CM332C – Introductory Quantum Theory
Compact Lecture Notes and Exercises

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$$i\hbar\frac{\partial}{\partial t}\Psi = -\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\Psi + V\Psi$$

'While it is never safe to affirm that the future of the Physical Sciences has no marvels in store even more astonishing than those of the past, it seems probable that *most of the grand unifying principles have been firmly established and that further advances are to be sought chiefly in the rigorous application of these principles to all the phenomena which come under our notice*' .... '*the future truths of Physical Science are to be looked for in the sixth place of decimals*'.

A.A. Michelson, Chicago, 1894

1. Historical Background

1.1. Classical Physics Around 1900

1.1.1. Newtonian Mechanics

- Position and momentum: $\boldsymbol{x} = (x_1, \ldots, x_N)$, $\boldsymbol{p} = (p_1, \ldots, p_N)$
  Hamilton's equations:

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2m_i} + V(\boldsymbol{x}) : \qquad \frac{dx_i}{dt} = \frac{\partial H}{\partial p_i} \qquad \frac{dp_i}{dt} = -\frac{\partial H}{\partial x_i}$$

- Poisson brackets for functions $A(\boldsymbol{x}, \boldsymbol{p})$ and $B(\boldsymbol{x}, \boldsymbol{p})$:

$$(A, B) \equiv \sum_{i=1}^{N} \left\{ \frac{\partial A}{\partial x_i}\frac{\partial B}{\partial p_i} - \frac{\partial A}{\partial p_i}\frac{\partial B}{\partial x_i} \right\} = \boldsymbol{\nabla_x} A \cdot \boldsymbol{\nabla_p} B - \boldsymbol{\nabla_p} A \cdot \boldsymbol{\nabla_x} B$$

  Properties:

$$(A, B) = -(B, A) \qquad \text{hence also } (A, A) = 0$$
$$(A, \lambda_1 B + \lambda_2 C) = \lambda_1 (A, B) + \lambda_2 (A, C)$$
$$(AB, C) = (A, C)B + A(B, C)$$

  Examples:

$$(x_i, x_j) = \boldsymbol{\nabla_x} x_i \cdot \mathbf{0} - \mathbf{0} \cdot \boldsymbol{\nabla_x} x_j = 0$$
$$(p_i, p_j) = \mathbf{0} \cdot \boldsymbol{\nabla_p} p_i - \boldsymbol{\nabla_p} p_j \cdot \mathbf{0} = 0$$
$$(x_i, p_j) = \boldsymbol{\nabla_x} x_i \cdot \boldsymbol{\nabla_p} p_j = \sum_{\ell} \delta_{i\ell}\delta_{j\ell} = \delta_{ij}$$

- Evolution of functions $f(\boldsymbol{x}, \boldsymbol{p}, t)$ in terms of Poisson brackets:

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + (f, H)$$

  Proof:

$$\begin{aligned} \frac{\partial f}{\partial t} + (f, H) &= \frac{\partial f}{\partial t} + \boldsymbol{\nabla_x} f \cdot \boldsymbol{\nabla_p} H - \boldsymbol{\nabla_p} f \cdot \boldsymbol{\nabla_x} H \\ &= \frac{\partial f}{\partial t} + \boldsymbol{\nabla_x} f \cdot \frac{d\boldsymbol{x}}{dt} + \boldsymbol{\nabla_p} f \cdot \frac{d\boldsymbol{p}}{dt} = \frac{df}{dt} \end{aligned}$$

  Examples:

$$\frac{dx_i}{dt} = (x_i, H) = \boldsymbol{\nabla_x} x_i \cdot \boldsymbol{\nabla_p} H = \frac{\partial H}{\partial p_i}$$
$$\frac{dp_i}{dt} = (p_i, H) = -\boldsymbol{\nabla_p} p_i \cdot \boldsymbol{\nabla_x} H = -\frac{\partial H}{\partial x_i}$$
$$\frac{dH}{dt} = (H, H) = 0$$

1.1.2. Maxwell Theory

- Electric and magnetic fields on $\boldsymbol{x} \in \mathbb{R}^3$: $\boldsymbol{E}(\boldsymbol{x},t)$ and $\boldsymbol{B}(\boldsymbol{x},t)$ (both $\in \mathbb{R}^3$)
  Electric charge density and current density (due to particles at $\boldsymbol{x}_i$ with charge e_i):
  $$\rho(\boldsymbol{x},t) = \sum_i e_i \delta[\boldsymbol{x} - \boldsymbol{x}_i(t)] \quad (\in \mathbb{R})$$
  $$\boldsymbol{j}(\boldsymbol{x},t) = \sum_i e_i \frac{d\boldsymbol{x}_i}{dt} \delta[\boldsymbol{x} - \boldsymbol{x}_i(t)] \quad (\in \mathbb{R}^3)$$
  Maxwell equations:
  $$\boldsymbol{\nabla} \times \boldsymbol{E} + \frac{1}{c}\frac{\partial \boldsymbol{B}}{\partial t} = \boldsymbol{0} \qquad \boldsymbol{\nabla} \cdot \boldsymbol{B} = 0$$
  $$\boldsymbol{\nabla} \times \boldsymbol{B} - \frac{1}{c}\frac{\partial \boldsymbol{E}}{\partial t} = \frac{4\pi}{c}\boldsymbol{j} \qquad \boldsymbol{\nabla} \cdot \boldsymbol{E} = 4\pi\rho$$
- Effects of electro-magnetic fields on charged particle at $\boldsymbol{x}_i \in \Re^3$ with momentum $\boldsymbol{p}_i \in \Re$:
  $$\boldsymbol{E} = -\boldsymbol{\nabla}\phi - \frac{1}{c}\frac{\partial \boldsymbol{A}}{\partial t}, \qquad \boldsymbol{B} = \boldsymbol{\nabla} \times \boldsymbol{A}$$
  $$V \to V + e_i\phi(\boldsymbol{x}_i), \qquad \boldsymbol{p}_i \to \boldsymbol{p}_i - \frac{e_i}{c}\boldsymbol{A}$$
  with $\phi(\boldsymbol{x},t)$ ($\in \mathbb{R}$) and $\boldsymbol{A}(\boldsymbol{x},t)$ ($\in \mathbb{R}^3$)

1.1.3. Extensions, Properties, Range of Verification

- Light: electro-magnetic waves with speed c, carried by an 'ether'
- Laws for solids, liquids, gases: derived from above ('statistical mechanics')
- Coordinates $\{x_i, p_i\}$ can in principle have *any* real value
- First order differential equations and partial differential equations:
  the present in principle determines the future, to unlimited accuracy
- Distance scales (experimentally accessible in 1900: $\star$):

10^{13} m	size of the solar system	–
10^{9} m	diameter of Saturn	–
10^{6} m	London – Rome	–
10^{3} m	King's – Trafalgar Square	$\star$
$10^{0} - 10^{-2}$ m	macroscopic scale	$\star$
10^{-5} m	cells	$\star$
10^{-8} m	large molecules (e.g. proteins)	–
10^{-10} m	atoms	–
10^{-15} m	atomic nuclei	–

- Two main scientific revolutions of 20th century:
  relativity theory (1905), initially for large scales, later also small scales
  quantum mechanics (1925), initially for small scales, later also large scales

1.2. The Three Main Clouds on the Horizon

1.2.1. *Black-body Radiation (1860, Kirchhof)*

- Electro-magnetic radiation inside a cavity with a (partially) absorbing interior ('black-body surface')
- Power distribution over radiation frequencies depends *only* on temperature T; not on shape or material of cavity
- Classical theory: intensity must increase monotonically with frequency (i.e. intensity $\uparrow \infty$ as wavelength $\downarrow 0$) ...

