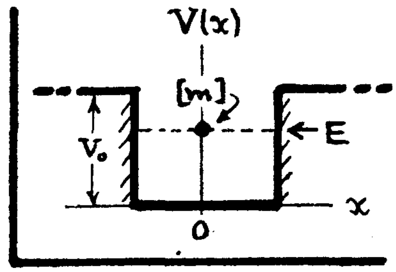
Schrödinger's Problem for a Rectangular Potential Well.

Examples: Solutions to Schrodinger's Eqtn in Simple Systems.

At long last, we shall actually use the QM theory we have invented to solve some simple problems for a particle interacting with an external potential. We do 3 examples: (A) a particle bound in a 1D rectangular potential well, (B) a particle "penetrating" a rectangular potential barrier in 1D, (C) a particle bound in a 1D simple harmonic oscillator (SHO) potential. Besides rediscovering the notion of discrete bound states, we shall find that a QM particle can behave quite non-classically... in example (B), the particle can climb over a mountain without ever going to the top.

A. Rectangular Potential Well [Davydov, Sec. 25].



1. We want a solution for the potential:

$$V(x) = \begin{cases} 0, & \text{for } -a < x < +a; \\ V_0, \text{ cnst}, & \text{for } |x| > a. \end{cases} \qquad (1)$$

We want solutions for m bound in V(x), i.e. at energy E such that $0 < E < V_0$. The fact that V(x) is symmetric in x, $V(-x) = V(x)$, can be used to classify possible solutions $\psi(x)$ according to their "parity" (i.e. reflection symmetry), as follows. The Schrödinger Eqtn is...

$$\rightarrow \frac{d^2}{dx^2}\psi(x) + \frac{2m}{\hbar^2}[E - V(x)]\,\psi(x) = 0. \qquad (2A)$$

Carry out a parity operation, i.e. reflection (mirror-imaging) of the space coordinates: $x \rightarrow (-)x$. Then $\psi(x) \rightarrow \psi(-x)$, and $V(x) \rightarrow V(-x) = V(x)$, so...

$$\rightarrow \frac{d^2}{dx^2}\psi(-x) + \frac{2m}{\hbar^2}[E - V(x)]\,\psi(-x) = 0. \qquad (2B)$$

Comparing (2B) with (2A), we see that $\psi(-x)$ & $\psi(x)$ are solutions each with eigenenergy E; both $\psi(-x)$ & $\psi(x)$ describe the same QM energy state. As such, $\psi(-x)$ must be a multiple of $\psi(+x)$; assume...

$$\psi(-x) = \epsilon\,\psi(+x),\ \epsilon = \text{cnst. Then } x \to (-)x \text{ again} \Rightarrow$$
$$\psi(+x) = \epsilon\,\psi(-x) = \epsilon^2\,\psi(x), \text{ so } \underline{\epsilon^2 = 1, \text{ or } \epsilon = \pm 1}. \tag{3}$$

Then solutions to Schrödinger's Eqtn in this case split into two classes:

$$\left.\begin{array}{l} \text{CLASS I } (\underline{\underline{+\text{ve parity}}}: \psi(x) \text{ even in } x): \underline{\underline{\psi(-x) = +\psi(+x)}} \Rightarrow (d\psi/dx)_0 = 0; \\ \text{CLASS II } (\underline{\underline{-\text{ve parity}}}: \psi(x) \text{ odd in } x): \underline{\underline{\psi(-x) = -\psi(+x)}} \Rightarrow \psi(0) = 0. \end{array}\right\} \tag{4}$$

All solutions ψ to this problem must show such a reflection symmetry. Then, since we know $\psi(-x)$ from $\psi(+x)$, we need only find solutions for $x \geq 0$. In times to come, we shall see that any symmetries in $\mathcal{H}$ [in the present case, $\mathcal{H}(x) = -(\hbar^2/2m)\frac{d^2}{dx^2} + V(x) = \mathcal{H}(-x)$] generate symmetries in ψ.

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2. Solutions inside and outside the well are...

INSIDE: $0 \leq x < a$.

$$\frac{d^2\psi}{dx^2} + \alpha^2\psi = 0, \text{ w/ } \alpha = (2mE/\hbar^2)^{1/2}; \tag{5A}$$

$\Rightarrow \psi(x) = A\cos\alpha x + B\sin\alpha x$, A & B cnsts, as general solution;

so CLASS I solutions (set $B=0$): $\underline{\underline{\psi(x) = A\cos\alpha x}}$, even (+ve parity);

CLASS II solutions (set $A=0$): $\underline{\underline{\psi(x) = B\sin\alpha x}}$, odd (−ve parity).

