1 May 2007, Quantum Mechanics, Problem 3

1.1 (a)

We have two independent potential wells, for the case $\lambda = \infty$. Then the solutions take the form:

$$\Psi = \sqrt{\frac{1}{L}} sin\left(\frac{\pi x}{L}\right) \quad Odd \tag{1}$$

$$\Psi = \frac{1}{\sqrt{L}} sin\left(\frac{\pi |x|}{L}\right) \quad Even \tag{2}$$

$$E = \left(\frac{\pi}{L}\right)^2 \frac{1}{2m} \tag{3}$$

1.2 (b)

We will solve Schrdinger's equation on either side of the well. Then the function should be continuous across the delta function, while the derivative is discontinuous, with a condition derived by integrating Schrdinger's equation around x=0:

$$\Psi(0) \equiv \Psi_{right}(0) = \Psi_{left}(0)$$

$$-\frac{1}{2m}\left(\Psi'_{right}(0) - \Psi'_{left}(0)\right) + \lambda\Psi(0) = 0$$

$$\Psi_{right}(L) = 0$$

$$\Psi_{left}(-L) = 0$$

Notice from the derivative condition that if the value of the function is 0 at x=0, then the derivative is continuous, i.e., the function doesn't "see" the delta function. Therefore, the sine solutions found in part a are still valid. It turns out that the other types of states, with $\Psi(0) \neq 0$, are of the form:

$$\Psi(x) = -\frac{\sqrt{2mE}B}{\lambda m}\cos(\sqrt{2mE}x) - Bsin(\sqrt{2mE}|x|)$$

Notice that these states are all even, so the lowest odd state will still be the one found in part a:

$$\Psi(x) = \frac{1}{\sqrt{L}} sin\left(\frac{\pi x}{L}\right) \quad Odd \tag{4}$$

$$E = \left(\frac{\pi}{L}\right)^2 \frac{1}{2m} \quad Odd \tag{5}$$

The energy for the other state can be derived from the derivative condition, together with one of the conditions of vanishing wavefunction at the ends. The transcendental equation is:

$$-\frac{\sqrt{2mE}L}{\lambda m L} = tan(\sqrt{2mE}L)$$

and to find the solution with lowest energy, one has to exploit the fact that $\lambda mL >> 1$, so the tangent must be small while its argument remains somewhat larger. The lowest-energy solution is:

$$\sqrt{2mE}L \approx \pi - \epsilon$$
$$\epsilon = \frac{\pi}{\lambda mL}$$
$$E = \frac{1}{2m}\left(\frac{\pi}{L}\right)^2\left(1 - \frac{2}{\lambda mL}\right) \quad Even \tag{6}$$

1.3 (c)

$$\Psi(x,0) = \begin{cases} 0, & x < 0 \\ \sqrt{\frac{2}{L}}sin\left(\frac{\pi x}{L}\right), & x > 0 \end{cases}$$

Notice that the even and odd functions are orthogonal to each other, since the integral from -L to L of the product of an even and an odd function must be 0. This will come in handy shortly. We express this initial state as a linear combination of other states:

$$\Psi(x,0) = \sum_n \alpha_n \Psi_e n + \sum_n \beta_n \Psi_o n$$
$$\Psi_{en} = n\pi B \frac{1}{mL\lambda} cos\left(\frac{n\pi x}{L}\right)\left(-1 + \frac{|x|}{L}\right) - Bsin\left(\frac{n\pi|x|}{L}\right)$$

where $\Psi_e n$ are the even states found earlier, and $\Psi_o n$ are the odd states, while the coefficients α_n and β_n need to be determined specifically for our $\Psi(x,0)$. We do this by taking the dot product with one of the even states, for instance:

$$< \Psi_e m|\Psi(x,0) >= \sum_n \alpha_n < \Psi_e m|\Psi_e n >$$
$$< \Psi_{om}|\Psi(x,0) >= \sum_n \beta_n < \Psi_{om}|\Psi_{on} >$$

