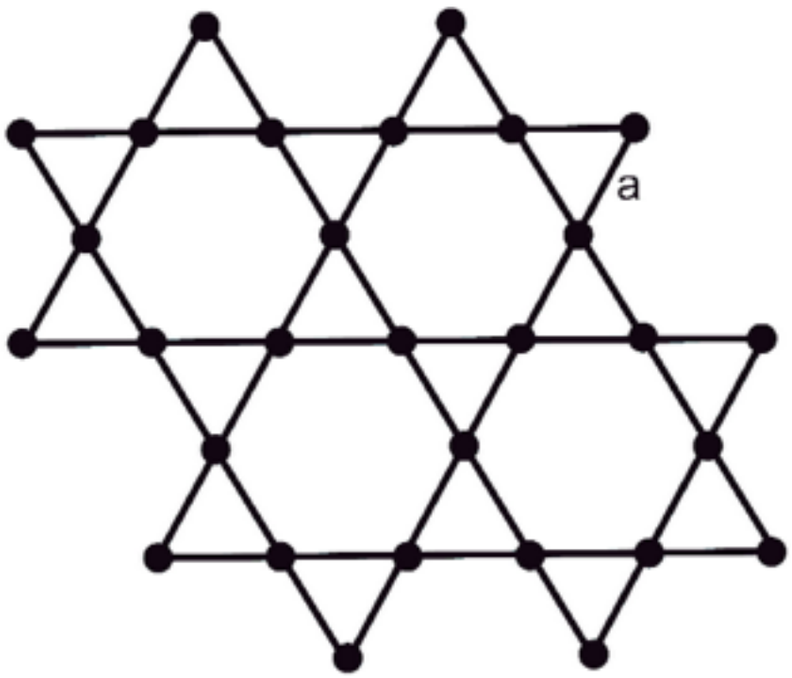
Kagome and pyrochlore lattice

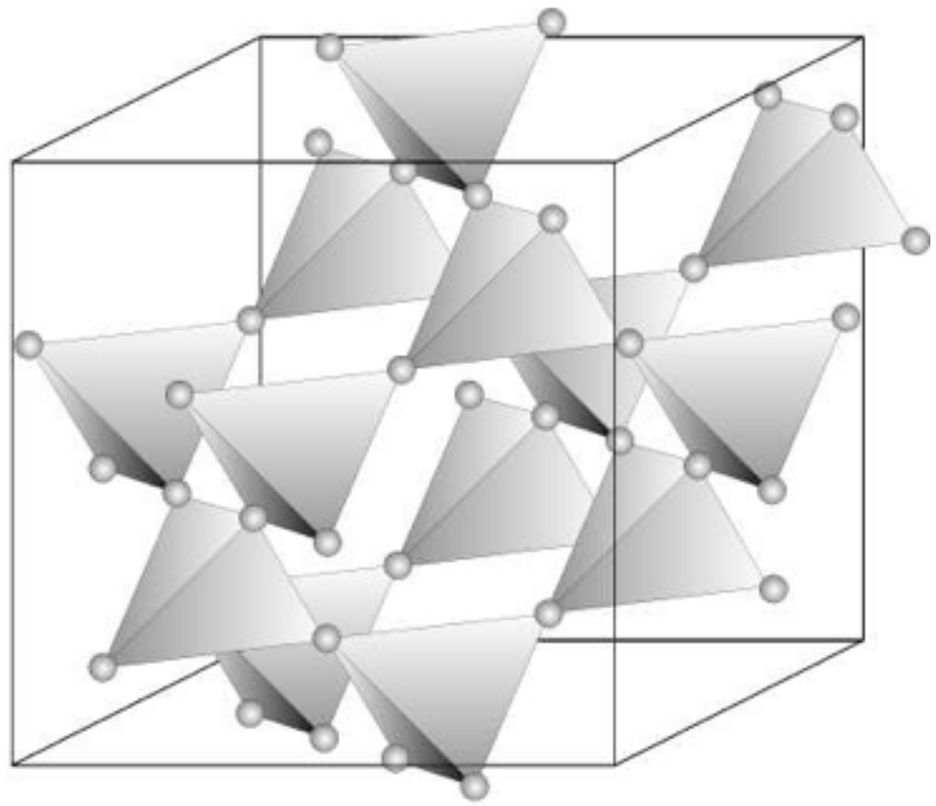
Calculate the band dispersion and density of states for the Kagome and pyrochlore lattices. We assume that there is one orbital on each lattice site. The hopping amplitude between nearest neighbors is t and 0 between any further neighbors, i.e. hopping take place only of the marked bonds in the lattice.

