LecturM03L07

PH101: Physics 1

Module 3: Introduction to Quantum Mechanics

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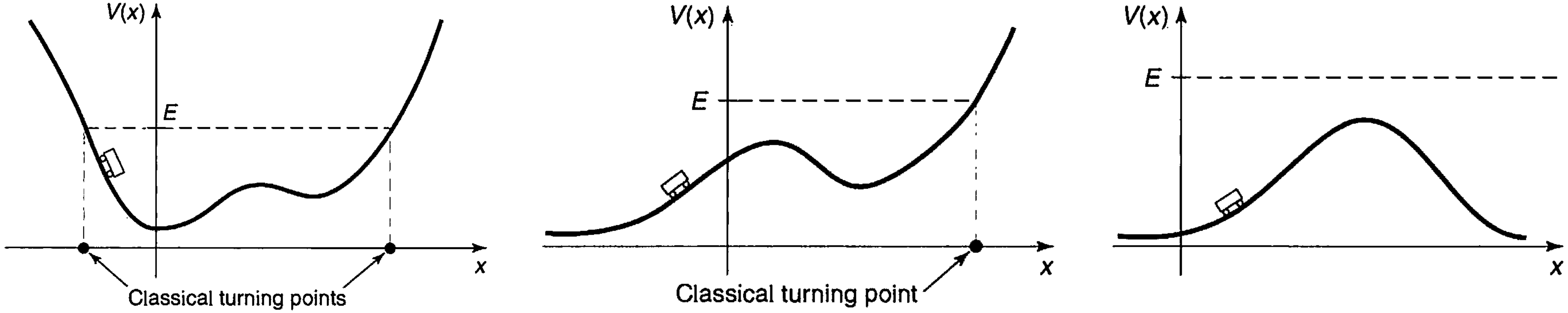
Bound and scattering states



(a) (b)

In classical mechanics a one-dimensional time-independent potential can give rise to two rather different kinds of motion. If V(x) rises higher than the particle's total energy (E) on either side (fig.(a)), then the particle is "stuck" in the potential well—it rocks back and forth between the turning points, but it cannot escape of its own. We call this a bound state. If, on the other hand, E exceeds V(x) on one side (or both), then the particle comes in from "infinity," slows down or speeds up under the influence of the potential, and returns to infinity (fig. (b)). (It can't get trapped in the potential unless there is some mechanism, such as friction, to dissipate energy, but again, we're not talking about that.) We call this a scattering state.

