Universität Regensburg
Institute for Theoretical Physics
Institute of Computational Condensed Matter Theory
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`http://www.physik.uni-regensburg.de/forschung/evers/courses/cscn.phtml`

Exercise Sheet No. 3
"Computational Condensed Matter Theory"

1 Tight-binding chain (1d) with disorder

Consider the tight-binding Hamiltonian

$$\hat{H} = -\sum_{\langle k,l \rangle} t_{kl} c_k^\dagger c_l + \sum_{l \in \mathcal{L}} \epsilon_l c_l^\dagger c_l \tag{1}$$

$c_l^\dagger, c_l$ denote fermionic creation and annihilation operators acting on site l of a 1d chain with $L = 500$ sites. The hopping matrix t_{kl} connects nearest neighbors, only. Assume periodic boundary conditions.

a) On-site disorder

First consider a uniform hopping $t_{kl} = t$ and random "on-site energies" ϵ_l. The values for ϵ_l are uniformly distributed random numbers from an interval $[-W/2, W/2]$ with $W = t = 1$.
Calculate, by exact diagonalization, the spectrum and the corresponding density of states (DOS) for three different disorder realizations. Visualize several eigenfunctions. Discuss your observations and the physical implications.
Calculate the DOS averaged over an ensemble of 1000 disorder realizations.

b) Off-diagonal disorder

Now consider pure off-diagonal disorder $\epsilon_l = 0$ and $t_{l,l+1} = t + \delta t_l$ at random values for δt_l chosen to be uniformly distributed from an interval $[-\frac{W}{2}, \frac{W}{2}]$. As disorder strength choose $W = t$
Again, average the DOS over 1000 disorder configurations. Compare your results with the previous on-site disorder case.

Useful functions:

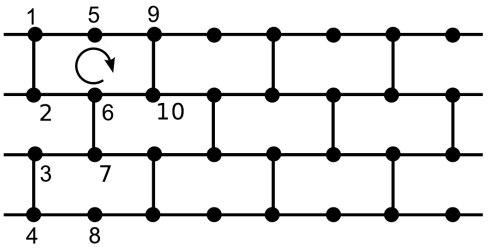
- numpy: `diag`
- numpy.random: `rand`
- scipy.linalg: `toeplitz`

2 Quantum Spin Hall Effect in Graphene

Now consider a graphene ribbon with spin-orbit interactions. A model describing this system has been studied in Ref. [1] by Kane and Mele. Since the Hamiltonian of their model is diagonal in spin-space, for simplicity we consider only one spin component. As previously discussed on exercise sheet 2 the lattice of graphene is again modelled by a brick-wall lattice. The Hamiltonian thus reads

$$H = -\sum_{\langle k,l\rangle} t c_k^\dagger c_l - \sum_{\langle\langle k,l\rangle\rangle} i t' \nu_{kl} c_k^\dagger c_l, \quad \nu_{kl} = -\nu_{lk} = \pm 1 \tag{2}$$

Here $\langle\langle k,l\rangle\rangle$ denotes pairs of next-nearest neighbours and $\nu_{kl} = +1$ if the electron encircles a plaquette clockwise to get to the second site (e.g. $\nu_{1,9} = \nu_{5,10} = \nu_{2,7} = \nu_{4,7} = \nu_{6,3} = +1$), and $\nu_{kl} = -1$ if it moves anti-clockwise (e.g. $\nu_{1,6} = \nu_{2,10} = \nu_{3,6} = \nu_{6,9} = \nu_{7,2} = -1$).



a) Construct the Hamiltonian Eq. (2) for a ribbon of size M x L with M=4 and L=64, and use a next-nearest neighbour hopping of $t' = 0.33t$. Assume periodic boundary conidtions in x- but not in y-direction.

b) Calculate and plot the dispersion relation $\epsilon(k_x)$, and compare the band structure to the case without next-nearest neighbour hopping.

c) Visualize the probability density ($|\Psi(x,y)|^2$) of a wavefunction with an energy eigenvalue of $\epsilon(k_x) \approx 0$ and discuss its spatial structure.

Hint: Use the `plt.imshow` function with the options `interpolation = 'none', aspect = 'auto'` to display the absolute square of the wave function.

References

[1] C.L. Kane and E.J. Mele, Phys. Rev. Lett. **95**, 226801 (2005), (arXiv:cond-mat/0411737)