Quantum Mechanics A PHY-319 Note Set No. 3

The Finite square well.

We have already solved the problem of the infinite square well. Let us now solve the more realistic finite square well problem. Consider the potential shown in fig.1, the particle has energy, E, less than V_0, and is bound to the well.

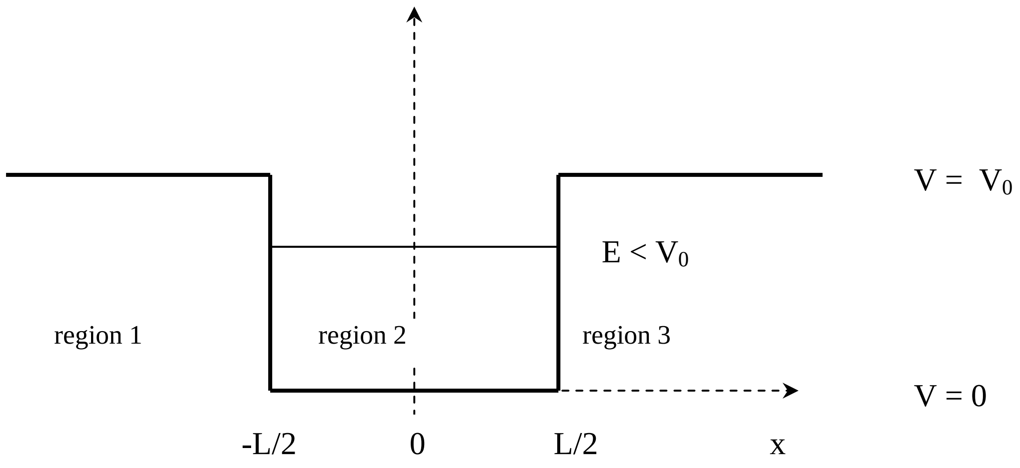

Figure 1: A finite square well, depth, V_0, width L.

Region 1

$x \le -\frac{L}{2}$, $V(x) = V_0$, substituting into TISE:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V_0\psi = E\psi \;\Rightarrow\; \frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2}(V_0 - E)\psi$$

yielding

$$\frac{d^2\psi}{dx^2} = \kappa^2\psi \quad \text{with } \kappa^2 = \frac{2m}{\hbar^2}(V_0 - E) > 0 \text{ ,so } \kappa = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)} \text{ ,which is real.}$$

The solutions to this differential equation are:

$\psi = Be^{\kappa x} + De^{-\kappa x}$ but since $\psi \to 0$ as $x \to -\infty$, $D = 0$

we get $\psi = Be^{\kappa x}$ for region 1…

Region 3

$x \ge \frac{L}{2}$, $V(x) = V_0$, .

similarly to region 1, the solutions are:

$\psi = Ae^{-\kappa x} + D'e^{\kappa x}$ but since $\psi \to 0$ as $x \to +\infty$, $D' = 0$
we get $\psi = Ae^{-\kappa x}$ for region 3…

<u>Region 2</u>

$-\frac{L}{2} \le x \le \frac{L}{2}$, $V(x) = 0$, substituting into TISE:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + 0 = E\psi \quad \Rightarrow \quad \frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2}E\psi$$

meaning

$$\frac{d^2\psi}{dx^2} = -k^2\psi \text{ with } k^2 = \frac{2mE}{\hbar^2} > 0, \text{ so } k = \sqrt{\frac{2m}{\hbar^2}E}$$, which is real.

…which we have already encountered in the infinite square well, since the potential is symmetric, we have even and odd parity solutions, namely:

$\psi = C\cos(kx)$ for even parity (n odd)
and $\psi = D\sin(kx)$ for odd parity (n even)

Parity +1 Even		Parity –1 Odd
Wavefunction	Region	Wavefunction
$\psi = Be^{\kappa x}$	1	$\psi = B'e^{\kappa x}$
$\psi = C\cos(kx)$	2	$\psi = D\sin(kx)$
$\psi = Ae^{-\kappa x}$	3	$\psi = A'e^{-\kappa x}$

Table 1: summary of wavefunctions of the finite potential well.