Hint: Identify the periodic lattice and its unit cell, perform the Fourier transformation, solve the eigenvalue problem for each k-vector. To calculate DOS for a uniform k-mesh in the primitive cell of reciprocal lattice and compute a histogram of the eigenenergies arising on this mesh. Use a finer mesh for smoother DOS.

kagome lattice (2D)



pyrochlore lattice (3D)



Nesting function

Derive a formula to calculate the nesting function (below). In analogy to the definition of DOS via a surface integral (lecture 1) derive a formula for the nesting function (joint density of states).

Hint: DOS with one Dirac delta in its definition leads to a surface integral. Nesting function with two Dirac delta functions leads to a line integral. Find out the line and define a suitable local coordinates along it.

One possible way to proceed is to define Dirac delta as a limit of Lorentzians with vanishing width. Evaluate the integrals for finite width and only then take the limit.

$$\Delta_{ij}(\mathbf{q}) = \sum_{\mathbf{k}} \delta(\epsilon_{i\mathbf{k}} - \epsilon_F)\delta(\epsilon_{j\mathbf{k}+\mathbf{q}} - \epsilon_F)$$

Fermi velocity in fcc Cu

Compute and visualize the distribution of the Fermi velocity on the Fermi surface of fcc Cu. Fermi velocity (group velocity at the Fermi level) is by definition perpendicular to the Fermi surface (why?), i.e. it can represented by a number (the length of the normal component).

Hint: The Wien2k code (OPTIC) allows computation of the group velocity for each band and k-point. Therefore we can generate two fields $\epsilon(\mathbf{k})$ and $|v(\mathbf{k})|$ on a chosen k-mesh. Choose a visualization software that can plot an isovalue surface of one field colored with values of another field.

$$\mathbf{v}_k = \nabla_k \epsilon_k$$

Remark: This problem is mostly about the visualization. In the past I was able to plot such figure with Open DX, but I am not sure whether this option is still available. I will not be able to provide you assistance with the visualization part. **So do not choose this project, unless you know how to do the plotting or know someone who can help you .**

Anti-ferromagnetic NiO with LDA and LDA+U

Study the magnetic ground state of NiO using Wien2k and LDA+U approach. NiO is a type II anti-ferromagent at room temperature. The unit cell of the AFM structure is larger than that of (paramagnetic) rock salt structure. The basis task is there for to set up the AFM unit cell. Note that the atomic positions in the larger unit cell are the same as in the rock salt structure, but the two Ni atoms in the AFM cell are not equivalent because they will have opposite spin polarization.

Use the LDA+U functional (see wien2k users guide) with U=8 eV and J=0.95 eV and perform two types of calculations (both for the AFM unit cell and with the same computational parameters): AFM structure with moments M and -M on the two Ni atoms and FM structure with the same M and M moments on Ni atoms. The two structures are selected during the initialization part of the calculation. Plot the DOS for the two solutions and compare their total energies. What conclusions can we draw from the results?

The lattice parameter of crystallographic unit cell is 4.1759 Å.

