HOMEWORK SET 04
Theory of Condensed Matter
UFV/TKL1/99 lecture by Martin Gmitra
Winter Semester 2021, room KNKTFA(Pa9-PKn)

1. [1 *point*] Show that matrix element of the momentum operator $\mathbf{p}$ in the basis of the Bloch states is $\mathbf{p}_{nn'} = \hbar\mathbf{k}\delta_{nn'} + \mathbf{p}^u_{nn'}$, where $\mathbf{p}^u_{nn'} = \langle u_n| - i\hbar\nabla|u_{n'}\rangle$.

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 $H' = \dfrac{\hbar}{m}\mathbf{k}\cdot(\mathbf{p} + \hbar\mathbf{k}_0)$ 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 $H(\mathbf{k}) = \dfrac{\hbar^2}{2m}(-i\nabla + \mathbf{k})^2 + U(\mathbf{r})$. 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 $f(\mathbf{r} - \mathbf{r}_0) = \exp(-\mathbf{r}\cdot\nabla)f(\mathbf{r})$. *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 $\epsilon(k) = \dfrac{\hbar^2}{ma^2}\left[\dfrac{7}{8} - \cos(ka) + \dfrac{1}{8}\cos(2ka)\right]$.
   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 $\phi_n(\mathbf{r} - \mathbf{R}_j) = \dfrac{1}{\sqrt{N}}\sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}_j}\psi_{n\mathbf{k}}(\mathbf{r})$, where *n* is the band index and $\psi_{n\mathbf{k}}(\mathbf{r})$ is the state describing fulfilling the Bloch theorem, prove 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 $\psi_{n\mathbf{k}}(\mathbf{r}) = \dfrac{1}{\sqrt{N}}\sum_j e^{i\mathbf{k}\cdot\mathbf{R}_j}\phi_n(\mathbf{r} - \mathbf{R}_j)$, show that dispersion $\epsilon(k) = \epsilon_0 + \sum_{\mathbf{R}} t(\mathbf{R})\mathrm{e}^{-i\mathbf{k}\cdot\mathbf{R}}$, 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 $(1/m)^* = 1/\hbar^2(\partial^2\epsilon(k)/\partial k^2)$.

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