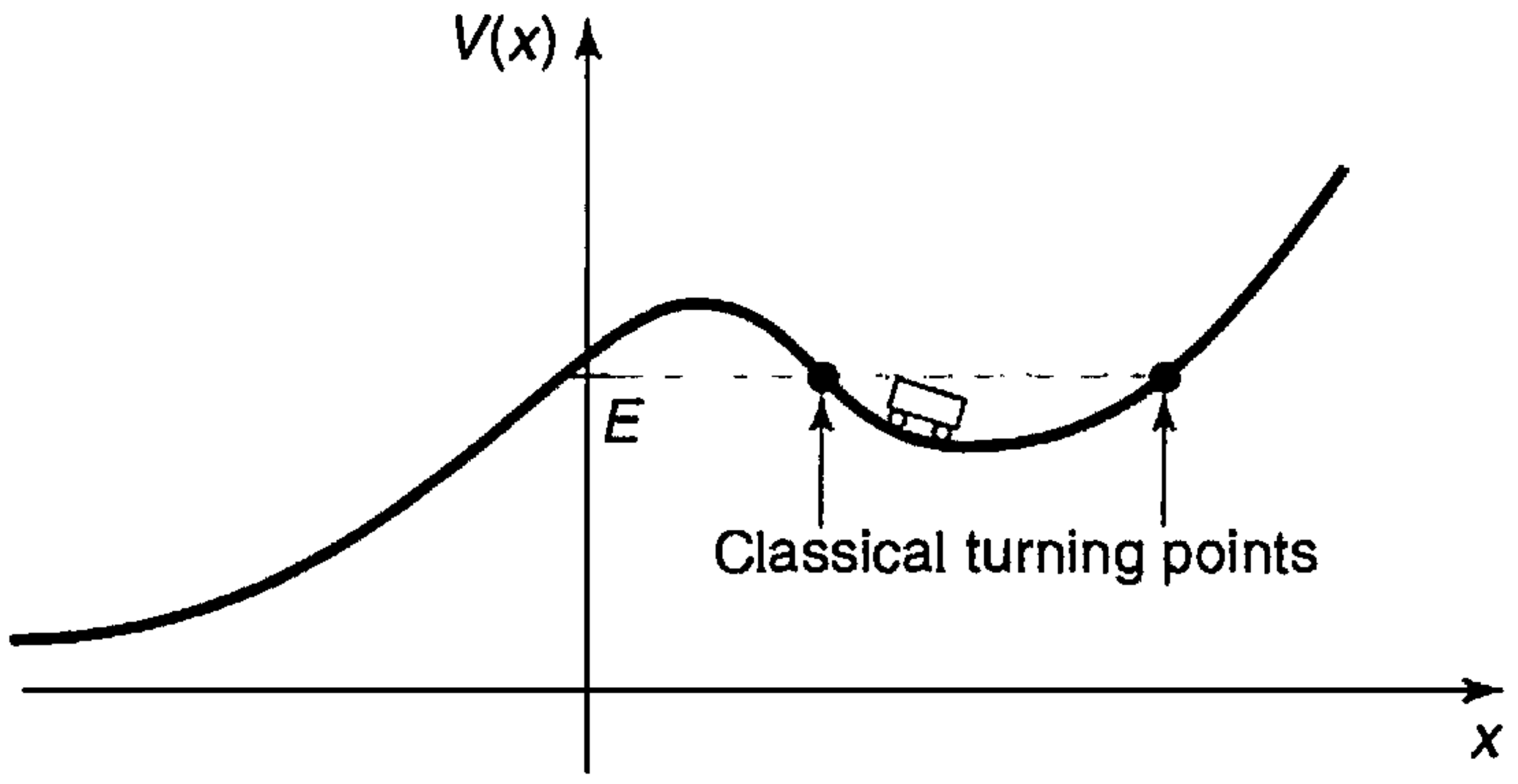
Some potentials admit only bound states (for instance, the harmonic oscillator); some allow only scattering states (a potential hill with no dips in it, for example); some permit both kinds, depending on the energy of the particle.

The two kinds of solutions to the Schroedinger equation correspond precisely to bound and scattering states. The only thing that matters is the potential at infinity (fig. (c)):

$$\begin{cases} E < [V(-\infty) \quad \text{and} \quad V(+\infty)] \Rightarrow & \text{bound state,} \\ E > [V(-\infty) \quad \text{or} \quad V(+\infty)] \Rightarrow & \text{scattering state.} \end{cases}$$

In "real life" most potentials go to zero at infinity, in which case the criterion simplifies even further:

$$\begin{cases} E < 0 \Rightarrow & \text{bound state,} \\ E > 0 \Rightarrow & \text{scattering state.} \end{cases}$$

