Lab 4 writeup, Numerical SE

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1 Pre-Lab exercises

Question 1.1. *Solve the two differential equations under the initial conditions* $(x(0), x'(0)) = (x_0, v_0)$.

$$\frac{d^2x}{dt^2} = \lambda^2 x \tag{1.1}$$

$$\frac{d^2x}{dt^2} = -\omega^2 x \tag{1.2}$$

Solution. Start with the first equation. The solution is some sum of regular exponentials. We express the solution as a sum of hyberbolic sin and cosine.

$$x = A\cosh(\lambda t) + B\sinh(\lambda t) \tag{1.3}$$

Imposing the initial condition $x(0) = x_0, x'(0) = v_0$, we obatin the following solution.

$$x = x_0\cosh(\lambda t) + v_0\sinh(\lambda t) \tag{1.4}$$

The solution for the second equation is similar. Change the hyperbolic trig functions to regular trig functions.

$$x = A\cos(\lambda t) + B\sin(\lambda t) \tag{1.5}$$

Imposing the initial condition $x(0) = x_0, x'(0) = v_0$, we obatin the following solution.

$$x = x_0\cos(\lambda t) + v_0\sin(\lambda t) \tag{1.6}$$

□

Question 1.2. *Consider a finite potential where the particle is bounded, i.e.* $E < V_0$. *What is the decay constant of the wavefunction of the particle outside the well? Also, what is the wavelength of the particle within the region?*

Proposition 1.1. *Let* k *be the decay constant and* λ *the wavelength.*

$$k = \frac{\sqrt{2m(V_0 - E)}}{\hbar} \tag{1.7}$$

$$\lambda = \frac{2\pi\hbar}{\sqrt{2mE}} \tag{1.8}$$

Proof. Solve the TISE.

$$E\psi(x) \;=\; -\frac{\hbar^2}{2m}\psi''(x) + V(x)\psi(x) \tag{1.9}$$

Assuming $V(x)$ is constant around the region, the equation simplifes to (1.1).

$$(E - V(x))\psi(x) \;=\; -\frac{\hbar^2}{2m}\psi''(x) \tag{1.10}$$

Within the well, the potential is zero. The solution is an harmonic oscillator. Following Robinett's notation, we label the wavenumber as q.

$$q \;=\; \frac{\sqrt{2mE}}{\hbar} \tag{1.11}$$

From the wavenumber, we derive the wavelength.

$$\lambda \;=\; \frac{2\pi}{q} \;=\; \frac{2\pi\hbar}{\sqrt{2mE}} \tag{1.12}$$

Outside the well, the potential has a value of V_0. Thus, the decay constant is

$$k \;=\; \frac{\sqrt{2m(V_0 - E)}}{\hbar}. \tag{1.13}$$

□

Question 1.3. *Take a moment to work out the scaled TISE, or reference past work you may have done on a problem set. We'll define an energy scale E_0 and a length scale x_0 and re-write the equation in terms of a dimensionless position $s = x/x_0$, energy $e = E/E_0$, and potential energy $v = V(x)/E_0$. If you do so, you should find that you can write the TISE in the form*

$$\frac{d^2\psi}{ds^2} = A(v(s) - e)\psi, \tag{1.14}$$

where A is a dimensionless constant.

Find A in terms of characteristic quantities, and then calculate its numerical value assuming that $x_0 = 1\,nm$, $m = m_e$, and $E_0 = 1\,eV$. You should find that for these parameters $A \approx 26.24$.

Solution. Faithfully applying the substitutions, we find the following formula for A.

$$A \;=\; \frac{2mE_0x_0^2}{\hbar^2} \;\approx\; 26.24 \tag{1.15}$$

□

Question 1.4. *Suppose that $V(x) = \frac{1}{2}m\omega^2 x^2$, as with a simple harmonic oscillator. Show that in this case we can write the TISE in the form*

$$\frac{d^2\psi}{ds^2} = A\left(\frac{1}{2}Bs^2 - e\right)\psi,$$

and find the constant B. You should see that for a suitable choice of scales x_0 and E_0 you can set both constants A and B to 1, allowing us to write the scaled TISE simply as

$$\frac{d^2\psi}{ds^2} = \left(\frac{1}{2}s^2 - e\right)\psi.$$

Proof. It is straightforward to see that

$$B = \frac{m\omega^2}{E_0}. \tag{1.16}$$

From (1.14), we purport that a subsitution $s = kl$ will simplify the equation into the desired form. Rewriting the equation in terms of l, we obtain the following.

$$\psi''(l) = k^2 A\left(\frac{1}{2}B(kl)^2 - e\right)\psi(l) \tag{1.17}$$

We wish

$$k^2 A = 1 \quad \text{and} \quad k^4 AB = 1 \tag{1.18}$$

which implies

$$k^2 B = 1 \quad \text{and} \quad A/B = 1 \tag{1.19}$$

and imposing $A/B = 1$, we derive an expression for the characteristic length with respect to the energy scale.

$$\boxed{x_0 = \frac{E_0}{\sqrt{2}\hbar}} \tag{1.20}$$

□

2 FSW with barriers

2.1 Solution for the wavefunction with barrier

Define our barrier potential to have width of 1, well height of $10V$, and barrier height of $5V$.

