Disordered Electron Systems: A Local Quantum Cluster Approach

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Motivation, Background, and Goal

- **Quantum materials** represent the **next major technological jump** for humanity.
- In order to utilize these materials, we must understand their fundamental properties.
- **Disorder** is ubiquitous in all real materials and can have **profound effects on materials' properties**.
- One such effect is the **metal-insulator transition (MIT)**, which is **caused by disorder driven Anderson localization of electrons** [1].
- Anderson localization is a quantum wave phenomenon and has been observed in microwaves, light [2], acoustic waves, and ultracold atoms [3]. **It may occur for any wave propagating through a disordered medium.**

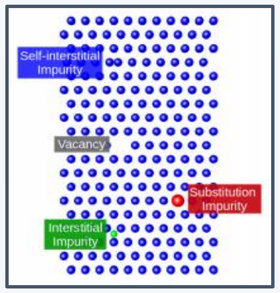


Figure 1: Examples of various types of disorder, including substitution and interstitial impurities, and vacancies.

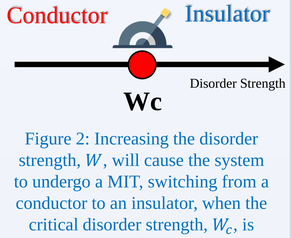


Figure 2: Increasing the disorder strength, W, will cause the system to undergo a MIT, switching from a conductor to an insulator, when the critical disorder strength, W_c, is reached.

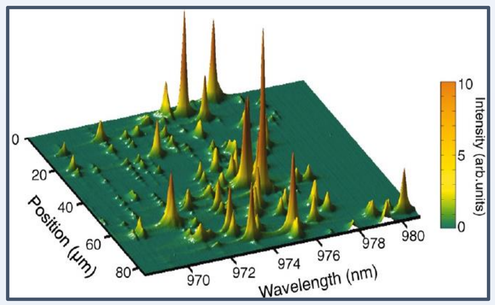


Figure 3: High intensity peaks show the random positions where the light emitted in a disordered photonic crystal waveguide becomes strongly localized [2]

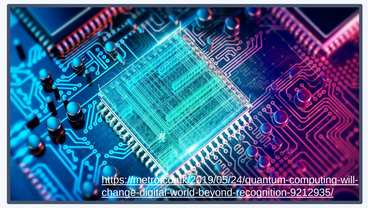
GOAL: To develop numerical tool **to simplify simulations involving disorder** so that more realistic systems can be modeled.

Applications

- Gaining a better understanding of disorder and its effects on quantum materials will lead to their application in an extensive range of fields:

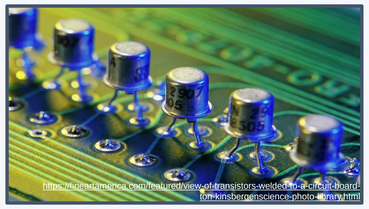
Understand Research the nature of interactions b/w electrons in solids ↔ **Control** Control the behavior of electrons in real materials ↔ **Design** Create materials with any desired set of characteristics

- **Quantum computing**, which will facilitate advances in **encryption** and consequently **national security.**



- In **energy generation**, **solar cells** that utilize disorder in their creation are more effective than their silicon counterparts [4].

- **Fabrication of new nano-electric circuits**, where they could be used as **ultra-fast switches to replace traditional transistors** [5].



- **Data and energy storage**, **fabrication of nano-materials**, **development of novel materials** (high-Tc superconductors), and much more.

Method

- We use quantum cluster typical medium theory (**QC-TMT**), a **computational numerical method** which employs typical density of states (TDOS) to determine when the MIT occurs [6].
- When the calculated TDOS(w=0) collapses to zero, the critical disorder, Wc, has been reached signaling the MIT

- Old models with this method used a complex initialization condition that led to high computation times.
- Here we propose a new initialization condition that neglects all non-local inter-site effects and is thus much simpler.

Results

- We tested the new model for a cluster size of 38 (Fig. 3) against previous results [6].
- The new model showed a very good agreement at larger disorders (W~1), and correctly predicted where the MIT occurs.
- Next, we checked the mobility edge behavior (Fig. 4). The local only model routinely undershot the correct edge value and showed only slight reentrance (the bowing out of the sides on the plot).

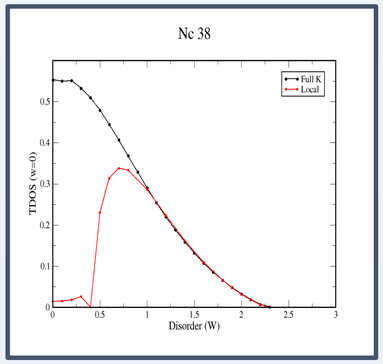


Figure 4: TDOS for both models (old - black, new - red) over increasing disorder strength for a cluster size of Nc=38.

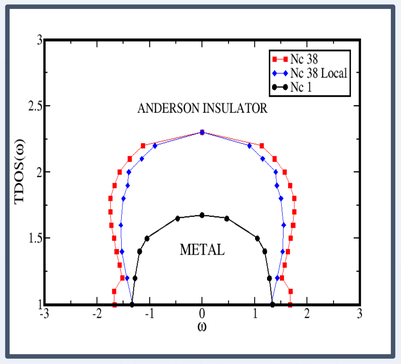


Figure 5: Mobility edge behavior of old and new models. The mobility edge marks the boundary between metal (inside) and insulator (outside).

Results (Cont.) and Conclusions

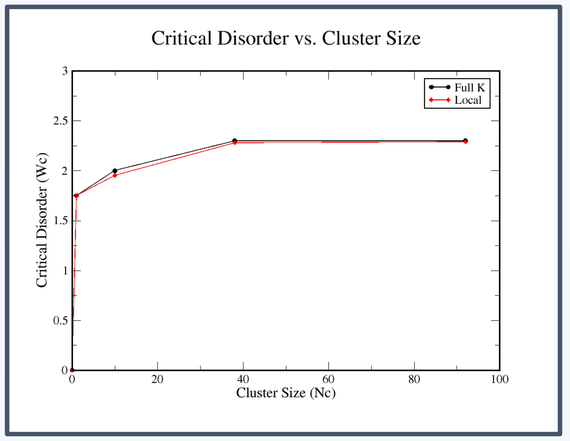


Figure 6: Comparison of calculated critical disorder (Wc) for the local and full models across a range of cluster sizes (Nc=1,10,38,92)

- Our local approx. agrees perfectly with full-K TM-DCA results at the band-center (TDOS w=0) for higher disorders, indicating that **the proposed local ansatz can be used to effectively capture the metal-insulator transition.**
- **This agreement increases with cluster size**.
- The local-only ansatz **underestimates the mobility edge values**. Performing a large cluster analysis may allow us to correctly capture the mobility edge behavior.
- Our results show that the **use of a local-only ansatz greatly reduces computation times**, and hence **can potentially be used to model disorder in realistic systems**.

References

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2) Sapienza, Luca & Thyrrestrup, Henri & Stobbe, Søren & Garcia, Pedro & Smolka, Stephan & Lodahl, Peter. (2010). Cavity Quantum Electrodynamics with Anderson-Localized Modes. Science (New York, N.Y.). 327. 1352-5. 10.1126/science.1185080.
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Acknowledgements

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