Disordered Three-Dimensional Weyl Electrons

Braga, 27th of July 2025

J. P. Santos Pires (U. Porto & CF-UM-UP)

U.PORTO
FACULDADE DE CIÊNCIAS
UNIVERSIDADE DO PORTO

CF-UM-UP

Presentation Outline

A. Emergence of Gapless Dirac/Weyl Physics: A bit of context.

B. Dirac/Weyl Semimetals with Potential Disorder

- Unconventional Semimetal-to-Metal Critical Point.
- Avoided Criticality: Smooth Region Mechanism
- Avoided Criticality: Large Potential Fluctuation Mechanism

C. Dirac/Weyl Semimetals with Point Defects

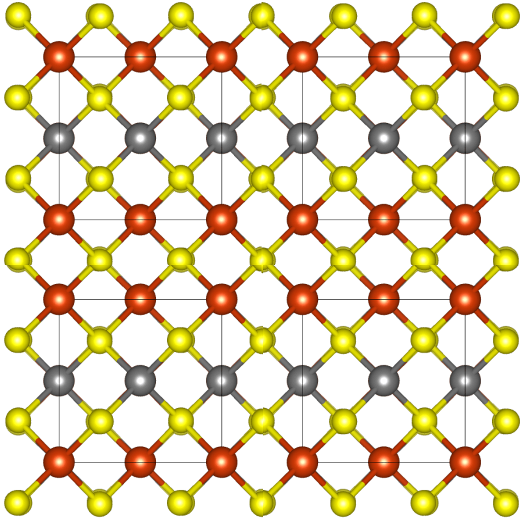
- Semimetal Phase Instability
- Signatures under Magnetic field
- DC-transport and Optical Absorption Signatures

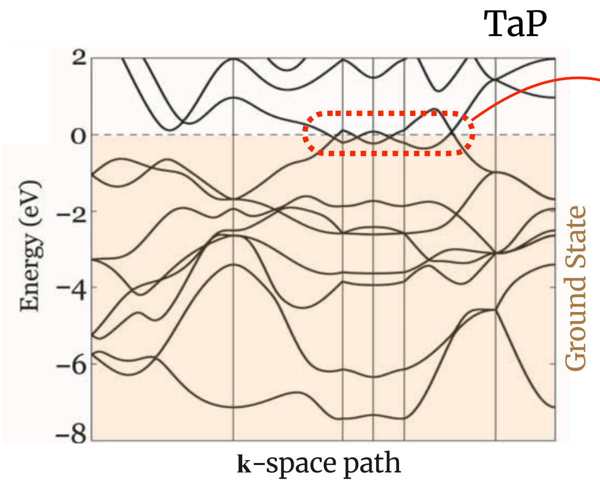
D. Outlook

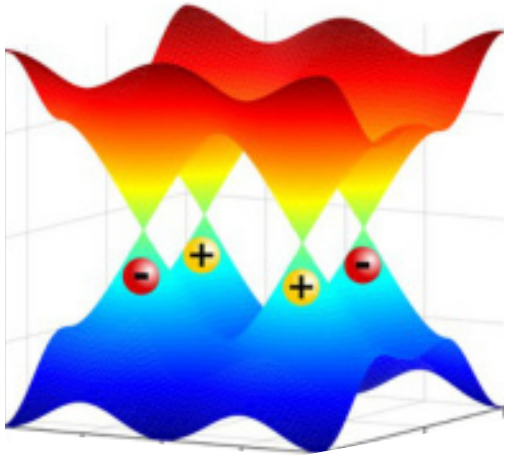
[In Slide Reference Text]

Emergent Massless Quasiparticles

A. Periodic Arrays of Orbitals (Periodic Potential)
B. Complex Energy Spectra (System Specific)
C. Low-energy phenomena dominated by elementary excitations over the ground state.
D. Elementary Excitation can display an emergent universality.







Xu et al. Sci. Adv. 1:e1501092 (2015)

3D Weyl and Dirac Quasiparticles

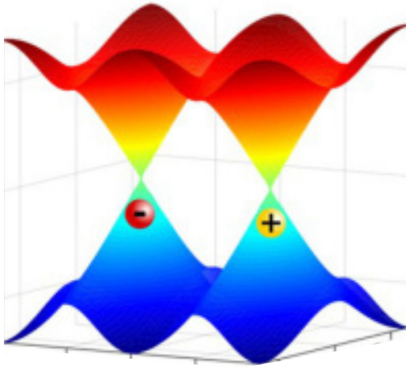
Point-like Band Crossings

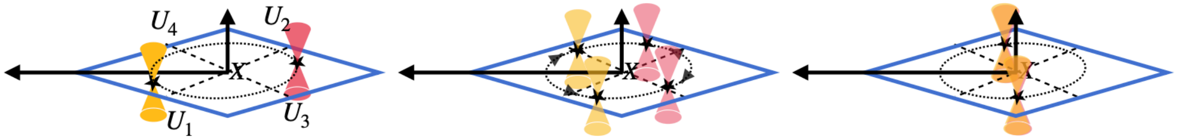
A. **PT-Symmetric Case:** Dirac Semimetal (DSM)

- Doubly-Degenerate bands
- Fine-tuned cases (Fu-Kane-Mele topological phase transition point)
- Symmetry-enforced band crossings (nonsymmophic space groups)
- Examples: Na_3Bi, Cd_3As_2, black phosphorous

