Quantum Mechanics and Atomic Physics 750:361

Prof. Sean Oh, Fall 2011

HW #4

1. Consider the semi-infinite potential well illustrated in Figure P3.11 of Reed Problem 3-11: Each of the following parts is worth one full HW problem for grading.

(a) Set up and solve the SE for this system; assume E < $V_0$. Apply the appropriate boundary conditions at x=0 and x=L, show that $\tan(\xi) = -\frac{\xi}{\sqrt{K^2-\xi^2}}$, where $K^2 \equiv \frac{2mV_0L^2}{\hbar^2}$ and $\xi = k_2L$ with $k_2 \equiv \sqrt{\frac{2mE}{\hbar^2}}$.

(b) As we did in class, sketch $f(\xi) = \tan(\xi)$ and $g(\xi) = -\frac{\xi}{\sqrt{K^2-\xi^2}}$, and find how many bound states exist for $K^2$=100.

(c) With $K^2$=100, find all real and positive roots of $\xi$ in the equation [ $\tan(\xi) = -\frac{\xi}{\sqrt{K^2-\xi^2}}$ ] using a numerical root-finder (such as FindRoot[] in Mathematica).

(a)

Define region 1 as that for which $x < 0$, region 2 as $0 \leq x \leq L$, and region 3 as $x > L$. Since $V = \infty$ in region 1, $\psi = 0$ there. We restrict attention to bound states, that is, $E < V_o$. In regions 2 and 3 the solutions of the Schrödinger equation take the usual sinusoidal and exponential forms:

$$\psi_2 = A\cos(k_2 x) + B\sin(k_2 x), \qquad k_2 = \sqrt{2mE/\hbar^2}$$

and

$$\psi_3 = C\exp(k_3 x) + D\exp(-k_3 x), \qquad k_3 = \sqrt{2m(V_o - E)/\hbar^2}\,.$$

At $x = 0$, we must have $\psi_2 = 0$, which forces $A = 0$. As $x \to \infty$, we must have $\psi_3 \to 0$, which forces $C = 0$. Demanding the continuity of $\psi_2$ and $\psi_3$ and their first derivatives at $x = L$ leads to

$$B\sin(k_2 L) = D\exp(-k_3 L)$$

and

$$k_2 B\cos(k_2 L) = -k_3 D\exp(-k_3 L).$$

Dividing the first of these conditions by the second (or vice-versa) gives the energy eigenvalue condition

$$-k_3 \tan(k_2 L) = k_2.$$

Defining dimensionless variables $\xi = k_2 L$ and $\eta = k_3 L$, this condition can be expressed as

