

II. FIRST APPLICATIONS

II.1 The Harmonic Oscillator

* Recall: A particle in 1-D of mass m subject to a potential energy

$$V(x) = \frac{1}{2} m \omega^2 x^2 \text{ is called a harmonic oscillator.}$$

This potential could be the result of an approximation of a more general potential $\tilde{V}(x)$ around a local minimum at $x = x_0$:

$$\tilde{V}(x) = \tilde{V}(x_0) + \underbrace{\frac{1}{2} \frac{d^2 \tilde{V}}{dx^2} \Big|_{x_0}}_{= m \omega^2} (x - x_0)^2 + \dots \text{ and a shift of coord. } x - x_0 \mapsto x$$

* Hamiltonian: $H = \frac{p^2}{2m} + \frac{m\omega^2}{2} x^2$

Equation of motion: $\frac{d^2 x}{dt^2} = -\omega^2 x$

II.1.1 Stationary States

* We solve the t -indep. Schrödinger eqn.

$$H\psi = E\psi \quad (1)$$

to obtain energy eigenvalues and eigenfcts.

* The Gaussian $\psi_0(x) = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}$ is a solution to (1).

$$\begin{aligned} \text{Why? } \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2\right) \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2} &= \\ &= \left(\frac{\hbar\omega}{2} - \frac{1}{2}m\omega^2 x^2 + \frac{1}{2}m\omega^2 x^2\right) \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2} = \frac{1}{2}\hbar\omega \psi_0 \quad \checkmark \end{aligned}$$

Normalization: $\int_{\mathbb{R}} |\psi_0|^2 dx = 1$ (check!)

The energy eigenvalue for ψ_0 is $E_0 = \frac{1}{2}\hbar\omega$

* We suspect that other solutions to (1) are also related to a Gaussian.

We choose the general ansatz $\psi(x) = e^{-\frac{m\omega}{2\hbar}x^2} v(x)$

Plugging into (1): $\frac{1}{2}\hbar\omega \psi + \hbar\omega x \frac{dv}{dx} e^{-\frac{m\omega}{2\hbar}x^2} - \frac{\hbar^2}{2m} \frac{d^2v}{dx^2} e^{-\frac{m\omega}{2\hbar}x^2} = E\psi$

$$\Rightarrow \frac{\hbar^2}{2m} \frac{d^2v}{dx^2} - \hbar\omega x \frac{dv}{dx} + (E - E_0)v = 0$$

$\sqrt{\frac{\hbar}{m\omega}}$ seems to be a "characteristic length scale" and we can introduce the

dimensionless variable $\xi = \sqrt{\frac{m\omega}{\hbar}} x$

$$\Rightarrow E_0 \frac{d^2v}{d\xi^2} - 2E_0 \xi \frac{dv}{d\xi} + (E - E_0)v = 0$$

$$(2) \quad \text{or} \quad \boxed{\frac{d^2v}{d\xi^2} - 2\xi \frac{dv}{d\xi} + 2nv = 0}$$

$$\text{with } n = \frac{E - E_0}{E_0}$$

$$\text{or } E = \left(n + \frac{1}{2}\right)\hbar\omega$$

Diff. equation for $v(x)$.

* Exercise: The parity operator \hat{P} represents inversions $\vec{r} \mapsto -\vec{r}$ ($x \rightarrow -x$ in 1-D)

in space. It acts on a Hilbert space \mathcal{H} by $\psi(\vec{r}) \mapsto \psi(-\vec{r})$.

Obviously its eigenvalues are $+1$ and -1 and the corresponding

eigenspaces are those of even and odd fcts $\psi(\vec{r})$ resp., i.e.

$$\psi(-\vec{r}) = +\psi(\vec{r}), \quad \psi(\vec{r}) = -\psi(\vec{r})$$

Why? $P\psi = \alpha\psi \Rightarrow P^2\psi = \alpha^2\psi = \psi \rightarrow \alpha^2 = 1$

Furthermore: $[P, H] = 0$ for the ^{1-D} harmonic oscillator. Why? $V(x) = V(-x)$

Theorem (later): For commuting operators a common set of orthonormal eigenfunctions can be found.

* Thus ^{energy} eigenfcts. ψ of the harm. osc. and therefore the fcts. $v(x)$ can be chosen to be either even or odd in x (or ξ).

Power series ansatz to solve (2): $v(\xi) = \sum_{k=0}^{\infty} c_k \xi^k$

into (2): $\sum_{k=2}^{\infty} c_k k(k-1) \xi^{k-2} - \sum_{k=1}^{\infty} 2c_k k \xi^k + \alpha n \sum_{k=0}^{\infty} c_k \xi^k = 0$

$$\Rightarrow \sum_{k=0}^{\infty} \xi^k (2(n-k)c_k + c_{k+2}(k+2)(k+1)) = 0$$

$$\Rightarrow c_{k+2} = -c_k \frac{2(n-k)}{(k+2)(k+1)}$$

odd and even coefficients decoupled, we can choose odd or even fcts!

even: $c_k = c_0 \frac{(-1)^{k/2}}{k!} n(n-2)\dots(n-k+2)$; even $v_n(\xi) = c_0 (1 - \frac{2n}{2!}\xi^2 + \frac{n(n-2)}{4!}\xi^4 \dots)$

odd: $c_k = c_1 \frac{(-1)^{(k+1)/2}}{k!} (n-1)(n-3)\dots(n-k+2)$; odd $v_n(\xi) = c_1 (\xi - \frac{2(n-1)}{3!}\xi^3 + \frac{4(n-1)(n-3)}{5!}\xi^5 \dots)$

* The series for the $v(\xi)$ terminates and v is a polynomial if n is a positive integer (even for even v , n odd for odd v).