B. **Non PT-Symmetric Case:** Weyl Semimetal (WSM)

- Non-degenerate bands.
- Topological Protection (Berry Curvature Monopoles)
- Broken Time-Reversal (e.g., spin split electronic bands)
- Broken Inversion-Symmetry (e.g., Fu-Kane-Mele with staggered mass)
- Examples: TaAs, TaP, NbAs, NbP (T-symmetric) or $RMnBi_2$, $R_2Ir_2O_7$ (P-Symmetric)





Murakami and Kuga PRB 78, 165313 (2008)
Young et al PRL 108, 140405 (2012)
Armitage, Mele and Vishwanath RMP 90, 15001 (2018)

Observable Signatures of Weyl Physics

Emergent Dirac/Weyl Quasiparticles Lead to Major Observable Consequences:

A. Chiral Magnetic Effect

B. Negative Longitudinal Magnetoresistance

$$\partial_t \rho(\mathbf{r},t) + \boldsymbol{\nabla}_{\mathbf{r}} \cdot \mathbf{J}(\mathbf{r},t) = \frac{E_F}{|E_F|} \frac{\chi e^3}{4\pi^2 \hbar^2} (\mathbf{E} \cdot \mathbf{B})$$

C. Planar Quantum Hall Effect

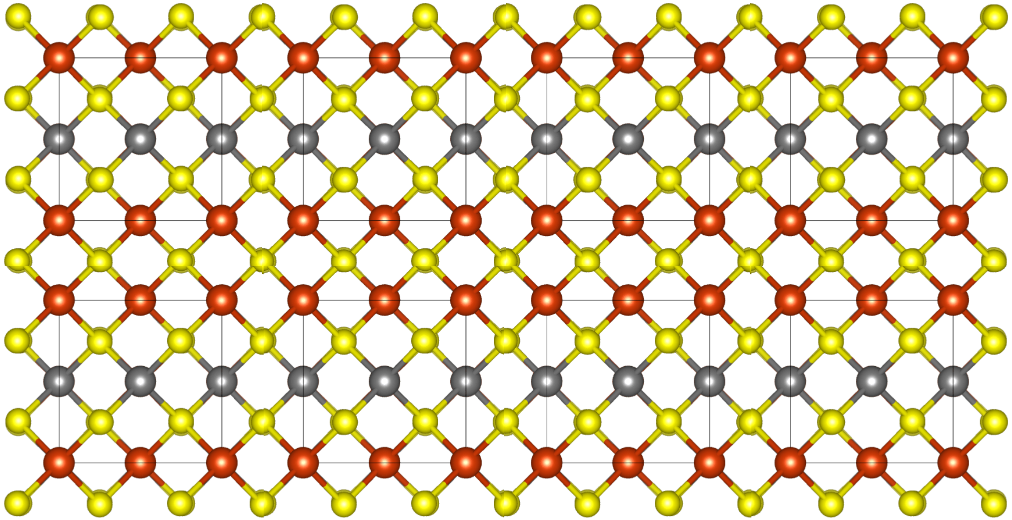
D. Chiral Zero Energy Landau Bands (under high Magnetic Fields)

E. Surface States of Topological Origin (Fermi-Arc States)

Topological Semimetals in Real Life

Interpreting Electronic Measurements in Real Materials always involve other effects beyond the Periodic Model

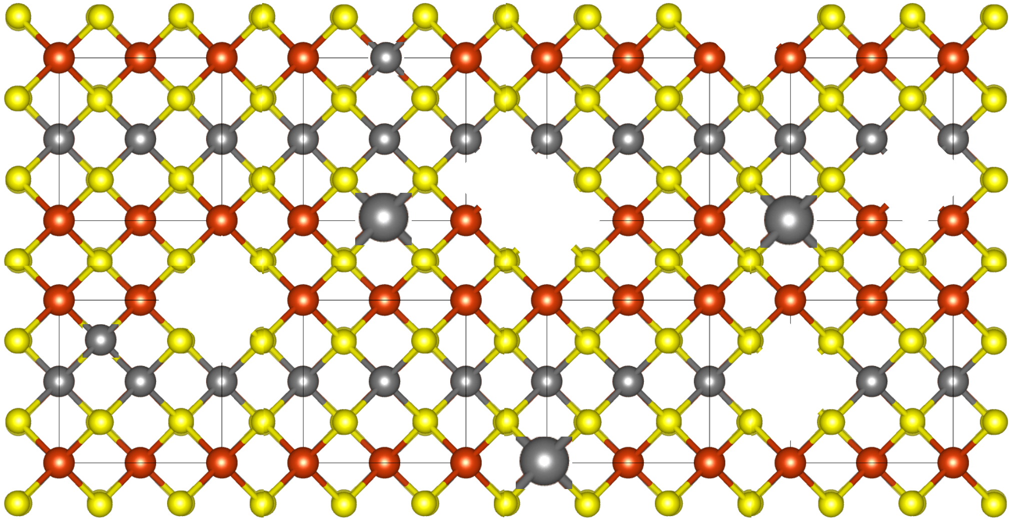
A. Atomic Impurities
B. Structural Disorder
C. Electron-Electron Interactions
D. Lattice Dynamics Effects
E. …



Topological Semimetals in Real Life

Interpreting Electronic Measurements in Real Materials always involve other effects beyond the Periodic Model

