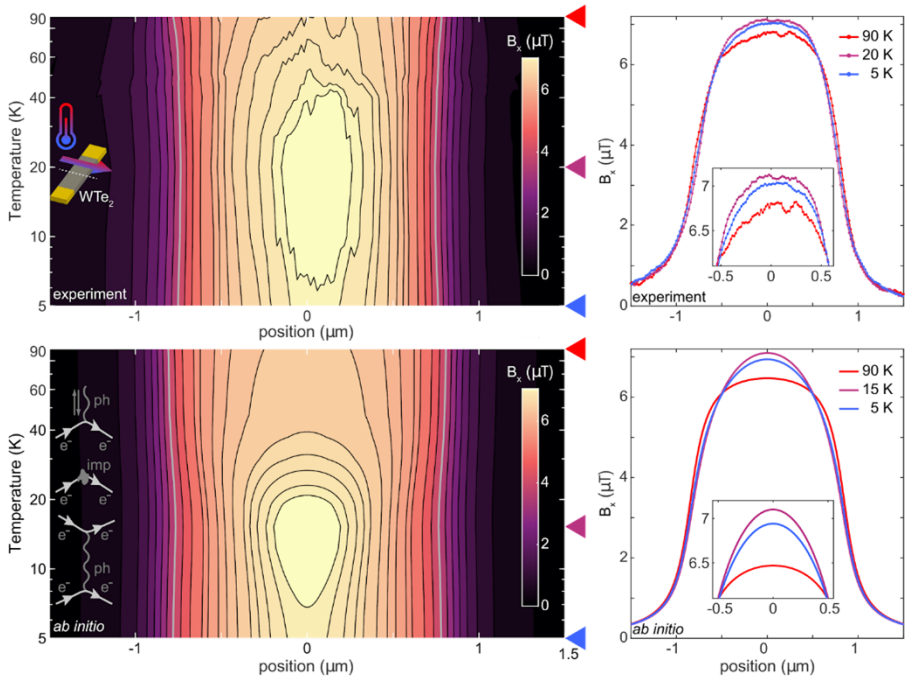

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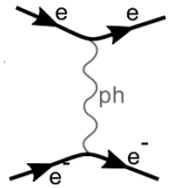
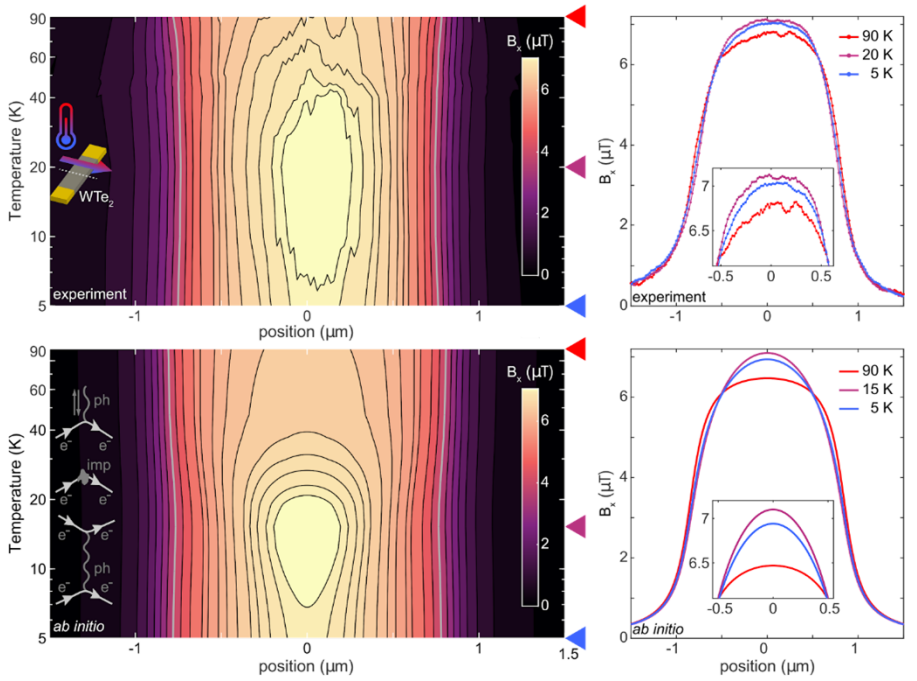
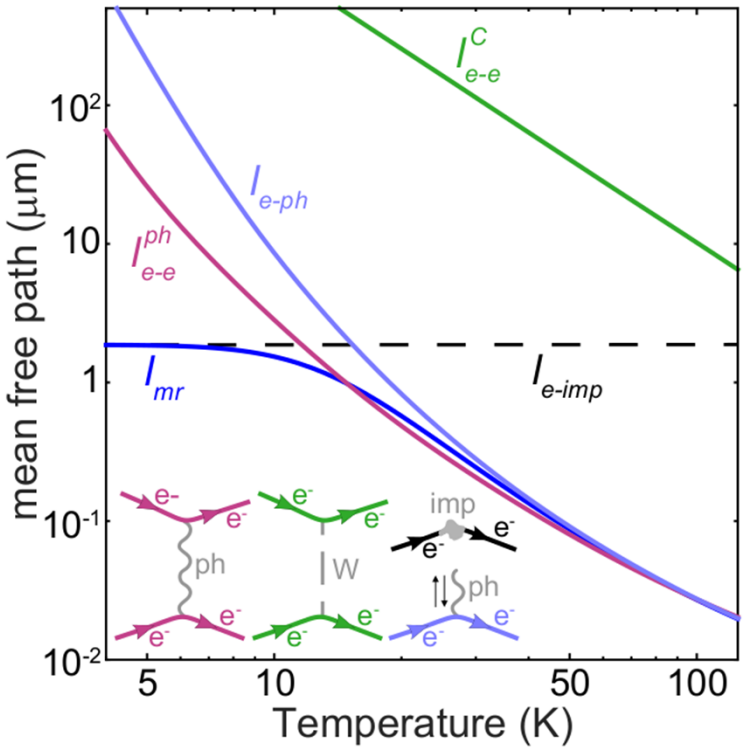
  - Predicted from first principles in a wider set of materials
    - PdCoO2
      Varnavides*, Wang*, et al., (2022), **Phys Rev Materials** 6, 045002
    - ZrSiS, TaAs2
      Wang*, Varnavides*, et al., (2022), **ArXiv**: 2109.00550 **Phys Rev Materials**





Populating transport regime diagram

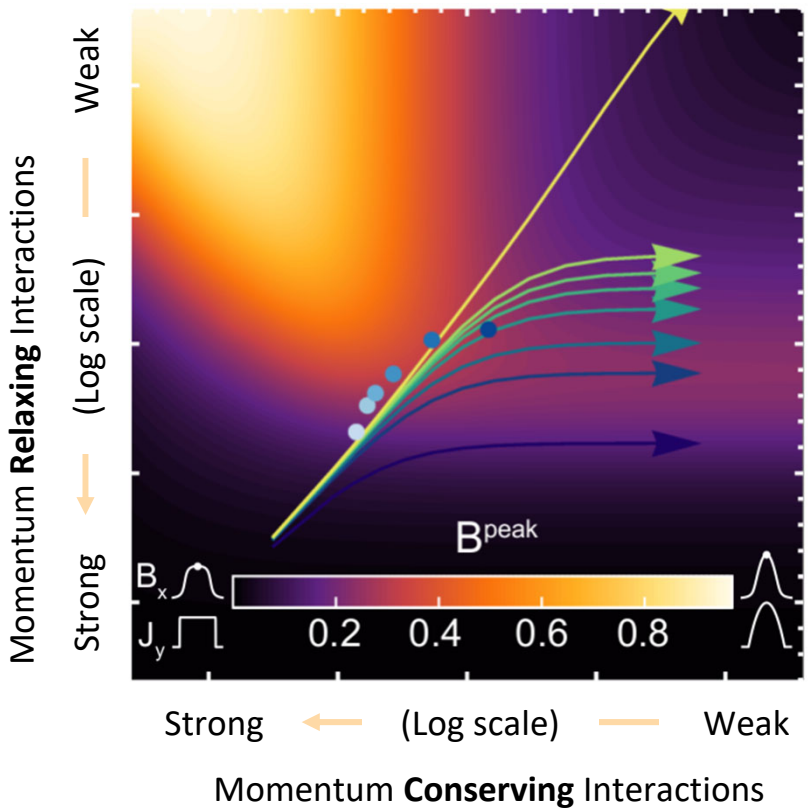
- WTe_2 is a semi-metal
  - Screened Coulomb interaction
- Ultrapure single-crystal samples
  - Impurity mean free path > 1 μm
- Phonon-mediated interaction
  - Dominates over 15-50K range



Vool*, Hamo*, Varnavides*, Wang*, et al. (2021), **Nat Phys**

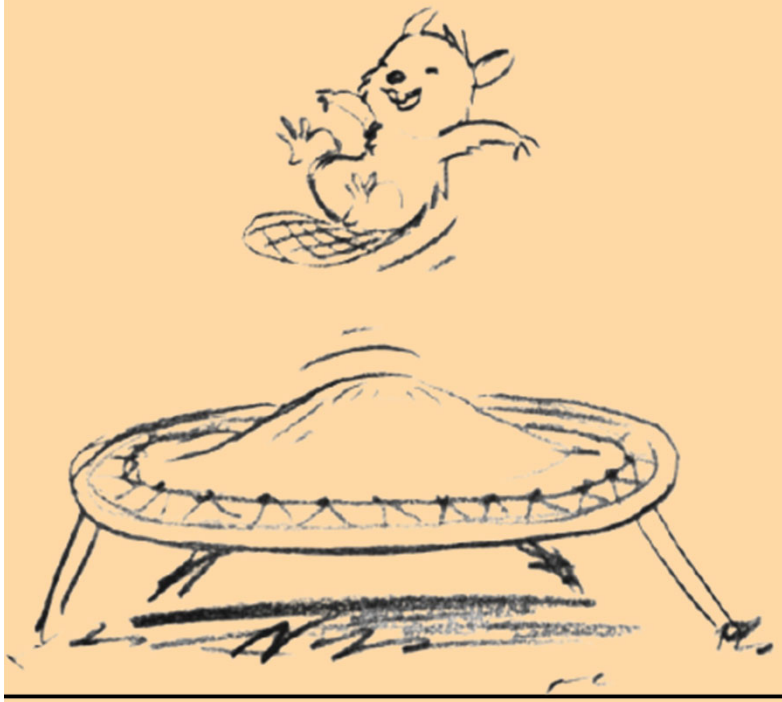
Populating transport regime diagram

- Compute current density for a range of momentum-relaxing / momentum-conserving values
- Calculate induced magnetic field
- Overlay experimental observations (blue points)
- Overlay first-principles calculations (arrows)



Vool*, Hamo*, Varnavides*, Wang*, et al. (2021), **Nat Phys**

More on this (general) mechanism



Osterhoudt, Narang *et al*, *Phys. Rev. X* 11, 011017 (**2021**)

van Delft, Wang,.., Narang *et al*, *Nat. Commun.*, **12**, 1-9 (**2021**)

Narang *et al. Nat. Mater.* (**2021**)

Nenno,.. Narang. *Nat. Rev Phy.* (**2020**)

Wang & Narang, *Phys. Rev. B* 102, 125122 (**2020**)

Garcia, Coulter, Narang. *Phys. Rev. Research* 2, 013073 (**2020**)

Coulter,.., Narang. *Phys. Rev. B* 100, 220301(R) (**2019**)

Coulter, Sundararaman, Narang, *Phys. Rev. B* 98 (11), 115130 (**2018**)

How general is this mechanism?

Empirically (ab-initio), a lot of materials show shorter phonon-mediated electron lifetimes.
Under what conditions does this hold?

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Empirically (ab-initio), a lot of materials show shorter phonon-mediated electron lifetimes. Under what conditions does this hold?

Electron-Phonon Linewidth

$$\tau_{\mathrm{eph}}^{-1} = \frac{\pi\beta}{2g(\epsilon_F)} \sum_{\nu} \int \frac{d\boldsymbol{q}}{\Omega_{\mathrm{BZ}}} G_{\boldsymbol{q}\nu} \frac{\omega_{\boldsymbol{q}\nu}}{\sinh^2(\hbar\beta\omega_{\boldsymbol{q}\nu}/2)}$$

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Phonon-Mediated Electron-Electron Linewidth

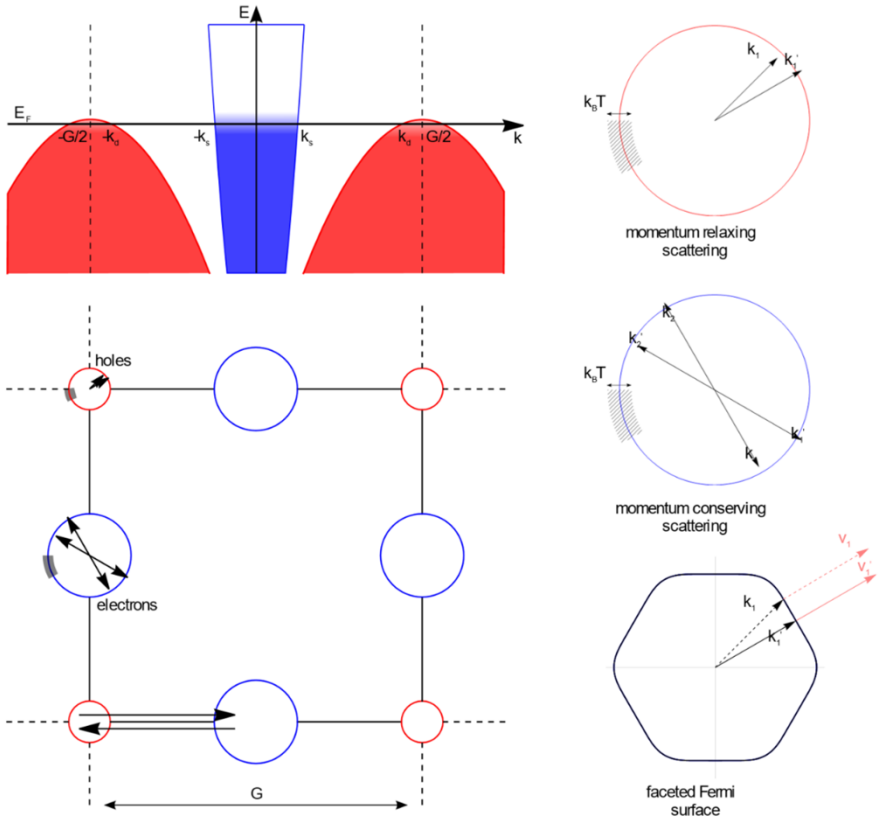
$$\tau_{\mathrm{ee(ph)}}^{-1} = \frac{2\pi}{\hbar g(\epsilon_F)} \sum_{\nu} \int \frac{d\boldsymbol{q}}{\Omega_{\mathrm{BZ}}} G_{\boldsymbol{q}\nu}^2 \gamma(\hbar\beta\bar{\omega}_{\boldsymbol{q}\nu})$$

Design Principles

- Approximations valid for electron-phonon couplings **G << 1**
  - True for non-superconducting materials
- Mechanism relies on ‘virtual’ phonon exchange
  - Temps below Debye temperature

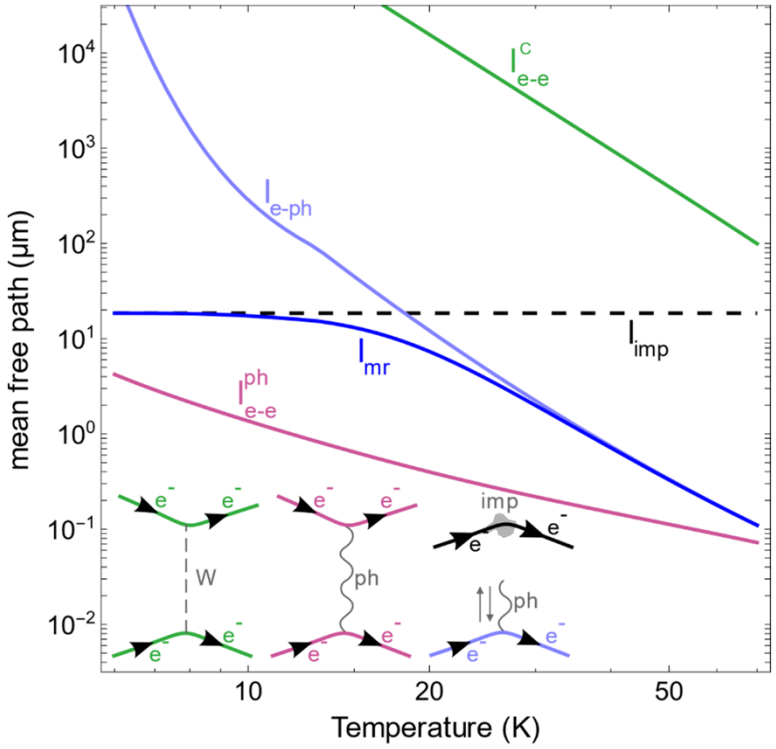
Design Principles

- Approximations valid for electron-phonon couplings **G << 1**
  - True for non-superconducting materials
- Mechanism relies on ‘virtual’ phonon exchange
  - Temps below Debye temperature
- Proposed candidates:
  - Semi-metals with separated pockets
  - Low-symmetry crystal (p/d orbitals)
  - Suppressed phonon scattering
  - Large Fermi velocity