On the other hand, for $n \notin \mathbb{N}$ the series is infinite and the coefficients grow faster than those for $e^{+\xi^2/2}$ (check, cf. Henkel p. 82)

Such wave fcts. diverging for $\xi \rightarrow \pm\infty$ are unphysical

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For integer n the $v_n(\xi)$ are called Hermite polynomials. They are

usually normalized by choosing $c_0 = (-1)^{\frac{n}{2}} \frac{n!}{(\frac{n}{2})!}$ for even n

$c_1 = (-1)^{\frac{n-1}{2}} \frac{2n!}{(\frac{n-1}{2})!}$ for odd n

i.e. $H_n(\xi) = (-1)^{\frac{n}{2}} \frac{n!}{(\frac{n}{2})!} \left(1 - \frac{2n}{2!} \xi^2 + \frac{2^2 n(n-2)}{4!} \dots \right)$ for n even

$H_n(\xi) = (-1)^{\frac{n-1}{2}} \frac{2n!}{(\frac{n-1}{2})!} \left(\xi - \frac{2(n-1)}{3!} \xi^3 + \frac{2^2 (n-1)(n-3)}{5!} \xi^5 \dots \right)$ for n odd

explicitly: $H_0(\xi) = 1$ $H_1(\xi) = 2\xi$

$H_2(\xi) = -2 + 4\xi^2$ $H_3(\xi) = -12\xi + 8\xi^3$

...

...

* Hence: The energy spectrum of the harm. oscillator is discrete, eigenvalues are not degenerate and

$$E_n = (n + \frac{1}{2}) \hbar \omega \quad n \in \mathbb{N}$$

$E_0 = \frac{1}{2} \hbar \omega$ is the ground state energy (zero-point energy); $E_{j.s.} > 0$ is clear

from the uncertainty principle: $\langle p^2 \rangle$ and $\langle x^2 \rangle$ cannot both vanish simultaneously.

The eigenfct. for E_n is

$$\Psi_n(x) = C_n H_n \left(\sqrt{\frac{m\omega}{\hbar}} x \right) e^{-\frac{m\omega}{2\hbar} x^2}$$

* Basic properties of Hermite polynomials:

$H_n(\xi)$ is a polynomial of degree n satisfying the DE

$$\frac{d^2}{d\xi^2} H_n(\xi) - 2\xi \frac{d}{d\xi} H_n(\xi) + 2n H_n(\xi) = 0 \quad (\text{clear!})$$

They can be derived from the power series of a generating function

$$F(\xi, s) = \sum_{n=0}^{\infty} \frac{1}{n!} H_n(\xi) s^n$$

One finds $F(\xi, s) = e^{\xi^2 - (s-\xi)^2}$

It follows that

$$H_n(\xi) = (-1)^n e^{\xi^2} \frac{d^n}{d\xi^n} e^{-\xi^2}$$

and $H_n(\xi)$ has n real roots.

Recursion for derivatives: $\frac{dH_n(\xi)}{d\xi} = 2n H_{n-1}(\xi)$

Integral representation: $H_n(\xi) = \frac{2^n}{\sqrt{\pi}} \int_{\mathbb{R}} (\xi + is)^n e^{-s^2} ds$

Proofs: HW or Merzbacher pp 85-88

* The $\psi_n(x)$, $n \in \mathbb{N}$ form an orthonormal basis of $L^2(\mathbb{R})$ with normalization

$$C_n = 2^{-\frac{n}{2}} \frac{1}{\sqrt{n!}} \left(\frac{m\omega}{\hbar\pi}\right)^{1/4}$$

Why? Consider $I = \int_{\mathbb{R}} F(\xi, s) F(\xi, t) e^{-\xi^2} d\xi = \int_{\mathbb{R}} e^{\xi^2 - (s-\xi)^2} e^{\xi^2 - (t-\xi)^2} e^{-\xi^2} d\xi$

$$= e^{2st} \int_{\mathbb{R}} e^{-(s+t-\xi)^2} d\xi = \sqrt{\pi} e^{2st} = \sum_{j=0}^{\infty} (st)^j \frac{2^j \sqrt{\pi}}{j!}$$

On the other hand $I = \sum_{j=0}^{\infty} \sum_{k=0}^{\infty} \frac{s^j t^k}{j! k!} \int_{\mathbb{R}} H_j(\xi) H_k(\xi) e^{-\xi^2} d\xi$

$$= \sqrt{\frac{m\omega}{\hbar\pi}} \int dx \psi_j(x) \psi_k(x) dx (C_j C_k)^{-1}$$

Compare both power series: $\int_{\mathbb{R}} dx \psi_j(x) \psi_k(x) dx \sqrt{\frac{m\omega}{\hbar\pi}} \frac{1}{C_j C_k} = \delta_{jk} j! 2^j \sqrt{\pi}$

$$\Rightarrow C_j^2 = \left(\frac{m\omega}{\hbar\pi}\right)^{1/2} \frac{1}{j! 2^j}$$

