

HOMEWORK SET 03
 Theory of Condensed Matter
 UFV/TKL1/99 lecture by Martin Gmitra
 Winter Semester 2021, room KNKTFA(Pa9-PKn)

- [2 points] Derive density of states for free-electrons in one, two and three dimensions.
- [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 $k_F = \left(\frac{\pi}{a}\right) \left(\frac{3z}{\pi}\right)^{1/3}$. Find Fermi wave vectors for
 - body-centered cubic crystal
 - face-centered cubic crystal
 - hexagonal close-packed structure

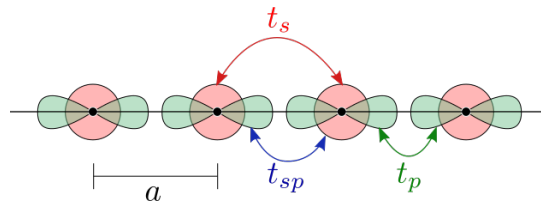
- [1 point] When seeking a Bloch state within tight-binding approximation in the form

$$\varphi_{\mathbf{k}\ell i}(\mathbf{r}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}'} e^{i\mathbf{k}\cdot\mathbf{R}'} \phi_{\ell}(\mathbf{r} - \mathbf{t}_i - \mathbf{R}')$$

show that

$$\langle \varphi_{\mathbf{k}m j} | \hat{H} | \varphi_{\mathbf{k}\ell i} \rangle = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} \langle \phi_m(\mathbf{r} - \mathbf{t}_j) | \hat{H} | \phi_{\ell}(\mathbf{r} - \mathbf{t}_i - \mathbf{R}) \rangle$$

- [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 $\int g(\epsilon) d\epsilon = 1$ that corresponds to the one electron per site.
- 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.



- [2 points] Calculate energy dispersion in 1st Brillouin zone.
 - [1 extra point] Plot bands dispersion for $\epsilon_s = -2$, $\epsilon_p = 0.5$, $t_s = -0.8$, $t_p = 1.0$, and $t_{sp} = 0$.
 - [1 extra point] Plot bands as in b) but for $t_{sp} = 0.2$ and discuss main difference.
- Assume square lattice with $\mathbf{a}_1 = a\hat{x}$, $\mathbf{a}_2 = a\hat{y}$ being the lattice vectors, and two atoms with s -orbitals at positions $\mathbf{t}_1 = (\mathbf{a}_1 + \mathbf{a}_2)/4$ and $\mathbf{t}_2 = 3(\mathbf{a}_1 + \mathbf{a}_2)/4$.
 - [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.
 - [2 extra points] Plot dispersion along the point $\mathbf{X} = \frac{2\pi}{a} \left(\frac{1}{2}, 0\right)$, $\Gamma = (0, 0)$, and $\mathbf{M} = \frac{2\pi}{a} \left(\frac{1}{2}, \frac{1}{2}\right)$
 - [2 extra points] Calculate velocity of the Bloch electrons.

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