# Fermi Surfaces from Many-Body Ground States

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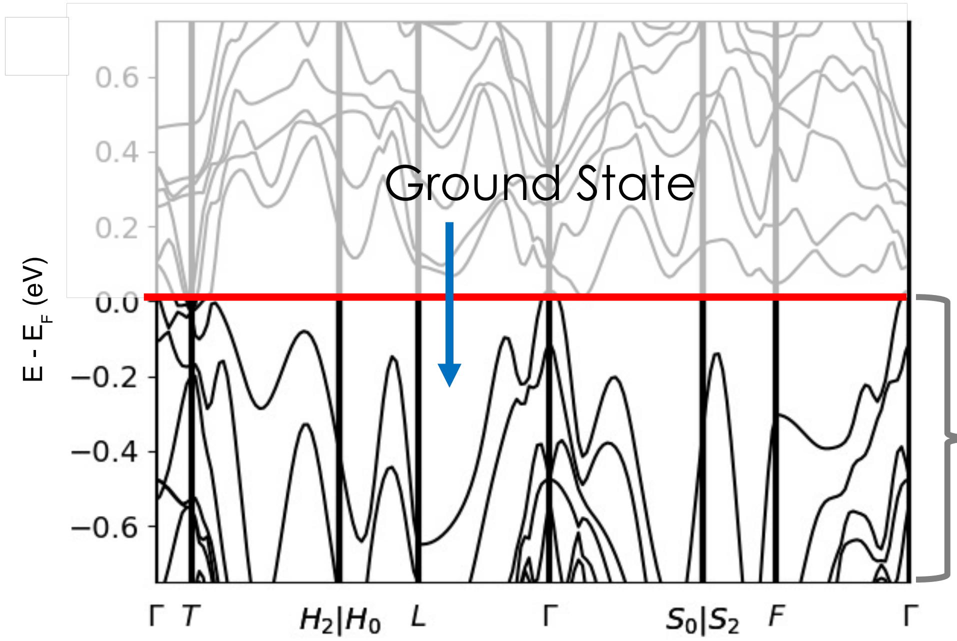
# Outline

- Formal connection between many body ground state and Fermi Surface
- Demonstration: $PdCoO_2$ delafossite Fermi Surface from quantum Monte Carlo and ARPES
- Future application domains

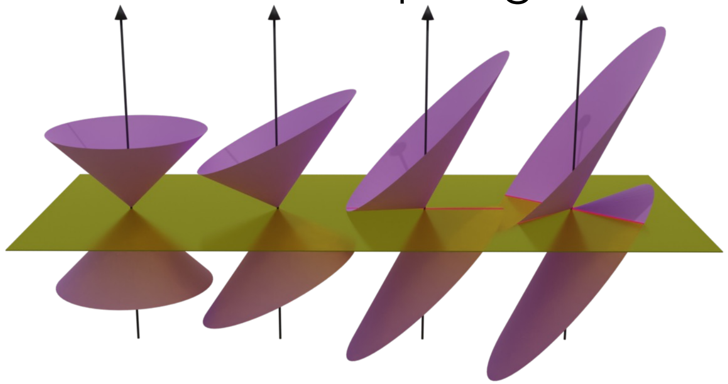
# The Fermi Surface and the Ground State Wavefunction

- Knowledge of Fermi surface is important for classification of many topological materials (relevant to DM, DSM, WSM, etc)
- Fermi surface is actually a ground state property
- But how to access it from the ground state?




$\Psi_0$

Fermi Surface and Topological States



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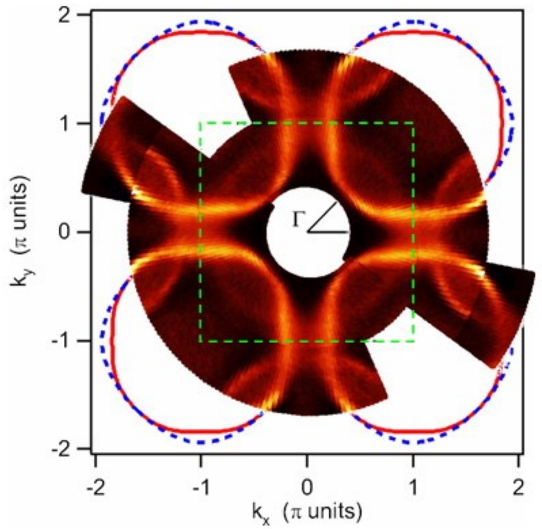
Fermi Surface from ARPES (BSCCO)

