HOMEWORK SET 03
Theory of Condensed Matter
UFV/TKL1/99 lecture by Martin Gmitra
Winter Semester 2024, room KNKTFA

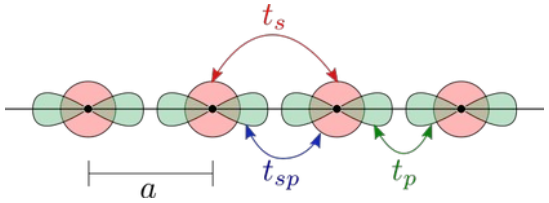
1. [*2 points*] Derive density of states for free-electrons in one, two and three dimensions.

2. [*3 points*] Fermi radius or Fermi wave vector of the Fermi sphere in free-electron model (or in the empty lattice) for simple cubic lattice with lattice constant a is $k_{\mathrm{F}} = \left(\frac{\pi}{a}\right)\left(\frac{3z}{\pi}\right)^{1/3}$. Find Fermi wave vectors for
   a) body-centered cubic crystal
   b) face-centered cubic crystal
   c) hexagonal close-packed structure

3. [1 *point*] When seeking a Bloch state within tight-binding approximation in the form
$$\varphi_{\mathbf{k}\ell i}(\mathbf{r}) = \frac{1}{\sqrt{N}}\sum_{\mathbf{R}'} e^{i\mathbf{k}\cdot\mathbf{R}'}\phi_\ell(\mathbf{r}-\mathbf{t}_i-\mathbf{R}')$$
show that
$$\langle\varphi_{\mathbf{k}mj}|\hat{H}|\varphi_{\mathbf{k}\ell i}\rangle = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}}\langle\phi_m(\mathbf{r}-\mathbf{t}_j)|\hat{H}|\phi_\ell(\mathbf{r}-\mathbf{t}_i-\mathbf{R})\rangle$$

4. [*2 points*] Calculate density of states $g(\epsilon)$ for one-dimensional linear chain with dispersion $\epsilon(k) = \epsilon_0 + 2t\cos(ka)$, where a is the lattice spacing, t is the hopping parameter and ϵ_0 is the on-site orbital energy. Test the result in terms of $\int g(\epsilon)\mathrm{d}\epsilon = 1$ that corresponds to the one electron per site.

5. Consider one-dimensional linear chain with one atom that have both an *s* and a *p* orbital. For hoppings assume t_s, t_p and t_{sp} between nearest-neighbor $s-s$ orbitals, $p-p$ orbitals and $s-p$ orbitals, as shows figure below. For on-site orbital energies assume ϵ_s and ϵ_p for the s and p orbitals respectively.



   a) [*2 points*] Calculate energy dispersion in 1st Brillouin zone.
   b) [1 *extra point*] Plot bands dispersion for $\epsilon_s = -2$, $\epsilon_p = 0.5$, $t_s = -0.8$, $t_p = 1.0$, and $t_{sp} = 0$.
   c) [1 *extra point*] Plot bands as in b) but for $t_{sp} = 0.2$ and discuss main difference.

6. Assume square lattice with $\mathbf{a}_1 = a\hat{\mathbf{x}}$, $\mathbf{a}_2 = a\hat{\mathbf{y}}$ being the lattice vectors, and two atoms with *s*-orbitals at positions $\mathbf{t}_1 = (\mathbf{a}_1+\mathbf{a}_2)/4$ and $\mathbf{t}_2 = 3(\mathbf{a}_1+\mathbf{a}_2)/4$.
   a) [4 *extra points*] Calculate in tight-binding approximation energy dispersion considering $\epsilon_s = 0$, orthogonal basis (no overlap) and hopping *t* between nearest-neighbors only.
   b) [*2 extra points*] Plot dispersion along the point $\mathbf{X} = \frac{2\pi}{a}\left(\frac{1}{2},0\right)$, $\mathbf{\Gamma} = (0,0)$, and $\mathbf{M} = \frac{2\pi}{a}\left(\frac{1}{2},\frac{1}{2}\right)$
   c) [*2 extra points*] Calculate velocity of the Bloch electrons.

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