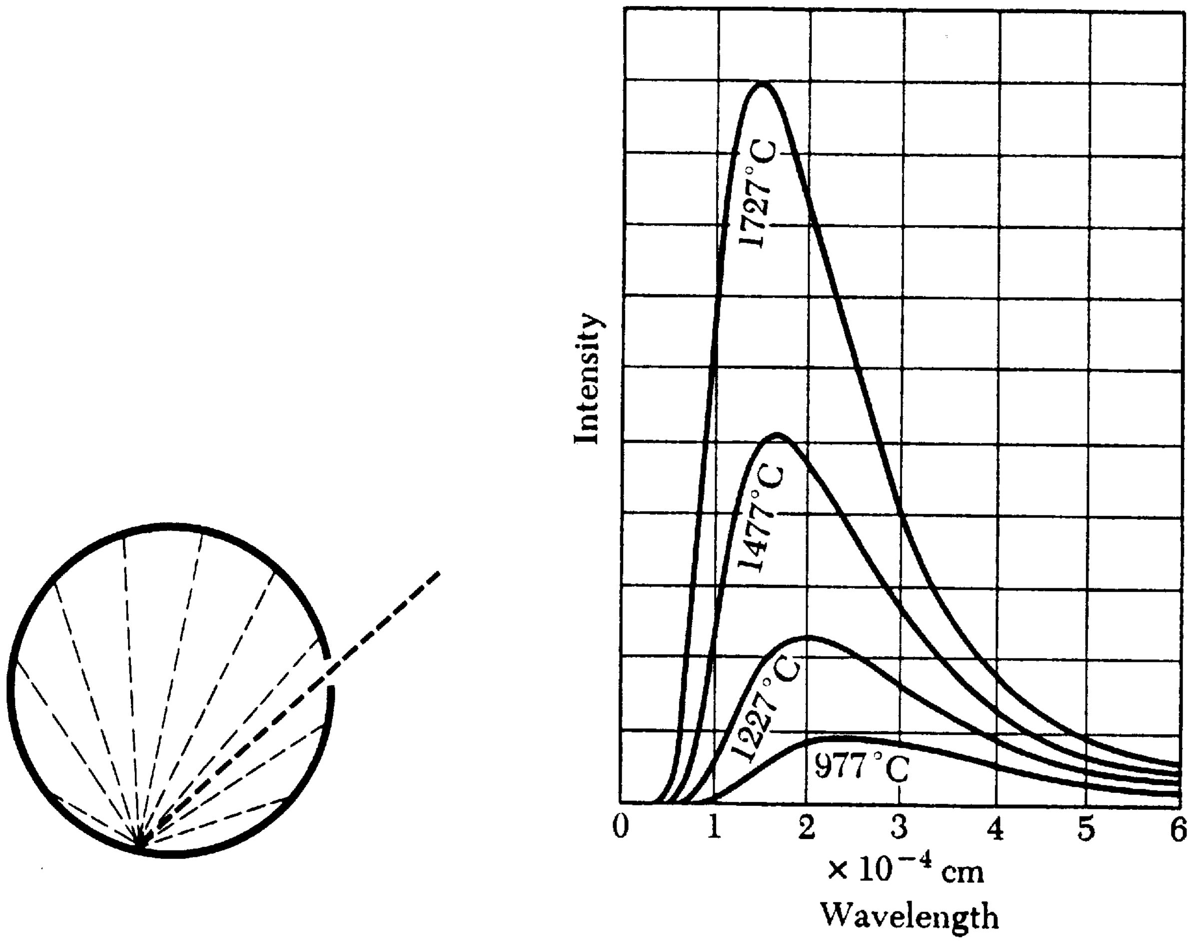


Figure 1. Left: electro-magnetic radiation inside a cavity with a (partially) absorbing interior ('black-body surface'). Right: power emitted by a black-body radiator, for different temperatures T.

1.2.2. The Photo-electric Effect (1887, Herz)

- When light is incident on a metal surface, electrons will be ejected
- The kinetic energy of these electrons is *independent* of the intensity of the light, but increases linearly with its frequency ...

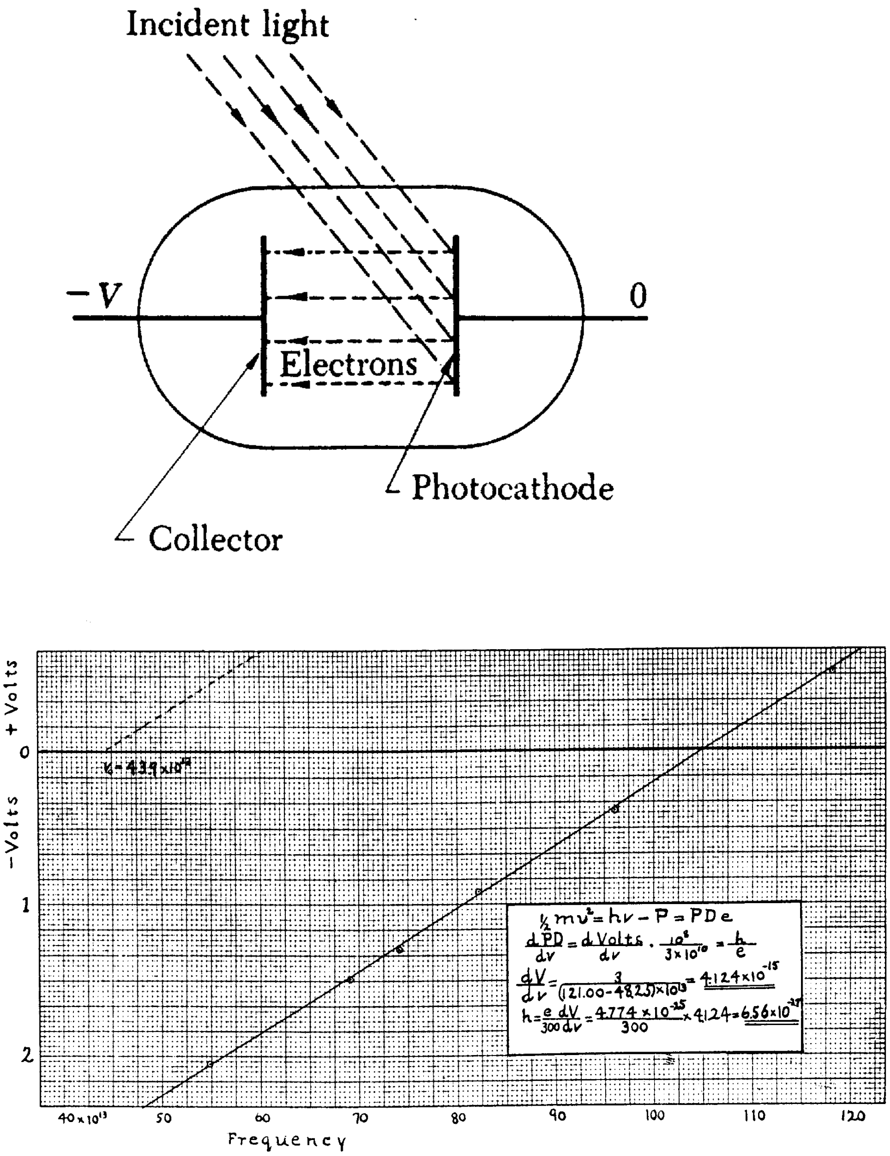


Figure 2. Top: measurement of the energy of electrons ejected from the cathode material due to incident light (the photo-electric effect). Bottom: resulting linear dependence on the frequency of the incident light.

1.2.3. The Problem of Atomic Stability (1911, Rutherford)

- Atom size: $\pm 10^{-10}$ m. Scattering experiments: a very small, positively charged, nucleus, surrounded by electrons. Size of nucleus and elctrons: $< \pm 10^{-13}$ m.
- Solar-system picture of the atom, with electrons moving along ellipsoidal trajectories around the nucleus (note: electric force proportional to r^{-2}, similar to gravitational force).
- Emission and absorption by atoms of electro-magnetic radiation occurs only in terms of discrete spectra. Balmer's expression for frequencies of hydrogen atom:

$$f_{nm} = R\left(\frac{1}{n^2} - \frac{1}{m^2}\right), \qquad n, m \in \{1, 2, 3, \ldots\}$$

- Why the spectral lines ? Why do atoms have a specific size ?
- Orbiting electrons are accelerating all the time (central force), so they emit radiation. Hence they lose energy continuously. Why do they not therefore collapse to the nucleus ?

Let us inspect spherical orbits of a charged electron (charge -e, mass m) around a nucleus (charge +Ze) located in the origin. We write its velocity as $v = |d\boldsymbol{x}/dt|$ and its distance from the nucleus as $r = |\boldsymbol{x}|$:

$$\text{Newton's law :} \qquad m\frac{d^2}{dt^2}\boldsymbol{x} = -\frac{e^2 Z}{|\boldsymbol{x}|^3}\boldsymbol{x}$$

$$\frac{1}{2}\frac{d^2}{dt^2}\boldsymbol{x}^2 = \frac{d}{dt}\left[\boldsymbol{x}\cdot\frac{d\boldsymbol{x}}{dt}\right] = \left[\frac{d\boldsymbol{x}}{dt}\right]^2 + \boldsymbol{x}\cdot\frac{d^2\boldsymbol{x}}{dt^2} = \left[\frac{d\boldsymbol{x}}{dt}\right]^2 - \frac{e^2 Z}{m|\boldsymbol{x}|}$$

Stable spherical orbits: $d\boldsymbol{x}^2/dt = 0$. Hence:

$$v^2 = \frac{e^2 Z}{mr}$$

Angular velocity ω: circumference $= 2\pi r$, so

$$\omega = \frac{v}{r}$$

Energy, $E = \frac{1}{2}mv^2 - e^2 Z/r$:

$$E = \frac{1}{2}\frac{e^2 Z}{r} - \frac{e^2 Z}{r} = -\frac{e^2 Z}{2r}$$

Angular momentum: $\boldsymbol{L} = \boldsymbol{x} \times \boldsymbol{p} = m\boldsymbol{x} \times (d\boldsymbol{x}/dt)$
Since $\boldsymbol{x} \cdot (d\boldsymbol{x}/dt) = 0$: $L \equiv |\boldsymbol{L}| = m|\boldsymbol{x}||d\boldsymbol{x}/dt|$, so

$$L^2 = m^2 r^2 \frac{e^2 Z}{mr} = e^2 Z m r$$

Expression of all characteristics in terms of L:

$$r = \frac{L^2}{Zme^2} \qquad v = \frac{Ze^2}{L} \qquad \omega = \frac{Z^2 m e^4}{L^3} \qquad E = -\frac{Z^2 m e^4}{2L^2}$$

Angular momentum is conserved (spherically symmetric potential), and hence L is determined purely by initial conditions and can take any value $L \in \mathbb{R}$. Therefore, so can r.

