

Frankfurt, June 19, 2012

Exercises for Computational Methods in Solid State Theory
 SS 2012

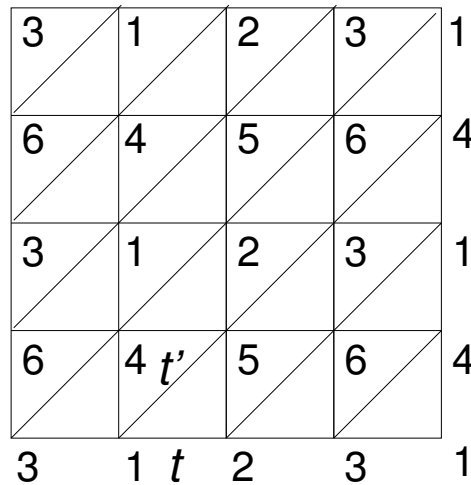
Exercise Set 8
 (Due date: Monday, June 25, 2012)

Exercise 8 (Exact diagonalization) (10 points)

The Hamiltonian of single-band Hubbard model with frustration is given as

$$(1) \quad H = -t \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} - t' \sum_{[i,j'], \sigma} c_{i\sigma}^\dagger c_{j'\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow},$$

where $c_{i\sigma}$ ($c_{i\sigma}^\dagger$) is the annihilation (creation) operator of an electron with spin σ at the i -th site, and U represents the Coulomb repulsion. Consider a 6-site toy model with periodic boundary condition as given in the figure below.



- Construct the Hamiltonian with $\frac{1}{3}, \frac{2}{3}$ and half-filling for $t = t' = 1$ and $U/t = 6$ using a programming language.
- Read the Hamiltonians obtained from a) into the Mathematica and calculate the eigenvectors and eigenvalues in the three cases.