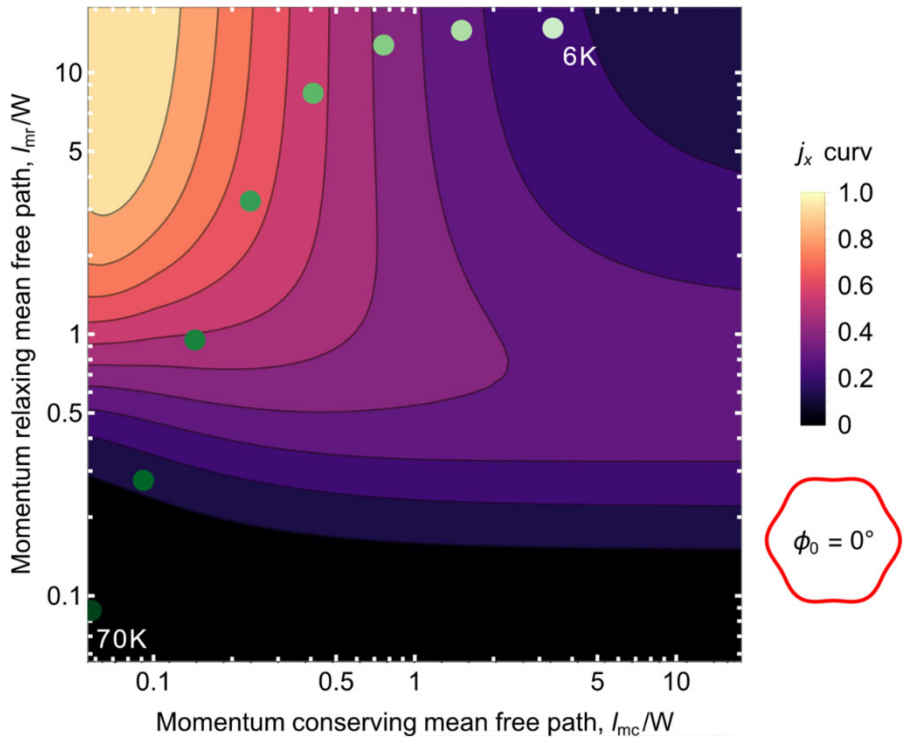
First Principles Lifetimes

- $PdCoO_2$ is a single band metal
  - Screened Coulomb interaction
- Ultrapure single-crystal samples
  - Impurity mean free path > 10 µm
- Phonon-mediated interaction
  - Dominates over 10-100K range



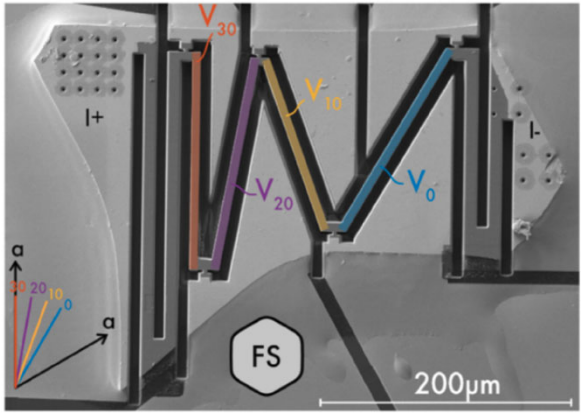
Transport Regimes

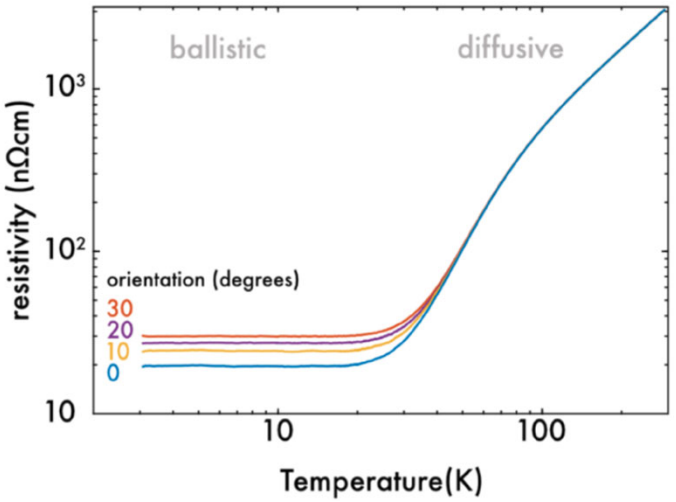
- More generally, electron transport regimes exist on a continuous spectrum
- Current density curvature
  - Related to the experimentally accessible magnetic field max
- Overlaid points trace the temperature-dependent trajectory in $PdCoO_2$



Fermi Surface Anisotropy

- Directional ‘ballistic’ transport in (highly-faceted) $PdCoO_2$
- What about Neumann’s Principle?
  - $PdCoO_2$ is hexagonal
  - Any rank-2 tensor → isotropic





See also work by Mackenzie, Moll, Bonn, others!

Fermi Surface Anisotropy

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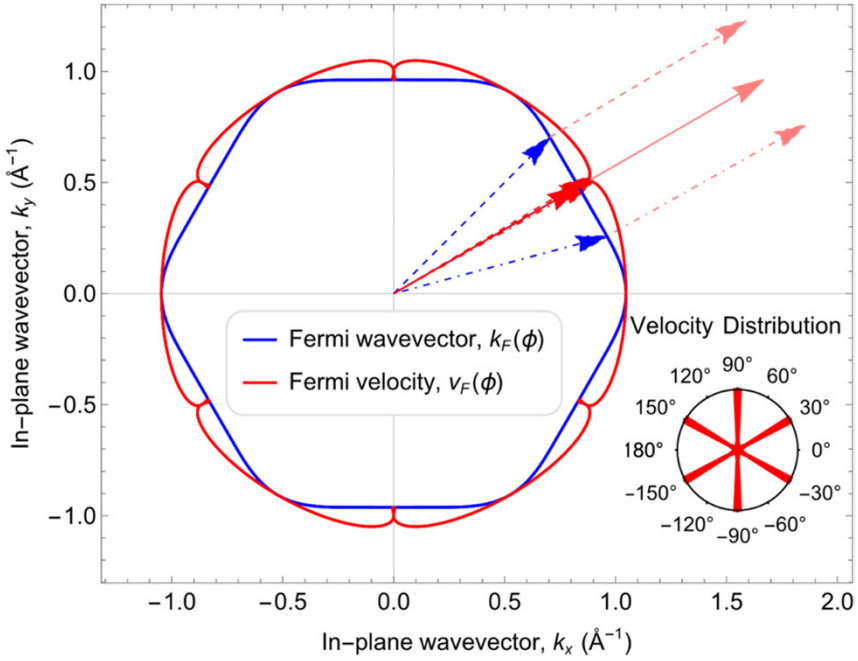
- What about Neumann’s Principle?
  - $PdCoO_2$ is hexagonal
  - Any rank-2 tensor → isotropic
- At these length-scales, relevant physical property → Fermi vel.
  - Which allows for ‘easy’ and ‘hard’ transport directions



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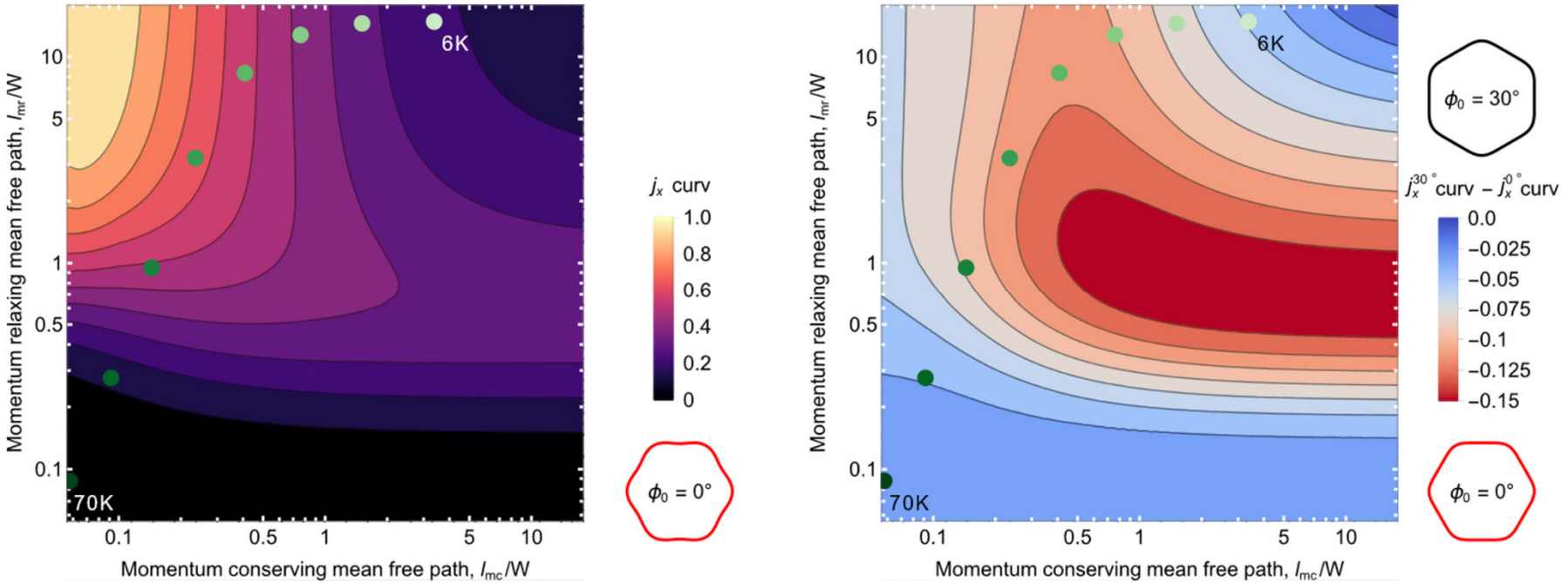

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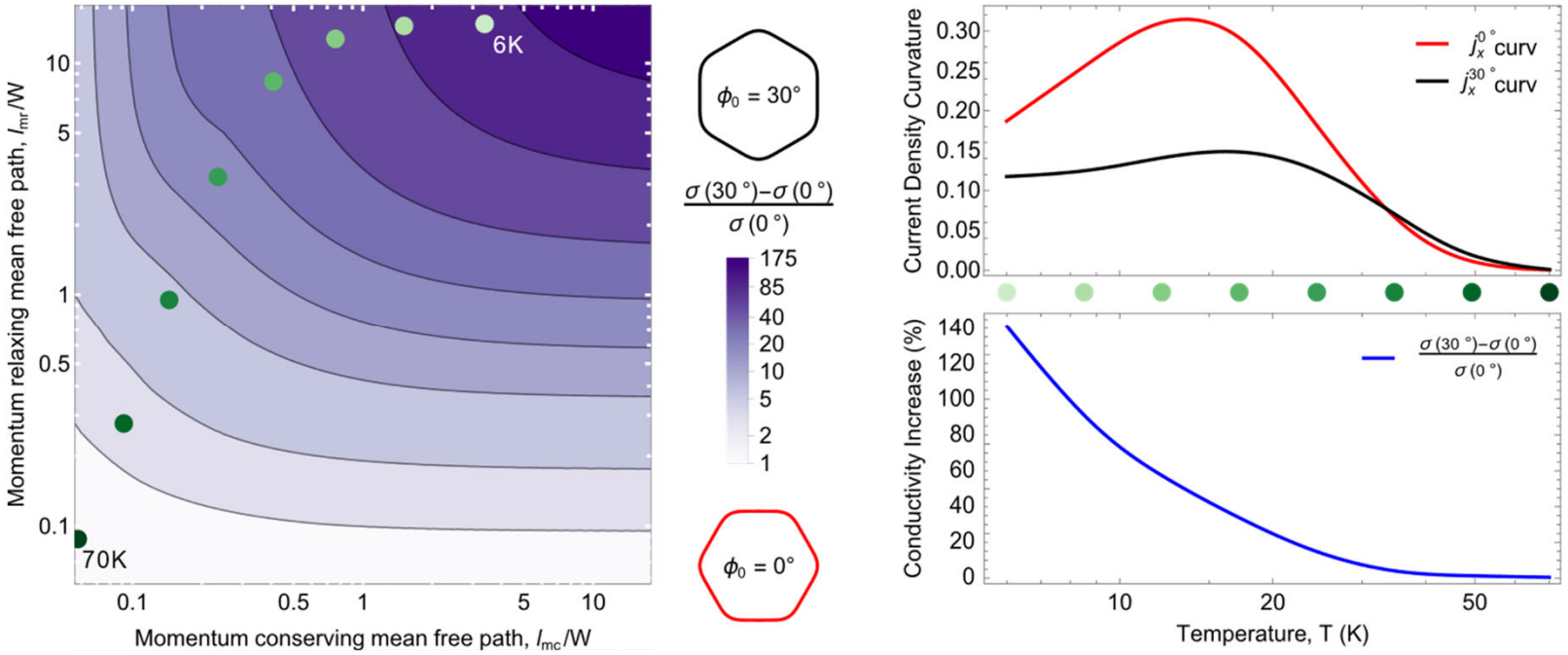
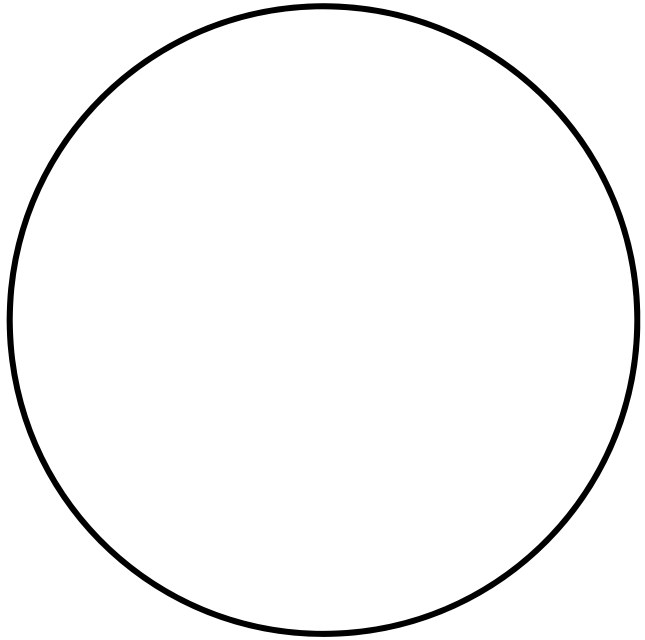


03. Anisotropic Electron Fluids

[Var20] Varnavides*, Jermyn*, et al. (2020), **Nat Commun** 11 (1)
See also work by L. Levitov, G. Falkovich, J. Moore, A. Stern, others!

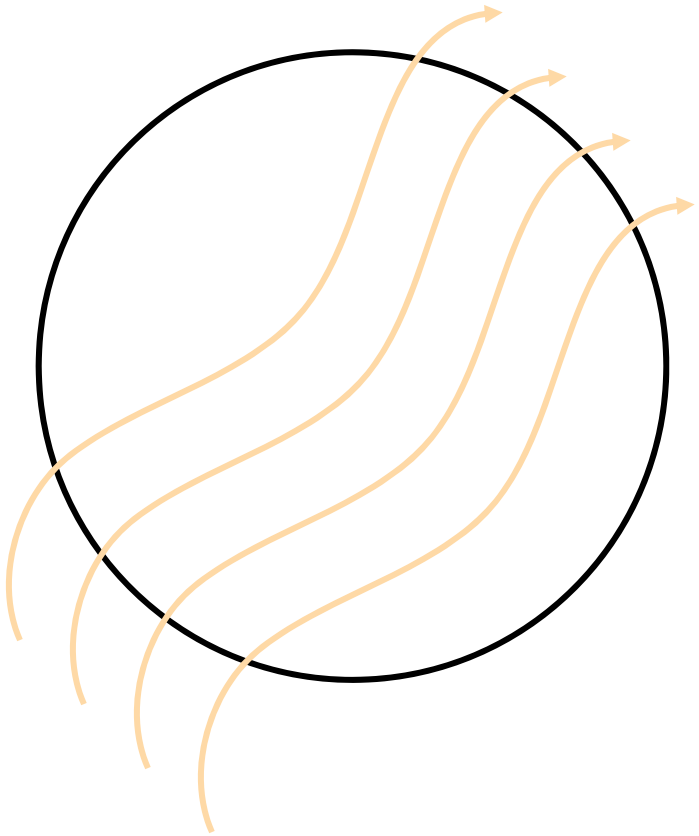
Navier Stokes Equation



Navier Stokes Equation

- Mass conservation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{V}) = 0$$