1.3. Quantum Mechanics: Revolution rather than Evolution

1.3.1. Impact of QM

Quantization
: Some observables (e.g. angular momentum) are *quantized* (can take only discrete values)

Probability
: Quantum state specifies *probabilities*; the uncertainty is intrinsic, not due to incomplete knowledge of the system

Uncertainty Principle
: There is a limit to how well one can jointly localize both position and momentum of a particle (so too for certain other observables)

Tunneling
: Quantum mechanics allows particles to be found in locations that are absolutely forbidden classically

Anti-matter
: Relativistic quantum mechanics predicts the existence if nearly identical anti-particles (electrons vs positrons), with opposite charge

Creation and Destruction of Matter
: Allowed, predicted and described by quantum mechanics

1.3.2. Comparison with Relativity Theory

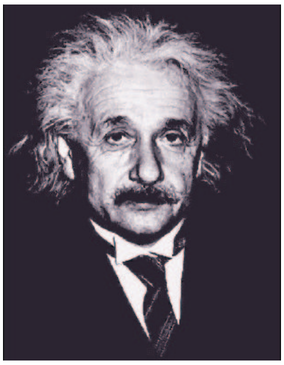
- Relativity: 1905 – 1916
  Quantum Mechanics: 1925
- Quantum Mechanics: triggered mainly by experiments
  Relativity: triggered mainly by thinking
- Relativity: mainly the solo project of Albert Einstein
  Quantum Mechanics: collective enterprise

1.3.3. Timing of the Revolution

1860: measurement of black-body radiation (Kirchhof)
1885: formula for spectral lines of hydrogen (Balmer)
1887: measurement of photo-electric effect (Herz)
Michelson-Morley experiment (ether ?)
1895: Lorentz transformations (problems with $v \sim c$ in Maxwell theory)
discovery of X-rays (Röntgen)
1896: discovery of radioactivity (Becqerel)
1897: discovery of the electron (Thomson)
1899: precise measurements of black-body radiation
1900: law of black-body radiation (Planck)

1905: light quantum explanation of photo-electric effect (Einstein)
special relativity theory (Einstein)
1911: discovery of the atomic nucleus (Rutherford)
precise measurement of electron charge (Millikan)
1913: Bohr's atom theory
1916: general relativity theory (Einstein)
1919: solar eclipse validation of general relativity
1923: matter waves postulated (De Broglie)

1925: matrix mechanics (Heisenberg)
exclusion principle (Pauli)
1926: Schrödinger equation
probabilistic interpretation of QM (Born)
equivalence with matrix mechanics (Schrödinger, Pauli, Eckart)
1927: Quantum electro-dynamics (Dirac)
uncertainty principle (Heisenberg)
1928: relativistic electron equation (Dirac)
1931: prediction of anti-matter (Dirac), experimental verification

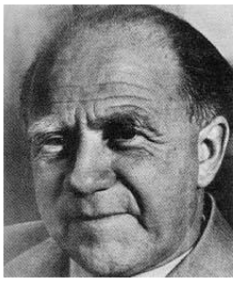


Albert Einstein

1879–1955

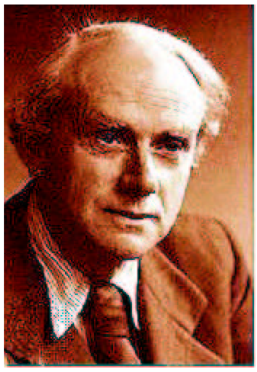
Niels Bohr

1885–1962



Werner Heisenberg

1901–1976



Paul Dirac

1902–1984

Photo-electric effect

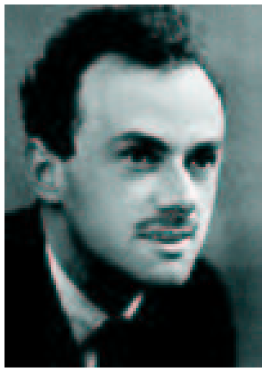
1905

Atom Theory

1913

Matrix Mechanics

1925

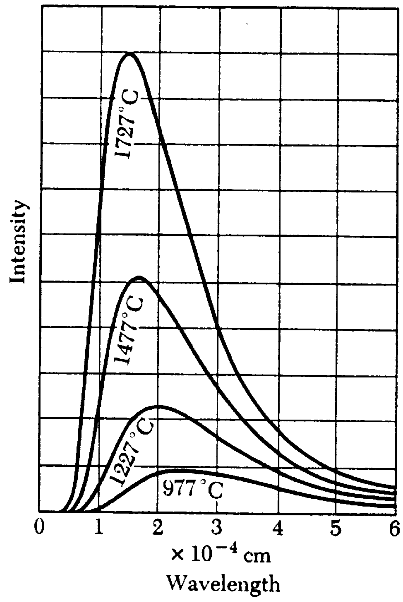


QED

1927

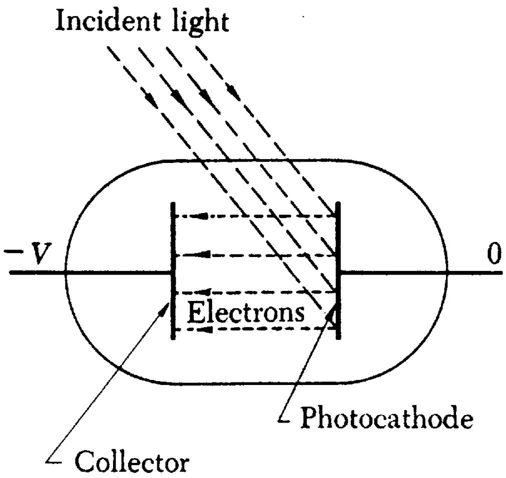
'Knaben-physik' ('Schoolboy-physics')

1.4. The Road Towards Quantum Theory



1.4.1. Explanation of Black-body Radiation (1900, Planck)

- Since black-body radiation independent of material of the wall:
  choose wall of harmonic oscillators, $V(x_i) = \frac{1}{2}m\omega^2 x_i^2$, interacting with the EM radiation.
- Assume that the energy E of each oscillator can only take the *discrete* values $E_n = nhf$ with $n \in \{0, 1, 2, 3, \ldots\}$, where f is the natural frequency of the oscillator ($f = \omega/2\pi$).
- It then follows (via classical statistical mechanics) that:
  $$W(\lambda, T) = \left(\frac{8\pi hc}{\lambda^5}\right) \frac{1}{e^{hc/\lambda kT} - 1}$$
  where k is Boltzmann's constant.
  (for $h \to 0$ one recovers the incorrect classical prediction)
- Perfect agreement with experiment, provided one chooses
  $$h \approx 6.626 \times 10^{-27} \text{ erg.sec.}$$
- Dimensions: kT = energy, λ = length, c = velocity, $hc/\lambda kT$ = dimensionless
  $$\dim h = \frac{m.kg.(m/s)^2}{m/s} = m^2 kg/sec$$
  Check angular momentum: dim L = dim $rp = m.kg.(m/s) = m^2.kg/sec$
  We conclude: h has dimension of *angular momentum*
- Alternative notation: $\hbar = h/2\pi$, $E_n = n\hbar\omega$
  Planck hoped and trusted that the quantization of energy would be a temporary fix ...

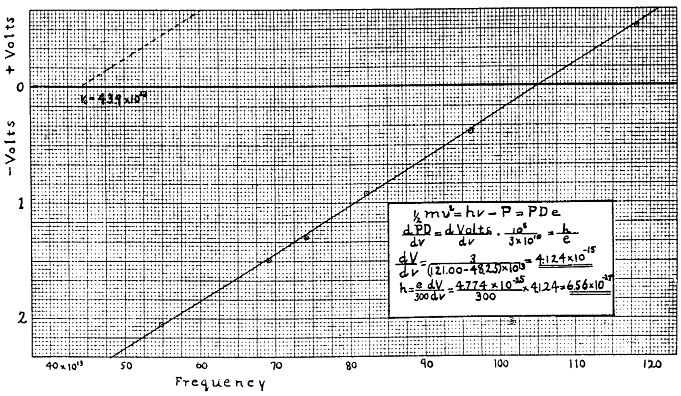


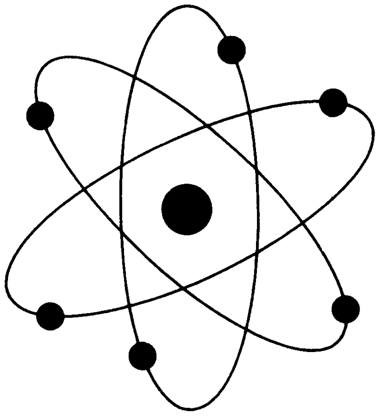
1.4.2. Explanation of the Photo-electric Effect (1905, Einstein)

