Quantum Mechanics

Solving the Schrödinger Equation

Time-independent Potential, $V = V(x)$

$$\boxed{i\hbar\frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V(x)\Psi}$$

Can we separate the variables? $\Psi(x,t) = \psi(x)\,\phi(t)$ $\rightarrow$ $\frac{\partial \Psi}{\partial t} = \psi\frac{d\varphi}{dt}, \quad \frac{\partial^2 \Psi}{\partial x^2} = \frac{d^2\psi}{dx^2}\varphi$

The Schrödinger equation can now be written as $i\hbar\frac{1}{\varphi}\frac{d\varphi}{dt} = -\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{d^2\psi}{dx^2} + V$

The only way this could be true is if both sides are equal to a constant.

So, we get two equations:

$$\boxed{\frac{d\varphi}{dt} = -\frac{iE}{\hbar}\varphi} \rightarrow \boxed{\varphi(t) = e^{-iEt/\hbar}} \rightarrow$$

Time-independent probabilities

$$|\Psi(x,t)|^2 = |\psi(x)|^2\phi^*(t)\phi(t) = |\psi(x)|^2$$

Steady states or stationary states

$$\boxed{-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi} \rightarrow \boxed{\hat{H}\psi = E\psi}$$

Time-independent Schrödinger Equation

The stationary states are eigenfunctions of the Hamiltonian operator.

Stationary States

The entire ensemble has the same energy, E

$$\langle H\rangle = \int \Psi^* \hat{H}\,\Psi\, dx = \int (\phi^*\phi)(\psi^*\hat{H}\psi)\, dx = E\int(\psi^*\psi)\, dx = E$$

$$\langle H^2\rangle = \int (\psi^*\hat{H}\hat{H}\psi)\, dx = E^2\int(\psi^*\psi)\, dx = E^2 \quad \longrightarrow \quad \sigma_H = 0$$

General solutions are linear combinations

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x) e^{-iE_n t/\hbar} = \sum_{n=1}^{\infty} c_n \Psi_n(x,t)$$

Example 2.1 Suppose a particle starts out in a linear combination of just *two* stationary states:

$$\Psi(x,0) = c_1\psi_1(x) + c_2\psi_2(x).$$

(To keep things simple I'll assume that the constants c_n and the states $\psi_n(x)$ are *real*.) What is the wave function $\Psi(x,t)$ at subsequent times? Find the probability density, and describe its motion.

Combinations can have dynamics

Solution: The first part is easy:

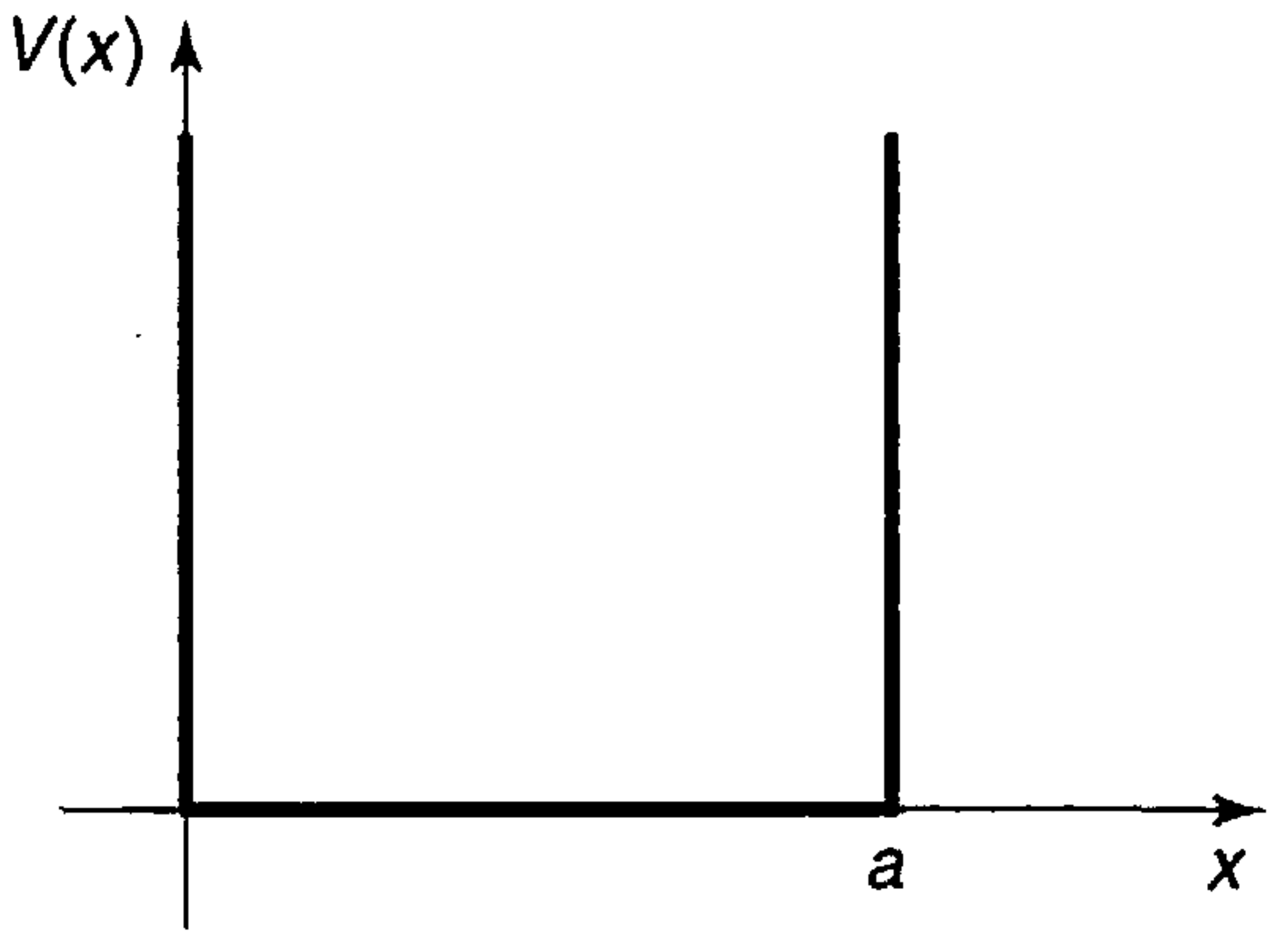
$$\Psi(x,t) = c_1\psi_1(x)e^{-iE_1t/\hbar} + c_2\psi_2(x)e^{-iE_2t/\hbar},$$

where E_1 and E_2 are the energies associated with ψ_1 and ψ_2. It follows that

$$|\Psi(x,t)|^2 = (c_1\psi_1 e^{iE_1t/\hbar} + c_2\psi_2 e^{iE_2/\hbar})(c_1\psi_1 e^{-iE_1t/\hbar} + c_2\psi_2 e^{-iE_2/\hbar})$$

$$= c_1^2\psi_1^2 + c_2^2\psi_2^2 + 2c_1c_2\psi_1\psi_2\cos[(E_2 - E_1)t/\hbar].$$

Particle in a Box



$$V(x) = \begin{cases} 0, & \text{if } 0 \le x \le a, \\ \infty, & \text{otherwise} \end{cases}$$

If $E < 0$, there is no normalisable solution to the Schrödinger equation

Outside the walls $\psi(x) = 0$. Inside,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \quad \rightarrow \quad \frac{d^2\psi}{dx^2} = -k^2\psi \quad \text{where} \quad k \equiv \frac{\sqrt{2mE}}{\hbar}$$

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) e^{-i(n^2\pi^2\hbar/2ma^2)t}$$

General solution

$$\psi(x) = A\sin kx + B\cos kx$$

Boundary conditions

ψ and $d\psi/dx$ are continuous unless $V = \infty$. In that case, only ψ is continuous

$$\psi(0) = B = 0$$

$$\psi(a) = A\sin(ka) = 0 \quad \rightarrow \quad ka = 0, \pm\pi, \pm 2\pi, \pm 3\pi, \ldots$$

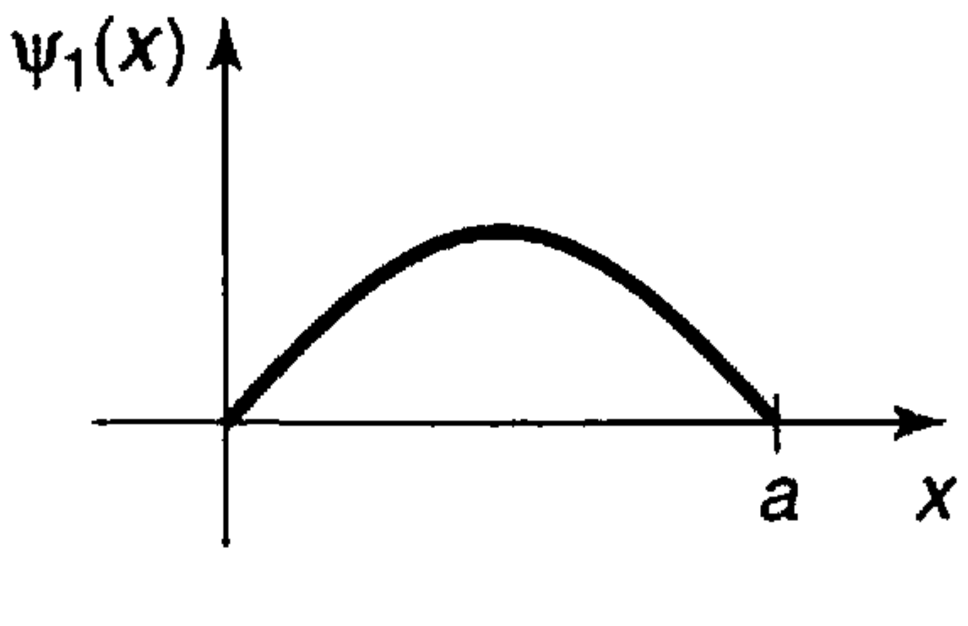
We can absorb the minus sign in A $\rightarrow$ $k_n = \dfrac{n\pi}{a}$ with $n = 1, 2, 3, \ldots$ $\rightarrow$