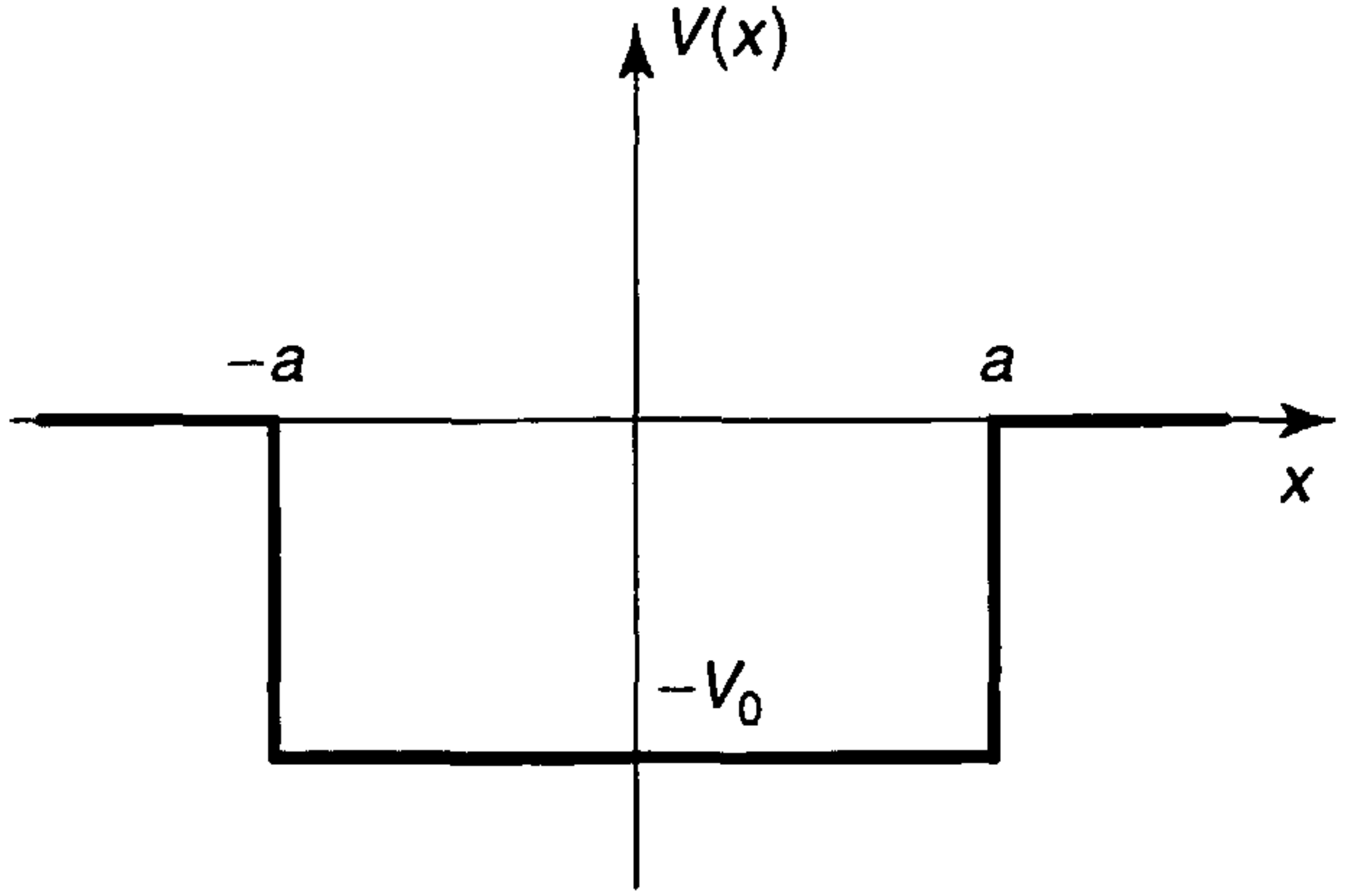


(c)

Finite square well potential

$$V(x) = \begin{cases} -V_0, & \text{for } -a \le x \le a, \\ 0, & \text{for } |x| > a, \end{cases}$$

where V_0 is a (positive) constant



Consider the case ***E* < 0 (bound states)**

In the region $x < -a$ the potential is zero, so the Schrödinger equation reads

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi, \quad \text{or} \quad \frac{d^2\psi}{dx^2} = \kappa^2\psi,$$

where $\kappa \equiv \dfrac{\sqrt{-2mE}}{\hbar}$ is real and positive.

The general solution is $\psi(x) = A\exp(-\kappa x) + B\exp(\kappa x)$

contd...

the first term blows up (as $x \to -\infty$), so

$$\psi(x) = Be^{\kappa x}, \quad \text{for } x < -a.$$

In the region $-a < x < a$, $V(x) = -V_0$, and the Schrödinger equation reads

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - V_0\psi = E\psi, \quad \text{or} \quad \frac{d^2\psi}{dx^2} = -l^2\psi,$$

where $\quad l \equiv \dfrac{\sqrt{2m(E+V_0)}}{\hbar}.$

***E* is negative (for bound states), it must be greater than — V_0, so *l* is also real and positive**.

The general solution is

$$\psi(x) = C\sin(lx) + D\cos(lx), \quad \text{for } -a < x < a,$$

where C and D are arbitrary constants.

contd…

In the region $x > a$, the potential is again zero; the general solution is of the form

$$\psi(x) = F\exp(-\kappa x) + G\exp(\kappa x),$$

second term blows up (as $x \to \infty$), so

$$\psi(x) = Fe^{-\kappa x}, \quad \text{for } x > a.$$

The boundary conditions are

$$\psi \text{ and } d\psi/dx \text{ continuous at } -a \text{ and } +a.$$

In order to solve for the wave functions, we are going to exploit the following property related to the given form of potential:

If $V(x)$ is an even function, $V(-x) = V(x)$, then $\psi(x)$ can always be taken to be either even or odd, that is, if $\psi(x)$ satisfies the time-independent Schrödinger equation for a given E, so too does $\psi(-x)$, and hence also the even and odd linear combinations $\psi(x) \pm \psi(-x)$.

