H4: one-dimensional examples

4.1 general formulae	
Particle in a potential V(x)	The Schrödinger eq: $$i\hbar \frac{\partial}{\partial t}\Psi(x,t) = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\Psi(x,t).$$ Since the potential is time-independent, we can look for stationary-state solutions: $$\Psi(x,t) = \psi(x)\exp(-iEt/\hbar)$$ the TISE is: $$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$$ Furthermore the probability density is: $$P(x) = \|\psi(x)\|^2.$$ with a probability current density: $$j = \frac{\hbar}{2im}\left[\psi^*(x)\frac{d\psi(x)}{dx} - \psi(x)\frac{d\psi^*(x)}{dx}\right]$$
4.2 the free particle	
free particle problem	Consider V(x) = V_0 > then F = dV/dx = 0 > no forces on the particle, thus a free particle Then the TISE: $$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x).$$ now for $k = \left(\frac{2m}{\hbar^2}E\right)^{1/2}$ we find two linearly independent solutions: > these form a linear combination: $$\boxed{\psi(x) = Ae^{ikx} + Be^{-ikx}}$$ We must have that k cannot have an imaginary part > otherwise ψ would increase exponentially at x=∞ > since E = $\hbar^2k^2/2m$ we find E≥0 > energy cannot remain lower than the potential over the entire interval Remark that the basic solutions may be written in the form: $$\psi_{k_x}(x) = C\exp(ik_x x)$$ or $$\psi_{p_x}(x) = C\exp(ip_x x/\hbar)$$
4.2.1 momentum eigenfunction	
momentum eigenfunctions	The eigenvalue equation for momentum operator reads: $$-i\hbar\frac{\partial}{\partial x}\psi_{p_x}(x) = p_x\psi_{p_x}(x)$$ > we still have the same solutions: $$\psi_{k_x}(x) = C\exp(ik_x x)$$ or $$\psi_{p_x}(x) = C\exp(ip_x x/\hbar)$$ with $p_x = \hbar k_x$ real, since the eigenfunctions must remain finite as x→∞ > spectrum of p_{op} is continuous

4.2.2 physical interpretation of the free-particle solution	
analysing free particle	Substitute the general solution ψ in the formula for Ψ: $$\begin{aligned}\Psi(x,t) &= (Ae^{ikx} + Be^{-ikx})e^{-iEt/\hbar} \\ &= Ae^{i(kx-\omega t)} + Be^{-i(kx+\omega t)}\end{aligned}$$ Now we will discuss four cases: - B = 0 - A = 0 - A = B - A = -B
case 1: B=0	<u>The solution then results in:</u> $$\Psi(x,t) = Ae^{i(kx-\omega t)}$$ > free particle with mass m moving along x-axis in positive direction: - definite momentum $p = \hbar k$ - energy $E = p^2/2m$ - angular frequency $\omega = E/\hbar = \hbar k^2/2m$ - wave number $k = p/\hbar = 2\pi/\lambda$ > vibration traveling in x-direction with phase velocity $v_{ph} = d\omega/dk$ <u>The corresponding position probability density :</u> $$P = \|\Psi(x,t)\|^2 = \|A\|^2$$ > time and position independent > in accordance with Heisenberg's uncertainty principle ie: particle moving along x-axis with well-defined momentum, $\Delta p = 0$, cannot be localised along its axis $\Delta x = \infty$ <u>The correspond probability current density:</u> $$\begin{aligned}j &= \frac{\hbar}{2im}(A^* e^{-ikx} Aik e^{ikx} - Ae^{ikx} A^*(-ik)e^{-ikx}) \\ &= \frac{\hbar k}{m}\|A\|^2 = \frac{p}{m}\|A\|^2 = v\|A\|^2\end{aligned}$$ > time and position independent
case 2: A=0	<u>The plane wave:</u> $$\Psi(x,t) = Be^{-i(kx+\omega t)}$$ <u>The corresponding position probability density:</u> $$P = \|\Psi(x,t)\|^2 = \|B\|^2$$ <u>The corresponding probability current density:</u> $$j = -\frac{\hbar k}{m}\|B\|^2 = -\frac{p}{m}\|B\|^2 = -v\|B\|^2.$$ >> same as case1, but traveling in opposite direction

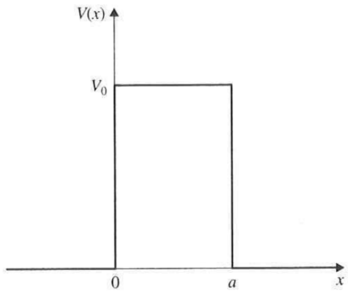
case3: A=B	<u>The plane wave, with C=2A:</u> $$\Psi(x,t) = A(e^{ikx} + e^{-ikx})e^{-i\omega t} = C\cos kx e^{-i\omega t}$$ > standing wave with fixed nodes at: $$x_n = \pm\left(\frac{\pi}{2} + n\pi\right)\Big/ k, \qquad n = 0, 1, 2, \ldots$$ for which cos(kx) vanishes <u>The corresponding position probability density:</u> $$P(x) = \lvert C\rvert^2 \cos^2 kx$$ <u>The corresponding probability current density:</u> $$j = \frac{\hbar}{2im}(-C^* \cos kx Ck \sin kx + C\cos kx C^* k \sin kx) = 0.$$ This is because the probability flux v|A|² from case1 is cancelled by -v|A|² from case2 > no net flux >> case3 describes a free particle whose momentum p is known precisely , but the direction is unknown
case4: A=-B	<u>The plane wave, with D=2iA:</u> $$\Psi(x,t) = A(e^{ikx} - e^{-ikx})e^{-i\omega t} = D\sin kx e^{-i\omega t},$$ > vanishes for: $x_n = \pm n\pi/k (n = 0, 1, 2, \ldots)$ for which $\sin kx = 0$. <u>The position probability density:</u> $$P(x) = \lvert D\rvert^2 \sin^2 kx$$ <u>j = 0</u>
case5: general free particle	<u>General position probability density:</u> $$P(x) = \lvert A\rvert^2 + \lvert B\rvert^2 + (AB^* e^{2ikx} + A^* B e^{-2ikx})$$ > interference of two plane waves <u>probability current density:</u> $$j = v[\lvert A\rvert^2 - \lvert B\rvert^2]$$
4.2.3 'normalisation' of the free-particle wave function	
normalisation problems	The integral: $$I = \int_{-\infty}^{+\infty} \lvert Ae^{ikx} + Be^{-ikx}\rvert^2 dx$$ is infinite for all values of A and B > the free-particle functions cannot satisfy the normalisation condition: $$\int_{-\infty}^{+\infty} \lvert\psi(x)\rvert^2 dx = 1.$$ > we can only speak of relative probabilities >> alternative: - box normalization - delta-function normalization