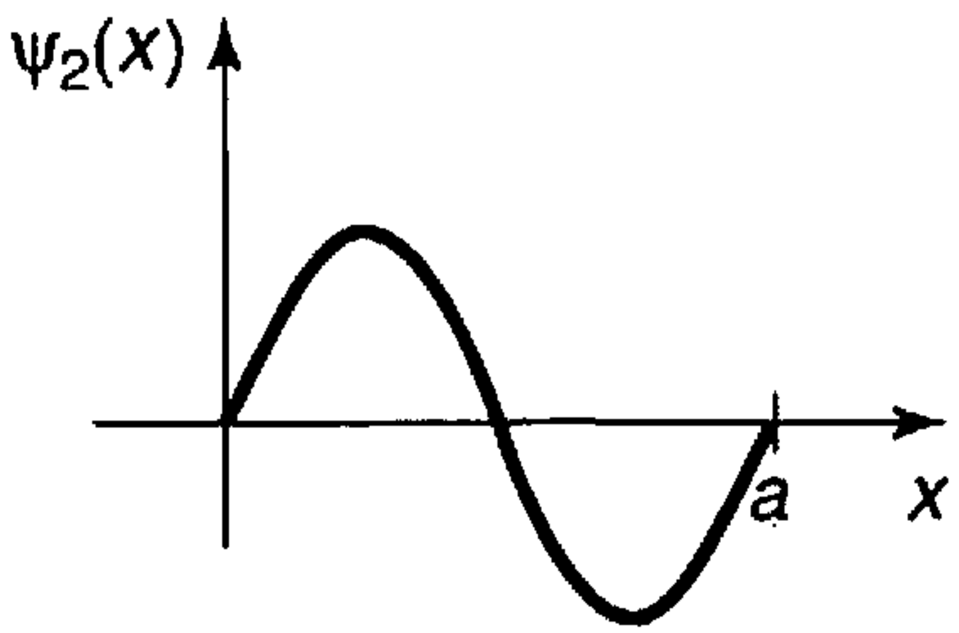
Discrete

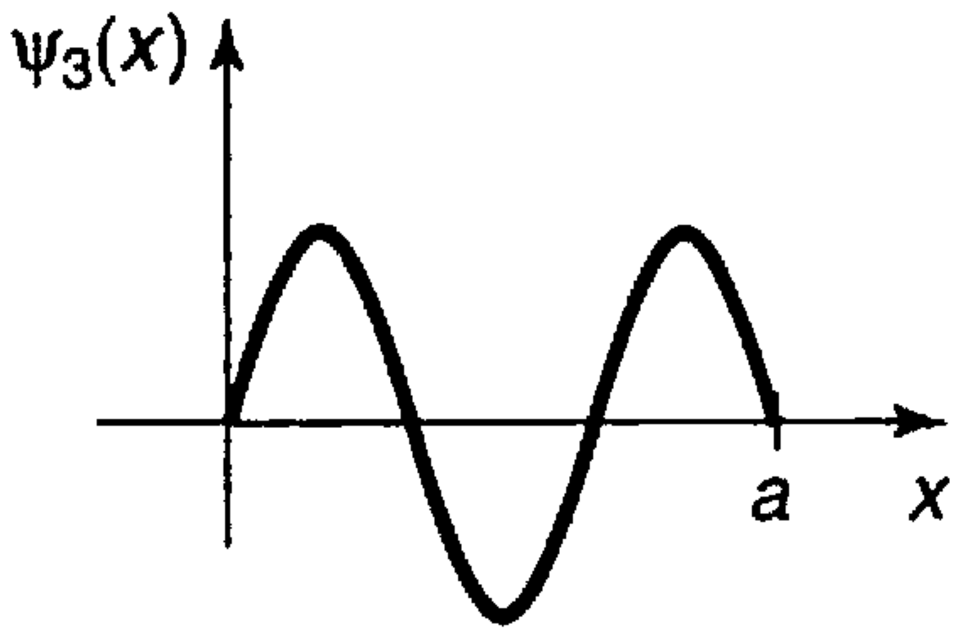
$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{n^2\pi^2\hbar^2}{2ma^2}$$

Normalise to get

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right)$$







Particle in a Box

$$E_n = \frac{n^2 h^2}{8ma^2}$$

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin(\frac{n\pi x}{a})$$

$$P_n(x) = \frac{2}{a}\sin^2(\frac{n\pi x}{a})$$

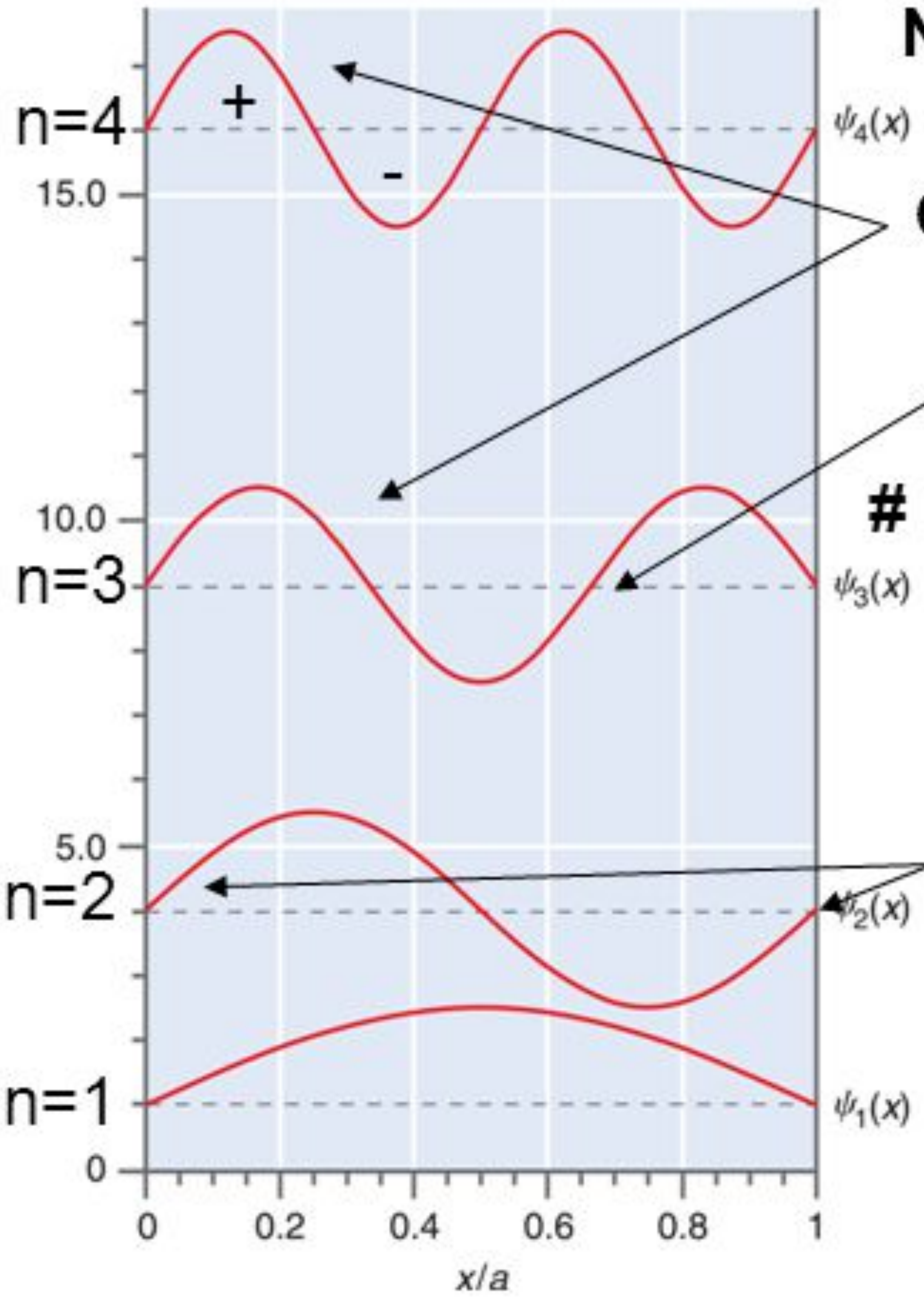
$$E_4 = \frac{16h^2}{8ma^2}$$

$$E_3 = \frac{9h^2}{8ma^2}$$

$$E_2 = \frac{4h^2}{8ma^2}$$

$$E_1 = \frac{h^2}{8ma^2} \neq 0$$

Ground state



Normalized

Orthogonal

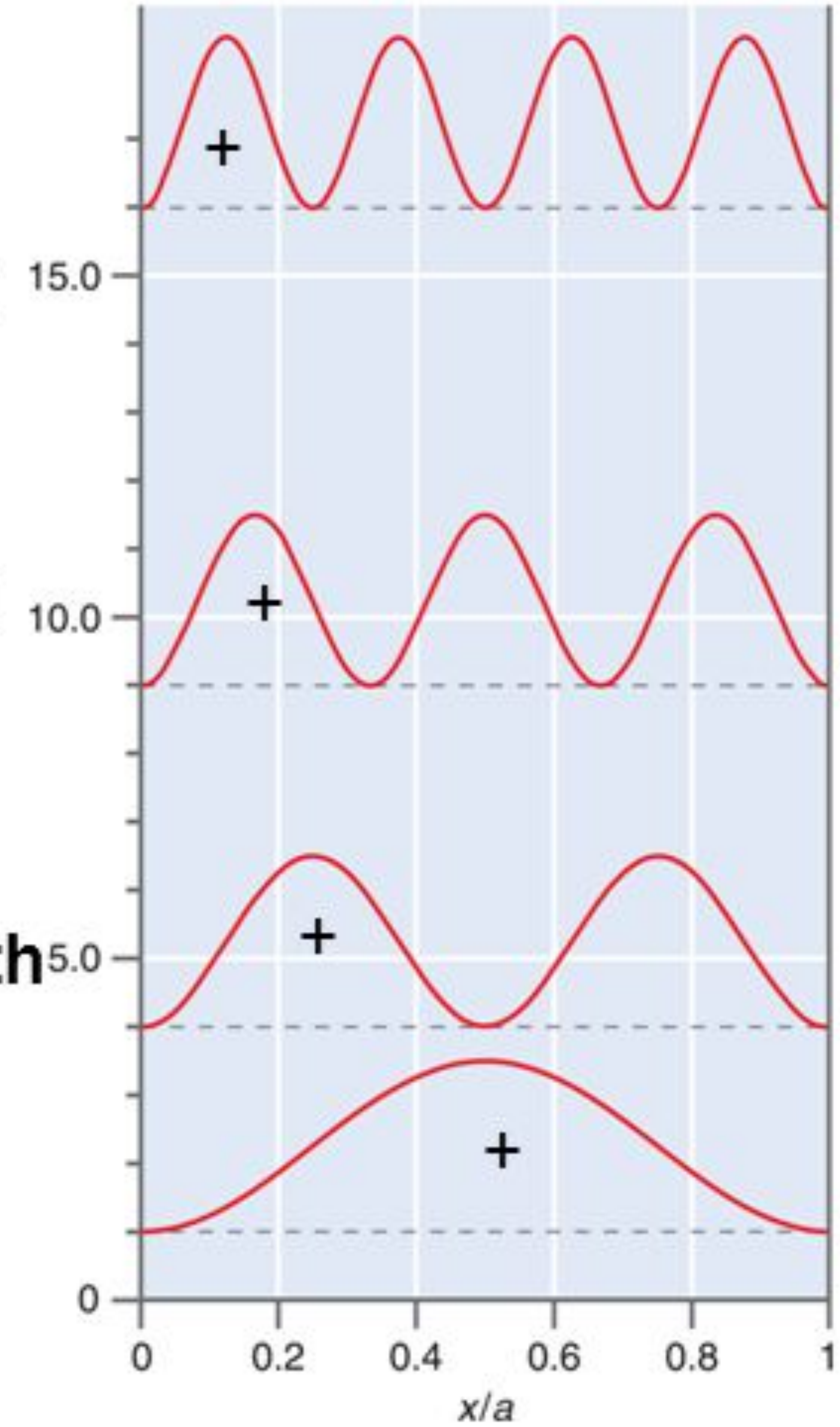
Node

 # nodes= n-1

n > 0

Wavelength

$$\lambda = \frac{2a}{n}$$



Particle in a Box

The states are mutually orthogonal (i.e. ⊥)

Kronecker delta

$$\int \psi_m(x)^* \psi_n(x)\,dx = \delta_{mn} \text{ where } \boxed{\delta_{mn} = \begin{cases} 0, & \text{if } m \neq n \\ 1, & \text{if } m = n \end{cases}}$$

If $m \neq n$

$$\int \psi_m(x)^* \psi_n(x)\,dx = \frac{2}{a}\int_0^a \sin\left(\frac{m\pi}{a}x\right)\sin\left(\frac{n\pi}{a}x\right)dx$$

$$= \frac{1}{a}\int_0^a \left[\cos\left(\frac{m-n}{a}\pi x\right) - \cos\left(\frac{m+n}{a}\pi x\right)\right]dx$$

$$= \left\{\frac{1}{(m-n)\pi}\sin\left(\frac{m-n}{a}\pi x\right) - \frac{1}{(m+n)\pi}\sin\left(\frac{m+n}{a}\pi x\right)\right\}\Bigg|_0^a$$

$$= \frac{1}{\pi}\left\{\frac{\sin[(m-n)\pi]}{(m-n)} - \frac{\sin[(m+n)\pi]}{(m+n)}\right\} = 0.$$

$$\boxed{\Psi(x,t) = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right) e^{-i(n^2\pi^2\hbar/2ma^2)t}}$$

The states are complete

Any function $f(x)$ can be expressed in terms of them

$$f(x) = \sum_{n=1}^{\infty} c_n \psi_n(x) = \sqrt{\frac{2}{a}}\sum_{n=1}^{\infty} c_n \sin\left(\frac{n\pi}{a}x\right)$$

$$\int \psi_m(x)^* f(x)\,dx = \sum_{n=1}^{\infty} c_n \int \psi_m(x)^* \psi_n(x)\,dx$$

$$= \sum_{n=1}^{\infty} c_n \delta_{mn} = c_m$$

$$\boxed{\begin{aligned} \Psi(x,0) &= \sum_{n=1}^{\infty} c_n \psi_n(x) \\ c_n &= \sqrt{\frac{2}{a}}\int_0^a \sin\left(\frac{n\pi}{a}x\right)\Psi(x,0)\,dx \end{aligned}}$$

The probability of getting E_n if you measure energy $= |c_n|^2$.

