Lecture by Professor Tigran Tchrakian

Quantum Mechanics I

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Contents

1 Introduction

Classical mechanics breaks down at (sub)atomic scales

- Black body radiation: physical system = (ideal) gas of photons; classical statistical mechanics → average energy $\langle E\rangle = \frac{\int Ef(E)dE}{\int f(E)dE}$ leads to wrong result:
  Max Planck:

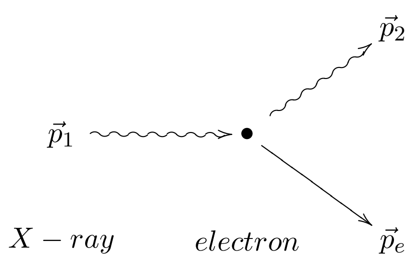
$$\int Ef(E)dE \to \sum_n E_n f(E_n)$$
$$\int f(E)dE \to \sum_n f(E_n)$$

  In subatomic mechanics the spectrum of energy is DISCRETE

$$E_n = n\hbar\omega$$

  i.e. energy comes in packets (quantum) of $\hbar$

- Compton Scattering



  From energy and momentum conservation, we get

$$\left(\frac{1}{\omega_1} - \frac{1}{\omega_2}\right) = \left(\frac{\hbar}{mc^2}\right)\sin^2\frac{\theta}{2}$$

  Louis deBroglie: particles = waves

$$\frac{\hbar}{mc^2} = \frac{1}{\omega_e}$$

2 Particle-wave-duality

0.
   - Radiation (photons) = waves propagating with speed of light
   - Maxwell waves are not localised in x-space

$$\psi(x,t) = e^{-i(\omega t - kx)}$$

1. de Broglie: also $m > 0$ particles are waves
   - $m > 0$ waves should be localised in x-space

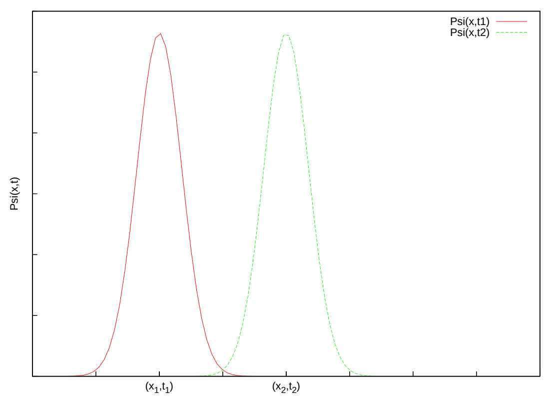


Figure 2.1: Wave function for a massive particle

   - $m > 0$: speed $u = \frac{|\vec{p}|c^2}{E}$
   -

$$\begin{aligned} m < 0 &\Rightarrow u > 0 && \text{tachyons} \\ m = 0 &\Rightarrow u = c && \text{photons} \\ m > 0 &\Rightarrow u < 0 && \text{massive particles} \end{aligned}$$

2.1 Model for a massive particles/waves:

0. massless particles (photons):

$$\psi_{plane}(x,t) = e^{-i(\omega t - kx)}$$

Most general solution to the wave equation is a linear superposition of plane waves, i.e. a Fourier superposition

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int a(k) e^{-i(\omega t - kx)} dk$$

where $\omega = ck$

1. Massive particles

   a) They are localised, i.e. peaked in x-space. Recall that

   $$\int |\psi(x)|^2 dx = \int |a(k)|^2 dk$$

   Then if $a(k)$ is peaked, $\psi(x)$ is also peaked, so to have a peaked profile for $\psi(x,t)$ we must employ a peaked $a(k)$.

   b) $u < c$, i.e. $\omega \neq ck$
   Using $E = \hbar\omega$ and $\vec{p} = \hbar\vec{k}$ yields

   $$u = \frac{pc^2}{E} = \frac{\hbar k c^2}{\hbar\omega} = \frac{kc^2}{\omega}$$

   so for massless particles with $\omega = kc \Rightarrow u = c$
   Let $\omega = \omega(k)$ which is a monotonic function of k. Since $a(k)$ is peaked, say to a narrow band around $k = k_0$, the integral for $\psi(x,t)$ gets its contribution mostly from this narrow range of integration. This allows us to approximate using the expansion of $\omega(k)$ around k_0, i.e. use

   $$\omega(k) = \omega(k_0) + (k - k_0)\frac{d\omega}{dk}|_{k=k_0} + \ldots$$

   i.e.

   $$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int dk\ a(k) e^{-i\left[\left(\omega(k_0)+(k-k_0)\frac{d\omega}{dk}|_{k=k_0}\right)t - kx\right]} =$$
   $$= \frac{1}{\sqrt{2\pi}} \underbrace{e^{-i\left(\omega(k_0)-k_0\frac{d\omega}{dk}|_{k=k_0}\right)t}}_{\text{Time dependent phase to be ignored}} \int dk\ a(k) e^{-i\left(k\frac{d\omega}{dk}{}_{k_0}t - kx\right)}$$
   $$\psi(x,t) \cong \frac{1}{\sqrt{2\pi}} \int dk\ a(k) e^{-ik\left(\frac{d\omega}{dk}|_{k_0}t - x\right)}$$

   whose speed of propagation is

   $$v_g = \frac{d\omega}{dk}$$

using a) and b) we get a peaked profile for $\psi(x,t)$ which propagates with speed

$$v = \frac{d\omega}{dk} = \frac{d\frac{E}{\hbar}}{d\frac{p}{\hbar}} = \frac{dE}{dp}$$

(Aside: in 3D $\vec{v} = \vec{\nabla}_p E$)

i) $u \ll c$ non relativistic particle $E = \frac{p^2}{2m}$

$$\Rightarrow v = \frac{dE}{dp} = \frac{2p}{2m} = \frac{p}{m} = \frac{mu}{m} = u$$

ii) u comparable to c: relativistic particle $E = c\sqrt{p^2 + m^2c^2}$

$$\Rightarrow v = \frac{dE}{dp} = \frac{1}{2}c(p^2 + m^2c^2)^{-1/2}2p = \frac{pc}{(p^2 + m^2c^2)^{1/2}} = \frac{pc^2}{E} = u$$

2.2 Time-evolution equation for $\psi(x,t)$

For massless particles we had

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int dka(k)e^{-i(\omega t - kx)}$$

Using $E = \hbar\omega$ and $p = \hbar k$ we get

$$\psi(x,t) \cong \frac{1}{\sqrt{2\pi\hbar}} \int dpa(p)e^{-\frac{i}{\hbar}(Et - px)}$$

To deduce the Time-evolution we calculate different derivatives of $\psi(x,t)$:

$$\frac{\partial\psi}{\partial t} = -\frac{i}{\hbar}E\psi \qquad \frac{\partial^2\psi}{\partial t^2} = \left(-\frac{i}{\hbar}E\right)^2\psi$$

$$\frac{\partial\psi}{\partial x} = \frac{ip}{\hbar}\psi \qquad \frac{\partial^2\psi}{\partial x^2} = \left(\frac{ip}{\hbar}\right)^2\psi$$

i) nonrelativistic (free) particle: $E - \frac{p^2}{2m} = 0$

$$i\hbar\frac{\partial\psi}{\partial t} + \frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = E\psi - \frac{p^2}{2m}\psi = 0$$

$$\Rightarrow i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}$$

Schrödinger-equation for a free particle

ii) relativistic (free) particle: $\frac{E^2}{c^2} - p^2 = m^2c^2$

$$-\frac{\hbar^2}{c^2}\frac{\partial^2\psi}{\partial t^2} + \hbar^2\frac{\partial^2\psi}{\partial x^2} = \frac{E^2}{c^2}\psi - p^2\psi = m^2c^2\psi$$

$$\Rightarrow \frac{1}{c^2}\frac{\partial^2\psi}{\partial t^2} - \frac{\partial^2\psi}{\partial x^2} = -\frac{m^2c^2}{\hbar^2}\psi$$

Klein-Gordon-Equation

2.3 Physical Interpretation of $\psi(x,t)$

Entirely different from that of Maxwell-waves, obeying

$$\frac{1}{c^2}\frac{\partial^2\psi}{\partial t^2} - \frac{\partial^2\psi}{\partial x^2} = 0$$

where ψ is complex, but because

$$\psi(x,t) = e^{-i(\omega t - kx)} = cos(\omega t - kx) - i\sin(\omega t - kx)$$

ψ is a physical observable.

This is not the case with Schrödinger-equation where the differential operator

$$i\hbar\frac{\partial}{\partial t} + \frac{\partial^2}{\partial x^2}$$

is itself comlex valued! $\Rightarrow$ solutions $\psi(x,t)$ are in general complex!

Max Born: Born's probabilistic interpretation of $\psi(x,t)$. The simplest real quantity of ψ is $|\psi(x,t)|^2 = \psi^*\psi \geq 0$. $|\psi|^2 \geq 0$ is like a probability density $\rho(x,t) \geq 0$. $(|\psi(x,t)|^2 dx)$ is the probability of finding the particle between x and $x + dx$

Remark.

