ELECTRON-PHONON SCATTERING
IN TOPOLOGICAL INSULATORS

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Motivation

- What limits the surface conductivity and the integrity of surface quasi-particles?
- Large static dielectric constant ($\epsilon \approx 50$ to 200) $\rightarrow$ drastic reduction of direct Coulomb interaction or charged impurity potentials.
- Consequences of the electron-phonon coupling on the TI surface state?
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Outline

- Model Hamiltonian for the surface state coupled to phonons
- Quasi-particle decay rate
- Surface resistivity
Effective model for surface electronic states

- Effective model Hamiltonian to describe the bulk of 3D TI – Bi$_2$Te$_3$ or Bi$_2$Se$_3$. Bulk gap: $\Delta_b \simeq 0.3$ eV, proposed by Zhang *et al.*, *Nat. Phys.* 5, 438 (2009).

- For a semi-infinite setup $z > 0$, with Dirichlet boundary condition at $z = 0$, the surface-state wave function is:

- Projection of the bulk Hamiltonian onto the surface state

\[ H_e = \sum_{k,s=\pm} \epsilon_{ks} c^\dagger_{ks} c_{ks}, \quad \epsilon_{ks} = s v_F |k| - \mu, \]

where $v_F \simeq 4.36 \times 10^5$ m/s and $k = (k_x, k_y)$ is the surface momentum. Helical operators $c_k = (c_{k+}, c_{k-})^T$ are connected to the usual spinful operators $d_k = (d_{k\uparrow}, d_{k\downarrow})^T$ by the unitary transformation:

\[ c_k = U_k d_k, \quad U_k = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\theta_k/2} & ie^{-i\theta_k/2} \\ e^{i\theta_k/2} & -ie^{-i\theta_k/2} \end{pmatrix}, \quad \tan \theta_k = k_y/k_x. \]
Effective model for surface electronic states

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  \[ \chi(z) \simeq 1.86 \text{ nm}, \text{ for Bi}_2\text{Te}_3 \]

  Liu et al., Phys. Rev. B 82, 045122 (2010)

- Projection of the bulk Hamiltonian onto the surface state

  $\Rightarrow$ massless 2D Dirac Hamiltonian:

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Acoustic phonon modes in a half space

- Isotropic elastic continuum theory for the displacement field $u$:
  \[ \frac{\partial^2 u}{\partial t^2} = c_i^2 \triangle u + (c_i^2 - c_t^2) \text{grad div } u, \quad c_i \simeq 2800 \text{ m/s}, \quad c_t \simeq 1600 \text{ m/s} \]
  in the half-space $z > 0$ with stress free boundary condition at $z = 0$.

- 4 types of phonon modes labeled by surface momentum $\mathbf{q} = (q_x, q_y)$ and frequency $\Omega$:
  - horizontal shear mode ($\lambda = H$): $\perp \mathbf{q}$ and $e_z \rightarrow$ divergence-free
  - longitudinal mode ($\lambda = L$): extended state, $\Omega > c_i q$.
  - transverse mode ($\lambda = T$): extended state, $\Omega > c_t q$.
  - Rayleigh surface wave ($\lambda = R$): localized state, $\Omega = c_R q$, $c_R \simeq 0.92 c_t$.

- Noninteracting phonon Hamiltonian:
  \[ H_p = \sum_{\Lambda} \Omega_{\Lambda} (b_{\Lambda}^\dagger b_{\Lambda} + 1/2). \]
  where $\Lambda = (\lambda, \mathbf{q}, \Omega)$ and $b_{\Lambda}$ is a bosonic operator.
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Electron-phonon coupling

- The electron-phonon coupling is dominated by the deformation potential:

\[ H_{ep} = \alpha \int d\mathbf{r} \, n(\mathbf{r}) \, \text{div} \, U(\mathbf{r}), \]

where \( n(\mathbf{r}) \) is the local electron density.

For \( \text{Bi}_2\text{Te}_3 \), \( \alpha \simeq 35 \text{ eV} \). Huang and Kaviany, \textit{PRB} 77, 125209 (2008) strong coupling constant!

- In the second quantized formalism:

\[ H_{ep} = \frac{\alpha}{\sqrt{A}} \sum_{\lambda q\Omega} M_{q\Omega}^{(\lambda)} \sum_{k,\sigma=\uparrow,\downarrow} d_{k+q,\sigma}^\dagger d_{k\sigma} b_{\lambda q\Omega} + \text{h.c.}, \]

where \( \lambda = L, T, R \) only, the coupling matrix elements \( M_{q\Omega}^{(\lambda)} \) may be calculated analytically and \( d_{k\sigma} \) has to be expressed in function of helical operators \( c_{k\sigma} \).

