PHYS-E0421 Solid-State Physics (5cr), Spring 2019
Exercise session 1
Model solutions

1. **Effective mass**

   a) For a free electron, $E(k) = \hbar^2 k^2/2m_e$ and

   $$m_e^* = \frac{\hbar^2}{\partial^2 E/\partial k^2} = m_e. \tag{1}$$

   b) For a 1D tight-binding band, $E(k) = \epsilon_i - \alpha_i - 2\beta_i \cos(ka)$, and

   $$m_e^* = \frac{\hbar^2}{\partial^2 E/\partial k^2} = \frac{\hbar^2}{2a^2\beta_i \cos(ka)}. \tag{2}$$

   At the zone boundary, $k = \pi/a$ and $\cos(ka) = -1$. Thus, $m_e^* = -\hbar^2/2a^2\beta_i$. The width of the band is $W = \max_k[E(k)] - \min_k[E(k)] = 4\beta_i$, so

   $$m_e^* = \frac{2\hbar^2}{a^2 W \cos(ka)}. \tag{3}$$

   The group velocity of an electron is

   $$v_g = \frac{1}{\hbar}\frac{\partial E}{\partial k} = \frac{1}{\hbar} 2a\beta_i \sin(ka). \tag{4}$$

   At $k = \pi/2a$, v_g is a maximum $2a\beta_i/\hbar$. At this point, $m_e^* = \infty$. However, v_g is well behaved, even if m_e^* is not, so there are no discontinuities in conductivity, for example.

   Consider that the current model describes a metal, i.e., the band is half-filled. Then, applying a DC electric field cause a shift in k according to $k(t) = k(0) - eEt/\hbar$, see, e.g., Elliott Eq. (6.22). Thus, an oscillating behaviour of $v_g(k)$ might imply oscillating behaviour with time, $v_g(t)$, giving an AC current. However, this will only be observed if the electron can travel a distance in k-space $\delta k > \pi/a$ between collisions. However, collisions in a normal metal are so frequent that this is not possible. For example, for $\tau \approx 10^{-14}\,\mathrm{s}$ and $E \approx 1\,\mathrm{Vm}^{-1}$, $\delta k = eE\tau/\hbar \approx 16\,\mathrm{m}^{-1}$ (compare $k = \pi/a \approx 10^{10}\,\mathrm{m}^{-1}$).

2. **Semiclassical theory**

   The Hamiltonian of the system is

   $$H_0(\mathbf{r}) = -\frac{\hbar^2}{2m}\nabla^2 + v(\mathbf{r}) \tag{5}$$

   where $v(\mathbf{r} + \mathbf{R}) = v(\mathbf{r})$ is a periodic potential. With this Hamiltonian, the solutions of the time-independent Schrödinger equation are Bloch wave functions satisfying

   $$\psi(\mathbf{r} + \mathbf{R}) = e^{i\mathbf{k}\cdot\mathbf{R}}\psi(\mathbf{r}). \tag{6}$$

   The time evolution $\psi(\mathbf{r}, t)$ can be obtained from time-dependent Schrödinger equation

   $$i\hbar\frac{\partial \psi}{\partial t} = H_0\psi \tag{7}$$

in the form of

$$\psi(\mathbf{r},t) = e^{-iH_0(\mathbf{r})t/\hbar}\psi(\mathbf{r},0). \tag{8}$$

Now, consider

$$\begin{aligned}
\psi(\mathbf{r}+\mathbf{R},t) &= e^{-iH_0(\mathbf{r}+\mathbf{R})t/\hbar}\psi(\mathbf{r}+\mathbf{R},0) &(9)\\
&= e^{-iH_0(\mathbf{r})t/\hbar}e^{i\mathbf{k}\cdot\mathbf{R}}\psi(\mathbf{r},0) &(10)\\
&= e^{i\mathbf{k}\cdot\mathbf{R}}e^{-iH_0(\mathbf{r})t/\hbar}\psi(\mathbf{r},0) &(11)\\
&= e^{i\mathbf{k}\cdot\mathbf{R}}\psi(\mathbf{r},t). &(12)
\end{aligned}$$

Thus, ($\mathbf{k}(t) = \mathbf{k}(0)$, i.e., the long wavelength factor remains unaffected during the time-evolution.

Now, consider the Hamiltonian with an electric field

$$H = H_0 + e\mathbf{E}\cdot\mathbf{r}. \tag{13}$$

Proceeding like above, the time-evolution of the wave function becomes

$$\begin{aligned}
\psi(\mathbf{r}+\mathbf{R},t) &= e^{-iH(\mathbf{r}+\mathbf{R})t/\hbar}\psi(\mathbf{r}+\mathbf{R},0) &(14)\\
&= e^{-i(H(\mathbf{r})t+e\mathbf{E}\cdot\mathbf{R}t)/\hbar}e^{i\mathbf{k}\cdot\mathbf{R}}\psi(\mathbf{r},0) &(15)\\
&= e^{i\mathbf{k}\cdot\mathbf{R}}e^{-ie\mathbf{E}\cdot\mathbf{R}t/\hbar}e^{-iH(\mathbf{r})t/\hbar}\psi(\mathbf{r},0) &(16)\\
&= e^{i(\mathbf{k}-e\mathbf{E}t/\hbar)\cdot\mathbf{R}}\psi(\mathbf{r},t). &(17)
\end{aligned}$$

Here, $\mathbf{r}$-dependent phase terms can be collected together to a wave vector that depends on time

$$\mathbf{k}(t) = \mathbf{k}(0) - e\mathbf{E}t/\hbar. \tag{18}$$

3. **Landau levels**

The energy separation between two Landau levels n and $n+1$ is

$$\begin{aligned}
\Delta E = E_{n+1} + E_n = \frac{\hbar^2 k_z^2}{2m} + (n+\frac{3}{2})\hbar\omega_c - \frac{\hbar^2 k_z^2}{2m} - &&(19)\\
-(n+\frac{1}{2})\hbar\omega_c = \frac{3}{2}\hbar\omega_c - \frac{1}{2}\hbar\omega_c = \hbar\omega_c = \frac{\hbar e B}{m} &&(20)
\end{aligned}$$

Under a strong magnetic field strength of 1 T, the energy separation is approximately 0.7 meV. The thermal energy at the room temperature is approximately equal 25.7 meV and at the 1K ($k_B T \approx 0.1$ meV). at this point we can conclude, that the effects of Landau levels are only observed when the mean thermal energy is smaller than the energy level separation, $kT \ll \hbar\omega_c$, meaning low temperatures and strong magnetic fields.