- QM is therefore an INDETERMINISTIC regime
- In QM x is not an explicit function of t
- In QM all the dynamical information (i.e. time-evolution) information is encoded in $\psi(x,t)$
- Total probability

  $$N = \int |\psi(x,t)|^2 dx < \infty$$

  Convention: Normalize ψ

  $$\int |\psi(x,t)|^2 dx = 1$$

- Convergence of this integral requires that $\psi \xrightarrow{x\to\pm\infty} 0$
- expectation value of x

  $$\langle x \rangle = \frac{\int x|\psi(x,t)|^2 dx}{\int |\psi|^2 dx}$$

- In general the integral is a function of time:

  $$\int_{x=a}^{x=b} f(x,t)dx = g(t)$$

but the total probability must be independent of t for ψ obeying the QM equation of motion. Check:

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\int|\psi|^2dx &= \int\left[\left(i\hbar\frac{\partial\psi^*}{\partial t}\right)\psi+\psi^*\left(i\hbar\frac{\partial\psi}{\partial t}\right)\right]dx \\ &= \frac{\hbar^2}{2m}\int\left[\frac{\partial^2\psi^*}{\partial x^2}\psi-\psi^*\frac{\partial^2\psi}{\partial x^2}\right]dx \\ &= \frac{\hbar^2}{2m}\int\left[\frac{\partial}{\partial x}\frac{\partial\psi^*}{\partial x}\psi-\psi^*\frac{\partial}{\partial x}\frac{\partial\psi}{\partial x}\right]dx \end{aligned}$$

using $\psi\frac{\partial}{\partial x}\frac{\partial\psi^*}{\partial x}=\frac{\partial}{\partial x}\left(\psi\frac{\partial\psi^*}{\partial x}\right)-\frac{\partial\psi}{\partial x}\frac{\partial\psi^*}{\partial x}$

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\int|\psi|^2dx &= \frac{\hbar^2}{2m}\int\left[\frac{\partial}{\partial x}\left(\psi\frac{\partial\psi^*}{\partial x}\right)-\frac{\partial}{\partial x}\left(\psi^*\frac{\partial\psi}{\partial x}\right)\right]dx \\ &= \frac{\hbar^2}{2m}\left[\psi\frac{\partial\psi^*}{\partial x}-\psi^*\frac{\partial\psi}{\partial x}\right]_{-\infty}^{+\infty} \\ &= 0 \end{aligned}$$

Klein-Gordon-Equation is no use for this purpose $\Rightarrow$ restrict to NONRELATIVISTIC QM

2.4 Quantum Mechanics → Classical Mechanics

For the size of the system going from micro to macro the Quantum Mechanical values shoul go to the classical values, i.e.

$$\langle x\rangle \xrightarrow{QM\to CM} x \quad \langle p\rangle \xrightarrow{QM\to CM} p$$

i.e.

$$\langle p\rangle \overset{Def}{=} m\frac{\partial}{\partial t}\langle x\rangle$$

$$\begin{aligned} i\hbar\langle p\rangle &= i\hbar m\frac{\partial}{\partial t}\int x|\psi|^2dx \\ &= m\int x\left(i\hbar\frac{\partial\psi^*}{\partial t}\psi+\psi^*i\hbar\frac{\partial\psi}{\partial t}\right)dx \\ &= \frac{m\hbar^2}{2m}\int x\left(\frac{\partial^2\psi^*}{\partial x^2}\psi-\psi^*\frac{\partial^2\psi}{\partial x^2}\right)dx \end{aligned}$$

using $x\psi\frac{\partial^2\psi^*}{\partial x^2}=\frac{\partial}{\partial x}\left(x\psi\frac{\partial\psi^*}{\partial x}\right)-\psi\frac{\partial\psi^*}{\partial x}-x\frac{\partial\psi}{\partial x}\frac{\partial\psi^*}{\partial x}$

$$\begin{aligned} i\hbar\langle p\rangle &= \frac{\hbar}{2}\int\left\{\frac{\partial}{\partial x}\left[x\psi\frac{\partial\psi^*}{\partial x}-x\psi^*\frac{\partial\psi}{\partial x}\right]-\psi\frac{\partial\psi^*}{\partial x}+\psi^*\frac{\partial\psi}{\partial x}\right\}dx \\ \frac{2i}{\hbar}\langle p\rangle &= \left[x\left(\psi\frac{\partial\psi^*}{\partial x}-\psi^*\frac{\partial\psi}{\partial x}\right)\right]_{-\infty}^{\infty}+\int\left(\psi^*\frac{\partial\psi}{\partial x}-\psi\frac{\partial\psi^*}{\partial x}\right)dx \\ \langle p\rangle &= \frac{i\hbar}{2}\int\left(\psi\frac{\partial\psi^*}{\partial x}-\psi^*\frac{\partial\psi}{\partial x}\right)dx \end{aligned}$$

Conventional choice

$$\int \psi \frac{\partial \psi^*}{\partial x} dx = \int \left[\frac{\partial}{\partial x} \left(\psi \psi^* \right) - \frac{\partial \psi}{\partial x} \psi^* \right] = [|\psi|^2]_{-\infty}^{\infty} - \int \psi^* \frac{\partial \psi}{\partial x} dx$$

$$\langle p \rangle = \int \psi^* \left(-i\hbar \frac{\partial \psi}{\partial x} \right) dx$$

i.e. p can be interpreted as the operator $-i\hbar \frac{\partial}{\partial x} = \hat{p}$

3 Formulation of QM

3.1 Prescription of canonical Quantisation

$$
\begin{aligned}
x(t) &\xrightarrow{CM\to QM} \hat{x} = x \\
p(t) &\xrightarrow{CM\to QM} \hat{p} = -i\hbar\frac{\partial}{\partial x} \\
\vec{x}(t) &\xrightarrow{CM\to QM} \hat{\vec{x}} = \vec{x} \\
\vec{p}(t) &\xrightarrow{CM\to QM} \hat{\vec{p}} = -i\hbar\vec{\nabla}
\end{aligned}
$$

ONLY FOR CARTESIAN COORDINATES
Energy

$$H(t) = \frac{p^2}{2m} + V(x) \xrightarrow{CM\to QM} \hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$$

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$$

The free particle Schrödinger-equation is

$$i\hbar\frac{\partial\psi}{\partial t} = \hat{H}_0\psi \qquad \hat{H}_0 = \frac{\hat{p}^2}{2m}$$

i.e. for a particle in the field of a force with potential $V(x)$ the full Schrödinger-equation is

$$i\hbar\frac{\partial\psi}{\partial t} = \hat{H}\psi$$

In general we define the expectation value of a Quantum mechanical observable represented by the operator $\hat{A}$ by

$$\langle A\rangle = \int \psi^*(\hat{A}\psi)dx$$

3.2 Compability QM $\leftrightarrow$ CM

Does $\frac{\partial}{\partial t}\langle p\rangle = \langle F\rangle \xrightarrow{QM\to CM} \frac{\partial}{\partial t}p = F$? where $\langle F\rangle = \int \psi^*(\hat{F}\psi)dx = \int \psi^*(-\frac{\partial V}{\partial x}\psi)dx$

$$\begin{aligned}
\frac{\partial}{\partial t}\langle p\rangle &= \frac{\partial}{\partial t}\int \psi^*\left(-i\hbar\frac{\partial}{\partial x}\right)\psi dx \\
&= \left[-i\hbar\frac{\partial\psi^*}{\partial t}\frac{\partial\psi}{\partial x} - i\hbar\psi^*\frac{\partial^2\psi}{\partial t\partial x}\right]dx \\
&= \int(\hat{H}\psi^*)\frac{\partial\psi}{\partial x} - \psi^*\frac{\partial}{\partial x}(\hat{H}\psi)dx \\
&= \int\left\{\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi^* + V\psi^*\right]\frac{\partial\psi}{\partial x} - \psi^*\frac{\partial}{\partial x}\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi + V\psi\right]\right\}dx
\end{aligned}$$

$$\begin{aligned}
\text{using } \int\psi^*\frac{\partial}{\partial x}\frac{\partial^2}{\partial x^2}\psi dx &= \underbrace{\int\frac{\partial}{\partial x}\left(\psi^*\frac{\partial^2}{\partial x^2}\psi\right)dx}_{=0} - \int\frac{\partial\psi^*}{\partial x}\frac{\partial^2\psi}{\partial x^2}dx = \\
&= -\int\frac{\partial}{\partial x}\left(\frac{\partial\psi^*}{\partial x}\frac{\partial\psi}{\partial x}\right) + \int\frac{\partial^2}{\partial x^2}\psi^*\frac{\partial\psi}{\partial x}
\end{aligned}$$

$$\begin{aligned}
\frac{\partial}{\partial t}\langle p\rangle &= \int\left\{-\frac{\hbar^2}{2m}\frac{\partial^2\psi^*}{\partial x^2}\frac{\partial\psi}{\partial x} + V\psi^*\frac{\partial\psi}{\partial x} + \frac{\hbar^2}{2m}\frac{\partial^2\psi^*}{\partial x^2}\frac{\partial psi}{\partial x} - \psi^*\frac{\partial}{\partial x}(V\psi)\right\}dx = \\
&= \int\left\{V\psi^*\frac{\partial\psi}{\partial x} - \psi^*\frac{\partial V}{\partial x}\psi + V\psi^*\frac{\partial\psi}{\partial x}\right\}dx \\
&= \int\psi^*\left(-\frac{\partial V}{\partial x}\right)\psi dx
\end{aligned}$$

So $\frac{\partial}{\partial t}\langle p\rangle = \left\langle -\frac{\partial V}{\partial x}\right\rangle$ like Newton's 2nd law.

3.3 Stationary State Schrödinger Equation

For time independent potentials, seek Separable solutions:

$$\psi(x,t) = u(x)v(t)$$

$$i\hbar\frac{\partial\psi}{\partial t} = i\hbar\frac{\partial}{\partial t}(uv) = i\hbar u\frac{\partial v}{\partial t} \qquad \hat{H}\psi = v(\hat{H}u)$$

$$
\begin{aligned}
i\hbar u\frac{\partial v}{\partial t} &= v(\hat{H}u) \\
i\hbar\frac{1}{v}\frac{\partial v}{\partial t} &= \frac{1}{u}\hat{H}u \\
i\hbar\frac{d}{dt}\ln(v)(t) &= u^{-1}(\hat{H}u)(x) \\
&= const = E \\
\frac{d}{dt}\ln v &= -\frac{i}{\hbar}E \\
\ln v &= -\frac{i}{\hbar}Et \\
v &= e^{-\frac{i}{\hbar}Et}
\end{aligned}
$$

Note.