OUTSIDE: $x > a$.

$$\frac{d^2\psi}{dx^2} - \beta^2\psi = 0, \text{ w/ } \beta = \left[\frac{2m}{\hbar^2}(V_0 - E)\right]^{1/2} \int \begin{array}{l} V_0 > E > 0 \text{ for bound states,} \\ \text{so } \beta = (+)\text{ve real cnst.} \end{array} \tag{5B}$$

$\Rightarrow \psi(x) = Ce^{-\beta x} + De^{+\beta x}$, C & D cnsts, as general solution;

but ψ finite as $x \to +\infty$, so choose $D=0$, and $\underline{\underline{\psi(x) = Ce^{-\beta x}}}$.

Now impose the continuity conditions for ψ & $\psi' = d\psi/dx$ at the boundary $x=a$. It is these conditions that end up requiring energy eigenvalues -- as we saw before (ref. CLASS NOTES, pp. Prop. 11-12). Here, for the two solution classes...

Rectangular Potential Well (cont'd).

CLASS I solutions (even parity)

ψ continuous at $x=a$: $A\cos\alpha a = Ce^{-\beta a}$
ψ' " " " : $-\alpha A\sin\alpha a = -\beta Ce^{-\beta a}$ } $\underline{\underline{\alpha\tan\alpha a = +\beta}}$. (6A)

CLASS II solutions (odd parity)

ψ continuous at $x=a$: $B\sin\alpha a = Ce^{-\beta a}$
ψ' " " " : $\alpha B\cos\alpha a = -\beta Ce^{-\beta a}$ } $\underline{\underline{\alpha\,\mathrm{ctn}\,\alpha = -\beta}}$. (6B)

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3. With $\alpha = [(2m/\hbar^2)E]^{1/2}$ and $\beta = [(2m/\hbar^2)(V_0 - E)]^{1/2}$, Eqs (6) are transcendental equations for the (discrete) system energies E. An instructive graphical method of solution proceeds as follows...

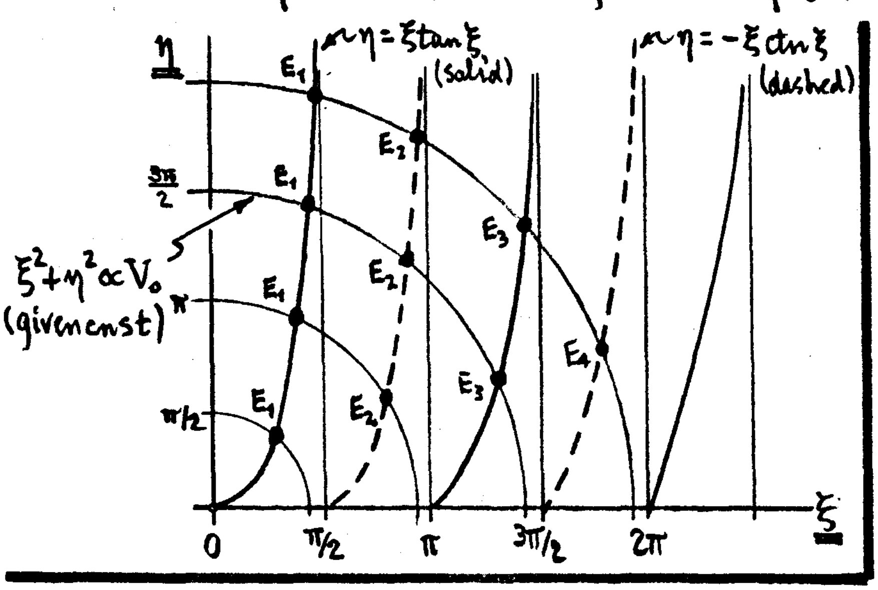
$$\text{Define}\begin{cases}\underline{\xi = \alpha a \geqslant 0}, & \text{w/ } \alpha = [(2m/\hbar^2)E]^{1/2};\\ \underline{\eta = \beta a \geqslant 0}, & \text{w/ } \beta = [(2m/\hbar^2)(V_0-E)]^{1/2}.\end{cases} \qquad (7)$$

Then // $\underline{\underline{\xi^2+\eta^2 = 2mV_0a^2/\hbar^2}}$ = cnst, determined by "well size" V_0a^2;

And // $\underline{\underline{\eta = +\xi\tan\xi}}$, for CLASS I energies [Eq. (6A)];

$\underline{\underline{\eta = -\xi\,\mathrm{ctn}\,\xi}}$, for CLASS II energies [Eq. (6B)]. } (8)

We now plot these three families of curves in the ξ-η plane. The curves



$\xi^2+\eta^2$ = cnst are a family of circles as shown; also shown are the curves $\eta = \xi\tan\xi$ and $\eta = -\xi\,\mathrm{ctn}\,\xi$ for the even & odd states. The points of intersection of the circles with the trig fcns determine discrete energies E_1, E_2, E_3 allowed for m bound in the well. As V_0 increases in size, we add energy states $(E_1, E_3, \ldots)$ of even, then $(E_2, E_4, \ldots)$ of odd parity.

