GRADUATE QUANTUM MECHANICS: 501 Fall 2001

Assignment 5. (Due weds 7th)

Read Sakurai p. 109- 143.

1. Consider an electron confined within a square "quantum coral" of side length L.

   (a) Write down the time-independent Schrödinger equation and by separating the variables $\psi(x,y) = X(x)Y(y)$, carefully present the arguments which show that X and Y must satisfy

   $$\begin{aligned} \frac{d^2X}{dx^2} + k_x^2 X &= 0, \\ \frac{d^2Y}{dx^2} + k_y^2 Y &= 0, \end{aligned} \tag{1}$$

   where $\frac{\hbar^2}{2m}(k_x^2 + k_y^2) = E$, the total energy.

   (b) Assuming the boundaries of the coral are completely inpenetrable, and $\psi = 0$ if $x \notin (0, L),\ y \notin (0, L)$, show that the wavefunctions for the quantum coral can be written

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

   (c) Suppose that the coral contained three, rather than one electron. The Exclusion principle forces each electron to go into different states. If the electrons go into the three lowest energy states, give an expression for the charge density in the coral and sketch or plot your results as a contour or 3D plot.

2. We have discussed how a single attractive delta-function attractive potential leads to a bound-state. This question asks: what happens when we have a periodic array attarctive delta-function potentials in 1D, uniformly spaced with separation a? Your answer will give you an insight into the way electrons in atoms hybridize to produce extended "Bloch" waves. This is a hard question, but I try to lead you through the steps. Go as far as you can and try to draw pictures for all your calculations

   (a) Consider first a single delta-function potential, $V(x) = -V_o\delta(x)$. Show that if

   $$\psi(x) = \begin{cases} A_L e^{-\kappa x} + B_L e^{\kappa x} & (x < 0) \\ A_R e^{-\kappa x} + B_R e^{\kappa x} & (x > 0) \end{cases} \tag{3}$$

   then the amplitudes on each side of the scattering potential are related by

   $$\begin{pmatrix} A_R \\ B_R \end{pmatrix} = \begin{pmatrix} 1+\lambda & \lambda \\ -\lambda & 1-\lambda \end{pmatrix} \begin{pmatrix} A_L \\ B_L \end{pmatrix}, \qquad \lambda = \frac{\kappa_o}{\kappa}, \qquad \kappa_o = \frac{mV_o}{\hbar^2}. \tag{4}$$

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

   $$V(x) = -V_0 \sum_{n=1,N} \delta(x - na) \tag{5}$$

   Suppose that the wavefunction in the nth segment is given by

   $$\psi(x) = A_n e^{-\kappa x} + B_n e^{\kappa(x-a)}, \qquad (x \in [na, (n+1)a]). \tag{6}$$

Show using the results of (a) that the wavefunction along successive segments of the "wire" is related by a "transfer matrix" according to

$$\begin{pmatrix} A_{n+1} \\ B_{n+1} \end{pmatrix} = T \begin{pmatrix} A_n \\ B_n \end{pmatrix}, \qquad T = \begin{pmatrix} (1+\lambda)e^{-\kappa a} & \lambda \\ -\lambda & (1-\lambda)e^{\kappa a} \end{pmatrix}. \tag{7}$$

(c) Since the potential is periodic, the problem is invariant under discrete translations. It is thus natural to look for solutions which are eigenstates of the translation operator: solutions that have got a definite "crystal momentum". Such a solution is called a "Bloch wave" and can be written

$$\begin{pmatrix} A_{n+1} \\ B_{n+1} \end{pmatrix} = e^{ik} \begin{pmatrix} A_n \\ B_n \end{pmatrix} = e^{ink} \begin{pmatrix} A_1 \\ B_1 \end{pmatrix} \tag{8}$$

Show that if we impose periodic boundary conditions $A_{N+1} = A_1$, $B_{N+1} = B_1$ that $k = 2n\pi/N$ where n is an integer. Convince yourself that changing $k \to k + 2\pi$ makes no difference, so that we can take $k \in [-\pi, \pi]$. This region of crystal momentum is called a "Brillouin zone".

(d) (Hard) By comparing the Bloch wave of (c) with the transfer matrix equation (b), write down an eigenvalue equation for e^{ik} and show that its solution is given by

$$\tan k = \frac{\sqrt{1 - [\cosh(\kappa a) - \lambda \sinh(\kappa a)]^2}}{\cosh(\kappa a) - \lambda \sinh(\kappa a)}, \qquad \lambda = \frac{\kappa_o}{\kappa}, \qquad \kappa_o = \frac{mV_o}{\hbar^2}. \tag{9}$$

(e) (Here: you may find it useful to consult a book on solid state physics, e.g. Ashcroft and Mermin) In the above equation, k may run from $-\pi$ to π, and corresponding to each k there is there is a band energy $E(\kappa) = -\frac{\hbar^2\kappa^2}{2m}$. For each value of k, there is a corresponding value of $E(k)$, corresponding to the band of allowed energies of the delocalized Bloch wavese. Sketch the wavefunction of states at the top and bottom of this energy band, and show qualitatively how $E(k)$ depends on the crystal momentum k.