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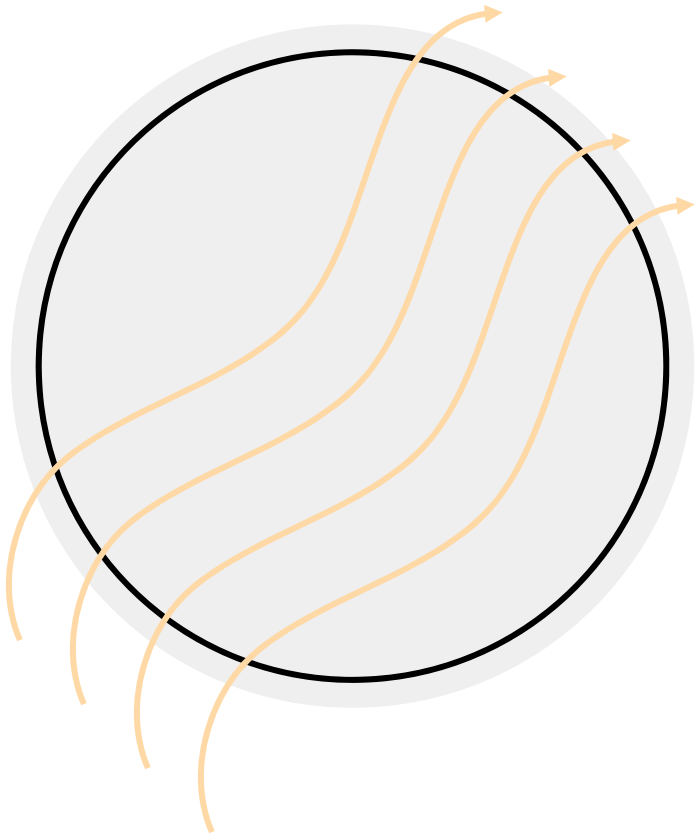
$$\frac{\partial (\rho \boldsymbol{V})}{\partial t} + \nabla \cdot (\rho \boldsymbol{V} \otimes \boldsymbol{V}) = -\nabla p + \nabla \cdot \boldsymbol{\tau}$$



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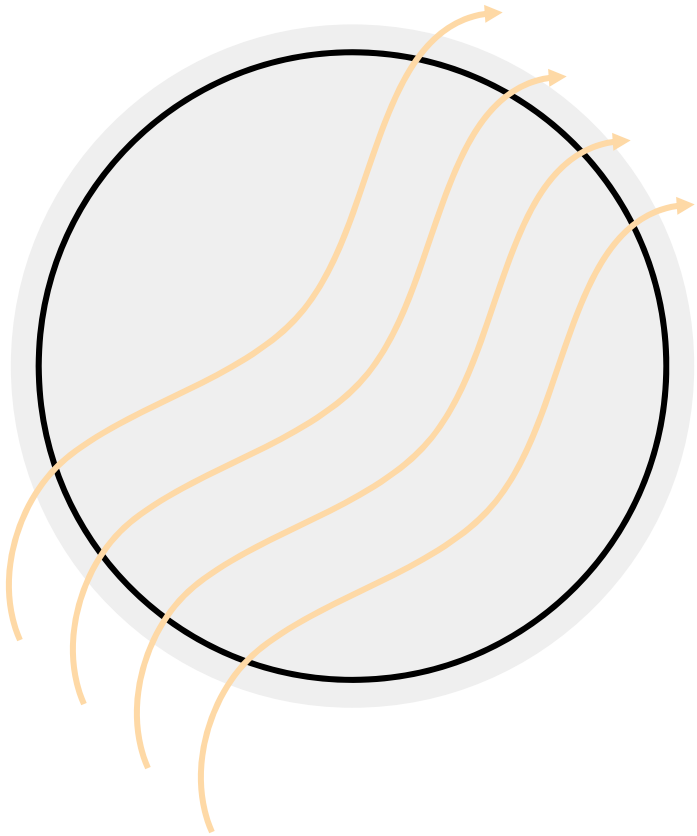

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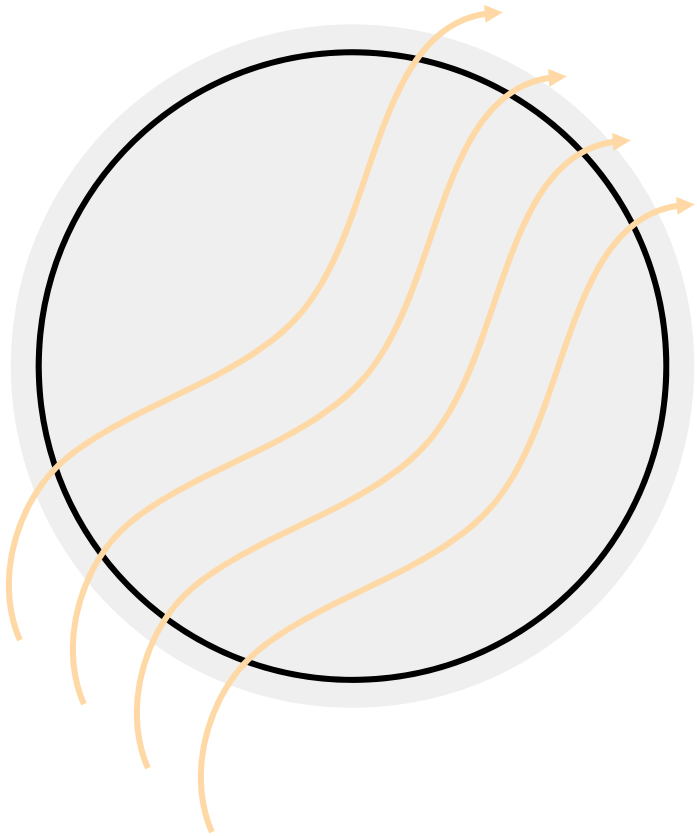
- Constitutive law (viscosity)

$$\tau_{ij} = \eta_{ijkl} \partial_l V_k$$



Classical Fluids

- Viscosity
  - Stress to gradient in fluid velocity
  - Rank 4 tensor

- Rotational Invariance

P( ) = P ( )

  - Incompressible fluids
    → 'scalar' (shear) viscosity

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Electron Fluids

- Viscosity constrained by **crystal** and **tensor symmetries**

"The symmetry elements of **any physical property** of a crystal must **include** the **symmetry** elements of the **point group** of the crystal"

Anisotropic behaviour (α)

Dissipationless (Hall) behaviour (β)

Asymmetric (Vorticity) behaviour (γ)

Varnavides*, Jermyn* et al. (2020), **Nat Commun** 11

Neumann's Principle

"The symmetry elements of **any physical property** of a crystal must **include** the **symmetry** elements of the **point group** of the crystal"

$$A'_{ijkl} = |s|^{\nu} s_{im} s_{jk} s_{ko} s_{lp} A_{mnop}$$

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Tensor Basis	Symmetries			Tensor Type	Independent Components	
	i ↔ j	k ↔ l	ij ↔ kl		2D	3D
$\alpha = \eta^{\text{dissipative}}_{((ij)(kl))}$	+	+	+	proper	6	21
$\beta = \eta^{\text{Hall}}_{[(ij)(kl)]}$	+	+	-	pseudo	3	15
$\gamma = \eta^{\text{vorticity}}_{(ij)[kl]}$	+	-	N/A	pseudo	3	18

Neumann's Principle

- Most general viscosity tensor in 3D (basal plane)

$$A^{(001)} = \begin{pmatrix} \begin{pmatrix} \alpha_{1111} & \alpha_{1112}+\beta_{1112}+\gamma_{1112} \\ \alpha_{1112}+\beta_{1112}-\gamma_{1112} & \alpha_{1122}+\beta_{1122} \end{pmatrix} & \begin{pmatrix} \alpha_{1112}-\beta_{1112} & \alpha_{1212}+\gamma_{1212} \\ \alpha_{1212}-\gamma_{1212} & \alpha_{1222}+\beta_{1222} \end{pmatrix} \\ \begin{pmatrix} \alpha_{1112}-\beta_{1112} & \alpha_{1212}+\gamma_{1212} \\ \alpha_{1212}-\gamma_{1212} & \alpha_{1222}+\beta_{1222} \end{pmatrix} & \begin{pmatrix} \alpha_{1122}-\beta_{1122} & \alpha_{1222}-\beta_{1222}+\gamma_{2212} \\ \alpha_{1222}-\beta_{1222}-\gamma_{2212} & \alpha_{2222} \end{pmatrix} \end{pmatrix}$$

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- Point Group Symmetries

Four-fold (C_4)

E	C_4	C_2	C_4^3

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- Point Group Symmetries

Four-fold (C_4)

E $\quad$ C_4 $\quad$ C_2 $\quad$ C_4^3

$$A'^{(001)} = \begin{pmatrix} \begin{pmatrix} \alpha_{2222} & -\alpha_{1222}+\beta_{1222}+\gamma_{2212} \\ -\alpha_{1222}+\beta_{1222}-\gamma_{2212} & \alpha_{1122}-\beta_{1122} \end{pmatrix} & \begin{pmatrix} -\alpha_{1222}-\beta_{1222} & \alpha_{1212}-\gamma_{1212} \\ \alpha_{1212}+\gamma_{1212} & \beta_{1112}-\alpha_{1112} \end{pmatrix} \\ \begin{pmatrix} -\alpha_{1222}-\beta_{1222} & \alpha_{1212}-\gamma_{1212} \\ \alpha_{1212}+\gamma_{1212} & \beta_{1112}-\alpha_{1112} \end{pmatrix} & \begin{pmatrix} \alpha_{1122}+\beta_{1122} & -\alpha_{1112}-\beta_{1112}+\gamma_{1112} \\ -\alpha_{1112}-\beta_{1112}-\gamma_{1112} & \alpha_{1111} \end{pmatrix} \end{pmatrix}$$

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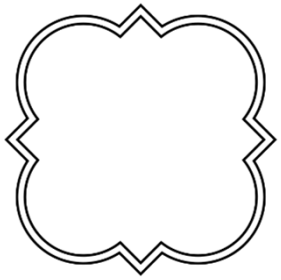
- Point Group Symmetries

Four-fold (C_4)

E C_4 C_2 C_4^3

$$A^{C_4^{(001)}} = \begin{pmatrix} \begin{pmatrix} \alpha_{1111} & \alpha_{1112}+\beta_{1112}+\gamma_{1112} \\ \alpha_{1112}+\beta_{1112}-\gamma_{1112} & \alpha_{1122} \end{pmatrix} & \begin{pmatrix} \alpha_{1112}-\beta_{1112} & \alpha_{1212} \\ \alpha_{1212} & \beta_{1112}-\alpha_{1112} \end{pmatrix} \\ \begin{pmatrix} \alpha_{1112}-\beta_{1112} & \alpha_{1212} \\ \alpha_{1212} & \beta_{1112}-\alpha_{1112} \end{pmatrix} & \begin{pmatrix} \alpha_{1122} & -\alpha_{1112}-\beta_{1112}+\gamma_{1112} \\ -\alpha_{1112}-\beta_{1112}-\gamma_{1112} & \alpha_{1111} \end{pmatrix} \end{pmatrix}$$

Neumann's Principle



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- Point Group Symmetries

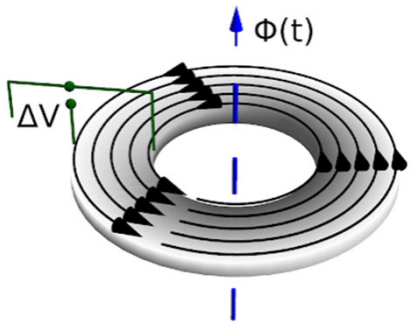
Square (D_4)

E	C_4	C_2	C_4^3	C_2^x	C_2^y	C_2^{x+y}	C_2^{x-y}

$$A^{D_4^{(001)}} = \begin{pmatrix} \begin{pmatrix} \alpha_{1111} & 0 \\ 0 & \alpha_{1122} \end{pmatrix} & \begin{pmatrix} 0 & \alpha_{1212} \\ \alpha_{1212} & 0 \end{pmatrix} \\ \begin{pmatrix} 0 & \alpha_{1212} \\ \alpha_{1212} & 0 \end{pmatrix} & \begin{pmatrix} \alpha_{1122} & 0 \\ 0 & \alpha_{1111} \end{pmatrix} \end{pmatrix}$$

Effect of Crystal Anisotropy

- Steady state **rotational flow** (corbino disk geometry)



Corbino Disk
Geometry

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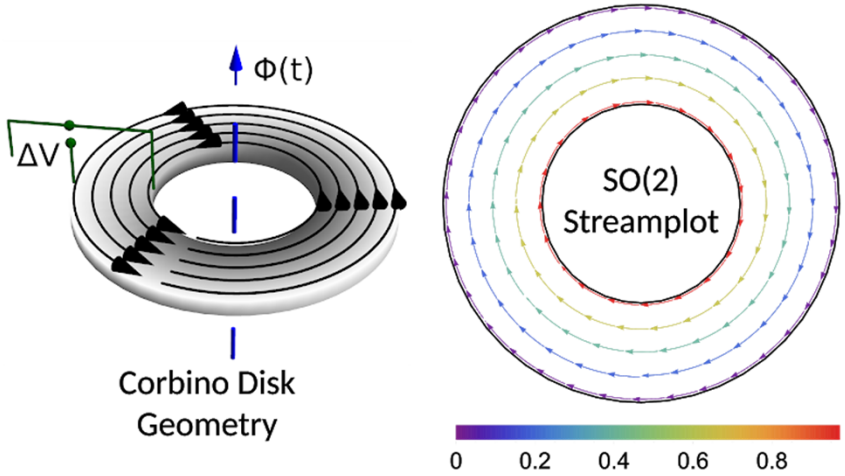

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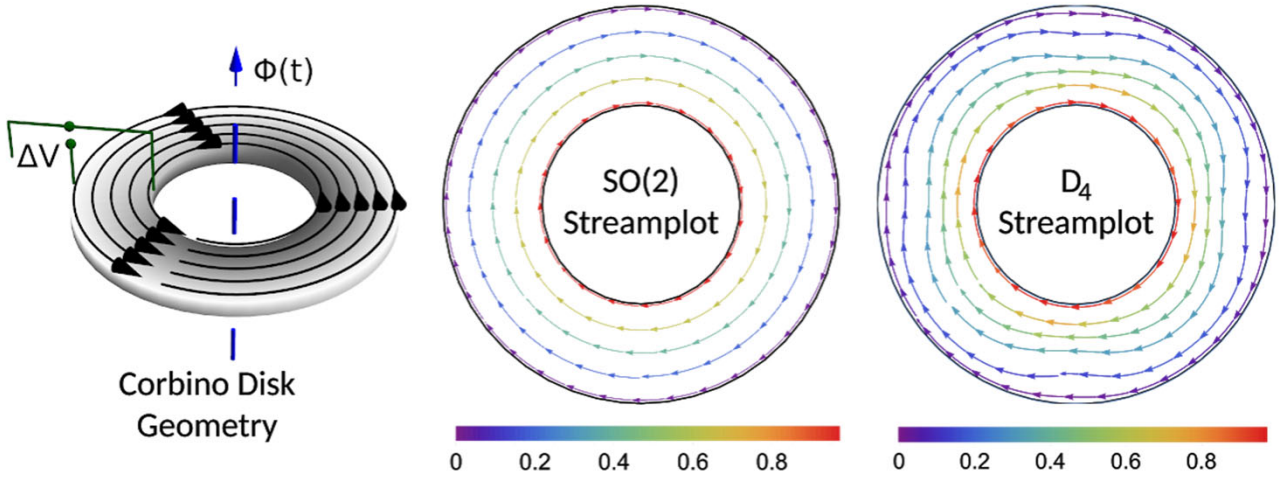
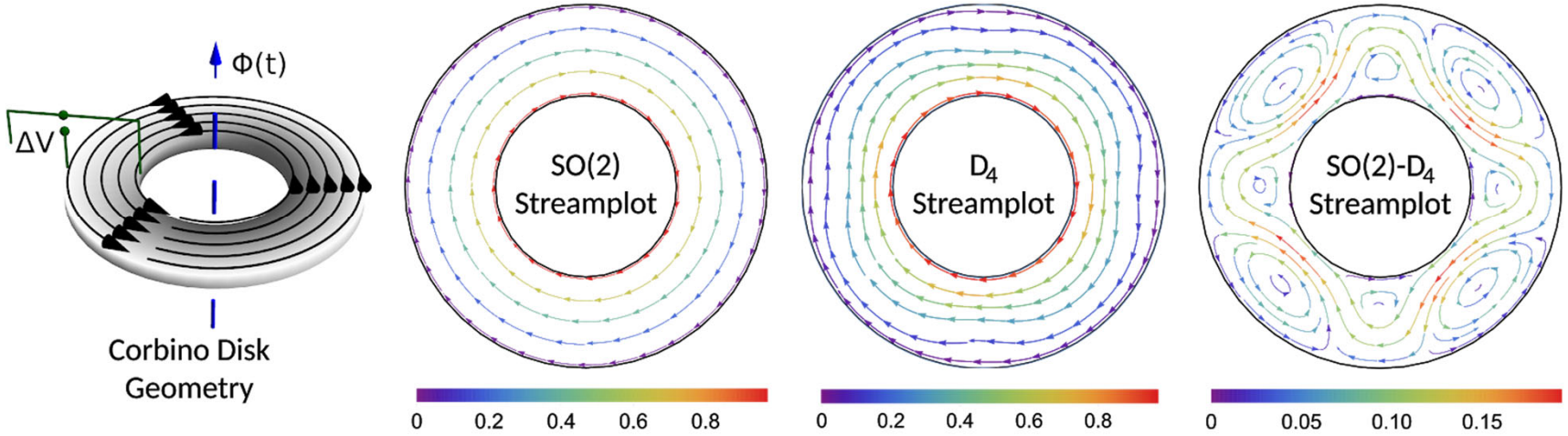


