QUANTUM MECHANICS A (SPA 5319)

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.

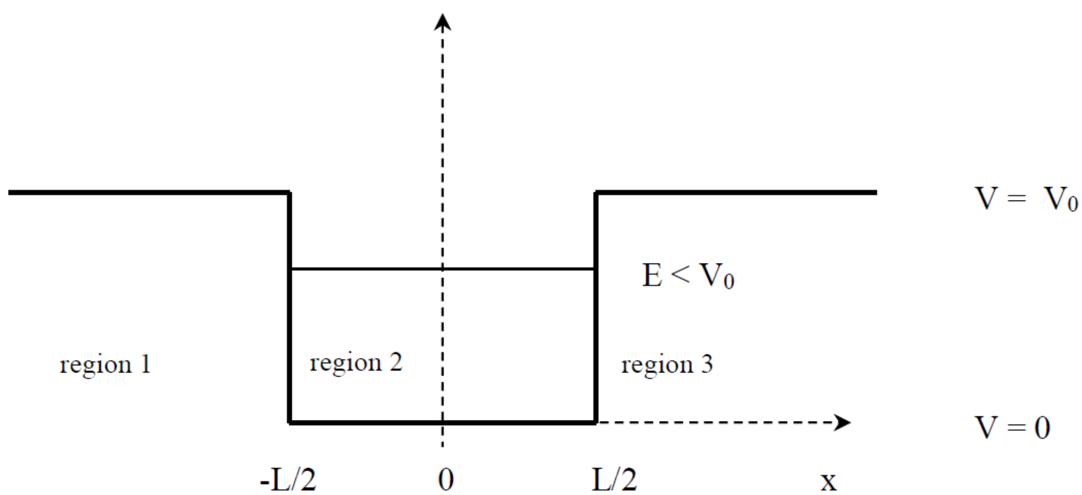

Figure 1: *A finite square well, with depth V_0 and width L.*

Region 1: $x \leq -\frac{L}{2}$, and $V(x) = V_0$, substituting into the TISE:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V_0\psi = E\psi \qquad \Longrightarrow \qquad \frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2}(V_0 - E)\psi \tag{1}$$

yielding

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

with $\kappa^2 = 2m(V_0 - E)/\hbar^2 > 0$. The solutions to this differential equation are:

$$\psi = Be^{\kappa x} + De^{-\kappa x} \tag{3}$$

but since $\psi \to 0$ as $x \to -\infty$, we have $D = 0$. We therefore get $\psi = Be^{\kappa x}$ for region 1.

Region 3: $x \geq -\frac{L}{2}$, and $V(x) = V_0$. Similarly to region 1, the solutions are:

$$\psi = Ae^{-\kappa x} + D'e^{\kappa x} \tag{4}$$

but since $\psi \to 0$ as $x \to +\infty$, we have $D' = 0$. We therefore have $\psi = Ae^{-\kappa x}$ for region 3.

Region 2: $-\frac{L}{2} \leq x \leq \frac{L}{2}$, and $V(x) = 0$. Substituting into the TISE:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + 0 = E\psi \qquad \Longrightarrow \qquad \frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi \tag{5}$$

This yields

$$\frac{d^2\psi}{dx^2} = -k^2\psi \tag{6}$$

with $k^2 = 2mE/\hbar^2 > 0$. As the potential is symmetric, we have even and odd parity solutions, namely:

$$\psi = C\cos(kx) \qquad \text{for even parity } (n \text{ odd})$$

and

$$\psi = D\cos(kx) \qquad \text{for odd parity } (n \text{ even})$$

Our results so far are summarized in table 1, below.

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 in the finite potential well.*

Clearly, for parity $+1$ we have $B = 1$, and for parity -1 we have $B' = -A'$. Now we have to match both the wavefunction, $\psi(x)$, and its derivative, $d\psi/dx$, at the well boundaries, where $x = \pm L/2$. Of course, we have to do this twice, since we have even and odd parity solutions.

