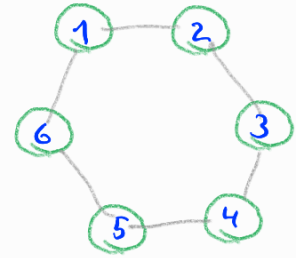


Homework 6a

The benzene molecule in Hückel model is described as six quantum dots.

The Hamiltonian for single electron in benzene ring is

$$H = -t (|1\rangle\langle 2| + |2\rangle\langle 3| + |3\rangle\langle 4| + |4\rangle\langle 5| + |5\rangle\langle 6| + |6\rangle\langle 1|) + \text{h.c.}$$



where h.c. is hermitian conjugation of previous terms.

- Find the single-particle energies and states

(assume $|\psi\rangle = \sum_n e^{i\alpha n} |n\rangle$ or $\sum_n \cos \alpha n |n\rangle = \text{Re} |\psi\rangle$ and $\sum_n \sin \alpha n |n\rangle = \text{Im} |\psi\rangle$)

- consider noninteracting electrons with spin $1/2$ occupying the ring. What is ground state and its energy?
- Consider simple coulomb interaction given by Hubbard term $\hat{V} = U \sum_n \hat{N}_n^+ \hat{N}_n^-$, where $\hat{N}_{n\sigma} = c_{n\sigma}^\dagger c_{n\sigma}$ is operator for number of electrons with spin σ in dot n .

Try to include this interaction either by perturbation theory or using the Hartree-Fock approach.