- E has dimensions of energy
- Provided $\frac{\partial V}{\partial t} = 0$, i.e. a "usual" potential
- time dependence is fixed, such that $\psi(x,t) = u(x)e^{-\frac{i}{\hbar}Et}$ and $\psi(x,t)$ is called a stationary State.

  $$\hat{H}u = Eu \tag{3.1}$$

  is called the stationary Schrödinger Equation.
- Expectation value of H, i.e. the energy

  $$
  \begin{aligned}
  \langle H\rangle &= \int \psi^*(\hat{H}\psi)dx \\
  &= \int u^* e^{\frac{i}{\hbar}Et}(\hat{H}ue^{-\frac{i}{\hbar}Et})dx \\
  &= \int u^*(\hat{H}u)dx \\
  &= \int |u|^2 E dx \\
  &= E
  \end{aligned}
  $$

  i.e. unlike p and x, E is an observable whose measurement is exact

3.4 Eigenvalues and eigenvalue equations

$$\hat{A}u = au$$

Question: Can several obserables be measured (exactly) simultaneously?

$$
\begin{aligned}
\hat{A}u &= au \\
\hat{B}u &= bu
\end{aligned}
$$

using the operators on the other equations we get

$$\hat{B}\hat{A}u = bau$$
$$\hat{A}\hat{B}u = abu$$
$$[\hat{B}\hat{A} - \hat{A}\hat{B}]u = 0$$

This has to be true for all u. We denote the condition for simultaneously observability as an operator expression (commutator brackets)

$$\hat{A}\hat{B} - \hat{B}\hat{A} = [\hat{A}, \hat{B}] = 0$$

Example.

i) Free particle, $V = 0$

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} \quad \hat{p} = -i\hbar\frac{\partial}{\partial x}$$

$$[\hat{H}, \hat{p}]f = \frac{i\hbar^3}{2m}\frac{\partial^2}{\partial x^2}\frac{\partial f}{\partial x} - \frac{i\hbar^3}{2m}\frac{\partial}{\partial x}\frac{\partial^2 f}{\partial x^2} = 0$$

energy and momentum of free particle are simultaneously observable

ii) Particle in potential $V(x) \neq 0$

$$[\hat{H}, \hat{p}]f = -i\hbar V(x)\frac{\partial f}{\partial x} + i\hbar\frac{\partial Vf}{\partial x} = fi\hbar\frac{\partial V}{\partial x}$$

i.e. in this case $[\hat{H}, \hat{p}] = -\hat{p}V \neq 0$

3.5 Canonical Commutation Relations (CCR)

Canonical Quantisation $\rightarrow \hat{x}$ and $\hat{p}$
CCR: $[\hat{x}, \hat{p}] = i\hbar$

$$[\hat{x}, \hat{p}]f = x(-i\hbar\frac{\partial f}{\partial x}) - (-i\hbar\frac{\partial}{\partial x})(xf) = i\hbar f$$

CCR $\Rightarrow \hat{x}$ and $\hat{p}$ are not simultaneously observable

3.6 Heisenberg uncertainty relation

$$\Delta x \Delta p \geq \frac{\hbar}{2}$$

$\Delta x, \Delta p$ "uncertainties":

$$(\Delta x)^2 = \langle x^2 \rangle - \langle x \rangle^2$$
$$(\Delta p)^2 = \langle p^2 \rangle - \langle p \rangle^2$$

Choice of $\langle x\rangle = \langle p\rangle = 0$.

$$(\Delta x)^2 = \left\langle x^2\right\rangle$$
$$(\Delta p)^2 = \left\langle p^2\right\rangle$$

Consider the integral

$$\begin{aligned}
I(\lambda) &= \int \left|\lambda\hbar\frac{\partial\psi}{\partial x} + x\psi\right|^2 dx \geq 0 = \\
&= \int \left(\lambda\hbar\frac{\partial\psi^*}{\partial x} + x\psi^*\right)\left(\lambda\hbar\frac{\partial\psi}{\partial x} + x\psi\right) dx = \\
&= \int \left(\lambda^2\hbar^2\frac{\partial\psi^*}{\partial x}\frac{\partial\psi}{\partial x} + \lambda\hbar x\psi\frac{\partial\psi^*}{\partial x} + \lambda\hbar x\psi^*\frac{\partial\psi}{\partial x} + x^2\psi^*\psi\right) dx = \\
&= \int \left[\lambda^2\hbar^2\frac{\partial}{\partial x}\left(\psi^*\frac{\partial\psi}{\partial x}\right) - \lambda^2\hbar^2\psi^*\frac{\partial^2\psi}{\partial x^2} + \lambda\hbar x\frac{\partial}{\partial x}|\psi|^2 + \psi^*(x^2\psi)\right] dx = \\
&= 0 + \lambda^2\int\psi^*\left(-i\hbar\frac{\partial}{\partial x}\right)^2\psi dx + 0 + \left\langle x^2\right\rangle + \lambda\hbar\int\left[\frac{\partial}{\partial x}(x|\psi|^2) - |\psi|^2\right] dx = \\
&= \lambda^2\left\langle p^2\right\rangle + \left\langle x^2\right\rangle - \lambda\hbar \\
I(\lambda) &= (\Delta p)^2\lambda^2 - \hbar\lambda + (\Delta x)^2 \geq 0
\end{aligned}$$

Quadratic in lambda and as $I(\lambda \geq 0)$ the determinant has to be ≤ 0:

$$[\hbar^2 - 4(\Delta p)^2(\Delta x)^2] \leq 0$$
$$4(\Delta p)^2(\Delta x)^2 \geq \hbar^2$$
$$\Delta x\Delta p \geq \frac{\hbar}{2}$$

$$[\hat{x},\hat{p}] = i\hbar \leftrightarrow \Delta x\Delta p \geq \frac{\hbar}{2}$$

Limiting case: $\Delta x\Delta p = \frac{\hbar}{2}$

$$\begin{aligned}
\lambda\hbar\frac{\partial\psi}{\partial x} + x\psi &= 0 \\
\frac{1}{\psi}\frac{\partial\psi}{\partial x} &= -\frac{1}{\lambda\hbar}x \\
\int\frac{\partial}{\partial x}\ln\psi dx &= -\frac{1}{\lambda\hbar}\int x dx \\
\ln\psi &\cong -\frac{x^2}{2\lambda\hbar} \\
\psi &\cong e^{-\frac{x^2}{2\sigma^2}} \quad \text{The Gaussian}
\end{aligned}$$

4 Applications

Start with 1-dimensional systems

1. Piecewise constant potential (i.e. discontinuous $V(x)$)
2. Simple Harmonic Oszillator (SHO) $V(x) = \frac{1}{2}m\omega^2 x^2$

4.1 Piecewise constant potential

4.1.1 Outstanding technical problems

- Normalisation of scattering states
- Boundary conditions for discontinuous $V(x)$

i) Scattering States
Initial State (Free particle state), Free particle $\equiv$ Superposition of plane waves

$$\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int dpa(p)e^{-\frac{i}{\hbar}(Et-px)}$$

$\langle p \rangle$ depends on $a(p)$ and has an average value, i.e. not exact. Only the plane wave

$$\psi_{plane} = e^{-\frac{i}{\hbar}(Et-px)}$$

has exact momentum

$$\hat{p}\psi_{plane} = -i\hbar \frac{\partial}{\partial x} e^{-\frac{i}{\hbar}(Et-px)} = p\psi_{plane}$$

$$\psi_{plane} = \psi_{stationary\ state} = e^{-\frac{i}{\hbar}Et} u(x)$$

Normalisation:

$$u_p(x) = e^{-\frac{i}{\hbar}Et}$$

$$\int |u_p(x)|^2 dx = \int 1 dx \to \infty$$

Not normalizable.
What happens to probability conservation i.e. $\frac{\partial}{\partial t} \int |\psi|^2 dx = 0$?

Define a probability current $\vec{J}(x,t)$ such that the continuity equation

$$\frac{\partial \rho}{\partial t} + \vec{\nabla}.\vec{J} = 0$$

is satisfied i.e. probability is conserved.

$$
\begin{aligned}
i\hbar\frac{\partial\rho}{\partial t} &= i\hbar(\frac{\partial\psi^*}{\partial\psi} + \psi^*\frac{\partial\psi}{\partial t}) = \\
&= \psi^*\hat{H}\psi - \psi\hat{\psi}^* \\
&= \psi^*(-\frac{\hbar^2}{2m}\nabla.\nabla\psi + V(x)\psi) - \psi(-\frac{\hbar^2}{2m}\nabla.\nabla\psi^* + V(x)\psi^*) = \\
&= -\frac{\hbar^2}{2m}(\psi^*\nabla.\nabla\psi - \psi\nabla.\nabla\psi^*) \\
&= -\frac{\hbar^2}{2m}\left[\nabla.(\psi^*\nabla\psi) - \nabla.(\psi\nabla\psi^*)\right] \\
\frac{\partial\rho}{\partial t} &= \frac{\hbar}{2im}\nabla.(\psi\nabla\psi^* - \psi\nabla\psi^*)
\end{aligned}
$$

i.e.