A. Atomic Impurities
B. Structural Disorder
C. Electron-Electron Interactions
D. Lattice Dynamics Effects
E. …



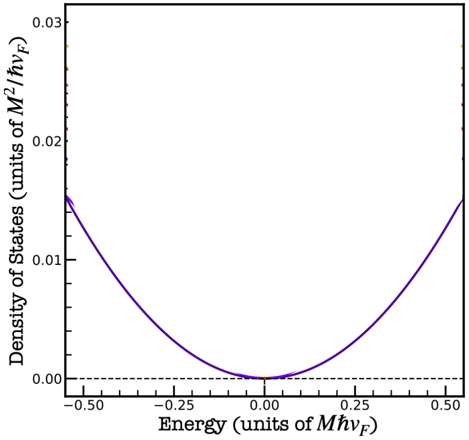
May change significantly observables even at low energies

Disorder-Driven Criticality

Simplest Static Disorder: Single Weyl Node with Random Scalar Field

$$\mathcal{H}=\mathcal{H}_c^0+\mathcal{V}_d=\hbar v_{\mathrm{F}}\int d\mathbf{k}\Psi_{a\mathbf{k}}^{\dagger}\left(\boldsymbol{\sigma}^{ab}\cdot\mathbf{k}\right)\Psi_{b\mathbf{k}}+\int d\mathbf{r}\Psi_{a\mathbf{r}}^{\dagger}V(\mathbf{r})\Psi_{a\mathbf{r}}$$

$$\overline{V(\mathbf{r})}=0 \text{ and } \overline{V(\mathbf{r}_1)V(\mathbf{r}_2)}=W^2 f\left(\frac{|\mathbf{r}_2-\mathbf{r}_1|}{\xi}\right)$$



Simplest Observable: Spectral Density of States

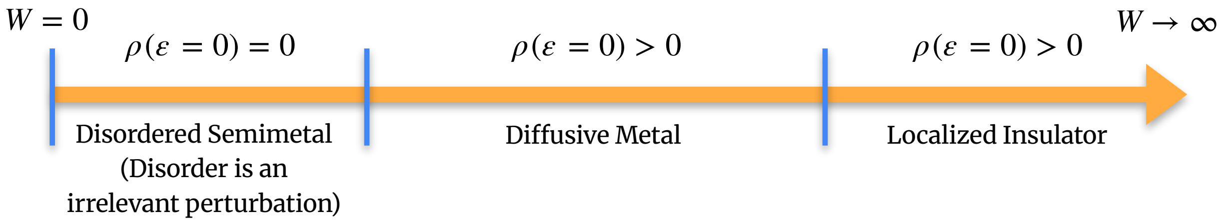
Disorder-Driven Criticality

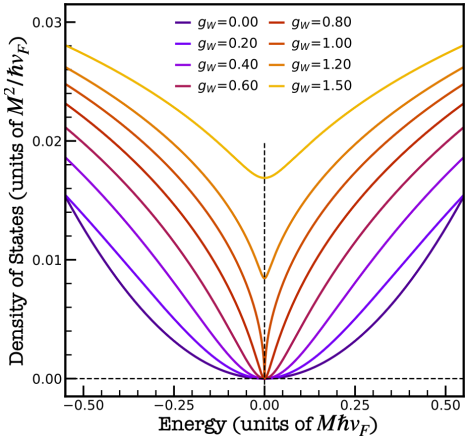
Simplest Static Disorder: Single Weyl Node with Random Scalar Field

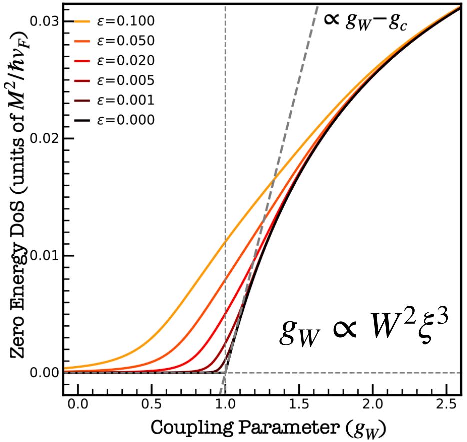
$$\mathcal{H}=\mathcal{H}_c^0+\mathcal{V}_d=\hbar v_{\mathrm{F}}\int d\mathbf{k}\Psi_{a\mathbf{k}}^{\dagger}\left(\boldsymbol{\sigma}^{ab}\cdot\mathbf{k}\right)\Psi_{b\mathbf{k}}+\int d\mathbf{r}\Psi_{a\mathbf{r}}^{\dagger}V(\mathbf{r})\Psi_{a\mathbf{r}}$$

$$\overline{V(\mathbf{r})}=0 \text{ and } \overline{V(\mathbf{r}_1)V(\mathbf{r}_2)}=W^2 f\left(\frac{|\mathbf{r}_2-\mathbf{r}_1|}{\xi}\right)$$

Simplest Observable: Spectral Density of States



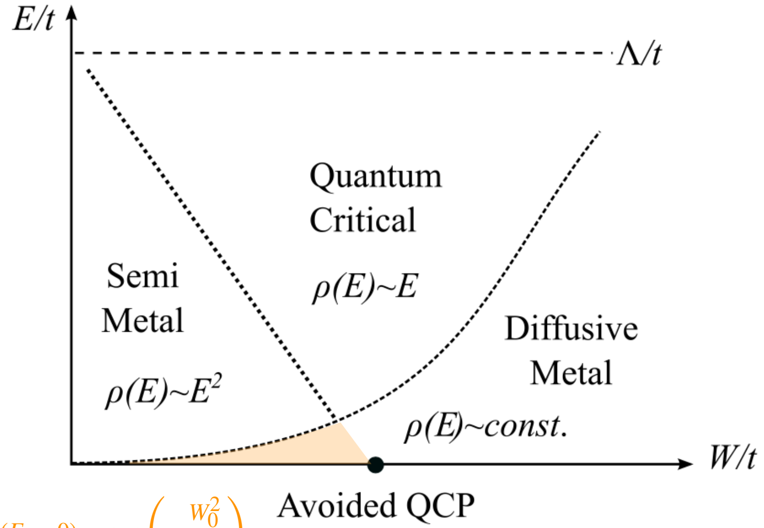




E. Fradkin PRB 33, 3257–3262 and 3263–3268 (1986)

Criticality Avoided by Rare Events

Mean-field theory misses non-perturbative effects arising from non-uniform solutions that lead to instantonic effects on the field propagators.