- Einstein took the quantization in Planck's formula $E_n = n\hbar\omega$ seriously. Assume that the energy of the Planck oscillators can only change in units of $\hbar\omega$, *because electro-magnetic waves come in quantized units (photons) with energy $\hbar\omega$ each.*
- Each photon with angular frequency ω carries energy $E_{\text{photon}} = \hbar\omega$.
  Part of this energy, W, is needed to disconnect the electron from the atom.
  The remainder will be carried away by the electron as kinetic energy:

$$\begin{array}{lll} \hbar\omega < W : & \text{nothing happens} & \\ \hbar\omega > W : & \hbar\omega = W + \frac{1}{2}mv^2 & \text{so} \quad \frac{1}{2}mv^2 = \hbar\omega - W \end{array}$$

- No dependence on intensity !
  Intensity determines only the *number* of electrons knocked out, hence





1.4.3. Bohr's Atom Model (1913, Bohr)

- Bohr also took Planck's quantization seriously, but emphasized that h has the dimension of *angular momentum*, so the key discrete physical quantity must be angular momentum: $L_n = n\hbar$ with $n \in \{0, 1, 2, 3, \ldots\}$
- Solar-system picture of the atom, with negatively charged electrons moving along ellipsoidal trajectories around the positively charged nucleus.
- Now combine the classical equations (circular orbits, for simplicity)

$$r = \frac{L^2}{Zme^2} \qquad v = \frac{Ze^2}{L} \qquad \omega = \frac{Z^2me^4}{L^3} \qquad E = -\frac{Z^2me^4}{2L^2}$$

with $L_n = n\hbar$:

$$r_n = \frac{n^2\hbar^2}{Zme^2} \qquad v_n = \frac{Ze^2}{n\hbar} \qquad \omega_n = \frac{Z^2me^4}{n^3\hbar^3} \qquad E_n = -\frac{Z^2me^4}{2n^2\hbar^2}$$

- **Atom size:**
  for Hydrogen ($Z = 1$) on finds $r_1 = \frac{\hbar^2}{me^2} \approx 0.529.10^{-10}\ m$!!
- **Spectral lines, Balmer's formula:**
  Electrons can be made to switch between the allowed orbits r_n by EM radiation. Energy is conserved, so the balance is carried away (if $E_n > E_m$) or supplied ($E_n < E_m$) by the EM radiation:

$$\hbar\omega = E_n - E_m = \frac{Z^2me^4}{2\hbar^2}\left[\frac{1}{m^2} - \frac{1}{n^2}\right]$$

- **atom stability:**
  Accept that electrons in atoms do not radiate continuously (reasons as yet unknown)

2. The Schrödinger Equation

2.1. Matter Waves

2.1.1. De Broglie's Proposal (1923)

- If light can exhibit particle behaviour (discrete energy quanta $E = \hbar\omega$), then perhaps particles can also have wave-like properties.
- Consider particle orbits in Bohr's model (radius r, momentum p), quantized according to $L = n\hbar$:

$$rp = n\hbar \qquad \Leftrightarrow \qquad n\lambda = 2\pi r \quad \text{with} \quad \lambda = \frac{2\pi\hbar}{p}$$

  The condition $n\lambda = 2\pi r$ can be interpreted as describing *standing waves* along the circular orbit of radius r, with λ denoting the wavelength
- Wave associated with particle: $\lambda = 2\pi\hbar/p$
- Experimental verification: interference patterns of diffracted electrons (Davisson & Germer, 1927)

2.1.2. The Search for the Wave Equation (in 1 Dimension)

- Wave function: $\psi(x,t)$
- Require plane wave solutions to represent free particles, obeying $\hbar\omega = p^2/2m$ (quantized energy) and $p = 2\pi\hbar/\lambda$ (De Broglie wavelength):

$$\psi(x,t) = e^{i(kx-\omega t)} \qquad k = \frac{2\pi}{\lambda} \quad \text{(wavevector)}$$

  The two conditions lead to a relation between ω and k (upon eliminating p):

$$\hbar\omega = \frac{1}{2m}\frac{4\pi^2\hbar^2}{\lambda^2} = \frac{\hbar^2 k^2}{2m} \quad \text{so} \quad \omega = \frac{\hbar k^2}{2m}$$

- Assume linearity (so superposition of solutions is allowed, as in Maxwell's equations): If $\psi_a(x,t)$ and $\psi_b(x,t)$ solve the wave equation, then also $\psi(x,t) = C_a\psi_a(x,t) + C_b\psi_b(t)$ $(\forall C_a, C_b \in \mathbb{C})$

$$\text{e.g.} \qquad \frac{\partial^u \psi(x,t)}{\partial t^u} = K\frac{\partial^v \psi(x,t)}{\partial x^v} \qquad (u, v \in \mathbb{N})$$

  Substitute plane wave into proposed wave equation:

$$(\forall x, t \in \mathbb{R}): \quad \{(-i\omega)^u - K(ik)^v\}\, e^{i(kx-\omega t)} = 0 \qquad \Rightarrow \qquad (-i\omega)^u = K(ik)^v$$

$$(-i\frac{\hbar k^2}{2m})^u = K(ik)^v \qquad \text{hence}: \quad 2u = v, \quad K = (\frac{i\hbar}{2m})^u$$

  Simplest choice: $u = 1$, now $K = i\hbar/2m$,

$$\frac{\partial\psi(x,t)}{\partial t} = \frac{i\hbar}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2}$$

$$\text{Equivalently :} \qquad i\hbar \frac{\partial \psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x,t)}{\partial x^2}$$

2.1.3. Wave Packets in 3 Dimensions

- Generalize the wave equation to 3 dimensions:
  ($\boldsymbol{x}, \boldsymbol{k} \in \mathbb{R}^3$)

$$\psi(\boldsymbol{x},t) = e^{i(\boldsymbol{k}\cdot\boldsymbol{x} - \omega t)} \qquad |\boldsymbol{k}| = \frac{2\pi}{\lambda} \qquad \omega = \frac{\hbar \boldsymbol{k}^2}{2m}$$

$$i\hbar \frac{\partial}{\partial t}\psi(\boldsymbol{x},t) = -\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\psi(\boldsymbol{x},t) \qquad \boldsymbol{\nabla}^2 = \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial x_3^2}$$

- Use the linearity of the wave equation (superposition of plane wave solutions):

$$\psi(\boldsymbol{x},t) = \int_{\mathbb{R}^3} \frac{d\boldsymbol{k}}{(2\pi)^{3/2}}\ \phi(\boldsymbol{k}) e^{i(\boldsymbol{k}\cdot\boldsymbol{x} - \omega_{\boldsymbol{k}} t)} \qquad \omega_{\boldsymbol{k}} = \frac{\hbar \boldsymbol{k}^2}{2m}$$

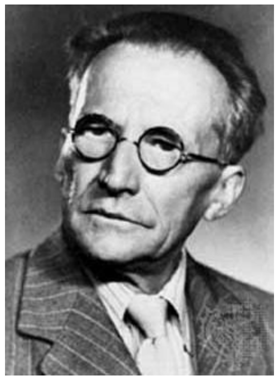
$$\psi(\boldsymbol{x},0) = \int_{\mathbb{R}^3} \frac{d\boldsymbol{k}}{(2\pi)^{3/2}}\ \phi(\boldsymbol{k}) e^{i\boldsymbol{k}\cdot\boldsymbol{x}} \qquad \text{(Fourier transform)}$$

If $\lim_{t\to 0} \psi \in L^2(\mathbb{R}^3)$:

$$\phi(\boldsymbol{k}) = \int_{\mathbb{R}^3} \frac{d\boldsymbol{x}}{(2\pi)^{3/2}}\ \psi(\boldsymbol{x},0) e^{-i\boldsymbol{k}\cdot\boldsymbol{x}} \qquad \text{(inverse Fourier transform)}$$

Note:
$L^2(\mathbb{R}^3)$ denotes the vector space of functions $f : \mathbb{R}^3 \to \mathbb{C}$ which are square integrable, i.e. $\int_{\mathbb{R}^3} d\boldsymbol{x}\ |f(\boldsymbol{x})|^2 < \infty$

2.2. The Schrödinger Equation and its Interpretation



$$i\hbar\frac{\partial}{\partial t}\psi(\boldsymbol{x},t) = -\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\psi(\boldsymbol{x},t) + V(\boldsymbol{x})\psi(\boldsymbol{x},t)$$

The wave equation for a particle with mass m moving in a potential $V(\boldsymbol{x}) \in \mathbb{R}$

2.2.1. Mathematical Properties

We define the real-valued objects

$$\rho(\boldsymbol{x},t) = |\psi(\boldsymbol{x},t)|^2 = \psi^*(\boldsymbol{x},t)\psi(\boldsymbol{x},t)$$
$$\boldsymbol{j}(\boldsymbol{x},t) = \frac{i\hbar}{2m}\left[\psi(\boldsymbol{x},t)\boldsymbol{\nabla}\psi^*(\boldsymbol{x},t) - \psi^*(\boldsymbol{x},t)\boldsymbol{\nabla}\psi(\boldsymbol{x},t)\right]$$

