1. Show that the Bloch wavefunction

$$\psi(\mathbf{r},\mathbf{t}) = \frac{\mathbf{1}}{\sqrt{\mathbf{V}}}\mathbf{u_k}(\mathbf{r})\mathrm{e}^{\mathrm{i}(\mathbf{k}\cdot\mathbf{r}-\omega\mathbf{t})}\,,$$

where $u_{\mathbf{k}}(\mathbf{r})$ is a periodic function with the period of the lattice is unchanged by a shift

$$\mathbf{k}' = \mathbf{k} + \mathbf{G_0}$$

where $\mathbf{G_0} = \mathbf{ha}^* + \mathbf{kb}^* + \mathbf{lc}^*$ is a reciprocal lattice vector.

2. Calculate the ratio k_F/k_m for metals of valency 1, for both the fcc and bcc structures, where k_F is the free electron Fermi wavenumber and k_m is the minimum distance in reciprocal space from the origin to the boundary of the first Brillouin zone.

3. Find the first Brillouin zone of the honeycomb/hexagonal lattice by considering the reciprocal lattice vectors and sketch it.

4. Consider $\mathrm{e}^{\mathrm{i}kx}$ and $\mathrm{e}^{-\mathrm{i}kx}$. What are the only orthogonal linear combinations, $\phi_1(x)$ and $\phi_2(x)$, of these functions which satisfy

$$\int \mathrm{d}x\phi_1^*(x)V(x)\phi_2(x) = 0\,,$$

for all k where $V(X)$ is a periodic potential which can be written as

$$V(x) = -\sum_{n=1}^{\infty} V_n \cos\left(\frac{2\pi n x}{a}\right)\,.$$

5. To be handed in. Near the boundary of the first Brillouin zone, for a one-dimensional chain of atoms, at $k = \pi/a$, the nearly free electron theory predicts that the most important term in the lattice potential is $V(x) \approx V_1 \cos[2\pi x/a]$. The wavefunction is then approximately

$$\psi(x) \approx \alpha\mathrm{e}^{\mathrm{i}kx} + \beta\mathrm{e}^{\mathrm{i}(k-2\pi/a)x}\,.$$

Substitute this wavefunction into Schrödinger's equation:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V(x)\psi(x) = \epsilon\psi(x)\,.$$

To find equations for α and β we can use that $\mathrm{e}^{\mathrm{i}kx}$ and $\mathrm{e}^{\mathrm{i}(k-2\pi/a)x}$ are *orthogonal*. Let us do this explicitly. Multiply the result of your substitution of the $\psi(x)$ into Schroödinger's equation by

   (a) $\mathrm{e}^{-\mathrm{i}kx}$, and
   (b) $\mathrm{e}^{-\mathrm{i}(k-2\pi/a)x}$.

Then integrate over all space to find two equations for α and β. Solve these equations and show that

$$\epsilon = \frac{\hbar^2 k^2}{2m} + \frac{\pi\hbar^2}{ma}\left[\frac{\pi}{a} - k \pm \sqrt{\left(\frac{\pi}{a} - k\right)^2 + \left(\frac{amV_1}{2\pi\hbar^2}\right)^2}\right]$$

is the energy. Show that this agree with our solution near $k = \pi/a$ and $k = 0$.

6. Calculate the variation with wavenumber of the electron effective mass m_e for the tight binding dispersion relation $\epsilon = B - 2t\cos(ka)$. Show that the value obtained at $k = \pi/a$ agrees with that obtained by expanding to second order in $k - \pi/a$ about $k = \pi/a$.