$\rho(E=0) \propto \exp\left(-\frac{W_0^2}{W^2}\right)$

Two instability Mechanisms:

A. Bound-States of Rare Smooth Potential Regions

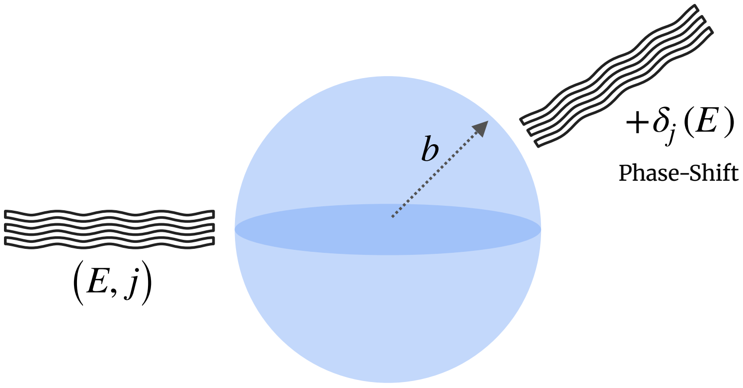
B. Bound-States of Large Potential Fluctuations

J. Pixley et al PRX 6, 021042 (2016)
M. Buchhold, S. Diehl and A. Altland PRL 121, 215301 (2018)
J. P. Santos Pires et al PRResearch 3, 013183 (2021)

Smooth Rare Regions

Model: Spherical Potential Wells/Plateaux

Scattering Theory in a Dirac Semimetal (irrelevant inter-valley mixing for large regions)

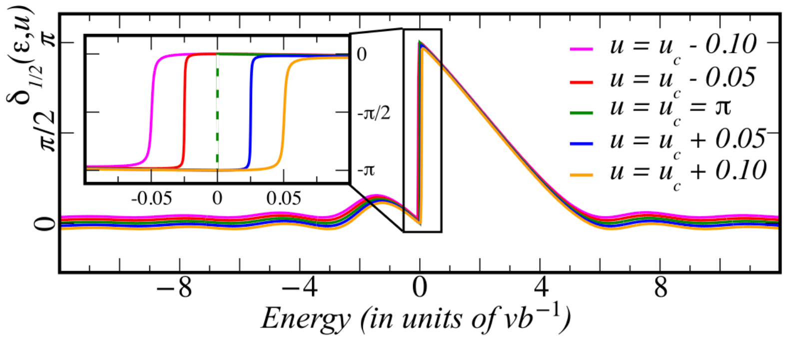


$$U(\mathbf{r}) = \lambda\,\Theta\big(|\mathbf{r}| - b\big)$$

Friedel Sum Rule >> Impact on Density of States

$$\overline{\delta\rho(E,b)} = \frac{2c}{\pi}\int d\lambda\, P(\lambda) \left[\sum_{j=\frac{1}{2}}^{\infty} (2j+1)\frac{\partial \delta_j(E,\lambda,b)}{\partial E}\right]$$

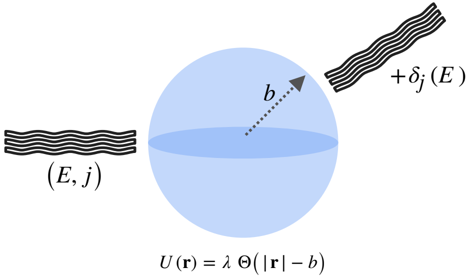
λ is a random potential strength



Discontinuity on the phase-shifts related to fine-tuned bound states.

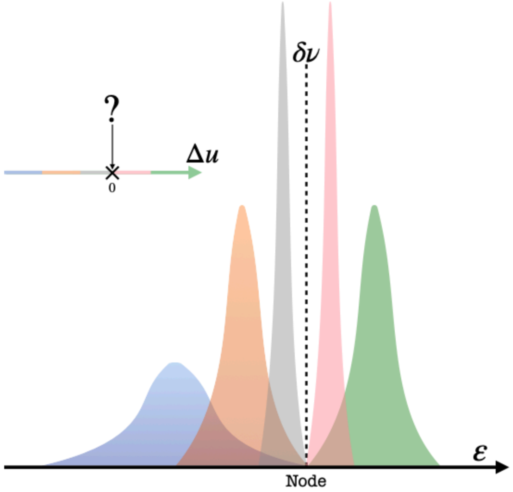
M. Buchhold, S. Diehl and A. Altland PRL 121, 215301 (2018)
J. P. Santos Pires et al PRResearch 3, 013183 (2021)