$$-\eta\tan\xi = \xi,$$

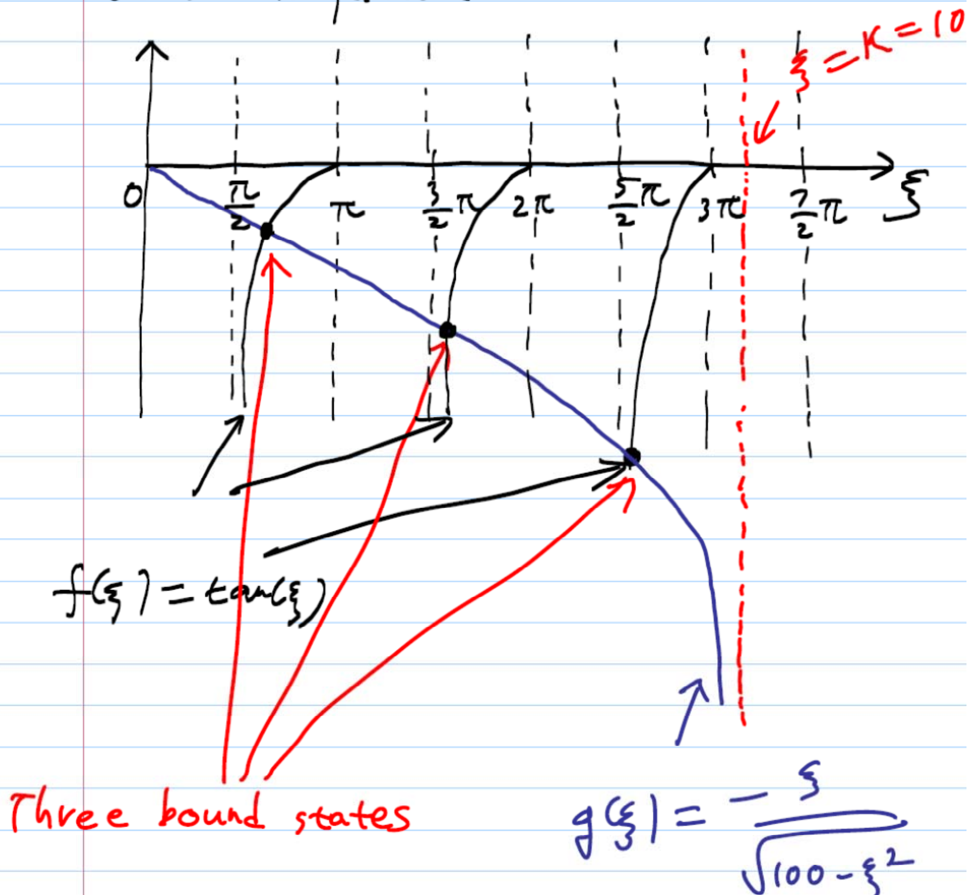
$\xi$ and $\eta$ also satisfy

$$\xi^2 + \eta^2 = \frac{2mV_o L^2}{\hbar^2} = K^2.$$

So $\tan(\xi) = -\frac{\xi}{\eta} = -\frac{\xi}{\sqrt{K^2 - \xi^2}}$.

(b) Because $\xi \equiv L\sqrt{\frac{2mE}{\hbar^2}}$,

Only positive $\xi$ values are valid solutions. Therefore, $f(\xi) = \tan(\xi)$ and $g(\xi) = -\frac{\xi}{\sqrt{K^2-\xi^2}}$ should be both negative




(c) $\xi_1 = 2.85234$, $\xi_2 = 5.67921$, $\xi_3 = 8.4232$ : See the Mathematica code below:

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FindRoot[Tan[y]==-y/√(100 - y²) ,{y,Pi}]
{y→2.85234}
FindRoot[Tan[y]==-y/√(100 - y²) ,{y,2Pi}]
{y→5.67921}
FindRoot[Tan[y]==-y/√(100 - y²) ,{y,3Pi}]
{y→8.4232}
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2. Reed. Prob. 3-17

**Problem 3-17**

Electrons of energy 10 eV are incident on a rectangular potential barrier of height 20 eV and width 50Å. What is the transmission coefficient?

First check that the thick barrier approximation is valid. This requires (MKS units)

$$\frac{2mL^2(V_o - E)}{\hbar^2} = \frac{2(9.109 \times 10^{-31})(5 \times 10^{-9})^2(1.602 \times 10^{-18})}{(1.055 \times 10^{-34})^2} = 6555.4$$

to be much greater than 1, which is so. Hence (again MKS units)

$$T_{Thick} \sim 16\left(\frac{E}{V_o}\right)\left(1 - \frac{E}{V_o}\right) \exp\left[-\frac{2L}{\hbar}\sqrt{2m(V_o - E)}\right]$$

$$\sim 4 \exp\left[-\frac{2(5 \times 10^{-9})}{1.055 \times 10^{-34}}\sqrt{2(9.109 \times 10^{-31})(1.602 \times 10^{-18})}\right]$$

$$\sim 4 \exp(-161.93) \approx 1.89 \times 10^{-70}.$$

3. Reed, Prob. 3-18

In quantum tunneling, the penetration probability is sensitive to slight changes in the height and/or width of the barrier. Consider an electron with $V(x) - E = 10$ eV incident on a barrier of width 20Å. By what factor does the penetration probability change if the width is increased to 21Å?