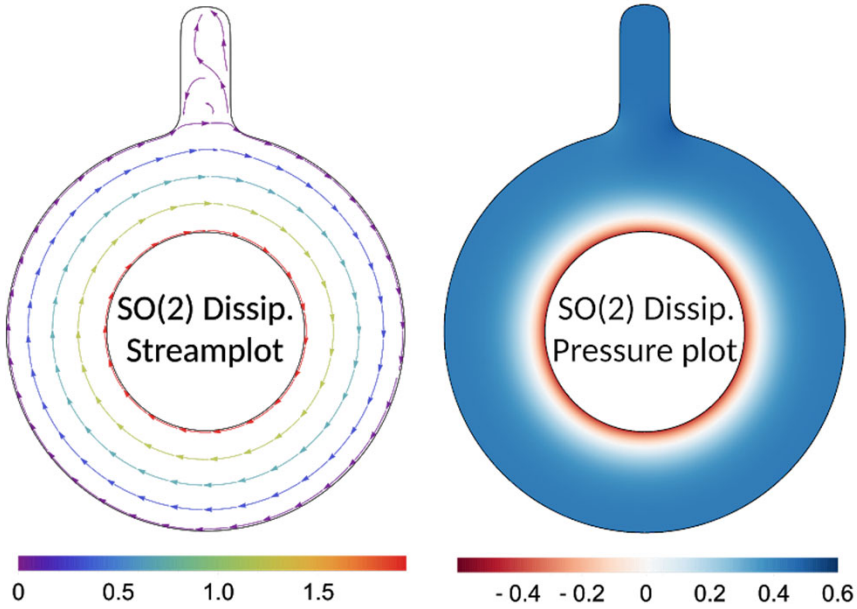
Effect of Crystal Anisotropy

- Steady state **rotational flow** (corbino disk geometry)
- **Square** symmetry (D_4) **breaks rotational symmetry**
- Introduces ~15% **steady state 'vortices'**



Varnavides*, Jermyn* et al. (2020), **Nat Commun** 11

Effect of Dissipation-Less Hall Viscosity



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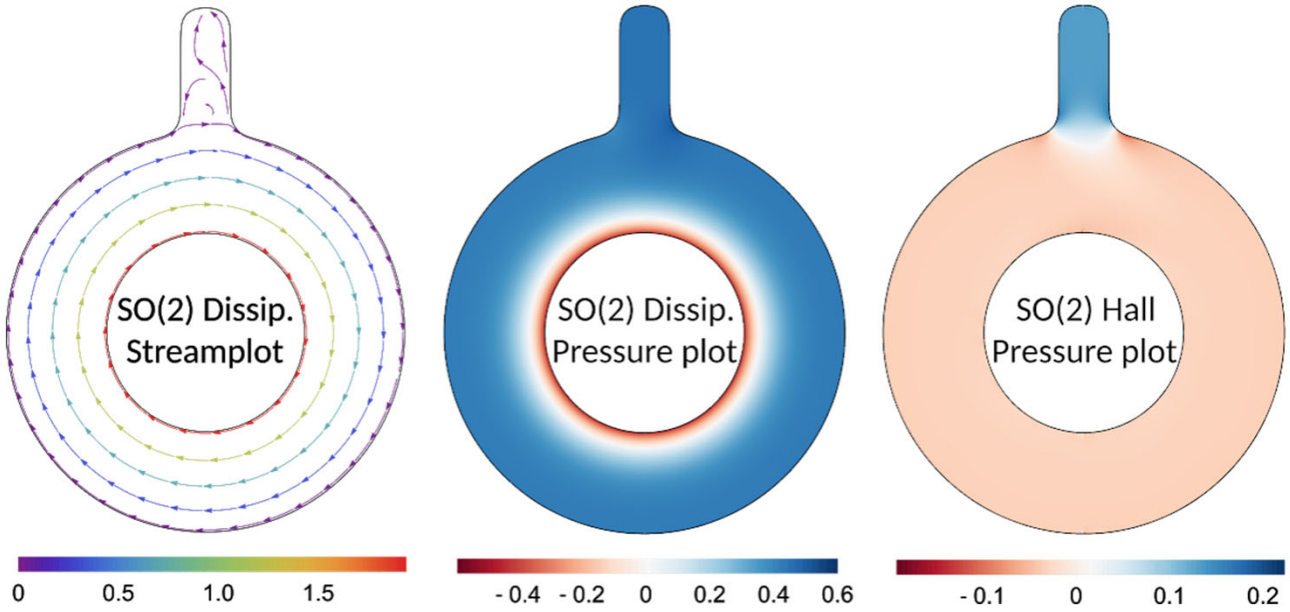
Effect of Dissipation-Less Hall Viscosity

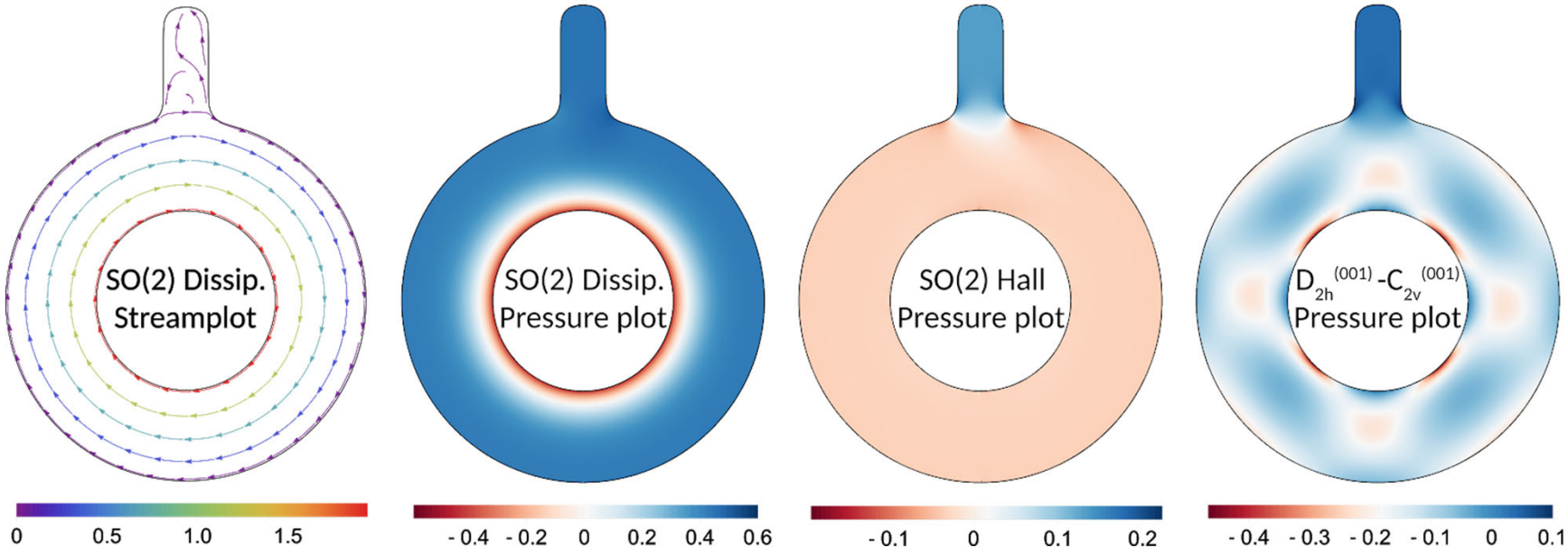
- **Hall viscosity** leads to measurable **voltage drop**



See corbino disk measurements by A. Kapitulnik and others!

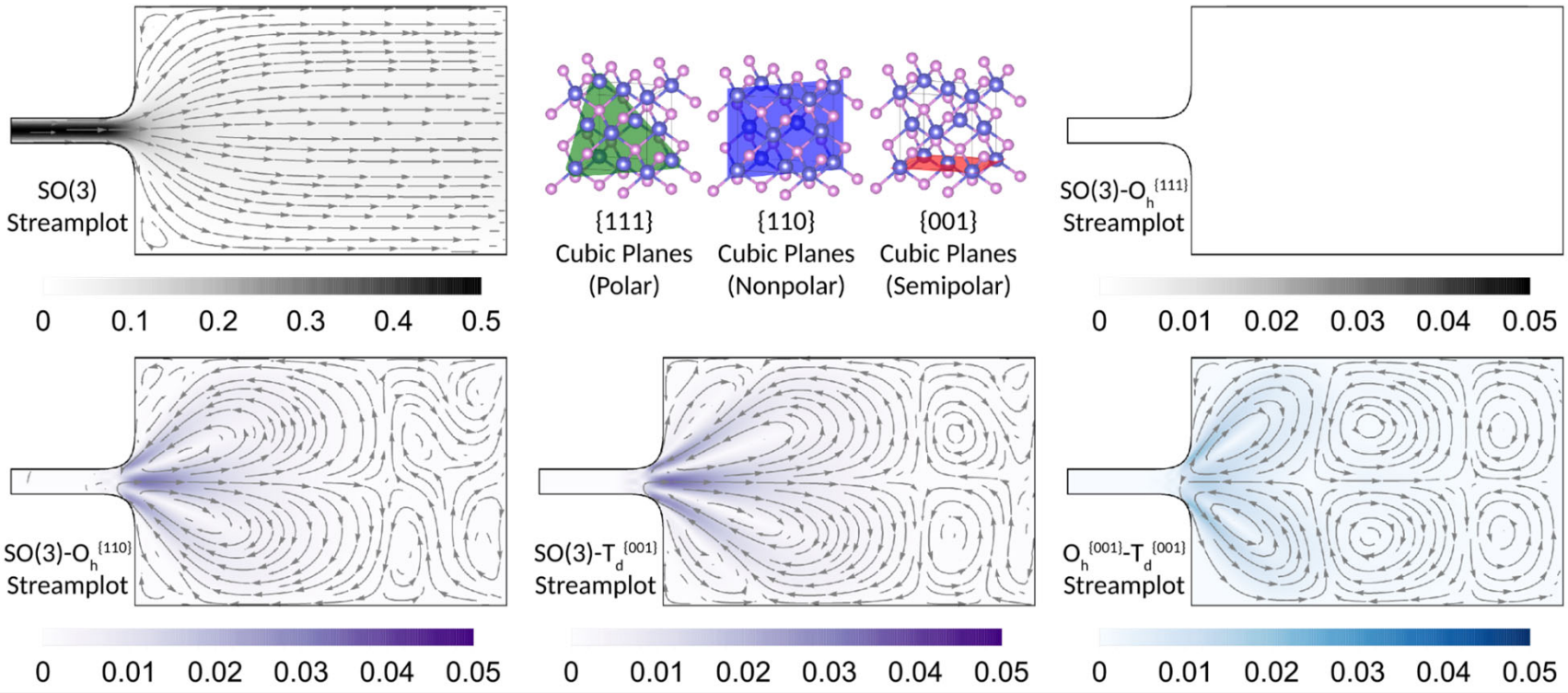
Effect of Dissipation-Less Hall Viscosity

- **Hall viscosity** leads to measurable **voltage drop**
- Effect **persists in 3D crystals** (e.g. basal plane WTe_2)



Varnavides*, Jermyn* et al. (2020), **Nat Commun** 11

Vorticity Coupling in 3D Crystals



Varnavides*, Jermyn* et al. (2020), **Nat Commun** 11

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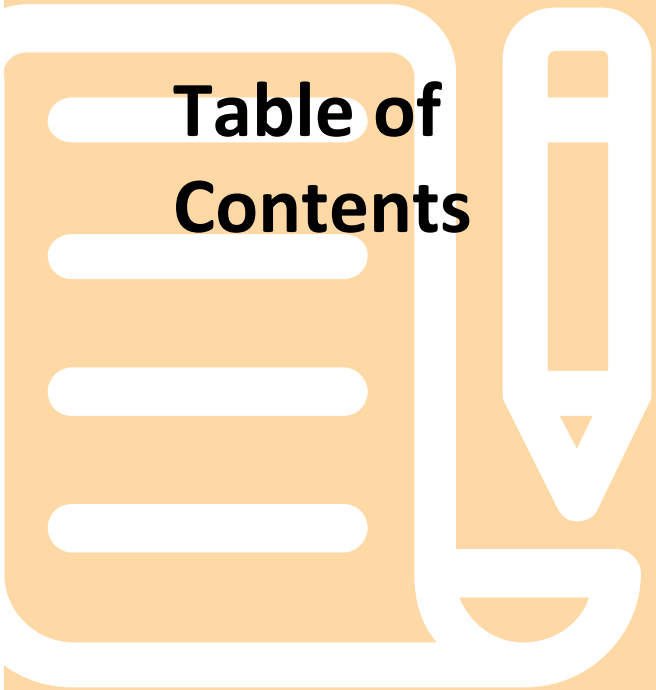

Background

01 Boltzmann Transport Equation Theory

02 Electron Transport Regimes

03 Anisotropic Electron Fluids

Results

04 Spatially-Resolved Transport Framework

05 Observables Sensitivity to Scattering Details

04. Spatially-Resolved Transport Framework

[Var19] Varnavides et al., (2019), **Phys Rev B.** 100, 115402.

[Var22b] Varnavides*, Jermyn*, et al. (2022, in preparation)

Rich Literature of Transport Methods

	DoF (q,r,t)	Accuracy	Method	Equation	Reference
EPRT	(3*,3,1)	RTA	Finite Differences	Boltzmann	Majumdar, J. Heat Transf. 1, 115 (1993)
I-BTE	(3,0,0)	Exact	Jacobi	Boltzmann	Omini & Sparavigna, Phys. Rev. B 53, 14 (1996)
V-BTE	(3,0,0)	Exact	Variational	Boltzmann	Fugallo et al, Phys. Rev. B 88, 4 (2013)
Relaxons	(3,0,0)	Exact	Direct	Boltzmann	Cepellotti & Marzari, Phys. Rev. X 6, 4 (2016)
aiWTE & Phoebe	(3,0,0)	Exact	Direct	Wigner	Simoncelli, Marzari, Mauri, Nat. Phys. 15 (2020) Cepellotti and Kozinsky, Mattod. Phys. 19 (2021)
Perturbo	(3,0,1)	Exact	Jacobi	Boltzmann	Zhou et al, Comput. Phys. Commun. 264, (2021)
Gen. MFPs	(3,3,0)	Exact	Jacobi / Finite Volume	Boltzmann	Romano, arXiv:2002.08940 (2020)
Bolt	(3*,2,1)	RTA	Finite Vol / Advective Semi-Lagrangian	Boltzmann	Chandra et al, Phys. Rev. B 99, 165409 (2019) Gupta et al, Nat Commun 12, 5048 (2021)
NESSE & SpaRTaNS	(3,3,1*)	Exact	Jacobi / Finite Element	Boltzmann	Jermyn et al, Phys. Rev. Mat. 3, 075201 (2019) **Varnavides** et al, Phys. Rev. B 100 (2019) **Varnavides***, Jermyn* et al, in preparation (2022)

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Linearizing BTE

- Collision integral is nonlinear in distribution function *f*

$$\left(\frac{\partial f}{\partial t}\right)_{\text{coll}} = f^0(\boldsymbol{k})\hat{A}\psi + \mathcal{O}(\psi^2)$$
$$f(\boldsymbol{k}) = f^0(\boldsymbol{k}) + f^0(\boldsymbol{k})\psi(\boldsymbol{k})$$

- At steady-state we write BTE as:

$$\boldsymbol{v}_i \cdot \nabla\psi_i(\boldsymbol{r}) = S_i^{(0)}(\boldsymbol{r}) + A_{ij}\psi_j(\boldsymbol{r})$$

  - $S^{(0)}$ is a source term used to approximate the external force

- Rearrange equation to **group** distribution **by scattering events**

$$A_{ij} \equiv M_{ij} - \tau_i^{-1}\delta_{ij}$$
$$\left(\tau_i^{-1} + \boldsymbol{v}_i \cdot \nabla\right)\psi_i(\boldsymbol{r}) = S_i^{(0)}(\boldsymbol{r}) + M_{ij}\psi_j(\boldsymbol{r})$$

- Split distribution at nth order in *M* and **solve recursively**

$$\left(\tau_i^{-1} + \boldsymbol{v}_i \cdot \nabla\right)\psi_i^{(n)}(\boldsymbol{r}) = S_i^{(n)}(\boldsymbol{r})$$
$$S_i^{(n+1)}(\boldsymbol{r}) = M_{ij}\psi_j^{(n)}(\boldsymbol{r})$$

Varnavides, Jermyn, et al. (2019), **Phys. Rev. B.**

Spatially **R**esolved **T**ransport of **N**on-equilibrium **S**pecies **(SpaRTaNS)**

- Massively-parallelized (collisions) — c++ (streaming) & python
- Spatial resolution → Finite Element Method
- State resolution → Full Scattering Matrix (beyond RTA)

Varnavides et al. (2019), **Phys. Rev. B.** 100, 115402
Varnavides*, Jermyn* et al. (2022), in preparation

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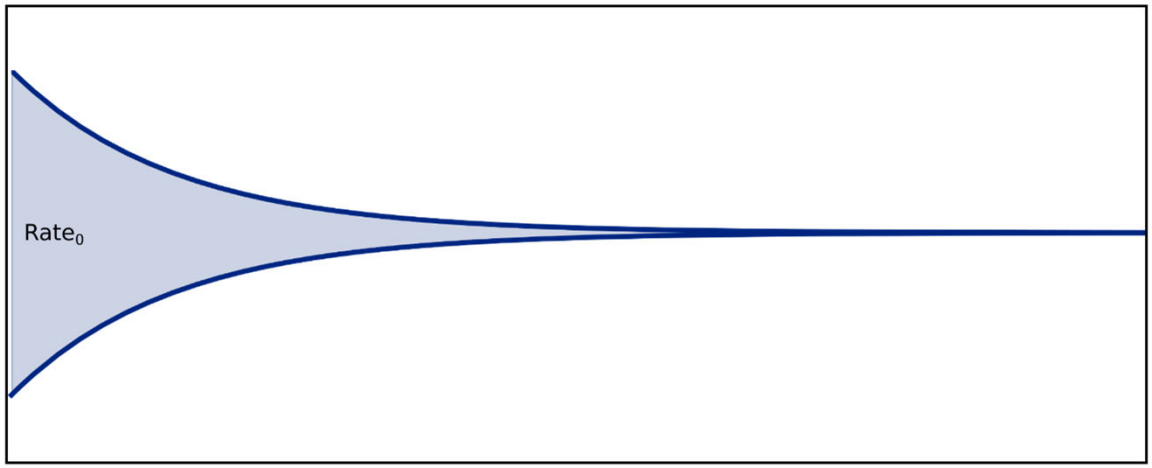