Properties of an ∞ly deep well.

4. We can track the sequence of allowed energy states as follows...

$$\left[\begin{array}{l} 0 < (2m/\hbar^2)V_0 a^2 < \left(\frac{\pi}{2}\right)^2, \text{ i.e. } 0 < V_0 < 1^2 \cdot \frac{\pi^2\hbar^2}{8ma^2} \Rightarrow 1 \text{ state } \left(\substack{\text{even}\\ \text{parity}}\right); \\ \vdots \\ 0 < (2m/\hbar^2)V_0 a^2 < \left(n\frac{\pi}{2}\right)^2, \text{ i.e. } 0 < V_0 < n^2 \cdot \frac{\pi^2\hbar^2}{8ma^2} \Rightarrow n \text{ states}; \\ \text{So a new state appears each time: } \underline{\underline{V_0 > n^2(\pi^2\hbar^2/8ma^2)}}, \quad n = 1, 2, 3, 4, 5, \ldots \end{array}\right. \quad (9)$$

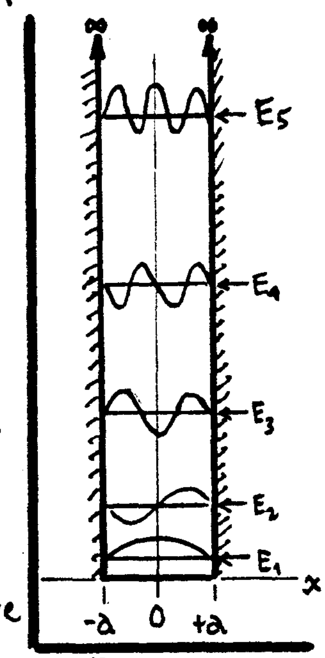
class I ($n = 1, 3, 5, \ldots$); class II ($n = 2, 4, \ldots$)

When $V_0 \to \infty$ (i.e. becomes very large compared with the scale $\pi^2\hbar^2/8ma^2$), then...

$$\left[\begin{array}{l} V_0 \to \infty \Rightarrow \text{a new state appears each time } \xi = n\frac{\pi}{2}, \; n = 1, 2, 3, \ldots \\ \text{So } \xi = \alpha a = [(2m/\hbar^2)E_n]^{1/2} a = n\frac{\pi}{2}, \text{ and } \boxed{E_n = n^2(\pi^2\hbar^2/8ma^2)} \end{array}\right. \quad (10)$$

These E_n are the energy levels for a very deep (formally: ∞ly deep) potential well of spatial extent $2a$. We have seen them before, in the 1D box example on pp. Prop. 6-7 of CLASS NOTES. The wavefcns for the present example are...

$$\left[\begin{array}{l} \text{CLASS I}: \; \psi_n(x) = A\cos(n\pi x/2a), \quad n = 1, 3, 5, \ldots; \\ \text{CLASS II}: \; \psi_n(x) = B\sin(n\pi x/2a), \quad n = 2, 4, 6, \ldots . \end{array}\right. \quad (11)$$



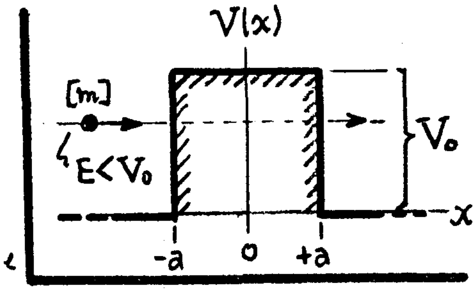
These ψ_n's are sketched at right, at the energies E_n allowed in the (deep) well -- they show the same features as in the previous semi-quantitative analysis (see p. Prop. 12): alternation of states of $\pm$ve parity, n^{th} state ψ_n has $(n-1)$ nodes, etc.

It is interesting to note that for the 1D box problem, the above energies E_n can be derived from de Broglie's relation: $p = 2\pi\hbar/\lambda$. Insist that an integral # of half-λ's "fit" into the box: $n \cdot \frac{\lambda}{2} = 2a$, so: $\lambda = 4a/n$. Then m^{s} allowed momenta are quantized: $p_n = 2\pi\hbar/\lambda_n = (\pi\hbar/2a)n$, and hence the energy (free motion for $|x| < a$): $\underline{\underline{E_n = p_n^2/2m = n^2(\pi^2\hbar^2/8ma^2)}}$, as in Eq. (10).

