Modeling Disorder in Materials: Anderson Localization

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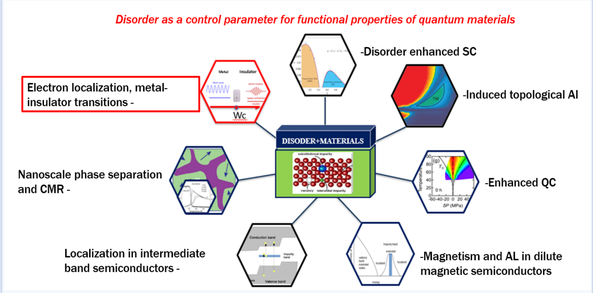
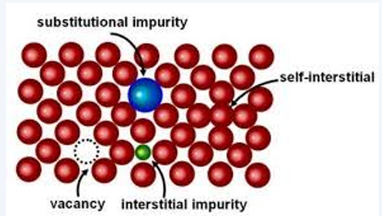
Motivation, background, and goal

Every real material contains some amount of imperfections or impurities. This is what we call disorder. Disorder affects a material's physical properties. Hence it is important to properly model it in numerical studies.



This figure shows that physics of disorder induced phenomena is very rich. It can induce multiple effects in materials: electron localization or metal-insulator transition, enhance super-conductivity, induce topological changes, have dramatic affects in semiconductors. Hence, studying effects of disorder in materials is very important for its better control and application.

What is disorder?



Disorder can be caused by any imperfection in a lattice, which arises during crystal growth or are during the doping procedure.

In general, disorder is any inconsistency in the potential created by the atoms in the material.

Goal of this project:

The most prominent effects of disorder is Anderson localization. [1]. This is a phenomena when electrons get trapped within some region of the material (get localized), and hence no longer carry electricity through the material.

Our Goal: Perform numerical simulation of such Anderson localization of electrons.

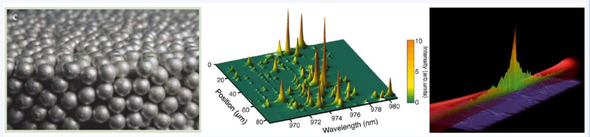
Anderson localization: a quantum effect

In a quantum mechanics class, we learn that the wavefunction of a particle determines all the particle's physical quantities and depends on the kinetic and potential energy of the particle.

In clean perfect crystal (left side), which is modeled by periodic potential, electrons are plane waves and extended, with finite probability of electrons to be found in any place of the crystal. i.e. the system behave as a metal (conductor).

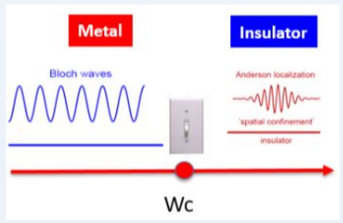
For not clean systems (right), the disorder is modeled by non-periodic potential. Such randomness in the potential causes electrons to localize in some region of the crystal. The electron wave function is not an extended plane wave anymore but is exponentially decaying function.

Anderson localization: a wave phenomenon



What is exciting about Anderson localization is that, because is a wave effect, it is not limited to electrons. It can occur for any waves (sound, light, etc) propagating through random/disordered medium. It has been experimentally shown to occur with sound (left) [3] and light (middle and right) [2], [4]. Hence, the study of disorder has wide reaching implications.

Application of Anderson localization: a conductor-to-nonconductor switch



At enough disorder, there is a transition from a metal/conductor to an insulator/non-conductor: a disorder-induced electric switch.

Theoretical model

The simplest model to study Anderson localization and model disorder in real materials is the Anderson Hamiltonian:

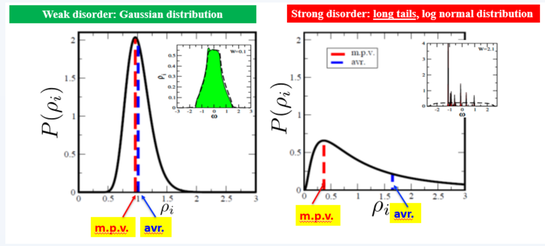
$$H = -\sum_{<ij>} t_{ij}(c_i^\dagger c_i + h.c.) + \sum_i V_i n_i$$

The first term describes kinetic hopping of electron between different lattice sites, and second term models disorder by random potential V.

Method and the main numerical challenge

We use two numerical methods to study disorder:
-the Coherent Potential Approximation (CPA).
-and the Typical Medium Method (TMT) [5].

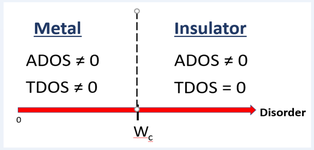
For years, it has been a great challenge to capture Anderson localization numerically. The roots of this stem from the fact that the Anderson transition is not a self-averaging phenomena, which is illustrated in Figure below.



This figure shows that for weak disorder (left panel), the system is self-averaged: the average and the most probable (the one we measure in experiment) are the same. While at large disorder (right panel), the system is not self-averaged, so the m.p.v. and the average values of the measure quantities, will differ dramatically.

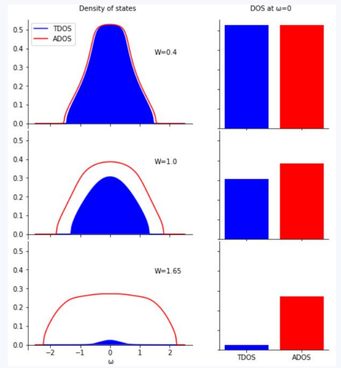
Our hypothesis

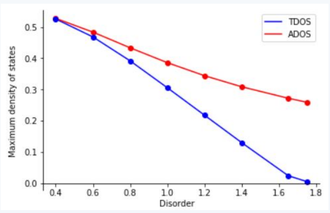
We propose to capture Anderson localization by calculating the typical density of states (TDOS) which should vanish above the transition, while the average density of states (ADOS) should remain finite.



Main results

Results: TDOS works as an order parameter





Disorder is represented by W. As we increase the amount of disorder in our model, TDOS goes to zero but ADOS remains finite. When $W \geq W_C$, every electron is localized and the material acts as an insulator. We can see that as W increases to W_C, TDOS=0 and ADOS is not critical. Therefore, we showed that TDOS is a valid order parameter for Anderson localization.

Conclusion

We study numerically the effect of disorder in three-dimensional lattice and showed that the typical DOS (TDOS) vanishes at large enough disorder strength (W>1.65) while the average DOS (ADOS) remans finite. Our findings convincingly show that TDOS can be used as a valid order parameter for numerical description of electron localization in disordered materials.

References

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[2] A. Aspect and M. Inguscio, *Physics Today*, 62, 30, 08 (2009).
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Acknowledgements

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