Mathematical Interlude

Wave functions are all square integrable (normalised).

Such functions ($\int |f(x)|^2 dx < \infty$) form a vector space called Hilbert space or L_2 space.

Inner product

A complex number

$$\langle \Phi | \Psi \rangle = \int \Phi^*(x,t)\,\Psi(x,t)\,dx$$

Dirac's bra(c)ket notation

Normalisation: $\langle \Psi | \Psi \rangle = 1$

Dual vector space
Bra space

Vector space
Ket space

Complex conjugation

If $|\Psi\rangle = c_0|\Psi_0\rangle + c_1|\Psi_1\rangle$

$\langle\Phi|\Psi\rangle = c_0\langle\Phi|\Psi_0\rangle + c_1\langle\Phi|\Psi_1\rangle$

If $|\Phi\rangle = c_0|\Phi_0\rangle + c_1|\Phi_1\rangle$

$\langle\Phi| = c_0^*\langle\Phi_0| + c_1^*\langle\Phi_1|$

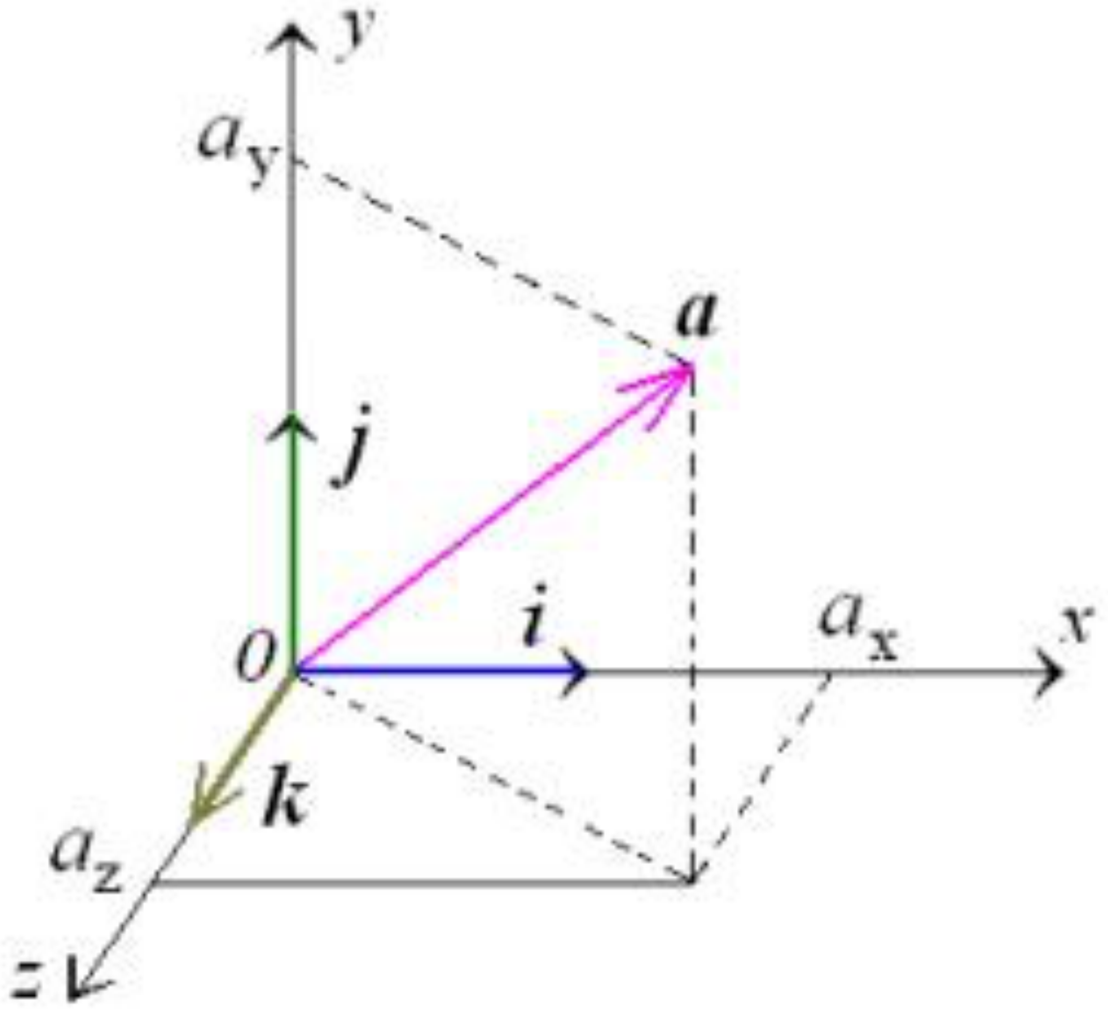
$\langle\Phi|\Psi\rangle = c_0^*\langle\Phi_0|\Psi\rangle + c_1^*\langle\Phi_1|\Psi\rangle$

$$\boxed{\langle\Psi|\Psi\rangle = |c_0|^2\langle\Psi_0|\Psi_0\rangle + |c_1|^2\langle\Psi_1|\Psi_1\rangle}$$

Resolving $\Psi(x,t)$ into mutually orthogonal components

n^{th} unit vector $|\Psi_n\rangle$

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \boxed{\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right) e^{-i(n^2\pi^2\hbar/2ma^2)t}}$$



Orthogonality $\equiv \langle\Psi_m|\Psi_n\rangle = \delta_{mn}$

$$c_n = \langle\Psi_n|\Psi\rangle$$

Mathematical Interlude

$\boxed{\langle f \,|\, g \rangle = \langle g \,|\, f \rangle^*}$

What about operators?

The expectation value of some observable $Q(x,p)$ is written as $\langle Q \rangle = \int \Psi^*(\hat{Q}\Psi)\,dx = \langle \Psi \,|\, \hat{Q}\Psi \rangle$

The dual vector of $|\,\hat{Q}\Psi\rangle$ is $\boxed{\langle \Psi\hat{Q}^\dagger\,|}$. Hence, $\langle \Psi\hat{Q}^\dagger \,|\, \Psi \rangle = \int (\hat{Q}^\dagger\Psi^*)\,\Psi\,dx = \int (\hat{Q}\Psi)^*\,\Psi\,dx = \langle Q \rangle^*$

Also written as $\langle \hat{Q}^\dagger\Psi\,|$

Observables $\equiv$ Hermitian operators

Since measurement outcomes are real, $\langle \Psi\hat{Q}^\dagger \,|\, \Psi \rangle = \langle \Psi \,|\, \hat{Q}\Psi \rangle$ or, simply, $\langle \Psi\hat{Q}^\dagger\Psi \rangle = \langle \Psi\hat{Q}\Psi \rangle$, i.e., $\hat{Q}^\dagger = \hat{Q}$

Momentum operator $\langle f|\hat{p}g\rangle = \int_{-\infty}^{\infty} f^* \frac{\hbar}{i}\frac{dg}{dx}\,dx = \frac{\hbar}{i} f^* g\Big|_{-\infty}^{\infty} + \int_{-\infty}^{\infty} \left(\frac{\hbar}{i}\frac{df}{dx}\right)^* g\,dx = \langle \hat{p}f|g\rangle$

Measuring an observable $\equiv$ Operating on the state vector with an (hermitian) operator

$\hat{Q}\,|\,\Psi\rangle = q_i\,|\,\Psi\rangle$ Normally, if measurements are done on an ensemble, different members return different outcomes

If $|\,\Psi\rangle$ is an eigenvector/eigenfunction of $\hat{Q}$ then we would get the same value, the eigenvalue, from all members

$\hat{Q}|\,\Psi\rangle = q|\,\Psi\rangle \Rightarrow \langle Q \rangle = \langle \Psi \,|\, \hat{Q} \,|\, \Psi \rangle = q\langle \Psi \,|\, \Psi \rangle = q$ and $\sigma_Q = 0$

Operator

Number

E.g., stationary states are eigenfunctions of the Hamiltonian operator with e.v. E_n

Mathematical Interlude

Two theorems for Hermitian operators $(\hat{Q} = \hat{Q}^\dagger)$ in linear algebra

Eigenvalues of Hermitian operators are real

Let $\hat{Q}\,|\,\Psi\rangle = q\,|\,\Psi\rangle$. Now, $q\,\langle\Psi\,|\,\Psi\rangle = \langle\Psi\,|\,\hat{Q}\Psi\rangle = \langle\Psi\hat{Q}^\dagger\,|\,\Psi\rangle = q^*\langle\Psi\,|\,\Psi\rangle$ ***QED***

Eigenvectors/eigenfunctions with different eigenvalues are orthogonal

Let $\hat{Q}\,|\,\Phi\rangle = q'\,|\,\Phi\rangle$. Now, $q'\,\langle\Psi\,|\,\Phi\rangle = \langle\Psi\,|\,\hat{Q}\Phi\rangle = \langle\Psi\hat{Q}^\dagger\,|\,\Phi\rangle = q^*\langle\Psi\,|\,\Phi\rangle = q\,\langle\Psi\,|\,\Phi\rangle$ ***QED***

The degenerate case: If two or more eigenvectors have the same eigenvalues we can find linear combinations that are orthogonal (remember **Gram-Schmidt orthogonalisation**?).

In many cases it is possible to prove that eigenvectors of a Hermitian operator form a complete basis (e.g. particle in a box). In some infinite dimensional cases it is not. There we consider only those operators as our observables for which this is true. Hence, we can span the Hilbert space with these vectors/functions, i.e., express any function in the Hilbert space with them.