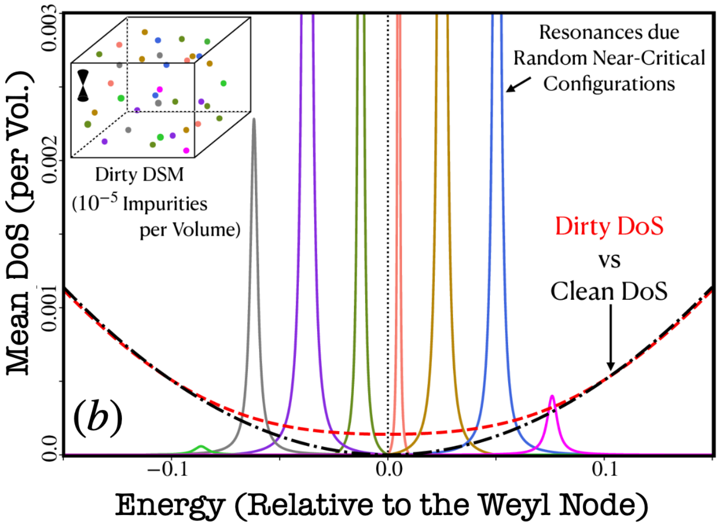
Smooth Rare Regions



Near-critical resonances give finite statistical weight to fine-tuned bound states.

$$\overline{\delta\rho(\varepsilon)} = \underbrace{N_v c_i \sum_{j=\frac{1}{2}}^{\infty} \int du\, P(u) \left(\frac{2j+1}{\pi} \frac{\partial}{\partial \varepsilon} \delta_j(\varepsilon, u) \right)}_{\text{Scattering States' Contribution}} + \underbrace{N_v\, c_i\, \delta_{\varepsilon,0} \sum_{j=\frac{1}{2}}^{\infty} \sum_{u_c^j} P(u_c^j)\, (2j+1)}_{\text{Bound States' Contribution}};$$





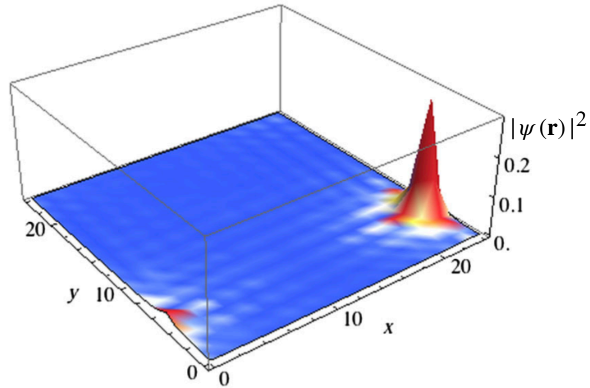
M. Buchhold, S. Diehl and A. Altland PRL 121, 215301 (2018)
J. P. Santos Pires et al PRResearch 3, 013183 (2021)

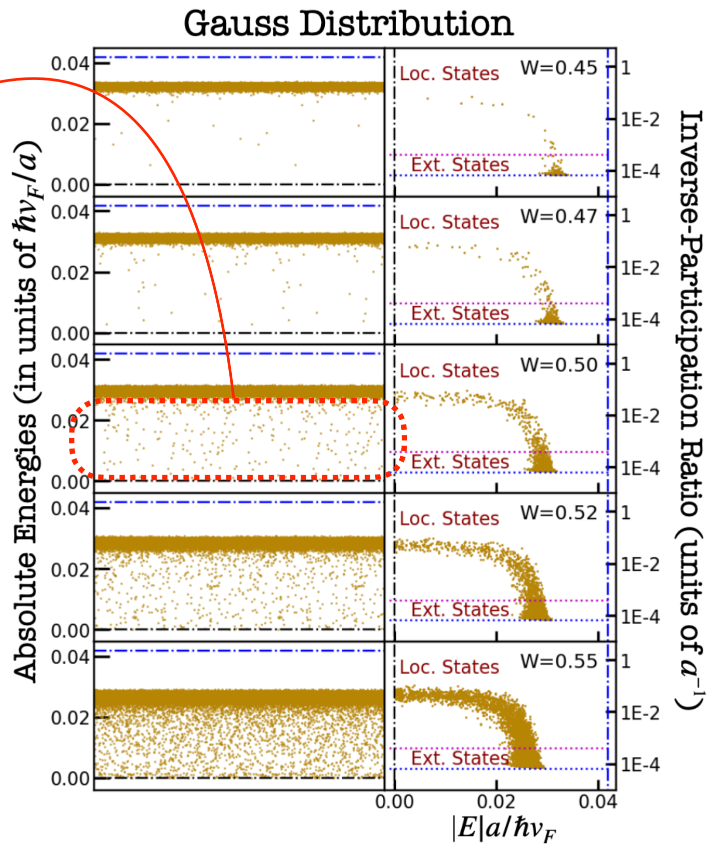
Large Potential Fluctuations

Model: Lattice Model with Gaussian Anderson Potential

$$P_{\rm GD}(V) = \frac{\exp\left[-\frac{V^2}{24W^2}\right]}{2\sqrt{6\pi}W}$$

Low-IPR states (localized or quasi-localized)
Contribute to the finite size gap DoS.