Completeness:

$$\begin{aligned} \sum_{n=0}^{\infty} \psi_n^*(x') \psi_n(x) &= \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{m\omega}{\hbar\pi}\right)^{1/2} H_n(\xi') H_n(\xi) e^{-\xi'^2/2} e^{-\xi^2/2} \\ &= \left(\frac{m\omega}{\hbar\pi}\right)^{1/2} \frac{1}{\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{1}{n!} \int_{-\infty}^{+\infty} (\xi'+is)^n H_n(\xi) e^{-s^2} e^{-\xi'^2/2} e^{-\xi^2/2} ds \\ &= \left(\frac{m\omega}{\hbar\pi}\right)^{1/2} \frac{1}{\pi} \int_{-\infty}^{+\infty} F(\xi, \xi'+is) e^{-s^2 - \frac{\xi'^2}{2} - \frac{\xi^2}{2}} ds \\ &= \left(\frac{m\omega}{\hbar\pi}\right)^{1/2} \frac{1}{\pi} \int_{-\infty}^{+\infty} e^{-(\xi'+is)^2 + 2\xi(\xi'+is) - s^2 - \frac{\xi'^2}{2} - \frac{\xi^2}{2}} ds \\ &= \left(\frac{m\omega}{\hbar\pi}\right)^{1/2} \frac{1}{\pi} e^{-\frac{3}{2}\xi'^2 - \frac{\xi^2}{2} + 2\xi\xi'} \int_{-\infty}^{+\infty} e^{-2is(\xi'-\xi)} ds \\ &= \delta(x-x') \end{aligned}$$

$$\begin{aligned} \xi &= \sqrt{\frac{m\omega}{\hbar}} x \\ \xi' &= \sqrt{\frac{m\omega}{\hbar}} x' \end{aligned}$$

* We find $\int_{-\infty}^{+\infty} \psi_n^*(x) x \psi_k(x) dx = \sqrt{\frac{\hbar}{m\omega}} \left(\sqrt{\frac{n}{2}} \delta_{k,n-1} + \sqrt{\frac{n+1}{2}} \delta_{k,n+1} \right)$ for $n, k \in \mathbb{N}$

II.1.2 Wave Packets and General Solutions

* Let $\psi(x,0)$ be the initial wave pkt. in a harmonic osc. potential at time $t=0$.

Let $c_n = \int_{\mathbb{R}} \psi_n(x) \psi(x,0) dx$ be the probability amplitudes

of $\psi(x,0)$ w.r.t. each eigenstate $\psi_n(x)$, i.e. $\psi(x,0) = \sum_{n \in \mathbb{N}} c_n \psi_n(x)$.

Then

$$\psi(x,t) = e^{-\frac{i}{\hbar} E_0 t} \sum_{n=0}^{\infty} c_n \psi_n(x) e^{-i n \omega t} \quad (*)$$

Why? Clear from I.9.6

* If $\langle x \rangle_0$ and $\langle p \rangle_0$ are the initial average position and momentum

then

$$\langle x \rangle(t) = \langle x \rangle_0 \cos \omega t + \frac{\langle p \rangle_0}{m\omega} \sin \omega t, \quad \langle p \rangle(t) = m \frac{d\langle x \rangle}{dt}$$

as for a classical particle, as expected from I.8

Why? from e.o.m. of expectation values HW5 [1]

directly from solution (*): HW7

II.2 Potential Steps and Barriers

* Prelude: Energy is bounded from below

Let $V(\vec{r})$ be a potential energy fct. If $V(\vec{r})$ has a lower bound, i.e. $V(\vec{r}) > V_0 \quad \forall \vec{r} \in \mathbb{R}^3$ then $E_0 > V_0$ and $\langle E \rangle > V_0$

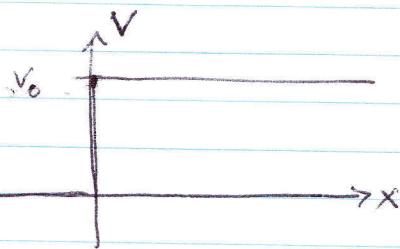
where E_0 is the lowest energy eigenvalue and $\langle E \rangle$ is the average energy in any state ψ . In particular: if V_0 is a global minimum of $V(\vec{r})$ then $E_0 > V_0$, $\langle E \rangle > V_0$.

Why? later.

II.2.1 Potential Step

* Consider a particle of mass m with pot. energy $V(x) = V_0 \theta(x)$

in 1-D.



↑
Heaviside step fct.

$$V = \begin{cases} 0 & x < 0 \\ V_0 & x > 0 \end{cases}$$

Solve $H\psi = E\psi$ to find stationary states.

→ CASE A: $E > V_0$

* We find e^{ikx} , e^{-ikx} (2-fold degeneracy) as solutions for $x < 0$

$$k = \frac{1}{\hbar} \sqrt{2mE}$$

$e^{2k'x}, e^{-ik'x}$ $k' = \frac{1}{\hbar} \sqrt{2m(E-V_0)}$ as solutions for $x > 0$

$$\Rightarrow \psi(x) = \begin{cases} A e^{ikx} + B e^{-ikx}, & x < 0 \\ C e^{ik'x} + D e^{-ik'x}, & x > 0 \end{cases}$$

is general form of stationary solutions with matching conditions (I.9.6)

ψ, ψ' continuous at $x = 0$.

