

Exercise set 4 (due Thursday Feb 19)

- 1 Consider a diatomic molecule with onsite energies E_A and $E_B > E_A$. The hopping integral t between the two orbitals ϕ_A and ϕ_B is negative, and we use $x = t/\Delta E$ where $\Delta E = E_B - E_A$. Neglect the overlap integrals. Write down the Hamiltonian matrix of the molecule and find its eigenvalues and eigenstates. (You might want to express them in terms of the variable θ defined by $x = \tan 2\theta$) Discuss the eigenvalues and eigenstates in the limits $x \rightarrow 0$ and $x \rightarrow \infty$.

Calculate the probabilities of finding the bonding electron on the A atom and the B atom respectively. What do you find in the limit $x \rightarrow 0$? What does it mean?

- 2 Consider a linear chain with two atoms A and B per unit cell. Call a the lattice constant, E_A and E_B the onsite energies and t_1 and t_2 the hopping integrals corresponding to the short and long $A - B$ bonds respectively. Neglect the overlap integrals.

Write down the Bloch basis associated with the atomic orbitals ϕ_A and ϕ_B , and calculate the Hamiltonian matrix in this basis.

Find the eigenvalues of the infinite chain and plot the band structure in the three following limits:

- 1- $E_A = E_B$ and $t_1 = t_2 = t$
- 2- $E_A = E_B$ and $t_1 = 2t_2 = 2t$
- 3- $E_A = 0$; $E_B = 2t$ and $t_1 = t_2 = t$

Calculate and plot the DOS in the first case on the same diagram as the band structure.

Can you do the same (only qualitatively, no calculations are required) for cases 2 and 3?