- box normalization	Enclose the particle in a box of length L > wave function must obey boundary conditions example: consider the wave functions 4.11a: $\psi_{k_x}(x) = C\exp(\mathrm{i}k_x x)$ its convenient to require ψ to satisfy the periodic boundary conditions at the walls > then: $\psi_{k_x}(x+L) = \psi_{k_x}(x)$ > this causes k_x to be restricted to: $k_x = \frac{2\pi}{L}n, \qquad n = 0, \pm 1, \pm 2, \dots .$ > the spectrum of energy eigenvalues of the Schrödinger eq. becomes discrete: $E_n = \frac{\hbar^2 k_x^2}{2m} = \frac{2\pi^2\hbar^2}{mL^2}n^2$ As L increases, the spacing of the successive energy levels decreases > for a macroscopic box the energy spectrum is essentially continuous Now we can normalise a free particle by requiring: $\int_{-L/2}^{+L/2} \lvert\psi_{k_x}(x)\rvert^2 \mathrm{d}x = 1$ Which gives us $C = L^{-1/2}$, thus the eigenfunctions: $\psi_{k_x}(x) = L^{-1/2}\exp(\mathrm{i}k_x x).$
- delta-function normalization	use Dirac delta functions for normalization > allows momentum eigenfunctions to retain their form over the entire x-axis for real k_x We have: $\int_{-\infty}^{+\infty} \exp[\mathrm{i}(k_x - k'_x)x]\mathrm{d}x = 2\pi\delta(k_x - k'_x).$ **(4.35)** Taking the arbitrary phase of the normalisation constant C in (4.11a) to be zero, we see that if we choose $C = (2\pi)^{-1/2}$, the momentum eigenfunctions $\psi_{k_x}(x) = (2\pi)^{-1/2}\exp(\mathrm{i}k_x x)$ **(4.36)** satisfy the orthonormality relation $\int_{-\infty}^{+\infty} \psi^*_{k'_x}(x)\psi_{k_x}(x)\mathrm{d}x = \delta(k_x - k'_x).$ **(4.37)** We also see with the help of (A.18) that the wave functions (4.36) satisfy the *closure relation* $\int_{-\infty}^{+\infty} \psi^*_{k_x}(x')\psi_{k_x}(x)\mathrm{d}k_x = \delta(x - x').$ **(4.38)** >> 4.37 is referred to as k-normalization We can do the same for momentum eigenfunctions: $\psi_{p_x}(x) = (2\pi\hbar)^{-1/2}\exp(\mathrm{i}p_x x/\hbar)$ are such that $\int_{-\infty}^{+\infty} \psi^*_{p'_x}(x)\psi_{p_x}(x)\mathrm{d}x = \delta(p_x - p'_x)$ > p-normalization
4.3 the potential step	
potential step	particle moving in a potential V(x) which has the form of an infinitely wide barrier: left: V(x) goes to zero right: V(x) goes to a constant value >0 >> quantummechical the particle gets both reflected as transmitted NIET IN DE LES BEHANDELD, MAAR KAN WEL OP HET EXAMEN GEVRAAGD WORDEN aka: kijk er eens vlug naar

4.4 the potential barrier

particle in potential barrier

consider a rectangular potential barrier:



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

classical for an incident particle with energy E:

- $E<V_0$: particle reflected
- $E>V_0$: particle transmitted

quantum: both reflection and transmission

There is no solution for the TDSE if E<0
> the energy of the particle must be positive: E>0
> general solution of the TDSE is given by:

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

since there, the particle is free

We will study particles incident on the barrier from the left
> nothing at large positive values of x
> D=0:

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

thus: -left: incident wave with amplitude A
reflected wave with amplitude B
- right: transmitted wave with amplitude C

The probability current density is then:

$$j = \begin{cases} v[|A|^2 - |B|^2], & x < 0 \\ v|C|^2, & x > a \end{cases}$$

Define the reflection and transmission coefficients as:

$$R = \frac{j(\text{gereflecteerd})}{j(\text{inkomend})} \qquad T = \frac{j(\text{doorgelaten})}{j(\text{inkomend})}$$

then:

$$R = \frac{|B|^2}{|A|^2}, \qquad T = \frac{|C|^2}{|A|^2}.$$

However, the nature of the TDSE in the internal region 0<x<a depends on energy:

- case 1: $E<V_0$
- case 2: $E>V_0$

case 1: $E<V_0$

$V(x) = V_0$ for $0<x<a$ and set $\kappa = [2m(V_0 - E)/\hbar^2]^{1/2}$
> TDSE for the internal region is given by:

$$\psi(x) = F e^{\kappa x} + G e^{-\kappa x}, \qquad 0 < x < a.$$

now A,B,C,F and G are related by th requirement: dψ/dx is continuous at x=0 and x=a
thus at x=0:

$$A + B = F + G$$
$$ik(A - B) = \kappa(F - G)$$

while at $x = a$ we find from (4.74b) and (4.77) that

$$Ce^{ika} = Fe^{\kappa a} + Ge^{-\kappa a}$$
$$ikCe^{ika} = \kappa(Fe^{\kappa a} - Ge^{-\kappa a}).$$

Now we can calculate T and R:

Eliminating F and G and solving for the ratios B/A and C/A, we obtain

$$\frac{B}{A} = \frac{(k^2+\kappa^2)(e^{2\kappa a}-1)}{e^{2\kappa a}(k+i\kappa)^2 - (k-i\kappa)^2} \qquad \textbf{(4.80a)}$$

and

$$\frac{C}{A} = \frac{4ik\kappa e^{-ika} e^{\kappa a}}{e^{2\kappa a}(k+i\kappa)^2 - (k-i\kappa)^2} \qquad \textbf{(4.80b)}$$

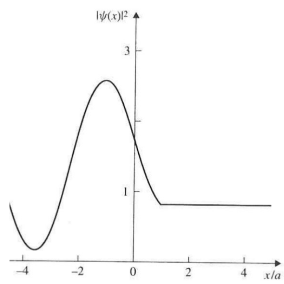
so that the reflection and transmission coefficients are given by

$$R = \frac{|B|^2}{|A|^2} = \left[1 + \frac{4k^2\kappa^2}{(k^2+\kappa^2)^2 \sinh^2(\kappa a)}\right]^{-1} = \left[1 + \frac{4E(V_0-E)}{V_0^2 \sinh^2(\kappa a)}\right]^{-1} \qquad \textbf{(4.81a)}$$

and

$$T = \frac{|C|^2}{|A|^2} = \left[1 + \frac{(k^2+\kappa^2)^2 \sinh^2(\kappa a)}{4k^2\kappa^2}\right]^{-1} = \left[1 + \frac{V_0^2 \sinh^2(\kappa a)}{4E(V_0-E)}\right]^{-1}. \qquad \textbf{(4.81b)}$$

We see that a particle has a chance of going through the barrier
= barrier penetration / tunnel effect



<u>relation to classical mechanics</u>:
1: for $E \to 0$, T goes to 0
2: when the E approaches the top of the barrier, we have

$$\lim_{E \to V_0} T = \left(1 + \frac{mV_0 a^2}{2\hbar^2}\right)^{-1}.$$

> consider $mV_0a^2/\hbar^2$ the opacity of the barrier
> in classical limit this becomes very large
> T is very small

3: $\kappa a \gg 1$ we can write $\sinh(\kappa a) \simeq 2^{-1}\exp(\kappa a)$
> T then becomes:

$$T \simeq \frac{16E(V_0-E)}{V_0^2} e^{-2\kappa a}$$

> which is very small

>> T is small in classical limit

case 2: E>V_0

solution in internal region is given by:

$$\psi(x) = F e^{ik'x} + G e^{-ik'x} \qquad 0 < x < a$$

where $k' = [2m(E - V_0)/\hbar^2]^{1/2}$ as in (4.59b).

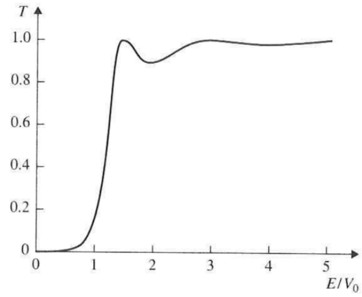
Via same steps as case 1 we find:

$$R = \frac{|B|^2}{|A|^2} = \left[1 + \frac{4k^2k'^2}{(k^2 - k'^2)^2 \sin^2(k'a)}\right]^{-1} = \left[1 + \frac{4E(E - V_0)}{V_0^2 \sin^2(k'a)}\right]^{-1}$$

$$T = \frac{|C|^2}{|A|^2} = \left[1 + \frac{(k^2 - k'^2)^2 \sin^2(k'a)}{4k^2k'^2}\right]^{-1} = \left[1 + \frac{V_0^2 \sin^2(k'a)}{4E(E - V_0)}\right]^{-1}$$

remarks:

1: T is in general less than unity
> only when k'a = π, 2π, 3π, ... is T=1
ie: when a = half number of Broglie wavelengths λ' = 2π/k'
> this is due to destructive interference between x=0 and x=a



2: when E tends to V_0, T joins smoothly to the value given by:

$$\lim_{E \to V_0} T = \left(1 + \frac{mV_0a^2}{2\hbar^2}\right)^{-1}.$$

when E is large compared to V_0, T becomes asymptotically equal to unity

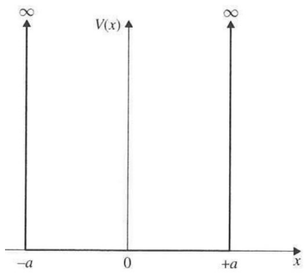
4.5 infinite square well

infinite square well

Consider a particle of mass m bound so that the classical motion is periodic
> we have a potential V(x) equal to:

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

with a = L/2, half the box



for |x|<a the TISE:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x).$$

with a general solution:

$$\psi(x) = A\cos kx + B\sin kx, \qquad k = \left(\frac{2m}{\hbar^2}E\right)^{1/2}.$$

