

Electron-Phonon Interaction

From a Symmetry Point of View

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October 12, 2026

Summary

1 Introduction

- Electron-Phonon Coupling
- Selection Rules
- Computational Validation with QE

2 Methodology

- Wigner-Mackey Little Group
- Projective Representation and Factor System
- Spin-Orbit Coupling

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Electron-Phonon Coupling

$|\psi_{n\mathbf{k}}\rangle$: Electronic Bloch state.

$\hat{V}_{\mathbf{v}\mathbf{q}}$: Phonon-induced perturbation for mode $(\mathbf{v}, \mathbf{q})$.

Electron–phonon scattering matrix element:

$$g_{mn\mathbf{v}}(\mathbf{k}, \mathbf{q}) = \langle \psi_{m\mathbf{k}+\mathbf{q}} | \hat{V}_{\mathbf{v}\mathbf{q}} | \psi_{n\mathbf{k}} \rangle. \quad (1)$$

Motivation: Eq. (1) governs charge and heat transport.

Main Result: I developed *spGroup* to identify symmetry-forbidden electron–phonon scattering channels at arbitrary momenta.

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Selection Rules

G : Space group (without SOC).

$\therefore g_{mn\nu}$ affords a representation of some symmetry.

$\therefore$ Symmetry can force $g_{mn\nu}(\mathbf{k}, \mathbf{q}) = 0$. Such scattering channels are **symmetry-forbidden**.

We are interested in such cases because important processes such as intervalley scattering can be strongly constrained by symmetry.

$G_{\mathbf{k}} := \text{Stab}_G(\mathbf{k})$: Stabilizer subgroup at $\mathbf{k}$, known as "little group".

The common symmetry group of the scattering process is

$$H_{\mathbf{k},\mathbf{q}} := G_{\mathbf{k}+\mathbf{q}} \cap G_{\mathbf{k}} \cap G_{\mathbf{q}}. \quad (2)$$

The three states form a tensor-product representation of $H_{\mathbf{k},\mathbf{q}}$, ie.

$$g_{mnv}(\bullet, \bullet) \in \text{Hom}_{H_{\mathbf{k},\mathbf{q}}}(V_{m\mathbf{k}+\mathbf{q}}^{\vee} \otimes V_{v\mathbf{q}} \otimes V_{n\mathbf{k}}, \mathbb{C}). \quad (3)$$

The scattering channel is allowed iff the trivial representation occurs:

$$\begin{aligned} a_1 &:= \dim_{\mathbb{C}} \text{Hom}_{H_{\mathbf{k},\mathbf{q}}} (V_{m\mathbf{k}+\mathbf{q}}^{\vee} \otimes V_{\nu\mathbf{q}} \otimes V_{n\mathbf{k}}, \mathbb{C}) \\ &\begin{cases} \geq 1, & \text{Symmetry-allowed} \\ = 0, & \text{Symmetry-forbidden} \end{cases} . \end{aligned} \quad (4)$$

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Computational Validation with QE

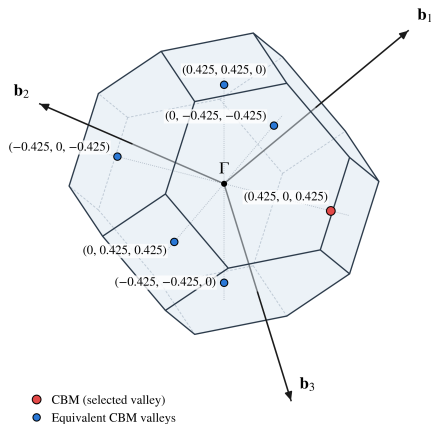


Figure: The first Brillouin zone and CBM of Si

We performed non-SOC ab-initio calculations of

Si (#227, $Fd\bar{3}m$)

using QE, locating the conduction-band minimum (CBM) at

$$\mathbf{k} = (0.425, 0.425, 0)$$

and showing all possible process channels of CBM intervalley scattering.

Process	$\mathbf{k}_i$	$\mathbf{q}$	$\mathbf{k}_f$	Mult.	Forbidden/Total
f	(0.425, 0, 0.425)	($\overline{0.425}, \overline{0.425}, 0.150$)	($0, \overline{0.425}, \overline{0.425}$)	4	2/4 (50%)
g	(0.425, 0, 0.425)	(0.150, 0, 0.150)	($\overline{0.425}, 0, \overline{0.425}$)	1	4/5 (80%)