Intercalated Kogome lattice

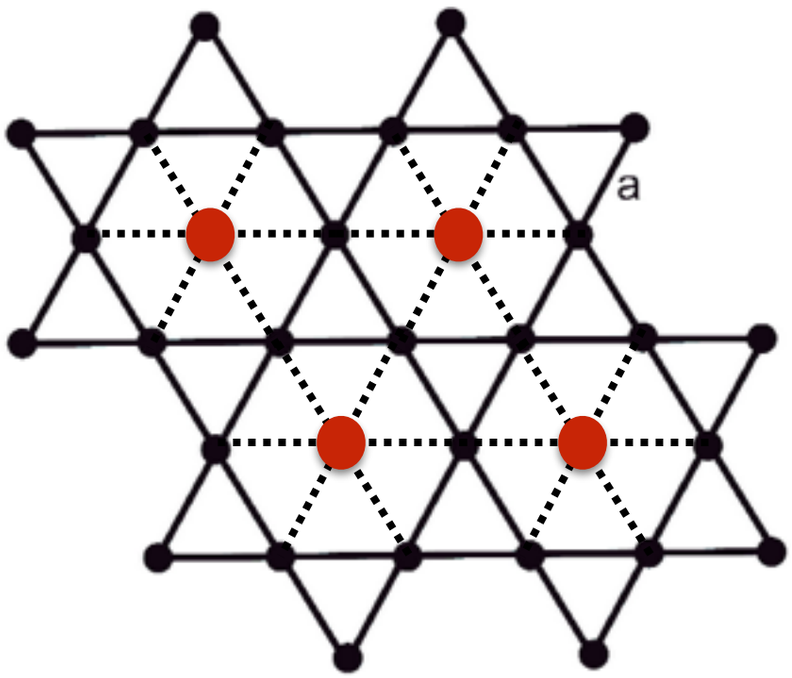
Calculate the band dispersion and density of states for the lattices in the picture. There are two distinct lattice sites with energies E_a (black) and E_b (red) and two hopping amplitudes t (full) and t' (dotted). Perform the calculation for

$E_a = E_b$ and t=t'

$E_a = E_b$ and t=2t'=1

$E_a = 2t+E_b$ and t=2t'=1

Hint: Identify the periodic lattice and its unit cell, perform the Fourier transformation, solve the eigenvalue problem for each k-vector. To calculate DOS for a uniform k-mesh in the primitive cell of reciprocal lattice and compute a histogram of the eigenenergies arising on this mesh. Use a finer mesh for smoother DOS.



Magnetic hcp Co

Study the magnetic ground state of hcp Co using Wien2k. Elemental cobalt is a collinear ferromagnet. The magnetic moment on Co is predominantly of spin character with small orbital contribution due to the spin-orbit coupling.

Calculate and compare the total energies in the non-magnetic and ferromagnetic structures. Include the spin-orbit coupling (see Wien2k user's guide) assuming the magnetization being parallel to the hexagonal c-axis. Determine the size of the spin and orbital moment (see LAPWDM chapter in Wien2k user's guide).

The lattice parameter are a=2.507 Å, c=4.069 Å

$SrVO_3$

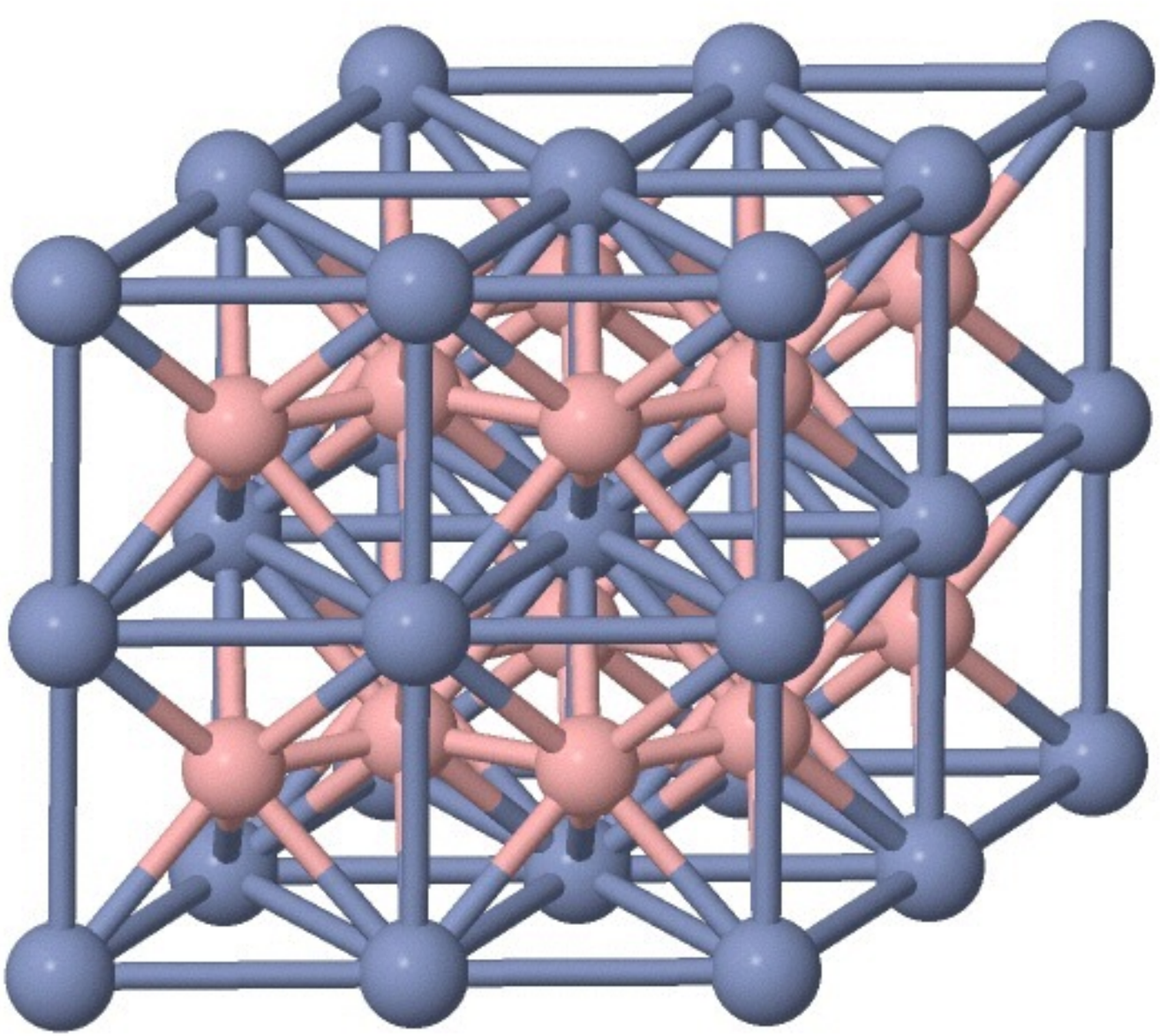
Construct a lattice model of $SrVO_3$ using Wien2k and wannier90. Find the structure of SrVO3 in the litereature. Construct Hamiltonians in the Wannier basis for the V d-bands and V-d+O-p bands. Prepare a table of nn and nun hoppings and discuss their symmetry. Plot several selected Wannier functions for both models.