$$\frac{\partial\rho}{\partial t} + \nabla.\vec{J} = 0 \tag{4.1}$$

where $\vec{J}$ is defined by

$$\vec{J} = \frac{\hbar}{2im}(\psi^*\nabla\psi - \psi\nabla\psi^*) \tag{4.2}$$

For stationary states

$$\vec{J} = \frac{\hbar}{2im}(u^*\nabla u - u\nabla u^*)$$

in which case the continuity equation is

$$
\begin{aligned}
\frac{\partial}{\partial t}u^*u + \nabla.\vec{J} &= 0 \\
\nabla.\vec{J} &= 0
\end{aligned}
$$

ii) Boundary conditions for discontinuous $V(x)$

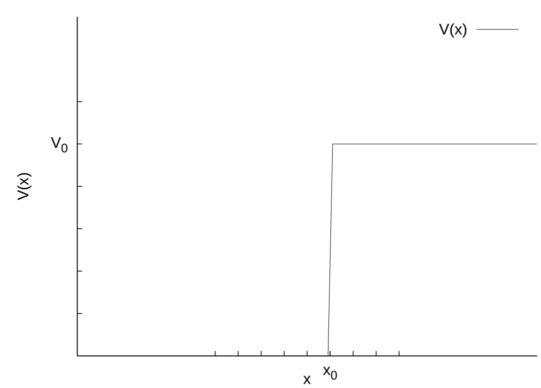


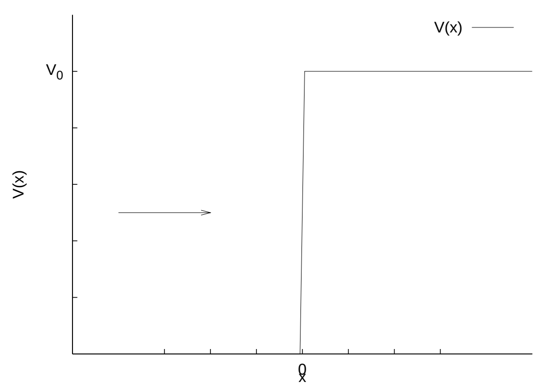
Figure 4.1: Potential with discontinuity at x_0

Starting with the 1-dim St. St. Schrödinger Equation we get

$$\hat{H}u = Eu$$
$$-\frac{\hbar^2}{2m}\frac{\partial^2 u}{\partial x^2} + Vu = Eu$$
$$u'' + \frac{2m}{\hbar^2}(E - V)u = 0$$
$$u'' + k^2 u = 0 \quad k = \frac{\sqrt{2m(E-V)}}{\hbar}$$

$V(x_0)$ is not single valued, i.e. u'' is not singlevalued. But if u' is discontinuous at x_0 $u'' \xrightarrow{x \to x_0} \infty$ i.e. $\hat{p}^2 u \to \infty$ unphysical: energy $< \infty \Rightarrow u'(x_0)$ must be continuous. Also if u is discontinuous at x_0 then $u' \xrightarrow{x \to x_0} \infty$ i.e. $\hat{p}u \to \infty$ unphysical: $\langle p \rangle < \infty$ i.e. $u(x_0)$ must be continuous

4.1.2 Scattering off a 1-dim step barrier



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

Choose initial conditions: Incoming particle wave is incident from $L \to R$ and has definite momentum p i.e.

$$\psi(x,t) = e^{-\frac{i}{\hbar}Et} u_p(x) \qquad u_p(x) = e^{\frac{i}{\hbar}px}$$

The Schrödinger equation in this case is:

$$u'' + k^2 u = 0 \quad k = \frac{\sqrt{2m(E-V)}}{\hbar} \tag{4.3}$$

- in $L, x < 0$

$$u_L'' + k_0^2 u_L = 0 \quad k_0 = \frac{\sqrt{2mE}}{\hbar}$$

i.e. $u_L \cong e^{\pm ik_0 x}$, but incoming from $L \to R$ so choose incident wave to be

$$e^{ik_0 x} \equiv e^{\frac{i}{\hbar}px}$$

General solution in L region is

$$u_L = Ae^{ik_0 x} + Re^{-ik_0 x}$$

i.e. there is a reflected wave

- in $R, x \geq 0$

$$u'' + k^2 u = 0 \quad k = \frac{\sqrt{2m(E - V_0)}}{\hbar}$$

so $u_R \cong e^{\pm ikx}$

$$u_R = Te^{ikx} + \underset{=0}{B}e^{-ikx}$$

transmitted wave only

$$\begin{aligned} u_L &= Ae^{ik_0 x} + Re^{-ik_0 x} \\ u_R &= Te^{ikx} \end{aligned}$$

Note. Plane waves are not normalizeable. One condition on A, R, T can/must be fixed arbitrarily. Natural choice: $A = 1$

1. $E > V_0$. In classical mechanics we would expect $R = 0, T \neq 0$, in QM we have both $R, T \neq 0$

$$\begin{aligned} u_L &= e^{ik_0 x} + Re^{-ik_0 x} \\ u_R &= Te^{ikx} \end{aligned}$$

$k = \frac{\sqrt{2m(E-V_0)}}{\hbar}$ real. Now impose boundary conditions

$$\begin{aligned} u_L(0) &= u_R(0) \\ 1 + R &= T \\ u'_L(0) &= u'_R(0) \\ ik_0 - ik_0 R &= Tik \\ 1 - R &= \frac{k}{k_0}T \\ 2 &= T + \frac{k}{k_0}T \end{aligned}$$

$$\begin{aligned} T &= \frac{2k_0}{k + k_0} \\ R &= \frac{k_0 - k}{k + k_0} \end{aligned}$$

2. $E < V_0$, in classical mechanics we would expect $R \neq 0, T = 0$

$$k = \frac{sqrt{-}2m(V_0 - E)}{\hbar} = \frac{i\sqrt{2m(V_0 - E)}}{\hbar} = i\kappa$$

pure imaginary

$$\begin{aligned} u_L &= e^{ik_0x} + Re^{-ik_0x} \\ u_R &= Te^{-\kappa x} \end{aligned}$$

BC:

$$\begin{aligned} u_L(0) &= u_R(0) \\ 1 + R &= T \\ u'_L(0) &= u'_R(0) \\ ik_0 - ik_0R &= -\kappa T \\ 1 - R &= \frac{i\kappa}{k_0}T \\ 2 &= T(1 + \frac{i\kappa}{k_0}) = T\left(\frac{k_0 + i\kappa}{k_0}\right) \end{aligned}$$

$$\begin{aligned} T &= \frac{2k_0}{k_0 + i\kappa} \\ R &= \frac{k_0 - i\kappa}{k_0 + i\kappa} \end{aligned}$$

$$|R|^2 = 1$$

Probability current

$$J = \frac{\hbar}{2mi}(\psi^* \nabla\psi - c.c) = \frac{\hbar}{2mi}(u^* u' - c.c.)$$

i)

$$
\begin{aligned}
J_L &= \frac{\hbar}{2im}\left\{(e^{-ik_0x}R^*e^{ik_0x})(ik_0e^{ik_0x} - ik_oRe^{-ik_0x}) - c.c.\right\} \\
&= \frac{\hbar}{2im}\left\{(ik_0)(1 - Re^{-2ik_0x} + R^*e^{2ik_0x} - |R|^2 - c.c.\right\} \\
&= \frac{\hbar}{2im}\left\{2ik_0(1-|R|^2)\right\} \\
&= \frac{\hbar}{m}k_0\{1-|R|^2\} \\
J_L &= \frac{\hbar k_0}{m}\left\{1 - \left(\frac{k_0-k}{k_0+k}\right)^2\right\} \\
&= \frac{\hbar k_0}{m}\left\{\frac{k_0^2 + 2kk_0 + k^2 - k_0^2 + 2k_0k - k^2}{(k_0+k^2)}\right\} \\
&= \frac{4\hbar k_0^2 k}{m(k_0+k)^2} \\
J_R &= \frac{\hbar}{2im}\left\{T^*e^{-ikx}T(ik)e^{ikx} - c.c.\right\} \\
&= \frac{\hbar}{2im}\left\{|T|^2 2ik\right\} \\
&= \frac{\hbar k}{m}|T|^2 \\
J_R &= \frac{\hbar k}{m}\frac{4k_0^2}{(k_0+k)^2} = J_L
\end{aligned}
$$

ii)

$$
\begin{aligned}
J_L &= \frac{\hbar k_0}{m}\left\{1-|R|^2\right\} = 0 \\
J_R &= \frac{\hbar}{2im}\left\{T^*e^{-\kappa x}T(-\kappa)e^{-\kappa x} - c.c.\right\} = 0 = J_L
\end{aligned}
$$

4.1.3 Tunneling example

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

$E < V_0$

- L: $u_L'' + k_0^2 u_L = 0$
- R: $u_R'' + k_0^2 u_R = 0$
- I: $u_I'' + k^2 u_I = 0 \quad k = \frac{i\sqrt{2m(V_0-E)}}{\hbar} = i\kappa$

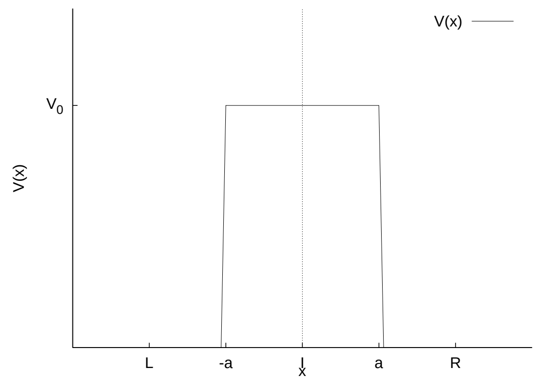


Figure 4.2: Potential step barrier for tunneling

Solutions:

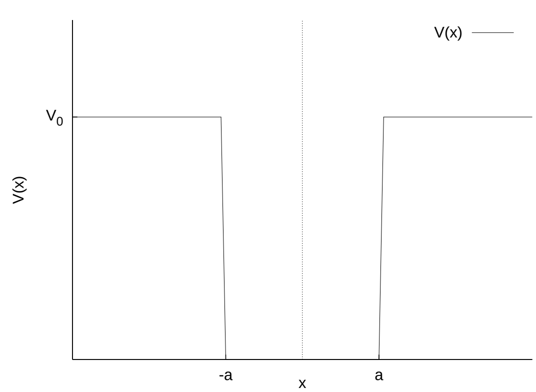
$$u_L = e^{ik_0x} + Re^{-ik_0x}$$
$$u_I = Be^{-\kappa x} + Ae^{\kappa x}$$
$$u_R = Te^{ik_0x}$$