The Harmonic Oscillator

$$\boxed{-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2x^2\psi = E\psi}$$

$$H = \frac{1}{2m}[p^2 + (m\omega x)^2]$$

Can we factorise the operator H (as usual, we are sloppy with the hat) like a number? $u^2 + v^2 = (iu+v)(-iu+v)$

Let us define two operators

$$\boxed{a_\pm \equiv \frac{1}{\sqrt{2\hbar m\omega}}(\mp ip + m\omega x)}$$

$$a_-a_+ = \frac{1}{2\hbar m\omega}(ip + m\omega x)(-ip + m\omega x) = \frac{1}{2\hbar m\omega}[p^2 + (m\omega x)^2 - im\omega\boxed{(xp - px)}]$$

$$= \frac{1}{2\hbar m\omega}[p^2 + (m\omega x)^2] - \frac{i}{2\hbar}[x, p]$$

Commutator $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$

$$\boxed{[x,p]f(x) = \left[x\frac{\hbar}{i}\frac{d}{dx}(f) - \frac{\hbar}{i}\frac{d}{dx}(xf)\right] = \frac{\hbar}{i}\left(x\frac{df}{dx} - x\frac{df}{dx} - f\right) = i\hbar f(x)} \Rightarrow \boxed{[x,p] = i\hbar}$$

$$\boxed{a_-a_+ = \frac{1}{\hbar\omega}H + \frac{1}{2}} \Rightarrow H = \hbar\omega\left(a_-a_+ - \frac{1}{2}\right)$$

$$\boxed{[a_-, a_+] = 1}$$

$$\boxed{a_+a_- = \frac{1}{\hbar\omega}H - \frac{1}{2}} \Rightarrow H = \hbar\omega\left(a_+a_- + \frac{1}{2}\right)$$

Schrödinger equation

$$\boxed{\hbar\omega\left(a_\pm a_\mp \pm \frac{1}{2}\right)\psi = E\psi}$$

The Harmonic Oscillator

$$\boxed{-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2x^2\psi = E\psi}$$

$$H = \frac{1}{2m}[p^2 + (m\omega x)^2]$$

$$\boxed{a_\pm \equiv \frac{1}{\sqrt{2\hbar m\omega}}(\mp ip + m\omega x)}$$

$$H(a_+\psi) = \hbar\omega\left(a_+a_- + \frac{1}{2}\right)(a_+\psi) = \hbar\omega\left(a_+a_-a_+ + \frac{1}{2}a_+\right)\psi$$

$$= \hbar\omega a_+\left(a_-a_+ + \frac{1}{2}\right)\psi = a_+\left[\hbar\omega\left(a_+a_- + 1 + \frac{1}{2}\right)\psi\right]$$

$$= a_+(H + \hbar\omega)\psi = a_+(E + \hbar\omega)\psi = (E + \hbar\omega)(a_+\psi).$$

$$H(a_-\psi) = (E - \hbar\omega)(a_-\psi).$$

If $a\_$ is applied again and again, we would reach a state with -ve energy!

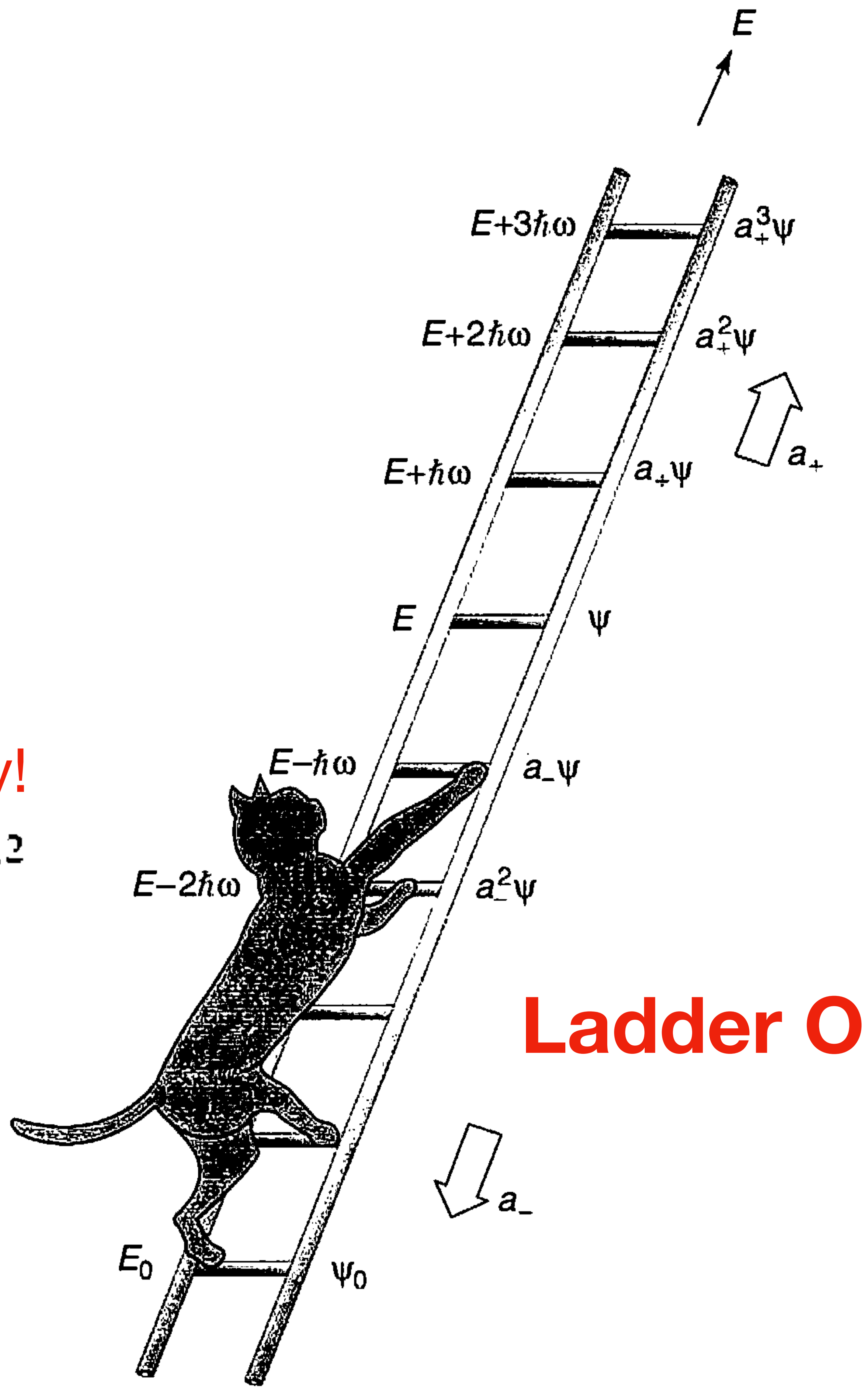
$a_-\psi_0 = 0$ or $\frac{1}{\sqrt{2\hbar m\omega}}\left(\hbar\frac{d}{dx} + m\omega x\right)\psi_0 = 0$ → $\psi_0(x) = Ae^{-\frac{m\omega}{2\hbar}x^2}$

$$1 = |A|^2\int_{-\infty}^{\infty} e^{-m\omega x^2/\hbar}\,dx = |A|^2\sqrt{\frac{\pi\hbar}{m\omega}}$$

Ground state

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}$$

$$E_0 = \frac{1}{2}\hbar\omega.$$



Ladder Operators

The Harmonic Oscillator

$$\boxed{\psi_n(x) = A_n(a_+)^n \psi_0(x), \quad \text{with } E_n = \left(n + \frac{1}{2}\right)\hbar\omega}$$

It is possible to figure out the constants with simple algebra

$$\boxed{\hbar\omega\left(a_\pm a_\mp \pm \frac{1}{2}\right)\psi = E\psi}$$

Let $\quad a_+\psi_n = c_n\psi_{n+1}, \quad a_-\psi_n = d_n\psi_{n-1}$

Notice

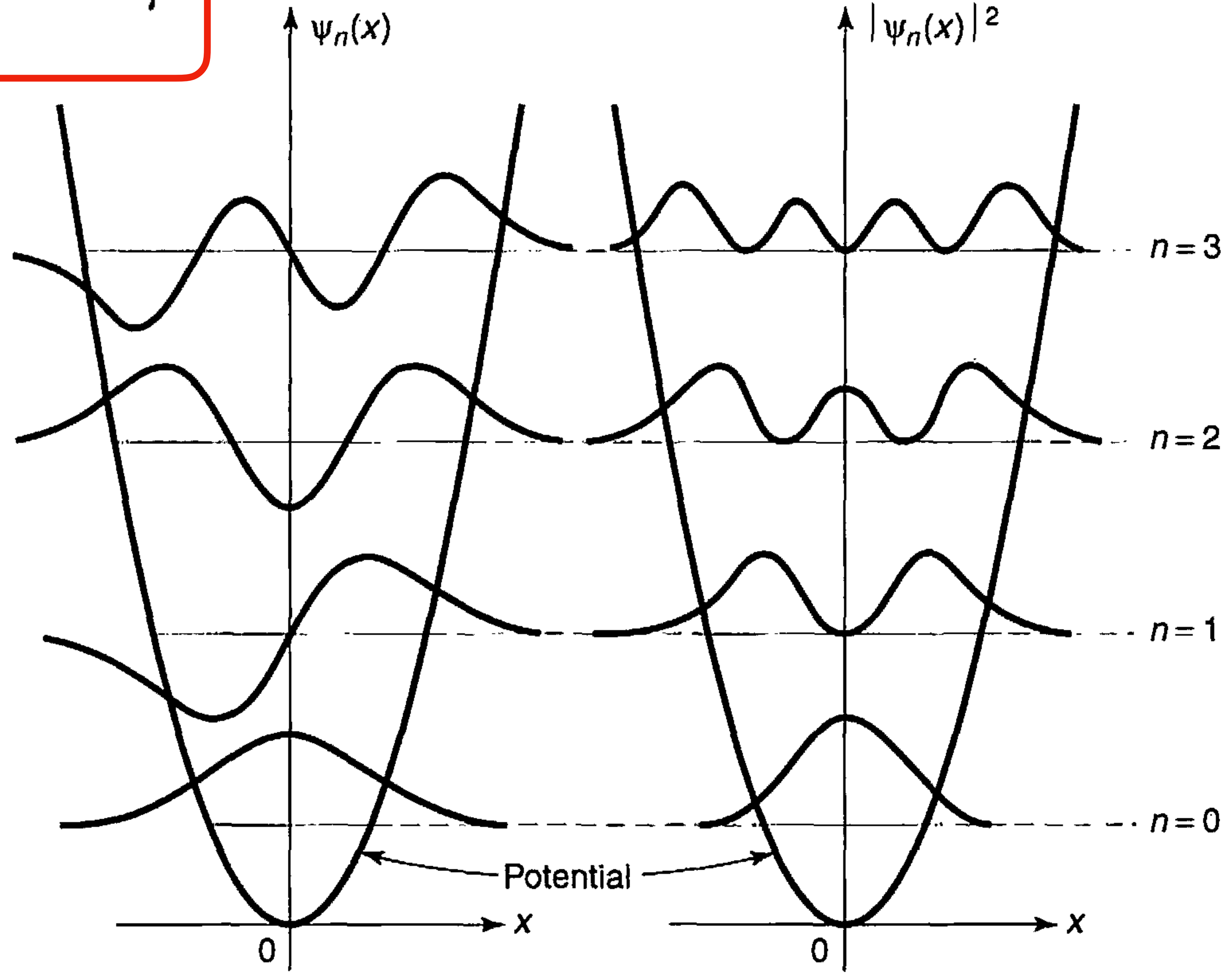
$$\int_{-\infty}^{\infty}(a_\pm\psi_n)^*(a_\pm\psi_n)\,dx = \int_{-\infty}^{\infty}(a_\mp a_\pm\psi_n)^*\psi_n\,dx$$

Now

$$a_+a_-\psi_n = n\psi_n, \quad a_-a_+\psi_n = (n+1)\psi_n$$

$$\int_{-\infty}^{\infty}(a_+\psi_n)^*(a_+\psi_n)\,dx = |c_n|^2\int_{-\infty}^{\infty}|\psi_{n+1}|^2\,dx = (n+1)\int_{-\infty}^{\infty}|\psi_n|^2\,dx$$

$$\int_{-\infty}^{\infty}(a_-\psi_n)^*(a_-\psi_n)\,dx = |d_n|^2\int_{-\infty}^{\infty}|\psi_{n-1}|^2\,dx = n\int_{-\infty}^{\infty}|\psi_n|^2\,dx.$$



$$\boxed{a_+\psi_n = \sqrt{n+1}\,\psi_{n+1}, \quad a_-\psi_n = \sqrt{n}\,\psi_{n-1}} \rightarrow \boxed{\psi_n = \frac{1}{\sqrt{n!}}(a_+)^n\psi_0}$$

