III ~~II~~. FIRST APPLICATIONS

Sections in these notes are now renumbered. New numbers are indicated in Courier font to the left.

III.1 ~~II~~.1 The Harmonic Oscillator

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

$V(x) = \frac{1}{2} m\omega^2 x^2$ 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 $x = x_0$:

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

* Hamilton fct. $H = \frac{p^2}{2m} + \frac{m\omega^2}{2} x^2$

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

II.1.1 Stationary States

* We solve the t-indep. Schrödinger eqn.

$$H\varphi = E\varphi \qquad (1)$$

to obtain energy eigenvalues and eigenfcts.

* The Gaussian $\varphi_0(x) = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}$ is a solution to (1).

Why? $\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2x^2\right)\left(\frac{m\omega}{\hbar\pi}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2} =$

$= \left(\frac{\hbar\omega}{2} - \frac{1}{2}m\omega^2x^2 + \frac{1}{2}m\omega^2x^2\right)\left(\frac{m\omega}{\hbar\pi}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2} = \frac{1}{2}\hbar\omega\,\varphi_0$ ✓

Normalization: $\int_{\mathbb{R}} |\varphi_0|^2 dx = 1$ (check!)

The energy eigenvalue for φ_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 $\varphi(x) = e^{-\frac{m\omega}{2\hbar}x^2} v(x)$

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

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

$\sqrt{\frac{\hbar}{m\omega}}$ 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) or $$\boxed{\frac{d^2v}{d\xi^2} - 2\xi\frac{dv}{d\xi} + 2n\,v = 0}$$ with $n = \frac{E - E_0}{E_0}$

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

Diff. equation for $v(x)$.

* Excursion: The parity operator $\mathcal{P}$ represents inversions $\vec{r} \mapsto -\vec{r}$ ($x \to -x$ in 1-D) in space. It acts on a Hilbert space $\mathcal{H}$ by $\varphi(\vec{r}) \mapsto \varphi(-\vec{r})$.

Obviously its eigenvalues are $+1$ and -1 and the corresponding eigenspaces are those of even and odd fcts $\varphi(\vec{r})$ resp., i.e.

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

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

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

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

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

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

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

* The series for the $v(\xi)$ terminates and v is a polynomial if n is a positive integer (n 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. Merzbacher p. 82)

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

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

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

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

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

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

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

$$\dots \qquad \dots$$

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

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

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

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

* Basic properties of Hermite polynomials:

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

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

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 $\varphi_n(x)$, $n \in \mathbb{N}$ 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 $I = \sum_{j=0}^{\infty}\sum_{k=0}^{\infty} \frac{s^j t^k}{j!\,k!} \underbrace{\int_{\mathbb{R}} H_j(\xi) H_k(\xi)\, e^{-\xi^2} d\xi}$

$$= \sqrt{\frac{m\omega}{\hbar}} \int dx\, \varphi_j(x)\varphi_k(x)\, dx\, (C_j C_k)^{-1}$$

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

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

Completeness:

$$\sum_{n=0}^{\infty} \psi_n^*(x')\,\psi_n(x) = \sum_{n=0}^{\infty} \frac{1}{2^n n!}\left(\frac{m\omega}{\hbar\pi}\right)^{1/2} H_n(\xi')\,H_n(\xi)\, e^{-\xi'^2/2}\, e^{-\xi^2/2}$$

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

$\xi' = \sqrt{\frac{m\omega}{\hbar}}\, x'$

$$= \left(\frac{m\omega}{\hbar\pi}\right)^{1/2} \frac{1}{\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{1}{n!} \int_{-\infty}^{+\infty} (\xi'+is)^n H_n(\xi)\, e^{-s^2} e^{-\xi'^2/2} e^{-\xi^2/2}\, ds$$

$$= \left(\frac{m\omega}{\hbar}\right)^{1/2} \frac{1}{\pi} \int_{-\infty}^{+\infty} F(\xi, \xi'+is)\, e^{-s^2 - \frac{\xi'^2}{2} - \frac{\xi^2}{2}}\, ds$$

$$= \left(\frac{m\omega}{\hbar}\right)^{1/2} \frac{1}{\pi} \int_{-\infty}^{+\infty} e^{-(\xi'+is)^2 + 2\xi(\xi'+is) - s^2 - \frac{\xi'^2}{2} - \frac{\xi^2}{2}}\, ds$$