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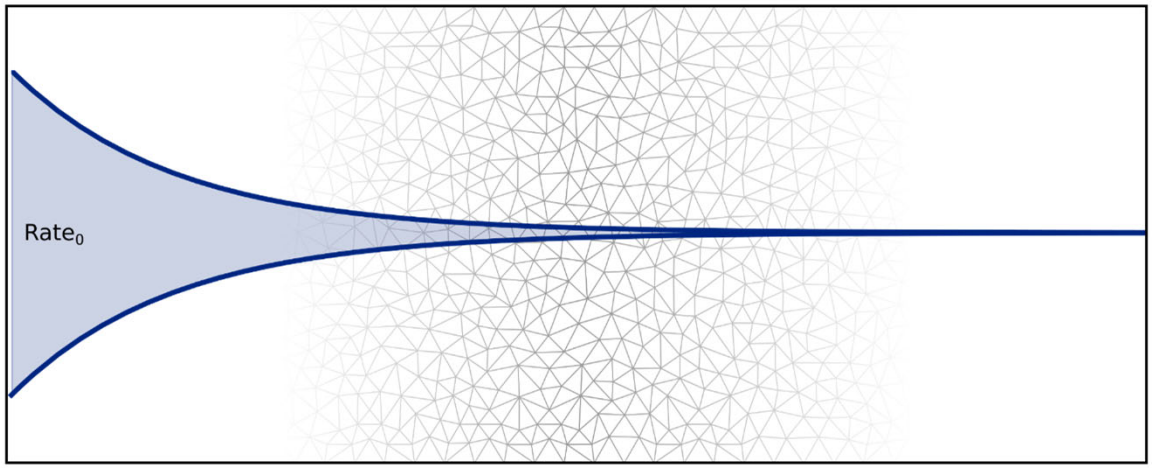

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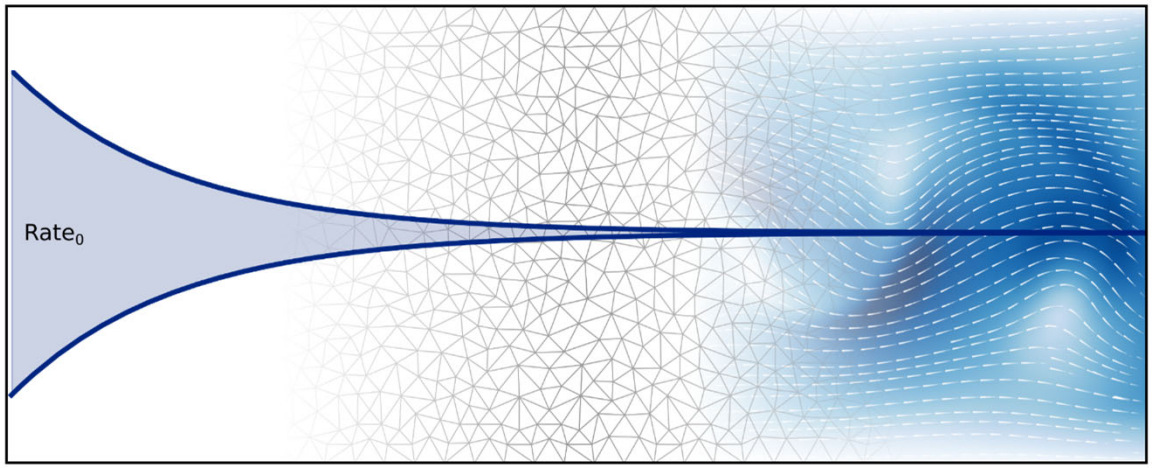

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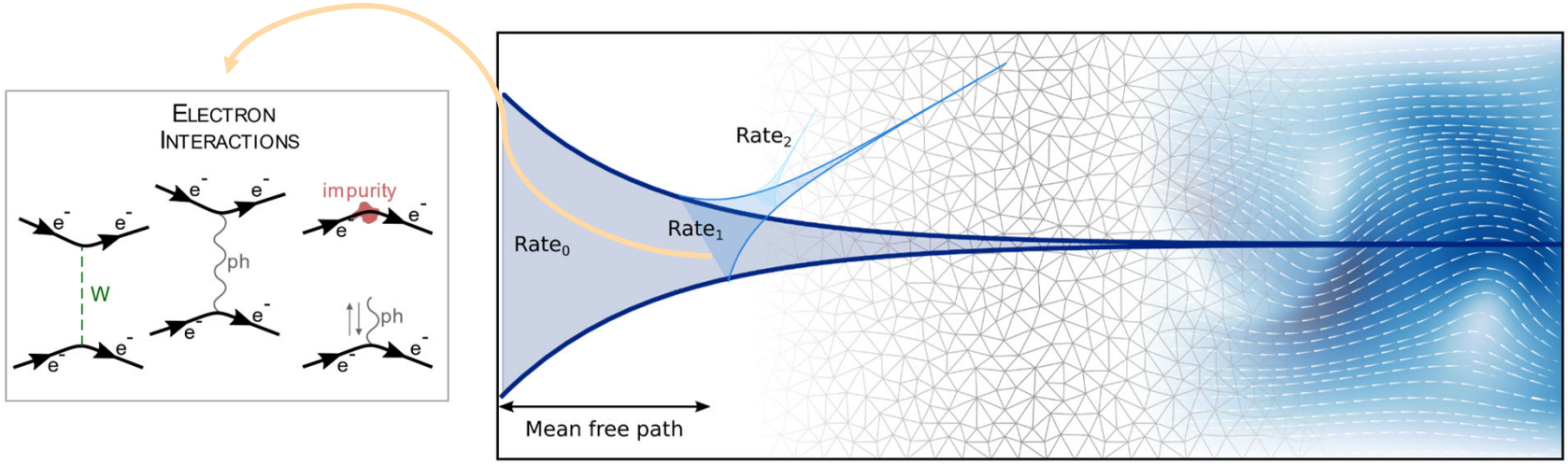

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Varnavides et al. (2019), **Phys. Rev. B.** 100, 115402
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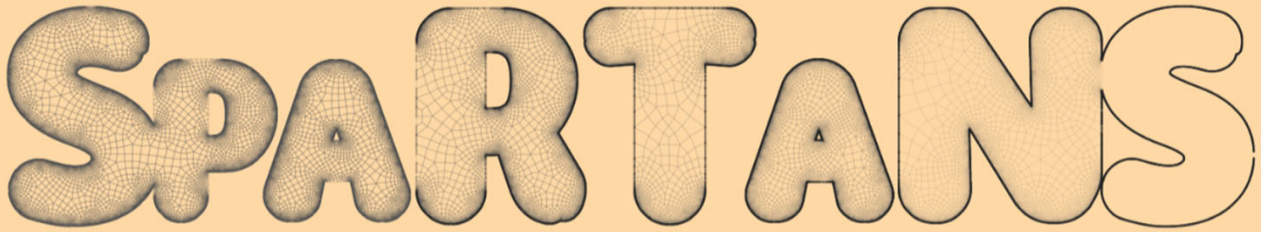
SpaRTaNS Docs News GitHub

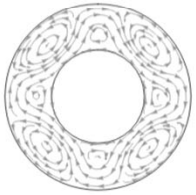
SpaRTaNS

Spatially Resolved Transport of Nonequilibrium Species



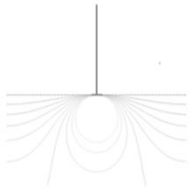
Get Started

https://narang-lab.github.io/spartans/



Spatially-Resolved, Momentum-Exact

SpaRTaNS solves the steady-state Boltzmann transport equation in three real-space and three momentum-space dimensions.



General Framework

SpaRTaNS is carrier-agnostic with applications in fields like phonon transport and "hydrodynamic" electron transport.

Open Source & Parallel

SpaRTanS makes use of multiple processors using the MPI framework, and is embarassingly-parallel across real-space tetrahedra.

05. Observables Sensitivity to Scattering Details

[Var22a] Varnavides*, Jermyn* et al. (2022), **ArXiv**:2204.06004
See our collaborative work with C. Felser, A. Yacoby, K. Burch, P. Moll, F. Tafti, more!

Physically Inspired Scattering Matrix

- SpaRTaNS requires the **full scattering matrix**
  - This is often **hard to obtain** from first principles
  - Can we obtain this using **crystal symmetries** and **conservation laws**?

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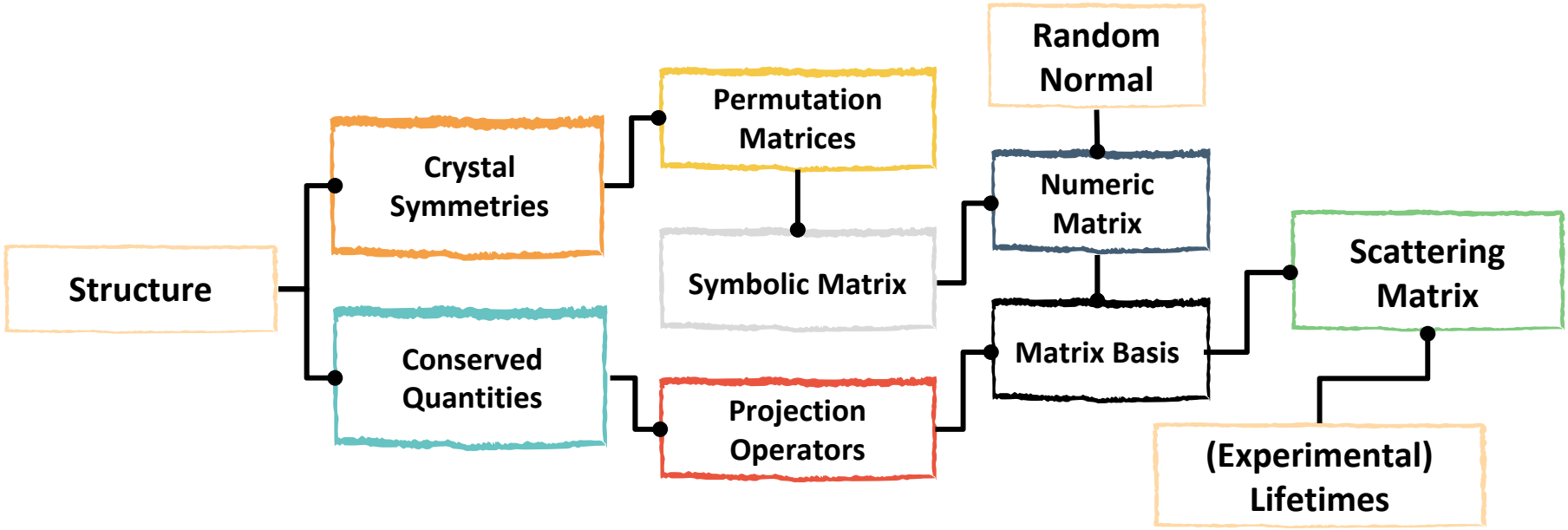
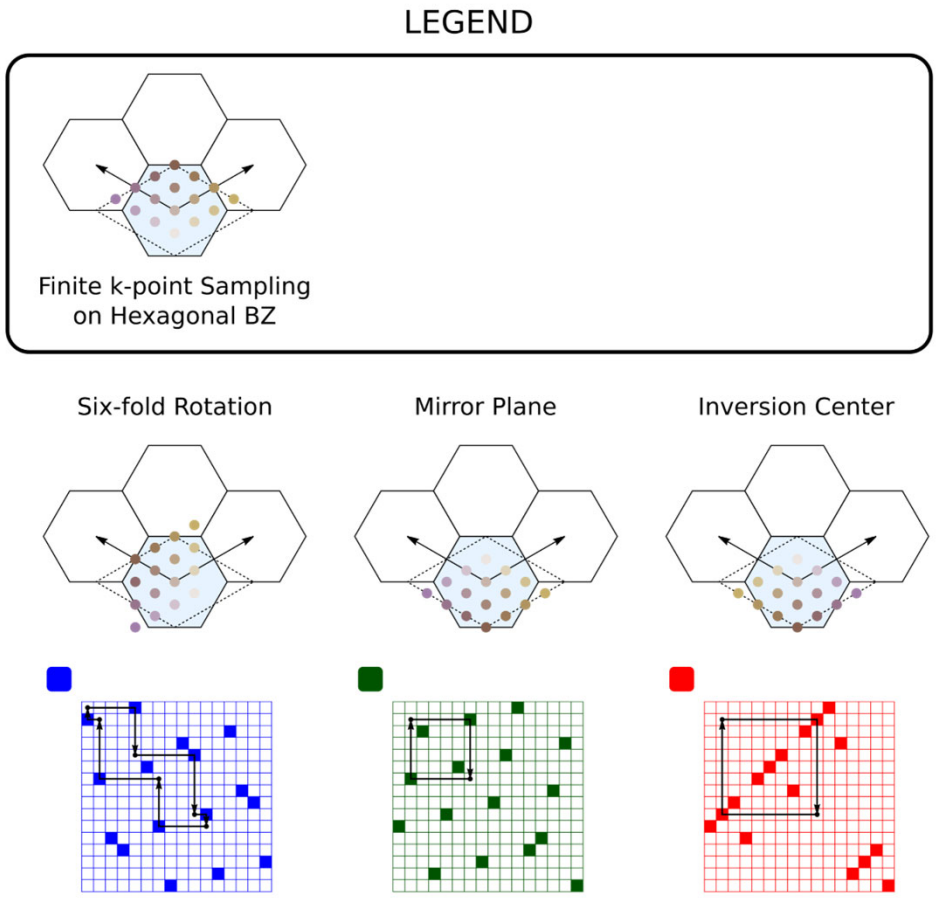