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# The Back-Folded Momentum Distribution: Mean Field

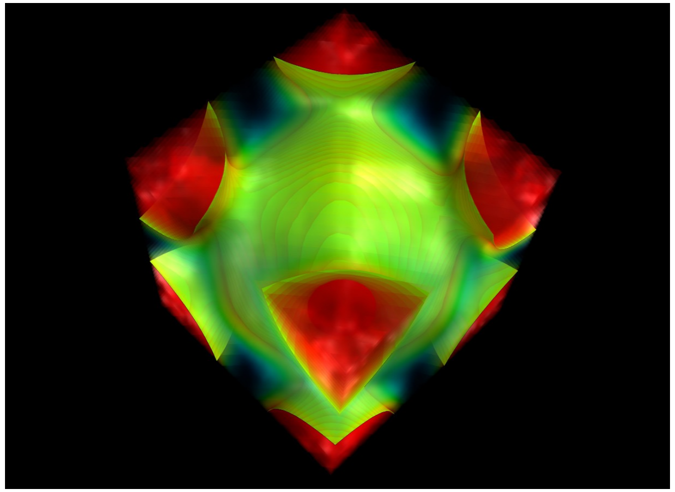
### Backfolding: Periodization in 1st BZ

$$n_b(k) = \sum_G n(k+G)$$

(Lock-Crisp-West procedure)

D. G. Lock *J. Phys. F: Met. Phys.* **3** 561 (1973)

### FS from Positron Annihilation (Cu)



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### Single Bloch Orbital Contribution to $n_b(k)$

$$\begin{aligned} n_{b\phi}(k) &= \sum_G n_\phi(k+G) \\ &= \sum_G |\phi(k+G)|^2 \\ &= \sum_{GG'} |\phi_{k_b+G'}|^2 \delta_{k+G,k_b+G'} \\ &= \sum_G |\phi_{k_b+G}|^2 \delta_{k,k_b} \quad \text{since} \quad k = k_b + G' \\ &= \delta_{k,k_b} \quad \text{since} \quad \sum_G |\phi_{k_b+G}|^2 = 1 \end{aligned}$$

- Much of the structure of the extended zone n(k) is removed via back-folding
- In particular, the k-space orbital structure is entirely erased, with each orbital collapsing to a single point in the 1st BZ
- Step discontinuities in $n_b(k)$ identify the FS

# The Back-Folded Momentum Distribution: Many Body

### 1RDM from Many Body Wavefunction

$$\hat{n}_1 = \int drdr'|r\rangle \int d\bar{R}\Psi(r,\bar{R})\Psi^*(r',\bar{R})\langle r|$$

### Bloch Natural Orbitals/Occupation Numbers

$$\hat{n}_1|\phi_{ik_b}\rangle = n_{ik_b}|\phi_{ik_b}\rangle$$

$$\hat{n}_1 = \sum_{ik_b}|\phi_{ik_b}\rangle n_{ik_b}\langle\phi_{ik_b}|$$

Non-integer with static/dynamic correlation

### Correlated Momentum Distribution

$$n(k) = \langle k|\hat{n}_1|k\rangle$$
$$= \sum_{ik_b} n_{ik_b}|\phi_{ik_b}(k)|^2$$

### Backfolded Correlated n(k)

$$n_b(k) = \sum_G n(k+G)$$
$$= \sum_{ik_b} n_{ik_b}\sum_G|\phi_{ik_b}(k+G)|^2$$
$$= \sum_{ik_b} n_{ik_b}\delta_{k,k_b}$$
$$= \sum_{k_b}\left(\sum_i n_{ik_b}\right)\delta_{k,k_b}$$

- $n_b(k)$ maps the distribution of electronic occupation throughout the 1st BZ (non-integer occupations)
- Insulators have ~uniform occupation
- Metals have steps in the occupation, generalizing the "band crossing the Fermi level" picture of the mean field
- The step locations fully define the Fermi surface
- Equally useful for simple and complex/topological metals

# Technical Issues: Trace Convergence

### QMC n(k) below cutoff due to cost

$$n(k) = \langle k|\hat{n}_1|k\rangle \quad k < k_{max}$$
$$n(k) = ? \quad k > k_{max}$$