Clearly, for parity +1 and for parity -1

$B = A$ $\qquad\qquad$ $B' = -A'$

Now we have to match both the wavefunction, $\psi(x)$, and its derivative, $\frac{d\psi(x)}{dx}$, at the well boundaries, namely at $x = \pm\frac{L}{2}$. Of course, we have to do this twice, since we have even and odd parity solutions…

So, at $x = \frac{L}{2}$, for even parity:

… equating ψ: $$C\cos\left(k\frac{L}{2}\right) = Ae^{-\kappa\frac{L}{2}} \qquad (1)$$

… and equating $\frac{d\psi}{dx}$: $$-Ck\sin\left(k\frac{L}{2}\right) = -A\kappa e^{-\kappa\frac{L}{2}} \qquad (2)$$

Dividing eq(2) by eq(1) to eliminate C and A gives:

$$\frac{\kappa}{k} = \tan\left(\frac{kL}{2}\right) \qquad (3)$$

We can carry out the same analysis for the negative parity solutions and obtain:

$$\frac{\kappa}{k} = -\cot\left(\frac{kL}{2}\right) \qquad (4a)$$

$$\frac{\kappa}{k} = \tan\left(\frac{kL}{2} + \frac{\pi}{2}\right) \qquad (4b)$$

Note that since $\kappa = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}$ and $k = \sqrt{\frac{2m}{\hbar^2}E}$, in both equations (3) and (4), there is only one unknown, the energy, E; so we should be able to solve for the energy. It transpires that both equation (3) and equation (4) are <u>transcendental</u>, that is, they cannot be solved *analytically*, we can, however, solve them *numerically*. In order to do so, we shall rewrite them in a more convenient form, using dimensionless parameters, η and ζ_0.

η is simply the argument of the trigonometric function:

$$\eta = \frac{kL}{2} = \frac{L}{2}\sqrt{\frac{2m}{\hbar^2}E}$$

and is the variable we will be solving for since it contains the energy…

Now, ζ_0 is defined by:

$$\zeta_0 = \frac{L}{2}\sqrt{\frac{2m}{\hbar^2}V_0}$$

and is called the **potential-strength parameter**, since it contains the depth of the potential well, V_0, (and its width, L).

Recall that $\kappa = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}$ and $k = \sqrt{\frac{2m}{\hbar^2}E}$, so…

$$\kappa^2 = \frac{2m}{\hbar^2}(V_0 - E) = \frac{2m}{\hbar^2}V_0 - k^2$$

$$\kappa^2 = k^2\left\{\zeta_0^2\left(\frac{2}{L}\right)^2\frac{1}{k^2}-1\right\}$$

$$\frac{\kappa^2}{k^2}=\left\{\frac{\zeta_0^2}{\eta^2}-1\right\} \qquad \Rightarrow \qquad \frac{\kappa}{k}=\sqrt{\frac{\zeta_0^2}{\eta^2}-1}$$

So our transcendental equations (3) and (4) become:

$$\tan(\eta)=\sqrt{\left(\frac{\zeta_0}{\eta}\right)^2-1} \qquad (5) \qquad \text{for even parity, and,}$$

$$-\cot(\eta)=\sqrt{\left(\frac{\zeta_0}{\eta}\right)^2-1} \qquad (6) \qquad \text{for odd parity, note that } -\cot(\theta)=\tan\left(\theta+\frac{\pi}{2}\right)$$

Reiterating, since $\eta=\frac{kL}{2}=\frac{L}{2}\sqrt{\frac{2m}{\hbar^2}E}$, if we can solve these for η, we will obtain the energy eigenvalues E_n for our finite well.

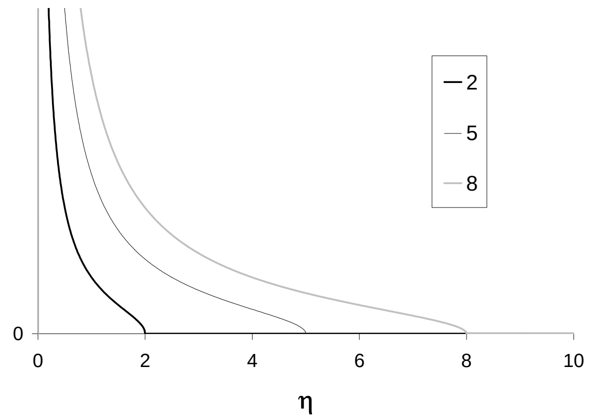

Figure 2: A plot of $\sqrt{\left(\frac{\zeta_0}{\eta}\right)^2-1}$ versus η for three values of ζ_0 (2, 5 and 8).

