

## **Presentation, text**

### **Slide 1:**

#### **Introduction:**

Hello, first I would like to thank the professor for the introduction. My name is Jan Suntajs, and today I'll be giving a seminar on the Anderson localization. My masters thesis under the supervision of Janez Bonca and Lev Vidmar is about the localization in many-body systems with disorder. In plain language, this means I am studying how certain systems can go from a metallic to an insulating state if interactions between particles are changed or if the disorder is changed. I will be using the term disorder quite a lot during this presentation, so I would like to clarify right away that you can associate disorder with the presence of impurities, defects, dislocations or other irregularities in an otherwise ideal crystalline solid.

My today's talk will actually not concern the interacting systems. Given that we haven't heard much about localization here at the faculty, I figured it would be probably nice and more enlightening if I started with a somewhat simpler case of localization in systems of non-interacting particles with disorder. In other words, with the Anderson localization.

### **Slide 2: What is it about**

#### **(non-interacting, disorder, DIFFERENT THAN DRUDE)**

In the next five minutes or so, I'll show you five short slides with which I'll try to motivate you as per why the topic is interesting and relevant today. Let me start with what the Anderson localization is about - as already stated, it is a mechanism which provides a description of **conduction** in systems of **non-interacting** particles with disorder. We know that up until now we have mostly been considering the Drude model of conduction, in which the electron conductivity  $\sigma$  is proportional to the electron's mean free path,  $l$ . That is, the distance the electron travels before colliding with an impurity. If concentration of impurities is increased, the mean free path and the conductivity both decrease. The Drude model therefore predicts lowering of the conductivity but not its vanishing.

### **Slide 3: What does it predict?**

#### **(vanishing conductivity, 1958, Nobel in 1977, Light cone plot)**

The Anderson model, on the other hand, does predict that the electron conductivity can vanish if the disorder is strong enough, and the system becomes an insulator. This is not merely a theoretical exercise ... (rephrase). The idea was formulated in a seminal paper by P.W. Anderson in 1958. The paper is a notoriously difficult read and was only cited for about 20 times in the first 10 years. Its significance was recognized later and it has now been cited for more than 6000 times and its author has been Awarded with the Nobel prize in 1977. Shown on the right are the results of the simulations I've done in the past few months. Here we see that for no disorder, an initial sharply localized wavefunction in one dimension spreads across the whole system with time in a ballistic manner. If disorder is sufficiently strong, however, the wave function remains more or less centered at its initial point even as times passes. We'll talk about the simulations more in detail at the end of the seminar.

### **Slide 4: Why does it still matter?**

#### **(two articles shown)**

Now, I've shown you some dates in the previous slide, and you might as well wonder why would something that was predicted in 1958 and already awarded with a Nobel prize in 1977 still be relevant today? Well, localization is a complex phenomenon and its complete and rigorous treatment is still lacking even today. Above is crop from the Anderson's 60-year old groundbreaking

paper, while a crop from a paper of a younger date is shown below. It shows how the interest in the field has all but vanished.

#### **Slide 5, go seamlessly - The hot topic – MBL**

**(article from 2015 shown, 672 citations as of April 2018)**

Furthermore, understanding the Anderson localization is of paramount importance in understanding the interacting systems with disorder. Currently, the MBL is the hot topic in the research community. As an illustration - an article published in 2015 has already been quoted more than 670 times as of April 2018 acc. to Google Scholar. As stated in the very beginning, the MBL itself is not the subject of this seminar.

#### **Slide 6: the Outline of the seminar**

**(The basics, models of disorder, simulations, conclusion ?)**

Finally, after I've hopefully managed to motivate you, we come to the outline of this seminar. In the beginning, I will explain the basic concepts of the Anderson localization.

Next, I will outline how different models of disorder can be constructed starting from the picture of an ideal translationally invariant crystal. We will focus on the Anderson Hamiltonian more in detail. Afterwards, the results of the numerical simulations I've done in the past few (two) months are presented and finally, the ideas for the follow-up discussion are presented in the conclusion.

#### **Slide 7: The basics**

**(Localized states, exponential localization, no transport)**

So, here are the basics of the Anderson localization. As you may recall from your favourite solid state physics class, wavefunctions in a perfect crystal are Bloch waves and are spatially extended across the whole crystal. As Anderson pointed out in his paper, disorder can cause these states to become exponentially localized, meaning their envelope decays exponentially from some point in space, as shown both in this equation and in the figure here where an extended and a localized state are compared. If electrons are in extended states, they can contribute to transport and conductivity, while the localized states cannot.

#### **Slide 8: The keynotes**

**(interference – back-scattering, dimensionality – scaling, energy – mobility edge)**

Before explaining them, I would like to emphasize three keynotes about localization. First, in order to explain it, one needs to consider it as an interference phenomenon which we'll do in a short while. Then, we must also realize that the localization phenomena strongly depend on the system dimensionality. This makes them particularly complex which is also the reason why a complete and comprehensive theoretical treatment is still lacking today. Lastly, I would like to stress that whether a state becomes localized also depends on its energy. In the following few slides, we'll consider each of the three keynotes more in detail.