Boundary conditions:

$$u_I(a) = u_R(a): \qquad Ae^{\kappa a} + Be^{-\kappa a} = Te^{ik_0a}$$
$$u'_I(a) = u'_R(a): \qquad \kappa(Ae^{\kappa a} - Be^{-\kappa a}) = ik_oTe^{ik_0a}$$
$$u_I(-a) = u_L(-a): \qquad Ae^{-\kappa a} + Be^{\kappa a} = e^{-ik_0a} + Re^{ik_0a}$$
$$u'_I(-a) = u'_L(-a): \qquad \kappa(Ae^{-\kappa a} - Be^{\kappa a}) = ik_o(e^{-ik_0a} - Re^{ik_0a})$$

4.1.4 Bound State system

Iniftely deep square well



$$V(x) = \begin{cases} 0 & |x| \le a \\ V_0 \to \infty & |x| > a \end{cases}$$

$$u_I'' + k_0^2 u_I = 0 \qquad k_0 = \frac{\sqrt{2mE}}{\hbar}$$

$$u_R'' - K^2 u_R = 0 \qquad K = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$$

Solutions:

$$\begin{aligned} u_I &= A\sin(k_0 x) + B\cos(k_0 x) \\ u_R &= Ce^{-Kx} + De^{Kx} \end{aligned}$$

$D = 0$ as otherwise $\psi \xrightarrow{x\to\infty} \infty$. Therefore $u_R = Ce^{-K(V_0)x} \xrightarrow{V_0\to\infty} 0$. $u_R = 0$.

Boundary conditions:

$$u_R(a) = u_I(a)$$

BUT: In 1-dim system with symmetric $V(x) = V(-x)$ $u(x) = \pm u(-x)$. As

$$\begin{aligned} (Hu)(x) &= Eu(x) \qquad H(x) = H(-x) \\ (Hu)(-x) &= Eu(-x) \\ u(-x) &= \alpha u(x) \quad u(x) = \alpha u(-x) = \alpha^2 u(x) \\ \Rightarrow \alpha &= \pm 1 \\ u(x) &= \pm u(-x) \end{aligned}$$

$$\begin{aligned} u^{(A)}(x) &= A\sin(k_0 x) \\ u^{(S)}(x) &= B\cos(k_0 x) \end{aligned}$$

Now impose the Boundary condition. For the antisymmetric case we get

$$\begin{aligned} &u^{(A)}(a) = u_R(a) = 0 \\ &\sin k_0 a = 0 \qquad \Rightarrow k_0 a = m\pi \quad m \in \mathbb{N} \\ &u_m^{(A)}(x) = A_m \sin\frac{m\pi}{a}x \end{aligned}$$

For the symmetric case we get

$$\begin{aligned} &u^{(S)}(a) = u_R(a) = 0 \\ &\cos k_0 a = 0 \qquad \Rightarrow k_0 a = n\frac{\pi}{2} \quad n \text{ odd int} \\ &u_m^{(S)}(x) = B_n \cos\frac{n\pi}{2a}x \end{aligned}$$

rewrite $u_n^{(A)} = A_n \sin \frac{n\pi}{2a}x \quad n =$even. Then

$$u_n(x) = A_n \sin \frac{n\pi}{2a}x + B_n \cos \frac{n\pi}{2a}x \tag{4.4}$$

Our boundary condition then set either $B_n = 0$ for even n or $A_n = 0$ for odd n.

$$\begin{aligned} k_0 = \frac{\sqrt{2mE}}{\hbar} &= \frac{n\pi}{2a} \\ \frac{2mE}{\hbar^2} &= \frac{n^2\pi^2}{4a^2} \\ E_n &= \frac{\hbar^2\pi^2}{8ma^2}n^2 \end{aligned}$$

Energy spectrum of bound-state system is DISCRETE!
Properties of bound state system:

1. Enery spectrum is discrete
2. Ground state energy > 0
   Lowest energy state is $n = 0$, i.e. $u_0^{(A)}(x) = A_0 \sin(0) = 0$, i.e. $|u_0^{(A)}(x)|^2 = 0$... vanishing probability ... forbidden state. $\Rightarrow$ Ground state is E_1: $u_1^{(S)} = B_1 \cos \frac{\pi}{2a}x \neq 0$
3. $V(x) = V(-x) \Rightarrow u(x) = \pm u(-x)$
4. Bound states are normalisable and mutually orthonormal

$$\int_{-\infty}^{\infty} u_n^* u_m dx = \delta_{nm}$$

$$\begin{aligned} 1 &= |A_n|^1 \int_{-a}^{a} \sin^2 \frac{n\pi}{2a}x \; dx \\ &= \frac{1}{2}|A_n|^2 \int_{-a}^{a} \left(1 - \cos \frac{n\pi}{a}x\right) dx \\ &= \frac{1}{2}|A_n|^2 \left[x - \frac{\sin \frac{n\pi}{a}x}{\frac{n\pi}{a}}\right]_{-a}^{a} \\ &= \frac{2a}{a}|A_n|^2 \\ A_n &= \frac{1}{\sqrt{a}} \\ 1 &= |B_n|^2 \int_{-a}^{a} \cos^2 \frac{n\pi}{2a}x \; dx = \\ &= \dots \\ B_n &= \frac{1}{\sqrt{a}} \end{aligned}$$

Orthonormality

$$\int_{-a}^{a} \sin\frac{n\pi}{2a}x \sin\frac{m\pi}{2a}x \; dx = \frac{1}{2}\int_{-a}^{a}\left[-\cos\frac{n+m}{2a}\pi x + \cos\frac{n-m}{2a}\pi x\right] dx$$

$$= \frac{1}{2}\left[\frac{-\sin\frac{n+m}{2a}\pi x}{\frac{n+m}{2a}\pi} + \frac{\sin n - m2a\pi x}{\frac{n-m}{2a}\pi}\right]_{-a}^{a}$$

$$= \frac{-\sin\frac{n+m}{2}\pi}{\frac{n+m}{2a}pi} + \frac{\sin n - m2\pi}{\frac{n-m}{2a}\pi}$$

$$= 0$$

as $m \neq nn$ and m, n even

$$\int_{-\infty}^{\infty} u_n^* u_m dx = \delta_{nm}$$

5. Ground state is the state with highest symmetry; with increasing energy symmetry decreases. number of nodes increases with energy

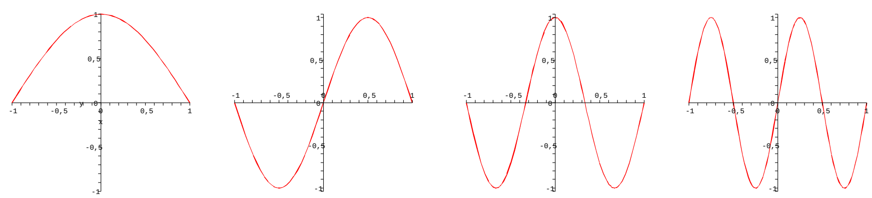
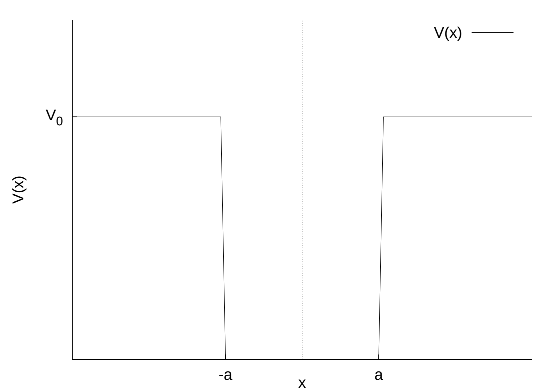


Figure 4.3: Eigenfunctions for $n = 1, 2, 3, 4$

Finitely deep square well



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

$$u_I'' + k_0^2 u_I = 0$$
$$u_R'' - K^2 u_R = 0$$

Solutions

$$u_I^{(S)} = B\cos k_0 x$$
$$u_I^{(A)} = A\sin k_0 x$$
$$u_R^{(S)} = Ce^{-Kx} \quad u_L^{(S)} = Ce^{-K|x|}$$
$$u_R^{(A)} = De^{-Kx} \quad u_L^{(A)} = -De^{-K|x|}$$

Boundary conditions:

$$u_I(a) = u_R(a)$$
$$u_I'(a) = u_R'(a)$$

1. Symmetric case

$$B\cos k_0 a = Ce^{-Ka}$$
$$-Bk_0 \sin k_0 a = -CKe^{-Ka}$$

Dividing gives

$$k_0 \tan k_0 a = K$$

$$K^2 = k_0^2 \tan^2 k_0 a$$
$$\frac{2m(V_0 - E)}{\hbar^2} = \frac{2mE}{\hbar^2} \tan^2 \frac{\sqrt{2mE}a}{\hbar}$$
$$\frac{V_0}{E} - 1 = \tan^2 \frac{\sqrt{2mE}a}{\hbar}$$
$$\frac{V_0}{E} = \frac{1}{\cos^2 \frac{\sqrt{2m}a}{\hbar}\sqrt{E}}$$
$$\frac{V_0}{\epsilon^2} = \frac{1}{\cos^2 \lambda\epsilon}$$
$$\epsilon^2 = V_0 \cos^2 \lambda\epsilon$$

This equation is only satisfied for some ϵ, i.e. discrete E. To see this we plot the two functions ϵ^2 and $\cos^2 \epsilon$ (Figure 4.4)