$$= \left(\frac{m\omega}{\hbar}\right)^{1/2} \frac{1}{\pi} \underbrace{e^{-\frac{3}{2}\xi'^2 - \frac{\xi^2}{2} + 2\xi\xi'}}_{=1 \text{ for } \xi'=\xi} \underbrace{\int_{-\infty}^{+\infty} e^{-2is(\xi'-\xi)}\, ds}_{\pi\,\delta(\xi'-\xi)}$$

$$= \delta(x - x')$$

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

II.1.2 Wave Packets and General Solutions

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

Let $c_n = \displaystyle\int_{\mathbb{R}} \psi_n(x)\, \psi(x,0)\, dx$ be the probability amplitudes of $\psi(x,0)$ w.r.t. each energy eigenstate $\psi_n(x)$, i.e $\psi(x,0) = \sum_{n\in\mathbb{N}} c_n \psi_n(x)$.

Then

$$\boxed{\psi(x,t) = e^{-\frac{i}{2}\omega t} \sum_{n=0}^{\infty} c_n \psi_n(x)\, e^{-in\omega t}} \qquad (*)$$

Why? Clear from I.9.6

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

then

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

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

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

directly from solution (*). HW7

III.2 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 $E_0 > V_0$, $\langle E \rangle > V_0$.

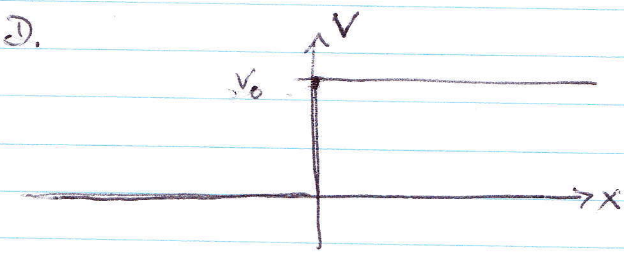
Why? later.

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 $x < 0$

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

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

$$\Rightarrow \psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx}, & x < 0 \\ Ce^{ik'x} + De^{-ik'x}, & x > 0 \end{cases}$$

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

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

(2) − k'(1)

(2) + k(1)

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

Interpretation: $\psi(x) = (Ae^{ikx} + Be^{-ikx})\Theta(-x) + Ce^{ik'x}\Theta(x)$

- Ae^{ikx}: incident plane wave (from left)
- Be^{-ikx}: reflected plane wave
- $Ce^{ik'x}$: transmitted plane wave

One can define reflection and transmission coefficients (probabilities):

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

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

$\frac{k'}{k}$ prefactor ensures that $\boxed{R + T = 1}$

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

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

$= \frac{\hbar k}{m}\left[|A|^2 - |B|^2\right]$ 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 $\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & (x<0) \quad k = \frac{1}{\hbar}\sqrt{2mE} \\ Ce^{-\kappa x} & (x>0) \quad \kappa = \frac{1}{\hbar}\sqrt{2m(V_0 - E)} \end{cases}$

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

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

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

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

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: $\psi(x) = A\left(e^{ikx} + e^{i\alpha} e^{-ikx}\right) = A e^{i\frac{\alpha}{2}}\left(e^{i(kx-\frac{\alpha}{2})} + e^{-i(kx-\frac{\alpha}{2})}\right)$

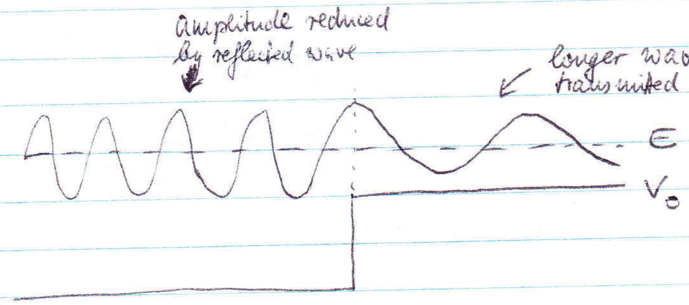
$$= 2A e^{i\frac{\alpha}{2}} \cos\left(kx - \frac{\alpha}{2}\right) \qquad \text{for } x<0$$

standing wave!