- ρ and $\boldsymbol{j}$ obey a continuity equation, which implies that $\rho(\boldsymbol{x},t)$ is the *density of a conserved quantity*, and $\boldsymbol{j}(\boldsymbol{x},t)$ is the *associated current density*:
$$\frac{\partial}{\partial t}\rho(\boldsymbol{x},t) + \boldsymbol{\nabla}\cdot\boldsymbol{j}(\boldsymbol{x},t) = 0$$
Proof:
$$\begin{aligned}
\frac{\partial}{\partial t}\rho(\boldsymbol{x},t) &= \frac{\partial\psi^*(\boldsymbol{x},t)}{\partial t}\psi(\boldsymbol{x},t) + \psi^*(\boldsymbol{x},t)\frac{\partial\psi(\boldsymbol{x},t)}{\partial t} \\
&= \frac{1}{i\hbar}\Bigg\{-[-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\psi(\boldsymbol{x},t) + V(\boldsymbol{x})\psi(\boldsymbol{x},t)]^*\psi(\boldsymbol{x},t) \\
&\qquad\qquad +\psi^*(\boldsymbol{x},t)[-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\psi(\boldsymbol{x},t) + V(\boldsymbol{x})\psi(\boldsymbol{x},t)]\Bigg\} \\
&= -\frac{i\hbar}{2m}\left\{\boldsymbol{\nabla}^2\psi^*(\boldsymbol{x},t).\psi(\boldsymbol{x},t) - \psi^*(\boldsymbol{x},t).\boldsymbol{\nabla}^2\psi(\boldsymbol{x},t)\right\} \\
&= -\frac{i\hbar}{2m}\{\boldsymbol{\nabla}\cdot[\boldsymbol{\nabla}\psi^*(\boldsymbol{x},t).\psi(\boldsymbol{x},t)] - \boldsymbol{\nabla}\psi^*(\boldsymbol{x},t)\cdot\boldsymbol{\nabla}\psi(\boldsymbol{x},t) \\
&\qquad\qquad -\boldsymbol{\nabla}\cdot[\psi^*(\boldsymbol{x},t).\boldsymbol{\nabla}\psi(\boldsymbol{x},t)] + \boldsymbol{\nabla}\psi(\boldsymbol{x},t)\cdot\boldsymbol{\nabla}\psi^*(\boldsymbol{x},t)\} \\
&= -\frac{i\hbar}{2m}\boldsymbol{\nabla}\cdot\{\boldsymbol{\nabla}\psi^*(\boldsymbol{x},t).\psi(\boldsymbol{x},t) - \psi^*(\boldsymbol{x},t).\boldsymbol{\nabla}\psi(\boldsymbol{x},t)\} \\
&= -\boldsymbol{\nabla}\cdot\boldsymbol{j}(\boldsymbol{x},t)
\end{aligned}$$
- If the integral $\int d\boldsymbol{x}\ \rho(\boldsymbol{x},t)$ exists, and the current $\boldsymbol{j}(\boldsymbol{x},t)$ vanishes sufficiently fast as $|\boldsymbol{x}| \to \infty$ then $\int d\boldsymbol{x}\ \rho(\boldsymbol{x},t)$ is a *conserved quantity*.
$$\begin{aligned}
\frac{d}{dt}\int d\boldsymbol{x}\ \rho(\boldsymbol{x},t) &= \int d\boldsymbol{x}\ \frac{\partial}{\partial t}\rho(\boldsymbol{x},t) = -\int d\boldsymbol{x}\ \boldsymbol{\nabla}\cdot\boldsymbol{j}(\boldsymbol{x},t) \\
&= -\lim_{R\to\infty}\int_{|\boldsymbol{x}|=R} dS\ \hat{\boldsymbol{n}}\cdot\boldsymbol{j}(\boldsymbol{x},t) = 0
\end{aligned}$$

- Solution by separation of variables: insert $\psi(\boldsymbol{x},t) = \phi(\boldsymbol{x})\chi(t)$ into SE:

$$i\hbar\phi(\boldsymbol{x})\frac{\partial}{\partial t}\chi(t) = -\frac{\hbar^2}{2m}\chi(t)\boldsymbol{\nabla}^2\phi(\boldsymbol{x}) + V(\boldsymbol{x})\phi(\boldsymbol{x})\chi(t)$$

Divide by $\psi(\boldsymbol{x},t)$:

$$i\hbar\frac{\partial}{\partial t}\log\chi(t) = -\frac{\hbar^2}{2m}\frac{1}{\phi(\boldsymbol{x})}\boldsymbol{\nabla}^2\phi(\boldsymbol{x}) + V(\boldsymbol{x})$$

LHS is a function of t only, RHS is a function of $\boldsymbol{x}$ only, hence both are constants:

$$i\hbar\frac{\partial}{\partial t}\log\chi(t) = E \qquad -\frac{\hbar^2}{2m}\frac{1}{\phi(\boldsymbol{x})}\boldsymbol{\nabla}^2\phi(\boldsymbol{x}) + V(\boldsymbol{x}) = E$$

$$\chi(t) = \chi(0)e^{-iEt/\hbar} \qquad \left[-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + V(\boldsymbol{x})\right]\phi(\boldsymbol{x}) = E\phi(\boldsymbol{x})$$

This (the time-independent Schrödinger equation) is a so-called Sturm-Liouville eigenvalue equation

differential operator :	$-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + V(\boldsymbol{x})$
eigenfunction :	$\phi(\boldsymbol{x})$
eigenvalue :	E

General solution (superposition):

$$\psi(\boldsymbol{x},t) = \sum_n c_n e^{-iE_n t/\hbar}\phi_n(\boldsymbol{x})$$

(or an integral, or a combination of integral and summation; depending on the spectrum $\{E_n\}$ found for the operator).

2.2.2. Statistical Interpretation of Schrödinger Equation

- $\rho(\boldsymbol{x},t)$ gives the *probability density* for finding the particle at position $\boldsymbol{x}$ at time t:
  - Continuity equation $\frac{\partial}{\partial t}\rho(\boldsymbol{x},t) + \boldsymbol{\nabla}\cdot\boldsymbol{j}(\boldsymbol{x},t) = 0$ expresses probability conservation
  - Solutions of SE must be normalized according to $\int d\boldsymbol{x}\ \psi^*(\boldsymbol{x},t)\psi(\boldsymbol{x},t) = 1$ for all $t \in \mathbb{R}$ ($\int d\boldsymbol{x}\ \rho(\boldsymbol{x},t)$ is conserved, so we just need to ensure normalization at $t = 0$)
- Physical (observable) quantities correspond to *operators*:

position :	$\boldsymbol{x}$	$[\boldsymbol{x}\psi](\boldsymbol{x}) = \boldsymbol{x}.\psi(\boldsymbol{x})$
momentum :	$\boldsymbol{p}$	$[\boldsymbol{p}\psi](\boldsymbol{x}) = -i\hbar\boldsymbol{\nabla}\psi(\boldsymbol{x})$
kinetic energy :	$\frac{\boldsymbol{p}^2}{2m}$	$[\frac{\boldsymbol{p}^2}{2m}\psi](\boldsymbol{x}) = -\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\psi(\boldsymbol{x})$
force :	$\boldsymbol{F}$	$[\boldsymbol{F}\psi](\boldsymbol{x},t) = -\boldsymbol{\nabla}V(\boldsymbol{x}).\psi(\boldsymbol{x})$
energy :	H	$[H\psi](\boldsymbol{x},t) = -\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\psi(\boldsymbol{x}) + V(\boldsymbol{x})\psi(\boldsymbol{x})$

- Expectation values of physical quantities are defined as follows:

$$\text{operator } A: \qquad \langle A\rangle = \int d\boldsymbol{x}\ \psi^*(\boldsymbol{x},t)\ A\psi(\boldsymbol{x},t)$$

- The correspondence principle: the equations relating expectation values in QM must be identical to the corresponding equations in classical mechanics, i.e.

$$\frac{d}{dt}\langle\boldsymbol{x}\rangle = m^{-1}\langle\boldsymbol{p}\rangle, \qquad \frac{d}{dt}\langle\boldsymbol{p}\rangle = \langle\boldsymbol{F}\rangle, \qquad \text{etc}$$

Note: sometimes (when there is a risk of ambiguity) operators are written as $\hat{\boldsymbol{x}}$, $\hat{\boldsymbol{p}}$, $\hat{H}$, etc.

We are automatically led to the study of *function spaces* and operators on such spaces. The natural function spaces in QM are found to be Hilbert spaces; see below.