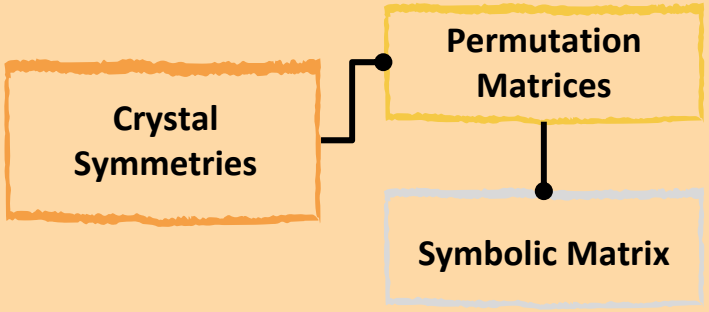
Physically Inspired Scattering Matrix

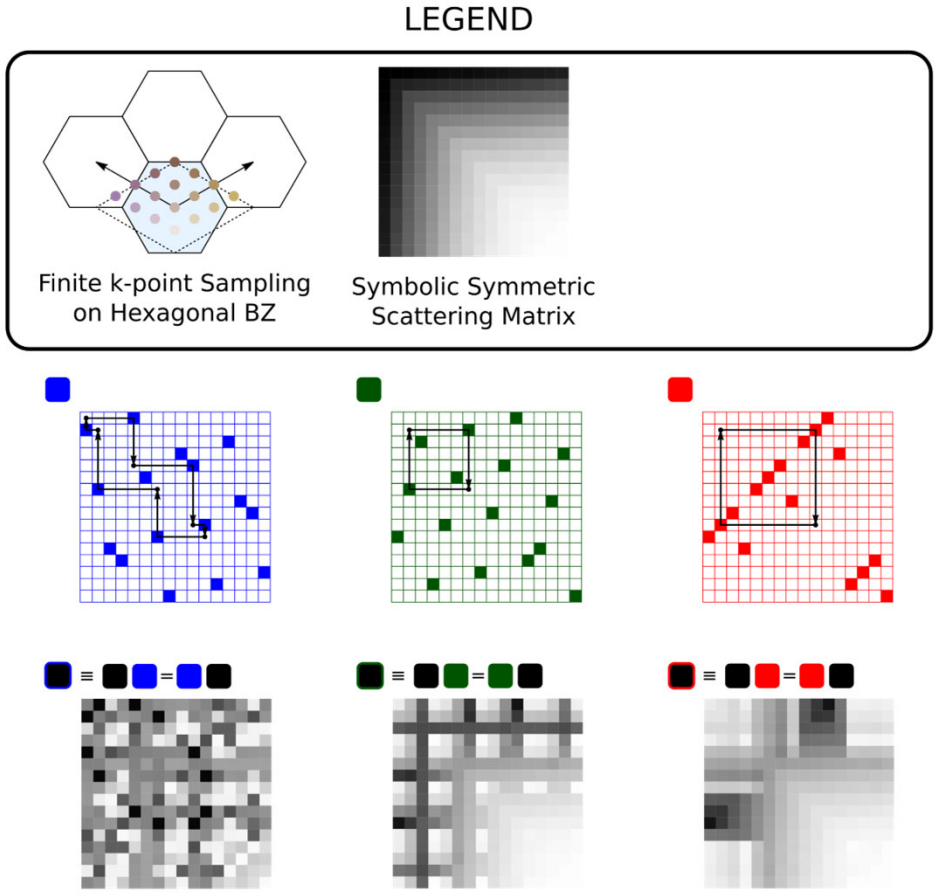
Crystal Symmetries

Permutation Matrices

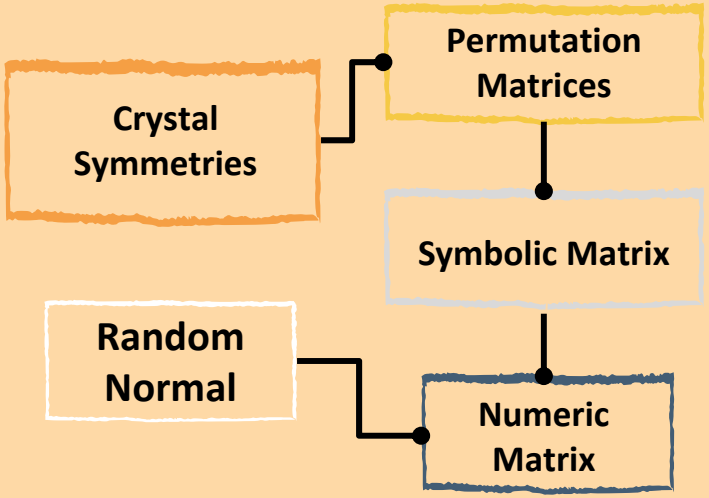


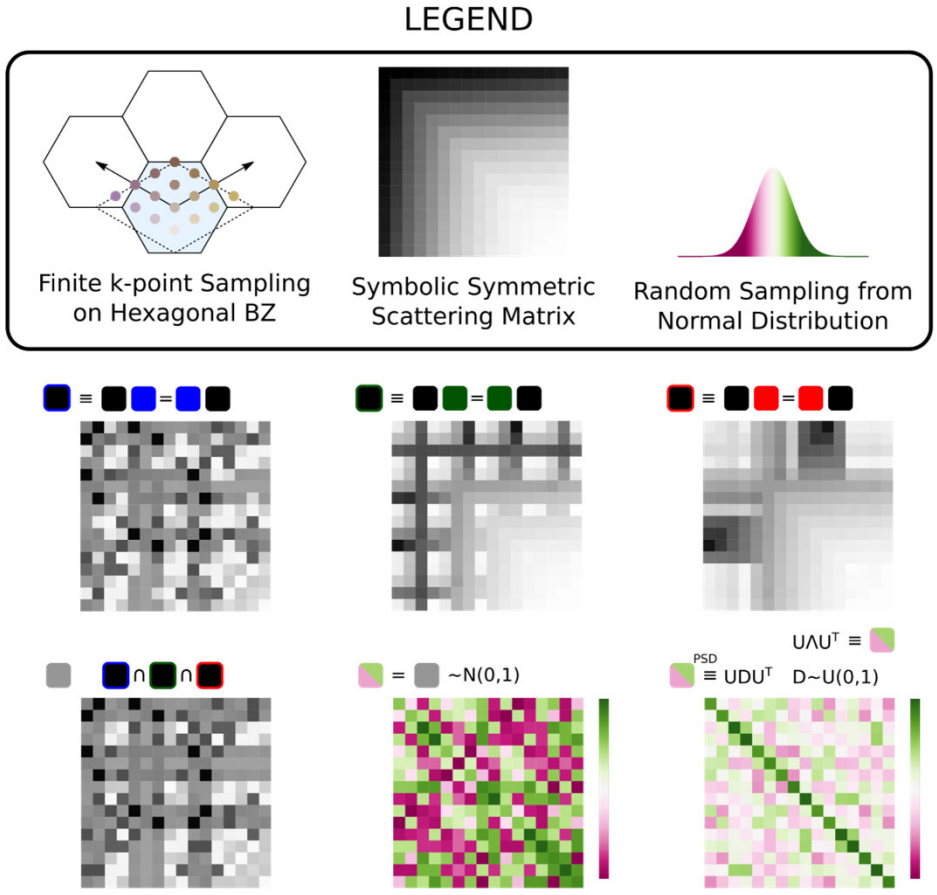
Physically Inspired Scattering Matrix





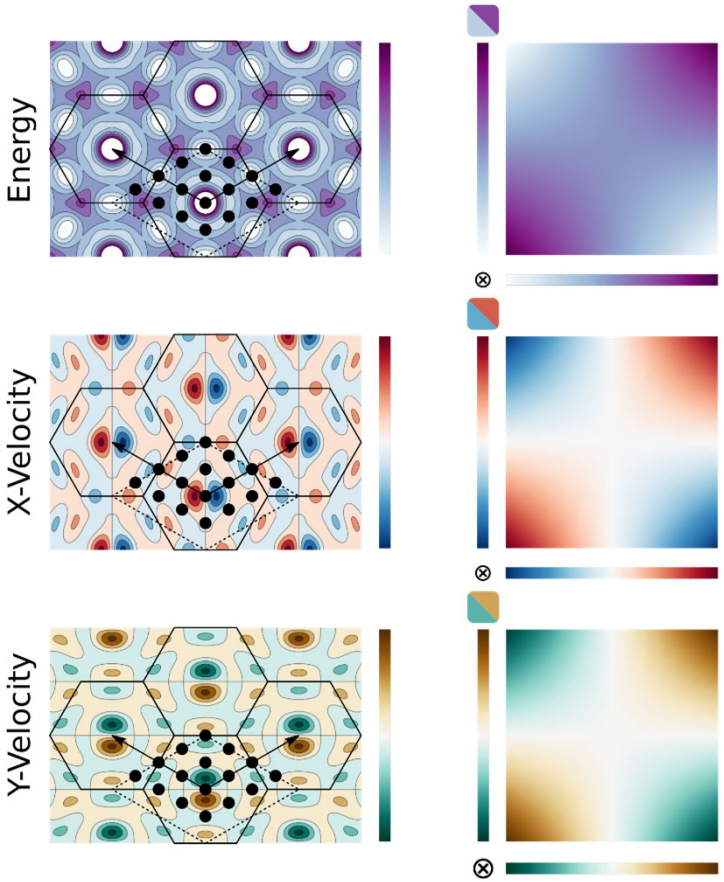
Physically Inspired Scattering Matrix





Physically Inspired Scattering Matrix

Conserved Quantities → Projection Operators



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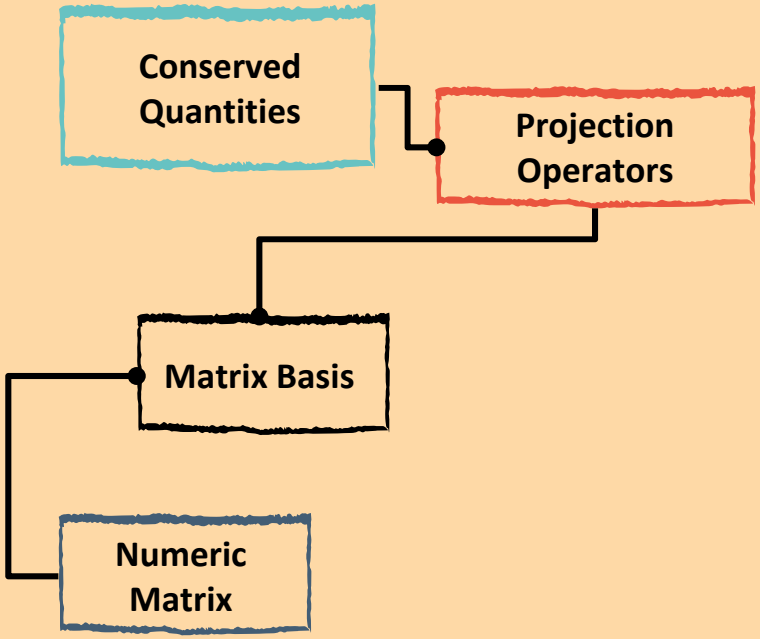
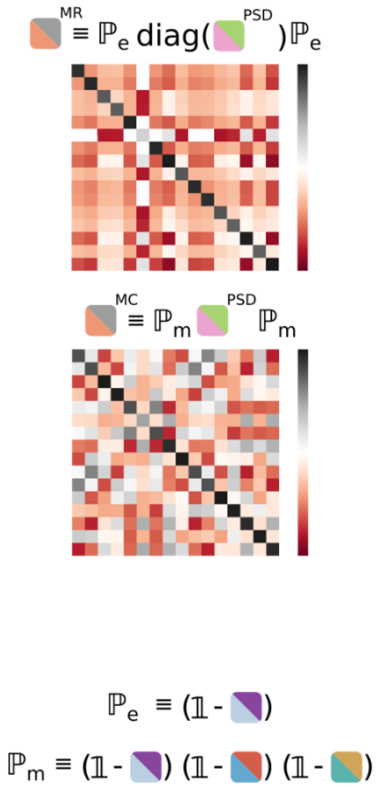
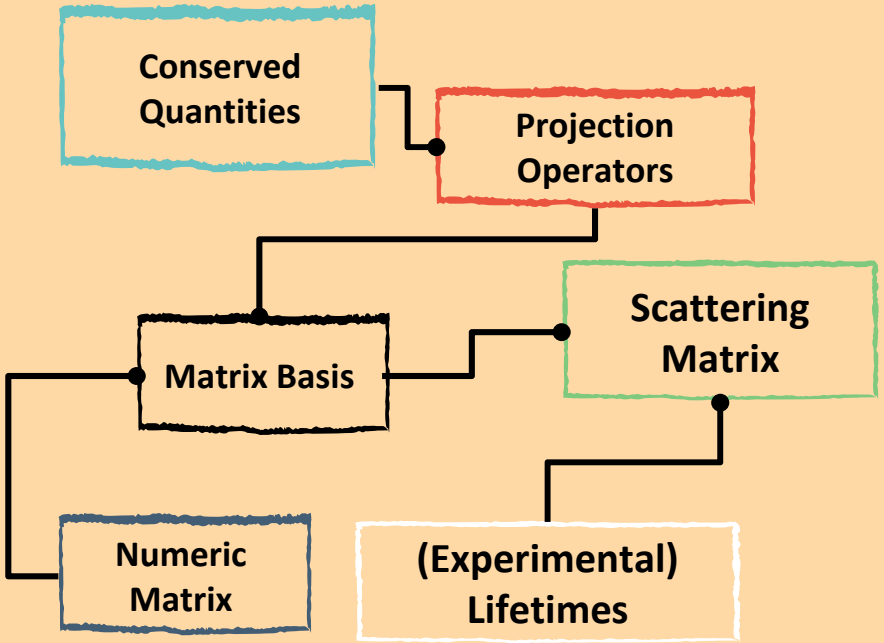


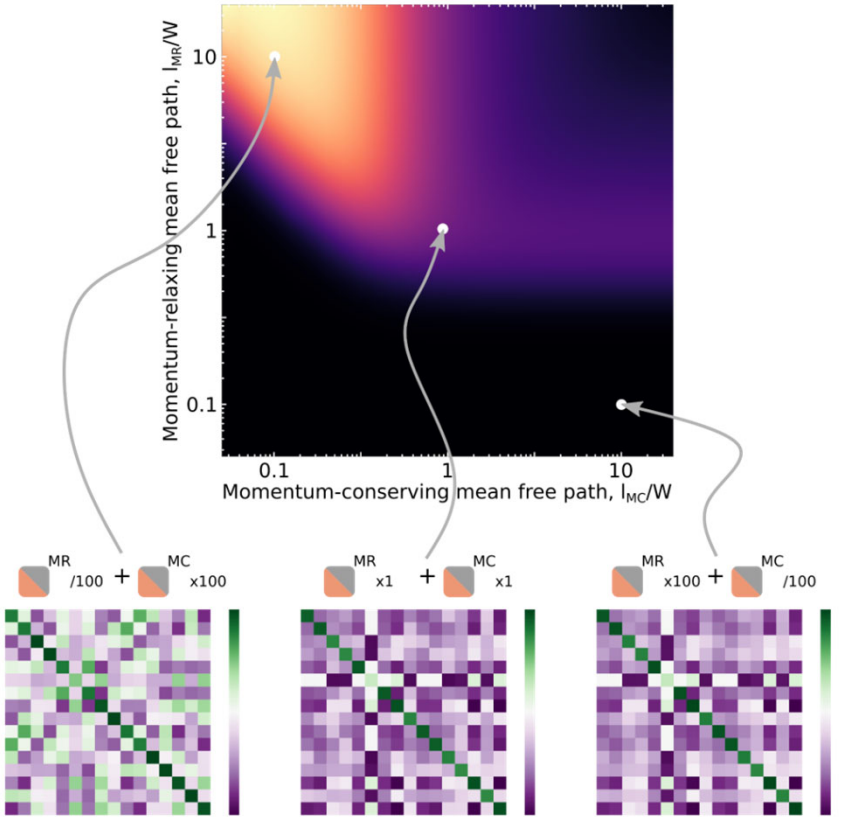


$\mathbb{P}_e \equiv (\mathbb{1} - \square)$

$\mathbb{P}_m \equiv (\mathbb{1} - \square)(\mathbb{1} - \square)(\mathbb{1} - \square)$

Physically Inspired Scattering Matrix





Isotropic SO(2)

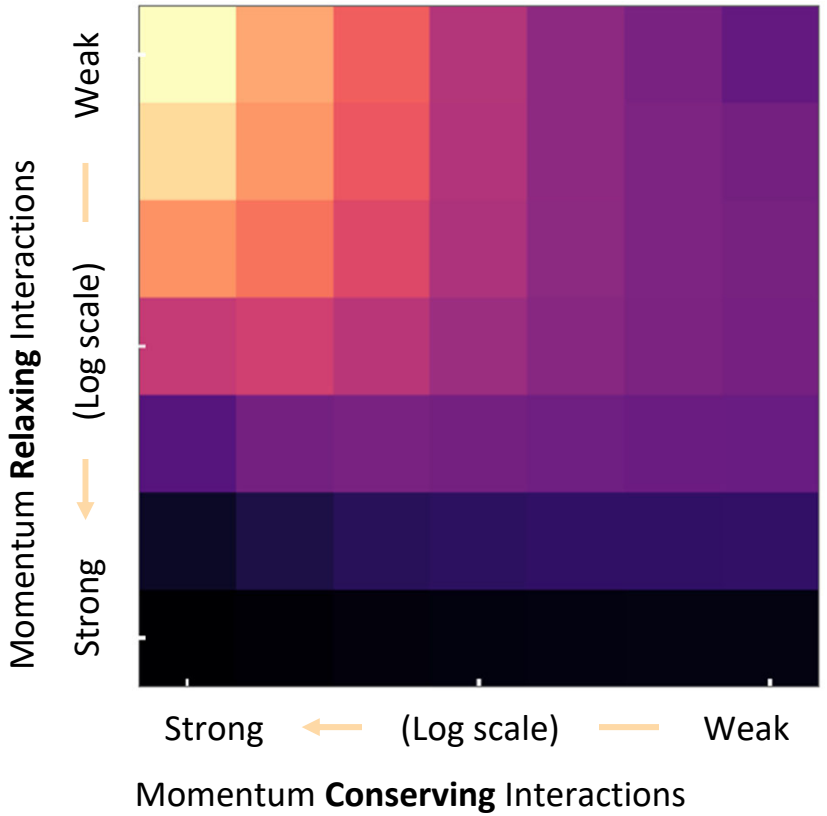
- Isotropic point group, SO(2)
  - no free parameters
  - i.e. single scattering matrix

Isotropic SO(2)

- Isotropic point group, SO(2)
  - no free parameters
  - i.e. single scattering matrix

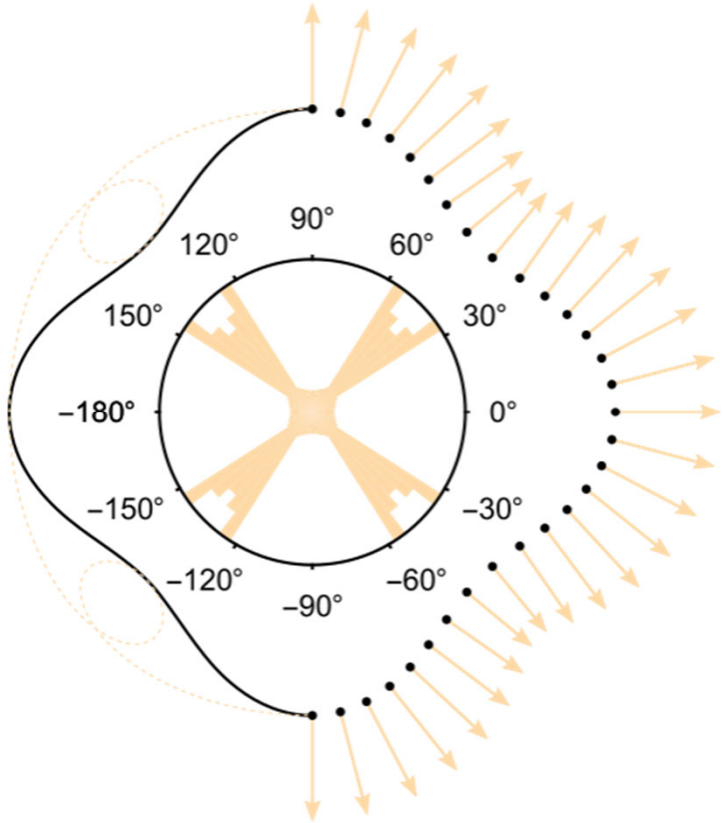
- Projection scheme recovers Callaway's hydrodynamic model!