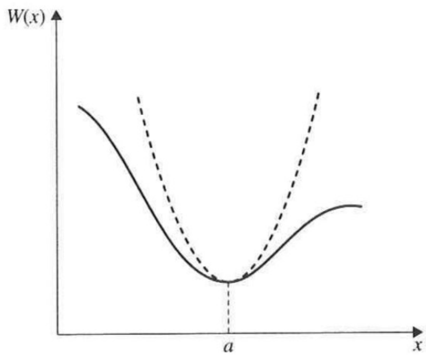
We have to impose boundary conditions:

$$\psi(x) = 0 \qquad \text{at} \qquad x = \pm a.$$

quantisation of energy due to boundary conditions	Because of the boundary condition, we find: $$A \cos ka = 0, \qquad B \sin ka = 0.$$ There are two possible solutions: 1: B=0 & cos(ka) = 0 2: A=0 & sin(ka) = 0 <u>case1:</u> For B=0 and cos(ka) we find the only possible solutions for k: $$k_n = \frac{n\pi}{2a} = \frac{n\pi}{L} \qquad \text{n = 1,3,5,...}$$ The eigenfunction $\psi_n(x) = A_n \cos k_n x$ can be normalized: $$\int_{-a}^{+a} \psi_n^*(x)\psi_n(x)\mathrm{d}x = 1$$ > from which we find that $A_n = a^{-1/2}$ > therefore the normalised eigenfunction is: $$\psi_n(x) = \frac{1}{\sqrt{a}} \cos \frac{n\pi}{2a} x, \qquad n = 1, 3, 5, \ldots .$$ <u>case2:</u> same steps as in case1: $$\psi_n(x) = \frac{1}{\sqrt{a}} \sin \frac{n\pi}{2a} x, \qquad n = 2, 4, 6, \ldots .$$ >> due to these two cases we conclude that k is quantise by: $$k_n = n\pi/L, \text{ with } n = 1, 2, 3, \ldots .$$ thus we have quantised energy levels: $$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2}{8m}\frac{\pi^2 n^2}{a^2} = \frac{\hbar^2}{2m}\frac{\pi^2 n^2}{L^2}, \qquad n = 1, 2, 3, \ldots$$ and quantised wavelengths: $$\lambda_n = 2\pi/k_n = 2L/n,$$ > energy spectrum consists of infinite number of discrete energy levels for each bound state now: for each level there is just one eigenfunction ie: the energy levels are non-degenerate
4.5.1 parity	
parity of eigenfunctions	for case1 we found even eigenfunctions, ie: $$\psi_n(-x) = \psi_n(x)$$ while for case2 we found uneven eigenfunctions: $$\psi_n(-x) = -\psi_n(x)$$ > this is caused by the symmetry of the potential V(x) about x=0 ie: V(x) is an even function: V(-x) = V(x)
parity of the Schrödinger eq.	if the potential is symmetric, the Hamiltonian doesn't change: $H = -(\hbar^2/2m)\mathrm{d}^2/\mathrm{d}x^2 + V(x)$ does not change when x is replaced by $-x$: > if we change the sign of x in the Schrödinger eq.: $$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi(-x)}{\mathrm{d}x^2} + V(x)\psi(-x) = E\psi(-x)$$ > both ψ(-x) and ψ(x) are solutions of the same equation > two wases: 1: eigenvalue E is non-degenerate 2: eigenvalue E is degenerate

case 1: E is non-degenerate	The two eigenfunctions $\psi(x)$ and $\psi(-x)$ can then differ only by a multiplicative constant $$\psi(-x) = \alpha\psi(x). \quad \textbf{(4.98)}$$ Changing the sign of x in this equation yields $$\psi(x) = \alpha\psi(-x) \quad \textbf{(4.99)}$$ and by combining these two equations we find that $\psi(x) = \alpha^2\psi(x)$. Hence $\alpha^2 = 1$ so that $\alpha = \pm 1$ and $$\psi(-x) = \pm\psi(x) \quad \textbf{(4.100)}$$ which shows that the eigenfunctions $\psi(x)$ have a *definite parity*, being either even or odd for the parity operation $x \to -x$. remarks: - bound states in 1D are degenerate > every 1D bound-state wave function in a symmetric potential must either be even or odd - even functions have even amount of nodes odd odd > if energy levels are ordered by increasing value, the eigenvalues are alternating even/odd > ground state is always even
case 2: E is degenerate	More than one linearly independent eigenfunction corresponds to the eigenvalue E > eigenfunctions don't need parity > construct lin. comb. of thes functions, such that it has parity: $$\psi(x) = \psi_+(x) + \psi_-(x) \quad \textbf{(4.101)}$$ where $$\psi_+(x) = \tfrac{1}{2}[\psi(x) + \psi(-x)] \quad \textbf{(4.102a)}$$ obviously has even parity, while $$\psi_-(x) = \tfrac{1}{2}[\psi(x) - \psi(-x)] \quad \textbf{(4.102b)}$$ is odd. Substituting (4.101) into the Schrödinger equation (4.3) we have $$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) - E\right]\psi_+(x) + \left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) - E\right]\psi_-(x) = 0. \quad \textbf{(4.103)}$$ Changing x to $-x$ and using the fact that $V(-x) = V(x)$, $\psi_+(-x) = \psi_+(x)$ and $\psi_-(-x) = -\psi_-(x)$, we find that $$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) - E\right]\psi_+(x) - \left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) - E\right]\psi_-(x) = 0. \quad \textbf{(4.104)}$$ > proves that: for a symmetric (even) potential the eigenfunctions ψ(x) of the 1D Schrödinger eq. can always be chosen to have definite parity

