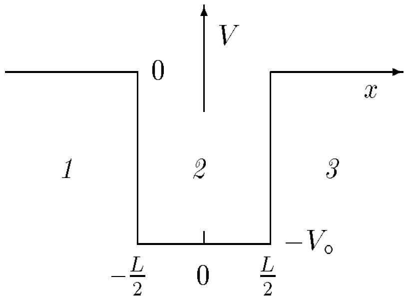
The Finite Square Well



Solutions of the time-independent Schrödinger Equation for a *finite square well* potential,

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi = E\psi\,, \quad V(x) = \begin{cases} -V_\circ, & |x| \le \frac{L}{2} \\ 0, & |x| > \frac{L}{2} \end{cases} \qquad (1)$$

reveal many of the qualitative characteristics of quantum mechanical ($\mathcal{QM}$) systems.

THINK FIRST! The first step in any problem is to gather together all your *qualitative* knowledge about the situation before you start working out any quantitative details. This is especially true in $\mathcal{QM}$, where the "blind calculation" approach is often not only a waste of effort but actually intractable!

SYMMETRY: In this case we save ourselves a mind-bogglingly difficult mathematical nightmare by making a few simple observations about SYMMETRY: the potential $V(x)$ is symmetric about $x = 0$; this implies that the probability of finding the particle on one side of the well must be equal to the probability of finding it on the other side. Since the wavefunction $\psi(x)$ is *squared* to get this probability, it follows that $\psi(x)$ can be *either* an EVEN function of x $[\psi(-x) = \psi(x)]$ *or* an ODD function of x $[\psi(-x) = -\psi(x)]$. This places lots of constraints on $\psi(x)$ for which we will soon be grateful.

BOUND or UNBOUND? A *potential well* generally has bound states of well-defined energy $E < 0$ unless the mass is too small (see below). There is also a continuum of *unbound* states with $E > 0$, whose behaviour we may also want to examine. [For instance, the classical particle will "pass over" the well and continue on the other side every time; this will not be the case for the $\mathcal{QM}$ result!] We will start with the *bound* state ($E < 0$). If $\psi(x)$ is localized around the potential well, then to be *normalizable* it must obey $\psi(x) \underset{|x|\to\infty}{\longrightarrow} 0$. [Moreover, we certainly expect $\psi \to 0$ as we get further into regions where the *classical* particle cannot penetrate *at all* due to its inadequate energy!] Our first guess for such functions is always the *decaying exponential* function, here $\boxed{\psi_1(x) = Ae^{\alpha x}}$ (2) for region *1* $\left(-\infty < x < -\frac{L}{2}\right)$. [Remember, $x = -|x|$ in this region.] Since we are always free to choose the *overall phase* of $\psi(x)$ arbitrarily [multiplying by a constant factor of $e^{i\phi}$ has no effect on the physics], we may do so immediately by choosing that $\boxed{A \text{ is real and positive}}$. In this case the $\left\{\begin{matrix}\text{EVEN}\\\text{ODD}\end{matrix}\right\}$ symmetry requirement gives two possible solutions for region *3* $\left(\frac{L}{2} < x < \infty\right)$: $\boxed{\psi_{3\pm}(x) = \pm Ae^{-\alpha x}}$ where the $+$ sign is for the symmetric (EVEN) solution and the $-$ sign is for the antisymmetric (ODD) solution.

On region *2* $\left(-\frac{L}{2} < x < \frac{L}{2}\right)$ we expect some sort of oscillatory function, for which the obvious $\left\{\begin{matrix}\text{EVEN}\\\text{ODD}\end{matrix}\right\}$ choices are $\boxed{\psi_{2\pm}(x) = B\left\{\begin{matrix}+\cos\\-\sin\end{matrix}\right\}(kx)}$ (3) where the $-$ sign is chosen for the (ODD) sin function for the following reason:

BOUNDARY CONDITIONS: We must always satisfy the matching condition for the wavefunction [ψ must be *continuous*] and the matching condition for its spatial derivative [$\partial\psi/\partial x$ must also be continuous (except where the potential is infinite)] at the boundaries $x_{12} \equiv -\frac{L}{2}$ and $x_{23} \equiv +\frac{L}{2}$. The first matching condition immediately implies that ψ_2 must be *positive* at x_{12}, since we chose ψ_1 positive. For the odd function this mandates the negative sign in Eq. (3) above. If we now explicitly apply the matching condition for ψ at the boundaries, we get $\boxed{\left\{\begin{matrix}\cos\\\sin\end{matrix}\right\}\left(\frac{kL}{2}\right) = \frac{A'}{B}}$ (4) where $\boxed{A' \equiv Ae^{-\alpha L/2}}$ is the magnitude of ψ *at the boundary*. The matching condition for the derivative gives

$\boxed{\left\{ \begin{array}{c} +\sin \\ -\cos \end{array} \right\} \left(\frac{kL}{2} \right) = \frac{\alpha}{k} \frac{A'}{B}}$ (5). Dividing Eq. (5) by Eq. (4) gives $\boxed{\left\{ \begin{array}{c} +\tan \\ -\cot \end{array} \right\} \left(\frac{kL}{2} \right) = \frac{\alpha}{k}}$ (6). Adding the squares of Eqs. (4) and (5) gives $\boxed{B^2 = A'^2 \left(1 + \frac{\alpha^2}{k^2} \right)}$ (7).

APPLYING the SCHRÖDINGER EQUATION: How do these guesses fare with our original equation? On regions *1* and *3* we get $-\frac{\hbar^2 \alpha^2}{2m} \psi = E\psi$, which ensures $\boxed{\hbar\alpha = \sqrt{-2mE}}$ (8) since $E < 0$ is the same throughout. On region *2* we have $\frac{\hbar^2 k^2}{2m} \psi_2 - V_\circ \psi_2 = E\psi_2$ or $\boxed{\hbar k = \sqrt{2m(V_\circ + E)}}$ (9). Substituting these values for α and k back into Eqs. (7) and (6) gives $\boxed{B = A' \sqrt{\frac{V_\circ}{V_\circ + E}}}$ (10) and

$$\boxed{\left\{ \begin{array}{c} +\tan \\ -\cot \end{array} \right\} \left(\sqrt{\frac{mL^2}{2\hbar^2}} \sqrt{V_\circ + E} \right) = \sqrt{\frac{-E}{V_\circ + E}}} \quad (11), \text{ respectively.}$$

Equation (11) implies restrictions on the allowed values of E. This is anticipated [remember, E is *quantized*] but you may be surprised to find a *transcendental* equation governing E. *There is no algebraic solution* to Eq. (11)! [Actually, Eq. (11) is *two* transcendental equations for $\left\{ \begin{array}{c} \text{EVEN} \\ \text{ODD} \end{array} \right\} \psi$. As n and E_n increase, we alternate between EVEN and ODD solutions.] If we define $\boxed{\theta \equiv \sqrt{\frac{mL^2(V_\circ + E)}{2\hbar^2}}}$ and $\boxed{\theta_\circ \equiv \sqrt{\frac{mL^2 V_\circ}{2\hbar^2}}}$ then Eq. (11) reads $\boxed{\left\{ \begin{array}{c} +\tan \\ -\cot \end{array} \right\} \theta = \sqrt{\frac{\theta_\circ^2}{\theta^2} - 1}}$, which one can plot up and solve graphically for the allowed values of θ_n (and therefore E_n). For a detailed description of how to do this, see pp. 156-162 of French & Taylor, *An Introduction to Quantum Physics.*