Some nasty algebra shows that:

$$< \Psi_{em}|\Psi_{en} >= \delta_{mn} B^2 L\left(1 + \frac{1}{\lambda mL}\right)$$
$$< \Psi_{om}|\Psi_{on} >= \delta_{mn}$$

to first order in $1/\lambda mL$. But we know by normalization that $< \Psi_{em}|\Psi_{em} >$ must be 1, so this gives us an expression for B:

$$B = \frac{1 - \frac{1}{2m\lambda L}}{\sqrt{L}}$$
$$\alpha_n =< \Psi_{en}|\Psi(x,0) >$$

$$\beta_n = < \Psi_{on}|\Psi(x,0) >$$

Letting $y = \frac{1}{m\lambda L}$, then we get the following expressions:

$$\alpha_n = -\delta_{n1} B\sqrt{\frac{2}{L}}\left(\frac{L}{2}+\frac{yL}{4}\right) + \sqrt{\frac{2}{L}}\frac{nBy}{L}(\delta_{n1}-1)\frac{L^2(-1)^{n-1}}{1-n^2}$$

$$\beta_n = \frac{\delta_{n1}}{2}$$

$$\Psi(x,t) = -B\sqrt{\frac{2}{L}}\left(\frac{L}{2}+\frac{Ly}{4}\right)\Psi_{e1}e^{-iE_{e1}t} + \sum_{n\neq 1}\sqrt{\frac{2}{L}}e^{-iE_{en}t}\frac{nBy}{L}\frac{L^2(-1)^{n-1}}{1-n^2}\Psi_{en} + \frac{1}{\sqrt{2L}}sin(\frac{\pi x}{L})e^{-iE_{o1}t}$$

$$\Psi(x,t) \approx -\frac{1}{\sqrt{2}}\left[\frac{\pi}{\sqrt{L}}ycos(\pi x/L)\left(-1+\frac{|x|}{L}\right) - Bsin(\frac{\pi|x|}{L})\right]e^{-iE_{e1}t}$$

$$+\sum_{n\neq 1}\sqrt{2}e^{-iE_{en}t}\frac{ny(-1)^n}{1-n^2}\frac{1}{\sqrt{L}}sin\left(\frac{n\pi|x|}{L}\right) + \frac{1}{\sqrt{2L}}sin\left(\frac{\pi x}{L}\right)e^{-iE_{o1}t} \quad First\,order$$

The probability we are looking for is:

$$P = \int_{-L}^{0}|\Psi(x,t)|^2\,dx$$

$$|\Psi(x,t)|^2 = -\frac{\pi y}{L}cos\left(\frac{\pi x}{L}\right)\left(-1+\frac{|x|}{L}\right)sin\left(\frac{\pi|x|}{L}\right)$$

$$-\frac{\pi y}{2L}cos\left(\frac{\pi x}{L}\right)\left(-1+\frac{|x|}{L}\right)2cos[(E_{o1}-E_{e1})t]sin\left(\frac{\pi x}{L}\right) + \frac{1}{2L}(1-y)sin^2\left(\frac{\pi x}{L}\right)$$

$$+\frac{1}{L}sin\left(\frac{\pi x}{L}\right)\left[\sum_{n\neq 1}2cos[(E_{en}-E_{e1})t]\frac{ny(-1)^n}{1-n^2}sin\left(\frac{n\pi x}{L}\right)\right]$$

$$+\frac{1-y/2}{2L}sin\left(\frac{\pi|x|}{L}\right)sin\left(\frac{\pi x}{L}\right)2cos[(E_{o1}-E_{e1})t]$$

$$+\left[\sum_{n\neq 1}2cos[(E_{o1}-E_{en})t]\frac{ny(-1)^n}{1-n^2}sin\left(\frac{n\pi|x|}{L}\right)\right]\frac{1}{L}sin\left(\frac{\pi x}{L}\right) + \frac{1}{2L}sin^2\left(\frac{\pi x}{L}\right)$$

After getting rid of all the terms that go away under the integral, this becomes:

$$|\Psi(x,t)|^2 = \frac{\pi yx}{L^2}sin\left(\frac{\pi x}{L}\right)cos\left(\frac{\pi x}{L}\right)(-1+cos[(E_{o1}-E_{e1})t])$$

$$+\frac{1}{2L}sin^2\left(\frac{\pi x}{L}\right)(2-y)(1-cos[(E_{o1}-E_{e1})t])$$

$$P = \frac{1-cos[(\frac{y}{m}\left(\frac{\pi}{L}\right)^2)t]}{2} \approx \frac{\pi^4 t^2\hbar^6}{4\lambda^2 m^4 L^6} \tag{7}$$