$$\left(\frac{\partial f}{\partial t}\right)_{\text{coll}} \equiv \frac{1}{\tau_{\text{mr}}}\left(\mathbb{P}_n - 1\right) f + \frac{1}{\tau_{\text{mc}}}\left(\mathbb{P}_m - 1\right) f$$



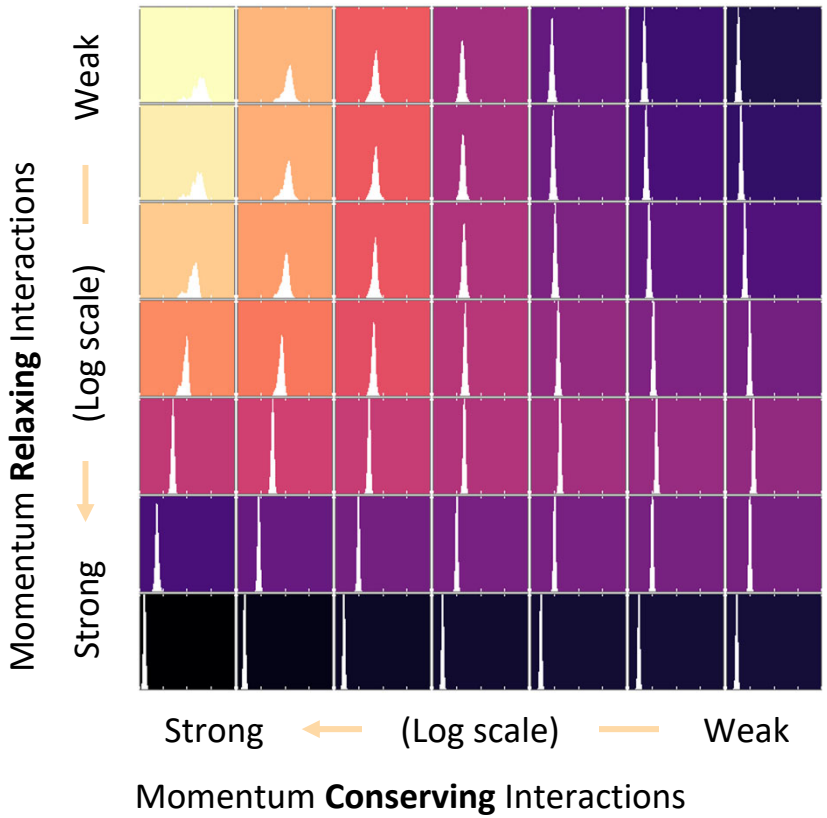
Square (D_4) Symmetry

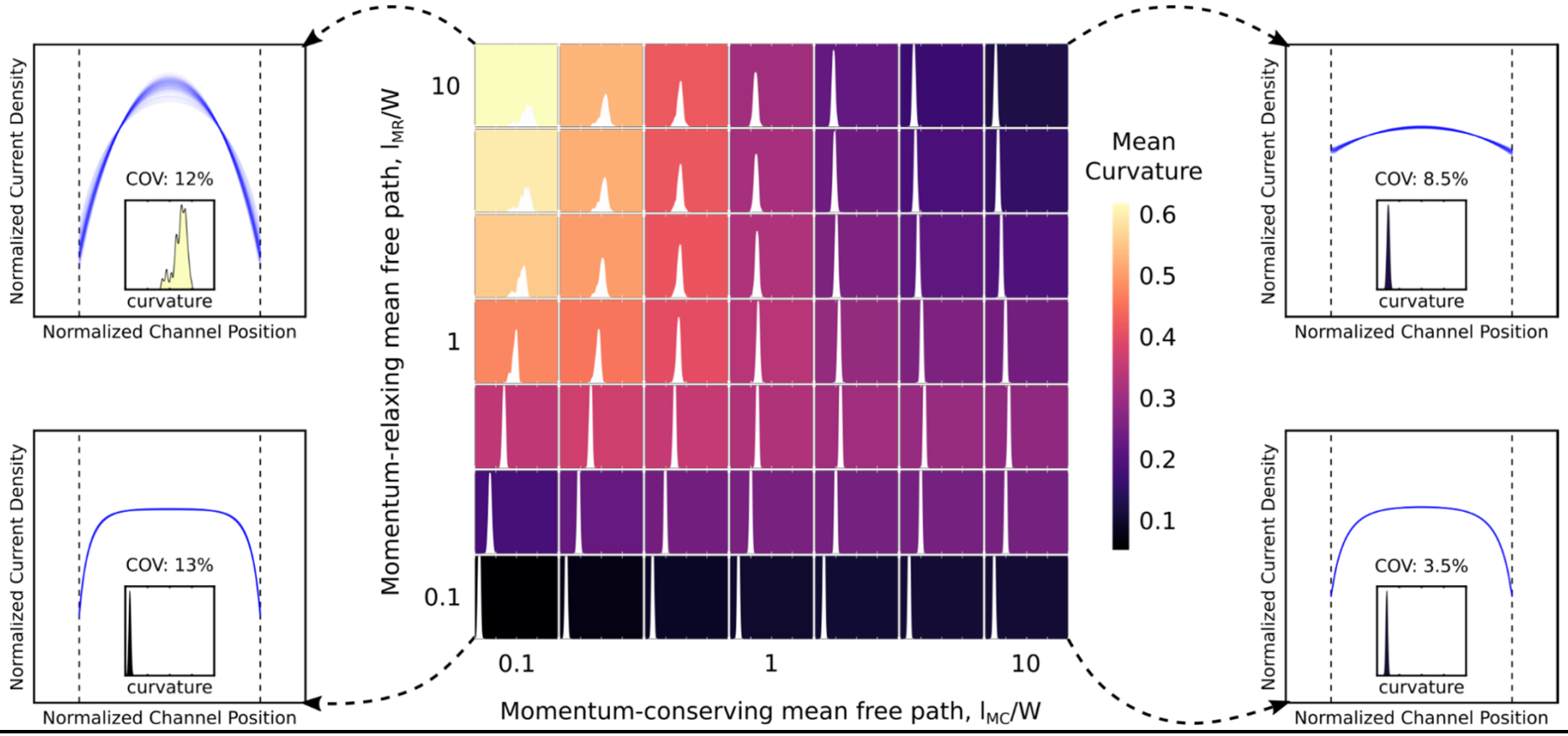
- 100 random* physically-inspired scattering matrices



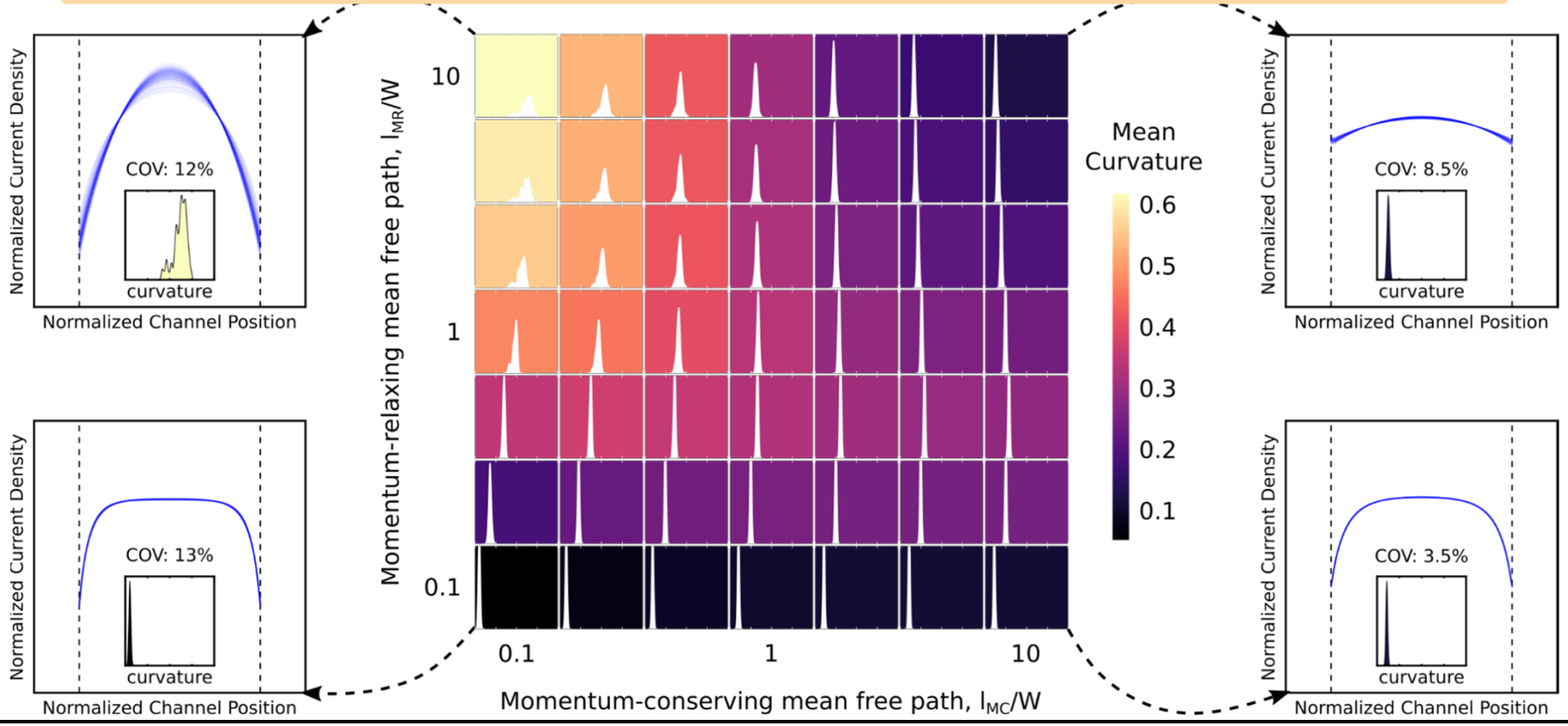
Square (D_4) Symmetry

- 100 random* physically-inspired scattering matrices
- Mean current curvature reproduces dual-relaxation lifetime dynamics
- Variability of current density profiles increases as we approach the hydrodynamic limit




Normalized Current Density
COV: 12%
curvature
Normalized Channel Position
Normalized Current Density
COV: 13%
curvature
Normalized Channel Position
Momentum-relaxing mean free path, l_{MR}/W
10
1
0.1
0.1
1
10
Momentum-conserving mean free path, l_{MC}/W
Mean Curvature
0.6
0.5
0.4
0.3
0.2
0.1
Normalized Current Density
COV: 8.5%
curvature
Normalized Channel Position
Normalized Current Density
COV: 3.5%
curvature
Normalized Channel Position

Maximum Coefficient of Variability < 15%



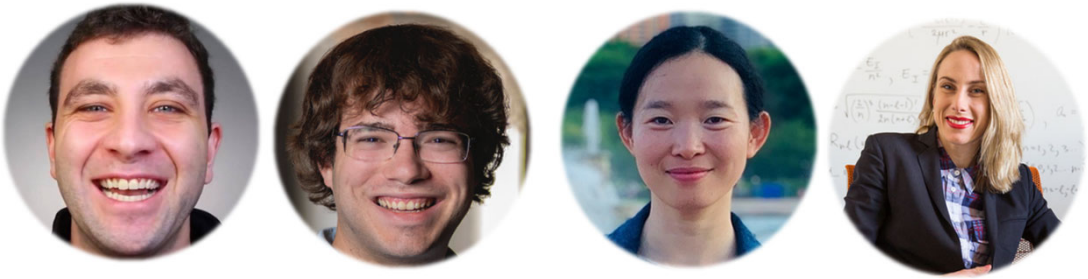
Varnavides*, Jermyn* et al. (2022), ArXiv:2204.06004

Summary and Outlook

Summary

- Proposed **indirect mechanism** for electron-electron interactions
  - **First** experimental **observation** of hydrodynamic flow **in 3D** material
- Incorporated effects of **crystal-lattice** on **electronic viscosity**
  - Investigated **anomalous landscape** of anisotropic/asymmetric viscous flow
- Developed an **efficient spatially-resolved BTE solver**
  - open-sourcing code: https://narang-lab.github.io/spartans/
- Formalized framework for **physically-plausible scattering matrices**
  - **Quantified the validity** of Callaway's model (~10-15%)

Acknowledgements



Theory & Computation

Spatially-Resolved Imaging

Hydrodynamic
Phenomena Measurements

Optional (Tutorial)

Installation

- Source code and examples: https://github.com/narang-lab/spartans
- Uses scikit-build and pybind11 to call performance-critical c++ streaming code from python
- Uses mpi4py to run c++ code using multiple cores
  - mpi4py installation can be tricky..
- In theory, all you need to do should be:

```
git clone https://github.com/narang-lab/spartans
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cd spartans
pip install .
```

- If this doesn't work, you can try installing all the dependencies globally:
  - "setuptools",
  - "wheel",
  - "pybind11",
  - "scikit-build",
  - "cmake",
  - "ninja",
  - "mpi4py==3.0.3",
  - "numpy",
  - "h5py",
  - "PyYAML",
  - "Parse",
- The culprit is likely mpi4py
  - Also note: the version pinning

SpaRTaNS datasets

- SpaRTaNS stores its data on a finite element mesh with linear interpolation
  - "Body" distribution functions defined on tetrahedra vertices
    - "Body in", Bi_{NxV}
    - "Body out", Bo_{NxV}
  - "Surface" fluxes defined on the vertices of surface triangles
    - "Surface in", Si_{NxTx3}
    - "Surface out", So_{NxTx3}
  - Dimensions:
    - N → State Index
    - V → Tet Vertex Index
    - T → Triangle Index

SpaRTaNS User Inputs

- All user inputs are specified using HDF5 datasets

- Material properties
  - carrier “velocities”
    - Dimensions: Nx3
  - carrier “frequencies” (i.e. energies)
    - Dimensions: Nx3
  - material scattering matrix
    - “diagonal”
      - Dimensions: N
    - “mixing_matrix”
      - Dimensions: NxN

- All should be under same HDF5 group
  - Although possibly in multiple files

A	velocities	NumericArray [Type: Real64 Dimensions: {48, 3}]
	frequencies	NumericArray [Type: Real64 Dimensions: {48}]
	diagonal	NumericArray [Type: Real64 Dimensions: {48}]
	mixing_matrix	NumericArray [Type: Real64 Dimensions: {48, 48}]

SpaRTaNS User Inputs

- All user inputs are specified using HDF5 datasets

- Mesh properties
  - tetrahedra “vertices”
    - Dimensions: Vx3
  - “tetrahedra_indices” (Integer)
    - Dimensions: Tet x 4
  - “triangle_indices” (Integer)
    - Dimensions”: T x 3
  - “surface_normals” [Optional]
    - Dimensions: T x 3

- All should be under same HDF5 group
  - Although possibly in multiple files

000	vertices	NumericArray [Type: Real64 Dimensions: {5658, 3}]
	tetrahedra_indices	NumericArray [Type: Integer64 Dimensions: {16 395, 4}]
	triangle_indices	NumericArray [Type: Integer64 Dimensions: {11 312, 3}]
	surface_normals	NumericArray [Type: Real64 Dimensions: {11 312, 3}]

SpaRTaNS User Inputs

- All user inputs are specified using HDF5 datasets

- Structure (injection) properties
  - “body_injection” (source term)
    - Dimensions: NxV
  - “surface_injection” (source term)
    - Dimensions: NxTx3

- Either (but not both) of the injection terms can be omitted

- All should be under same HDF5 group
  - Although possibly in multiple files

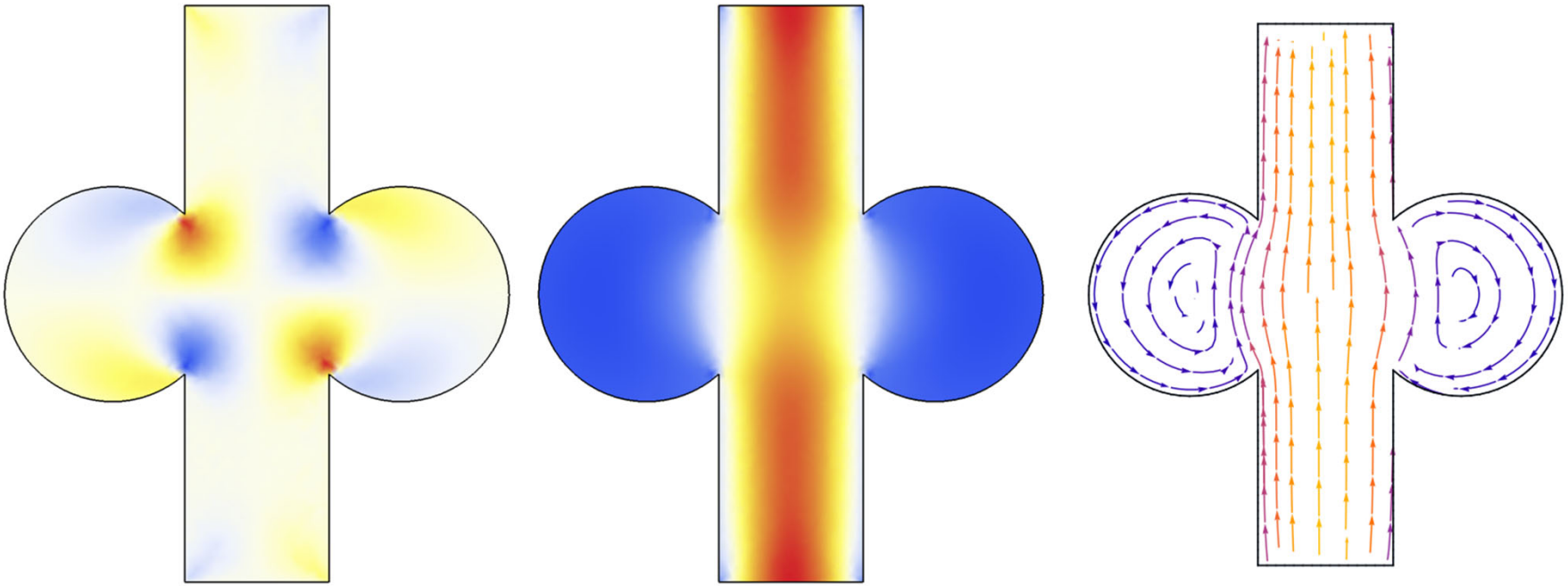
000--A	surface_injection	NumericArray [Type: Real64 Dimensions: {48, 11312, 3}]
	body_injection	NumericArray [Type: Real64 Dimensions: {48, 5658, 3}]

SpaRTaNS User Inputs

- All user inputs are specified using HDF5 datasets

- Connectivity information
  - "connectivity"
    - Dimensions: mxm
      - m → # of meshes
  - For each "interface"
    - For each "bounce_tensor"
      - Triangle mapping

Step-by-step example walk-through



Questions?