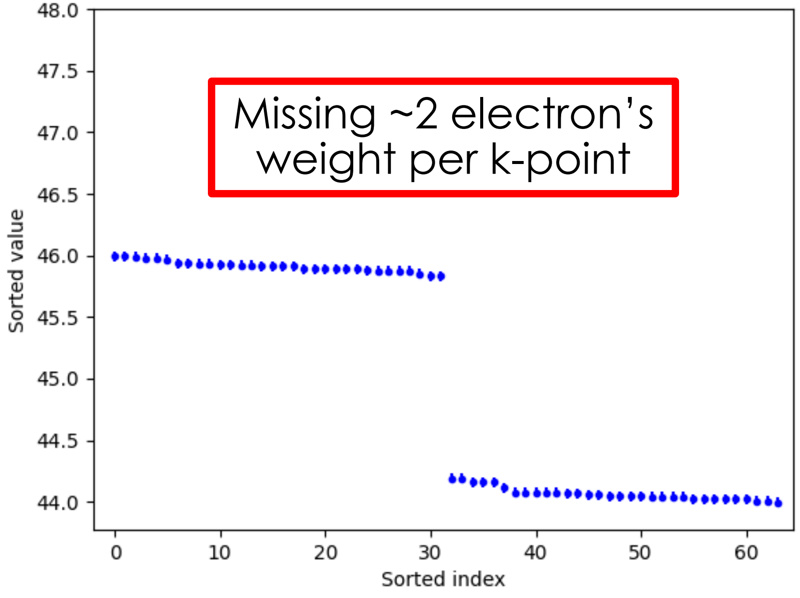
### How to extrapolate?

$$n(k) = n_{QMC}(k) \quad k < k_{max}$$
$$n(k) = n_{DFT}(k) \quad k > k_{max}$$

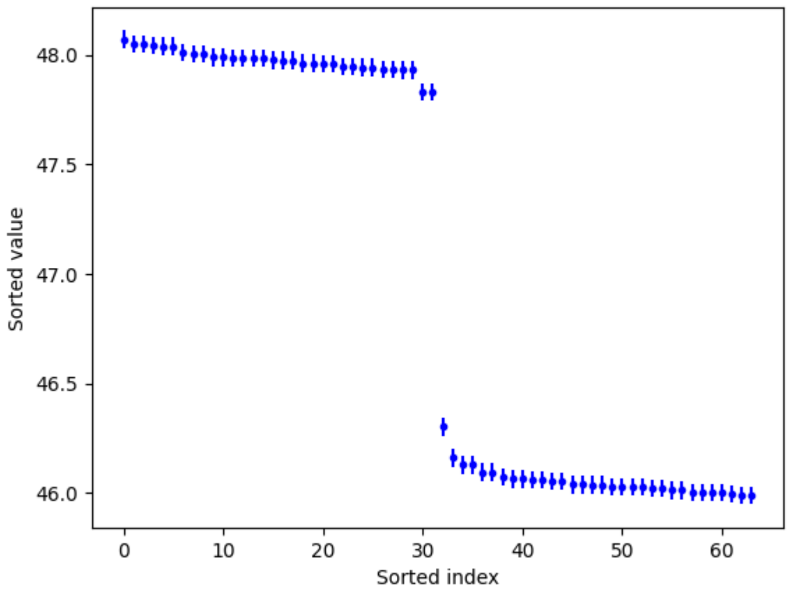
### Accelerating Convergence

$$n_b(k_b) = Tr_{k_b}(\hat{n}_1) \approx \sum_{i=0}^{M} \langle \phi_{ik_b}^{DFT}|\hat{n}_1|\phi_{ik_b}^{DFT}\rangle$$

### VMC n(k) with $k_{max}$ = 5.0

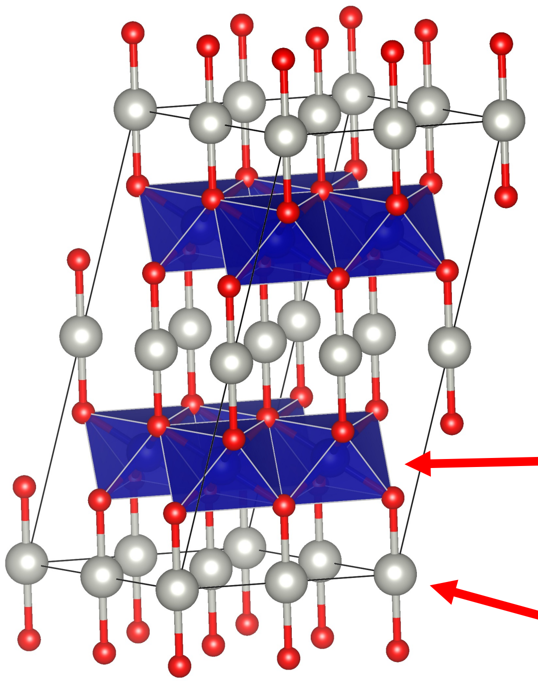



### VMC n(k) with DFT Asymptotics




- Perform trace in basis of DFT/etc Bloch states
- Convergence will be very rapid
- Perhaps only way forward for advanced wavefunctions when DFT asymptotics match poorly