* Here we restrict ourselves to $D = 0$ (i.e. no wave coming in from right)

from matching:
$$\begin{cases} A + B = C & (1) \\ k(A - B) = k'C & (2) \end{cases}$$

$$\Rightarrow \frac{B}{A} = \frac{k - k'}{k + k'} = \frac{\sqrt{E} - \sqrt{E - V_0}}{\sqrt{E} + \sqrt{E - V_0}}$$

$$\frac{C}{A} = \frac{2k}{k + k'} = \frac{2\sqrt{E}}{\sqrt{E} + \sqrt{E - V_0}}$$

Interpretation: $\psi(x) = \underbrace{(A e^{ikx})}_{\substack{\uparrow \\ \text{incident plane} \\ \text{wave (from left)}}} + \underbrace{B e^{-ikx}}_{\substack{\uparrow \\ \text{reflected} \\ \text{plane wave}}} \Theta(-x) + \underbrace{C e^{ik'x}}_{\substack{\uparrow \\ \text{transmitted} \\ \text{plane wave}}} \Theta(x)$

One can define reflection and transmission coefficients (probabilities):

$$R = \frac{|B|^2}{|A|^2} = \frac{(k - k')^2}{(k + k')^2}$$

$$T = \frac{k'}{k} \frac{|C|^2}{|A|^2} = \frac{4kk'}{(k + k')^2}$$

probability ensures that $R + T = 1$

Particle
* Current: $\vec{j} = \frac{\hbar}{2mi} \left[\psi^* \frac{d\psi}{dx} - \frac{d\psi^*}{dx} \psi \right]$

$x < 0$: $\vec{j}(x) = \frac{\hbar}{2mi} [ik|A|^2 - ik|B|^2] \cdot 2$ (mixed terms cancel) (check!)

$$= \frac{\hbar k}{m} [|A|^2 - |B|^2]$$

reflected wave generates current to the left, diminishing incident current!

$x > 0$: $\vec{j}(x) = \frac{\hbar k'}{m} |C|^2$

From $R + T = 1 \Rightarrow 1 - \frac{|B|^2}{|A|^2} = \frac{k'}{k} \frac{|C|^2}{|A|^2} \Rightarrow \vec{j}$ continuous (and constant!)

→ CASE B: $E < V_0$ (but $E > 0$ according to prelude)

* General solution $\psi(x) = \begin{cases} A e^{ikx} + B e^{-ikx} & (x < 0) \quad k = \frac{1}{\hbar} \sqrt{2mE} \\ C e^{-\kappa x} & (x > 0) \quad \kappa = \frac{1}{\hbar} \sqrt{2m(V_0 - E)} \end{cases}$

$e^{+\kappa x}$ would not be a physical solution.

* Matching conditions: $\begin{cases} A + B = C \\ ik(A - B) = -\kappa C \end{cases}$

$\Rightarrow \frac{B}{A} = \frac{ik + \kappa}{ik - \kappa}$; $k, \kappa \in \mathbb{R} \Rightarrow \frac{B}{A} = e^{i\alpha}$ is complex number of modulus 1 ($\alpha \in \mathbb{R}$)

$$\frac{C}{A} = \frac{2ik}{ik - \kappa} = 1 + e^{i\alpha}$$

Note: $R = \frac{|B|^2}{|A|^2} = 1$: incident wave is 100% reflected with just an exponential tail penetrating the barrier.

In particular: $\vec{j} = 0$ for $x < 0$

$\vec{j} = 0$ for $x > 0$ as well (check!)

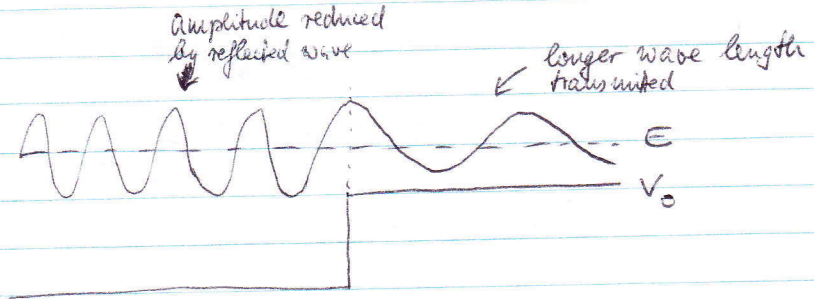
* Stationary
 Wave function: $\psi(x) = A(e^{ikx} + e^{i\alpha} e^{-ikx}) = A e^{i\frac{\alpha}{2}} (e^{i(kx - \frac{\alpha}{2})} + e^{-i(kx - \frac{\alpha}{2})})$
 $= 2A e^{i\frac{\alpha}{2}} \cos(kx - \frac{\alpha}{2})$ for $x < 0$

standing wave!