4.5.2 wave function regeneration	
wave regeneration for inf. sq. well	The general solution of the TDSE is given by: $$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x) \exp(-iE_n t/\hbar)$$ with E_n the energy eigenvalues fir eigenfunctions that can be odd or even We can determine c_n by: $$c_n = \int_{-a}^{+a} \psi_n^*(x)\Psi(x, t=0)\mathrm{d}x$$ As time passes, the wave packet changes > however, after a time $T = 2\pi\hbar/E_1$ the wave function is the same: $$\Psi(x, t=T) = \Psi(x, t=0).$$ We can show this via: with $E_n = n^2E_1$ $$\Psi(x, t=T) = \sum_{n=1}^{\infty} c_n \psi_n(x) \exp\left(-in^2 E_1 \frac{2\pi}{E_1}\right)$$ $$= \sum_{n=1}^{\infty} c_n \psi_n(x) \exp(-i2\pi n^2). \qquad \textbf{(4.108)}$$ Since $2n^2$ is an even integer, it follows that $\exp(-i2\pi n^2) = 1$, and hence $$\Psi(x, t=T) = \sum_{n=1}^{\infty} c_n \psi_n(x) = \Psi(x, t=0). \qquad \textbf{(4.109)}$$ By repeating this argument, we see that the wave function is completely regenerated at times sT, where $s = 1, 2, 3, \ldots$ is a positive integer.
reflection wave of inf. sq. well	After a time $t = (2s-1)T/2$ the wave function is a reflection of t=0: $$\Psi(x, t=(2s-1)T/2) = -\Psi(-x, t=0)$$ We can see this in: $$\Psi(x, t=(2s-1)T/2) = \sum_{n=1}^{\infty} c_n \psi_n(x) \exp[-i\pi n^2(2s-1)]. \qquad \textbf{(4.111)}$$ When n is odd, n^2 is odd and $\exp[-i\pi n^2(2s-1)] = -1$. On the other hand, when n is even, n^2 is even and $\exp[-i\pi n^2(2s-1)] = 1$. Thus $$\Psi(x, t=(2s-1)T/2) = \sum_{n=1}^{\infty} c_n(-1)^n \psi_n(x). \qquad \textbf{(4.112)}$$ Since $\psi_n(x) = \psi_n(-x)$ when n is odd, and $\psi_n(x) = -\psi_n(-x)$ when n is even, the result (4.110) follows.

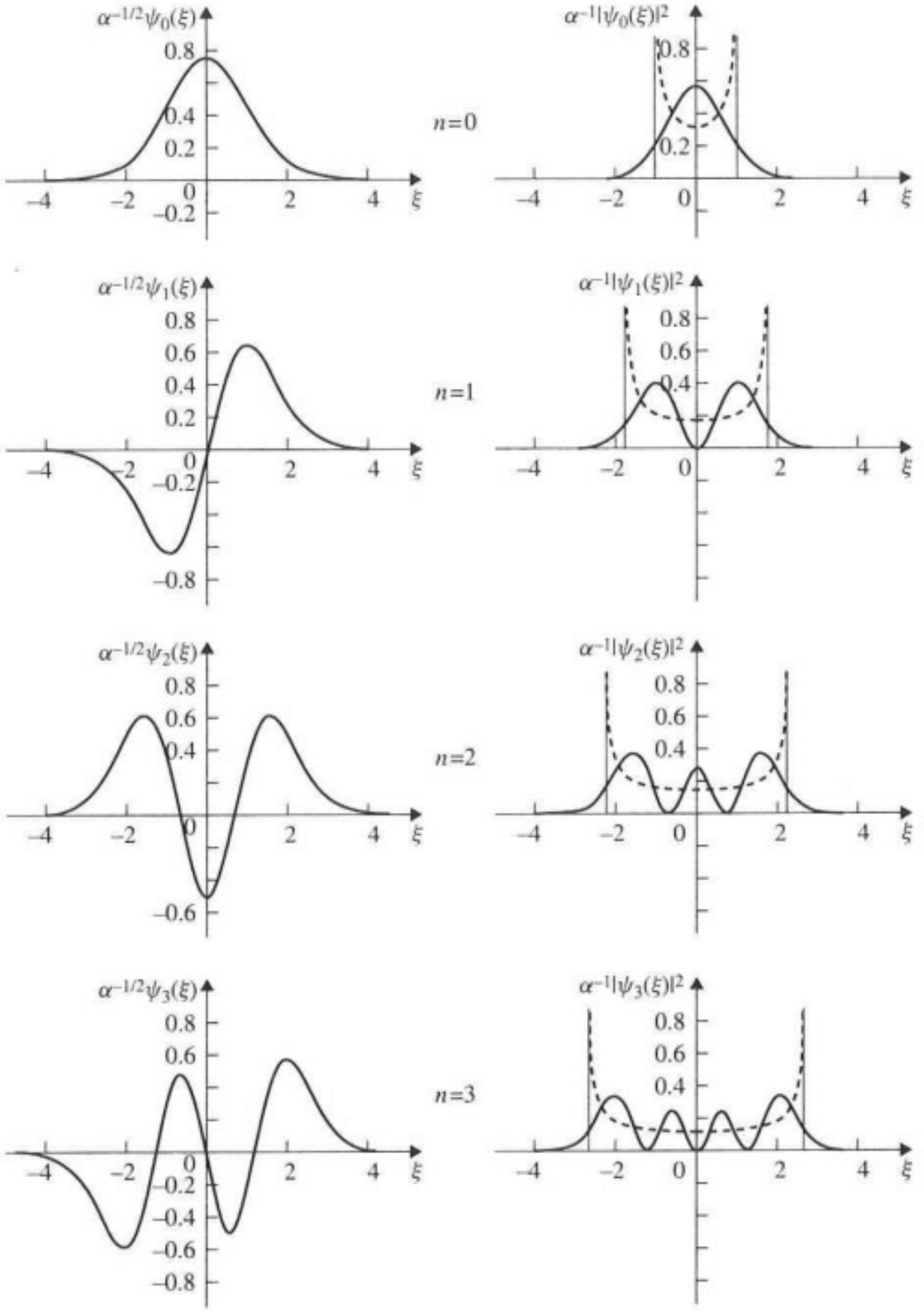
4.7 the linear harmonic oscillator	
lin. harmonic oscillator problem in quantum	consider a particle with mass m attracted to a fixed centre by a force F = -kx > the potential energy is given by: $V(x) = \frac{1}{2}kx^2$ Consider an arbitrary continuous potential W(x) with a minimum at x=a > at x=a we can approximate W(x) via a potential like V(x) > we can show this by taking the Taylor series of W(x) at x=a: $W(x) = W(a) + (x-a)W'(a) + \frac{1}{2}(x-a)^2W''(a) + \cdots$ Since x=a is a minimum, W'(a) = 0 and W''(a) > 0 > choose x=a as the origin of coordinates (a=0) choose W(a) as the origin of energy scale (ie: W(a) = 0) > all the expansions cancel, except for W''(a) > ie: $W(x) = \frac{1}{2}x^2W''(a)$ We now see that at a minimum for any arbitrary potential W(x), we can approximate this potential by V(x), the potential of an attractive force > in that case: $W(x) = \frac{1}{2}x^2W''(a),\ thus\ W''(x) = k$ 
TISE for harmonic osc.	For a potential V(x) = 1/2kx² the Hamiltonian is: $H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}kx^2$ (and the Schrödinger eigenvalue equation reads $-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + \frac{1}{2}kx^2\psi(x) = E\psi(x).$ (Clearly, all eigenfunctions correspond to bound states of positive energy. Rewrite the TISE in terms of dimensionless quantities > introduce the dimensionless eigenvalues: $\lambda = \frac{2E}{\hbar\omega}$ with the angular frequency ω of the corresponding classical oscillator: $\omega = \left(\frac{k}{m}\right)^{1/2}$ also introduce the dimensionless variable: $\xi = \alpha x$ where $\alpha = \left(\frac{mk}{\hbar^2}\right)^{1/4} = \left(\frac{m\omega}{\hbar}\right)^{1/2}.$ then the TISE becomes: $\frac{d^2\psi(\xi)}{d\xi^2} + (\lambda - \xi^2)\psi(\xi) = 0.$