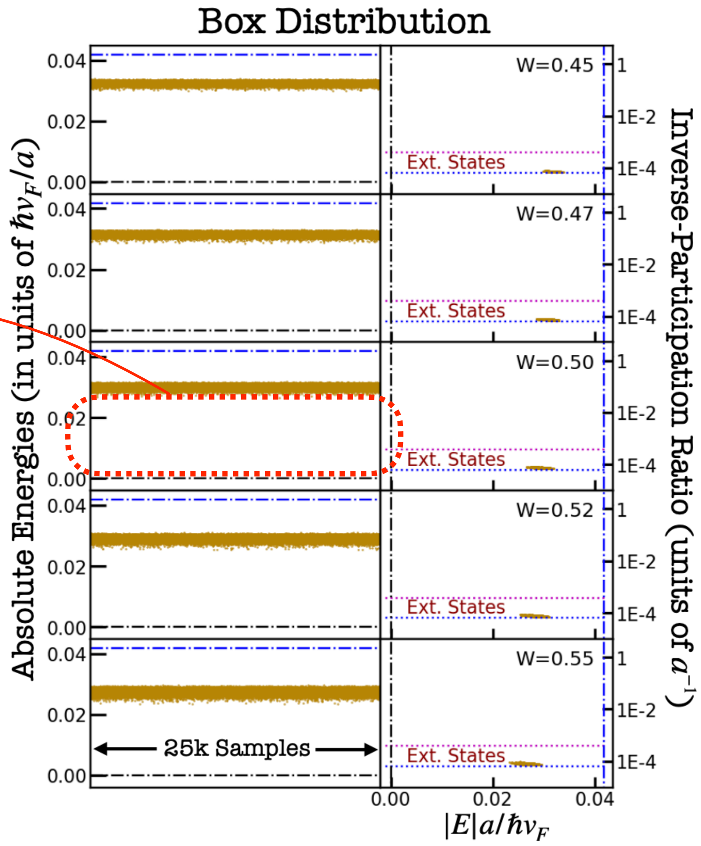
J. Pixley et al PRX 6, 021042 (2016)
J. P. Santos Pires PhD Thesis, arXiv:2212.11384 (2022)

Large Potential Fluctuations

Model: Lattice Model with Box Anderson Potential

$$P_{\text{BD}}(V) = \frac{1}{W}\Theta_H\left(|V| - \frac{W}{2}\right)$$

No quasi-localized states.

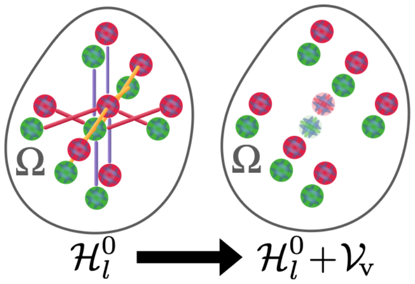


J. Pixley et al PRX 6, 021042 (2016)

J. P. Santos Pires PhD Thesis, arXiv:2212.11384 (2022)

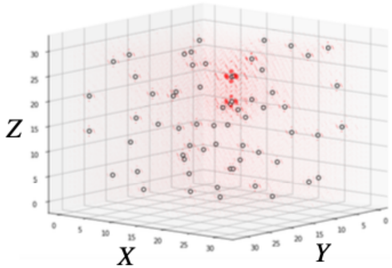
Point Defects | Semimetal Instability

Alternative Disorder Model: Point-like defects

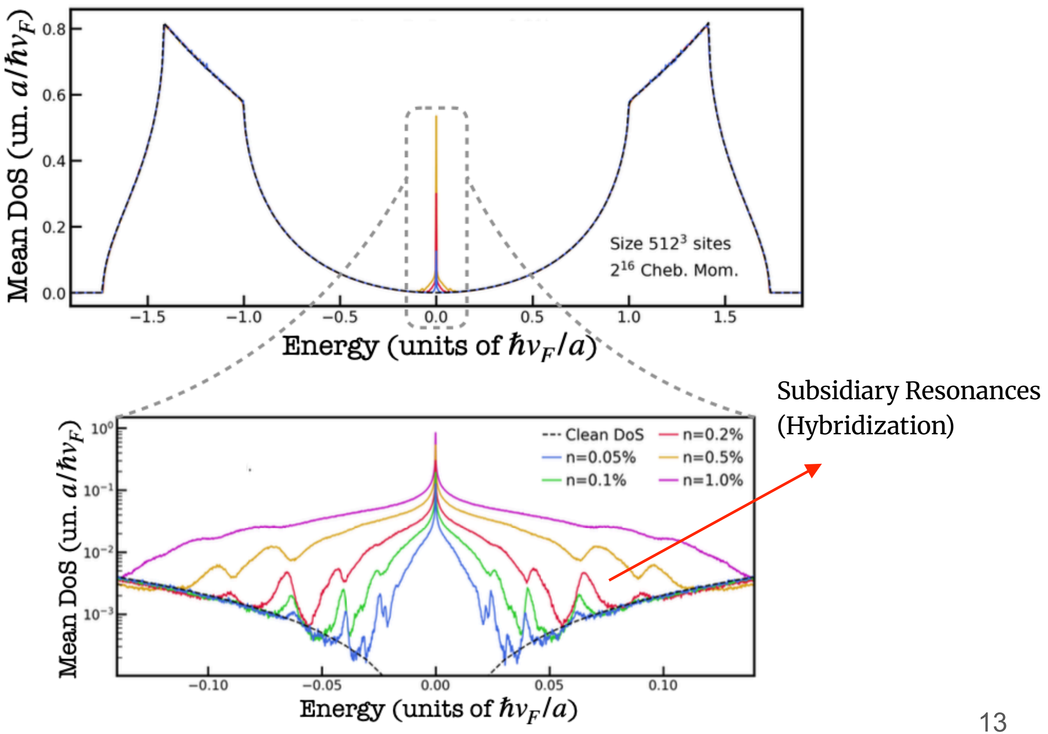


Each vacancy supports two zero-energy bound states around it.