The penetration probability for a barrier of width x is given by $P = e^{-kx}$, where

$$k = \frac{2\sqrt{2m_e}}{\hbar}\sqrt{V(x) - E}.$$

If x is changed to $x + \Delta x$, then

$$\frac{P_x}{P_{x+\Delta x}} = e^{k\Delta x}.$$

For an electron with $V(x)\text{-}E = 10$ eV,

$$k = \frac{2\sqrt{2(9.1094 \times 10^{-31} kg)}}{(1.0546 \times 10^{-34} J-sec)}\sqrt{10(1.6022 \times 10^{-19} J)} = 3.240 \times 10^{10} m^{-1}.$$

For $\Delta x = 10^{-10}$ m,

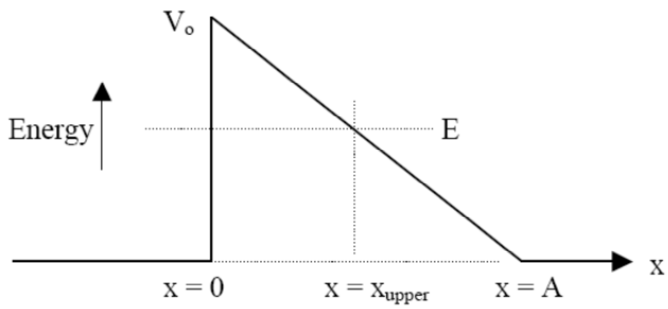
$$\frac{P_x}{P_{x+\Delta x}} = e^{3.24} = 25.5.$$

A 5% increase in the barrier width leads to a drop in the penetration probability by a factor of over 25.

4. Reed, Prob. 3-21

A potential barrier is defined by $V(x) = V_o (1 - x/A)$ for $0 \le x \le A$; $V(x) = 0$ otherwise. A particle of mass m and energy E ($< V_o$) is incident on this barrier from the left. Derive an expression for the penetration probability. Evaluate your result numerically for an electron incident on such a barrier with $V_o = 5$ eV, E = 2 eV, and A = 12 Å. Potentials of this form are used to model the spontaneous escape of electrons from metal surfaces subjected to electric fields, a process known as cold emission. The expression for the transmission probability is known as the *Fowler-Nordheim* formula.

A sketch of the potential is shown below. An particle of energy E ( $< V_o$) will cut the barrier at x = 0 and at the upper limit $x_{upper} = A(1-E/V_o)$.




The penetration probability is given by

$$\ln P \approx -\frac{2\sqrt{2m}}{\hbar}\int_0^{x_{upper}}\sqrt{V_o(1-x/A)-E}\,dx \approx -\frac{2\sqrt{2mV_o}}{\hbar}\int_0^{x_{upper}}\sqrt{(1-E/V_o)-x/A}\,dx.$$

Defining the new variable y = x/A transforms the integral to

$$\ln P \approx -\frac{2A\sqrt{2mV_o}}{\hbar}\int_0^{1-E/V_o}\sqrt{\alpha-y}\,dy\,,$$

where $\alpha = 1 - E/V_o$.

Solving the integral gives

$$\ln P \approx -\frac{2A\sqrt{2mV_o}}{\hbar}\left[-\frac{2}{3}(\alpha-y)^{3/2}\right]_0^{\alpha} \approx -\frac{4A\sqrt{2mV_o}}{3\hbar}(1-E/V_o)^{3/2}.$$

Substituting the given values (MKS units) yields

$$\ln P \approx -\frac{4(1.2 \text{ x } 10^{-9})\sqrt{2(9.109 \text{ x } 10^{-31})(8.010 \text{ x } 10^{-19})}}{3(1.055 \text{ x } 10^{-34})}(0.6)^{3/2} \approx -8.515,$$

or $P \sim 2.0 \text{ x } 10^{-4}$.

