Solution to Assignment 5.

1. (a) The time-independent Schrödinger equation for this problem is

$$\frac{-\hbar^2}{2m} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \psi = E \psi.$$ 

by separating the variables $$\psi(x,y) = X(x)Y(y)$$, we obtain

$$\frac{-\hbar^2}{2m} \left( \frac{1}{X} \frac{d^2X}{dx^2} + \frac{1}{Y} \frac{d^2Y}{dy^2} \right) = E$$

But since $$\frac{1}{X} \frac{d^2X}{dx^2}$$ is independent of $$y$$ and $$\frac{1}{Y} \frac{d^2Y}{dy^2}$$ is independent of $$x$$, both of these quantities must be constants, which we denote by

$$-\frac{\hbar^2}{2m} \frac{d^2X}{dx^2} = k_x^2, \quad -\frac{\hbar^2}{2m} \frac{d^2Y}{dy^2} = k_y^2$$

so that $$E = -\frac{\hbar^2}{2m} (k_x^2 + k_y^2)$$ is the total energy and

$$\frac{d^2X}{dx^2} + k_x^2 X = 0, \quad \frac{d^2Y}{dy^2} + k_y^2 Y = 0 \quad (1)$$

so that

$$\frac{\hbar^2}{2m} (k_x^2 + k_y^2) = E$$

is the total energy.

(b) The general solution of 1 is given by $$X(x) = A e^{ik_x x} + B e^{-ik_x x},$$ but the boundary conditions $$X(0) = X(L) = 0$$ imply that

$$A + B = 0, \quad A e^{ik_x L} + B e^{-ik_x L} = 0,$$

so that $$B = -A$$ and then the second condition becomes

$$\sin k_x L = 0,$$

so that $$k_x = \frac{\pi m}{L}$$ and thus $$X(x) = X_m(x) \equiv \sqrt{\frac{2}{L}} \sin \frac{\pi mx}{L}$$ is the normalized form for $$X$$. Similar reasoning holds for $$Y(y) = Y_n(y) \equiv \sqrt{\frac{2}{L}} \sin \frac{\pi ny}{L}$$ so that the wavefunctions for the quantum coral can be written

$$\psi_{mn}(x,y) = \sqrt{\frac{2}{L}} \sin \left( \frac{m\pi x}{L} \right) \sin \left( \frac{n\pi y}{L} \right), \quad E_{nm} = \frac{\hbar^2 \pi^2}{2m^2 L^2} (m^2 + n^2), \quad (m,n \geq 1). \quad (2)$$

(c) Suppose we ignore spin, so that each electron goes into a different state. The three lowest states are then $$\psi_{11}, \psi_{12}$$ and $$\psi_{21}.$$
The corresponding charge density is then

\[
\rho(x, y) = e(|\psi_{11}(x, y)|^2 + |\psi_{21}(x, y)|^2 + |\psi_{12}(x, y)|^2) \\
= \frac{4e}{L^2} \left( \sin^2 \frac{\pi x}{L} \sin^2 \frac{\pi y}{L} + \sin^2 \frac{2\pi x}{L} \sin^2 \frac{\pi y}{L} + \sin^2 \frac{\pi x}{L} \sin^2 \frac{2\pi y}{L} \right) \\
= \frac{4e}{L^2} \sin^2 \frac{\pi x}{L} \sin^2 \frac{\pi y}{L} \left[ 1 + 4(\cos^2 \frac{\pi x}{L} + \cos^2 \frac{\pi y}{L}) \right] 
\]

(3)

The density of charge looks something like:

![Figure 1: Density \(\rho(x, y)\) for three electrons in a quantum coral of unit side length. Spin is ignored in this example.](image)

Had you included electron spin, then you would have two electrons in the \(\psi_{11}\) state, and one in the \(\psi_{12}\) or \(\psi_{21}\) state, giving rise to a charge density of the form

\[
\rho(x, y) = \frac{8e}{L^2} \sin^2 \frac{\pi x}{L} \sin^2 \frac{\pi y}{L} \left[ 1 + 2\cos \frac{\pi x}{L} \right] 
\]

or

\[
\rho(x, y) = \frac{8e}{L^2} \sin^2 \frac{\pi x}{L} \sin^2 \frac{\pi y}{L} \left[ 1 + 2\cos \frac{\pi y}{L} \right] 
\]

corresponding to the asymmetric charge distributions:

![Figure 2: Density \(\rho(x, y)\) for three electrons in a quantum coral of unit side length, taking spin into account.](image)
2. (a) For a single delta function potential \( V(x) = -V_0 \delta(x) \) the Schrödinger equation is

\[
\left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} - V_0 \delta(x)\right] \psi(x) = E \psi(x)
\]

which implies that

\[
\psi(x) = \begin{cases} 
AL e^{-\kappa x} + BR e^{\kappa x} & (x < 0) \\
AR e^{-\kappa x} + BL e^{\kappa x} & (x > 0)
\end{cases}
\] (4)

where \( E = -\frac{\hbar^2 \kappa^2}{2m} \), subject to the boundary conditions

\[
\psi(0^+) = \psi(0^-), \quad \psi'(0^+) + \kappa_0 \psi(0^+) = \psi'(0^-) - \kappa_0 \psi(0^-),
\]

or

\[
\begin{pmatrix} 1 & 1 \\
-(\kappa + \kappa_0) & (\kappa - \kappa_0)
\end{pmatrix} \begin{pmatrix} AL \\
BL
\end{pmatrix} = \begin{pmatrix} 1 & 1 \\
-(\kappa - \kappa_0) & (\kappa + \kappa_0)
\end{pmatrix} \begin{pmatrix} AR \\
BR
\end{pmatrix}
\]