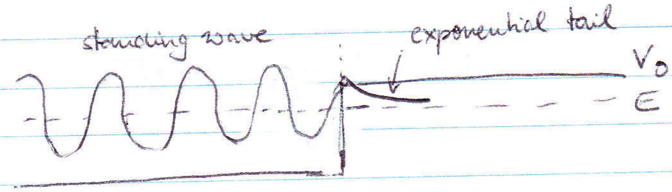
$$\psi(x) = 2A e^{i\frac{\alpha}{2}} \cos\frac{\alpha}{2}\, e^{-\varkappa x}$$

⇒ SUMMARY:

Case $E > V_0$:



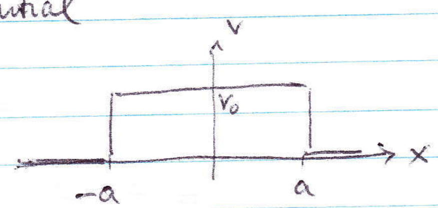
Case $0 < E < V_0$:



II 2.2 Potential Barrier

* Consider a rectangular "barrier" potential

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



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

For case $E > V_0$: maybe homework

(8)

* 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)

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

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 @ $x = +a$:

(check!)

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

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

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

$$+ \left(\frac{1}{4}\left(\frac{i\kappa}{k} + \frac{ik}{\kappa}\right) e^{2\kappa a} + \frac{1}{4}\left(-\frac{i\kappa}{k} - \frac{ik}{\kappa}\right) e^{-2\kappa a}\right) F$$

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

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

In matrix form:

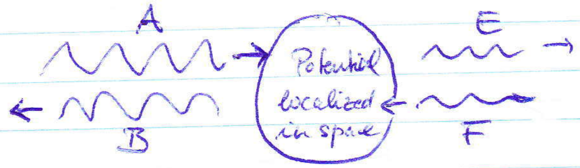
$$\begin{pmatrix} A \\ B \end{pmatrix} = \underbrace{\begin{pmatrix} \left(\cosh 2\kappa a + \frac{i\varepsilon}{2} \sinh 2\kappa a\right) e^{2ika} & \frac{i\eta}{2} \sinh 2\kappa a \\ -\frac{i\eta}{2} \sinh 2\kappa a & \left(\cosh 2\kappa a - \frac{i\varepsilon}{2} \sinh 2\kappa a\right) e^{-2ika} \end{pmatrix}}_{=: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

The matrix is called the M-matrix.

ingoing wave $x \to -\infty$; outgoing wave $x \to +\infty$

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

outgoing wave $x \to -\infty$; ingoing wave $x \to +\infty$



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 <u>S-matrix</u>

outgoing @ $x \to -\infty$; ingoing @ $x \to -\infty$

$$\begin{pmatrix} B \\ E \end{pmatrix} = S \begin{pmatrix} A \\ F \end{pmatrix} \quad ; \quad S = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix}$$

outgoing @ $x \to +\infty$; ingoing @ $x \to +\infty$

"scattering matrix"

<u>Generally</u>: Any interaction with a spatially localized potential that allows free-particle solutions (plane waves) for $x \to \pm\infty$ 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 $\Rightarrow \vec{j}(x \to -\infty) = \vec{j}(x \to +\infty)$

$$\underset{\text{II.2.1}}{\Rightarrow} |A|^2 - |B|^2 = |E|^2 - |F|^2 \Rightarrow |B|^2 + |E|^2 = |A|^2 + |F|^2$$

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

norms conserved thus S is unitary.

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 ($x<0$))

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

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

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

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

$$R = \frac{|B|^2}{|A|^2} = |S_{11}|^2 = \frac{|M_{21}|^2}{|M_{11}|^2}$$

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

For the rectangular barrier

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

Two special cases:

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

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

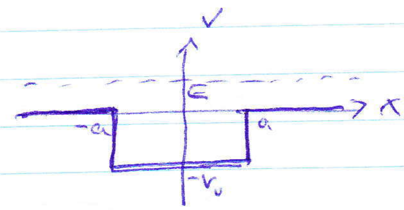
- Very tall and very narrow barrier: $V_0 \gg E \Rightarrow \kappa \gg k$ and $\kappa a \ll 1$

$$\Rightarrow T \approx \frac{k^2}{k^2 + \kappa^4 a^2} = \frac{E}{E + \frac{2m}{\hbar^2} V_0^2 a^2}$$