#### **Slide 9: The enhanced back-scattering:**

**(transmission probability, sum paths in a pairwise manner, coherent summation returns two times greater return probability – Stress the importance of randomness)**

We'll first address the role of interference effects in the onset of Anderson localization, where I will give a rather intuitive argument as per why can the interference importantly contribute towards the onset of localization. We start with elementary wave mechanics, where we want to find the probability that a propagating electron starting at point A arrives at point B. You probably recall from the nanophysics class, that in order to calculate electron's transmission probability, one needs to sum all the complex valued probability amplitudes for various possible paths between the two points, then take the sum's absolute value and square it, as shown in this equation for an example of

two possible paths. In general, the end result contains the classical term, which is the sum of the squares of individual probability amplitudes, together with the cross-product, interference terms. Since we are in a random disordered medium, the phases of the probability amplitudes are also random and one can with great possibility argue that the interference terms average out once a large number of all possible paths between the points is considered. This way, we are only left with the classical term which gives us the Drude model description and which obviously cannot explain localization.

It turns out that the above reasoning is correct in all cases but one – but this one is important – if we take a path from A along B back to A and its time-reversed path and calculate the transmission probability, we obtain a result which is two times greater than the one obtained in a classical manner. In simpler terms, this means that the probability of an electron scattering back to its initial place is greater than the probabilities of all other scattering outcomes.

### Slide 10: the scaling theory

**(the scaling laws, ohmic, insulating, two beta limits, what beta means, transition at some critical disorder)**

Now, the theory of Anderson localization is actually incredibly complex. In fact, a complete and rigorous treatment of it is still lacking even today. For the most part, this is due to the localization's strong dimensionality dependence. As we'll soon show, in 1 and 2D, all the eigenstates of a system can become localized for any nonzero disorder, while in 3D there exists some critical disorder strength above which all eigenstates are localized while for subcritical disorder both extended and localized states coexist in the system. Explaining this in full is really complex, however, some rather phenomenological theories exist which provide great insight into the role the dimensionality plays here. One such theory is the scaling theory, which was developed in 1979 and it treats the localization in the language of continuous quantum phase transitions, meaning it describes various quantities of interest in terms of some scaling laws which you may recall from the statistical physics class. Among those scaling laws, we'll only consider the one for the conductance  $g$ .

We recall from physics one, that for an ohmic conductor, the conductance  $g$  of a **hypercube** of side-length  $L$  is related to the conductivity  $\sigma$  like this  $\rightarrow$  put in  $d=3$  in three dimensions and you've got the OHM's law in its well known form. The other well known limit is the one of an insulating system, in which the conductance decays exponentially with its size like this. What the scaling theory does, is that it describes the scaling of conductance with respect to the system size in terms of a logarithmic derivative  $\beta$  defined here. If  $\beta$  is positive, this means that the conductance increases with system size, which is a hallmark of metallic behaviour. In the opposite case, the system is an insulator.

In the conducting limit, one simply has  **$\beta = d-2$** , which is only greater than zero in three dimensions. In the insulating limit, one has  **$\beta = \log g$** , which is a negative quantity since  $g$  is a small quantity close to zero in the insulating regime. The intermediate values are, within the framework of the scaling theory, interpolated assuming  $\beta$  is a smooth and monotonically increasing function of  $g$ . As we can see from the graph, the transition can only occur in 3D, where  $\beta$  can assume both positive and negative values. Critical value of  $\beta=0$  occurs for some critical amount of disorder. Above this critical amount, the system is an insulator, below it a conductor.

### Slide 11: the scaling theory 2

**(SCALING SUMMARY)**

In short, this is to summarize the most important results of the scaling theory. In 1D and 2D,  $\beta$  is always negative, which is why for any finite disorder the system is an insulator and its eigenstates are localized. In 3D, the system only becomes an insulator if some critical value of disorder is exceeded for which all states become localized.

## SLIDE 12: THE MOBILITY EDGE:

So, we've established that in 3D all states are localized if the disorder is strong enough. But what happens if it isn't? Then, the conductivity is nonvanishing, which means the extended states must surely be present in the system. It turns out that also the localized states are present then, however, they cannot coexist with the extended ones at the same energies. This means that there must be some critical energy  $E_c$  separating them and this critical energy is called the **mobility edge**. If this is a schematic of the density of states for some 3D system with a fixed amount of disorder, the states with the energy below the mobility edge are localized and thus cannot contribute to transport and electron conductions, while the extended states can. For those of you more into solid state physics, if the system's Fermi energy is in the region of the localized states, then the system is an insulator.

We'll return to this more in detail soon once we consider the Anderson model.