2. antisymmetric case

$$A\sin k_0 a = De^{-Kx}$$
$$Ak_0 \cos k_0 a = -KDe^{-Kx}$$

Dividing gives

$$k_0 \cot k_0 a = -K$$

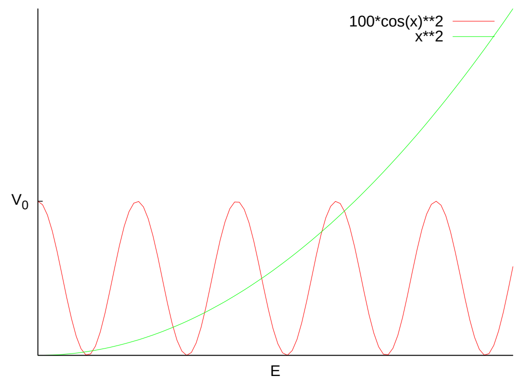


Figure 4.4: Discrete energy spectrum for symmetric case

$$
\begin{aligned}
K^2 &= k_0^2 \cot^2 k_0 a \\
\frac{V_0}{E} - 1 &= \cot^2 \frac{\sqrt{2ma}}{\hbar}\sqrt{E} \\
\frac{V_0}{\epsilon^2} &= \frac{1}{\sin^2 \lambda\epsilon} \\
\epsilon^2 &= V_0 \sin^2 \lambda\epsilon
\end{aligned}
$$

Figure 4.5 again shows the discrete energies

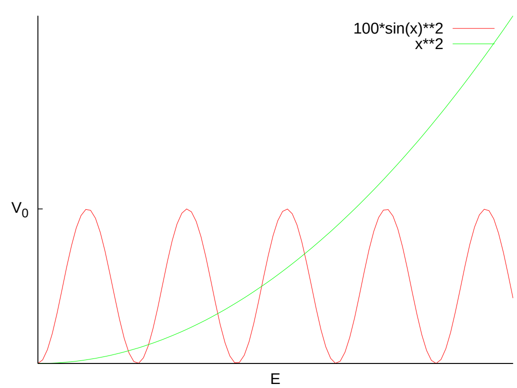


Figure 4.5: Discrete energy spectrum for assymetric case

Note the ground state is the most symmetric state:

4.2 Quantum mechanical harmonic Oscillator

$$V(x) = \frac{1}{2}kx^2 \qquad k = m\omega^2$$

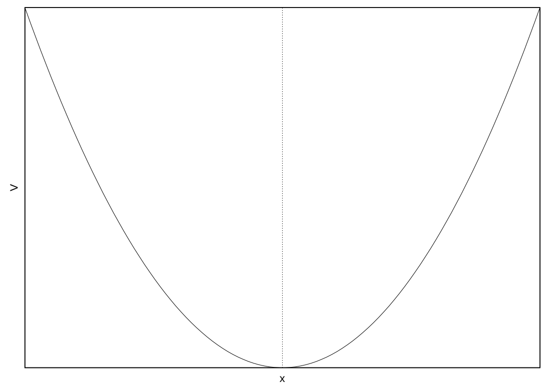


Figure 4.6: Potential for harmonic oscillator

Canonical quantisation and V being time-independent leads to Stationary State Schrödinger-equation:

$$Hu = Eu$$
$$H = \frac{\hat{p}^2}{2m} + V(x) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2 \tag{4.5}$$

4.2.1 Reduce Schrödinger equation

Seek to make the eigen-value dimensionless

$$\frac{1}{\hbar\omega}\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2\right)u = \underbrace{\frac{E}{\hbar\omega}}_{\epsilon}u$$
$$\frac{1}{2}\left(-\frac{\hbar}{m\omega}\frac{d^2}{dx^2} + \frac{m\omega}{\hbar}x^2\right)u = \epsilon u$$

Let $y = \sqrt{\frac{m\omega}{\hbar}}x$ Now we have the new Schrödinger equation

$$\left[-\frac{d^2}{dy^2} + y^2\right]u = 2\epsilon u$$
$$\left[\frac{d^2}{dy^2} - y^2\right]u = -2\epsilon u \tag{4.6}$$

4.2.2 Factorization of differential operators

"factorize" the differential operators

$$\left(\frac{d}{dy} \pm y\right)\left(\frac{d}{dy} \mp y\right)f = \frac{d^2}{dy^2}f \mp y\frac{d}{dy}f \mp f \pm y\frac{d}{dy}f - y^2 f =$$
$$= \left(\frac{d^2}{dy^2} - y^2\right)f \mp f \quad \left(\frac{d}{dy} \pm y\right)\left(\frac{d}{dy} \mp y\right) \quad = \left(\frac{d^2}{dy^2} - y^2\right) \mp 1$$

So we can express our Schrödinger equation in terms of our new factorisation:

$$\left(\frac{d}{dy}+y\right)\left(\frac{d}{dy}-y\right)u_n = -(2\epsilon_n+1)u_n \tag{4.7}$$

$$\left(\frac{d}{dy}-y\right)\left(\frac{d}{dy}+y\right)u_n = -(2\epsilon_n-1)u_n \tag{4.8}$$

where n is a quantum number.

4.2.3 Eigenvalues

Act on (4.7) with $\left(\frac{d}{dy}-y\right)$ and on (4.8) with $\left(\frac{d}{dy}+y\right)$:

$$\left(\frac{d}{dy}-y\right)\left(\frac{d}{dy}+y\right)\left[\left(\frac{d}{dy}-y\right)u_n\right] = -(2\epsilon_n+1)\left[\left(\frac{d}{dy}-y\right)u_n\right] \tag{4.9}$$

$$\left(\frac{d}{dy}+y\right)\left(\frac{d}{dy}-y\right)\left[\left(\frac{d}{dy}+y\right)u_n\right] = -(2\epsilon_n-1)\left[\left(\frac{d}{dy}+y\right)u_n\right] \tag{4.10}$$

(4.9) and (4.10) are Schrödinger equations too, but for different functions

$$u_m \propto \left(\frac{d}{dy}-y\right)u_n \tag{4.11}$$

Find the corresponding eigenvalue by identifying (4.9) with (4.8). So we get $2\epsilon_m - 1 = 2\epsilon_n + 1$

$$\epsilon_m = \epsilon_n + 1 \tag{4.12}$$

The same for (4.10) and (4.7) yields

$$u_m \propto \left(\frac{d}{dy}+y\right)u_n \tag{4.13}$$

and

$$\epsilon_m = \epsilon_n - 1 \tag{4.14}$$

So by using $\left(\frac{d}{dy}-y\right)$ and $\left(\frac{d}{dy}+y\right)$ we can jump between our eigen-functions.

$$\left(\frac{d}{dy}-y\right) \qquad \text{raising operator} \tag{4.15}$$

$$\left(\frac{d}{dy}+y\right) \qquad \text{lowering operator} \tag{4.16}$$

From this we deduce, that our eigen-values have to obey

$$\epsilon_n = \epsilon_0 + n \tag{4.17}$$

4.2.4 Eigenfunctions

When lowering operator acts on u_0 it annihilates it

$$\left(\frac{d}{dy} + y\right) u_0 = 0 \tag{4.18}$$

$$\begin{aligned}
\int \frac{1}{u_0} du_0 &= -\int y dy \\
\ln u_0 &\cong -\frac{1}{2} y^2 \\
u_0 &\cong e^{-\frac{1}{2}y^2}
\end{aligned}$$

Write (4.8) for $n = 0$:

$$\begin{aligned}
0 &= -(2\epsilon_0 - 1) u_0 \\
\epsilon_0 &= \frac{1}{2} \\
\epsilon_n &= n + \frac{1}{2}
\end{aligned}$$

$$E_n = \left(n + \frac{1}{2}\right) \hbar\omega \tag{4.19}$$

Properties of bound states:

1. Discrete energy spectrum: $\epsilon_n = n + \frac{1}{2}$
2. Ground state energy > 0: $\epsilon_0 = \frac{1}{2}$
3. $V(x) = V(-x) \Rightarrow u(x) = \pm u(-x)$

$$\begin{aligned}
u_0(y) &= u_0(-y) \\
u_1 &\cong \left(\frac{d}{dy} - y\right) u_0 \\
\Rightarrow u_1(y) &= -u_1(-y) \\
u_2(y) &= u_2(-y)
\end{aligned}$$

4. $\int u_n^* u_m = \delta_{mn}$ mutually orthonormal

$$
\begin{aligned}
u_1 &= A_1 \left(\frac{d}{dy} - y \right) e^{-\frac{1}{2}y^2} \\
&= A_1 \left(-ye^{-\frac{1}{2}y^2} - ye^{-\frac{1}{2}y^2} \right) \\
&= -2A_1 y e^{-\frac{1}{2}y^2} \\
u_2 &= -A_2 \left(\frac{d}{dy} - y \right) ye^{-1\frac{1}{2}y^2} \\
&= -A_2 \left(e^{-\frac{1}{2}y^2} - y^2 e^{-\frac{1}{2}y^2} - y^2 e^{-\frac{1}{2}y^2} \right) \\
&= A_2 (2y^2 - 1) e^{-\frac{1}{2}y^2} \\
& etc
\end{aligned}
$$

Normalise:

$$
\begin{aligned}
\int |u_0|^2 dy &= A_0^2 \int_{-\infty}^{\infty} e^{-y^2} dy = A_0^2 \sqrt{\pi} \\
\int |u_1|^2 dy &= A_1^2 \int_{-\infty}^{\infty} y^2 e^{-y^2} dy = -\frac{1}{2} \int y \frac{d}{dy} e^{-y^2} dy \\
&= -\frac{1}{2} \left[ye^{-y^2} \Big|_{-\infty}^{\infty} - \int e^{-y^2} dy \right] \\
&= \frac{\sqrt{\pi}}{2} A_1^2
\end{aligned}
$$

