

1. Suppose you had a 1d quantum well with depth $V_0 = 13.6\text{eV}$ and width $L = 1\text{\AA}$. How many bound states are possible? How does the energy of the lowest state compare with the bound state for a delta function potential $V(x) = -|V_0|L\delta(x)$. ?
2. For the potential $V(x) = -|V_0|L(\delta(x) + \delta(x - a))$, solve for the two possible eigenfunctions and sketch them . Derive a condition for which the higher energy state becomes unbound.
3. Try to modify the code given (in your lecture notes) and generate numerically the density of states $D(E)$ and plot it vs E .
4. This is somewhat open ended...Can you guess the limitations of the code? How can you improve it? Suppose the strengths of the delta function are not all same, but they are chosen from a random distribution (with a given mean and width). How do you think the answer would be modified?
5. A 2 dimensional lattice (of graphite) is defined by the two vectors, where a is some length

$$\mathbf{a}_1 = a \begin{pmatrix} 1 \\ 2, \frac{\sqrt{3}}{2} \end{pmatrix}$$

$$\mathbf{a}_2 = a \begin{pmatrix} -1 \\ 2, \frac{\sqrt{3}}{2} \end{pmatrix}$$

Calculate the two reciprocal lattice vectors.

6. Now consider a more generic problem. The unit vectors of a 2D lattice are \mathbf{a}_1 and \mathbf{a}_2 . The included angle between them is θ . For convenience take \mathbf{a}_1 to be along x axis. Calculate the reciprocal vectors \mathbf{b}_1 and \mathbf{b}_2 explicitly. What are the possible angles between the reciprocal vectors?

Show that the expression for the reciprocal vectors would be the following in 3D: (This is the form most textbooks will give you)

$$\begin{aligned} \mathbf{b}_1 &= 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)} \\ \mathbf{b}_2 &= 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)} \\ \mathbf{b}_3 &= 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)} \end{aligned} \quad (1)$$

7. What does $\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)$ imply? Work out the relevant expression for two dimensions.
8. find a relation between the volumes $\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)$ and the reciprocal unit cell volume $\mathbf{b}_1 \cdot (\mathbf{b}_2 \times \mathbf{b}_3)$
9. Consider a finite chain with N particles of mass m with spacing a , such that the density may be written as

$$\rho(x) = \sum_{n=0}^{N-1} m\delta(x - na)$$

Calculate the fourier transform of its density $\rho(k)$. What is the half width of each peak? How does your result differ from that of an infinite chain?

10. A lattice is built up of many atoms arranged in a periodic manner. Consider a function $f(\mathbf{r})$ that gives the electron density contributed by each atom (say). The full density at a point is the sum total of all the contributions from all the atoms.

$$\rho(\mathbf{r}) = \sum f(\mathbf{r} - \mathbf{R}_n)$$

Show that the fourier transform of this is a product of two distinct terms, irrespective of whether the sum is finite or infinite. What is the physical significance of each term?

11. Many semiconductors, like Si, Ge, GaAs, Diamond crystallise in a lattice called the Face centred cubic (FCC) lattice. The primitive unit vectors of the FCC lattice are given by

$$\begin{aligned} \mathbf{a}_1 &= \frac{a}{2}(\hat{x} + \hat{y}) \\ \mathbf{a}_2 &= \frac{a}{2}(\hat{y} + \hat{z}) \\ \mathbf{a}_3 &= \frac{a}{2}(\hat{z} + \hat{x}) \end{aligned}$$

- (a) Here a is some unit of length. What is the physical significance of a ?
- (b) Calculate the reciprocal lattice vectors.
- (c) Sketch the Wigner Seitz cell of the direct lattice and the reciprocal lattice (first Brillouin zone).
- (d) How many faces does the Wigner Seitz cell have? How many faces does the first Brillouin zone have?
12. • This problem is meant to guide you step by step, to understand how diffraction (of X ray, by a *finite sized crystal*) provides a way to deduce the crystal's reciprocal space.
- Consider a mono-atomic crystal with unit vectors \mathbf{a}_1 , \mathbf{a}_2 , \mathbf{a}_3 , the size of the crystal is such that it is a parallelopiped with dimensions $N_1 a_1 \times N_2 a_2 \times N_3 a_3$. A (plane wave) beam of x-ray is incident on it with wavevector \mathbf{k}_0 .
- Then write down an expression for the scattered wave at a point far enough from the crystal, so that the outgoing wave can be treated as a plane wave. This is not hard to achieve in practice - for a crystal of $\sim 1\text{mm}$, this means placing the detector at $\sim 1\text{m}$, for example.
- Now sum over the scattered waves from all the sites, associating the correct phases with each.

Finally express the scattered/diffracted intensity in some direction \mathbf{k} , taking into account the finite size of the crystal. Show that

$$I(\mathbf{k}) \propto \frac{\sin^2 \left[(\mathbf{k} - \mathbf{k}_0) \cdot \frac{N_1 \mathbf{a}_1}{2} \right]}{\sin^2 \left[(\mathbf{k} - \mathbf{k}_0) \cdot \frac{\mathbf{a}_1}{2} \right]} \times \frac{\sin^2 \left[(\mathbf{k} - \mathbf{k}_0) \cdot \frac{N_2 \mathbf{a}_2}{2} \right]}{\sin^2 \left[(\mathbf{k} - \mathbf{k}_0) \cdot \frac{\mathbf{a}_2}{2} \right]} \times \frac{\sin^2 \left[(\mathbf{k} - \mathbf{k}_0) \cdot \frac{N_3 \mathbf{a}_3}{2} \right]}{\sin^2 \left[(\mathbf{k} - \mathbf{k}_0) \cdot \frac{\mathbf{a}_3}{2} \right]}$$

When will this be non-zero? Explain the connection of the reciprocal lattice vectors with the expression you have derived. How would your answer be modified if the lattice was *not* mono-atomic?