The lattice parameter are a=3.838 Å.

Band structure and Fermi surface of CrB_2

Calculate the nonmagnetic (NM) and ferromagnetic (FM) band structure of CrB2 using Wien2k. Plot all sheets of the Fermi surface. Using the fat band plot determine the dominant character (atomic and orbital) of the states contributing to the given sheet. Does the Fermi surface depend on magnetic state (is it different for NM and FM solution)? Which sheets are and which not, why?

The lattice parameters are a=2.975 Å, c=3.070 Å. Space group P6/mmm (#191)



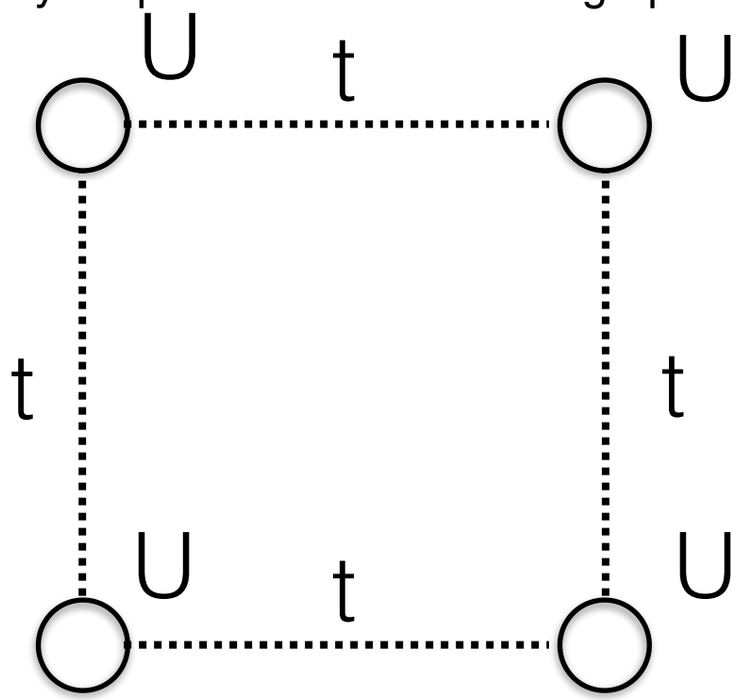
Hubbard 4-ring

Study the Hubbard model on a 4-ring using exact diagonalization. Calculate the spectrum the eigenstates of the problem in the 4 electron sector. Use U (t=1) as a variable parameter from U=0 to U=4. Calculate the spin-spin correlation functions *S* in the ground state (states in case of degeneracy). Extend the calculation to the finite temperature and calculate *S*(U=1) for temperatures from T=0.01 to T=1.

