University of Regensburg Summer Term 2018

Quantum Theory of Condensed Matter I

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Mo. 08:00-10:00 c.t., PHY 5.0.21

Sheet 3

1. Electronic Band Structure Within the Tight Binding Model ..... [10P]

The tight-binding model is typically used for calculations of the electronic band structure in presence of a periodic potential. When an atom is placed in a crystal, the atomic wave functions overlap adjacent atomic sites, and so are not true eigenfunctions of the crystal Hamiltonian. The overlap is less when electrons are tightly bound, which is the source of the descriptor "tight-binding".

The Hamiltonian describing the electron motion in a crystal can be written as

$$H = \frac{\mathbf{p}^2}{2m} + \sum_{\mathbf{R}} U(\mathbf{r}-\mathbf{R}) \quad \text{and} \quad H^{\text{at}}_{\mathbf{R}} = \frac{\mathbf{p}^2}{2m} + U(\mathbf{r}-\mathbf{R}), \tag{1}$$

where m is the free electron mass and $H^{\text{at}}_{\mathbf{R}}$ the Hamiltonian of an isolated atom placed on site $\mathbf{R}$ with potential $U(\mathbf{r}-\mathbf{R})$. Now, the small perturbation is given by $\Delta U(\mathbf{r}-\mathbf{R})$, defined by $H = H^{\text{at}}_{\mathbf{R}} + \Delta U(\mathbf{r}-\mathbf{R})$.

(a)(2P) The solution $\psi_{\alpha,\mathbf{k}}(\mathbf{r})$ to the time-independent single electron Schrödinger equation with the Hamiltonian H can be approximated as a linear combination of atomic orbitals $\varphi_\alpha(\mathbf{r}-\mathbf{R})$ which are the eigenstates of H_{at} (here α is a set of quantum numbers) with $H^{\text{at}}_{\mathbf{R}}\varphi_\alpha(\mathbf{r}-\mathbf{R}) = E_\alpha\varphi_\alpha(\mathbf{r}-\mathbf{R})$. Show that $\psi_{\alpha,\mathbf{k}}(\mathbf{r})$ which is given by

$$\psi_{\alpha,\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}} \exp(i\mathbf{k}\cdot\mathbf{R})\varphi_\alpha(\mathbf{r}-\mathbf{R}) \tag{2}$$

is of the Bloch form. Here, N is the number of atoms in the system.

(b)(4P) A good approximation for the eigenvalues of H is given by the Ritz method

$$\varepsilon_\alpha(\mathbf{k}) = \frac{\int \mathrm{d}^3r\, \psi^*_{\alpha,\mathbf{k}}(\mathbf{r}) H \psi_{\alpha,\mathbf{k}}(\mathbf{r})}{\int \mathrm{d}^3r\, \psi^*_{\alpha,\mathbf{k}}(\mathbf{r})\psi_{\alpha,\mathbf{k}}(\mathbf{r})}. \tag{3}$$

Show that $\varepsilon_\alpha(\mathbf{k})$ can be written in the tight-binding model as

$$\varepsilon_\alpha(\mathbf{k}) = E_\alpha + \frac{I_1 + \sum_{\mathbf{R}\neq 0} e^{-i\mathbf{k}\cdot\mathbf{R}} I_2(\mathbf{R})}{1 + \sum_{\mathbf{R}\neq 0} e^{-i\mathbf{k}\cdot\mathbf{R}} I_3(\mathbf{R})} \tag{4}$$

with

$$I_1 = \int \mathrm{d}^3r\, \varphi^*_\alpha(\mathbf{r}) \sum_{\mathbf{R}\neq 0} U(\mathbf{r}-\mathbf{R})\varphi_\alpha(\mathbf{r}), \tag{5}$$

$$I_2(\mathbf{R}) = \int \mathrm{d}^3r\, \varphi^*_\alpha(\mathbf{r}-\mathbf{R}) U(\mathbf{r}-\mathbf{R})\varphi_\alpha(\mathbf{r}), \tag{6}$$

$$I_3(\mathbf{R}) = \int \mathrm{d}^3r\, \varphi^*_\alpha(\mathbf{r}-\mathbf{R})\varphi_\alpha(\mathbf{r}). \tag{7}$$

Hint: Eq. 3 contains integrands of the form $\varphi^*_\alpha(\mathbf{r}-\mathbf{R}_2)U(\mathbf{r}-\mathbf{R}_3)\varphi_\alpha(\mathbf{r}-\mathbf{R}_1)$. Assume, that contributions from integrands with $\mathbf{R}_1 \neq \mathbf{R}_2 \neq \mathbf{R}_3 \neq \mathbf{R}_1$ (three center integrals) can be neglected.

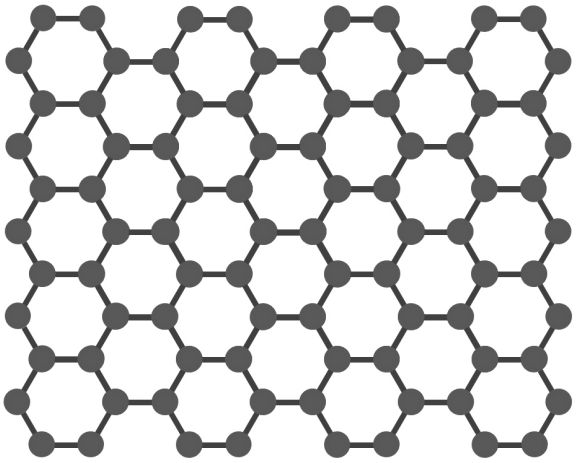
(c)(4P) Instead of atomic wave functions, use Wannier states to calculate the spectrum of a simple cubic crystal within the nearest neighbor approximation. Assume only s-bands so that the index α can be dropped. Calculate the effective electron mass for small k.

2. Graphene ..... [10P]

In graphene each carbon atom has three neighbours. Three electrons of a carbon atom are bound by a covalent σ-bond. The fourth electron is delocalized in the π-band and can propagate through the lattice. Every carbon atom contributes one electron to the π-band, which is therefore half-filled. We describe the system of delocalized electrons by the following Hamiltonian which includes only nearest neighbour hopping,

$$H = t \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle, \sigma} (c^\dagger_{\mathbf{r},\sigma} c_{\mathbf{r}',\sigma} + c^\dagger_{\mathbf{r}',\sigma} c_{\mathbf{r},\sigma})$$

where t is the hopping amplitude (overlap integral), $\langle \mathbf{r}, \mathbf{r}' \rangle$ are neighbouring sites and $c^\dagger_{\mathbf{r},\sigma}$ ($c_{\mathbf{r},\sigma}$) the creation (annihilation) operator of an electron on site $\mathbf{r}$ with spin σ in a Wannier state.



(a)(2P) Write down the primitive vectors of the spatial $(\mathbf{a_1}, \mathbf{a_2})$ and reciprocal lattice $(\mathbf{b_1}, \mathbf{b_2})$.

(b)(2P) Show the first Brillouin zone for this kind of lattice.

(c)(4P) Diagonalize the tight-binding Hamiltonian H and plot the energy spectrum. Why has graphene semimetallic properties?
Hint: Fourier-transform H into k-space and distinguish between the two different sublattices.

(d)(2P) Calculate the effective mass and Fermi velocity for Bloch electrons close to the corner of the first Brillouin zone with $k_x = \frac{4\pi}{3\sqrt{3}a}$ and $k_y = 0$. Here, a is the interatomic distance. Expand the dispersion relation in terms of $k_{x,y}a$ until the first non-zero order.