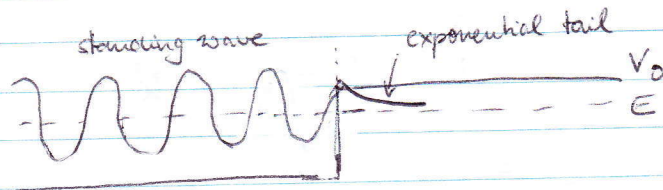
$$\psi(x) = 2A e^{i\frac{\alpha}{2}} \cos \frac{\alpha}{2} e^{-\kappa x}$$

⇒ SUMMARY:

Case $E > V_0$:



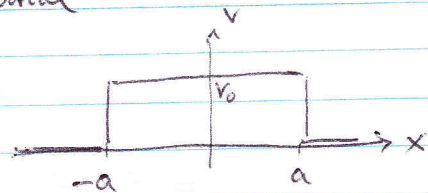
Case $0 < E < V_0$:



II.2.2 Potential Barrier

* Consider a rectangular "barrier" potential

$$V(x) = \begin{cases} V_0 & -a \leq x \leq a \\ 0 & \text{elsewhere} \end{cases}$$



Here: case $E < V_0$ ($E > 0$ of course)

For case $E > V_0$: maybe homework

* General solution

$$\psi(x) = \begin{cases} A e^{ikx} + B e^{-ikx} & k = \frac{1}{\hbar} \sqrt{2mE} \quad \text{for } x < -a \\ C e^{-\kappa x} + D e^{\kappa x} & \kappa = \frac{1}{\hbar} \sqrt{2m(V_0 - E)} \quad \text{for } -a < x < a \\ E e^{ikx} + F e^{-ikx} & \text{for } x > a \end{cases}$$

Matching @ $x = -a$: $A e^{-ika} + B e^{ika} = C e^{\kappa a} + D e^{-\kappa a}$ (1)

$$A e^{-ika} - B e^{ika} = \frac{i\kappa}{k} (C e^{\kappa a} - D e^{-\kappa a})$$
 (2)

Solving for A, B:

$$(1) + (2): A = \frac{1}{2} \left(1 + \frac{i\kappa}{k}\right) e^{\kappa a + ika} C + \frac{1}{2} \left(1 - \frac{i\kappa}{k}\right) e^{-\kappa a + ika} D$$

$$(1) - (2): B = \frac{1}{2} \left(1 - \frac{i\kappa}{k}\right) e^{\kappa a - ika} C + \frac{1}{2} \left(1 + \frac{i\kappa}{k}\right) e^{-\kappa a - ika} D$$

Matching @ $x = +a$:

$$C = \frac{1}{2} \left(1 - \frac{i\kappa}{\kappa}\right) e^{\kappa a + ika} E + \frac{1}{2} \left(1 + \frac{i\kappa}{\kappa}\right) e^{\kappa a - ika} F$$

(check!)

$$D = \frac{1}{2} \left(1 + \frac{i\kappa}{\kappa}\right) e^{-\kappa a + ika} E + \frac{1}{2} \left(1 - \frac{i\kappa}{\kappa}\right) e^{-\kappa a - ika} F$$

* Eliminate C, D:
$$A = \left(\frac{1}{4} \left(2 + \frac{i\kappa}{k} - \frac{i\kappa}{\kappa}\right) e^{2\kappa a + 2ika} + \frac{1}{4} \left(2 + \frac{i\kappa}{\kappa} - \frac{i\kappa}{\kappa}\right) e^{-2\kappa a + 2ika} \right) E + \left(\frac{1}{4} \left(\frac{i\kappa}{k} + \frac{i\kappa}{\kappa}\right) e^{2\kappa a} + \frac{1}{4} \left(-\frac{i\kappa}{k} - \frac{i\kappa}{\kappa}\right) e^{-2\kappa a} \right) F$$

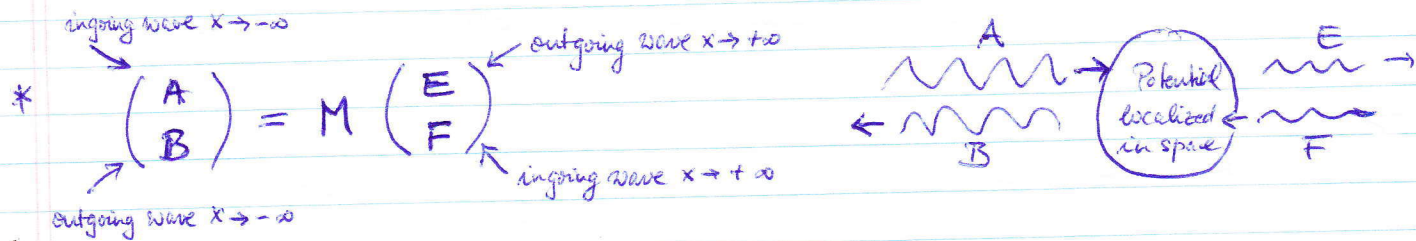
$$= \left(\cosh 2\kappa a + \frac{i\kappa}{2} \sinh 2\kappa a \right) e^{2ika} E + \frac{i\kappa}{2} \sinh 2\kappa a F$$

with $\epsilon = \frac{\kappa}{k} - \frac{k}{\kappa}$, $\eta = \frac{\kappa}{k} + \frac{k}{\kappa}$; similar for B.

In matrix form:

$$\begin{pmatrix} A \\ B \end{pmatrix} = \underbrace{\begin{pmatrix} \left(\cosh 2\kappa a + \frac{i\kappa}{2} \sinh 2\kappa a \right) e^{2ika} & \frac{i\kappa}{2} \sinh 2\kappa a \\ -\frac{i\kappa}{2} \sinh 2\kappa a & \left(\cosh 2\kappa a - \frac{i\kappa}{2} \sinh 2\kappa a \right) e^{-2ika} \end{pmatrix}}_{=: M} \begin{pmatrix} E \\ F \end{pmatrix}$$

The matrix is called the M -matrix.



A, B, E, F contain amplitude and overall phase of the asymptotic free plane waves.