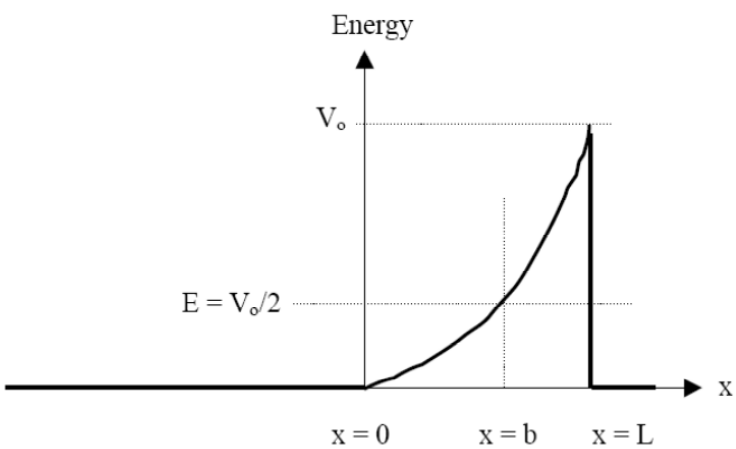
5. Reed, Prob. 3-22

A potential barrier is defined as

$$V(x) = \begin{cases} (V_o/L^2)x^2 & 0 \le x \le L \\ 0 & x < 0;\ x > L. \end{cases}$$

A particle of mass m and energy $V_o/2$ is incident on this barrier from $x < 0$. Derive an expression for the penetration probability. Evaluate your expression numerically for an electron striking such a barrier with L = 10Å and $V_o$ = 5 eV.

The situation is sketched below.




The barrier penetration integral is

$$\ln P \sim -\frac{2\sqrt{2m}}{\hbar} \int_b^L \sqrt{V(x) - E}\ dx .$$

With $E = V_o/2$, the lower limit of integration is $b = L/\sqrt{2}$, hence

$$\ln P \sim -\frac{2\sqrt{2mV_o}}{\hbar L} \int_{L/\sqrt{2}}^{L} \sqrt{x^2 - L^2/2}\ dx .$$

This integral is standard (see Appendix C); the result is

$$\ln P \sim -\frac{\sqrt{2mV_o}\,L}{\hbar} \left\{ \frac{1}{\sqrt{2}} - \frac{1}{2}\ln\left(1+\sqrt{2}\right) \right\} \sim -0.3768 \frac{\sqrt{mV_o}\,L}{\hbar} .$$

For an electron with L = 10Å and $V_o$ = 5 eV, P ~ 0.0473.

6. Reed, Prob. 3-23

A sprinter of mass 70 kg running at 5 m/s does not have enough kinetic energy to leap a wall of height 5 meters, even if all of that kinetic energy could be directed into an upward leap. If the wall is 0.2 meters thick, estimate the probability of the sprinter being able to "quantum tunnel" through it rather than attempting to leap over it.

The kinetic energy of the sprinter is

$$E = \frac{1}{2}mv^2 = \frac{1}{2}(70\ \text{kg})(5\ \text{m/s})^2 = 875\ \text{Joules}$$

The sprinter's potential energy at the top of the wall would be

$$V_o = mgh = (70\ \text{kg})(9.8\ \text{m/s}^2)(5\ \text{m}) = 3430\ \text{Joules},$$

showing that the sprinter does not possess sufficient energy to classically leap the wall. We therefore examine the problem as a quantum tunneling issue with a particle of mass 70 kg and energy E = 875 J incident on a barrier of height 3430 J and thickness 0.2 meters. This easily satisfies the condition for a thick barrier,

$$\frac{2mL^2(V_o - E)}{\hbar^2} >> 1,$$

since

$$\frac{2mL^2(V_o - E)}{\hbar^2} \sim 1.29 \times 10^{72}.$$

The penetration probability for a thick barrier is

$$T_{THICK} \approx 16\left(\frac{E}{V_o}\right)\left(1-\frac{E}{V_o}\right)\exp\left(-\frac{2\,L}{\hbar}\sqrt{2m(V_o-E)}\right).$$

This evaluates as

$$T \sim 3.04\exp(-2.268 \text{ x } 10^{36}).$$

To put this in a more convenient form, invoke the identity ln(x) = 2.303$\log_{10}$(x), from which we find $\log_{10}$(T) ~ -0.98 x $10^{36}$, which we can safely round to ~ -$10^{36}$, or $T \sim 10^{-10^{36}}$.