Backup Design Principles Slides

How general is this mechanism?

Empirically (ab-initio), a lot of materials show shorter phonon-mediated electron lifetimes. Under what conditions does this hold?

Electron-Phonon Linewidth

$$\tau_{\mathrm{eph}}^{-1} = \frac{\pi\beta}{2g(\epsilon_F)} \sum_{\nu} \int \frac{d\boldsymbol{q}}{\Omega_{\mathrm{BZ}}} G_{\boldsymbol{q}\nu} \frac{\omega_{\boldsymbol{q}\nu}}{\sinh^2(\hbar\beta\omega_{\boldsymbol{q}\nu}/2)}$$

Phonon-Mediated Electron-Electron Linewidth

$$\tau_{\mathrm{ee(ph)}}^{-1} = \frac{2\pi}{\hbar g(\epsilon_F)} \sum_{\nu} \int \frac{d\boldsymbol{q}}{\Omega_{\mathrm{BZ}}} G_{\boldsymbol{q}\nu}^2 \gamma(\hbar\beta\bar{\omega}_{\boldsymbol{q}\nu})$$

Wang*, Varnavides*, et al., (2021), ArXiv: 2109.00550

Functional Approximation

$$\gamma(x) \equiv \int_{-\infty}^{\infty} dy \frac{1}{4} \frac{y^2}{\sinh^2(y/2)|x-y|^2}$$

Wang*, Varnavides*, et al., (2021), ArXiv: 2109.00550

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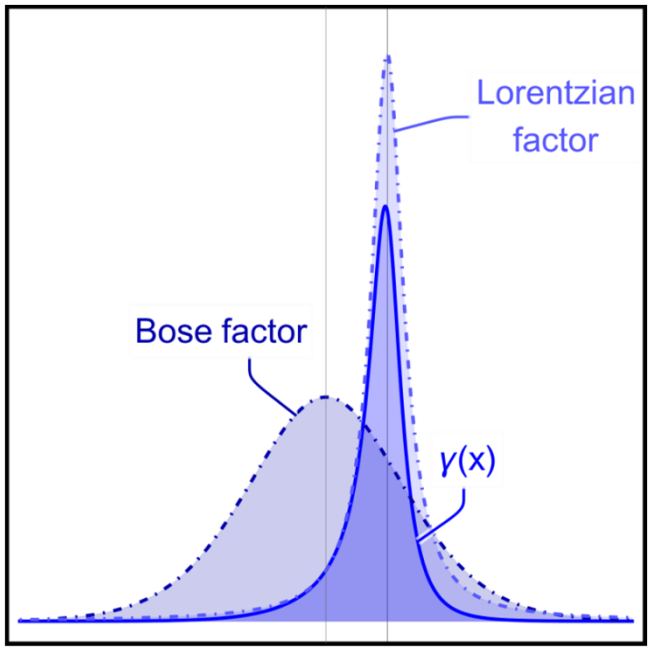
- Bose factor (temperature) times Lorentzian factor (on-shell)



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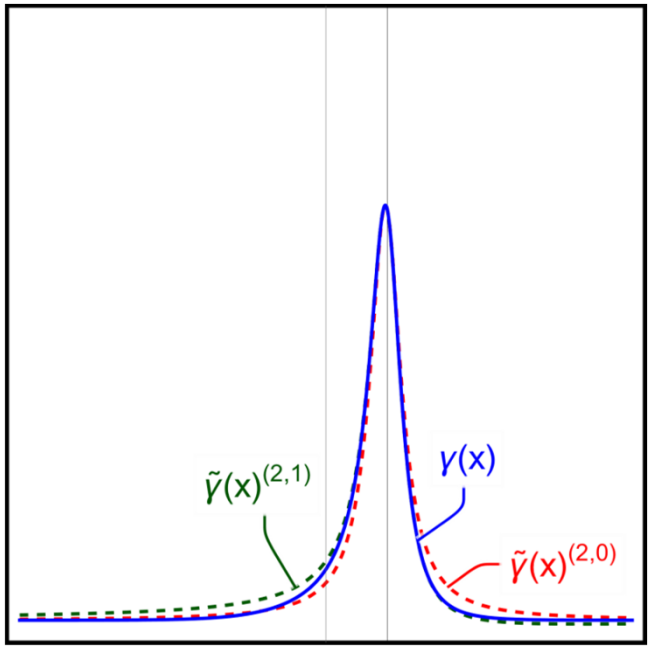
- Bose factor (temperature) times Lorentzian factor (on-shell)
- Approximate w/ (2,0) Padé approx.



Wang*, Varnavides*, et al., (2021), ArXiv: 2109.00550

How general is this mechanism?

Functional Approximation

$$\gamma(\hbar\beta\bar{\omega}_{\boldsymbol{q}\nu}) \approx \frac{\hbar\beta\omega_{\boldsymbol{q}\nu}}{2G_{\boldsymbol{q}\nu}\sinh^{\frac{3}{2}}\left(\frac{\hbar\beta\omega_{\boldsymbol{q}\nu}}{2}\right)\sqrt{4\sinh\left(\frac{\hbar\beta\omega_{\boldsymbol{q}\nu}}{2}\right)+\mathcal{O}\left(G^2\right)}}$$

Keeping terms linear in G

$$\gamma(\hbar\beta\bar{\omega}_{\boldsymbol{q}\nu}) \approx \frac{\hbar\beta\omega_{\boldsymbol{q}\nu}}{4G_{\boldsymbol{q}\nu}\sinh^2(\hbar\beta\omega_{\boldsymbol{q}\nu}/2)}$$

Two rates are identical (at linear order in G)
Any additional (higher order) scattering will reduce $\tau_{ee(ph)}$

Wang*, Varnavides*, et al., (2021), ArXiv: 2109.00550

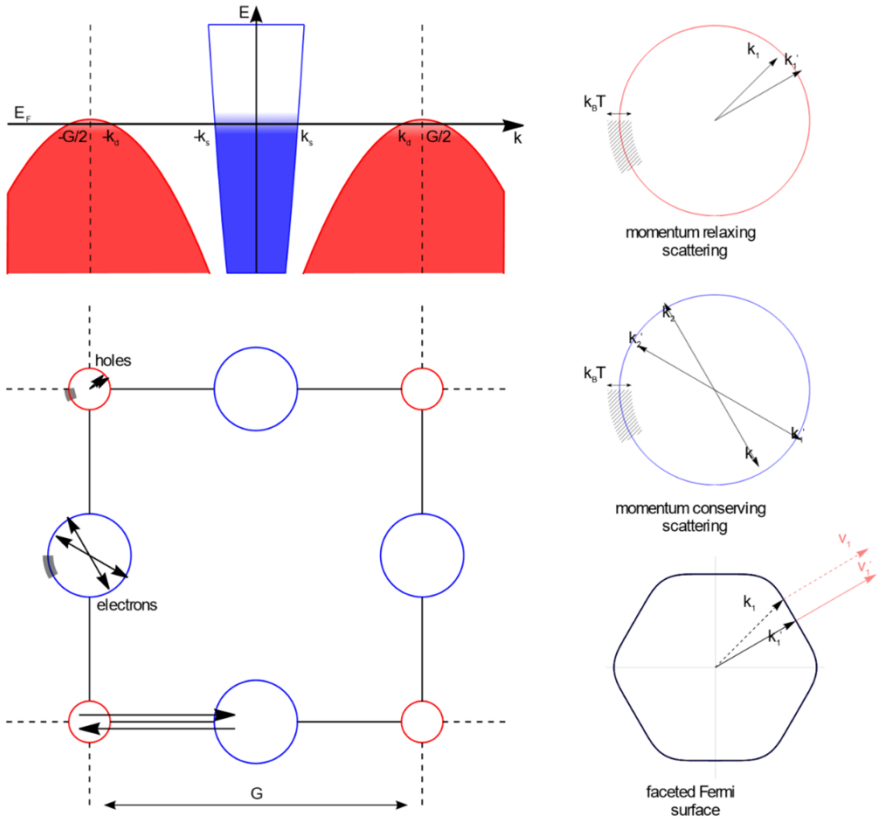
Design Principles

- Approximations valid for electron-phonon couplings **G << 1**
  - True for non-superconducting materials
- Mechanism relies on ‘virtual’ phonon exchange
  - Temps below Debye temperature

Wang*, Varnavides*, et al., (2021), ArXiv: 2109.00550

Design Principles

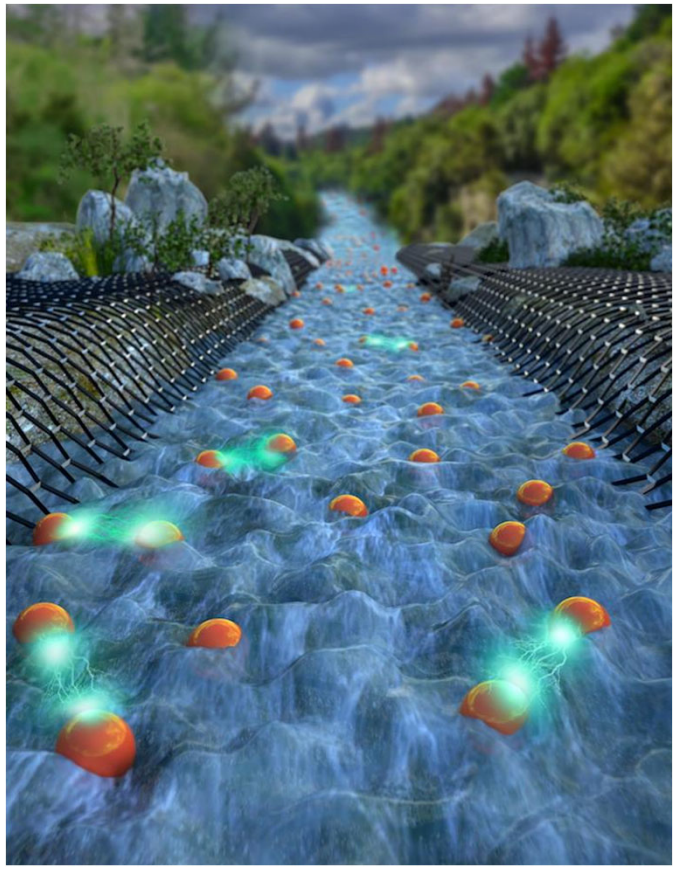
- Approximations valid for electron-phonon couplings **G << 1**
  - True for non-superconducting materials
- Mechanism relies on ‘virtual’ phonon exchange
  - Temps below Debye temperature
- Proposed candidates:
  - Semi-metals with separated pockets
  - Low-symmetry crystal (p/d orbitals)
  - Suppressed phonon scattering
  - Large Fermi velocity



Wang*, Varnavides*, et al., (2021), ArXiv: 2109.00550

Current Density Imaging Measurements

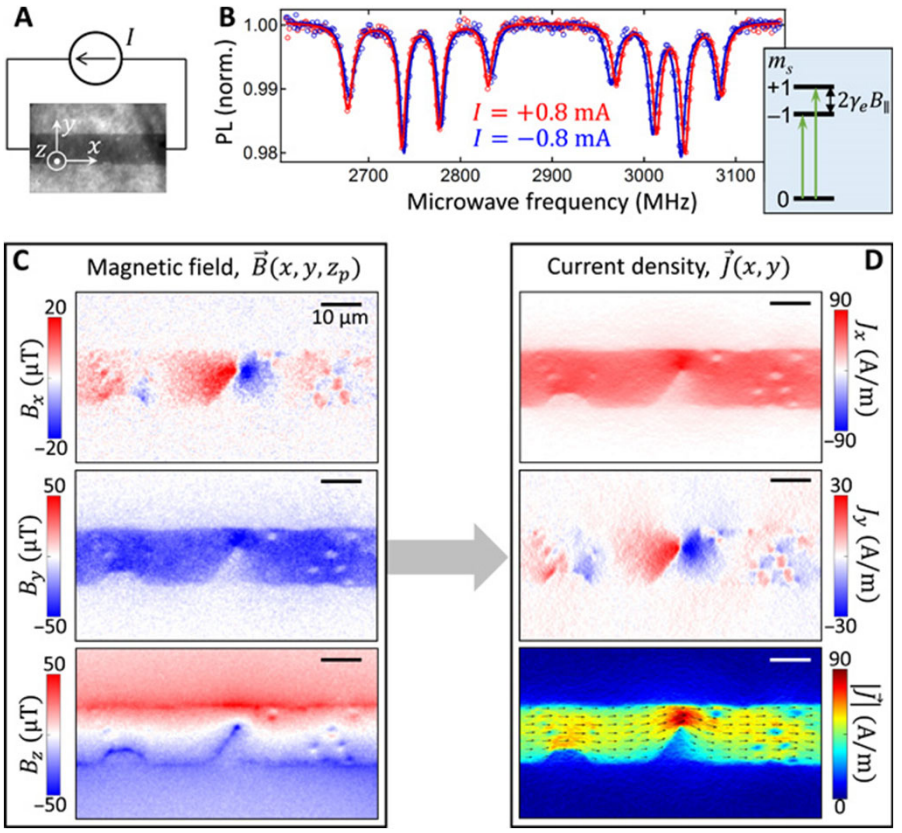
- Scanning SQUID microscopy
  - Measures induced magnetic flux
- Scanning CNT electron transistor
  - Measures Hall voltage (field)
- Nitrogen-vacancy magnetometry
  - Measures induced magnetic field
- Limitations:
  - Require specialized equipment
    - Limiting field's development
  - Limited spatial resolution (~80 nm)
    - Hard to correlate w/ structure



Courtesy: Ryan and Peter Allen, Second Bay Studios

Imaging Current Flows Around Defects

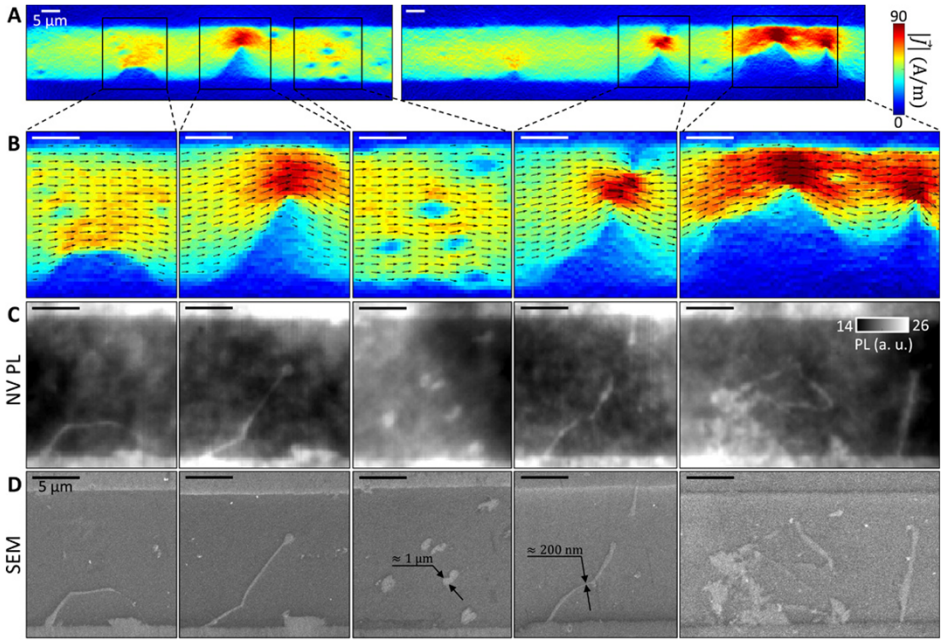
- Nitrogen-Vacancy magnetometry platform
  - 2D layer of near-surface NVs
- Used to image induced magnetic fields and reconstruct current density



Tetienne et al., (2017) **Sci. Adv**. 3: e1602429

Imaging Current Flows Around Defects

- Nitrogen-Vacancy magnetometry platform
  - 2D layer of near-surface NVs
- Used to image induced magnetic fields and reconstruct current density
- Correlated current irregularities around graphene “tears” using photoluminesce (PL) and SEM



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Predicting And Probing Carrier Interactions In Quantum Matter Using Electron Hydrodynamics

Prineha Narang

School on Quantum Materials | July 2022

NARANGLAB

Contact me for Ph.D & Postdoctoral Positions!