Alternatively we can solve these linear equations to obtain the S -matrix

outgoing @ $x \rightarrow -\infty$ $\begin{pmatrix} B \\ E \end{pmatrix} = S \begin{pmatrix} A \\ F \end{pmatrix}$ $\begin{matrix} \text{incoming} \\ \text{@ } x \rightarrow -\infty \end{matrix}$ $\begin{matrix} \text{incoming} \\ \text{@ } x \rightarrow +\infty \end{matrix}$

$$S = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix}$$

outgoing @ $x \rightarrow +\infty$ "scattering matrix"

Generally: Any interaction with a spatially localized potential that allows free-particle solutions (plane waves) for $x \rightarrow \pm\infty$ can be expressed via a M - or S -matrix for the complex amplitudes.

* Theorem: In such a general situation, if the potential is real-valued the S -matrix is unitary.

Why? V real \Rightarrow current conservation $\Rightarrow \vec{j}(x \rightarrow -\infty) = \vec{j}(x \rightarrow +\infty)$

$$\Rightarrow |A|^2 - |B|^2 = |E|^2 - |F|^2 \Rightarrow |B|^2 + |E|^2 = |A|^2 + |F|^2$$

$$\Rightarrow \left| \begin{pmatrix} B \\ E \end{pmatrix} \right| = \left| \begin{pmatrix} A \\ F \end{pmatrix} \right| \quad \text{for any } A, B, E, F$$

norms conserved thus S is unitary.

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Recall: for unitarity of matrices it is necessary and sufficient that row and column vectors form orthonormal basis vector (here in \mathbb{C}^2)

* Back to the special case of the rectangular barrier.

Consider $F=0$ (incident particles only from one side ($x < 0$))

$$\Rightarrow A = M_{11} E ; B = M_{12} E$$

$$\Rightarrow E = \frac{1}{M_{11}} A = S_{21} A ; B = \frac{M_{12}}{M_{11}} A = S_{11} A$$

$S_{11} = \frac{M_{12}}{M_{11}}$, $S_{21} = \frac{1}{M_{11}}$ are the only relevant coefficients of the S-matrix in this case.

* We can define reflection and transmission coefficients in the usual way

$$R = \frac{|B|^2}{|A|^2} = |S_{11}|^2 = \frac{|M_{12}|^2}{|M_{11}|^2}$$

$$T = \frac{|E|^2}{|A|^2} = |S_{21}|^2 = \frac{1}{|M_{11}|^2}$$

For the rectangular barrier

$$T = \frac{1}{|\cosh 2\kappa a + \frac{iE}{2} \sinh 2\kappa a|^2}$$

Two special cases:

• Tall and wide barrier: $\kappa a \gg 1$, i.e. $\cosh 2\kappa a \approx \sinh 2\kappa a \approx \frac{1}{2} e^{2\kappa a}$

$$\left|1 + \frac{iE}{2}\right|^2 = 1 + \frac{1}{4} \left(\frac{\kappa^2 - k^2}{\kappa k}\right)^2 = \left(\frac{\kappa^2 + k^2}{2\kappa k}\right)^2 \Rightarrow T \approx 16 e^{-4\kappa a} \left(\frac{\kappa k}{\kappa^2 + k^2}\right)^2$$

• Very tall and ^{very} narrow barrier: $V_0 \gg E \Rightarrow \kappa \gg k$ and $\kappa a \ll 1$

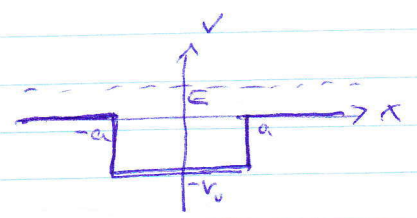
$$\Rightarrow T \approx \frac{k^2}{k^2 + \kappa^2 a^2} = \frac{E}{E + \frac{2m}{\hbar^2} V_0 a^2}$$

II.3 Potential Well

* Consider the finite square potential

$$V(x) = \begin{cases} -V_0 & -a < x < a \\ 0 & \text{elsewhere} \end{cases} \quad \text{with } V_0 > 0$$

→ CASE A: $E > 0$ i.e. scattering solution.



Same as potential barrier (II.2.2) with $E > V_0$; just replace $V_0 \leftrightarrow -V_0$ (see homework)

M-matrix in this case:

$$\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} (\cos 2k'a - \frac{iE}{2} \sin 2k'a) e^{2ika} & -\frac{iV_0'}{2} \sin 2k'a \\ \frac{iV_0'}{2} \sin 2k'a & (\cos 2k'a + \frac{iE}{2} \sin 2k'a) e^{-2ika} \end{pmatrix} \begin{pmatrix} E \\ F \end{pmatrix}$$

↑ complex amplitudes of in-/outgoing plane waves for $x < -a$
 k, k' wave vectors of plane waves outside and inside the square well
 ↑ complex ampl. for out-/ingeing plane waves for $x > a$

$$E' = \frac{k'}{k} + \frac{k}{k'} \quad \eta' = \frac{k'}{k} - \frac{k}{k'}$$

cf. HW III [4]