So, at $x = L/2$, for even parity:

$$\text{equating } \psi: \qquad C\cos\left(k\tfrac{L}{2}\right) = Ae^{-\kappa L/2} \tag{7}$$

$$\text{equating } \tfrac{d\psi}{dx}: \qquad -Ck\sin\left(k\tfrac{L}{2}\right) = -A\kappa e^{-\kappa L/2} \tag{8}$$

Dividing eq. (8) by eq. (7) to eliminate C and A gives:

$$\frac{\kappa}{k} = \tan\left(\frac{kL}{2}\right) \tag{9}$$

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

$$\frac{\kappa}{k} = -\cot\left(\frac{kL}{2}\right) \tag{10}$$

Note that as $\kappa^2 = 2m(V_0 - E)/\hbar^2$ and $k^2 = 2mE/\hbar^2$, in both equations (9) and (10), there is only one unknown, the energy, E. This means we should be able to solve for the energy. It transpires that both equation (9) and equation (10) are *transcendental* (meaning 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, and η and ζ.

$$\text{We define } \eta \text{ as}: \qquad \eta = \frac{kL}{2} = \frac{L}{2}\sqrt{\frac{2mE}{\hbar^2}}$$

$$\text{We define } \zeta \text{ as}: \qquad \zeta = \frac{L}{2}\sqrt{\frac{2mV_0}{\hbar^2}}$$

The first is the variable we will be solving for, and is called the "dimensionless energy", as it contains the energy. Likewise, the second is called the "dimensionless potential", as it contains the depth of the potential well, V_0.

Recall that $\kappa^2 = 2m(V_0 - E)/\hbar^2$ and $k^2 = 2mE/\hbar^2$, so that

$$\frac{\kappa^2}{k^2} = \frac{\zeta^2}{\eta^2} - 1$$

This means that our transcendental equations, (9) and (10), become:

$$\tan(\eta) = \sqrt{\tfrac{\zeta^2}{\eta^2} - 1} \qquad \text{for even parity} \tag{11}$$

$$-\cot(\eta) = \sqrt{\tfrac{\zeta^2}{\eta^2} - 1} \qquad \text{for odd parity} \tag{12}$$

Reiterating: as $\eta = (L/2)\sqrt{2mE/\hbar^2}$, if we can solve for η then we will also obtain the energy eigenvalues, E_n, for our finite well.

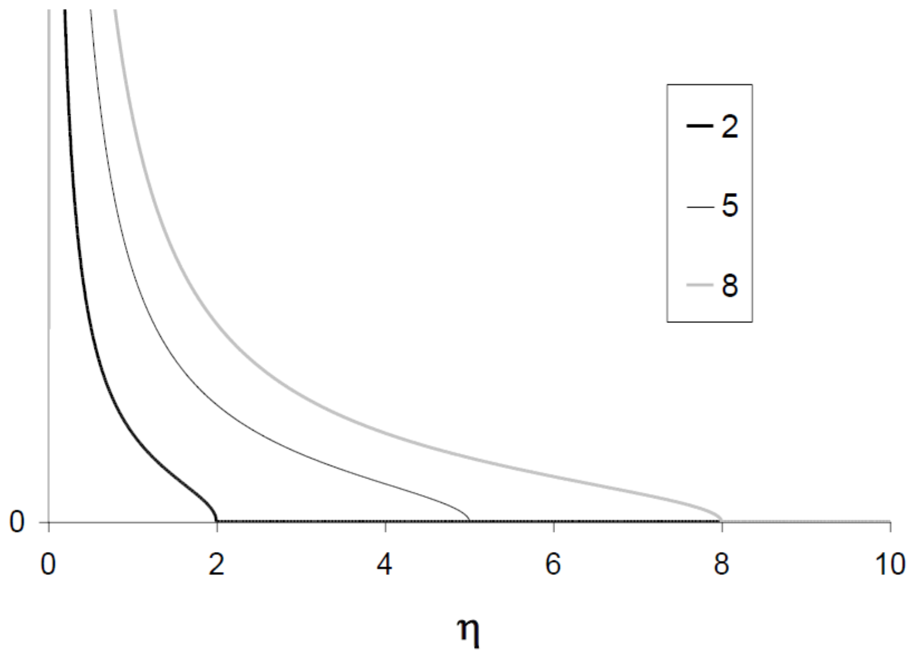

Figure 2: *A plot of* $\sqrt{\frac{\zeta^2}{\eta^2} - 1}$ *versus* η *for three values of* ζ *(2, 5 and 8).*