$$S = \tfrac{1}{4}(S_1^z S_2^z + S_2^z S_3^z + S_3^z S_4^z + S_4^z S_1^z)$$

$$\langle S \rangle_T = \frac{1}{Z} \sum_X \langle X|S|X\rangle \exp(-\tfrac{E_X}{T})$$

Hint: Diagonalize the different S_z sector separately. Represent the results as graphs E_i vs U, S vs U, S vs T



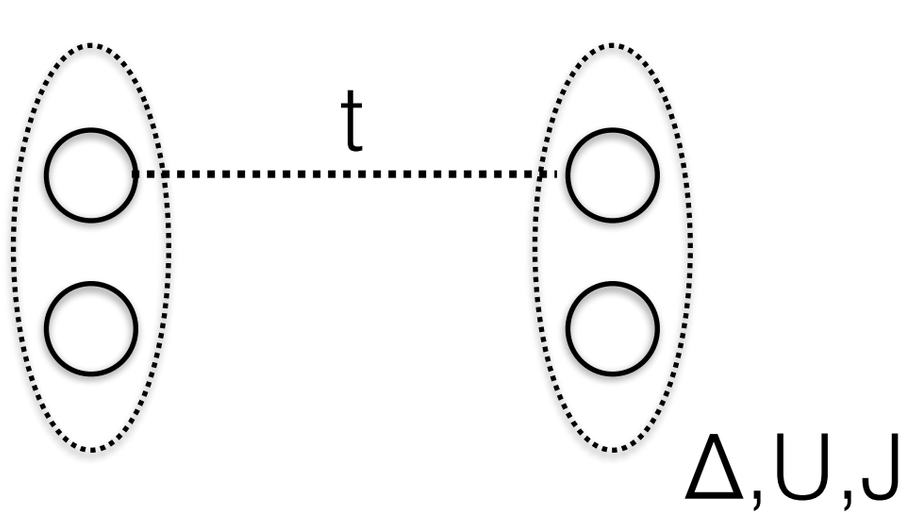
Hubbard molecule

Study the Hubbard molecule built from 2-orbital atoms. Calculate the spectrum the eigenstates of the problem in the **3 electron sector.** Calculate the spin-spin correlation function *S* in the ground state (states in case of degeneracy) for J form J=0 to J=1. Extend the calculation to the finite temperature and calculate *S*(J=0.2) for temperatures from T=0.01 to T=1. (t=1, U=4, U'=U-2J, J'=J, Δ=3)

$$S = S_1^z S_2^z + S_1^x S_2^x + S_1^y S_2^y$$

$$\langle S \rangle_T = \frac{1}{Z} \sum_X \langle X|S|X\rangle \exp(-\tfrac{E_X}{T})$$

Hint: Diagonalize the different S_z sector separately. Represent the results as graphs E_i vs J, S vs J, S vs T



Atomic Hamiltonian:

$$H_2 = U \sum_i n_{i\uparrow} n_{i\downarrow} + U' \sum_{\sigma\sigma'} \sum_{i>j} n_{i\sigma} n_{i\sigma'}$$
$$- J \sum_\sigma \sum_{i>j} (n_{i\sigma} n_{j\sigma} + c^\dagger_{i\sigma} c_{i\bar{\sigma}} c^\dagger_{j\bar{\sigma}} c_{j\sigma}) + J' \sum_{i>j} (c^\dagger_{i\uparrow} c^\dagger_{i\downarrow} c_{j\downarrow} c_{j\uparrow} + h.c.) + \frac{\Delta}{2}(n_a - n_b)$$