So, we can assume with no loss of generality that the solutions are either even or odd. The advantage of this is that we need only impose the boundary conditions on one side (say, at +*a*); the other side is then automatic, since $\psi(-x) = \pm\,\psi(x)$.

Let's work out the even solutions.

$$\psi(x) = \begin{cases} Fe^{-\kappa x}, & \text{for } x > a, \\ D\cos(lx), & \text{for } 0 < x < a, \\ \psi(-x), & \text{for } x < 0. \end{cases}$$

The continuity of $\psi(x)$, at $x = a$,

$$\Rightarrow \ Fe^{-\kappa a} = D\cos(la),$$

and the continuity of $d\psi/dx$,

$$\Rightarrow \ -\kappa Fe^{-\kappa a} = -lD\sin(la).$$

Dividing we find that

$$\kappa = l\tan(la).$$

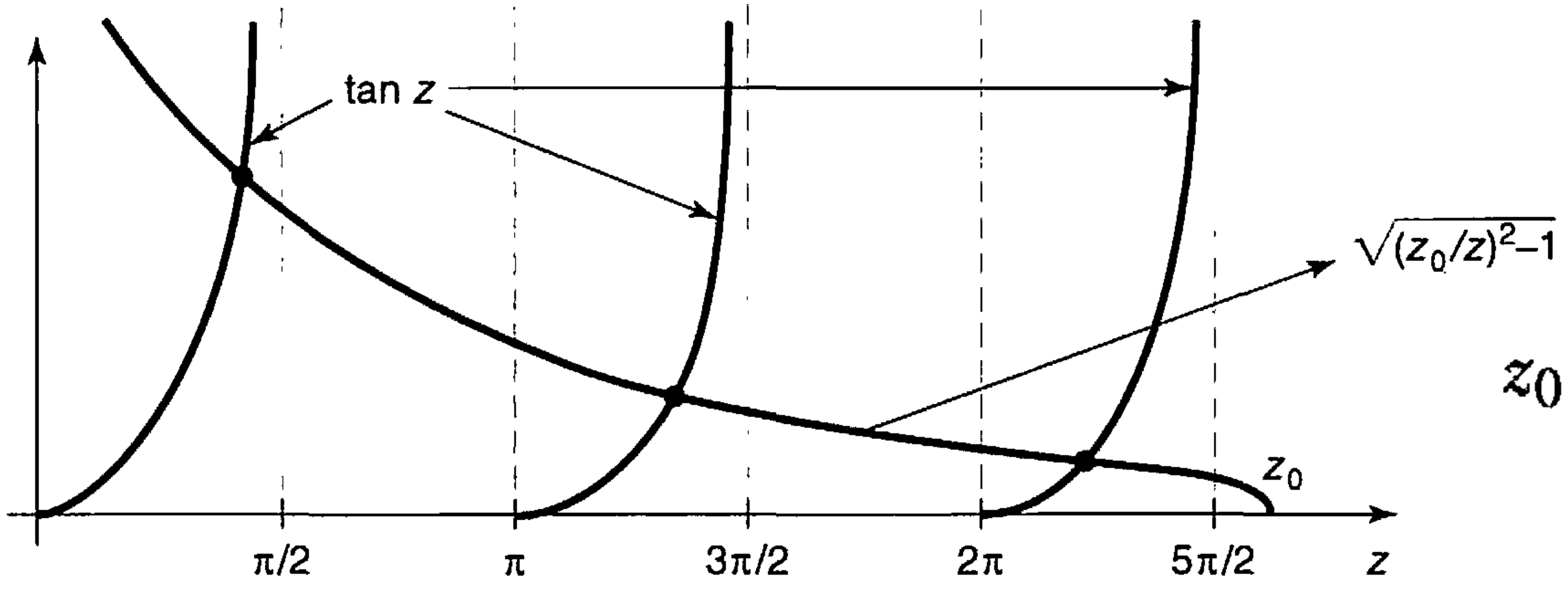
This is a formula for the allowed energies, since *k* and *l* are both functions of *E*. To solve for *E*, let us define

$$z \equiv la, \quad \text{and} \quad z_0 \equiv \frac{a}{\hbar}\sqrt{2mV_0}.$$

$$\text{so}, (\kappa^2 + l^2) = 2mV_0/\hbar^2 \Rightarrow \kappa a = \sqrt{z_0^2 - z^2}$$

$$\Rightarrow \tan z = \sqrt{(z_0/z)^2 - 1}.$$

This is a transcendental equation for *z* (and hence for *E*) as a function of z_o (which is a measure of the "size" of the well). Solved numerically, using a computer, or graphically, by plotting tanz and $\sqrt{(z_o/z)^2 - 1}$ on the same grid, and look for points of intersection.