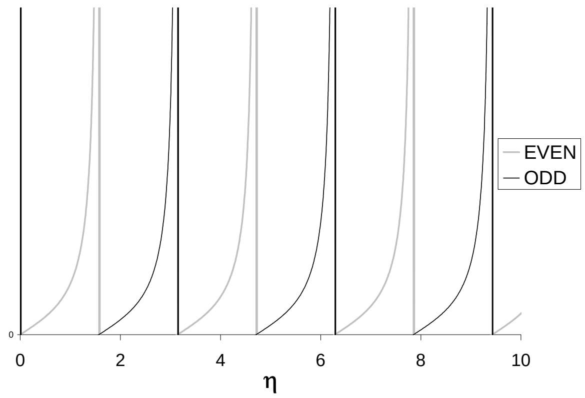

Figure 3: Plots of $\tan(\eta)$ for <u>even</u> parity solutions and of $-\cot(\eta)=\tan\left(\eta+\frac{\pi}{2}\right)$ for <u>odd</u> parity solutions versus η.

We can superimpose a plot of $\sqrt{\left(\frac{\zeta_0}{\eta}\right)^2 - 1}$ onto plots of $\tan(\eta)$ and $-\cot(\eta) = \tan\left(\eta + \frac{\pi}{2}\right)$ to graphically solve the two equations. For example taking an electron in a well, width 4Å and depth to be 14eV we can calculate $\zeta_0 = 3.83$. A plot of $\sqrt{\left(\frac{\zeta_0}{\eta}\right)^2 - 1}$ for $\zeta_0 = 3.83$ is shown in figure 4, together with the trigonometric function plots. The curves intersect at three values of η (circled), corresponding to the energy levels of the three bound states.

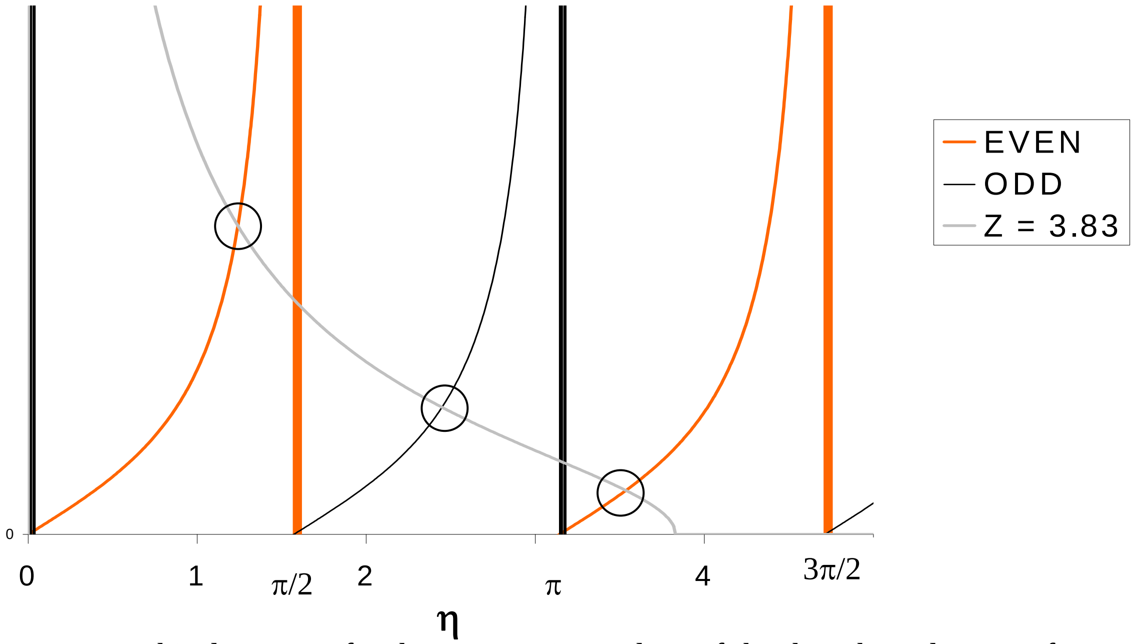

Figure 4: a graphical solution for the energy eigenvalues of the three bound states of an electron in a 4Å, 14eV finite potential well.