Orthogonal stationary states

The Harmonic Oscillator

$$\boxed{\psi_n = \frac{1}{\sqrt{n!}}(a_+)^n \psi_0}$$

$$\boxed{a_+\psi_n = \sqrt{n+1}\,\psi_{n+1}, \quad a_-\psi_n = \sqrt{n}\,\psi_{n-1}}$$

$$\int_{-\infty}^{\infty} \psi_m^*(a_+a_-)\psi_n\,dx = n\int_{-\infty}^{\infty} \psi_m^*\psi_n\,dx = \int_{-\infty}^{\infty} (a_-\psi_m)^*(a_-\psi_n)\,dx = \int_{-\infty}^{\infty} (a_+a_-\psi_m)^*\psi_n\,dx = m\int_{-\infty}^{\infty} \psi_m^*\psi_n\,dx.$$

Orthogonal stationary states $$\boxed{\int_{-\infty}^{\infty} \psi_m^*\psi_n\,dx = \delta_{mn}}$$

Example 2.5: $\langle V \rangle$ in the n^{th} state: $\langle V \rangle = \left\langle \frac{1}{2}m\omega^2x^2 \right\rangle = \frac{1}{2}m\omega^2 \int_{-\infty}^{\infty} \psi_n^* x^2 \psi_n\,dx$

$$\boxed{a_\pm \equiv \frac{1}{\sqrt{2\hbar m\omega}}(\mp ip + m\omega x)}$$

$$= \frac{\hbar\omega}{4}\int \psi_n^*\left[(a_+)^2 + (a_+a_-) + (a_-a_+) + (a_-)^2\right]\psi_n\,dx$$

But $(a_+)^2\psi_n$ is (apart from normalization) ψ_{n+2}, which is orthogonal to ψ_n, and the same goes for $(a_-)^2\psi_n$, which is proportional to ψ_{n-2}.

$$\boxed{\langle V \rangle = \frac{\hbar\omega}{4}(n+n+1) = \frac{1}{2}\hbar\omega\left(n+\frac{1}{2}\right)}$$

The Free Particle

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$$

$$\frac{d^2\psi}{dx^2} = -k^2\psi, \quad \text{where } k \equiv \frac{\sqrt{2mE}}{\hbar}$$

$$\Psi(x,t) = Ae^{ik\left(x-\frac{\hbar k}{2m}t\right)} + Be^{-ik\left(x+\frac{\hbar k}{2m}t\right)}$$

$$\Psi_k(x,t) = Ae^{i\left(kx-\frac{\hbar k^2}{2m}t\right)}$$

$$k \equiv \pm\frac{\sqrt{2mE}}{\hbar}, \quad \text{with} \begin{cases} k > 0 \Rightarrow & \text{traveling to the right,} \\ k < 0 \Rightarrow & \text{traveling to the left.} \end{cases}$$

Fixed profile wave traveling right/left

Wavelength $\lambda = 2\pi/|k|$

Momentum $p = \hbar k$

Speed of the waves: $v_{\text{quantum}} = \frac{\hbar|k|}{2m} = \sqrt{\frac{E}{2m}}$.

$$v_{\text{classical}} = \sqrt{\frac{2E}{m}} = 2v_{\text{quantum}}$$

Problem: Solutions are not normalisable!

wave packet

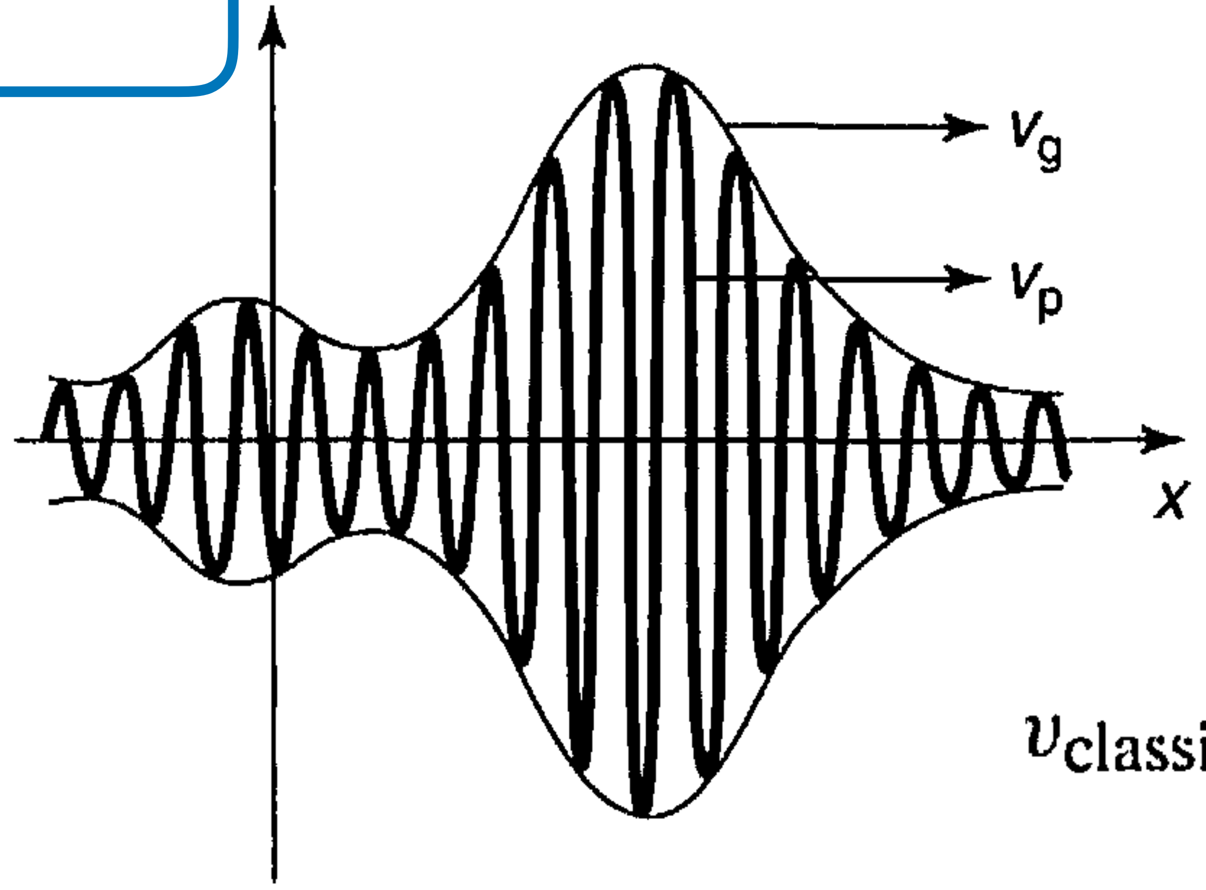
$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\phi(k)e^{i\left(kx-\frac{\hbar k^2}{2m}t\right)}\,dk$$

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\phi(k)e^{ikx}\,dk$$

Plancherel's theorem

$$f(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}F(k)e^{ikx}\,dk \iff F(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}f(x)e^{-ikx}\,dx$$

$$\phi(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\Psi(x,0)e^{-ikx}\,dx$$

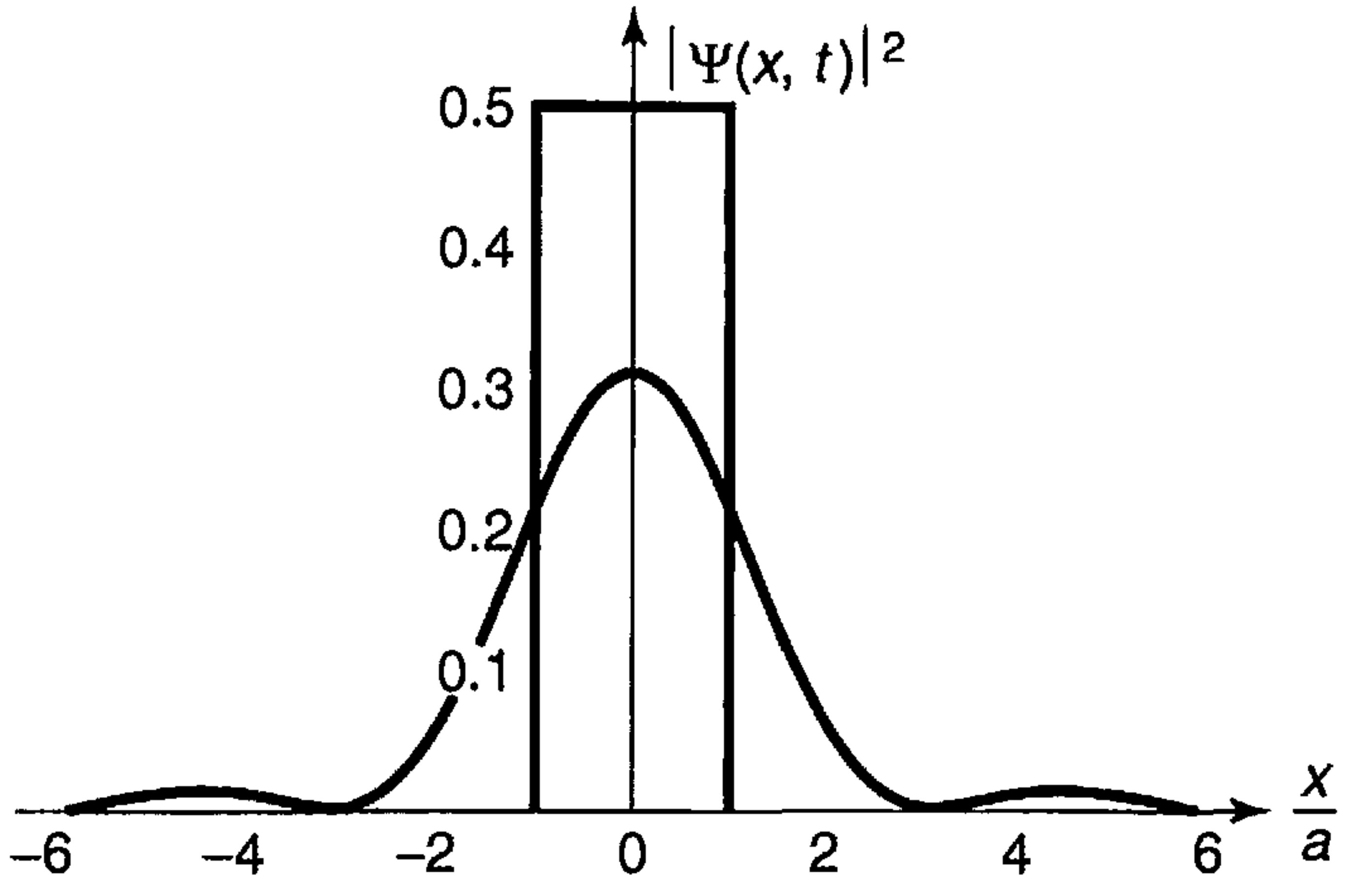


$$v_{\text{group}} = \frac{d\omega}{dk}$$

$$v_{\text{phase}} = \frac{\omega}{k}$$

$$v_{\text{classical}} = v_{\text{group}} = 2v_{\text{phase}}$$

The Free Particle



Example 2.6 A free particle, which is initially localized in the range $-a < x < a$, is released at time $t = 0$:

$$\Psi(x,0) = \begin{cases} A, & \text{if } -a < x < a, \\ 0, & \text{otherwise,} \end{cases}$$

where A and a are positive real constants. Find $\Psi(x,t)$.

