1 Problem Set 4

1. **Finite Well - Bound States**

We are tasked to find bound states of a finite well. Recall that solving the wavefunction is tantamount to solving a boundary value problem. The boundary conditions are continuity of the function, smoothness of derivatives, and square-integrability. The potential of a finite well is given as

$$V = \begin{cases} -V_0, & -a \leq x \leq a \\ 0, & |x| > a \end{cases} \tag{1}$$

We are after the bound states. Hence, $E > 0$. Our task is to solve for the time-independent Schrodinger equation (TISE) for each region. at $x < a$, TISE reads

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = \kappa^2\psi \tag{2}$$

where $\kappa := \sqrt{-2mE}/\hbar$. The solution is an exponential function $\psi(x) = A\exp(-\kappa x) + B\exp(\kappa x)$. Square integrability (normalizability) condition disposes the first term as it blows up as $x \to -\infty$. Hence, in the region $x < a$, the wavefunction is

$$\boxed{\psi(x) = B\exp(-\kappa x)} \tag{3}$$

Inside the well, in the region $-a < x < a$, TISE reads

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = -l^2\psi \tag{4}$$

where $l := \sqrt{2m(E + V_0)}/\hbar$. The solution is an oscillating function $\psi(x) = C\sin(lx) + D\cos(lx)$. Both terms do not explode and we can't dispose any term. Hence,

$$\boxed{\psi(x) = C\sin(lx) + D\cos(lx)} \tag{5}$$

Lastly, at the region $x > a$, we solve Eq. (2) again. This time, as we approach $x \to \infty$, the exponential with the positive parameter explodes. This gives us the solution.

$$\boxed{\psi(x) = F\exp(-\kappa x)} \tag{6}$$

The wavefunction can be summarized as

$$\psi(x) = \begin{cases} B\exp(-\kappa x) & x < a \\ C\sin(lx) + D\cos(lx) & -a < x < a \\ F\exp(\kappa x) & x > a \end{cases} \tag{7}$$

Normally, we impose four boundary conditions for the remaining four coefficients: continuity and smoothness at point $x = -a$ and continuity and smoothness at point $x = a$. However, there exists a quick way of doing stuff - it is to exploit symmetry of the system. This can be done since the potential is an even function which assures that the solution must be either even or odd. Griffith's took care of the even solution. Now, it is our duty to solve for the odd parity. Symmetrizing the system for odd parity, the wave function takes the form

$$\psi(x) = \begin{cases} B\exp(-\kappa x) & x < a \\ C\sin(lx) & -a < x < a \\ -\psi(-x) & x > a \end{cases} \tag{8}$$

where, of course, negating the parameter of an odd function negates the function itself. Imposing continuity condition at $x = a$, we get

$$F\exp(-\kappa a) = C\sin(la) \tag{9}$$

Imposing smoothness condition at $x = a$, we get

$$-\kappa F\exp(-\kappa a) = lC\cos(la) \tag{10}$$

where we simply take the derivative of the continuity condition. Now, we proceed to divide the smoothness condition Eq. (9) by the continuity conditon Eq. (10) (we take divide the LHS by LHS, and the RHS by RHS of the said equations). This gives us

$$\frac{-\kappa F\exp(-\kappa a)}{F\exp(-\kappa a)} = \frac{lC\cos(la)}{C\sin(la)} \tag{11}$$

Simplifying this gives us

$$\kappa = -l\cot(la) \tag{12}$$

As we foresee some numerical work, we introduce some parameters for convenience: $z := la$ amd $z_0 = (a/\hbar)(\sqrt{2mV_0})$. From the definitions of the parameters κ and l, we see that

$$k^2 + l^2 = \frac{2mV_0}{\hbar^2} \tag{13}$$

and so

$$\kappa a = (z_0^2 - z^2)^{1/2} \tag{14}$$

then,

$$\kappa = -l\cot(la) = -\frac{z}{a}\cot(z) \iff \kappa a = -z\cot(z) \tag{15}$$

Hence,

$$\boxed{-\cot(z) = \left(\left(\frac{z_0}{z}\right)^2 - 1\right)^{1/2}} \tag{16}$$