$$|\psi(\mathbf{r})| \propto 1/r^2$$



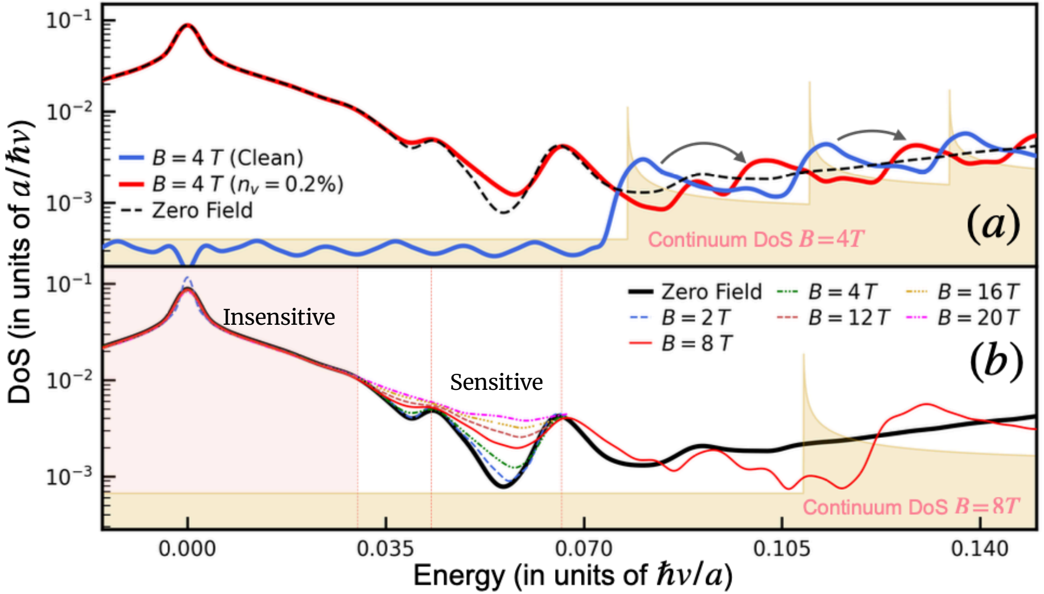
Nodal DoS becomes finite for any defect concentration

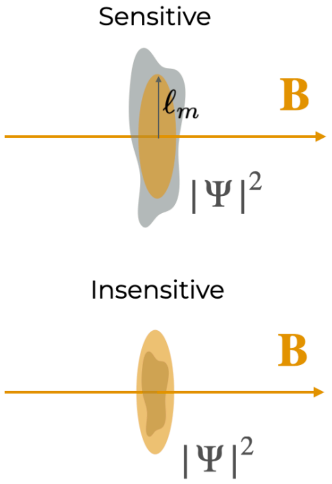


J. P. Santos Pires et al PRB 106, 184201 (2022)
J. P. Santos Pires PhD Thesis, arXiv:2212.11384 (2022)

Point Defects | Strong Magnetic Fields

WSM under strong magnetic fields (with point defects)

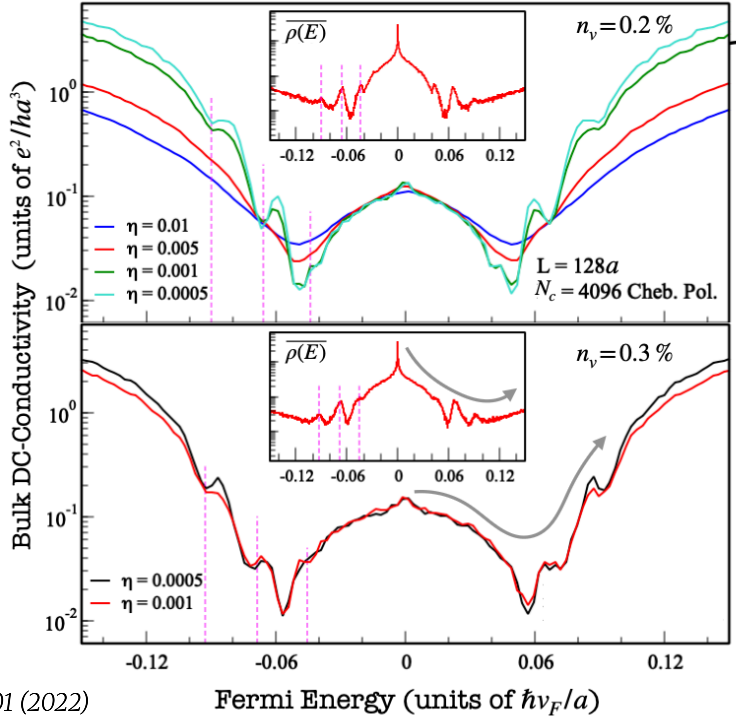




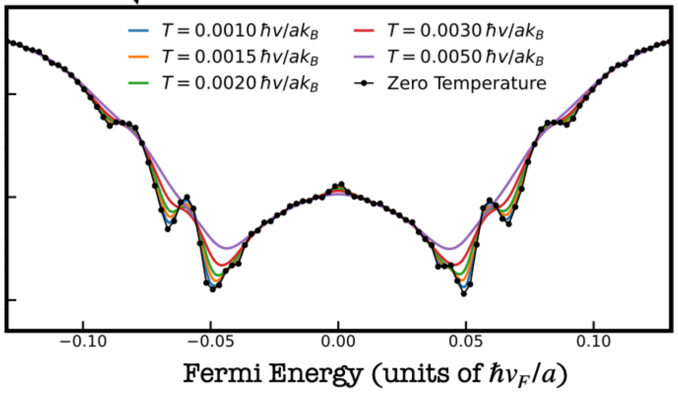
J. P. Santos Pires et al PRL 129, 196601 (2022)
J. P. Santos Pires PhD Thesis, arXiv:2212.11384 (2022)