2.2.3. Technical Subtleties

- We will generally assume ψ to be twice continuously differentiable in $\boldsymbol{x}$ (exception: potentials with δ-distributions, see later)
- Boundary conditions in $\mathbb{R}^3$: existence of integrals requires suitable behaviour for ψ as $|\boldsymbol{x}| \to \infty$. We may assume

$$\lim_{R\to\infty}\int_{|\boldsymbol{x}|<R} d\boldsymbol{x}\ |\psi(\boldsymbol{x},t)|^2 = 1$$

In polar coordinates (r,θ,ϕ), where $d\boldsymbol{x} \to r^2\sin(\theta)drd\theta d\phi$, this gives

$$\int_0^\pi d\theta \int_0^{2\pi} d\phi \left\{\lim_{R\to\infty}\int_0^R dr\ r^2\ |\psi|^2\right\} = 1$$

Hence $\lim_{r\to\infty} r^3|\psi|^2 = 0$ (since $\int_0^\infty dr\ r^{-1} = \infty$). Equivalently: $\psi(\boldsymbol{x},t) = |\boldsymbol{x}|^{-3/2}\epsilon(\boldsymbol{x},t)$ with $\lim_{|\boldsymbol{x}|\to\infty}\epsilon(\boldsymbol{x},t) = 0$.

Implications for $\boldsymbol{j}(\boldsymbol{x},t)$: $\boldsymbol{\nabla}\cdot\boldsymbol{j} = -|\boldsymbol{x}|^{-3}\frac{\partial}{\partial t}|\epsilon(\boldsymbol{x},t)|^2$, so $\lim_{|\boldsymbol{x}|\to\infty}[|\boldsymbol{x}|^2\boldsymbol{j}(\boldsymbol{x},t)] = 0$. This immediately leads to our previously encountered condition for probability conservation

$$\lim_{R\to\infty}\int_{|\boldsymbol{x}|=R} dS\ \hat{\boldsymbol{n}}\cdot\boldsymbol{j}(\boldsymbol{x},t) = 0$$

since $\int_{|\boldsymbol{x}|=R} dS = \mathcal{O}(R^2)$ (surface of a sphere with radius R in $\mathbb{R}^3$)

- The δ-function (for proper definitions and details see textbooks on *distribution theory*):
  - Defn. 1: $\delta[x] = 0$ for $x \neq 0$, $\delta[0] = \infty$, $\int dx\ \delta(x)f(x) = f(0)$ for all well-behaved f
  - Defn. 2: $\delta(x) = \lim_{\epsilon\to 0} G_\epsilon(x)$, with $G_\epsilon(x) = [\epsilon\sqrt{2\pi}]^{-1}e^{-\frac{1}{2}x^2/\epsilon^2}$
  - Defn. 3: $\delta(x) = (2\pi)^{-1}\int_{-\infty}^{\infty} dk\ e^{ikx}$

  Note the property $\int_{-\infty}^{\infty} dx\ f(x)\delta[x-y] = f(y)$ for all well-behaved f.

3. A More Formal Look at Quantum Theory

3.1. Function Spaces and Operators

3.1.1. Hilbert Spaces

Definition: A Hilbert space $\mathcal{H}$ is a vector space with the following properties:

(i) $\mathcal{H}$ is equipped with an inner product $\langle | \rangle : \mathcal{H} \times \mathcal{H} \to \mathbb{C}$
  (a) $(\forall u_1, u_2, v \in \mathcal{H}) : \langle u_1 + u_2 | v \rangle = \langle u_1 | v \rangle + \langle u_2 | v \rangle$
  (b) $(\forall u, v \in \mathcal{H})(\forall c \in \mathbb{C}) : \langle u | cv \rangle = c \langle u | v \rangle$
  (c) $(\forall u, v \in \mathcal{H}) : \langle u | v \rangle = \langle v | u \rangle^*$
  (d) $(\forall u \in \mathcal{H}) : \langle u | u \rangle \geq 0$, with equality if and only if $u = \mathbf{0}$

(ii) The metric on $\mathcal{H}$ is defined by the inner product: $|u| = \sqrt{\langle u | u \rangle}$

(iii) $\mathcal{H}$ is complete, i.e. every Cauchy sequence $\{u_n\}$ in $\mathcal{H}$ converges in $\mathcal{H}$:

$$\text{Cauchy sequence}: \quad (\forall \epsilon > 0)(\exists N \in \mathbb{N}) : |u_n - u_m| < \epsilon \quad (\forall n, m \geq N)$$

$$\text{convergence in } \mathcal{H}: \quad (\exists u \in \mathcal{H}) : \lim_{n \to \infty} |u_n - u| = 0$$

Why do we study Hilbert spaces in QM ?

- The SE is linear, so we are interested in *linear combinations* of complex functions $\psi : \mathbb{R}^n \to \mathbb{C}$, i.e. in vector spaces where the elements are functions
- We require $\int_{\mathbb{R}^n} d\boldsymbol{x}\ \psi^*(\boldsymbol{x})\psi(\boldsymbol{x}) = 1$. This is the statement $|\psi| = 1$, if we use the conventional (complex) inner product $\langle f | g \rangle = \int_{\mathbb{R}^n} d\boldsymbol{x}\ f^*(\boldsymbol{x}) g(\boldsymbol{x})$ in the function space $L^2(\mathbb{R}^n)$

Thus the natural space within which to solve the SE is the Hilbert space $L^2(\mathbb{R}^n)$.

3.1.2. Definitions and Properties of Operators on Hilbert Spaces

- Definition: the commutator of two operators A and B is $[A, B] \equiv AB - BA$
  Properties:

$$[A, B] = -[B, A] \qquad \text{hence also } [A, A] = 0$$
$$[A, \lambda_1 B + \lambda_2 C] = \lambda_1 [A, B] + \lambda_2 [A, C]$$
$$[AB, C] = [A, C]B + A[B, C]$$

  Examples:

$$[x_i, x_j]\psi = x_i x_j \psi - x_j x_i \psi = (x_i x_j - x_j x_i)\psi = 0$$
$$[p_i, p_j]\psi = (-i\hbar \frac{\partial}{\partial x_i})(-i\hbar \frac{\partial \psi}{\partial x_i}) - (-i\hbar \frac{\partial}{\partial x_i})(-i\hbar \frac{\partial \psi}{\partial x_i}) = -\hbar^2 [\frac{\partial^2 \psi}{\partial x_i \partial x_j} - \frac{\partial^2 \psi}{\partial x_j \partial x_i}] = 0$$
$$[x_i, p_j]\psi = x_i[-i\hbar \frac{\partial \psi}{\partial x_j}] - [-i\hbar \frac{\partial}{\partial x_j}](x_i \psi) = i\hbar \left\{ -x_i \frac{\partial \psi}{\partial x_j} + x_i \frac{\partial \psi}{\partial x_j} + \psi \frac{\partial x_i}{\partial x_j} \right\} = i\hbar \delta_{ij} \psi$$

Thus: $$[x_i, x_j] = [p_i, p_j] = 0, \qquad [x_i, p_j] = i\hbar\delta_{ij}$$

(note similarity with classical relations for Poisson brackets, under $(,) \to (i\hbar)^{-1}[,]$!)

- Definition: the (Hermitian) adjoint $A^\dagger$ of an operator A is defined by

  $$(\forall\phi, \psi \in \mathcal{H}): \quad \langle\phi|A\psi\rangle = \langle A^\dagger\phi|\psi\rangle$$

  Properties (with $\lambda \in \mathbb{C}$):

  $$(A^\dagger)^\dagger = A, \qquad (A+B)^\dagger = A^\dagger + B^\dagger, \qquad (AB)^\dagger = B^\dagger A^\dagger \qquad (\lambda A)^\dagger = \lambda^* A^\dagger$$

- Definition: a self-adjoint (or 'Hermitian') operator obeys $A^\dagger = A$

  Properties of Hermitian operators $A: \mathcal{H} \to \mathcal{H}$:

  (i) All eigenvalues of Hermitian operators are real-valued
  Proof: let $A^\dagger = A$ and let $A\phi = a\phi$, with $a \in \mathbb{C}$ and $\phi \neq \mathbf{0}$

  $$0 = \langle\phi|A\phi\rangle - \langle A\phi|\phi\rangle = \langle\phi|a\phi\rangle - \langle a\phi|\phi\rangle = a\langle\phi|\phi\rangle - a^*\langle\phi|\phi\rangle = (a - a^\star)|\phi|^2$$

  (ii) Every A can be written as the sum of an Hermitian and an anti-Hermitian part:

  $$A = \frac{1}{2}(A+A^\dagger) + \frac{1}{2}(A-A^\dagger)$$

  since $(A+A^\dagger)^\dagger = A+A^\dagger$ and $(A-A^\dagger)^\dagger = -(A-A^\dagger)$

  (iii) Eigenfunctions of Hermitian operators corresponding to different eigenvalues are *orthogonal*: if $A\phi_n = a_n\phi_n$ and $A\phi_m = a_m\phi_m$, then $\langle\phi_n|\phi_m\rangle = 0$ if $a_n \neq a_m$
  Proof:

  $$0 = \langle\phi_n|A\phi_m\rangle - \langle A\phi_n|\phi_m\rangle = \langle\phi_n|a_m\phi_m\rangle - \langle a_n\phi_n|\phi_m\rangle = (a_n - a_m)\langle\phi_n|\phi_m\rangle$$