$$\bullet \overline{0.425} \equiv -0.425$$

Process	Initial irrep (dim.)	Phonon irrep (dim.)	Final irrep (dim.)	a_1	Phonon branch(es)
f	$\Delta_1(A_1)$ (1)	$\Sigma_3(B_2)$ (1)	$\Delta_4(B_2)$ (1)	0	169.9 cm ⁻¹ (TA), 390.0 cm ⁻¹ (TA)
f	$\Delta_1(A_1)$ (1)	$\Sigma_2(A_2)$ (1)	$\Delta_4(B_2)$ (1)	0	461.0 cm ⁻¹ (LO)
f	$\Delta_1(A_1)$ (1)	$\Sigma_4(B_1)$ (1)	$\Delta_4(B_2)$ (1)	1	144.4 cm ⁻¹ (LA)
f	$\Delta_1(A_1)$ (1)	$\Sigma_1(A_1)$ (1)	$\Delta_4(B_2)$ (1)	1	387.7 cm ⁻¹ (TO), 470.9 cm ⁻¹ (TO)
g	$\Delta_1(A_1)$ (1)	$\Delta_4(B_2)$ (1)	$\Delta_4(B_2)$ (1)	1	507.5 cm ⁻¹ (LO)
g	$\Delta_1(A_1)$ (1)	$\Delta_3(B_1)$ (1)	$\Delta_4(B_2)$ (1)	0	not realized
g	$\Delta_1(A_1)$ (1)	$\Delta_5(E)$ (2)	$\Delta_4(B_2)$ (1)	0	85.2 cm ⁻¹ (TA), 496.7 cm ⁻¹ (TO)
g	$\Delta_1(A_1)$ (1)	$\Delta_1(A_1)$ (1)	$\Delta_4(B_2)$ (1)	0	150.9 cm ⁻¹ (LA)
g	$\Delta_1(A_1)$ (1)	$\Delta_2(A_2)$ (1)	$\Delta_4(B_2)$ (1)	0	not realized

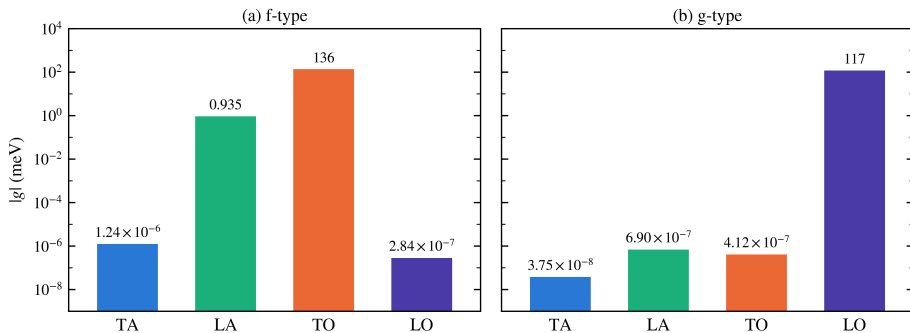


Figure: The electron-phonon CBM intervalley scattering rate by EPW and QE

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Wigner-Mackey Little Group

Bottleneck: G is infinite, so finite-group methods cannot be applied directly.

Wigner-Mackey method: For a space group, short exact sequence

$$0 \rightarrow L \rightarrow G \rightarrow P \rightarrow 1 \quad (5)$$

describes the extension of point group P by lattice L , with action on dual lattice $P \curvearrowright \hat{L} = \text{Hom}(L, \text{U}(1))$.

Prototype: Wigner used the same idea to classify relativistic one-particle states through representations of the Poincaré group

$$\mathcal{P}_+^\uparrow = \mathbb{R}^{1,3} \rtimes \text{SO}^+(1,3). \quad (6)$$

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Projective Representation and Factor System

Short exact sequence

$$0 \rightarrow L \rightarrow G_{\mathbf{k}} \rightarrow P_{\mathbf{k}} \rightarrow 1. \quad (7)$$

Correspondence

$$\text{Irr}_{\mathbf{k}}(G_{\mathbf{k}}) \leftrightarrow \text{PIrr}_{\omega_{\mathbf{k}}}(P_{\mathbf{k}}). \quad (8)$$

The extension in Eq. (7), together with the translation character at $\mathbf{k}$, induces

$$[\omega_{\mathbf{k}}] \in H^2(P_{\mathbf{k}}, \text{U}(1)). \quad (9)$$

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Spin-Orbit Coupling

Spin- $\frac{1}{2}$ states transform under the double cover

$$0 \rightarrow \mathbb{Z}_2 \rightarrow \mathrm{SU}(2) \rightarrow \mathrm{SO}(3) \rightarrow 1. \quad (10)$$

Therefore, when it comes to SOC we need to add one more factor system contributed by spin.

By $H^2(\mathrm{SO}(3), \mathrm{U}(1)) = \mathbb{Z}_2 = \{1, [\omega_{\mathrm{spin}}]\}$:

- Trivial class: single-valued representations;
- Nontrivial class: **double-valued (spinorial) representations**, one more factor system.

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