GRADUATE QUANTUM MECHANICS: 501 Fall 2001

Solution to Assignment 5.

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

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

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

$$-\frac{1}{X}\frac{d^2X}{dx^2} = k_x^2, \quad -\frac{1}{Y}\frac{d^2Y}{dx^2} = k_y^2$$

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

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

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 $X(x) = Ae^{ik_xx}+Be^{-ik_xx}$, but the boundary conditions $X(0) = X(L) = 0$ imply that

$$A+B = 0, \qquad Ae^{ik_xL}+Be^{-ik_xL} = 0,$$

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

$$\sin k_xL = 0,$$

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

$$\begin{aligned}\psi_{mn}(x,y) &= \left(\frac{2}{L}\right)\sin\left(\frac{m\pi x}{L}\right)\sin\left(\frac{n\pi y}{L}\right),\\ E_{nm} &= \frac{\hbar^2\pi^2}{2m^2L^2}(m^2+n^2), \qquad (m,n\geq 1).\end{aligned} \tag{2}$$

(c) Suppose we ignore spin, so that each electron goes into a different state. The three lowest states are then ψ_{11}, ψ_{12} and ψ_{21}.

The corresponding charge density is then

$$\begin{aligned}
\rho(x,y) &= e(|\psi_{11}(x,y)|^2 + |\psi_{21}(x,y)|^2 + |\psi_{12}(x,y)|^2) \\
&= \frac{4e}{L^2}\left(\sin^2\frac{\pi x}{L}\sin^2\frac{\pi y}{L} + \sin^2\frac{2\pi x}{L}\sin^2\frac{\pi y}{L} + \sin^2\frac{\pi x}{L}\sin^2\frac{2\pi y}{L}\right) \\
&= \frac{4e}{L^2}\sin^2\frac{\pi x}{L}\sin^2\frac{\pi y}{L}\left[1 + 4(\cos^2\frac{\pi x}{L} + \cos^2\frac{\pi y}{L})\right] \qquad (3)
\end{aligned}$$

The density of charge looks something like:

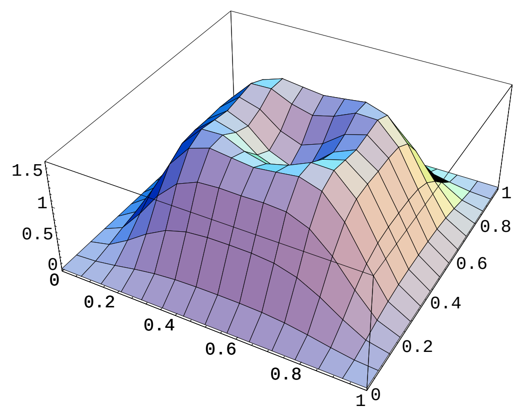

Figure 1: Density $\rho(x,y)$ for three electrons in a quantum coral of unit side length. Spin is ignored in this example.

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

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

or

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

corresponding to the asymmetric charge distributions:

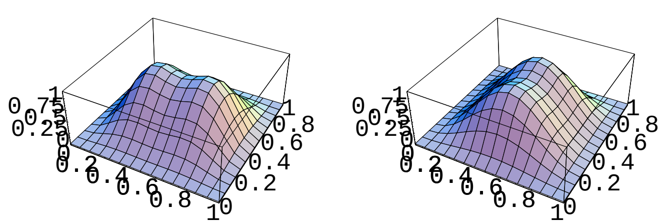

Figure 2: Density $\rho(x,y)$ for three electrons in a quantum coral of unit side length, taking spin into account.