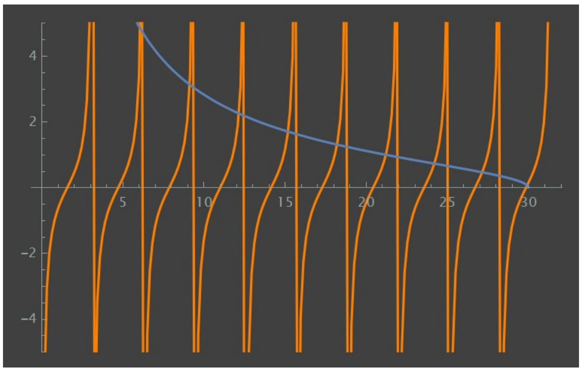

Figure 1: Orange lines represent -cot(z) while blue line represents the square root term for $z_0 = 30$

Observe from the figure above that for a wide well, the intersection always almost occur at the asymptotes. Finding the coordinates of these asymptotes, one can observe that this is π-periodic This gives us the solution

$$z_n = \frac{n\pi}{2} \tag{17}$$

for odd values of n. Note that we have followed closely from even derivations such that our introduced parameters are basically the same. From the definition of z and l, the found graphical solutions for z_n then corresponds to

$$E_n + V_0 \approx \frac{n^2\pi^2\hbar^2}{2m(2a)^2} \tag{18}$$

where n is even and z_0 is made large enough for a wide well limiting case. Even if there is a lot of similarities, observe the following significant difference. As we turn the dial down for z_0, it failed to intersect with the RHS equation.

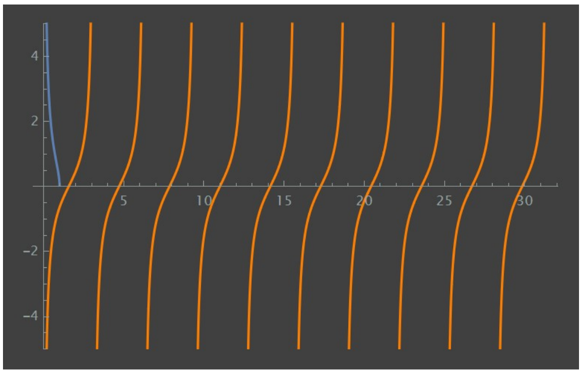

Figure 2: The -cot(z) function fails to intersect with RHS square root term at $z_0 = 1$

$\boxed{\text{Hence, for odd states, a bound state is not assured.}}$

Now, we have both odd and even states. Their energies can be summarized as the solutions of the following:

$$\begin{cases} \tan(z_n) = \left(\left(\frac{z_0}{z_n}\right)^2 - 1\right)^{1/2} & n \text{ is even} \\ -\cot(z_n) = \left(\left(\frac{z_0}{z_n}\right)^2 - 1\right)^{1/2} & n \text{ is odd} \end{cases} \tag{19}$$

2. **Bound state of a specific finite well configuration**

Now, we are tasked to determine the bound states of a system with specific numerical parameters. What we can do is to plug in the values directly, solving for the graphical plot, and eyeballing the intersections as solutions. However, I think more insight would be gained if we reparametrize the system by introducing some dimensionless parameters. We start with the odd states. Recall that z and z_0 was defined as

$$z = \frac{\sqrt{2m(E+V_0)}L}{2\hbar} \qquad z_0 = \frac{\sqrt{2mV_0}L}{2\hbar} \tag{20}$$

Then,

$$\frac{z_0}{z} = \sqrt{\frac{V_0}{E+V_0}} \iff \sqrt{\left(\frac{z_0}{z}\right)^2 - 1} = \sqrt{\frac{V_0}{E+V_0} - 1} = \sqrt{-\frac{E}{E+V_0}} \tag{21}$$

Recall that $E < 0$ but $|E| < V_0$ so the square root is real. Then, we can express Eq. (19) into its more primitive form

$$\begin{cases} \tan\left(\frac{\sqrt{2m(E+V_0)}L}{2\hbar}\right) = \sqrt{-\frac{E}{E+V_0}} & n \text{ is even} \\ -\cot\left(\frac{\sqrt{2m(E+V_0)}L}{2\hbar}\right) = \sqrt{-\frac{E}{E+V_0}} & n \text{ is odd} \end{cases} \tag{22}$$