→ CASE B: $-V_0 < E < 0$: bound states

* Symmetric $V(x) \Rightarrow$ eigenstates of H can be chosen to be parity eigenstates

as well, i.e. even or odd functions. Thus

$$\psi_+(x) = \begin{cases} C \cos kx & -a < x < a \\ B e^{-\kappa|x|} & \text{elsewhere} \end{cases} \quad ; \quad \psi_-(x) = \begin{cases} D \sin kx & \text{for } -a < x < a \\ -B e^{-\kappa|x|} & \text{for } x > a \\ B e^{-\kappa|x|} & \text{for } x < -a \end{cases}$$

for even parity

with $k' = \frac{1}{\hbar} \sqrt{2m(E+V_0)}$, $\kappa = \frac{1}{\hbar} \sqrt{-2mE}$

* Matching conditions:

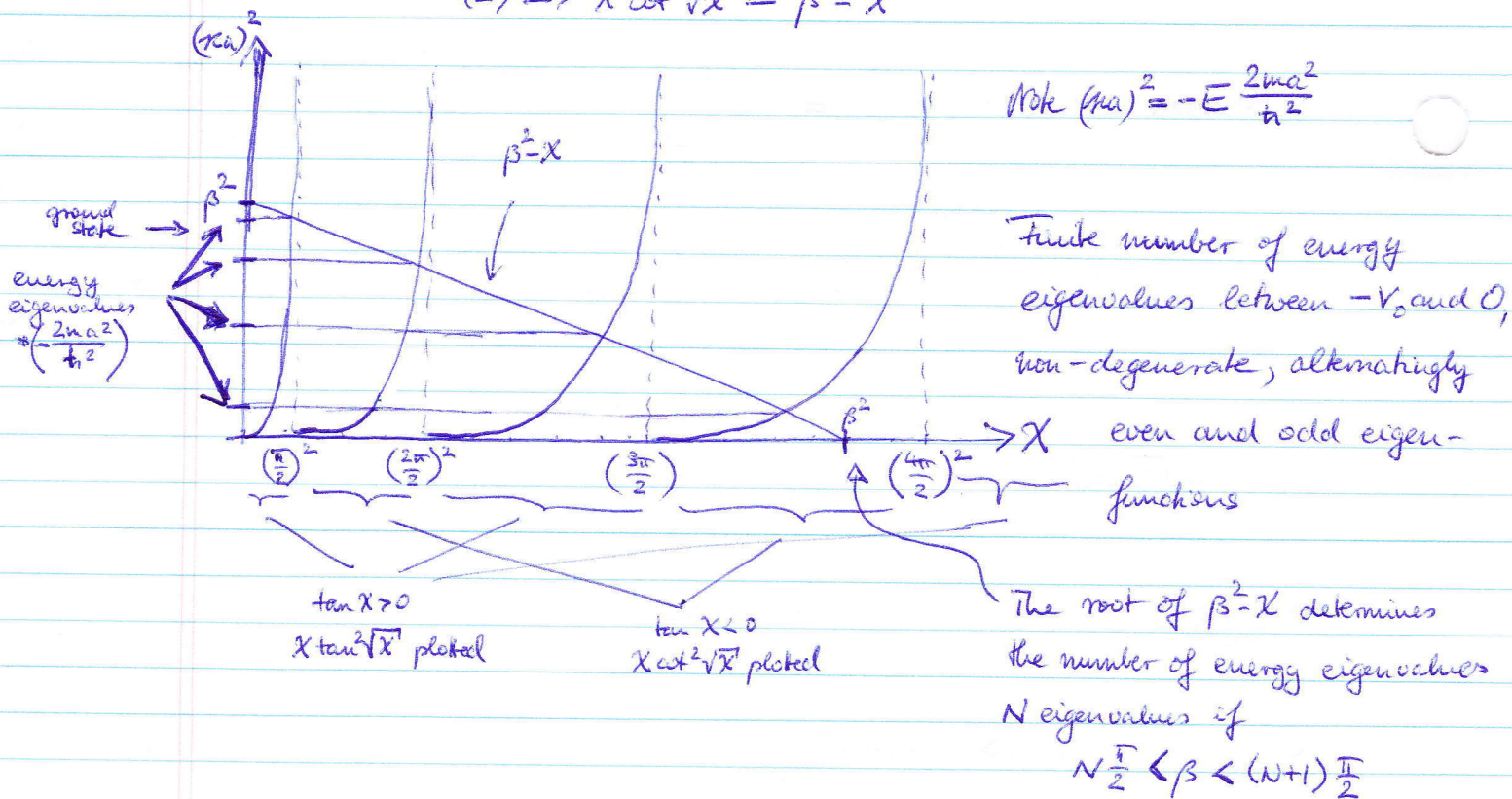
For ψ_+ $\begin{cases} C \cos ka = e^{-\kappa a} \\ -k' C \sin ka = -\kappa A e^{-\kappa a} \end{cases} \Leftrightarrow \begin{cases} C \cos ka = e^{-\kappa a} \\ k' \tan ka = \kappa \quad (1) \end{cases}$
 (for $\tan ka > 0$)

For ψ_- $\begin{cases} D \sin ka = -e^{-\kappa a} \\ k' \cot ka = -\kappa \quad (2) \end{cases}$
 ($\Rightarrow \tan ka < 0$)

Eqs. (1) + (2) determine the energy spectrum for even + odd eigenfunctions.