derivation of Hermite equation	Analyse ψ in the asymptotic region $\|\xi\|\to\infty$ > for any finite E, the value of λ becomes negligible with respect to ξ^2 > we can reduce the TISE to: $$\left(\frac{d^2}{d\xi^2}-\xi^2\right)\psi(\xi)=0.$$ the functions that satisfy this eq.: $$\psi(\xi)=\xi^p e^{\pm\xi^2/2}$$ since ψ must be bounded everywhere, only negative values of p are accepted: > should have the form: $$\psi(\xi)=e^{-\xi^2/2}H(\xi)$$ with H(ξ) functions that mustn't affect the asymptotic behaviour of ψ If we substitute this into the TISE, we have the *hermite equation:* $$\frac{d^2H}{d\xi^2}-2\xi\frac{dH}{d\xi}+(\lambda-1)H=0$$ in order to solve this eq., expand H(ξ) in a power series in ξ > However V(-x) = V(x), we know that the eigenfunctions ψ(x) have parity > consider even and odd states separately
4.7.1 even states	
solution for even states	Since ψ(-ξ) = ψ(ξ) we have H(-ξ) = H(ξ), thus the power series: $$H(\xi)=\sum_{k=0}^{\infty}c_k\xi^{2k},\qquad c_0\neq 0 \qquad (4.140)$$ with even powers of ξ Substitute this into the Hermite eq.: $$\sum_{k=0}^{\infty}[2k(2k-1)c_k\xi^{2(k-1)}+(\lambda-1-4k)c_k\xi^{2k}]=0$$ or $$\sum_{k=0}^{\infty}[2(k+1)(2k+1)c_{k+1}+(\lambda-1-4k)c_k]\xi^{2k}=0.$$ The eq. will be satisfied if the coefficient of each power of ξ separately vanishes > we obtain a recursion relation: $$c_{k+1}=\frac{4k+1-\lambda}{2(k+1)(2k+1)}c_k.$$ thus we can determine each c_k from a given c_0
H(ξ) must be polynomial	If the series c_{k+1} does not terminate, we find for large enough k: $$\frac{c_{k+1}}{c_k}\sim\frac{1}{k}.$$ which is the same ratio as the series for $\xi^{2p}\exp(\xi^2)$, where p has a finite value. > however, we find that the wave function ψ(ξ) has asymptotic behaviour of the form: $$\psi(\xi)\underset{\|\xi\|\to\infty}{\sim}\xi^{2p}e^{\xi^2/2}$$ thus the series H(ξ) should terminate ie: H(ξ) is a polynomial in variable ξ^2 Let the highest power of ξ^2 appearing in the polynomial be ξ^{2N} with N = 0,1,2,… > thus in (4.140) we have $c_N\neq 0$ while the coefficient c_{N+1} must vanish > using the recursion relation we find that this happens if λ takes on discrete values: $$\lambda=4N+1,\qquad N=0,1,2,\ldots.$$ >> for each N there corresponds an even function H(ξ) which is a polynomial of order 2N in ξ

