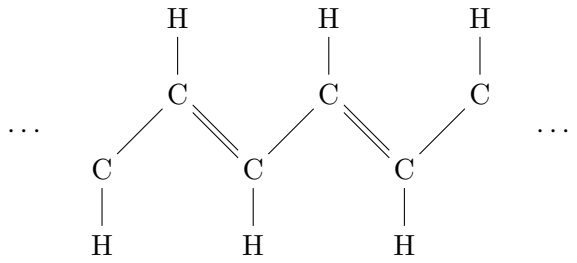
Polyacetylene

Polyacetylene is a polymer with the following chemical structure:



Chemistry tells us that each carbon will contribute 4 electrons to the chain, but 3 of them will be bound up in the sp^2-hybridized orbitals, oriented in the plane of the molecule. The remaining free electrons occupy weaker π orbitals, perpendicular to the plane of the molecule. Weak overlap of these π orbitals allows electrons from different atoms to interact, and this suggests that these electrons will delocalize.

To be more precise, let us denote by $c_{n\sigma}$ and $c^\dagger_{n\sigma}$ the fermionic annihilation/creation operators for the electron on carbon n in the chain, assuming the electron has spin σ, which can take 2 values (up or down). For simplicity, we will assume that the chain of carbons is an infinitely long 1D chain. If we denote the classical variable u_n to be the displacement of carbon atom n, a toy model for the effective Hamiltonian seen by the electrons is given by:

$$H = -t\sum_{n,\sigma}(1+u_n)\left[c^\dagger_{n\sigma}c_{(n+1)\sigma} + c^\dagger_{(n+1)\sigma}c_{n\sigma}\right] + \sum_n \frac{K}{2}\left(u_{n+1}-u_n\right)^2 .$$

Now, as we said earlier, the electrons will delocalize, so we would naïvely expect the polymer to be a good conductor. However, as we will show in this problem, the polymer chain is actually unstable to the deformation

$$u_n = (-1)^n U$$

with $U > 0$ some constant. We will see that this instability actually implies that this material is not metallic.

(a) Using the ansatz for u_n given above, find explicitly the eigenvectors and eigenvalues of H.[1] You should find that the energy spectrum of the electrons alone is given by

$$E(k) = \pm 2t\sqrt{1-(1-U^2)\sin^2 k}.$$

(b) Show that the polyacetylene is not a good conductor if $U > 0$. Remember that each carbon atom contributes exactly one electron, when determining where the Fermi energy is.

[1] Note that the ansatz for u_n breaks some of the translation symmetry. What translation symmetry is left? Exploit the remaining symmetry to diagonalize H.

(c) Now, let's see for what value of U the energy of the polymer is minimized. By exploiting the identity

$$\int_{-\pi/2}^{\pi/2} \mathrm{d}k \, \sqrt{1-(1-U^2)\sin^2 k} \approx 2 + \left(c_1 - c_2 \log U^2\right) U^2 + \cdots ,$$

valid for small values of U, show that the energy per carbon of the atomic chain is always minimized when $U > 0$.