Define $X = (k'a)^2$. (1) $\Rightarrow X \tan^2 \sqrt{X} = (\kappa a)^2 = \underbrace{\left(\frac{a}{\hbar} \sqrt{2mV_0}\right)^2}_{=\beta} - X$

(2) $\Rightarrow X \cot^2 \sqrt{X} = \beta^2 - X$



* The N eigenvalues /-states correspond to bound states in the potential well. We can still formally define the N - and

S-matrix using suitable asymptotic states

$$\psi(x) = \begin{cases} A e^{-kx} + B e^{kx} & (x < -a) \\ E e^{-kx} + F e^{kx} & (x > a) \end{cases}$$

and $\begin{pmatrix} A \\ B \end{pmatrix} = M \begin{pmatrix} E \\ F \end{pmatrix}$

Since $A = 0, F = 0$ for physical solutions: $M_{11} = 0$ and


$$S_{11} = \frac{M_{12}}{M_{21}}, S_{21} = \frac{1}{M_{11}} = \infty$$

i.e. bound states correspond to poles in the S-matrix.

II.4 Summary of Scattering in 1-D

* In retrospect, the potential well + barrier can be described by the same

M-/S-matrix formalism irrespective of whether the potential is attractive 

or repulsive : $\begin{pmatrix} B \\ E \end{pmatrix} = S \begin{pmatrix} A \\ F \end{pmatrix}$
outgoing ingoing

The amplitude for transmission is

$$S_{12} = \frac{E}{A} = \frac{1}{M_{11}} = \sqrt{T} e^{-i\phi}$$

↑
transmission coefficient

and for reflection

$$S_{11} = \frac{B}{A} = \frac{M_{21}}{M_{11}} = \sqrt{1-T} e^{-i\phi'}$$

ϕ is called the phase shift. It can be interpreted as a delay or speeding up of the ^{plane}wave due to the potential and the change in kinetic energy corresponding to it.

Since M_{21} always imaginary $\phi' = \phi \pm \frac{\pi}{2}$

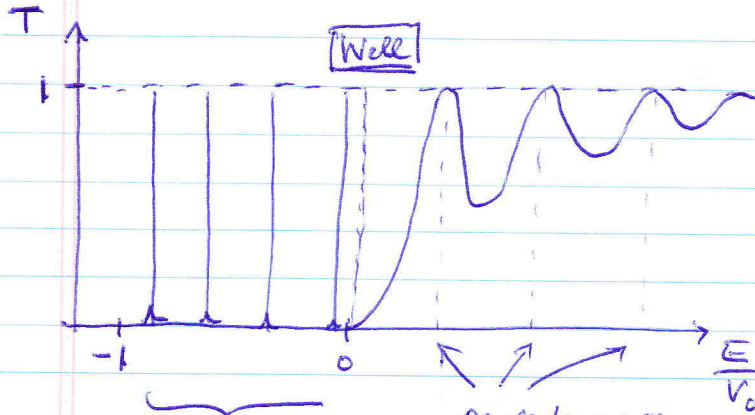
* II.2+II.3: $T = |S_{12}|^2 = \frac{1}{\cos^2 2k'a + \frac{E'^2}{4} \sin^2 2k'a}$

for both well and barrier as long as $E > V_0$ and $E > 0$

$\phi = 2ka - \arctan\left(\frac{E'}{2} \tan 2k'a\right)$

II.2: $T = \frac{1}{\cosh^2 2ka + \frac{E'^2}{4} \sinh^2 2ka}$

for $0 < E < V_0$



Bound states correspond to narrow δ -pts. in T (S-matrix poles)

Oscillations with maxima having $T=1$ at $k'a = n\pi$

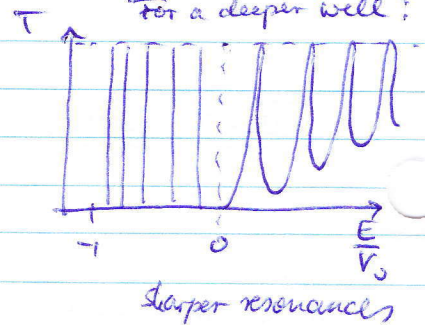
Peaks of pronounced enough are called resonances

Oscillations for $E > 0$

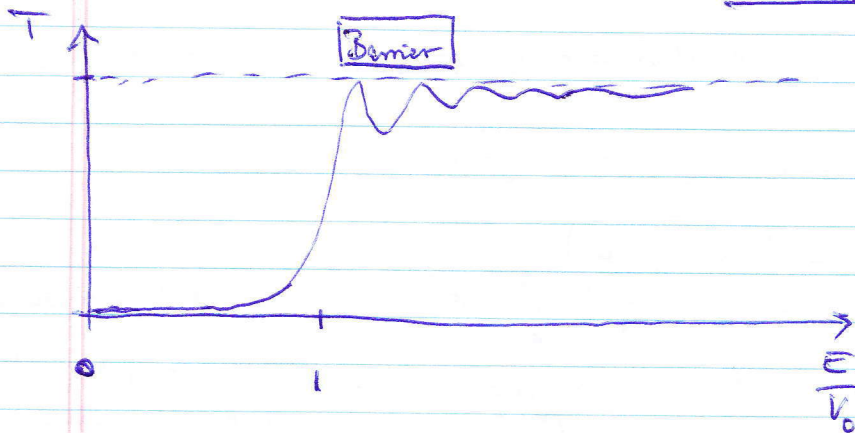
$T \rightarrow 1$ for $E \rightarrow \infty$ since $E' \rightarrow 2$

$T=1$ also for $k'a = n\pi$

For a deeper well:



Sharper resonances



* All of these features are also qualitatively true for more complicated potentials.