# Application to Delafossites: $PdCoO_2$



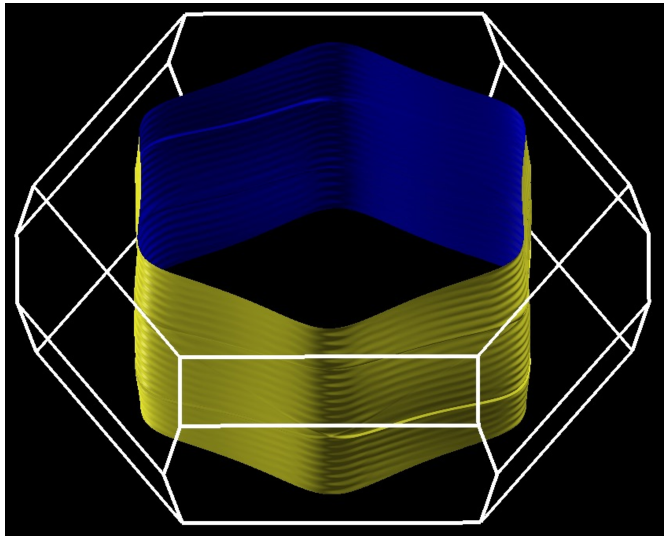
Mott insulating $CoO_2$ octahedral layer

Metallic triangular Pd lattice

**High conductivity quasi-2D metal**

- Highest in plane conductivity among oxides
- 1000x greater in plane vs out of plane conductivity