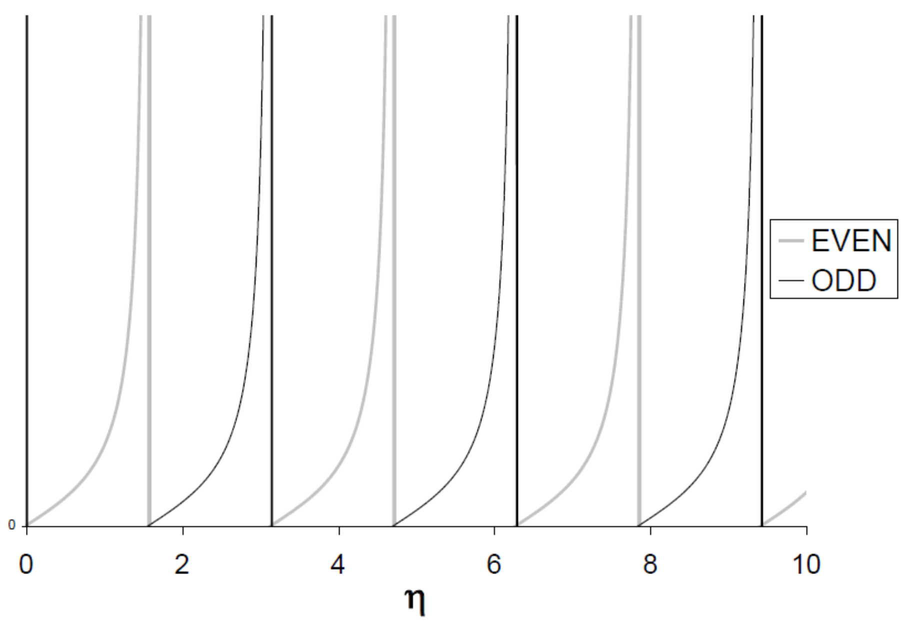

Figure 3: *Plots of* $\tan(\eta)$ *for even parity solutions, and* $-\cot(\eta)$ *for odd parity solutions.*

We can superimpose a plot of $\sqrt{\zeta^2/\eta^2 - 1}$ onto plots of $\tan(\eta)$ and $-\cot\eta$ to graphically solve the two equations. For example, taking an electron in a well, width 4Å and depth to be 14eV we can calculate $\zeta = 3.83$. A plot of $\sqrt{\zeta^2/\eta^2 - 1}$ for $\zeta = 3.83$ 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.

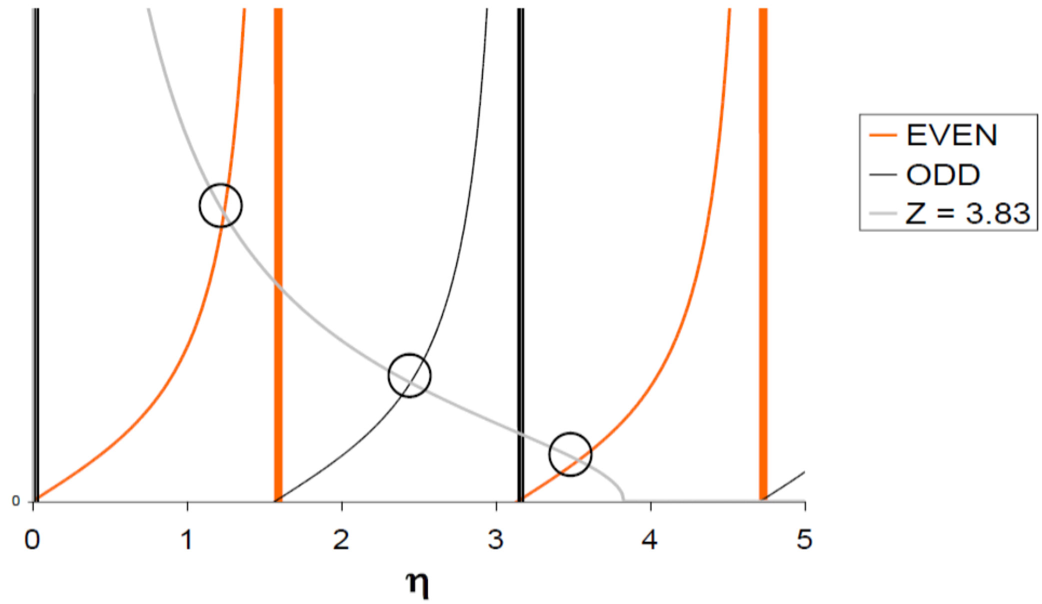

Figure 4: *A graphical solution for the energy eigenvalues of the three bound states of an electron in a 4Å, 14eV finite potential well.*

The values of η obtained are:

$$\eta = 1.24, \text{ corresponding to } n = 1, \text{ even parity} \tag{13}$$

$$\eta = 2.45, \text{ corresponding to } n = 2, \text{ odd parity} \tag{14}$$

$$\eta = 3.54, \text{ corresponding to } n = 3, \text{ even parity} \tag{15}$$

and the corresponding energy eigenvalues are: $E_1 = 1.47$eV, $E_2 = 5.74$eV and $E_3 = 11.99$eV. Note that these are much lower than the corresponding energy eigenvalues for an infinite square well of the same width (which has $E_1 = 2.36$eV, $E_2 = 9.43$eV and $E_3 = 21.24$eV). This is not surprising as the wavefunction in the finite potential well extends into the classically forbidden region, so the corresponding wavelengths are longer than those in the infinite well, resulting in lower energies (see figure 5).