4.7.2 odd states	
solution for odd states	Now we have $\psi(-\xi) = -\psi(\xi)$, and hence $H(-\xi) = -H(\xi)$. > in similar fashion we find: $$H(\xi) = \sum_{k=0}^{\infty} d_k \xi^{2k+1}, \qquad d_0 \neq 0$$ with recursion: $$d_{k+1} = \frac{4k+3-\lambda}{2(k+1)(2k+3)} d_k.$$ For similar reasons we find that H(ξ) must terminate > we find: $$\lambda = 4N + 3, \qquad N = 0, 1, 2, \ldots .$$ >> for each N corresponds an odd function H(ξ) which is a polynomial of order 2N+1 in ξ and an odd, physically acceptable wave function ψ(ξ)
4.7.3 energy levels	
quantisation of energy levels in LHO	Putting together the results of the even and odd cases we find for the eigenvalue λ: $$\lambda = 2n + 1, \qquad n = 0, 1, 2, \ldots$$ so for the energy spectrum: $$E_n = \left(n + \tfrac{1}{2}\right)\hbar\omega = \left(n + \tfrac{1}{2}\right)h\nu, \qquad n = 0, 1, 2, \ldots$$ with ν = ω/2π the frequency of the corresponding classical operator > these are non-degenerate ie: for each quantum number there is just one eigenvalue >> energy spectrum of a LHO consists of infinite sequence of discrete levels > for any finite eigenvalue the particle is bound
zero-point energy	at its lowest state (n=0) the energy of a LHO is ħω/2 > is due to the uncertainty principle
4.7.4 Hermite polynomials	
the Hermite polynomials	We know the acceptable solutions are given by the equation: $$\psi_n(\xi) = e^{-\xi^2/2} H_n(\xi)$$ with - $H_n(\xi)$ are polynomials of order n - $\psi_n(\xi)$ and $H_n(\xi)$ have parity n - $H_n(\xi)$ satisfy the Hermite equation with λ=2n+1: $$\frac{d^2 H_n}{d\xi^2} - 2\xi \frac{dH_n}{d\xi} + 2n H_n = 0.$$ The $H_n(\xi)$ are uniquely defined, except for an arbitrary multiplicative constant > choose this constant such that the highest power ξ appears with coeff. 2^n > these are defined by: $$H_n(\xi) = (-1)^n e^{\xi^2} \frac{d^n e^{-\xi^2}}{d\xi^n} = e^{\xi^2/2}\left(\xi - \frac{d}{d\xi}\right)^n e^{-\xi^2/2}.$$ The first few Hermite polynomials, obtained from (4.154), are $$\begin{aligned} H_0(\xi) &= 1 \\ H_1(\xi) &= 2\xi \\ H_2(\xi) &= 4\xi^2 - 2 \\ H_3(\xi) &= 8\xi^3 - 12\xi \\ H_4(\xi) &= 16\xi^4 - 48\xi^2 + 12 \\ H_5(\xi) &= 32\xi^5 - 160\xi^3 + 120\xi. \end{aligned}$$

Hermite polynomials through generating function	Consider a generating function G(ξ,s): $$G(\xi, s) = e^{-s^2+2s\xi} = \sum_{n=0}^{\infty} \frac{H_n(\xi)}{n!} s^n.$$ ie: if the function exp(-s²+2sξ) is expanded in a power series in s then the coeff. of successive powers of s are just 1/n! times the Hermite polyn. $H_n(\xi)$ Using this, we prove that the Hermite polyn. satisfy the recursion relations: $$H_{n+1}(\xi) - 2\xi H_n(\xi) + 2n H_{n-1}(\xi) = 0$$ and $$\frac{dH_n(\xi)}{d\xi} = 2n H_{n-1}(\xi).$$
4.7.5 the wave functions for the linear harmonic oscillator	
eigenfunction for a discrete E_n	For each discrete E_n the corresponding unique physically acceptable eigenfunction is: $$\psi_n(x) = N_n e^{-\alpha^2 x^2/2} H_n(\alpha x)$$ with ψ_n and H_n having parity n and n zeros N_n is a constant yet to be determined via the normalization requirement: $$\int_{-\infty}^{+\infty} \|\psi_n(x)\|^2 dx = \frac{\|N_n\|^2}{\alpha} \int_{-\infty}^{+\infty} e^{-\xi^2} H_n^2(\xi) d\xi = 1. \quad \textbf{(4.160)}$$ In order to evaluate the integral on the right of (4.160), we consider the generating function $G(\xi, s)$ given by (4.156) as well as the second generating function $$G(\xi, t) = e^{-t^2+2t\xi} = \sum_{m=0}^{\infty} \frac{H_m(\xi)}{m!} t^m. \quad \textbf{(4.161)}$$ Using (4.156) and (4.161), we may then write $$\int_{-\infty}^{+\infty} e^{-\xi^2} G(\xi, s) G(\xi, t) d\xi = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{s^n t^m}{n!m!} \int_{-\infty}^{+\infty} e^{-\xi^2} H_n(\xi) H_m(\xi) d\xi. \quad \textbf{(4.162)}$$ Since $$\int_{-\infty}^{+\infty} e^{-x^2} dx = \sqrt{\pi} \quad \textbf{(4.163)}$$ the integral on the left-hand side of (4.162) is simply $$\int_{-\infty}^{+\infty} e^{-\xi^2} e^{-s^2+2s\xi} e^{-t^2+2t\xi} d\xi = e^{2st} \int_{-\infty}^{+\infty} e^{-(\xi-s-t)^2} d(\xi - s - t) = \sqrt{\pi} e^{2st} = \sqrt{\pi} \sum_{n=0}^{\infty} \frac{(2st)^n}{n!}. \quad \textbf{(4.164)}$$ Equating the coefficients of equal powers of s and t on the right-hand sides of (4.162) and (4.164), we find that $$\int_{-\infty}^{+\infty} e^{-\xi^2} H_n^2(\xi) d\xi = \sqrt{\pi} 2^n n! \quad \textbf{(4.165)}$$ and $$\int_{-\infty}^{+\infty} e^{-\xi^2} H_n(\xi) H_m(\xi) d\xi = 0, \qquad n \neq m. \quad \textbf{(4.166)}$$ From (4.160) and (4.165) we see that apart from an arbitrary complex multiplicative factor of modulus one the normalisation constant N_n is given by $$N_n = \left(\frac{\alpha}{\sqrt{\pi} 2^n n!} \right)^{1/2} \quad \textbf{(4.167)}$$ so that the normalised linear harmonic oscillator eigenfunctions are given by $$\psi_n(x) = \left(\frac{\alpha}{\sqrt{\pi} 2^n n!} \right)^{1/2} e^{-\alpha^2 x^2/2} H_n(\alpha x). \quad \textbf{(4.168)}$$