Solution: First we need to normalize $\Psi(x, 0)$:

$$1 = \int_{-\infty}^{\infty} |\Psi(x,0)|^2\,dx = |A|^2 \int_{-a}^{a} dx = 2a|A|^2 \;\Rightarrow\; A = \frac{1}{\sqrt{2a}}.$$

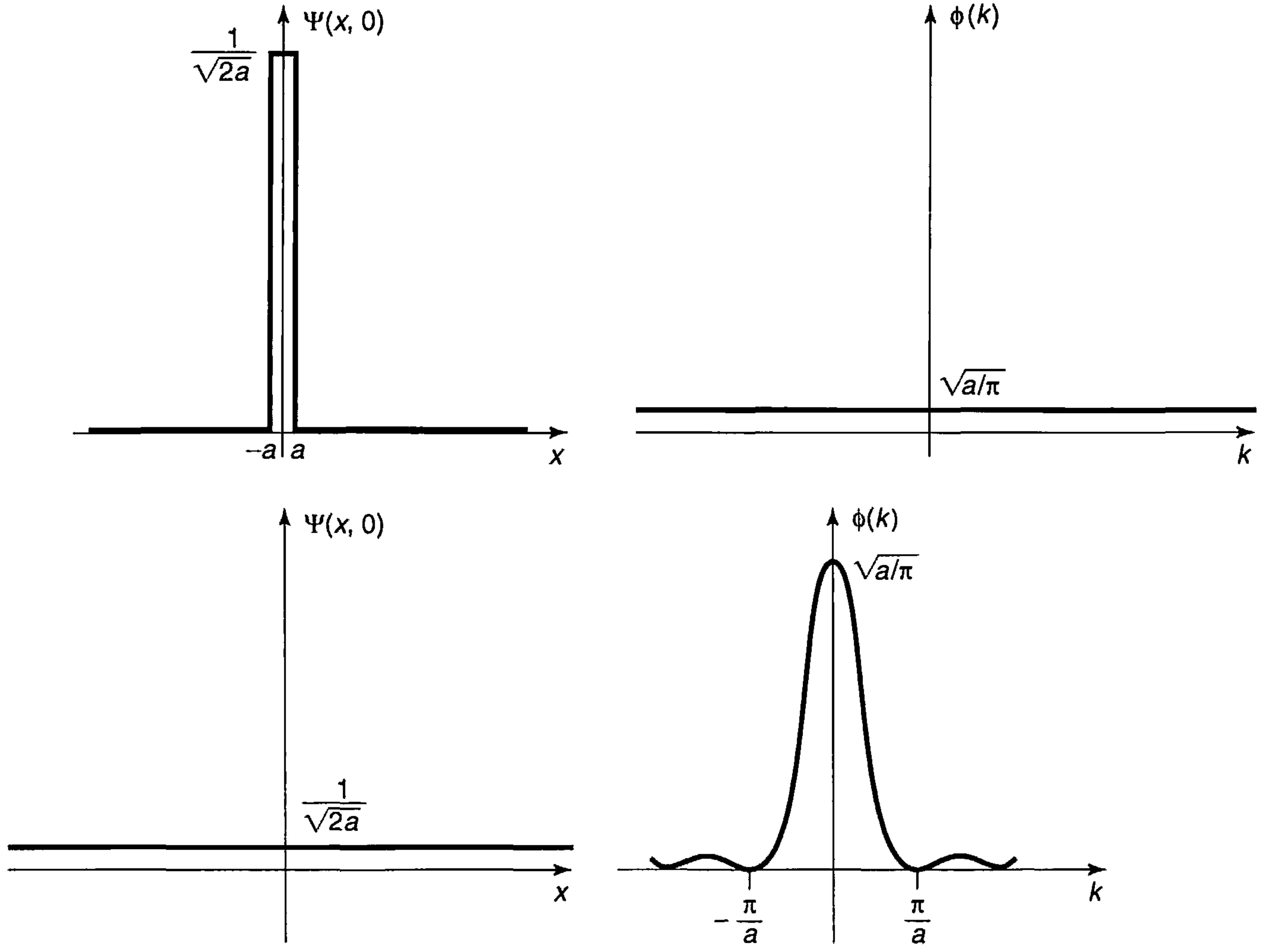
Next we calculate $\phi(k)$,

$$\phi(k) = \frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{2a}}\int_{-a}^{a} e^{-ikx}\,dx = \frac{1}{2\sqrt{\pi a}}\left.\frac{e^{-ikx}}{-ik}\right|_{-a}^{a}$$

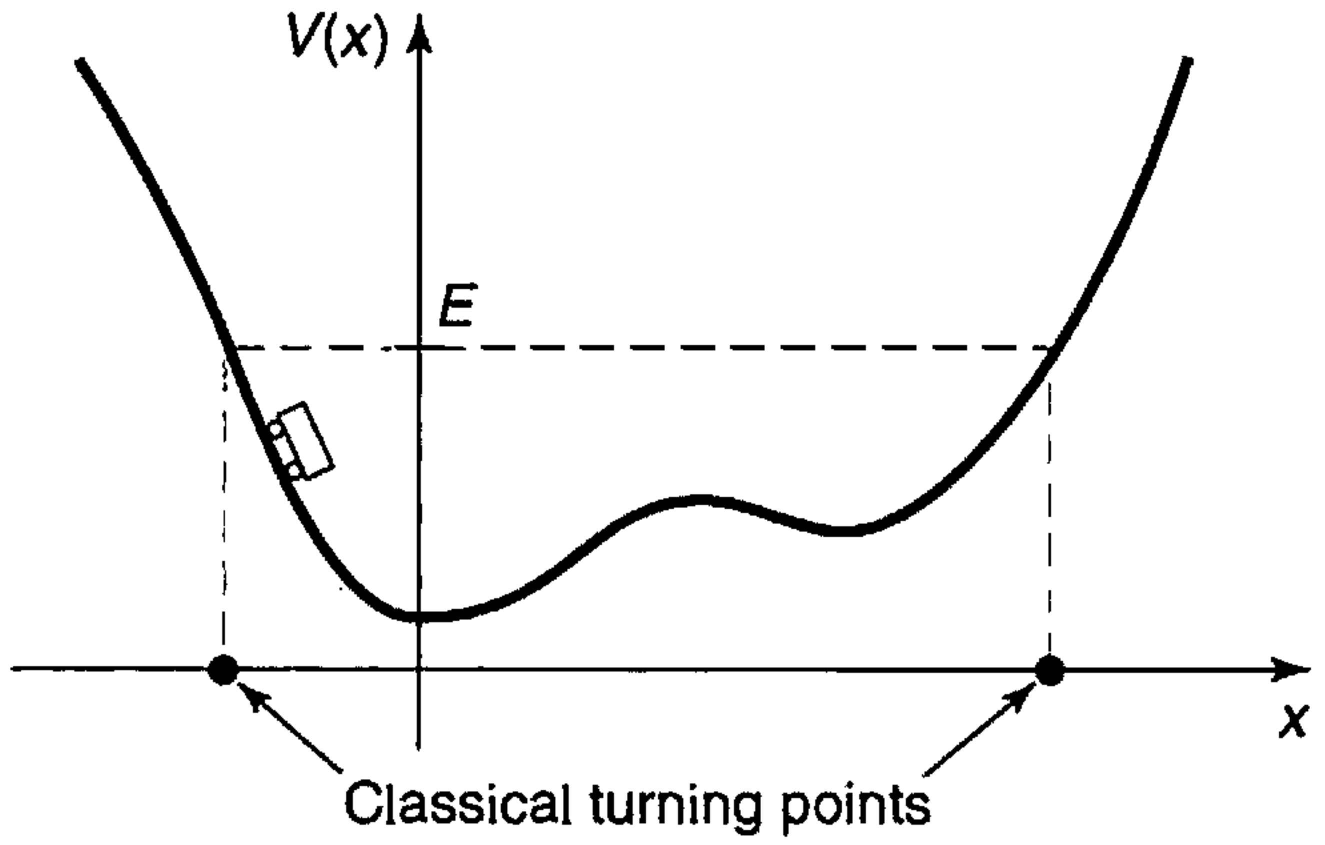
$$= \frac{1}{k\sqrt{\pi a}}\left(\frac{e^{ika}-e^{-ika}}{2i}\right) = \frac{1}{\sqrt{\pi a}}\frac{\sin(ka)}{k}.$$