$z_0 = 8$

Two limiting cases are of special interest:

1. Wide, deep well. If z_o is very large, the intersections occur just slightly below $z_n = n\pi/2$, with n odd; it follows that

$$E_n + V_0 \cong \frac{n^2\pi^2\hbar^2}{2m(2a)^2}.$$

The finite square well goes over to the infinite square well, as V_0 —> ∞; however, for any finite V_0 there are only a finite number of bound states.

2. Shallow, narrow well. As z_o decreases, **there are fewer and fewer bound states**, until finally (for $z_o < \pi/2$, where the lowest odd state disappears) only one remains. It is interesting to note, however, that **there is always one bound state, no matter how "weak" the well becomes.**

contd...

Consider the case **E > 0 (scattering states)**

$$\psi(x) = Ae^{ikx} + Be^{-ikx}, \quad \text{for } (x < -a).$$

where $$k \equiv \frac{\sqrt{2mE}}{\hbar}.$$

$$\psi(x) = C\sin(lx) + D\cos(lx), \quad \text{for } (-a < x < a),$$

where $$l \equiv \frac{\sqrt{2m(E+V_0)}}{\hbar}.$$

$$\psi(x) = Fe^{ikx} \text{ for } x > a.$$

A : incident amplitude.

B : reflected amplitude.

F : transmitted amplitude.

Continuity of $\psi(x)$ at $-a$

$$\Rightarrow Ae^{-ika} + Be^{ika} = -C\sin(la) + D\cos(la),$$

continuity of $d\psi/dx$ at $-a$

$$\Rightarrow ik[Ae^{-ika} - Be^{ika}] = l[C\cos(la) + D\sin(la)]$$

continuity of $\psi(x)$ at $+a$

$$\Rightarrow C\sin(la) + D\cos(la) = Fe^{ika}.$$

and continuity of $d\psi/dx$ at $+a$

$$\Rightarrow l[C\cos(la) - D\sin(la)] = ikFe^{ika}.$$

contd…

Eliminating C and D from the previous equations, we get

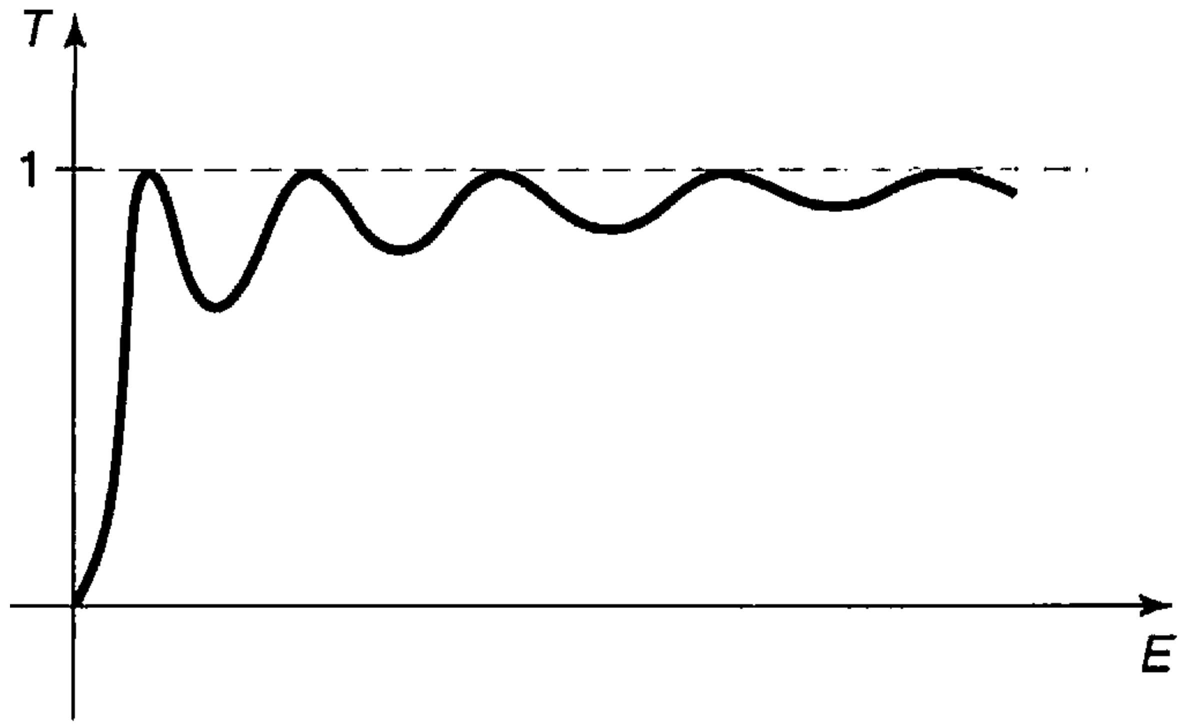
$$B = i\frac{\sin(2la)}{2kl}(l^2 - k^2)F.$$

