HOMEWORK SET 01

Selected Topic in Solid State Physics: Computational Physics Applications

UFV/VTFTL/20 lecture by Martin Gmitra

Winter Semester 2022, room KNKTFA

1. *[1 points]* Consider the following effective low energy Hamiltonian describing two band model of free-like electron and localized electron
$$\mathcal{H} = \begin{pmatrix} \frac{\hbar^2 k^2}{2m} & V \\ V^\dagger & \epsilon_c \end{pmatrix}$$
   a) diagonalize the Hamiltonian analytically.

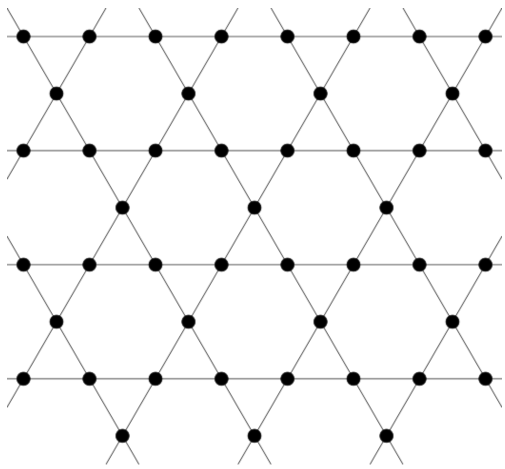
   b) plot the band structure for zero hybridization V and for positive and negative energy of localized state ϵ_c.

   c) analyze the band structure for positive ϵ_c and real, complex and pure imaginary hybridization V.

2. *[1 points]* Derive dispersion relation in tight-binding approximation for one-dimensional chain of atoms separated by the lattice constant a with s-orbital (follow derivation from Kaxiras' book)
   a) considering only nearest-neighbor hopping t.
   b) considering nearest-neighbor hopping t and next nearest-neighbor hopping t'.
   c) plot the band dispersion for the cases of $t = t'$, $t = 2t'$, and $t = t'/2$.
   d) consider finite chain length containing 3, 4, 5, ..., 20 atoms, calculate energy spectra and inspect the maximal and minimal eigenvalue for $t' = 1$.

3. *[2 points]* Derive tight-binding Hamiltonian for two-dimensional square lattice considering nearest-neighbor hopping t between two atoms in the unit-cell, the atom A is at (0,0) and atom B at (1/2,1/2) in units of lattice constant a.
   a) write computer program to diagonalize the Hamiltonian.
   b) calculate dispersion relation along high symmetry lines in k-space connecting Γ=(0,0), X=(1,0), M=(1,1) and Γ points in the 1st Brillouin zone. The coordinates of the high symmetry points are given in units of π/a.
   c) analyze bands width for small and large hopping t.

4. *[6 points]* Derive tight-binding Hamiltonian for the kagome lattice shown in the figure right considering nearest-neighbor hopping only. Plot band structure along the high symmetry points in the 1st Brillouin zone.



HOMEWORK SET 01

Selected Topic in Solid State Physics: Computational Physics Applications

UFV/VTFTL/20 lecture by Martin Gmitra

Winter Semester 2022, room KNKTFA

5. *[1 extra point]* From definition of the Wannier functions $\phi_n(\mathbf{r}-\mathbf{R}_j) = \dfrac{1}{\sqrt{N}}\sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}_j}\psi_{n\mathbf{k}}(\mathbf{r})$, where *n* is the band index and $\psi_{n\mathbf{k}}(\mathbf{r})$ is the state describing fulfilling the Bloch theorem, prove
   a) orthogonality $\langle\phi_n(\mathbf{r}-\mathbf{R}_j)|\phi_{n'}(\mathbf{r}-\mathbf{R}_{j'})\rangle = \delta_{nn'}\delta_{jj'}$
   b) that the original normalized Bloch state can be reconstructed from them in the form $\psi_{n\mathbf{k}}(\mathbf{r}) = \dfrac{1}{\sqrt{N}}\sum_{j} e^{i\mathbf{k}\cdot\mathbf{R}_j}\phi_n(\mathbf{r}-\mathbf{R}_j)$
6. *[1 extra point]* Show by means of the Wannier functions, defined in task 4, that the relation between energy dispersion of the Bloch electrons and the hopping matrix elements $t_{n,ji} = \int \psi_n^*(\mathbf{r}-\mathbf{R}_i)\mathcal{H}(\mathbf{r})\psi_n(\mathbf{r}-\mathbf{R}_j)\mathrm{d}\mathbf{r}$ can be expressed in the form $\epsilon_{n\mathbf{k}} = \sum_{\mathbf{R}_i} t_{n,ji}e^{-i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j)}$.