Orthogonality

$$
\begin{aligned}
&\int u_0^* u_1 dy = \int_{-\infty}^{\infty} e^{-\frac{1}{2}y^2} ye^{-\frac{1}{2}y^2} dy = \int ye^{-y^2} = 0 \\
&\int u_m^* u_n dy = 0 \quad \text{if } n = odd/even \ m = even/odd \\
&\int u_0^* u_2 dy = A_0 A_2 \int (2y^2 - 1) e^{-y^2} dy = A_0 A_2 \left(2\frac{\sqrt{\pi}}{2} - \sqrt{\pi} \right) = 0
\end{aligned}
$$

5. Number of nodes increases with ϵ_n, see Figure 4.7

4.3 General properties of Quantum mechanical states

(States are solutions of eigenvalue equation)

1. Orthonormal (immediately/manifest for bound state) e.g. for Scattering: $\int u_p^*(x) u_{p'}(x) dx = \delta(p - p')$
2. a) Energy (and all other observables') eigenstates are real
   b) all expectation values are also real

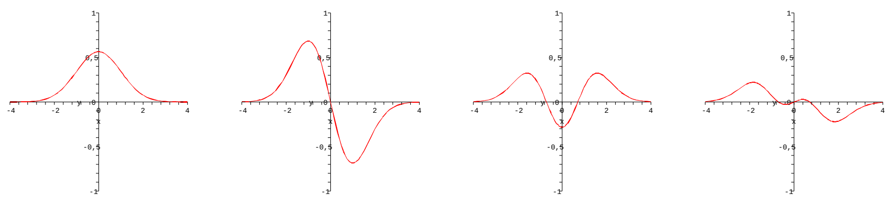


Figure 4.7: Eigenfunctions for Simple Harmonic Oszillator for $n = 0, 1, 2, 3$

5 New Formalism (Hilbert space)

- QM state functions are elements of a (finite or infinite) dimensional space $\mathcal{H}$
- $\mathcal{H}$ is spanned by an orthonormal basis $u_n(x)$ or $u_p(x)$

$$\int u_n^*(x)u_m(x)dx = \delta_{mn} \tag{5.1}$$

$$\int u_p^*(x)u_k(x)dx = \delta_D(p-k) \tag{5.2}$$

A general state is

$$\psi(x) = \sum_n c_n u_n(x) \qquad \text{or} \tag{5.3}$$

$$\psi(x) = \int c_p u_p(x)dp \tag{5.4}$$

- Definition of an inner product in $\mathcal{H}$

$$\langle\psi,\phi\rangle = \int \psi^*(x)\phi(x)dx \tag{5.5}$$

It has no geometric meaning. The Schwarz inequality holds:

$$\langle\psi,\psi\rangle\langle\phi,\phi\rangle \geq |\langle\psi,\phi\rangle|^2$$

Definition of matrix element of an operator

$$A_{mn} = \langle u_m, Au_n\rangle = \int u_m^*(\hat{A}u_n)dx \tag{5.6}$$

More generally $\langle\psi, A\phi\rangle = \int \psi^*\hat{A}\phi$

5.1 Hermiticity

Physical measurements must be real, i.e. expectation value of an operator representing an observable must be real. For a Hermitian operator holds:

$$\langle\psi, A\psi\rangle = \langle A\psi, \psi\rangle \tag{5.7}$$

Stronger condition of Hermiticity. $\psi, \phi \in \mathcal{H}$

$$\langle\psi, A\phi\rangle = \langle A\psi, \phi\rangle \tag{5.8}$$

Both conditions are equivalent: 1) $\Rightarrow$ 2) clear; 2) $\Rightarrow$ 1): $\psi, \phi \in \mathcal{H} \Rightarrow (\psi + \lambda\phi) \in \mathcal{H}$

$$\begin{aligned}
\langle \psi + \lambda\phi, A(\psi + \lambda\phi) \rangle - avA(\psi + \lambda\phi), \psi + \lambda\phi = 0 \\
\langle \psi, A\psi \rangle + \lambda \langle \psi, A\phi \rangle + \lambda^* \langle \phi, A\psi \rangle + |\lambda|^2 \langle \phi, A\phi \rangle - \\
- \langle A\psi, \psi \rangle - \lambda \langle A\psi, \phi \rangle - \lambda^* \langle A\phi, \psi \rangle - |\lambda|^* \langle A\phi, \phi \rangle = 0 \\
\lambda \left(\langle \psi, A\phi \rangle - \langle A\psi, \phi \rangle \right) + \lambda^* \left(\langle \phi, A\psi \rangle - \langle A\phi, \psi \rangle \right) = 0
\end{aligned}$$

As λ is arbitrary and λ and λ^* are in general linearly independent:

$$\begin{aligned}
\langle \psi, A\phi \rangle - \langle A\psi, \phi \rangle = 0 \\
\langle \phi, A\psi \rangle - \langle A\phi, \psi \rangle = 0
\end{aligned}$$

and therefore

$$\langle \psi, A\phi \rangle = \langle A\psi, \phi \rangle$$

If operator is not Hermitian this defines the Hermitian conjugate:

$$\langle \psi, A\psi \rangle = \left\langle A^\dagger \psi, \psi \right\rangle$$

Examples: $\hat{x}, \hat{p}, \hat{H}$

1. $\langle x \rangle = \int \psi^* x \psi dx = \langle x \rangle^*$

2. $$\begin{aligned}
\langle p \rangle &= \int \psi^* (\hat{p}\psi) dx = \int \psi^* \left(-i\hbar \frac{\partial}{\partial x} \psi \right) dx \\
\langle p \rangle^* &= \left(\int \psi^* \left(-i\hbar \frac{\partial}{\partial x} \psi \right) dx \right)^* = \int \psi \left(-i\hbar \frac{\partial}{\partial x} \psi \right)^* dx = \int i\hbar \frac{\partial \psi^*}{\partial x} \psi dx = \\
&= \int i\hbar \frac{\partial}{\partial x} |\psi|^2 dx - \int i\hbar \psi^* \frac{\partial \psi}{\partial x} dx = \langle p \rangle
\end{aligned}$$

3. $\hat{H} = \frac{\hat{p}^2}{2m} + V(x)$ and therefore hermitian

examples of non-hermitian Operator: the raising/lowering operator

$$A = \sqrt{\frac{\hbar}{m}} \frac{d}{dx} \mp \sqrt{\frac{m\omega}{\hbar}} x = \frac{d}{dy} \mp y$$

Hermitian conjugate:

$$\begin{aligned}
\left\langle A^\dagger\psi,\phi\right\rangle &= \langle\psi,A\phi\rangle = \\
&= \int\psi^*\left(\frac{d\phi}{dy}\mp x\phi\right)dx = \\
&= \int\psi^*\frac{d\phi}{dx}dx\mp\int(x\psi)^*\phi dx = \\
&= \int\frac{d}{dx}(\psi^*\phi)-\int\frac{d\psi^*}{dx}\phi dx\mp\int(x\psi)^*\phi dx \\
&= \int\left(\left(-\frac{d}{dx}\mp x\right)\psi\right)^*\phi dx \\
&= \left\langle\left(-\frac{d}{dx}\mp x\right)\psi,\phi\right\rangle
\end{aligned}$$

i.e. $A^\dagger = -\frac{d}{dx}\mp x \neq \frac{d}{dx}\mp x = A$
Hermitian conjugate of a matrix:

$$\left\langle e_{(\alpha)}, Me_{(\beta)}\right\rangle = \left\langle Me_{(\alpha)}, e_{(\beta)}\right\rangle \Rightarrow M^\dagger = (M^T)^*$$

5.2 Dirac's Notation

$$\begin{aligned}
,\psi \to |\psi\rangle &\quad \text{ket} \\
\psi, = \psi^* \to \langle\psi| &\quad \text{bra}
\end{aligned}$$

bra-ket $= \langle\psi|\phi\rangle$

$$\begin{aligned}
u_n &\to |n\rangle \\
u_n^* &\to \langle n|
\end{aligned}$$

5.3 Completness

$$\sum_\alpha e_i^{(\alpha)}\bar{e}_j^{(\alpha)} = \delta_{ij}$$

$$\sum_n u_n u_n^* = \mathbf{1}$$
$$\sum_n |n\rangle\langle n| = \mathbf{1} \tag{5.9}$$

5.4 Preparation for Matrix mechanics, Operators

Harmonic Oszillator:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2$$

We had the raising (and lowering) operator:

$$\begin{aligned}
\frac{d}{dy} - y &= \sqrt{\frac{\hbar}{\omega m}}\frac{d}{dx} - \sqrt{\frac{m\omega}{\hbar}}x = \\
&= \frac{i}{\hbar}\sqrt{\frac{\hbar}{m\omega}}\hat{p} - \sqrt{\frac{m\omega}{\hbar}}\hat{x} = \\
&= \sqrt{\frac{m\omega}{\hbar}}\left(\frac{i}{m\omega}\hat{p} - \hat{x}\right)
\end{aligned}$$

Define new operators:

$$a = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i}{m\omega}\hat{p}\right) \qquad \text{lowering operator} \tag{5.10}$$

$$a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - \frac{i}{m\omega}\hat{p}\right) \qquad \text{raising operator} \tag{5.11}$$

a and $a^\dagger$ are up to sign and const the lowering and raising operators respectively.