$$F = \frac{e^{-2ika}A}{\cos(2la) - i\frac{(k^2+l^2)}{2kl}\sin(2la)}.$$

The transmission coefficient ($T = |F|^2/|A|^2$) is given by

$$T^{-1} = 1 + \frac{V_0^2}{4E(E+V_0)}\sin^2\left(\frac{2a}{\hbar}\sqrt{2m(E+V_0)}\right).$$

$T = 1$ when $\frac{2a}{\hbar}\sqrt{2m(E_n + V_0)} = n\pi$, where n is any integer.



The energies for perfect transmission are given by

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

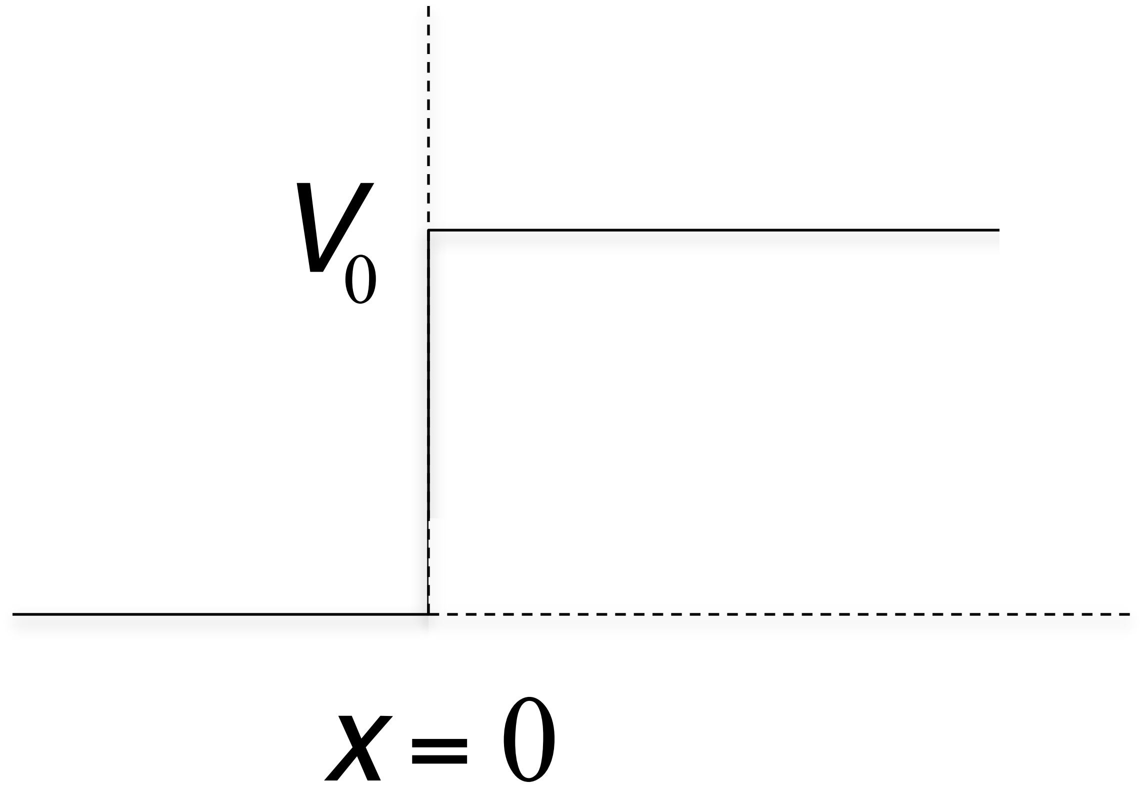
precisely the allowed energies for the *infinite* square well.