- Total Hamiltonian: \( H = H_e + H_p + H_{ep} \).

- For the numerics, published values for \( \text{Bi}_2\text{Te}_3 \). No free parameters!
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Quasi-particle decay rate – lifetime broadening measurable by ARPES!

- To lowest order in $H_{ep}$, the self-energy for a helical state $s = \pm$ is:

$$\Sigma_s(k, \omega) = \lambda, q, \Omega_s \pm \lambda, 0, 0$$

- The contribution from mode $\lambda$ to the decay rate $\Gamma^{(\lambda)}$ may be written as:

$$\Gamma^{(\lambda)}(k, \omega) = \sum_{\nu = \pm} \alpha^2 \int_0^\infty d\Omega \; F^{(\lambda \nu)}_{ks, \omega}(\Omega) \left[ n_B(\Omega) + n_F(\Omega + \nu \omega) \right]$$

where $F^{(\lambda \nu)}_{ks, \omega}(\Omega)$ is the Eliashberg function.

- On-the-shell $\omega = \epsilon_{ks}$

- $\mu = 0.05$ eV
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Quasi-particle decay rate – lifetime broadening

\[ T_{BG} = 2k_F c_R / k_B = 3.9 \text{ K} \]

\[ \sim \text{ maximal phonon momentum is } 2k_F \]

\[ \mu = 0.05 \text{ eV, } T_F = 580 \text{ K} \]
Quasi-particle decay rate – lifetime broadening

\[ \Gamma_k(T) = \frac{28\zeta(3)C}{\pi} \frac{\alpha^2 c_R k_F^3}{\rho_M v_F c_l^4} \left( \frac{T}{T_{BG}} \right)^3 \]

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\[ \lambda = R + L + T \]
\[ \lambda = R \]
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Quasi-particle decay rate – lifetime broadening

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For \( T = 0 \), \( \Gamma_k \sim |k - k_F|^3 \)

\[ \mu = 0.05 \text{ eV}, \ T_F = 580 \text{ K} \]
Phonon contribution to the surface resistivity

► Quasiclassical Boltzmann transport theory as employed for graphene:

\[ \rho = \frac{2}{e^2 v_F^2 D(\mu)} \frac{1}{\langle \tau \rangle}, \quad \langle \tau \rangle = \frac{\int d\epsilon (-\partial_\epsilon n_F) D(\mu + \epsilon) \tau(\epsilon)}{\int d\epsilon (-\partial_\epsilon n_F) D(\mu + \epsilon)}, \]

with \( D(E) = |E|/(2\pi v_F^2) \) the density of states.

→ valid for \( G_Q\rho \ll 1 \) (\( G_Q = e^2/h \)), i.e. \( |\mu|\langle \tau \rangle \gg 1 \).

► The inverse of the electron-phonon transport scattering time \( 1/\tau(\epsilon) \) is obtained by the Fermi’s golden rule as a sum over independent phonon mode contributions, with a “transport” Eliashberg function:

\[ \frac{1}{\tau(\epsilon_{ks})} = \sum_{\lambda,\nu = \pm} \alpha^2 \int_0^\infty d\Omega \mathcal{F}_{ks}^{(\lambda \nu)}(\Omega) \nu n_B(\nu \Omega) \frac{1 - n_F(\epsilon_{ks} + \nu \Omega)}{1 - n_F(\epsilon_{ks})}. \]
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Phonon contribution to the surface resistivity

\[ \rho (\Omega) \]

\[ T (K) \]

\[ \lambda = R \]
\[ \lambda = L \]
\[ \lambda = T \]
\[ \lambda = R + L + T \]

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Phonon contribution to the surface resistivity

\[ \rho = \frac{1488 \zeta(5) C}{\pi} \frac{\alpha^2 c_R^3 k_F^2}{\rho_M v_F^2 c_i^4} \left( \frac{T}{T_{BG}} \right)^5 \frac{h}{e^2} \]

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Phonon contribution to the surface resistivity

\[ \rho \sim T^5 \]

Graphene: \( \rho \sim T^4 \)
2D electron gas: \( \rho \sim T^7 \)
Bulk 3D metals: \( \rho \sim T^5 \)

\[
\rho = \frac{1488\zeta(5) C}{\pi} \frac{\alpha^2 c^3 R k^2_F}{\rho_M v_F^2 c^4_l} \left( \frac{T}{T_{BG}} \right)^5 \frac{h}{e^2}
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Conclusion and outlook

- Analytically tractable low-energy theory of the surface state in TI coupled to phonons.

- Temperature dependent contribution of phonons to the decay rate and surface resistivity.

- Physics near the Dirac point? Superconducting instabilities?