## SLIDE 13: THE MODELS OF DISORDER

In the following few slides, I'll briefly explain how different models of disorder can be constructed where I'll focus a bit more on the Anderson model since this is the model I have also used in my numerical simulations. When we want to model disorder in the solid state systems, we usually take the ideally ordered and translationally invariant crystal structure as the starting point and then distort it in some way. Here in the picture, we've got the ideal crystal structure shown first. If we want to simulate compositional disorder, which is typical for alloys, we can retain the lattice array, however we put different entities on the lattice sites. Pictorially, this is basically the scheme I have been using in my simulations. Then, if we wish to simulate structural disorder, which is the closest to what we are doing in the nanophysics class, we relax the lattice structure as shown here and place the crystal entities randomly. Lastly, this schematic shows an example of disorder in kinetic energies which I will not address into more detail here. A generic one-particle Hamiltonian for such systems is given by this expression, where  $V_j$ ,  $R_j$  or both can be taken at random according to some probability distribution.

## SLIDE 14: THE ANDERSON MODEL

In my simulations, I have been using the Anderson model, which is most often used in the literature because it's relatively mathematically tractable and at the same time retains all the features of the localization phenomena I have described so far. It is used to describe compositionally disordered solids, such as alloys, hence it is defined on a regular lattice and disorder is introduced by the randomly varying potential terms as shown in this expression. Here,  $c_j$  and  $c_j^\dagger$  are the fermionic creation and annihilation operators. The  $\epsilon_j$  in the diagonal term are the random site potential energies which tell what is the energy cost of an electron being localized at some site  $j$  in the lattice. In the kinetic part, only the nearest neighbour hopping is allowed and the hopping rate  $V$  was set to 1 in all of my calculations. A schematic representation of the model in 2D is shown here, where the cones denote the random potential energies and the arrows represent the hopping possibilities of this electron. The random energies are sampled according to the box distribution shown here.

## SLIDE 15: THE ANDERSON MODEL SCHEMATIC OF DOS

As already stated, the Anderson Hamiltonian retains all the basic features of the localization phenomena I've stated in the introduction. All of the Hamiltonian's eigenstates become localized for

any finite disorder in 1 and 2D, while the extended and localized states are both present in 3D for some subcritical disorder. What's interesting, is that there are in fact two mobility edges in the Anderson model, where their energies are symmetric with respect to the band center. This is shown in this figure here, where a schematic of the 3D Anderson density of states is shown.  $E_c$  and  $E_c$  dash are disorder dependent – for small disorder, only states in the tails of this distribution are localized. As we increase the disorder, the two critical energies move closer and closer to the band center. Full localization occurs once they merge at some critical disorder strength. In any case, bear in mind that the localized states first appear near the band extrema with those in between remaining extended.

## **SLIDE 16**

### **THE NUMERICS – INTRO**

#### **BULLET ONE: HOW TO EXTRACT SOMETHING – WHAT I DID**

#### **BULLET TWO: THE CRITERIA STATED, NOT ELABORATED UPON**

Finally, after all this theory, we come to the part when I can show you the results of my numerical simulations. My numerical inquiries started with a simple question of how can I extract some of the Anderson's localization distinguishing features by means of numerical work. What I did was, I implemented the Anderson Hamiltonian in 1,2 and 3D and then ran calculations for different parameter values at the F1 cluster at the Jožef Stefan Institute. I was doing the full diagonalization studies as well as time-evolutions of initial wave functions, those of you who have attended the advanced numerical methods classes should be well familiar with the techniques. In order to characterize whether the localization occurred, I have considered two criteria, namely the inverse participation ratio and the absence of diffusion which I will explain in the next slides together with the results.

## **SLIDE 17:**

In my numerical studies, I have been performing the full diagonalization studies in which I have used numerical diagonalization to find the eigenstates of the Anderson Hamiltonian. Then, in order to find whether the eigenstates are localized or not, I've used the criterion of the INVERSE PARTICIPATION RATIO, which is defined as follows: (show the equation) → its meaning is: we take some wavefunction in the site occupation basis, where each basis vector corresponds to an occupation of a particular lattice site. Given that the wave function is normalized to 1, we take the modulus of the probability at each site to the fourth power and sum over all the lattice sites. For example, this should be equal to 1 if the wavefunction only has a probability amplitude of 1 at one site and zero elsewhere, while  $P^{-1}$  should be small for states with nonvanishing probability amplitudes in considerable portions of the lattice. For a sufficiently large lattice, the scaling goes like this (show equation).

## **SLIDE 18:**

Here are the results of the IPR studies in the 1 and 2D. (left, above) Here, on the x-axis, we've got the index of each of the Hamiltonian's eigenstates where the states are ordered with respect to their energy and on the y-axis we've got the values of the IPR for each of the states. For  $W=0$ . or no disorder, all states are delocalized, resulting in the smallest values of the IPR. For nonzero disorder, the states in the band extrema have the largest values of IPR, which means they are the most localized. Even though there is no mobility edge in 1 and 2D, the disorder still affects the states with the energy near the band edges the most. In order to test how IPR scales with the system size, I've also performed the scaling analysis in which I've repeated the procedure for various system sizes and then plotted the average IPR versus  $1/L^d$ .