The values of η obtained are:
$\eta = 1.24$, corresponding to $n = 1$,even parity
$\eta = 2.45$, corresponding to $n = 2$,odd parity
$\eta = 3.54$, corresponding to $n = 3$,even parity
and the corresponding energy eigenvalues are:
$E_1 = 1.47eV$, $E_2 = 5.74eV$ and $E_3 = 11.99eV$
Note that these are much lower than the corresponding energy eigenvalues for an infinite square well of the same width ($E^{\infty}{}_1 = 2.36eV$, $E^{\infty}{}_2 = 9.43eV$ and $E^{\infty}{}_3 = 21.24eV$). This is not surprising as the wavefunction in the finite potential well extends into the classically forbidden region, so the corresponding wavelengths are <u>longer</u> than those in the infinite well, resulting in lower energies (see figure 5).

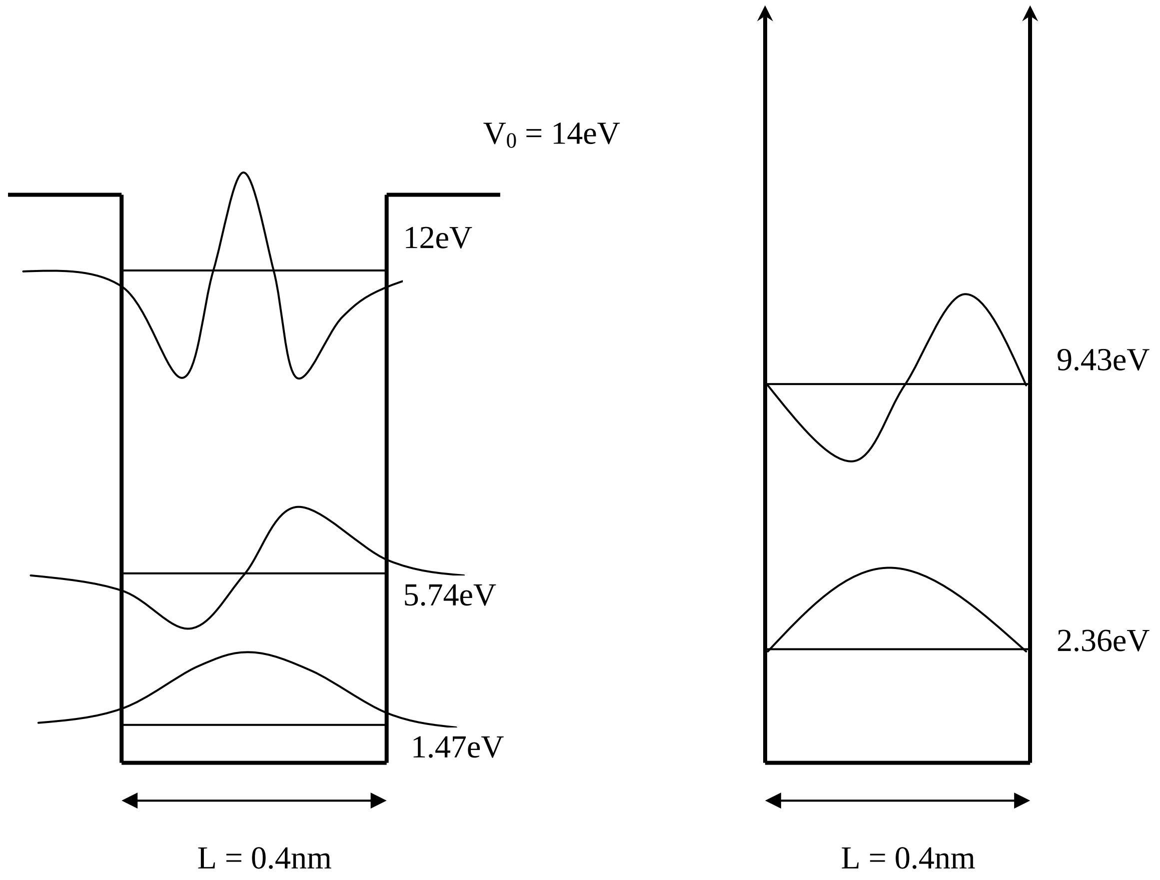

Figure 5: The three bound states in a 0.4nm, 14eV one-dimensional finite quantum well. The wavefunctions are shown schematically. Note how the corresponding energy levels of an infinite well are much higher.