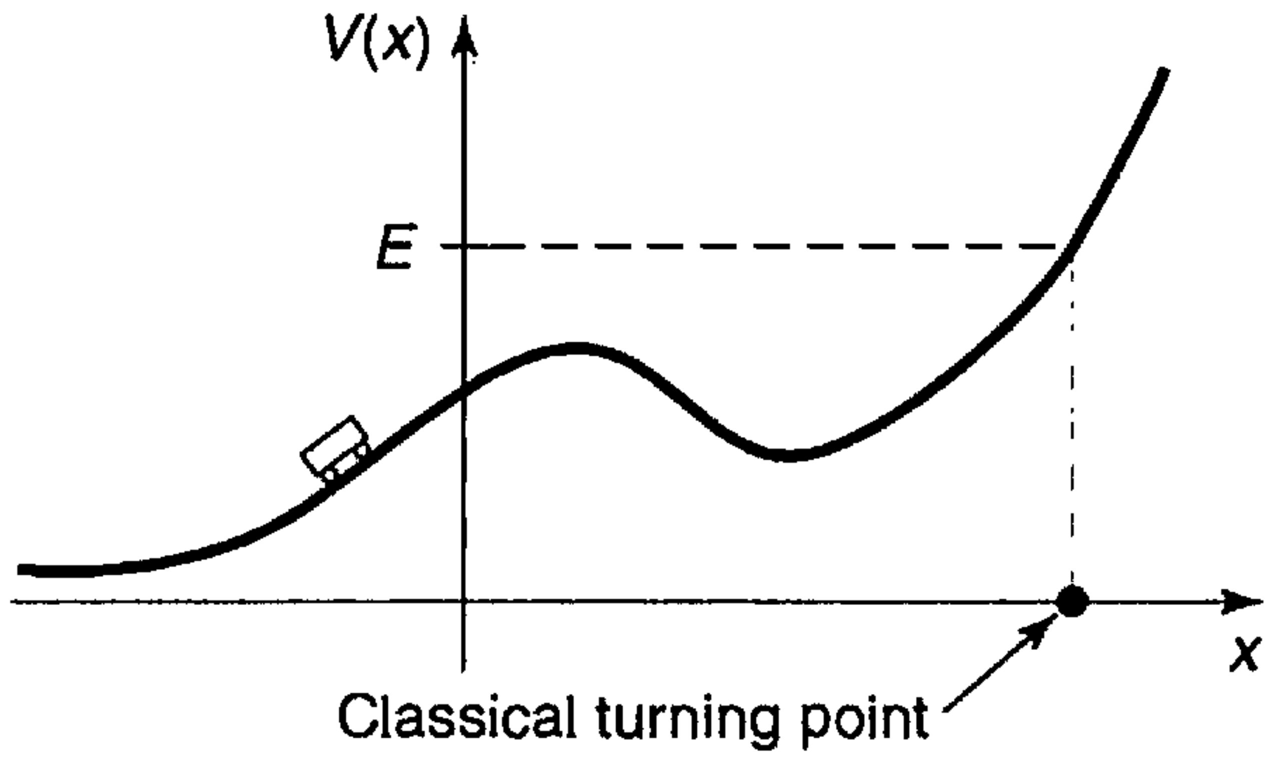
Finally, we plug this back

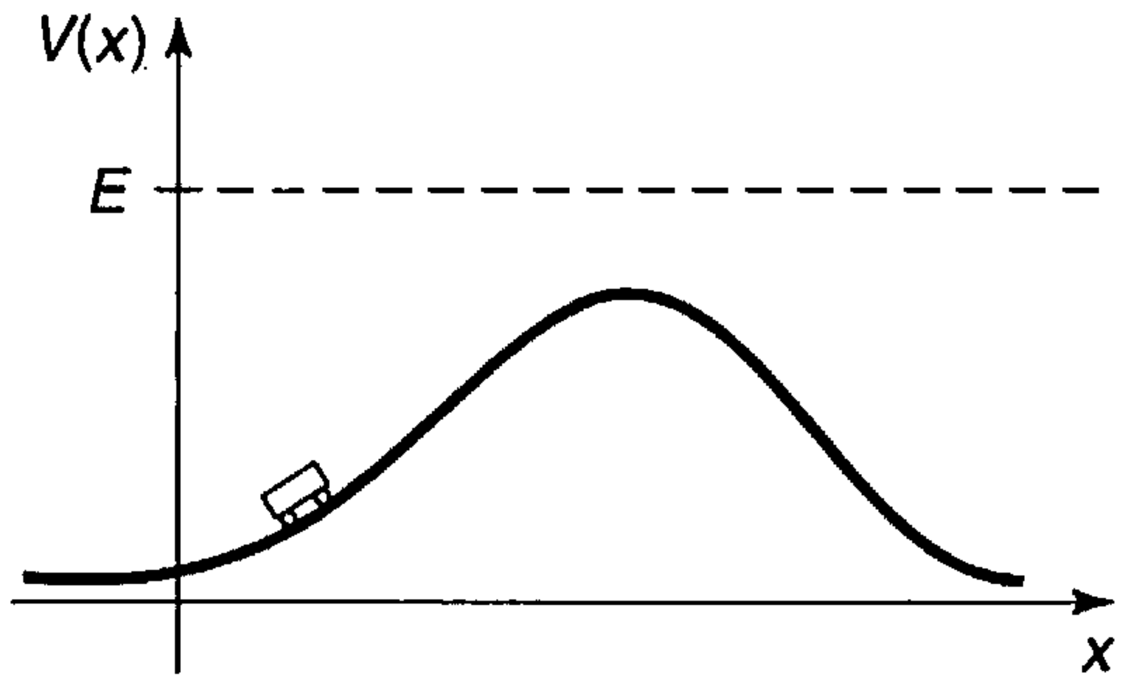
$$\Psi(x,t) = \frac{1}{\pi\sqrt{2a}}\int_{-\infty}^{\infty}\frac{\sin(ka)}{k}e^{i(kx-\frac{\hbar k^2}{2m}t)}\,dk.$$

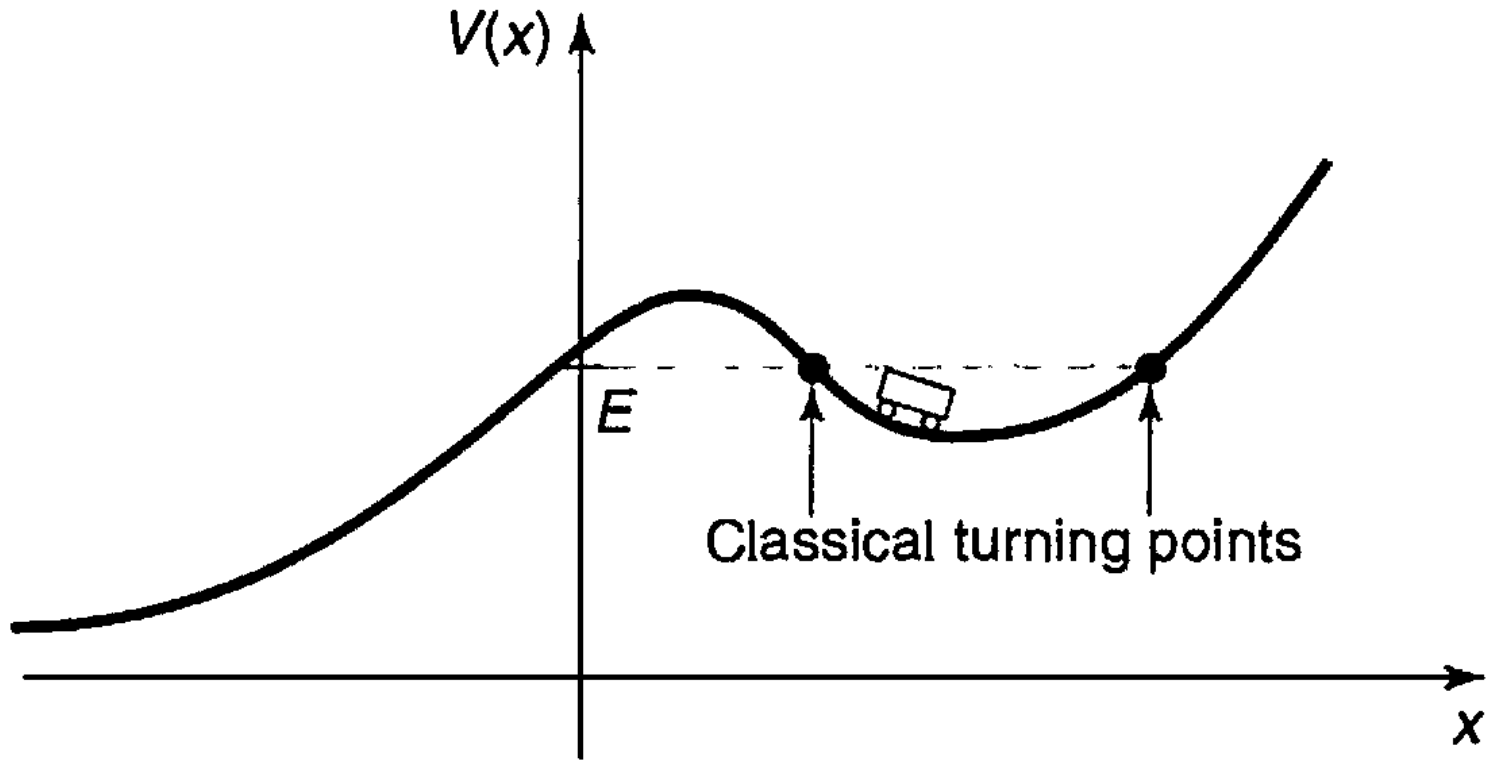


Bound States & Scattering States









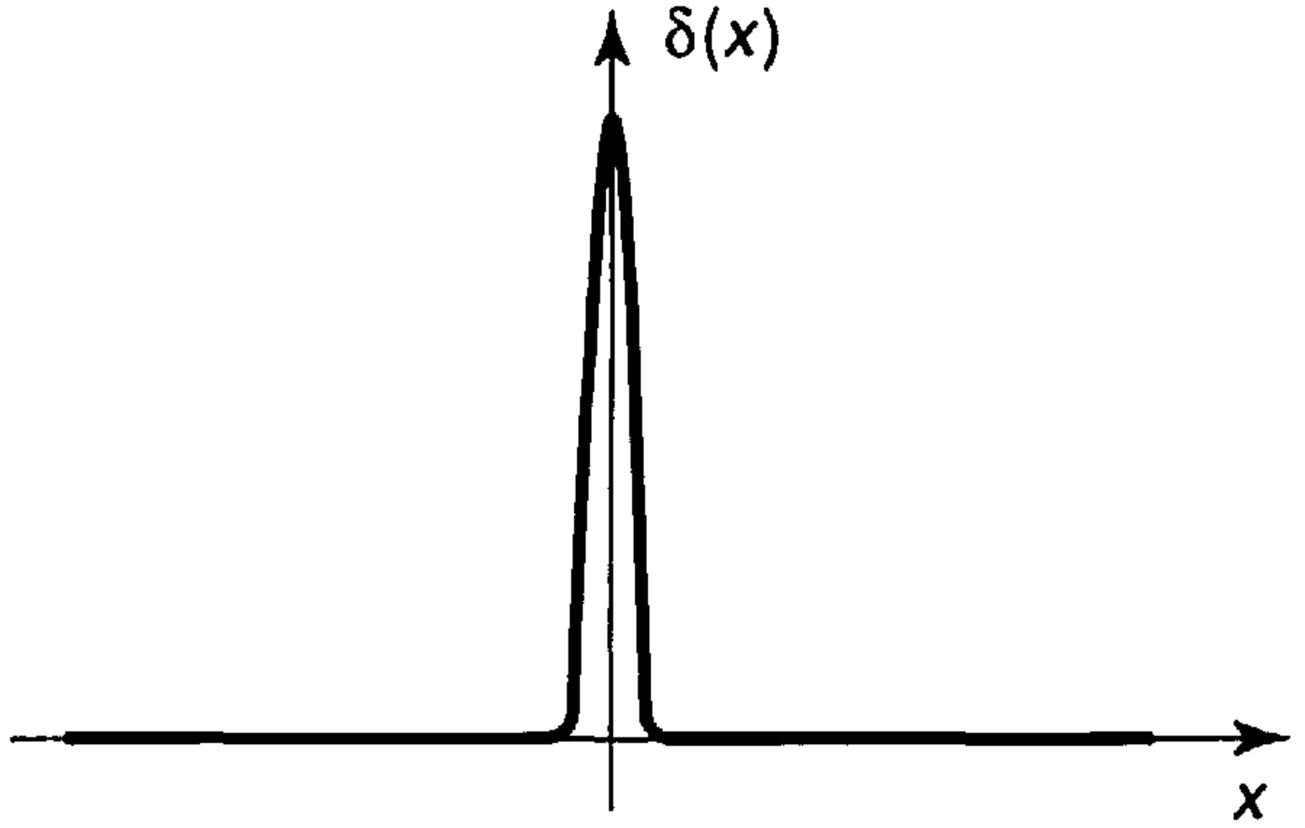
Tunneling

Normalisable discrete states

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

Non-normalisable; states with continuous index

Delta Well



Dirac delta function $\delta(x) \equiv \left\{ \begin{array}{ll} 0, & \text{if } x \neq 0 \\ \infty, & \text{if } x = 0 \end{array} \right\}$, with $\int_{-\infty}^{+\infty} \delta(x)\, dx = 1.$

$$\boxed{\int_{-\infty}^{+\infty} f(x)\delta(x-a)\, dx = f(a)\int_{-\infty}^{+\infty} \delta(x-a)\, dx = f(a).}$$

$$\boxed{-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - \alpha\delta(x)\psi = E\psi} \rightarrow \boxed{\text{both bound states } (E < 0) \text{ and scattering states } (E > 0)}$$

Bound States

the first term blows up as $x \to -\infty$, so we must choose $A = 0$:

