

HOMEWORK SET 04
 Theory of Condensed Matter
 UFV/TKL1/99 lecture by Martin Gmitra
 Winter Semester 2024, room KNKTFA

1. [1 point] Show that matrix element of the momentum operator \mathbf{p} in the basis of the Bloch states is $\mathbf{p}_{nn'} = \hbar \mathbf{k} \delta_{nn'} + \mathbf{p}_{nn'}^u$, where $\mathbf{p}_{nn'}^u = \langle u_n | -i\hbar \nabla | u_{n'} \rangle$.
2. [1 point] Show that $\langle u_{n,\mathbf{k}_0} | H' | u_{n,\mathbf{k}_0} \rangle = 0$ for $\mathbf{k}_0 = 0$, where the perturbation $H' = \frac{\hbar}{m} \mathbf{k} \cdot (\mathbf{p} + \hbar \mathbf{k}_0)$ and $u_{n,\mathbf{k}}(\mathbf{r})$ is the periodic part of the Bloch function.
3. [2 points] We know that the Schrödinger equation for a periodic potential $U(\mathbf{r})$ can be written in the form $H(\mathbf{k})u_{n\mathbf{k}}(\mathbf{r}) = \varepsilon_{n\mathbf{k}}u_{n\mathbf{k}}(\mathbf{r})$ where $H(\mathbf{k}) = \frac{\hbar^2}{2m}(-i\nabla + \mathbf{k})^2 + U(\mathbf{r})$. Suppose we know energies for the Bloch states at the $\mathbf{k} = 0$, that is the solution of $H(0)u_{n0}(\mathbf{r}) = \varepsilon_{n0}u_{n0}(\mathbf{r})$. Since $u_{n0}(\mathbf{r})$ form a complete basis of functions periodic with lattice, we can expand $u_{n\mathbf{k}}(\mathbf{r}) = \sum_{n'} c_{nn'}(\mathbf{k})u_{n'0}(\mathbf{r})$. Find the eigenvalue problem for the coefficients $c_{nn'}(\mathbf{k})$, that is, find the Hamiltonian matrix $H(\mathbf{k})_{nn'} = \langle u_{n0} | H(\mathbf{k}) | u_{n'0} \rangle$.
4. [1 point] Calculate effective mass for 1D linear chain with one orbital in unit cell and find k -vectors within the 1st Brillouin zone where the inverse effective mass is zero. What would be the effective mass in case of isolated atoms?
5. [1 point] Show that $f(\mathbf{r} - \mathbf{r}_0) = \exp(-\mathbf{r}_0 \cdot \nabla)f(\mathbf{r})$. *Hint:* use Taylor expansion of the $f(\mathbf{r} - \mathbf{r}_0)$ around \mathbf{r}_0 .
6. [2 points] Suppose 1D crystal with a lattice constant a and dispersion relation $\epsilon(k) = \frac{\hbar^2}{ma^2} \left[\frac{7}{8} - \cos(ka) + \frac{1}{8} \cos(2ka) \right]$.
 a) Determine effective masses at the bottom and top of the band.
 b) Express Bloch velocities at the bottom and top of the band in terms of effective mass.
7. [1 point] From definition of the Wannier functions $\phi_n(\mathbf{r} - \mathbf{R}_j) = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\mathbf{k} \cdot \mathbf{R}_j} \psi_{n\mathbf{k}}(\mathbf{r})$, where n is the band index and $\psi_{n\mathbf{k}}(\mathbf{r})$ is the state describing fulfilling the Bloch theorem, prove the orthogonality $\langle \phi_n(\mathbf{r} - \mathbf{R}_j) | \phi_{n'}(\mathbf{r} - \mathbf{R}_{j'}) \rangle = \delta_{nn'} \delta_{jj'}$.
8. [1 point] The original normalized Bloch state can be reconstructed in the form $\psi_{n\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{N}} \sum_j e^{i\mathbf{k} \cdot \mathbf{R}_j} \phi_n(\mathbf{r} - \mathbf{R}_j)$, show that dispersion $\epsilon(k) = \epsilon_0 + \sum_{\mathbf{R}} t(\mathbf{R})e^{-i\mathbf{k} \cdot \mathbf{R}}$, and define ϵ_0 and $t(\mathbf{R})$.
9. [5 extra points] Low energy electrons in graphene are called Dirac or massless electrons and are described by the linear dispersion in momentum $\epsilon(\mathbf{k}) = v_F |\mathbf{k}|$, where v_F is the Fermi velocity, a material constant. Find an alternative definition of the effective mass to cure the diverging problem when using the standard definition $(1/m)^* = 1/\hbar^2 (\partial^2 \epsilon(k) / \partial k^2)$.

HOMEWORK SET 04
Theory of Condensed Matter
UFV/TKL1/99 lecture by Martin Gmitra
Winter Semester 2024, room KNKTFA