III.3 II.3 Potential Well

* Consider the finite square potential

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



→ 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:

$$\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} \left(\cos 2k'a - \frac{i\varepsilon'}{2}\sin 2k'a\right)e^{2ika} & -\frac{i\eta'}{2}\sin 2k'a \\ \frac{i\eta'}{2}\sin 2k'a & \left(\cos 2k'a + \frac{i\varepsilon'}{2}\sin 2k'a\right)e^{-2ika} \end{pmatrix} \begin{pmatrix} E \\ F \end{pmatrix}$$

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-/ingoing plane waves for $x>a$

$$\varepsilon' = \frac{k'}{k} + \frac{k}{k'} \qquad \eta' = \frac{k'}{k} - \frac{k}{k'}$$

cf. HW VII [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

$$\psi_+(x) = \begin{cases} C\cos k'x & \text{f. } -a<x<a \\ Be^{-\kappa|x|} & \text{elsewhere} \end{cases} \quad ; \quad \psi_-(x) = \begin{cases} D\sin k'x & \text{for } -a<x<a \\ -Be^{-\kappa|x|} & \text{for } x>a \\ Be^{-\kappa|x|} & \text{for } x<-a \end{cases}$$

for even parity

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

* Matching conditions:

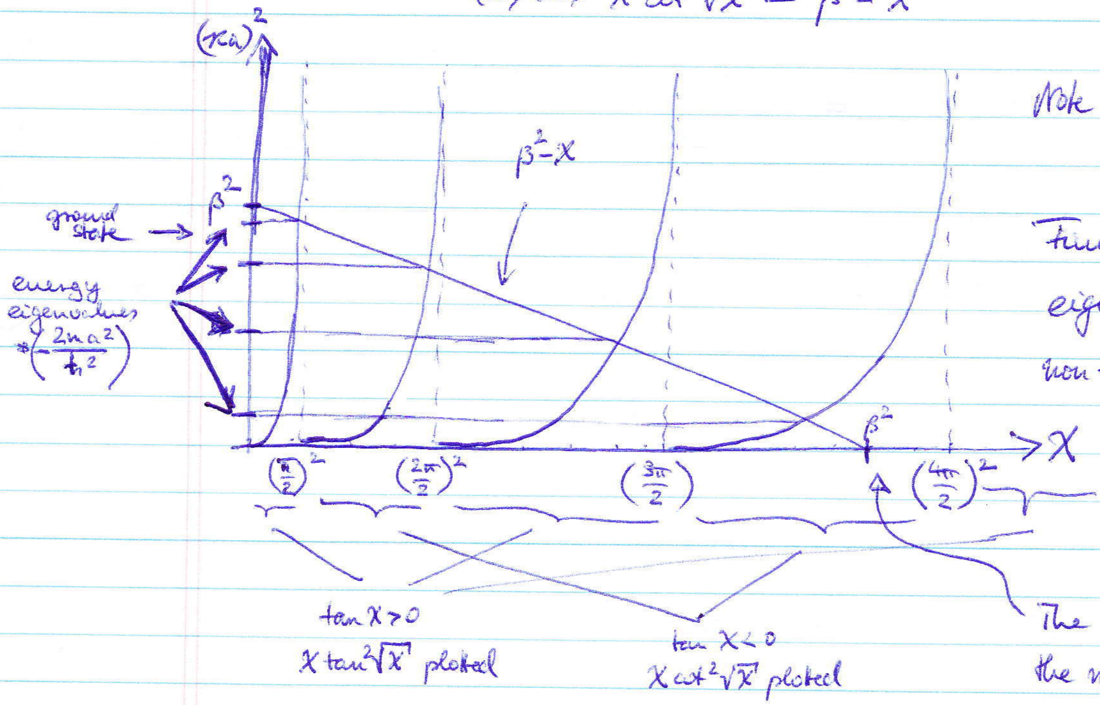
For ψ_+ $\begin{cases} C\cos k'a = e^{-\kappa a} \\ -k'C\sin k'a = -\kappa A e^{-\kappa a} \end{cases} \Leftrightarrow \begin{cases} C\cos k'a = e^{-\kappa a} \\ k'\tan k'a = \kappa \quad (1) \end{cases}$ ($\tan k'a > 0$)