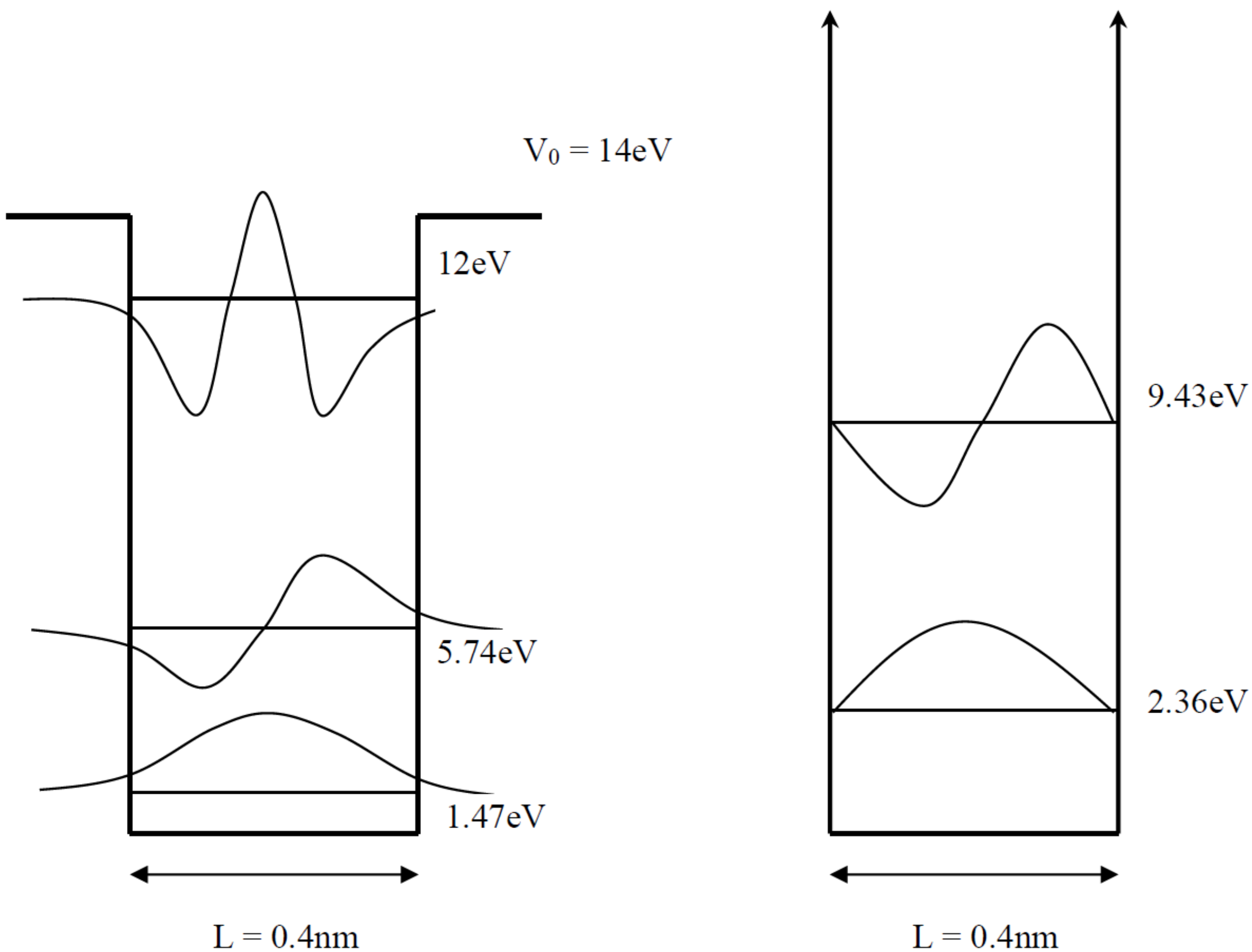

Figure 5: *The three bound states in a 0.4nm, 14eV one-dimensional finite quantum well. Note how the corresponding energy levels of an infinite well are much higher.*