$$\begin{aligned}
\left[a, a^\dagger\right] &= \frac{m\omega}{2\hbar}\left[\left(\hat{x} + \frac{i}{m\omega}\hat{p}\right), \left(\hat{x} - \frac{i}{m\omega}\hat{p}\right)\right] = \\
&= \frac{m\omega}{2\hbar}\left(0 - \frac{i}{m\omega}[\hat{x}, \hat{p}] + \frac{i}{m\omega}[\hat{p}, \hat{x}] + 0\right) = \\
&= \frac{m\omega}{2\hbar}\frac{-2i}{m\omega}[\hat{x}, \hat{p}] = \\
&= \frac{-i}{\hbar}(i\hbar) = 1
\end{aligned}$$

$$\left[a, a^\dagger\right] = 1 \tag{5.12}$$

$$\begin{aligned}
aa^\dagger &= \frac{m\omega}{2\hbar}\left(\hat{x} + \frac{i}{m\omega}\hat{p}\right)\left(\hat{x} - \frac{i}{m\omega}\hat{p}\right) = \\
&= \frac{m\omega}{2\hbar}\left(\hat{x}^2 - \frac{i}{m\omega}[\hat{x}, \hat{p}] - \frac{i^2}{m^2\omega^2}\hat{p}^2\right) = \\
&= \frac{m\omega}{2\hbar}\left(\frac{\hat{p}^2}{m^2\omega^2} + \hat{x}^2 - \frac{i^2\hbar}{m\omega}\right) = \\
&= \frac{1}{\hbar\omega}\left\{\frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 + \frac{\hbar\omega}{2}\right\}
\end{aligned}$$

So therefore

$$aa^\dagger\hbar\omega = \hat{H} + \frac{\hbar\omega}{2}$$

analogue we get

$$a^\dagger a\hbar\omega = \hat{H} - \frac{\hbar\omega}{2}$$

$$\left(aa^\dagger - \frac{1}{2}\right) u_n = \epsilon u_n \tag{5.13}$$

$$\left(a^\dagger a + \frac{1}{2}\right) u_n = \epsilon u_n \tag{5.14}$$

i) Act on au_n

$$\begin{aligned}\left(aa^\dagger - \frac{1}{2}\right) au_n &= a(a^\dagger a)u_n - \frac{1}{2}au_n = \\ &= a(aa^\dagger - \left[a, a^\dagger\right])u_n - \frac{1}{2}au_n = \\ &= a(aa^\dagger - 1)u_n - \frac{1}{2}au_n = \\ &= a(aa^\dagger - \frac{1}{2})u_n - au_n = \\ &= \epsilon_n au_n - au_n = (\epsilon_n - 1)(au_n)\end{aligned}$$

i.e. the eigenvalue of au_n is $\epsilon - 1$

ii) Act on $a^\dagger$

$$\begin{aligned}\left(a^\dagger a + \frac{1}{2}\right) a^\dagger u_n &= a^\dagger(aa^\dagger)u_n + \frac{1}{2}a^\dagger u_n = \\ &= a^\dagger(a^\dagger a + 1)u_n + \frac{1}{2}a^\dagger u_n = \\ &= a^\dagger(a^\dagger a + \frac{1}{2})u_n + a^\dagger u_n = \\ &= a^\dagger \epsilon_n u_n + a^\dagger u_n = \\ &= (\epsilon_n + 1)(a^\dagger u_n)\end{aligned}$$

i.e $a^\dagger u_n$ has eigenvalue $\epsilon_n + 1$

iii) $(a^\dagger a + \frac{1}{2})u_0 = \epsilon_0 \Rightarrow \epsilon_0 = \frac{1}{2}$ and $\epsilon_n = n + \frac{1}{2}$

Calculate the scaling factors for the raising and lowering operators.

$$au_n = \kappa_n^- u_{n-1}$$
$$a^\dagger u_n = \kappa_n^+ u_{n+1}$$

Take the inner product

$$\begin{aligned}\langle au_n, au_n\rangle &= \left\langle \kappa_n^- u_{n-1}, \kappa_n^- u_{n-1}\right\rangle = |\kappa_n^-|^2\\ \left\langle a^\dagger u_n, a^\dagger u_n\right\rangle &= \left\langle \kappa_n^+ u_{n+1}, \kappa_n^+ u_{n+1}\right\rangle = |\kappa_n^+|^2\\ \left\langle u_n, a^\dagger a u_n\right\rangle &= |\kappa_n^-|^2\\ \left\langle u_n, a a^\dagger u_n\right\rangle &= |\kappa_n^+|^2\end{aligned}$$

But $\left(aa^\dagger - \frac{1}{2}\right) u_n = (n+\frac{1}{2})u_n$ and $\left(a^\dagger a + \frac{1}{2}\right) u_n = (n+\frac{1}{2})u_n$

$$\begin{aligned}|\kappa_n^-|^2 &= \langle u_n, n u_n\rangle = n\\ |\kappa_n^+|^2 &= \langle u_n, (n+1) u_n\rangle = n+1\end{aligned}$$

$$au_n = \sqrt{n}u_{n-1} \tag{5.15}$$

$$a^\dagger u_n = \sqrt{n+1}u_{n+1} \tag{5.16}$$

Repeat this calculation in Dirac notation:

$$\begin{aligned}a\left|n\right\rangle &= \kappa_n^- \left|n-1\right\rangle\\ a^\dagger\left|n\right\rangle &= \kappa_n^+ \left|n+1\right\rangle\end{aligned}$$

Take inner product:

$$\begin{aligned}\left\langle n\right| a^\dagger a \left|n\right\rangle &= |\kappa_n^-|^2 \left\langle n-1|n-1\right\rangle = |\kappa_n^-|^2\\ \left\langle n\right| a a^\dagger \left|n\right\rangle &= |\kappa_n^+|^2 \left\langle n+1|n+1\right\rangle = |\kappa_n^+|^2\end{aligned}$$

$$\begin{aligned}\left(aa^\dagger - \frac{1}{2}\right)\left|n\right\rangle &= (n + \frac{1}{2}\left|n\right\rangle\\ \left(a^\dagger + \frac{1}{2}\right)\left|n\right\rangle &= (n + \frac{1}{2}\left|n\right\rangle\end{aligned}$$

$$\begin{aligned}|\kappa_n^-|^2 &= (n)\left\langle n|n\right\rangle\\ |\kappa_n^+|^2 &= (n+1)\left\langle n|n\right\rangle\end{aligned}$$

Fock space

6 Matrix Mechanics

QM formulated as wave-mechanics (particles $\leftrightarrow$ waves), operator representation of observables.
But operators can be employed also abstractly! Also they can be represented by matrices. The Matrix element of an operator was defined as

$$A_{mn} = \langle u_m, A u_n \rangle$$

If A satisfies an eigen-value equation, i.e. $Au_n = a_n u_n$ we get: $A_{mn} = a_n \delta_{mn}$
N.B. much more useful when spectrum of eigenvalues is discrete

6.1 Properties of operators

$\langle A \rangle$ is real if A is hermitian, i.e. if $A = A^\dagger$. If A is hermitian it can be diagonalised (i.e. the eigen-functions and eigen-values be found). If A is not hermitian, then $\langle \psi, A\phi \rangle = \left\langle A^\dagger \psi, \phi \right\rangle$. The hermitian conjugate of a matrix element is

$$(A^\dagger)_{mn} = \left\langle u_m, A^\dagger u_n \right\rangle = \langle A u_m, u_n \rangle = \langle u_n, A u_m \rangle^* = ((A^*)^T)_{mn})$$

6.2 Re-calculation of some result

6.2.1 QM Harmonic Oscillator

$$\begin{aligned} H &= \hbar\omega(aa^\dagger - \tfrac{1}{2}) \\ &= \hbar\omega(a^\dagger a + \tfrac{1}{2}) \\ \left[a, a^\dagger\right] &= 1 \end{aligned}$$

Solve the eigenvalue problem

$$(aa^\dagger - \tfrac{1}{2}) u_n = \epsilon_n u_n$$

From before:

$$\epsilon_n = n + \frac{1}{2}$$

and for the raising and lowering operators:

$$\begin{aligned} a u_n &= \sqrt{n} u_{n-1} \\ a^\dagger &= \sqrt{n+1} u_{n+1} \end{aligned}$$

Matrix Representation of $H, a, a^\dagger$

$$H_{mn} = \langle u_m, Hu_n \rangle = \langle u_m, E_n u_n \rangle = \hbar\omega(n + \frac{1}{2})\delta_{mn}$$

$$H = \hbar\omega \begin{bmatrix} \frac{1}{2} & & & \\ & \frac{3}{2} & & 0 \\ & & \frac{5}{2} & \\ & 0 & & \ddots \end{bmatrix} \tag{6.1}$$

$$a_{mn} = \langle u_m, au_n \rangle = \left\langle u_m, \sqrt{n}u_{n-1} \right\rangle = \sqrt{n}\delta_{m,n-1}$$

$$a = \begin{bmatrix} 0 & \sqrt{1} & 0 & & \\ & 0 & \sqrt{2} & 0 & \\ & & 0 & \sqrt{3} & 0 \\ & & & 0 & \ddots \end{bmatrix} \tag{6.2}$$

$$a^\dagger = \sqrt{n+1}\delta_{m,n+1}$$

$$a^\dagger = \begin{bmatrix} 0 & & & & \\ \sqrt{1} & 0 & & & \\ 0 & \sqrt{2} & 0 & & \\ & 0 & \sqrt{3} & 0 & \\ & & 0 & \ddots & \end{bmatrix} \tag{6.3}$$

What about eigen-functions?

eigen-functions $\rightarrow$ eigen-vectors

$$u_0 = \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix} \qquad u_1 = \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix} \qquad \cdots$$

$$\langle u_n, u_m \rangle = \delta_{nm}$$

6.2.2 Infinitely deep square well

$$Hu_n = \frac{\hbar^2\pi^2}{8ma^2}n^2 u_n$$

$$H_{mn} = \langle u_m, Hu_n \rangle = \frac{\hbar^2\pi^2}{8ma^2}n^2\delta_{mn}$$

$$H = \frac{\hbar^2\pi^2}{8ma^2} \begin{bmatrix} 1 & & & \\ & 4 & & 0 \\ & & 9 & \\ & 0 & & \ddots \end{bmatrix} \tag{6.4}$$

6.3 Outlook

When are matrix representations indispensible? When describing intrinsic angular momentum $\equiv$ spin (no classical analogue), otherwise cannot go beyond orbital angular momentum (Orbital has classical analogue).