Exercise-sheet 2 (November 2, 2015)

1 In-class exercises

1.1 Floquet's theorem

Consider the second-order differential equation

$$\frac{d^2y}{dx^2}+\big(\epsilon+f(x)\big)y=0, \tag{1}$$

with $f(x+a)=f(x)$ and ϵ a constant.

(a) Show that one can always find a solution of the form

$$y(x+a)=k\,y(x), \tag{2}$$

where k is a (complex) constant.

(b) Given

$$\phi(x)=e^{-\mu x}y(x), \tag{3}$$

with $\mu=\frac{1}{a}\ln k$. Show that $\phi(x)$ is a periodic function with period a.

(c) What can you say about $y(x)$ depending on the values of μ?

1.2 Mathieu's equation

Consider Schrödinger's equation for an electron in a chain of atoms with lattice spacing a, where the potential felt by the electron and due to the atoms is modelled by the function $V(x)=V_0\cos\left(\frac{2\pi}{a}x\right)$.

(a) Use Floquet's theorem to write the electronic wavefunction as $\psi(x)=e^{ikx}u_k(x)$ and substitute a Fourier series for the periodic function $u_k(x)$. Show that the coefficients of the series satisfy a three-term recurrence relation.

(b) Assuming that $V_0 << 1$, find an approximate expression for the electronic wavefunction and its energy.

2 Homework - due date: November 9, 2015 (25 points).

2.1 Atoms as Dirac delta potentials

Consider a one-dimensional lattice of atoms with lattice spacing a, where each atom is represented by the potential $V(x) = V_0\delta(x)$.

(a) Assuming that between the atoms the electronic wavefunction is given by

$$\psi(x) = A\,e^{iKx} + Be^{-iKx}, \tag{4}$$

where A and B are two constants and $K = \sqrt{\frac{2mE}{\hbar^2}}$, with m the electron mass and E its energy, show that the derivative of $\psi(x)$ is discontinuous at the location of the atoms.

(b) One can extend the solution (4) to the full lattice by using Floquet's theorem, i.e. by writing $\psi(x) = e^{ikx}u_k(x)$ which implies

$$u_k(x) = Ae^{i(K-k)x} + Be^{-i(K+k)x}. \tag{5}$$

Use the fact that at the location of the atoms $\psi(x)$ is continuous and $\frac{d\psi}{dx}(x)$ is discontinuous to show that the electron energy E and the wavenumber k satisfy the relation

$$\cos ka = \frac{\alpha}{K}\sin Ka + \cos Ka, \tag{6}$$

where $K = \sqrt{\frac{2mE}{\hbar^2}}$ and α is to be determined.

(c) Plot the function $f(E) = \frac{\alpha}{K(E)}\sin K(E)a + \cos K(E)a$.

Given that $|f(E)| \leq 1$, do all values of E satisfy this condition?

(d) Consider the nearly free electron limit at $k = \frac{\pi}{a}$, i.e. assume $K = \frac{\pi}{a} + \nu$ with $\nu << 1$. Use the relation (6) to find some approximate value for ν. What is the electron energy to first order in ν?