Schrödinger's Problem for a Rectangular Potential Barrier.

B. Rectangular Potential Barrier [Davydov, Sec. 24].

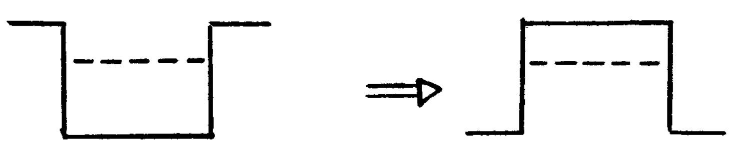
1. We want a solution for the potential:



$$V(x) = \begin{cases} V_0, & \text{for } -a < x < a; \\ 0, & \text{for } |x| > a; \end{cases} \qquad (1)$$

for the case of a particle of mass m incident from the left @ energy $E < V_0$.* Since $V(x)$ is a repulsive potential (w/ $-dV/dx \to -\infty$ @ $x = -a$), then--classically--m would just be reflected at the left-hand edge, and would never be found inside the barrier... since, inside (with $E < V_0$), its kinetic energy would have to be (−)ve. QMly, however, it is possible for m to penetrate the barrier and to travel beyond $x = +a$.

The above problem is just an upside-down square well. Symmetry suggests the following solution...



$$\psi(x) = A\cos\left(\frac{n\pi x}{2a}\right)$$

This is a rare instance where a symmetry argument does not work. The suggested $\psi(x)$ obeys Schrödinger's Eqtn, but not Schrödinger's Eqtn.

2. Schrödinger's Eqtn again has simple solutions...

$$\begin{cases} |x| > a: \ \psi'' + k^2\psi = 0, \ \text{w/ } k = \sqrt{2mE/\hbar^2} \Rightarrow \psi(x) \propto e^{\pm ikx}; \ \{\text{outside barrier} \\ |x| < a: \ \psi'' - \kappa^2\psi = 0, \ \text{w/ } \kappa = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)} \Rightarrow \psi(x) \propto e^{\pm \kappa x}. \ \{\text{inside barrier} \end{cases} \qquad (2)$$

ψ & ψ' will be finite everywhere. The labor in the problem is to make ψ & ψ' continuous at the boundary points $x = \pm a$. The general solutions in the

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* We do this problem without an explicit time-dependence. So we should imagine a steady stream of m's incident from the left, thus achieving a steady-state situation.

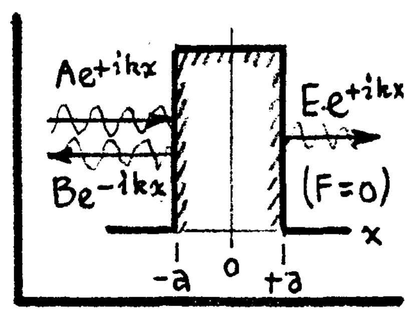
Rectangular Potential Barrier (cont'd)

various regions are (with $A, B, \ldots, F$ = cnsts):

$$\begin{cases} x < -a & : \psi(x) = A e^{+ikx} + B e^{-ikx}; \\ -a < x < +a : & \psi(x) = C e^{-\kappa x} + D e^{+\kappa x}; \\ x > +a & : \psi(x) = E e^{+ikx} + F e^{-ikx}. \end{cases} \qquad \frac{k = \sqrt{(2m/\hbar^2)E},}{\kappa = \sqrt{(2m/\hbar^2)(V_0 - E)}.} \tag{3}$$

4 of the 6 cnsts here can be fixed by the continuity conditions on ψ & ψ' at $x = \pm a$. A 5^{th} cnst can be fixed by imposing normalization -- e.g. requiring unit incident intensity. The 6^{th} cnst is free -- we can adjust it to fit the physics. We do that as follows...

$$\left[\begin{array}{l} \left.\begin{array}{c}\text{probability}\\ \text{current}\end{array}\right\} J = \frac{\hbar}{2im}\left[\psi^*\left(\frac{\partial\psi}{\partial x}\right) - \left(\frac{\partial\psi^*}{\partial x}\right)\psi\right]; \\ \ldots \text{for } \psi \propto e^{+ikx} : J = +(\hbar k/m)|\psi|^2 \Rightarrow m \text{ travels to } \underline{\underline{\text{right}}}; \\ \ldots \text{for } \psi \propto e^{-ikx} : J = -(\hbar k/m)|\psi|^2 \Rightarrow m \text{ travels to } \underline{\underline{\text{left}}}. \end{array}\right. \tag{4}$$



