Problems

1. Describe the energy for:
   (a) a free electron;
   (b) a strongly bound electron; and
   (c) an electron in a periodic potential.
   Why do we get these different band schemes?

2. *Computer problem*. Plot $\psi\psi^*$ for an electron in a potential well. Vary n from 1 to ~100. What conclusions can be drawn from these graphs? (*Hint*: If for large values for n you see strange periodic structures, then you need to choose more data points!)

3. State the two Schrödinger equations for electrons in a periodic potential field (Kronig–Penney model). Use for their solutions, instead of the Bloch function, the trial solution

$$\psi(x) = Ae^{ikx}.$$

   Discuss the result. (*Hint*: For free electrons $V_0 = 0$.)

*4. When treating the Kronig–Penney model, we arrived at four equations for the constants A, B, C, and D. Confirm (4.61).

5. The differential equation for an undamped vibration is

$$a\frac{d^2u}{dx^2} + bu = 0, \quad (1)$$

   whose solution is

$$u = Ae^{ikx} + Be^{-ikx}, \quad (2)$$

   where

$$k = \sqrt{b/a}. \quad (3)$$

   Prove that (2) is indeed a solution of (1).

6. Calculate the "ionization energy" for atomic hydrogen.

7. Derive (4.18a) in a semiclassical way by assuming that the centripetal force of an electron, mv^2/r, is counterbalanced by the **Coulombic attraction force**, $-e^2/4\pi\varepsilon_0 r^2$, between the nucleus and the orbiting electron. Use Bohr's postulate which states that the angular momentum $L = mvr$ (v = linear electron velocity and r = radius of the orbiting electron) is a multiple integer of Planck's constant (i.e., $n \cdot \hbar$). (*Hint*: The kinetic energy of the electron is $E = \frac{1}{2}mv^2$.)

8. *Computer problem*. Plot equation (4.67) and vary values for P.

9. *Computer problem*. Plot equation (4.39) for various values for D and γ.

10. The width of the potential well (Fig. 4.2) of an electron can be assumed to be about 2 Å. Calculate the energy of an electron (in Joules and in eV) from this information for various values of n. Give the zero-point energy.