orthogonality of wave functions	The result implies: $$\int_{-\infty}^{+\infty} \psi_n^*(x)\psi_m(x)\mathrm{d}x = 0, \qquad n \neq m$$ so the harmonic oscillator wave functions for n and m are orthogonal > we can write: $$\int_{-\infty}^{+\infty} \psi_n^*(x)\psi_m(x)\mathrm{d}x = \delta_{nm}$$ > hence they are orthonormal
integrals of LHO	we can evaluate integrals involving harmonic oscillators using the generating function > for example: see p178
4.7.6 comparison with classical theory	
quantum to classical theory	Classical: - position x given by $x = x_0\sin(\omega t)$ - speed v : $\omega x_0\cos(\omega t)$ - energy $E = m\omega^2 x_0^2/2$ > motion takes place between turning points such that E=V(x) is located at $\pm x_0 = \pm(2E/m\omega^2)^{1/2}$. classically define $P_c(x)dx$ as the probability that the classical particle will be found in the interval dx in a random observation: $$P_c(x)\mathrm{d}x = \frac{1}{T}\frac{2\mathrm{d}x}{v} = \frac{\mathrm{d}x}{\pi(x_0^2 - x^2)^{1/2}}.$$ this is the largest at the turning points $\pm x_0$, where the speed vanishes > in terms of ξ, this becomes: $$P_c(\xi) = \frac{1}{\pi(\xi_0^2 - \xi^2)^{1/2}}.$$ with: $\pm\xi_0 = \pm\alpha x_0 = \pm\lambda^{1/2}$ <u>Analyse the graphs in next page:</u> for low values of n, the quantum probability densities don't math the classical one > as n increases the quantum theory shifts towards the classical one > in accordance to the correspondence principle
expectation value of V and T in LHO	The expectation value of the potential energy in a state ψ_n is given by: $$\langle V\rangle = \int_{-\infty}^{+\infty} \psi_n^*(x)\frac{1}{2}kx^2\psi_n(x)\mathrm{d}x = \frac{1}{2}k\langle x^2\rangle$$ where $$\langle x^2\rangle = \int_{-\infty}^{+\infty} \psi_n^*(x)x^2\psi_n(x)\mathrm{d}x.$$ we can solve the integral via a generating function or via the recursion relation > either way we find: $$\langle x^2\rangle = \frac{2n+1}{2\alpha^2} = \left(n + \frac{1}{2}\right)\frac{\hbar}{m\omega}$$ so that, using (4.132), (4.178) and (4.151), we have $$\langle V\rangle = \tfrac{1}{2}(n + \tfrac{1}{2})\hbar\omega = \tfrac{1}{2}E_n.$$ the kinetic energy is then the operator $T = p_x^2/2m = -(\hbar^2/2m)\mathrm{d}^2/\mathrm{d}x^2$ in the state ψ_n. $$\langle T\rangle = E_n - \langle V\rangle = \tfrac{1}{2}E_n.$$ for any eigenstate ψ_n, the expectation of T and V are half the energy
expectation value of p	we have seen that for any eigenfunction ψ_n it holds: $\langle x\rangle = 0$ > thus: $$\langle p_x\rangle = \int \psi_n^*(x)\left(-\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}x}\right)\psi_n(x)\mathrm{d}x = 0$$ and from (4.182) we also deduce that $$\langle p_x^2\rangle = 2m\langle T\rangle = mE_n = (n + \tfrac{1}{2})m\hbar\omega.$$



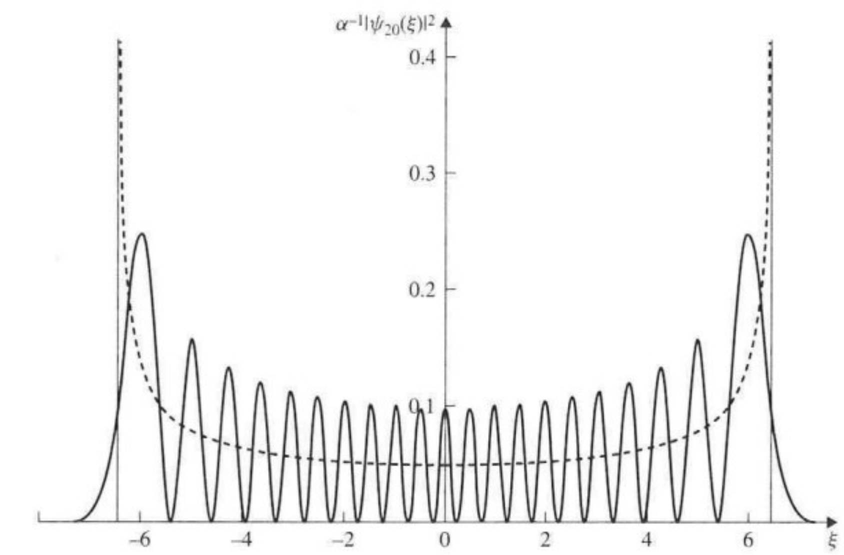


Figure 4.19 Comparison of the quantum mechanical position probability density for the state $n = 20$ of a linear harmonic oscillator (solid curve) with the probability density of the corresponding classical oscillator (dashed curve), having a total energy $E_{n=20} = (41/2)\hbar\omega$.