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

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



Note $(\kappa a)^2 = -E\frac{2ma^2}{\hbar^2}$

Finite number of energy eigenvalues between $-V_0$ and 0, non-degenerate, alternatingly even and odd eigenfunctions

The root of $\beta^2 - X$ determines the number of energy eigenvalues
N eigenvalues if
$N\frac{\pi}{2} < \beta < (N+1)\frac{\pi}{2}$

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

S-matrix using suitable asymptotic states

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

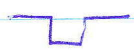
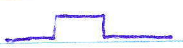
and $\begin{pmatrix} A \\ B \end{pmatrix} = M \begin{pmatrix} E \\ F \end{pmatrix}$

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

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

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

III.4 ~~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)

; 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.

and for reflection

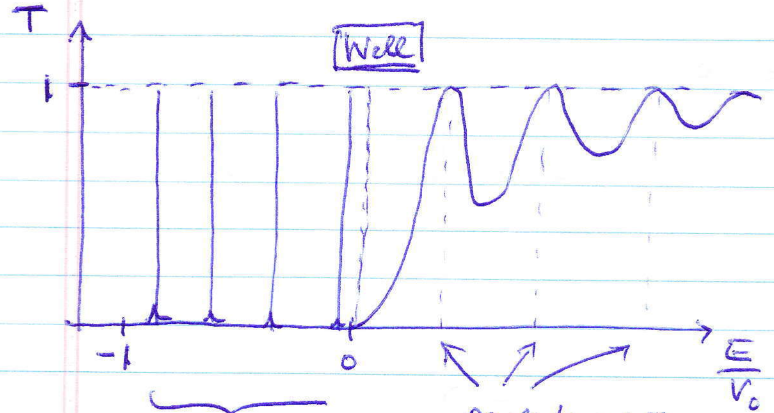
$$S_{11} = \frac{B}{A} = \frac{M_{21}}{M_{11}} = \sqrt{1-T}\, e^{-i\phi'}$$

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

* II.2 + II.3: $T = |S_{12}|^2 = \dfrac{1}{\cos^2 2k'a + \frac{\varepsilon'^2}{4}\sin^2 2k'a}$ for both well and barrier as long as $E > V_0$ and $E > 0$

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

II.2: $T = \dfrac{1}{\cosh^2 2\kappa a + \frac{\varepsilon^2}{4}\sinh^2 2\kappa a}$ for $0 < E < V_0$

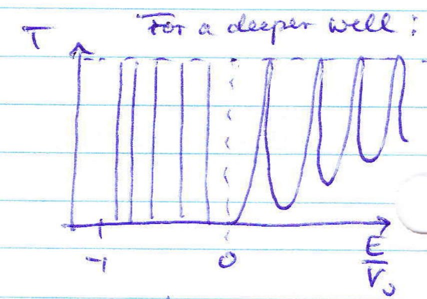


Oscillations for $E > 0$

$T \to 1$ for $E \to \infty$ since $\varepsilon' \to 2$

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

For a deeper well:

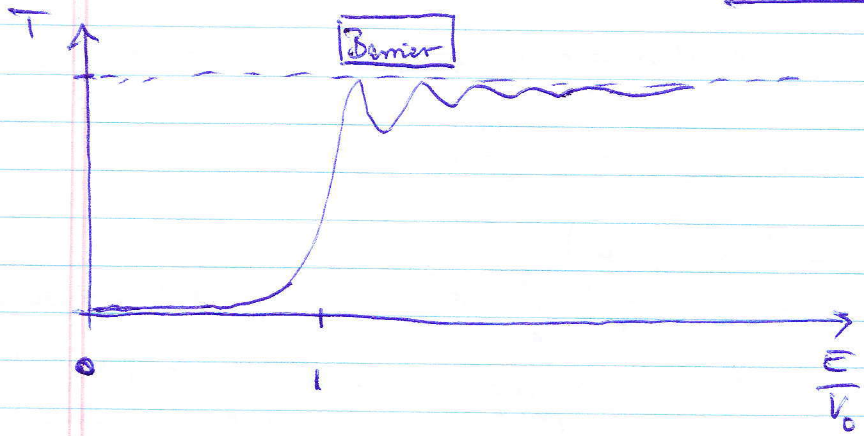


Sharper resonances

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

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

Peaks of pronounced enough are called <u>resonances</u>



* All of these features are also <u>qualitatively</u> true for more complicated potentials.