We first verify that there exists a case where the classical interpretation is violated. If the energy of the particle is less than the barrier potential of $5V$,

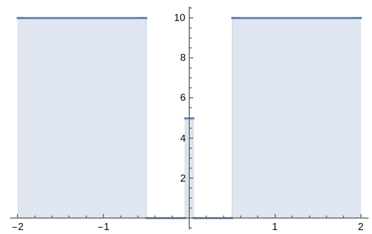


Figure 1: Figure of the FSW with Barrier Potential

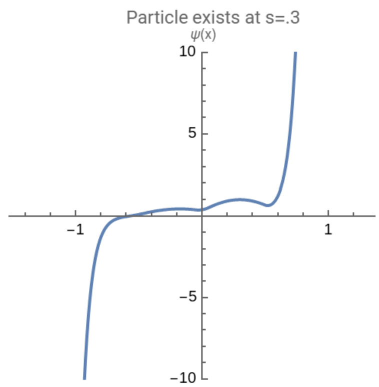


Figure 2: $E = 1, \psi(.3) = 1, \psi'(.3) = 0$. Apparently, the particle has spilled over the well.

then a particle confined in one side of the well should stay confined and not 'spill' to the neighboring well.

We also list out the first four energy eigenstates.

$$\begin{aligned} E_1 &= .83 & E_3 &= 3.45 \\ E_2 &= 1.21 & E_4 &= 4.73 \end{aligned} \tag{2.1}$$

Comparison with the FSW to be added

2.2 Taller and Wider Wells

In this section, we investigate potentials that have varying barrier dimensions.

We notice that the taller and the wider the barrier, the dimple of the first energy eigenstate gets bigger.

2.3 Limiting case

As we increase the height of the well and the width, the energy of the first eigenvalue approaches that of an infinite square well.

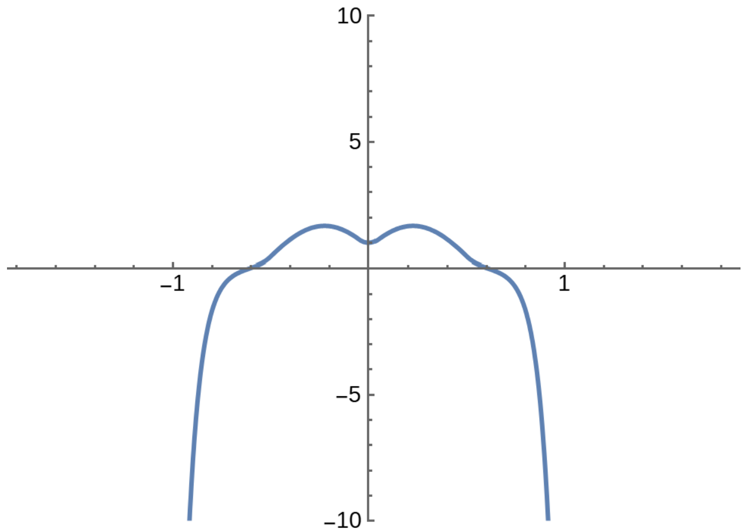
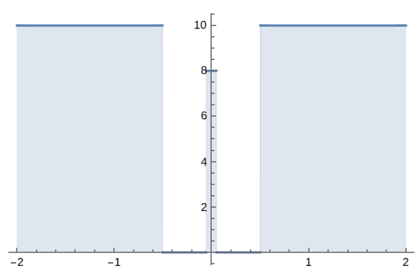
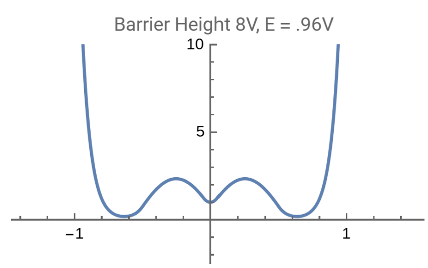


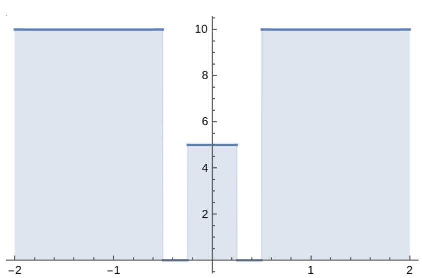
Figure 3: Wavefunction of the lowest energy eigenstate. Notice the 'dimple' on $s = 0$.



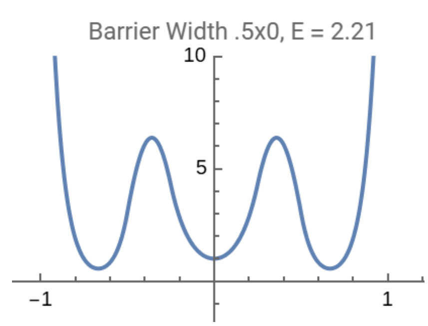
(a) h increased from $5V$ to $8V$



(b) Solution for the taller barrier



(c) Wider barrier, $w = .5x_0$



(d) Solution for wider barrier