Hubbard triangle

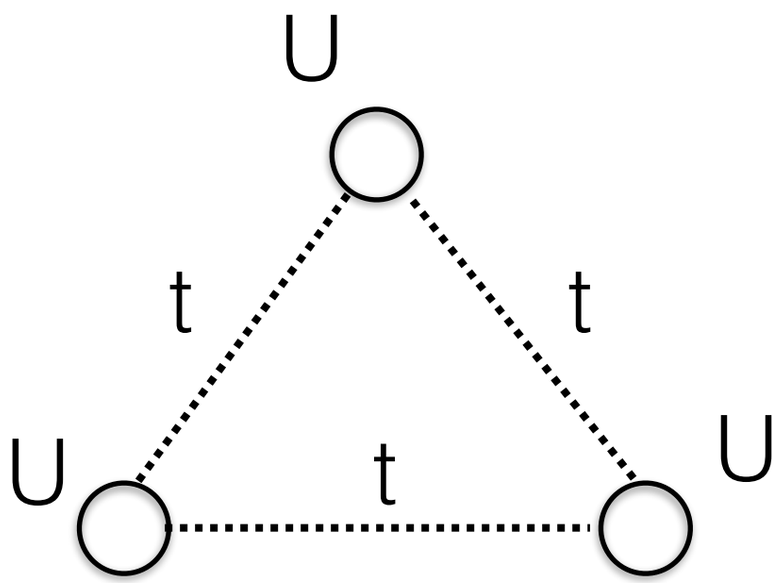
Study the Hubbard model on a triangle using exact diagonalization. Calculate the spectrum the eigenstates of the problem in the 2 and 3 electron sectors. Use U (t=1) as a variable parameter from U=0 to U=4. Calculate the spin-spin correlation functions *S* and double occupancy d in the ground state (states in case of degeneracy). Extend the calculation to the finite temperature and calculate *S*(U=1) for temperatures from T=0.01 to T=1.

$$S = \tfrac{1}{3}(S_1^z S_2^z + S_2^z S_3^z + S_3^z S_1^z)$$

$$\langle S \rangle_T = \frac{1}{Z} \sum_X \langle X|S|X\rangle \exp(-\tfrac{E_X}{T})$$

$$d = \tfrac{1}{3}(n_{1\uparrow} n_{1\downarrow} + n_{2\uparrow} n_{2\downarrow} + n_{3\uparrow} n_{3\downarrow})$$

Hint: Diagonalize the different S_z sector separately. Represent the results as graphs E_i vs U, S vs U, d vs U, S vs T



Strong coupling expansion

Derive the strong coupling expansion. Perform the Schrieffer-Wolff transformation to the order t^2 of the below model. We are interested in the filling of one electron per atom. The low-energy Hilbert space on each site contains two states: $b^\dagger_{i\uparrow}|0\rangle, b^\dagger_{j\downarrow}|0\rangle$

All constants in the Hamiltonian are assumed to be positive. The resulting low-energy model should have Heisenberg form, i.e., one has to derive the formula for the exchange constant. Can it be ferromagnetic for some parameters?

$$
\begin{aligned}
H =& t_a \sum_{ij\sigma} a^\dagger_{i\sigma} a_{j\sigma} + t_b \sum_{ij\sigma} b^\dagger_{i\sigma} b_{j\sigma} + V \sum_{ij\sigma} (a^\dagger_{i\sigma} b_{j\sigma} + b^\dagger_{i\sigma} a_{j\sigma}) \\
&+ \Delta \sum_{i\sigma} a^\dagger_{i\sigma} a_{i\sigma} \\
&+ U \sum_{i} (n^a_{i\uparrow} n^a_{i\downarrow} + n^b_{i\uparrow} n^b_{i\downarrow}) + (U - 2J) \sum_{i\sigma\sigma'} n^a_{i\sigma} n^b_{i\sigma'} - J \sum_{i\sigma} (n^a_{i\sigma} n^b_{i\sigma'} + a^\dagger_{i\sigma} a_{i-\sigma} b^\dagger_{i-\sigma} b_{i\sigma})
\end{aligned}
$$

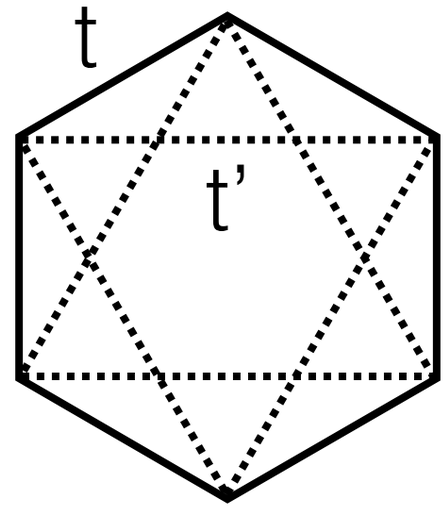
Hint: Generalization of the SW transformation of single-band Hubbard model derived in the class (with a-orbitals there are more intermediate states to sum over.