Inverting this equation, we have

\[
\begin{pmatrix} AR \\
BR
\end{pmatrix} = \begin{pmatrix} 1 + \lambda & \lambda \\
-\lambda & 1 - \lambda
\end{pmatrix} \begin{pmatrix} AL \\
BL
\end{pmatrix}, \quad \lambda = \frac{\kappa_0}{\kappa}, \quad \kappa_0 = \frac{mV_0}{\hbar^2}.
\] (5)

(b) We now consider a 1D “wire” with a whole line of such scattering potentials,

\[
V(x) = -V_0 \sum_{n=1,N} \delta(x - na)
\] (6)

There was a miss-print in the problem sheet. A more appropriate form for the wave-function in each segment is

\[
\psi(x) = An e^{-\kappa(x-na)} + Bn e^{\kappa(x-(n+1)a)}, \quad (x \in [na, (n+1)a]).
\] (7)

By examining the amplitudes of the wavefunction just before, and just after the \( n + 1 \)st potential spike, we can read off

\[
AR = An_{n+1}, \quad BR = B_{n+1} e^{-\kappa a}, \quad AL = An e^{-\kappa a}, BL = B_n,
\]

so that

\[
\begin{pmatrix} An_{n+1} \\
B_{n+1} e^{-\kappa a}
\end{pmatrix} = \begin{pmatrix} 1 + \lambda & \lambda \\
-\lambda & 1 - \lambda
\end{pmatrix} \begin{pmatrix} An e^{-\kappa a} \\
B_n
\end{pmatrix},
\]

which implies that the wavefunction along successive segments of the “wire” is related by a “transfer matrix” according to

\[
\begin{pmatrix} An_{n+1} \\
B_{n+1}
\end{pmatrix} = T \begin{pmatrix} An \\
B_n
\end{pmatrix}, \quad T = \begin{pmatrix} (1 + \lambda) e^{-\kappa a} & \lambda \\
-\lambda & (1 - \lambda) e^{\kappa a}
\end{pmatrix}.
\] (8)

(c) Clearly, if we introduce \( k \to k + 2\pi \) into the Bloch wave solution, the phase factor \( e^{ik} = e^{i(k+2\pi)} \) is unchanged, thus \( k \) is only defined up to multiples of \( 2\pi \).

(d) Comparing the Bloch wave solution with the results of section (c), we obtain the eigenvalue equation:

\[
\begin{pmatrix} (1 + \lambda) e^{-\kappa a} & \lambda \\
-\lambda & (1 - \lambda) e^{\kappa a}
\end{pmatrix} \begin{pmatrix} A_0 \\
B_0
\end{pmatrix} = e^{ik} \begin{pmatrix} A_0 \\
B_0
\end{pmatrix}.
\] (9)

which leads to the characteristic equation

\[
\begin{vmatrix} (1 + \lambda) e^{-\kappa a} - e^{ik} \\
-\lambda & (1 - \lambda) e^{\kappa a} - e^{ik}
\end{vmatrix} = 0
\]
or

\[(1 + \lambda)e^{-\kappa a} - e^{ik})(1 - \lambda)e^{\kappa a} - e^{ik}) + \lambda^2 = 0\]

or

\[1 - 2(\cosh \kappa a - \lambda \sinh \kappa a)e^{ik} + e^{2ik} = 0\]

and by completing the square:

\[e^{ik} = (\cosh \kappa a - \lambda \sinh \kappa a) \pm \sqrt{\cosh \kappa a - \lambda \sinh \kappa a} - 1\]

Recognizing that the argument inside the square root must be purely imaginary, we obtain

\[e^{ik} = (\cosh \kappa a - \lambda \sinh \kappa a) \pm i\sqrt{1 - (\cosh \kappa a - \lambda \sinh \kappa a)^2}\]

so that

\[\cos(k) = (\cosh \kappa a - \lambda \sinh \kappa a),\]
\[\tan(k) = \frac{\sqrt{1 - (\cosh \kappa a - \lambda \sinh \kappa a)^2}}{\cosh \kappa a - \lambda \sinh \kappa a}.

(e) To get an idea of the solutions, it is helpful to consider the case when \(\kappa_o a\) is large, corresponding to a small overlap between neighboring atoms. In this case, you can convince yourself that \(\kappa = \kappa_0 + \delta\) where \(\delta\) is a small quantity. Substituting this into the expression for \(\cos k\) obtained above, we derive

\[\cos k = e^{-\kappa_0 a} + \frac{\delta}{2} e^{\kappa_0 a}\]

so that we can solve for \(\delta\), which gives \(\delta = 2\cos k e^{-\kappa_0 a}\). The energy is then given by

\[E(k) = -\frac{\hbar^2 \kappa_0^2}{2m} (1 + 2\delta) = E_0 - 2t \cos k\]

where

\[t = -\frac{\hbar^2 \kappa_0^2}{m} e^{-\kappa_0 a}, \quad E_0 = -\frac{\hbar^2 \kappa_0^2}{2m}.

This defines an energy band of extended Bloch wave solutions. The lowest energy state corresponds to the uniform wavefunction

\[k=0 \quad \text{Uniform solution.}\]

\[k=\pi \quad \text{Staggered Solution.}\]

Figure 3:

whereas the highest energy state corresponds to the staggered solution.