In the first of Eqs. (3), we shall allow both A & B to be non-zero... this means that in the region $x < -a$, there is both an <u>incident</u> wave Ae^{+ikx} (traveling from left to right) and a <u>reflected</u> wave Be^{-ikx} (going from right to left). On the other hand, in the third of Eqs. (3), we allow $E \neq 0$, but set $F = 0$... this means that at $x > +a$, there is just a wave Ee^{+ikx} that is <u>transmitted</u> (and traveling to the right); there is no wave incident on the barrier at $x = +a$ from the right. So the solutions are now:

$$\rightarrow x < -a : \psi(x) = \underbrace{A}_{\text{incident}} e^{+ikx} + \underbrace{B}_{\text{reflected}} e^{-ikx}; \quad x > +a : \psi(x) = \underbrace{E}_{\text{transmitted}} e^{+ikx} \tag{5}$$

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3. Now we impose the boundary conditions on ψ & ψ' @ $x = \pm a$... (next page)

Rectangular Potential Barrier (cont'd)

$x=-a$: ψ & ψ' continuous

$$Ae^{-ika}+Be^{+ika}=Ce^{+\kappa a}+De^{-\kappa a},$$

&

$$ik(Ae^{-ika}-Be^{+ika})=-\kappa(Ce^{+\kappa a}-De^{-\kappa a});$$

call this matrix $\underline{M}$.

w/ $$\begin{pmatrix}A\\B\end{pmatrix}=\frac{1}{2}\begin{pmatrix}\left(1+\frac{i\kappa}{k}\right)e^{\kappa a+ika} & \left(1-\frac{i\kappa}{k}\right)e^{-\kappa a+ika}\\ \left(1-\frac{i\kappa}{k}\right)e^{\kappa a-ika} & \left(1+\frac{i\kappa}{k}\right)e^{-\kappa a-ika}\end{pmatrix}\begin{pmatrix}C\\D\end{pmatrix}. \quad (6)$$

$x=+a$: ψ & ψ' continuous

call this matrix $\underline{N}$.

$$\begin{pmatrix}C\\D\end{pmatrix}=\frac{1}{2}\begin{pmatrix}\left(1-\frac{ik}{\kappa}\right)e^{\kappa a+ika} & \left(1+\frac{ik}{\kappa}\right)e^{\kappa a-ika}\\ \left(1+\frac{ik}{\kappa}\right)e^{-\kappa a+ika} & \left(1-\frac{ik}{\kappa}\right)e^{-\kappa a-ika}\end{pmatrix}\begin{pmatrix}E\\F\end{pmatrix},\ \text{w/}\ F=0. \quad (7)$$

These two eqtns relate the amplitudes A (incident) & B (reflected), at $x<-a$, to the amplitude E (transmitted), at $x>+a$. We have...

$$\rightarrow \begin{pmatrix}A\\B\end{pmatrix}=\underline{M}\,\underline{N}\begin{pmatrix}E\\F\end{pmatrix},\ \text{w/}\ F=0. \quad (8)$$

The matrix product is:

$$\rightarrow \underline{M}\,\underline{N}=\begin{pmatrix}\left(\cosh 2\kappa a+\frac{1}{2}i\lambda\sinh 2\kappa a\right)e^{+2ika} & +\frac{1}{2}i\mu\sinh 2\kappa a\\ -\frac{1}{2}i\mu\sinh 2\kappa a & \left(\cosh 2\kappa a-\frac{1}{2}i\lambda\sinh 2\kappa a\right)e^{-2ika}\end{pmatrix},$$

where/ $$\underline{\lambda=\frac{\kappa}{k}-\frac{k}{\kappa}},\quad \underline{\mu=\frac{\kappa}{k}+\frac{k}{\kappa}}. \quad (9)$$

With $F=0$ in Eq. (8), this result immediately gives an expression for E, as...

$$A=(\underline{M}\,\underline{N})_{11}E,\ \text{w/}\ \underline{E/A=e^{-2ika}\big/\left(\cosh 2\kappa a+\tfrac{1}{2}i\lambda\sinh 2\kappa a\right)}. \quad (10)$$

And, for the reflected wave, some minor algebra gives...

$$\underline{B/A=-\tfrac{1}{2}i\mu\,(E/A)\sinh 2\kappa a}. \quad (11)$$

$|E/A|^2$ & $|B/A|^2$ give the fractional transmitted & reflected intensities, resp.