ARE THERE ANY BOUND STATES? Under what circumstances does Eq. (11) *have* a solution? On the one hand, the general rule that *confinement costs energy* would seem to dictate that a narrower well must be deeper in order to "hang on to" a particle: smaller L (or m) should require larger $V_\circ$. The definition of $\theta_\circ$ reflects this aspect of the problem: $\theta_\circ$ is smaller for smaller $V_\circ$ and/or smaller mL^2. However, $\tan\theta \left\{ \begin{array}{ll} \to 0 & \text{as } \theta \to 0 \\ \to \infty & \text{as } \theta \to \pi/2 \end{array} \right.$ while $\sqrt{\frac{\theta_\circ^2}{\theta^2} - 1} \left\{ \begin{array}{ll} \to \infty & \text{as } \theta \to 0 \\ \to 0 & \text{as } \theta \to \theta_\circ \end{array} \right.$, so that the two must intersect somewhere, no matter how small $\theta_\circ$ is. Thus *there is always at least one (even) bound state* for this potential! The apparent paradox is resolved when we realize that the exponentially decaying "tails" of $\psi(x)$ penetrate deeper and deeper into the classically forbidden region as $\theta_\circ$ gets smaller and smaller, until the region where $\psi(x)$ is sinusoidal (inside the well) becomes a negligible point at the centre of a wavefunction that decays away exponentially from a central cusp. The stability of this solution is extremely sensitive to the "flatness" of $V = 0$ in regions far from the well, for obvious reasons.

An interesting limit is obtained by allowing the well to shrink ($L \to 0$) while holding constant the ratio $L^2 V_\circ$ (so that $V_\circ \to \infty$ in compensation). This is called the DELTA FUNCTION POTENTIAL.

IS THAT THE WHOLE STORY?? After all this work, what have we learned? We know ψ everywhere to within a normalization constant A which can be found by applying $\int_{-\infty}^{\infty} \psi^* \psi dx = 1$ if we need it (*e.g.* if we want to calculate expectation values) and we have what we need to find E_n (and therefore k_n and α_n) for the stationary states allowed in this potential well. It would be nice to have a tidy algebraic solution, but even simple problems are not necessarily nice! If you want exact solutions, you will have to solve the transcendental equations each time you specify the parameters $V_\circ$, L and m which govern the physics of this problem. However, it is possible to make many qualitative obervations (see class notes) based on simple right-hemisphere graphical arguments. We may also examine some LIMITING CASES:

<u>DEEPLY BOUND STATES</u>: If $\frac{\hbar^2\pi^2}{2mL^2} \ll V_\circ$, the lowest few eigenstates will have energies E_n that are only a little above the bottom of the well [$E_n = -V_\circ + \varepsilon_n$, where $\varepsilon_n \ll V_\circ$]. Then Eq. (11) reads approximately $\boxed{\left\{\begin{matrix} +\tan \\ -\cot \end{matrix}\right\} \theta \approx \frac{\theta_\circ}{\theta}\left(1 - \frac{1}{2}\frac{\theta^2}{\theta_\circ^2}\right)}$ or, even more approximately, $\boxed{\left\{\begin{matrix} -\tan \\ +\cot \end{matrix}\right\} \theta \sim \frac{\theta}{\theta_\circ}}$. You may want to play with this approximation to see the spectrum of deeply-bound states. Note that $\theta_\circ \underset{V_\circ \to \infty}{\longrightarrow} \infty$, so in the limit of the INFINITE SQUARE WELL the solutions are simply $\boxed{\left\{\begin{matrix} \tan \\ \cot \end{matrix}\right\} \theta = 0}$, which is satisfied for $\boxed{\theta_n = n\frac{\pi}{2}}$. Check that this agrees with the formula you know already, bearing in mind that here we have defined the *top* of the well to have $V = 0$....

<u>UNBOUND STATES</u>: In all the equations above we have assumed $E < 0$ (bound states). *What happens when $E > 0$?* Taking the equations at face value, we would conclude that α is *imaginary*, meaning that our initial assumption of exponentially decaying solutions outside the well was incorrect and that ψ must be *sinusoidal* (oscillatory) *everywhere*. This is precisely the case. See how far you can get assuming that what we have written so far still applies....