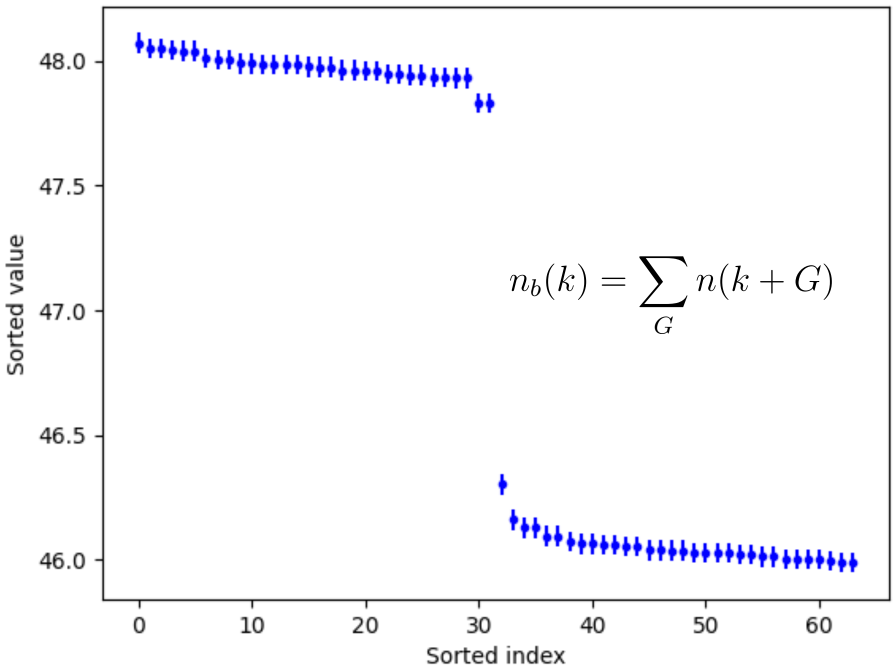
**Fermi Surface from DFT**

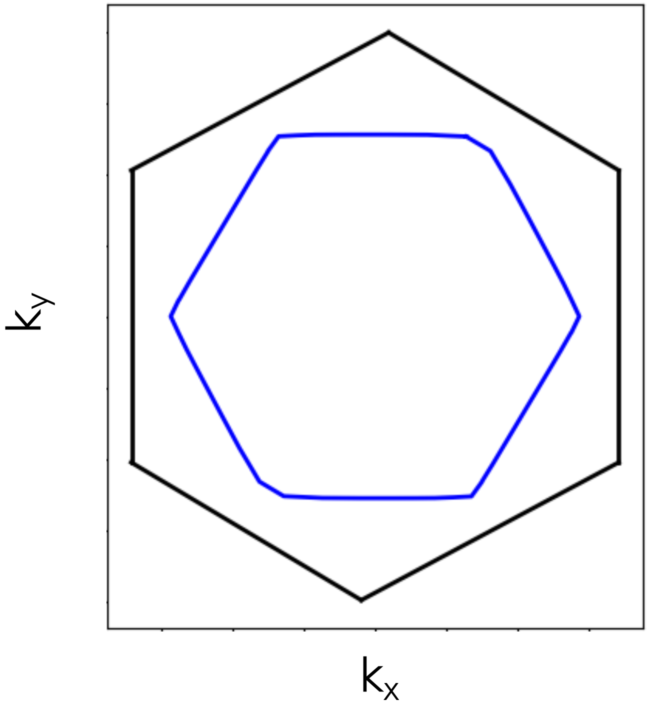


- Quasi-2D nature of metallic conduction in $PdCoO_2$ clearly evident in Fermi Surface
- $1^{st}$ Brillouin zone is essentially hexagonal, Fermi surface nearly hexagonal also
- Next: results from many body wavefunction and ARPES

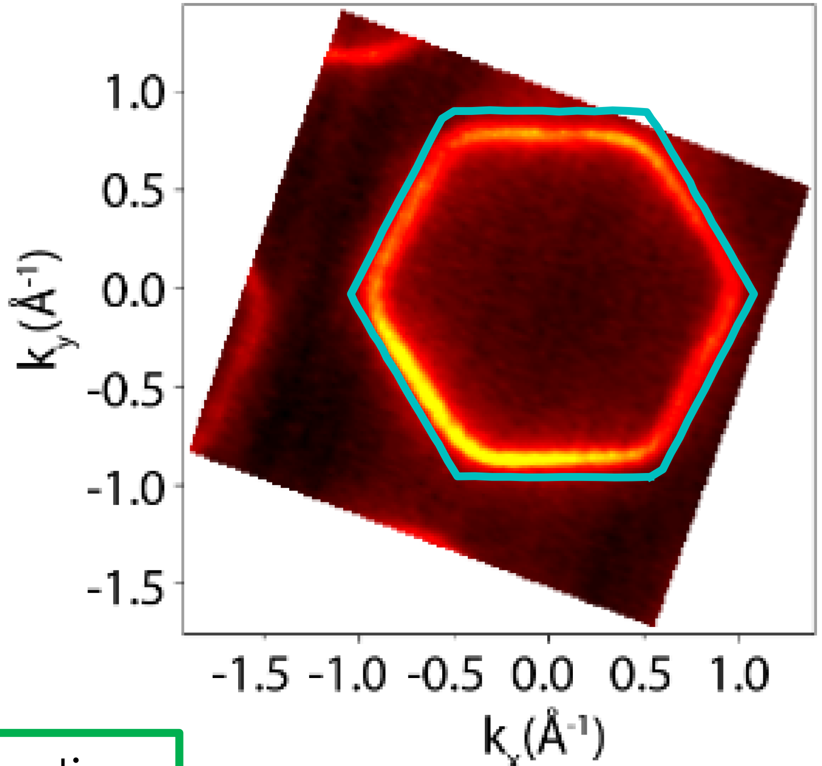
# Application to Delafossites: $PdCoO_2$ Theory and Experiment

## QMC FS: Backfolded n(k)




## ARPES




- Dynamic correlation (wavefunction) leads to fractional occupation
- QMC predicts low curvature FS relative to mean field DFT
- Overall good agreement found between (bulk) Fermi surface from wavefunction theory and (surface) ARPES

M. Brahlek, A. Mazza, A. Annaberdiyev, M. Chilcote, G. Rimal, G. Halasz, A. Pham, Y. Pai, J. Krogel, J. Lapano, H.N. Lee, B. Lawrie, G. Eres, J. McChesney, T. Prokscha, A. Suter, S. Oh, J. Freeland, Y. Cao, J. Gardner, Z. Salman, R. Moore, P. Ganesh, T. Z. Ward (Submitted)

# Summary and Outlook

- Shown how to obtain Fermi Surface from many body ground state
- Shown connection between Lock-Crisp-West backfolding procedure and partial traces of the k-partitioned one body density matrix
- Demonstrated effectiveness of the procedure in highly conductive quasi-2D oxide $PdCoO_2$ with good agreement with ARPES
- Future: applications of wavefunction-based methods to strongly correlated and topological metals providing a needed link between benchmark quality theory and experimental ARPES

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CADES

## Electronic Structure Packages

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## Institutional Support

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