2. (a) For a single delta function potential $V(x) = -V_o\delta(x)$ the Schrödinger equation is

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

which implies that

$$\psi(x) = \begin{cases} A_L e^{-\kappa x} + B_L e^{\kappa x} & (x < 0) \\ A_R e^{-\kappa x} + B_R e^{\kappa x} & (x > 0) \end{cases} \tag{4}$$

where $E = -\frac{\hbar^2\kappa^2}{2m}$, subject to the boundary conditions $\psi(0^+) = \psi(0^-)$, $\psi'(0^+) + \kappa_0\psi(0^+) = \psi'(0^-) - \kappa_0\psi(0^-)$, or

$$\begin{pmatrix} 1 & 1 \\ -(\kappa+\kappa_0) & (\kappa-\kappa_0) \end{pmatrix}\begin{pmatrix} A_L \\ B_L \end{pmatrix}\begin{pmatrix} 1 & 1 \\ -(\kappa-\kappa_0) & (\kappa+\kappa_0) \end{pmatrix}\begin{pmatrix} A_R \\ B_R \end{pmatrix}$$

Inverting this equation, we have

$$\begin{pmatrix} A_R \\ B_R \end{pmatrix} = \begin{pmatrix} 1+\lambda & \lambda \\ -\lambda & 1-\lambda \end{pmatrix}\begin{pmatrix} A_L \\ B_L \end{pmatrix}, \qquad \lambda = \frac{\kappa_o}{\kappa}, \qquad \kappa_o = \frac{mV_o}{\hbar^2}. \tag{5}$$

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

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

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

$$\psi(x) = A_n e^{-\kappa(x-na)} + B_n e^{\kappa(x-(n+1)a)}, \qquad (x \in [na,(n+1)a]). \tag{7}$$

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

$$A_R = A_{n+1}, \quad B_R = B_{n+1}e^{-\kappa a}, \quad A_L = A_n e^{-\kappa a}, B_L = B_n$$

so that

$$\begin{pmatrix} A_{n+1} \\ B_{n+1}e^{-\kappa a} \end{pmatrix} = \begin{pmatrix} (1+\lambda) & \lambda \\ -\lambda & (1-\lambda) \end{pmatrix}\begin{pmatrix} A_n e^{-\kappa a} \\ B_n \end{pmatrix},$$

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

$$\begin{pmatrix} A_{n+1} \\ B_{n+1} \end{pmatrix} = T\begin{pmatrix} A_n \\ B_n \end{pmatrix}, \qquad T = \begin{pmatrix} (1+\lambda)e^{-\kappa a} & \lambda \\ -\lambda & (1-\lambda)e^{\kappa a} \end{pmatrix}. \tag{8}$$

(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 2π.

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

$$\begin{pmatrix} (1+\lambda)e^{-\kappa a} & \lambda \\ -\lambda & (1-\lambda)e^{\kappa a} \end{pmatrix}\begin{pmatrix} A_o \\ B_0 \end{pmatrix} = e^{ik}\begin{pmatrix} A_o \\ B_0 \end{pmatrix}. \tag{9}$$

which leads to the characteristic equation

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

or

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

or

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

and by completing the square:

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

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

$$\begin{aligned} \cos(k) &= (\cosh\kappa a - \lambda\sinh\kappa a), \\ \tan(k) &= \frac{\sqrt{1 - (\cosh\kappa a - \lambda\sinh\kappa a)^2}}{\cosh\kappa a - \lambda\sinh\kappa a}. \end{aligned}$$

(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 δ 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 δ , which gives $\delta = 2\cos k e^{-\kappa_0 a}$. The energy is then given by

$$E(k) = -\frac{\hbar^2\kappa_0^2}{2m}(1+2\delta) = E_0 - 2t\cos k \tag{10}$$

where

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

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

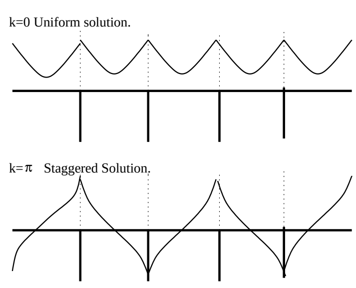

Figure 3:

whereas the highest energy state corresponds to the staggered solution