Potential Barriers

Consider the following two examples:

Ex.1

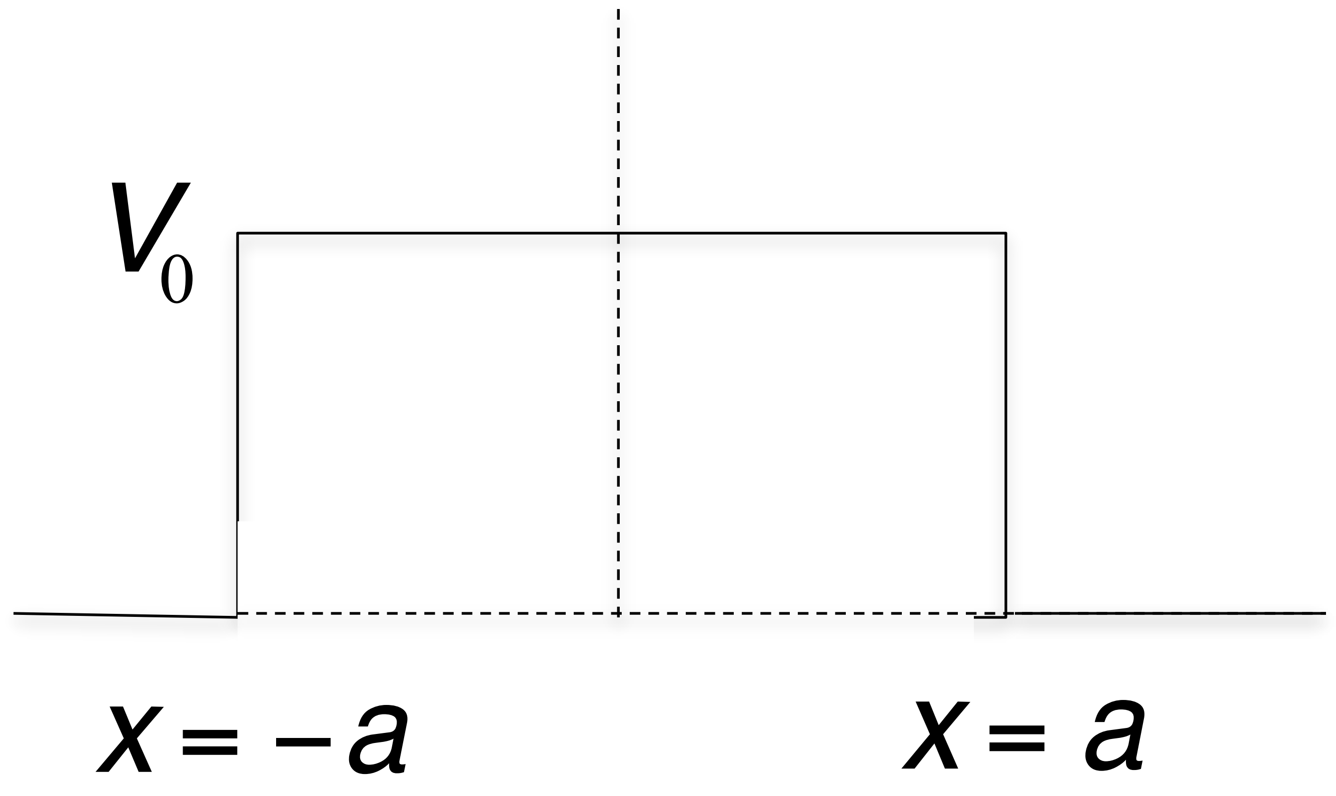
$$V(x) = \begin{cases} 0, & x < 0 \\ V_0, & x \geq 0 \end{cases}$$



Two regions of interest

Ex.2

$$V(x) = \begin{cases} 0, & x < -a \\ V_0, & -a \leq x \leq a \\ 0, & x > a \end{cases}$$



Three regions of interest