Fermions vs hard-core bosons

Calculate and compare the spectra of non-interacting spinless fermions and had-core bosons on a hexagon and 3x3 square lattice with periodic boundary conditions. For hexagon consider the nearest-neighbor (nn) hopping t and next-neighbor hopping t'=0 and t'=t. For the 3x3 lattice consider only nn hopping. Study all possible charge sectors, i.e., N=0,1,….,6 (or up to 9). Hard-core boson obey bosonic anti-commutation relations:

$$[b_i, b_j] = [b_i, b_j^\dagger] = 0 \quad i \neq j$$

$$\{b_i, b_i\} = \{b_i^\dagger, b_i^\dagger\} = 0, \quad \{b_i, b_i^\dagger\} = 1$$

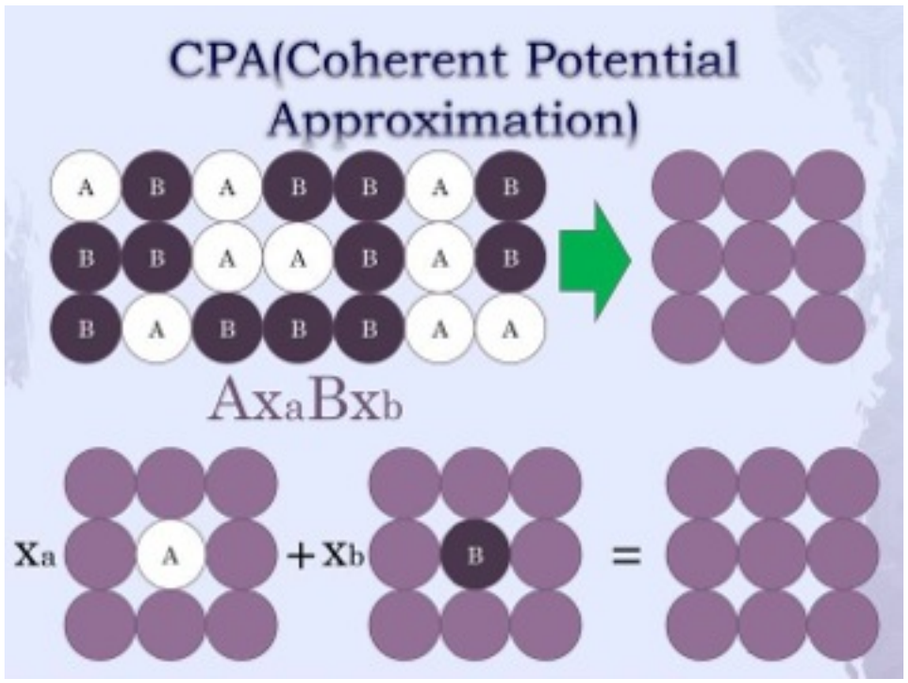


Hint: The Hilbert space of hard-core bosons is isomorphic to the Hilbert space of fermions (site double occupancy is forbidden). The fermionic and 'bosonic' Hamiltonian in occupation-number basis has the same zeros, but possibly different signs of the non-zero terms.

Coherent potential approximation (CPA)

A. Study convergence w.r.t. to the ***k***-, ω-grid and δ on a square lattice.
B. Consider other disorder distributions or other lattices (triangular, honeycomb, Kagome).
C. Study a doped model and/or adjust μ to a fixed number of particles.
D. Determine the self energy in the limit of strong disorder strength and compare CPA with this exact solution.
E. Compare CPA to the exact solution on a finite lattice.
F. Treat the Hubbard model with local interaction *U* instead of disorder ε_i using the dynamical mean field theory (DMFT). Here the impurity problem becomes an Anderson impurity model (AIM) instead of a resonant level model (RLM) (see lecture Jan. 7th).

$$H = \sum_{\mathbf{k}} \varepsilon_k c^\dagger_{\mathbf{k}} c_{\mathbf{k}} + \sum_i \epsilon_i c^\dagger_i c_i$$



Each letter is a separate project called 14A, 14B, … **Pick one**!