Topology of SmB$_6$ determined by DFT+DMFT

based on arXiv:1907.03899

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ERC workshop, Zoom, 8/5-2020
Outline

• Motivation
  - SmB$_6$ a strongly correlated topological insulator?
  - Experimental
    - Surface bands, but trivial or not?
  - Theoretical
    - Multiplet derived bands with fractional weights
    - Pole Expanded vs "Topological" Hamiltonian

• Theory and results
  - DFT + Dynamical Mean Field Theory
    - Nice agreement ⇒ Enough with a local self-energy
      - Topology
        - Pole Expanded Hamiltonian
        - Symmetry analysis
        - Pole Expanded Hamiltonian vs "Topological" Hamiltonian

• Summary and conclusion
Motivation

• Experimental motivation
  - Huge body of work, driven by the theoretical model prediction by [1]
  - Transport: insulating bulk but conducting surface states [2]
  - ARPES: Metallic surface bands, but trivial or not?
    - Even number of Fermi surface pockets? [3]
    - Rachba + Umklapp? [4]

Motivation

- Theoretical motivation

- Topological invariant $Z_2$ [1,2] is fundamentally connected to an effective $H_k$
  - Inversion and time-rev.: Count occupied bands and their parity at the TRIM points
- SmB$_6$ has multiplet derived bands with fractional weights
  - Bands can smear out or gradually disappear and reappear with shifted energy
  - How to even count the bands?

Theory and Results

- **DFT + Dynamical Mean Field Theory**
  - Sm 4f strongly correlated ($U = 8$, large $F_2$, $F_4$, and $F_6$ slater parameters)
  - Include spin-orbit, crystal fields, and a few bath states (hybridization)
  - Exact diagonalization impurity solver
  - Temperature: 100 K
  - Intermediate valence ground state: $N_f = 5.48$, Eigenstates $\Gamma_1$ and $\Gamma_8$ [1]

![Graph](image)

<table>
<thead>
<tr>
<th>Sym.</th>
<th>$N_f$</th>
<th>$E$ (eV)</th>
<th>Weight</th>
<th>$S_l[\rho]$</th>
<th>$J$</th>
<th>$L$</th>
<th>$S$</th>
<th>$J_z$</th>
<th>$L_z$</th>
<th>$S_z$</th>
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<tbody>
<tr>
<td>$\Gamma^+_1$</td>
<td>6.002</td>
<td>0.000</td>
<td>0.46</td>
<td>3.0</td>
<td>0.06</td>
<td>2.95</td>
<td>2.94</td>
<td>0.00</td>
<td>0.00</td>
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</tr>
<tr>
<td>$\Gamma^-_8$</td>
<td>5.016</td>
<td>0.012</td>
<td>0.12</td>
<td>1.9</td>
<td>2.52</td>
<td>4.95</td>
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<td>0.48</td>
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<td>-3.17</td>
<td>1.35</td>
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<tr>
<td>$\Gamma^-_7$</td>
<td>5.018</td>
<td>0.024</td>
<td>0.03</td>
<td>2.5</td>
<td>2.53</td>
<td>4.94</td>
<td>2.46</td>
<td>0.78</td>
<td>1.11</td>
<td>-0.33</td>
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<td>1.02</td>
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Theory and Results

• Take home message: DFT+DMFT work well! (local self-energy)
• For more details: arXiv:1907.03899
Theory and Results

• Topology outline
  - The Pole Expansion Hamiltonian!\([1,2]\) \(H_{\text{PE}}\)
  - Rigorous starting point, an effective Hamiltonian that fully captures \(G_k(v)\)
  - Based on
    - The pole expansion of the self-energy \(\Sigma_k\) (Pedagogical intro: \texttt{arXiv:1907.03899})
    - A mathematical identity for projections of Green's functions

\[
\Sigma(z) = \Sigma(\infty) + \Sigma_V \left[ z \mathbb{1} - \Sigma_E \right]^{-1} \Sigma_V^\dagger
\]

Theory and Results

- Topology
  - The dynamical term of $\Sigma(z)$ has the form of a hybridization function [1]
    \[
    \Sigma_k(z) = \Sigma_k(\infty) + \Sigma_{V_k} \left[ z \mathbf{1} - \Sigma_{E_k} \right]^{-1} \Sigma_{V_k}^{\dagger} \quad \Delta(z) = V \left[ z \mathbf{1} - E \right]^{-1} V^{\dagger}
    \]
  - Poles of the self-energy equivalent to auxiliary orbitals
  - Matrix form of the Green's function

\[
G_k(z) = \left( \begin{array}{ccc}
z \mathbf{1} & -H_k & \Sigma_{V_k} \\
+\Sigma_k(\infty) & \mathbf{1} & \mathbf{0} \\
\mathbf{0} & \mathbf{0} & \mathbf{1}
\end{array} \right)^{-1}
\]