We start the nondimensionalization process by expressing these as

$$\begin{cases} \tan\left(\frac{\sqrt{2mV_0}L}{2\hbar}\sqrt{1+\frac{E}{V_0}}\right) = \sqrt{-\frac{E}{V_0}\frac{1}{E/V_0+1}} & n \text{ is even} \\ -\cot\left(\frac{\sqrt{2mV_0}L}{2\hbar}\sqrt{1+\frac{E}{V_0}}\right) = \sqrt{-\frac{E}{V_0}\frac{1}{E/V_0+1}} & n \text{ is odd} \end{cases} \tag{23}$$

we introduce the scaling $E = E_c\bar{E}$, where E_c is the characteristic scaling on the system and $\bar{E}$ is dimensionless. Then,

$$\begin{cases} \tan\left(\frac{\sqrt{2mV_0}L}{2\hbar}\sqrt{1+\frac{E_c}{V_0}\bar{E}}\right) = \sqrt{-\frac{E_c}{V_0}\bar{E}\frac{1}{(E_c/V_0)\bar{E}+1}} & n \text{ is even} \\ -\cot\left(\frac{\sqrt{2mV_0}L}{2\hbar}\sqrt{1+\frac{E_c}{V_0}\bar{E}}\right) = \sqrt{-\frac{E_c}{V_0}\bar{E}\frac{1}{(E_c/V_0)\bar{E}+1}} & n \text{ is odd} \end{cases} \tag{24}$$

Introducing the following dimensionless groups,

$$\Pi_1 = \frac{\sqrt{2mV_0}L}{2\hbar} \qquad \Pi_2 = \frac{E_c}{V_0} \tag{25}$$

Observe that Π_1 represents that size of the well and Π_2 represents that energy of the particle. For convenience of notation we set $\Pi_1 = \varepsilon$ and $\Pi_2 = 1$. In this scaling, we are plotting energies as a fraction of the given potential restricting the domain at $(-1, 0)$. Hence, $E_c = V_0$ and our system is now

$$\begin{cases} \tan\left(\varepsilon\sqrt{1+\bar{E}}\right) = \sqrt{\frac{-\bar{E}}{\bar{E}+1}} & n \text{ is even} \\ -\cot\left(\varepsilon\sqrt{1+\bar{E}}\right)\sqrt{\frac{-\bar{E}}{\bar{E}+1}} & n \text{ is odd} \end{cases} \tag{26}$$

which is now fully non-dimensional and solution is governed by the dimensionless parameter ε. To find the bound states of the specified system, we must calculate ε for that system and find the roots of the plot of the dimensionless equation. We are given the following parameters:

$$U_0 = 240 \text{ meV} \tag{27}$$
$$m = 0.06 \text{ m}_e \tag{28}$$
$$L = 90 \text{ A} \tag{29}$$

Our next task is to perform dimensional analysis on Planck's constant for us to utilize the experimental units. Planck's constant has dimensions

$$[[\hbar]] = \frac{ML^2}{T} \tag{30}$$

To transfer the SI units $[[\alpha]]_s$ to experimental units $[[\alpha]]_x$, we aim find the appropriate transformation T where

$$[[\hbar]]_x = X[[\hbar]]_s \tag{31}$$

Expanding,

$$\frac{M_xL_x^2}{T_x} = \left(\frac{M_sL_s^2}{T_s}\right)\frac{M_x}{M_s}\cdot\frac{T_s}{T_x}\cdot\frac{L_x^2}{L_s^2} \iff X = \frac{L_x^2M_x}{T_x} \tag{32}$$

where $[[\alpha]] = 1$ for all units in S. In this units, $T_x^2 = (M_xL_x^2)/[[V_x]])$. Hence,

$$X = L_x^2M_x\cdot\frac{[[V_x]]^{1/2}}{M_x^{1/2}L_x} = L_xM_x^{1/2}[[V_x]]^{1/2} \tag{33}$$

