Unconventional quasiparticle scattering in disordered 2D TMDs

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Mathematical Modeling of 2D materials
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Atomic disorder in 2D TMDs

S vacancy

Komsa et al., PRL 109, 035503 (2012)

Mo vs S vacancies?

Lin et al., Nature Communications 6, 6736 (2014)
Scanning tunneling spectroscopy (WSe$_2$)

Yankowitz et al., PRL 115, 136803 (2015)

Liu et al., Nature Comm. 6, 8180 (2015)

They argue that they don't tunnel into the states at K, K', and therefore don't consider scattering between them.
FT of the LDOS: \[ A(r) = -1/\pi \text{Im} G(r, r; \varepsilon) \]

\[ A(q + G, \varepsilon) = \int dr \, e^{-i(q + G) \cdot r} A(r) \]

\[ = -\frac{1}{2\pi i} \sum_{mn} \sum_k n_{k, q}^{mn}(G) \times \left[ G_{k, k+q}^{mn}(\varepsilon) - G_{k+q, k}^{mn}(\varepsilon)^* \right] \]

Single-impurity Green’s function:

\[ G_{kk'}(\varepsilon) = \delta_{k, k'} G_k^0(\varepsilon) + G_k^0(\varepsilon) T_{kk'}(\varepsilon) G_{k'}^0(\varepsilon) \]

JDOS:

\[ A_{\text{JDOS}}(q, \varepsilon) \propto \sum_k A_0(k, \varepsilon) A_0(k + q, \varepsilon) \]

\[ A_0(k, \varepsilon) \propto \text{Im} \left[ \text{Tr} \{ G_k^0(\varepsilon) \} \right] \]
Disorder $T$ matrix

$$T_{kk'}(\varepsilon) = V_{kk'} + \sum_{k''} V_{kk''} G_{k''}(\varepsilon) T_{k''k'}(\varepsilon)$$

Ingredients:

- band structure:
  $$G_0^{\sigma n}(k, \varepsilon) = [\varepsilon - \varepsilon_{\sigma n}(k) + i\eta]^{-1}$$
- disorder matrix elements (next slide)

$N \times N$ BZ sampling $\rightarrow N^2 \times N^2$ matrices:

$$T(\varepsilon) = [1 - V G_0(\varepsilon)]^{-1} V$$

Take-home message
Don’t invert that matrix!
Atomistic supercell method

Scattering due to perturbations in the crystal potential:

\[ V^i_{kk'} = \langle k | V^i(r) | k' \rangle \]

Disorder scattering potential:

\[ V^i(r) = V^i_{\text{dis}}(r) - V^i_{\text{pris}}(r) \]

Atomic disorder (substitutional, vacancies, etc), impurities, phonons:

- Disorder potential \( V^i \) and Bloch functions calculated with DFT-LDA (PAW).
- Momentum conservation: \( k' \rightarrow k + q \).
Atomic monovacancies (MoS$_2$)

Mo vacancy:  \[ V_{kk'}^i = \langle k | V_i(r) | k' \rangle \]

\[ V_i(r) = V_0 \delta(r - R_i) \]
\[ \rightarrow V_{kk'}^i = V_0 \]
FT-STS: Mo vacancy

\[ \varepsilon = 5 \text{ meV} \]

\[ q_x (2\pi / a) \]

\[ q_y (2\pi / a) \]
FT-STS: Mo vacancy

\[ \varepsilon = 30 \text{ meV} \]

\( q_y (2\pi/a) \)

\( q_x (2\pi/a) \)

\( k_y \)

\( k_x \)
FT-STS: Mo vacancy

\( \varepsilon = 60 \text{ meV} \)

\( q = 2k \)
FT-STS: Mo vacancy

\[ \varepsilon = 225 \text{ meV} \]
FT-STS: S vacancy

$\varepsilon = 5 \text{ meV}$
FT-STS: S vacancy

\[ \varepsilon = 30 \text{ meV} \]
FT-STS: S vacancy

\[ \varepsilon = 60 \text{ meV} \]

Diagram 1: 
- A hexagonal Brillouin zone
- Two-dimensional momentum space
- Wave vector \( q_1 \)

Diagram 2: 
- Surface state dispersion
- Label \( q_1 \)
\section*{Selection rule: \( C_3 \) symmetry}

\begin{equation*}
\langle n_\tau | V_i | n_\tau' \rangle = \langle n_\tau | C_3^+ V_i C_3 | n_\tau' \rangle \equiv \gamma_{i,c} \langle n_\tau | V_i | n_\tau' \rangle
\end{equation*}

- \( \gamma_{i,c} = 1 \) for Mo centered disorder
- \( \gamma_{i,c} \neq 1 \) for S centered disorder

\( C_3 \) symmetry:

\( \langle n_\tau | V_i | n_\tau' \rangle = \langle n_\tau | C_3^+ V_i C_3 | n_\tau' \rangle \equiv \gamma_{i,c} \langle n_\tau | V_i | n_\tau' \rangle \)
FT-STS: S vacancy

\[ \varepsilon = 225 \text{ meV} \]
Midgap states

Gated TMDs

<table>
<thead>
<tr>
<th>$V_g = 0$</th>
<th>$V_g &gt; 0$</th>
<th>$V_g &gt;&gt; 0$</th>
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</thead>
<tbody>
<tr>
<td>Conduction band</td>
<td></td>
<td></td>
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<tr>
<td>Valence band</td>
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</tbody>
</table>

- Mo vacancy
- S vacancy

![DOS plots for Mo vacancy and S vacancy](Image)

![Gated TMDs](Image)
Summary

• FT-STS provides a unique fingerprint of vacancy type and their scattering properties.

• Symmetry-induced suppression ($C_3$) of intervalley scattering in addition to spin-valley coupling.

• Long valley lifetimes even in disordered TMDs.

• FT-STS useful tool for resolving band-structure issues (K vs Q valley ordering) in mono- and multilayer systems.

• Further STS studies on TMD systems.

• Impact of atomic vacancies on transport in TMDs.