Theory and Results

- Well-known matrix identity

\[ G_k(z) = \begin{bmatrix} z1 & -H_k + \Sigma_k(\infty) & \Sigma_{Vk} \\ \Sigma_{Ek} & -1 \\ \Sigma_{Vk} \end{bmatrix} \]

\[ = \begin{bmatrix} 1 & 0 \\ \Sigma_{Vk} & \Sigma_{Ek} \end{bmatrix} \]
Theory and Results

• Pole expanded Hamiltonian
  - Poles of the self-energy corresponds to auxiliary orbitals
  - Full Green's function reproduced by projecting upon the physical orbitals
    - All bands in $G_k(v)$ corresponds to eigenstates of $H^{PE}$
    - The *projection* reduces their weight in the spectral function
  - Topological surface states in $G_k \Leftrightarrow$ topological surface states from $H^{PE}$

$$H^{PE}_k = H_k + \Sigma_k(\infty) + \Sigma_{V_k} + \Sigma_{V_k}^\dagger + \Sigma_{E_k}$$
Theory and Results

• $Z_2$ well-defined on $H^{PE}$ [1]
• **Problem**: $\Sigma_{V_k}$ and $\Sigma_{E_k}$ are difficult (but not impossible) to obtain in practice!
• Can we be clever?
  - Symmetries
  - The self-energy of DMFT is local

\[ H^\text{PE}_k = H_k + \Sigma(\infty) + \Sigma_V \]

Theory and Results

- The self-energy has no poles in the bulk band gap
  - zero valued eigenstates of $H_{PE}$ has to have a finite physical weight
  - Bulk spectral function shows a band gap $\Rightarrow H_{PE}$ is gapped!

$$H_{PE} = H_k + \Sigma(\infty)$$

$$\Sigma_V$$

$$\Sigma_V^\dagger$$

$$\Sigma_E \neq 0$$
Theory and Results

- Two local orbitals will only hybridize if they share the same irreducible repr.
  - The auxiliary orbitals will transform as the Sm 4f orbitals.
  - Odd parity at the TRIM points!

- Enough to count the *non-interacting* bands in the *even* parity channel
  - Close to the DFT starting point. Odd number = **NON-TRIVIAL**!

\[
\begin{array}{c|cc}
H_k & \Sigma(\infty) & 0 \\
\hline
0 & H_k & 0 \\
\hline
\Sigma V^\dagger & 0 & \Sigma E \\
\end{array}
\]

At TRIM points: \( H_k^{PE} = \)
Theory and Results

- Pole expanded Hamiltonian vs "Topological" Hamiltonian

\[ H_{k} + \sum_{k(\infty)} \delta H_{k} + \sum_{k(0)} \delta H_{k} \]

\[ \sum_{V_{k}} \]

\[ \sum_{E_{k}} \]

\[ H_{k} \]
Theory and Results

- Pole expanded Hamiltonian \( \text{vs} \) "Topological" Hamiltonian
  - Continuous interpolation between \( H^{PE} \) and \( H_k + \Sigma_k(0) \) plus auxiliary \( \Sigma_{Ek} \) without closing the band gap! (assuming \( \Sigma_k(0) < \infty \))
    \[ \Rightarrow \text{Topologically equivalent!} \]

- Topological Hamiltonian works iff the detached auxiliary orbitals gives \( Z_2 = 1 \)
  - Always OK for a local self-energy, but not for a non-local self-energy!

\[
\begin{align*}
H(\lambda) &= \lambda \\
H^{PE} &= H_{FF} + \Sigma(\infty) \\
& \quad H_{FA} \\
& \quad H_{AF} \\
& \quad H_{AA} \\
H^{T}(\lambda) + H_{AA} &= H_{FF} + \Sigma(0, \lambda) \\
& \quad 0 \\
& \quad 0 \\
& \quad H_{AA}
\end{align*}
\]
Summary

- DFT+DFMT[ED] does a good job for SmB\textsubscript{6}
  - Intermediate valence ground state at 100K
  - Gap in bulk
  - *Topological* spin-polarized surface states

- Topology rigorously defined using $H^\text{PE}$
  - Topological Hamiltonian $H_k + \Sigma_k(0)$ breaks for topologically non-trivial pole structures in $\Sigma_k(z)$
  - More details + explicit examples in arXiv:1907.03899