  Hence: if $a_n - a_m \neq 0$ it follows that $\langle\phi_n|\phi_m\rangle = 0$

  (iv) The operator $B \equiv A^\dagger A$ is Hermitian, for any operator A,
  and it can have only non-negative eigenvalues.
  Proof: $B^\dagger = (A^\dagger A)^\dagger = A^\dagger(A^\dagger)^\dagger = A^\dagger A = B$.
  Let $B\phi = b\phi$ with $\phi \neq \mathbf{0}$: now

  $$b|\phi|^2 = \langle\phi|B\phi\rangle = \langle\phi|A^\dagger A\phi\rangle = \langle A\phi|A\phi\rangle = |A\phi|^2 \geq 0$$

  (v) If an Hermitian operator has a *complete* set of orthogonal eigenfunctions $\{\phi_n\}$, i.e. $(\forall\psi \in \mathcal{H})(\exists\{c_n \in \mathbb{C}\}): \ \psi = \sum_n c_n\phi_n$ (the sum could be an integral, or a combination of both, dependent on eigenvalue spectrum), then the *closure relation* holds:

  $$\sum_n \phi_n(\boldsymbol{x})\phi_n^*(\boldsymbol{x}') = \delta[\boldsymbol{x} - \boldsymbol{x}']$$

  Proof: we normalize the eigenfunctions according to $|\phi_n| = 1$ $(\forall n)$, hence $\langle\phi_m|\phi_n\rangle = \delta_{nm}$. For every $\psi \in \mathcal{H}$ we may write $\psi = \sum_n c_n\phi_n$. Take the inner product with ϕ_m:

  $$\langle\phi_m|\psi\rangle = \sum_n c_n\langle\phi_m|\phi_n\rangle = c_m$$

  Hence $$\psi(\boldsymbol{x}) = \sum_n \phi_n(\boldsymbol{x})\langle\phi_n|\psi\rangle = \int d\boldsymbol{x}' \left[\sum_n \phi_n(\boldsymbol{x})\phi_n^*(\boldsymbol{x}')\right]\psi(\boldsymbol{x}')$$

  This must be true for *every* $\psi \in \mathcal{H}$, so $\sum_n \phi_n(\boldsymbol{x})\phi_n^*(\boldsymbol{x}') = \delta[\boldsymbol{x} - \boldsymbol{x}']$

3.2. Operators in Quantum Mechanics

3.2.1. The Ehrenfest Theorem

If a QM system evolves according to the Schrödinger equation $i\hbar\frac{d}{dt}\psi = H\psi$, with $H^\dagger = H$, then for any operator A one has

$$\frac{d}{dt}\langle A\rangle = \langle\frac{\partial A}{\partial t}\rangle + \frac{1}{i\hbar}\langle[A,H]\rangle$$

(note similarity with classical relations for Poisson brackets, under $(,) \to (i\hbar)^{-1}[,]$)

Proof:

$$\begin{aligned}\frac{d}{dt}\langle A\rangle &= \frac{d}{dt}\langle\psi|A\psi\rangle = \langle\psi|\frac{\partial A}{\partial t}\psi\rangle + \langle\frac{d}{dt}\psi|A\psi\rangle + \langle\psi|A\frac{d}{dt}\psi\rangle \\ &= \langle\frac{\partial A}{\partial t}\rangle + \langle\frac{1}{i\hbar}H\psi|A\psi\rangle + \langle\psi|\frac{1}{i\hbar}AH\psi\rangle = \langle\frac{\partial A}{\partial t}\rangle + \frac{1}{i\hbar}\{-\langle H\psi|A\psi\rangle + \langle\psi|AH\psi\rangle\} \\ &= \langle\frac{\partial A}{\partial t}\rangle + \frac{1}{i\hbar}\{-\langle\psi|HA\psi\rangle + \langle\psi|AH\psi\rangle\} = \langle\frac{\partial A}{\partial t}\rangle + \frac{1}{i\hbar}\langle\psi|[A,H]\psi\rangle \\ &= \langle\frac{\partial A}{\partial t}\rangle + \frac{1}{i\hbar}\langle[A,H]\rangle\end{aligned}$$

3.2.2. QM Expectation Values of Hermitian Operators

We now interpret the expression for expectation values of operators describing a particle in space V in terms of inner products in $L^2(V)$: $\langle A\rangle = \int_V d\boldsymbol{x}\ \psi^* A\psi = \langle\psi|A\psi\rangle$. Note that normalization of the wave-function implies $\langle\psi|\psi\rangle = 1$.

- Hermitian operators have real-valued expectation values: if $A^\dagger = A$ then $\langle A\rangle \in \mathbb{R}$.
  Proof: $\langle A\rangle = \langle\psi|A\psi\rangle = \langle A\psi|\psi\rangle = \langle\psi|A\psi\rangle^* = \langle A\rangle^*$
- If $A^\dagger = A$, then also $[A - \langle A\rangle]^\dagger = A - \langle A\rangle$. Hence $[A - \langle A\rangle]^2$ has non-negative real-valued expectation values. This allows us to define the *uncertainty* $\Delta A \geq 0$ of observable A:
  $$\Delta A \equiv \sqrt{\langle[A - \langle A\rangle]^2\rangle} = \sqrt{\langle A^2\rangle - \langle A\rangle^2}$$
- $\Delta A = 0$ if and only if the system state ψ is an eigenfunction of A.
  Proof of the IF part, assume $A\psi = a\psi$:
  $$(\Delta A)^2 = \langle\psi|A^2\psi\rangle - \langle\psi|A\psi\rangle^2 = a^2\langle\psi|\psi\rangle - (a\langle\psi|\psi\rangle)^2 = a^2 - a^2 = 0$$
  Proof of the ONLY IF part, assume $\Delta A = 0$:
  $$0 = \langle[A-\langle A\rangle]^2\rangle = \langle\psi|[A-\langle A\rangle]^2\psi\rangle = \langle[A-\langle A\rangle]\psi|[A-\langle A\rangle]\psi\rangle = |[A-\langle A\rangle]\psi|^2$$
  Thus $A\psi - \langle A\rangle\psi = 0$, or, equivalently: $A\psi = \langle A\rangle\psi$
- If A has a *complete* set of eigenfunctions $\{\phi_n\}$ in $\mathcal{H}$, with corresponding eigenvalues $\{a_n\}$ and with $\langle\phi_m|\phi_n\rangle = \delta_{mn}$, then
  $$\langle A\rangle = \sum_n |\langle\phi_n|\psi\rangle|^2 a_n, \qquad \sum_n |\langle\phi_n|\psi\rangle|^2 = 1$$

Proof: first use closure relation

$$\psi = \sum_n \phi_n \langle \phi_n | \psi \rangle$$

Use this expression to calculate $\langle A \rangle$, using $A\phi_n = a_n \phi_n$:

$$\langle A \rangle = \sum_{nm} \langle \phi_n | \psi \rangle \langle \phi_m | \psi \rangle^* \langle \phi_m | A \phi_n \rangle = \sum_n a_n |\langle \phi_n | \psi \rangle|^2$$

Finally, use the expansion of ψ to re-write $|\psi| = 1$:

$$1 = \sum_{nm} \langle \phi_n | \psi \rangle \langle \phi_m | \psi \rangle^* \langle \phi_m | \phi_n \rangle = \sum_n |\langle \phi_n | \psi \rangle|^2$$

3.2.3. Position, Momentum and Energy

Let us check, in one spatial dimension, whether the main operators encountered so far (a) are Hermitian, and (b) have a complete set of orthogonal eigenfunctions. We observe the importance of *boundary conditions*. Let us assume $x \in [a, b]$, so the relevant Hilbert space is $L^2(a, b)$ with $\langle \phi | \psi \rangle = \int_a^b dx\ \phi^*(x)\psi(x)$, and use the notation convention $\hat{x}$, $\hat{p}$ etc for operators:

- Position operator: $(\hat{x}\phi)(x) = x\phi(x)$
  - Hermitian ?
  $$\langle \phi | \hat{x}\psi \rangle - \langle \hat{x}\phi | \psi \rangle = \int_a^b dx\, [x\phi^*(x)\psi(x) - \phi^*(x)x\psi(x)] = 0$$
  - Eigenfunctions ?
  $$(\forall x \in [a, b]) : \ x\phi_\lambda(x) = \lambda\phi_\lambda(x) \qquad (\lambda \text{ denotes eigenvalue})$$
  $$(\forall x \in [a, b]) : \ (x - \lambda)\phi_\lambda(x) = 0$$
  Apparently, $\phi_\lambda(x) = 0$ unless $x = \lambda$. Hence: $\phi_\lambda(x) = \delta[x - \lambda]$
  - Eigenvalue spectrum: $\lambda \in [a, b]$; associated eigenfunctions: $\phi_\lambda(x) = \delta[x - \lambda]$
  - Orthogonality:
  $$\langle \phi_\lambda | \phi_{\lambda'} \rangle = \int_a^b dx\ \delta[x - \lambda]\delta[x - \lambda'] = \delta[\lambda - \lambda']$$
  - Completeness:
  $$(\forall x \in (a, b)) : \quad f(x) = \int_a^b dy\ \delta[x - y]f(y) = \int_a^b d\lambda\ f(\lambda)\phi_\lambda(x)$$
- Momentum operator: $(\hat{p}\phi)(x) = -i\hbar\phi'(x)$
  - Hermitian ?
  $$\begin{aligned} \langle \phi | \hat{p}\psi \rangle &= -i\hbar \int_a^b dx\ \phi^*(x)\frac{\partial}{\partial x}\psi(x) \\ &= -i\hbar\,[\phi^*(x)\psi(x)]_a^b + \int_a^b dx\ \psi(x)\left[-i\hbar\frac{\partial}{\partial x}\phi(x)\right]^* \\ &= \langle \hat{p}\phi | \psi \rangle - i\hbar\,[\phi^*(x)\psi(x)]_a^b \end{aligned}$$
  Hermitian *only if* we impose boundary conditions such that $\phi(b) = \phi(a)$