Point Defects | DC Transport

Resonances in DoS = Suppressed Quantum Diffusivity >> Non-Monotonic / Oscillating Conductivity with Fermi Energy



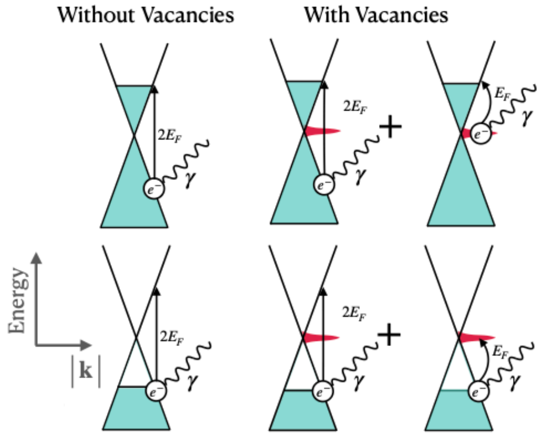
Finite Temperatures
$(0.001\hbar v_F/ak_B \approx 100K)$

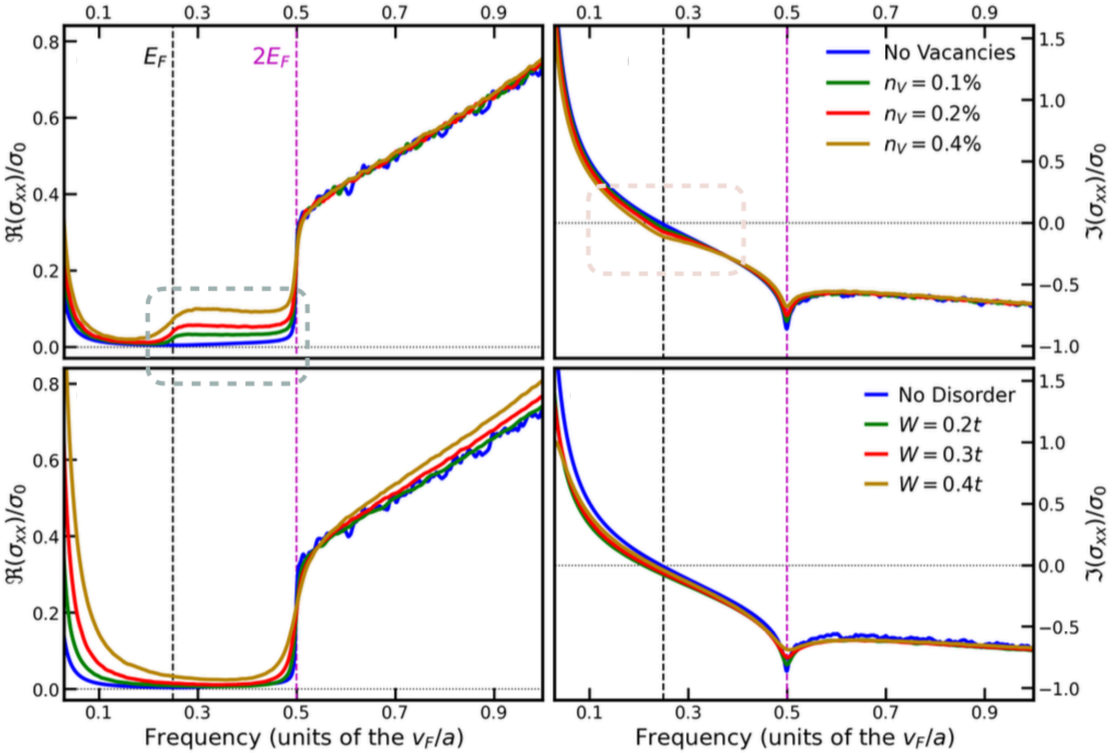


J. P. Santos Pires et al PRL 129, 196601 (2022)
J. P. Santos Pires PhD Thesis, arXiv:2212.11384 (2022)

Point Defects | Optical Absorption

Non Momentum Conserving Transitions from/to bound states lead to a plateau in the optical conductivity and inside the optical gap.





J. P. Santos Pires et al PRL 129, 196601 (2022)
J. P. Santos Pires PhD Thesis, arXiv:2212.11384 (2022)

New Steps

CF-UM-UP

Towards Local Measurements

- Probing Local Density of States (e.g., Structure of the Wavefunctions in the Presence of Disorder)
- Probing Local Currents (e.g., Mesoscopic Transport Effects in Real Space)
- Probing Local Topological Markers (Robustness, ??)

Crucial if we wish to Study Impact of Disorder in Surface States

Thank you

Colaborators:

J. Viana Lopes
(U. Porto)

Bruno Amorim
(U. Porto)

Aires Ferreira
(U. Of York)

Eduardo Mucciolo
(U. Central Florida)

Simão M. João
(Imperial College)

Inanc Adagideli
(U. Sabanci)

U.PORTO
FACULDADE DE CIÊNCIAS
UNIVERSIDADE DO PORTO

J. P. Santos Pires et al PRL 129, 196601 (2022)
J. P. Santos Pires et al PRB 106, 184201 (2022)
J. P. Santos Pires et al PRResearch 3, 013183 (2021)
J. P. Santos Pires PhD Thesis, arXiv:2212.11384 (2022)

CF-UM-UP