LMU München
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Lehrstuhl für Theoretische Nanophysik
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10. Exercise Sheet TA1: Theoretical Solid State Physics

To be discussed on Tuesday, January 31, 2017.

Exercise 1: Bloch electrons in 1D

Consider the Hamiltonian:

$$H = \frac{p^2}{2m} + U_0 \sin^2(\kappa x)$$

in a one dimensional box of length L with periodic boundary conditions, where $\kappa = \pi/a$. Discretize the space variable x. Use the central difference approximation for the second derivative:

$$\psi''(x) \approx \frac{\psi(x - \Delta x) - 2\psi(x) + \psi(x + \Delta x)}{\Delta x^2}.$$

This leads to a matrix representation of the Hamiltonian. Set $\hbar = 1$ and $m = 1$ and Diagonalize the Hamiltonian matrix numerically. Plot the eigenvalues and compare the spectrum for different depths of the potential $U_0 = 0.1, 1, 5$ and different discretisations $\Delta x = a, a/2, a/4$.

Exercise 2: Wannier-Stark states

Consider a tight-binding Hamiltonian of electrons in 1D with open boundary conditions and hopping matrix element t. For simplicity, assume that the electrons all have the same spin. The particles are subject to a linear potential proportional to $V_i = -Ei/L$ on site i.

a. Write down the Hamiltonian in 2nd quantization.

b. Write down H in the single-particule subspace as a matrix for a large system of $L = 100$.

c. Use your favorite software/ programming language to diagonalize the matrix from (b) for

   i. E=0
   ii. E=2t
   iii. E= 6t

   Plot the eigenenergies in ascending order. Discuss the structure.

d. Analyze the eigenstates. Plot their amplitudes as a function of i.

Bonus: In the case $E = 0$, how would the matrix from (b) be modified in the case of periodic boundary conditions?

Exercise 3: 1D Anderson model

In this exercise we want to study the effect of disorder on the electronic eigenstates. We consider a 1D model of L sites with hopping matrix elements $-t$ and onsite energies ϵ_i. We model the disorder by drawing the ϵ_i at random from a flat and uncorrelated disorder distribution $\epsilon_i \in [-W/2, W/2]$ of width W. In 2nd quantization, the Hamiltonian is:

$$H = \sum_{i=1}^{L} \left[-t(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i) + \epsilon_i c_i^\dagger c_i \right]$$

a. Diagonalize the Hamiltonian for W=0.2 and W=8 for L=1000 sites. Choose $t = 1$ thereby setting the energy scale and assume periodic boundary conditions. Plot some of the eigenstates $|\phi_\mu|^2$ ($\mu = 1, ..., L$) vs site i in a log-linear plot. Describe your observations.

b. The difference between localized and extended wave-functions can be quantified by the inverse participation ratio IPR:

$$1/IPR = \sum_{i=1}^{L} |\phi_\mu|^4$$

What do you obtain in limiting cases, i.e., for W=0 or for the extreme case where the wave-function is fully localized onto a single site ($W \gg t$)? Plot the IPR vs W for (i) single realization and for (ii) an average over 100 realizations (i.e., different choices for the random potentials). Use a state from the middle of the spectrum.

Note: the maximal and minimal eigenenergies will vary from realization to realization. Use the energy density $e = (e_\mu - e_{min})/(e_{max} - e_{min})$ and plot the IPR for a fixed $e = 0.5$ (i.e., pick the state that is the closest to e).

Then plot the IPR vs e for a single realization and for an average over disorder realizations for $W = 4$.

Note: The fact that the eigenstates become localized implies that the system any filling becomes an insulator. This state of matter is called the Anderson insulator.