Again, note that $[[\alpha]]_x$ is the conversion factor from SI units to experimental units. That is,

$$L_x = 1.000\times10^{10}\,\frac{\ddot{\text{A}}}{\text{m}} \tag{34}$$
$$M_x = 1.098\times10^{30}\,\frac{\text{m}_E}{\text{kg}} \tag{35}$$
$$[[V_x]] = 6.242\times10^{21}\,\frac{\text{meV}}{\text{J}} \tag{36}$$

Then,

$$X = 4.279 \times 10^{35} \tag{37}$$

Observe that the given experimental quantities have friendly values (which are in typical everyday scales). Hence, we should expect that $\hbar$ must also be have friendly a friendly value. From, Eq. (31), we have

$$[[\hbar]]_s = 87.340 \tag{38}$$

which is, indeed, friendly. One may ask why should we go through the trouble of converting into this experimental scale since we are only tasked to find a dimensionless parameter that is actually units-independent. We converted the Planck's constant such that we can reuse it again in tasks that do not require nondimensionalization. Now, we calculate the dimensionless parameter in terms of experimental units as "basis". From Eq. (25),

$$\varepsilon = \frac{\sqrt{2mV_0}L}{2\hbar} = \frac{\sqrt{2 * 0.06 * 240} * 90}{2 * 87.340} \tag{39}$$

Hence, in this specific system,

$$\boxed{\varepsilon = 2.765} \tag{40}$$

Observe that, in this scale, we can immediately assess the energy relative to our system without any reference to any units. Finally, plotting both odd and even states, we get

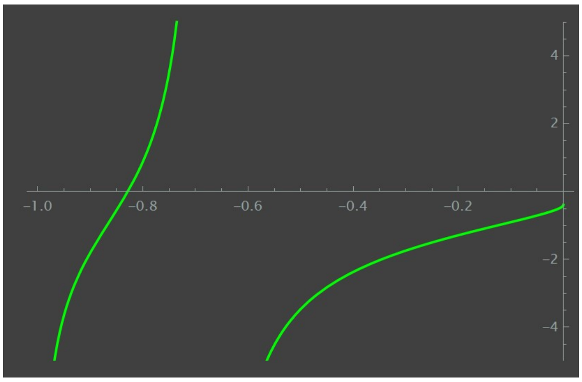

Figure 3: Plot of Eq. (26) even state, RHS is made zero where $\varepsilon = 2.75$

Finding the coordinates of the zeroes of the plot, we have $\bar{E} = -0.83$ for the even state. This is -0.83 times the well depth $U_0 = 240$ meV. Approximately, that is

$$\boxed{E = -199 \text{ meV}} \tag{41}$$

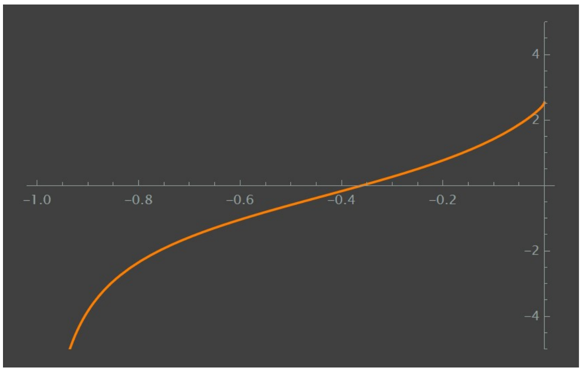

Figure 4: Plot of Eq. (26) even state, RHS is made zero where $\varepsilon = 2.75$

Finding the coordinates of the zeroes of the plot, we have $\bar{E} = -0.36$ for the odd state. This is -0.36 times the well depth $U_0 = 240$ meV. Approximately, that is

$$\boxed{E = -86 \text{ meV}} \tag{42}$$

Some accuracy might have been compromised due to numerous conversions and approximation errors. However, it is easier to generalize this to any arbitrary finite well configurations and easier to analyze global characteristics of a system. Of course, this can be arbitrarily made more accurate by using a more accurate conversion factors.