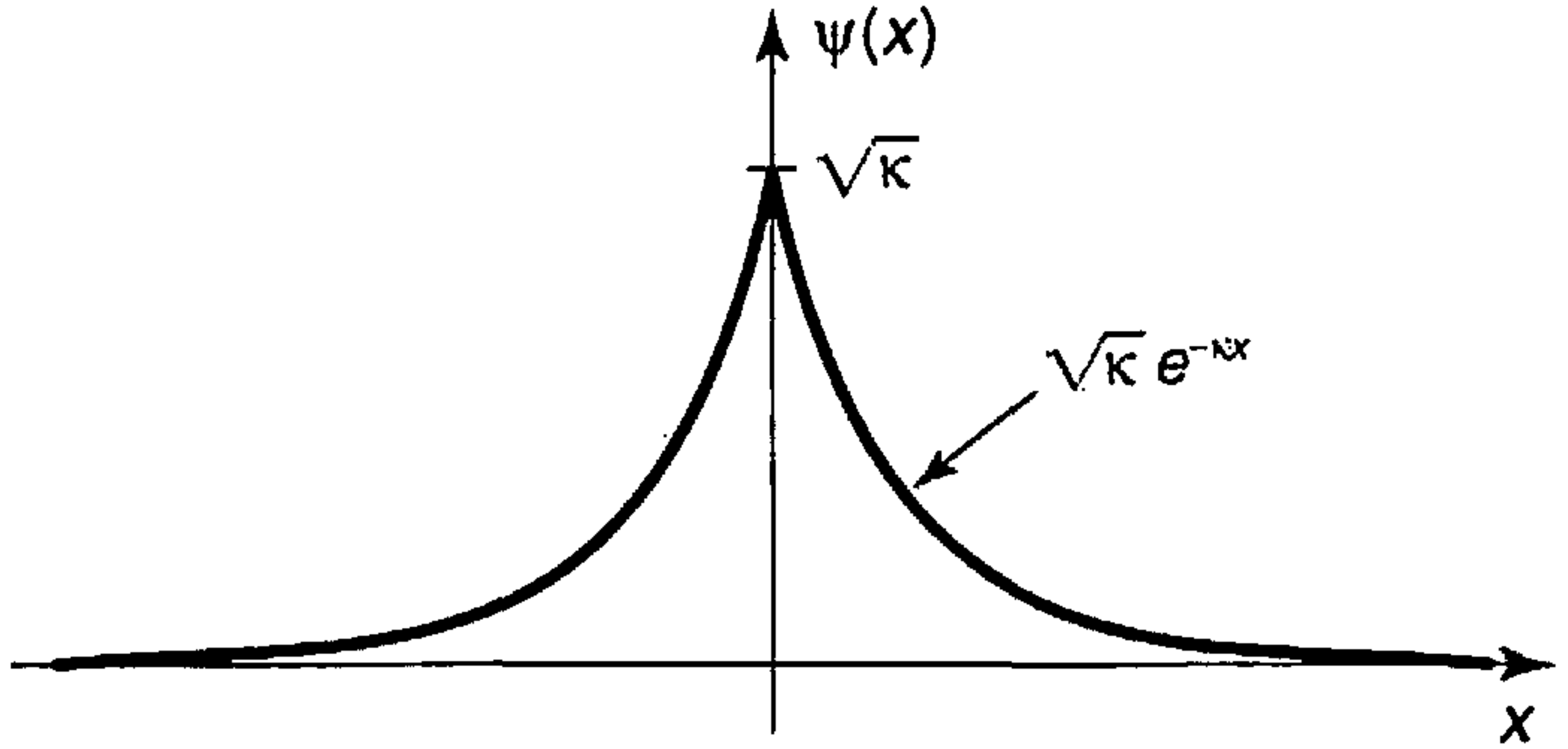
At $x < 0$ $\quad \boxed{\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi = \kappa^2\psi, \quad \kappa \equiv \frac{\sqrt{-2mE}}{\hbar}.} \rightarrow \boxed{\psi(x) = Ae^{-\kappa x} + Be^{\kappa x}}$ $\quad \boxed{\psi(x) = Be^{\kappa x}, \quad (x < 0)}$

At $x > 0$ $\quad \boxed{\psi(x) = Fe^{-\kappa x}, \quad (x > 0)}$

Boundary conditions

1. ψ is always continuous;
2. $d\psi/dx$ is continuous except at points where the potential is infinite.

$$\psi(x) = \begin{cases} Be^{\kappa x}, & (x \le 0), \\ Be^{-\kappa x}, & (x \ge 0); \end{cases}$$



Delta Well

To determine κ we shall integrate Schrödinger equation about the delta well

$$-\frac{\hbar^2}{2m}\int_{-\epsilon}^{+\epsilon}\frac{d^2\psi}{dx^2}\,dx+\int_{-\epsilon}^{+\epsilon}V(x)\psi(x)\,dx=E\int_{-\epsilon}^{+\epsilon}\psi(x)\,dx$$

$$\Delta\left(\frac{d\psi}{dx}\right)\equiv\lim_{\epsilon\to0}\left(\left.\frac{d\psi}{dx}\right|_{+\epsilon}-\left.\frac{d\psi}{dx}\right|_{-\epsilon}\right)=\frac{2m}{\hbar^2}\lim_{\epsilon\to0}\int_{-\epsilon}^{+\epsilon}V(x)\psi(x)\,dx. \longrightarrow \Delta\left(\frac{d\psi}{dx}\right)=-\frac{2m\alpha}{\hbar^2}\psi(0).$$

$$\begin{cases} d\psi/dx=-B\kappa e^{-\kappa x}, & \text{for } (x>0), \quad \text{so } d\psi/dx\big|_{+}=-B\kappa, \\ d\psi/dx=+B\kappa e^{+\kappa x}, & \text{for } (x<0), \quad \text{so } d\psi/dx\big|_{-}=+B\kappa. \end{cases} \longrightarrow \Delta(d\psi/dx)=-2B\kappa.\ \text{And } \psi(0)=B.$$

$$\kappa=\frac{m\alpha}{\hbar^2}. \longrightarrow E=-\frac{\hbar^2\kappa^2}{2m}=-\frac{m\alpha^2}{2\hbar^2}.$$

Normalisation $$\int_{-\infty}^{+\infty}|\psi(x)|^2\,dx=2|B|^2\int_0^{\infty}e^{-2\kappa x}\,dx=\frac{|B|^2}{\kappa}=1.$$

Single bound state $$\boxed{\psi(x)=\frac{\sqrt{m\alpha}}{\hbar}e^{-m\alpha|x|/\hbar^2};\qquad E=-\frac{m\alpha^2}{2\hbar^2}.}$$

Delta Well

Scattering States

At $x < 0$

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi = -k^2\psi, \qquad k \equiv \frac{\sqrt{2mE}}{\hbar}$$

The general solution is $\psi(x) = Ae^{ikx} + Be^{-ikx}$

At $x > 0$ $\quad \psi(x) = Fe^{ikx} + Ge^{-ikx}$

The continuity of $\psi(x)$ at $x = 0$ requires that $F + G = A + B$

The derivatives are
$$\begin{cases} d\psi/dx = ik\left(Fe^{ikx} - Ge^{-ikx}\right), & \text{for } (x > 0), \quad \text{so } d\psi/dx\big|_+ = ik(F-G), \\ d\psi/dx = ik\left(Ae^{ikx} - Be^{-ikx}\right), & \text{for } (x < 0), \quad \text{so } d\psi/dx\big|_- = ik(A-B). \end{cases}$$

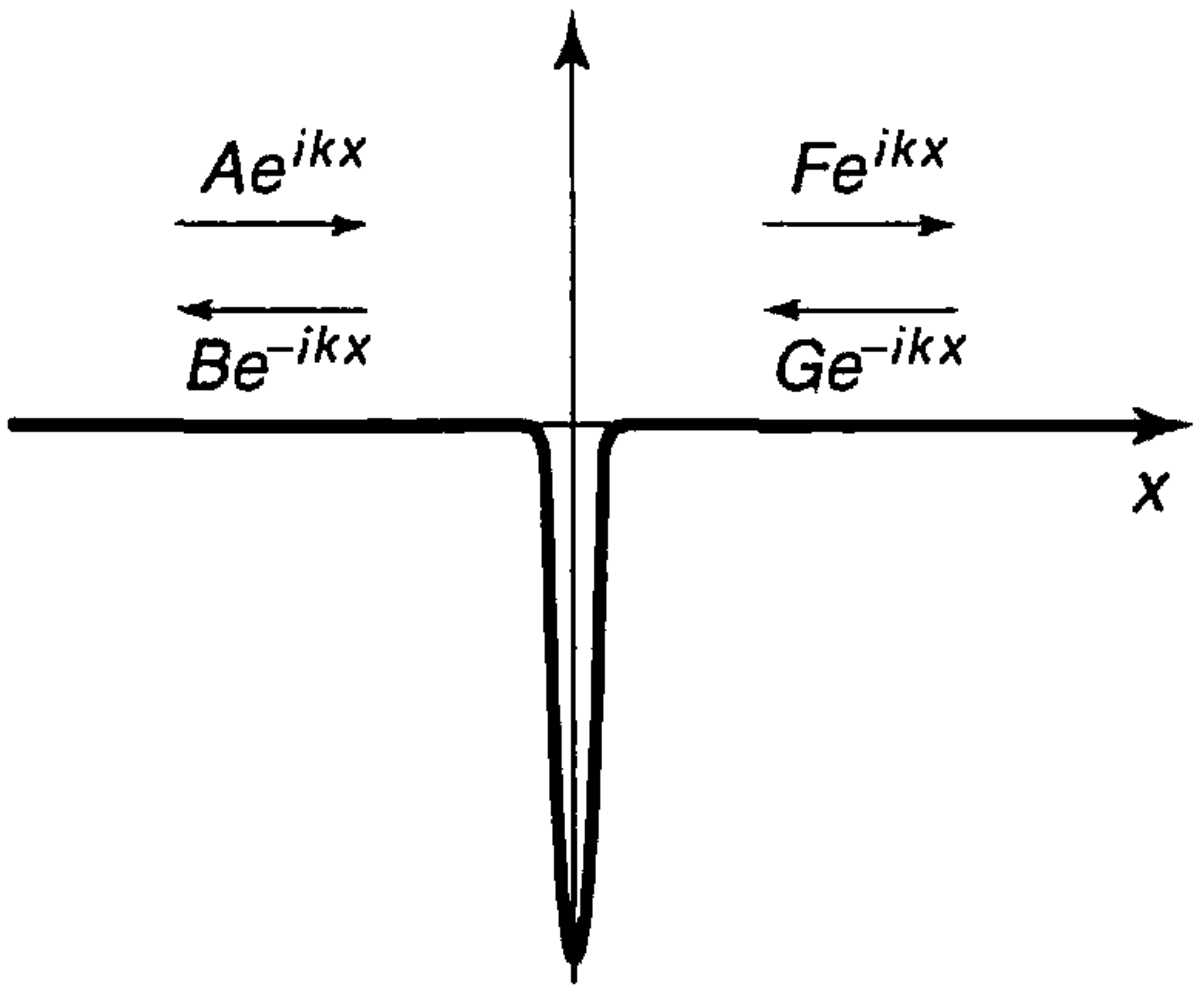
$$\Delta\left(\frac{d\psi}{dx}\right) = -\frac{2m\alpha}{\hbar^2}\psi(0).$$

$$ik(F - G - A + B) = -\frac{2m\alpha}{\hbar^2}(A + B)$$

$$F - G = A(1 + 2i\beta) - B(1 - 2i\beta), \quad \text{where } \beta \equiv \frac{m\alpha}{\hbar^2 k}.$$

Delta Well

Scattering States



Let's assume $G = 0,$ (for scattering from the left)

$$B = \frac{i\beta}{1 - i\beta} A, \quad F = \frac{1}{1 - i\beta} A.$$

Reflection coefficient: $R \equiv \frac{|B|^2}{|A|^2} = \frac{\beta^2}{1 + \beta^2}.$

Transmission coefficient: $T \equiv \frac{|F|^2}{|A|^2} = \frac{1}{1 + \beta^2}$

$$\boxed{R = \frac{1}{1 + (2\hbar^2 E / m\alpha^2)}, \quad T = \frac{1}{1 + (m\alpha^2 / 2\hbar^2 E)}}$$

Tunnelling

If $\alpha < 0$, i.e., a delta barrier instead of a delta well: The bound state vanishes. R and T remain the same.