– Eigenfunctions:

$$(\forall x \in [a,b]): \quad -i\hbar\frac{\partial}{\partial x}\phi_\lambda(x) = \lambda\phi_\lambda(x) \qquad (\lambda \text{ denotes eigenvalue})$$

$$\phi'_\lambda(x) = (i\lambda/\hbar)\phi_\lambda(x) \qquad \Rightarrow \qquad \phi_\lambda(x) = e^{i\lambda x/\hbar}$$

Impose acceptable boundary conditions (see above)
(more than one choice !):

$$\phi_\lambda(b) = \phi_\lambda(a): \quad e^{i\lambda(b-a)/\hbar} = 1, \quad \text{so} \quad \frac{\lambda(b-a)}{\hbar} = 2\pi n \quad (n \in \mathbb{Z})$$

– Eigenvalue spectrum & associated eigenfunctions:

$$\lambda_n = \frac{2\pi\hbar n}{b-a}, \qquad \phi_n(x) = e^{2\pi i n x/(b-a)}, \qquad (n \in \mathbb{Z})$$

– Orthogonality:

$$\langle\phi_n|\phi_m\rangle = \int_a^b dx\ [e^{-2\pi i n x/(b-a)}][e^{2\pi i m x/(b-a)}] = \int_a^b dx\ e^{2\pi i(m-n)x/(b-a)}$$

$$m = n: \quad \langle\phi_n|\phi_n\rangle = \int_a^b dx\ 1 = b-a$$

$$\begin{aligned} m \neq n: \quad \langle\phi_n|\phi_m\rangle &= \frac{b-a}{2\pi i(m-n)}\ e^{2\pi i(m-n)x/(b-a)}\Big|_a^b \\ &= \frac{b-a}{2\pi i(m-n)}\left[e^{2\pi i(m-n)b/(b-a)} - e^{2\pi i(m-n)a/(b-a)}\right] \\ &= \frac{b-a}{2\pi i(m-n)} e^{2\pi i(m-n)a/(b-a)}\ [1-1] = 0 \end{aligned}$$

– Completeness:
The set $\{\phi_n\}$ = Fourier expansion for functions in $L^2(a,b)$, which is complete

- Energy operator: $(\hat{H}\phi)(x) = -(\hbar^2/2m)\phi''(x) + V(x)\phi(x)$

– Hermitian ?
First inspect kinetic part. Note that $\hat{H}_{\rm kin} = \hat{p}^2/2m$, so

$$\begin{aligned} \langle\phi|\hat{H}\psi\rangle - \langle\hat{H}\phi|\psi\rangle &= \frac{1}{2m}[\langle\phi|\hat{p}^2\psi\rangle - \langle\hat{p}^2\phi|\psi\rangle] \\ &= \frac{1}{2m}[\langle(\hat{p}^\dagger)^2\phi|\psi\rangle - \langle\hat{p}^2\phi|\psi\rangle] \end{aligned}$$

So $\hat{H}_{\rm kin}$ is Hermitian if and only if $(\hat{p}^\dagger)^2 = p^2$. For boundary conditions such that $\hat{p}^\dagger = \hat{p}$ (see above).

Next inspect potential energy part $\hat{V}$:

$$\langle\phi|\hat{V}\psi\rangle - \langle\hat{V}\phi|\psi\rangle = \int_a^b dx\, [V(x)\phi^*(x)\psi(x) - \phi^*(x)V(x)\psi(x)] = 0$$

Thus, given suitable boundary conditions, $\hat{H}$ is Hermitian

– Eigenfunctions:

$$(\forall x \in (a,b)): \quad -\frac{\hbar^2}{2m}\phi''_\lambda(x) + V(x)\phi_\lambda(x) = \lambda\phi_\lambda(x)$$

Sturm-Liouville problem, generally complicated; solution depends on choice of $V(x)$

3.3. The Postulates of Quantum Mechanics

These are motivated by the properties of the SE and of Hermitian operators
(i.e. real eigenvalues, expression for $\langle A \rangle$ in terms of eigenvalues of A)

I: Every physical system describing a particle moving in Ω is described by a wave-function $\psi \in L^2(\Omega)$, which contains *all the information* about the state of the particle

II: The wave function ψ evolves in time according to the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t}\psi(\boldsymbol{x}, t) = -\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\psi(\boldsymbol{x}, t) + V(\boldsymbol{x})\psi(\boldsymbol{x}, t)$$

III: Every observable physical quantity corresponds to a Hermitian operator $A : \mathcal{H} \to \mathcal{H}$ with a complete set of eigenfunctions $\{\phi_n\}$. The corresponding eigenvalues $\{a_n\}$ of A are the possible outcomes of a measurement of this quantity.

IV: The probability P_n that a measurement of A leads to the observation a_n equals $P_n = |\langle \phi_n | \psi \rangle|^2$, given normalization $\langle \phi_n | \phi_m \rangle = \delta_{nm}$ and $\langle \psi | \psi \rangle = 1$ (if a_n is not degenerate)

If a_n is degenerate, the probability that a measurement of A leads to the observation a_n equals $P_n = \sum_{m|a_m = a_n} |\langle \phi_m | \psi \rangle|^2$.

V: At the instance of a measurement of A, leading to observation a_n, the wave function 'collapses' to the eigenspace of the operator A corresponding to the eigenvalue a_n.

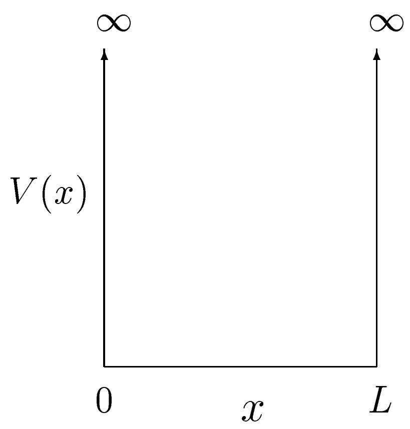
Note:
Since H has complete set of othogonal eigenfunctions:
solution obtained by separation of variables is *general* and *unique*

$$H = -\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + V(\boldsymbol{x}) \qquad H\phi_n = E_n\phi_n$$

$$\psi(\boldsymbol{x}, t) = \sum_n c_n e^{-iE_n t/\hbar}\phi_n(\boldsymbol{x}) \qquad c_n = \langle \phi_n | \psi_{t=0} \rangle$$

4. Examples of Simple Systems

4.1. Free Particle in a Box



4.1.1. Solution of the Schrödinger Equation

- Construct solution of SE in $[0, L]$ by separation of variables:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\phi(x) = E\phi(x)$$
$$\psi(x,t) = \sum_n c_n e^{-iE_n t/\hbar}\phi_n(x)$$

(or integral, dependent on spectrum $\{E_n\}$)

To be solved: $\phi''(x) + k^2\phi(x) = 0$, with $k^2 = 2mE/\hbar^2$

General solution:

$$\phi(x) = A_k e^{ikx} + B_k e^{-ikx}, \qquad A_k, B_k \in \mathbb{C}$$

- Boundary conditions: $\phi(0) = \phi(L) = 0$
This gives:

$$A_k + B_k = 0, \quad A_k e^{ikL} + B_k e^{-ikL} = 0 \quad \Rightarrow \quad B_k = -A_k, \quad \sin(kL) = 0$$

Hence: $kL = n\pi$ $(n \in \mathbb{N})$, or $k_n = n\pi/L$

$$\phi_n(x) = \sin(\frac{n\pi x}{L}), \qquad E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}, \qquad n = 1, 2, 3, \ldots$$

- Normalize ϕ_n:
$\phi_n \to C_n \sin(n\pi x/L)$

$$1 = |C_n|^2 \int_0^L dx\ \sin^2(\frac{\pi n x}{L}) = |C_n|^2(\frac{L}{\pi n})\int_0^{\pi n} dz\ \sin^2(z)$$
$$= |C_n|^2(\frac{L}{\pi n})(\frac{\pi n}{2}) = \frac{1}{2}L|C_n|^2$$

Thus $C_n = \sqrt{2/L}$

$$\phi_n(x) = \sqrt{\frac{2}{L}}\ \sin(\frac{n\pi x}{L})$$

- General solution of SE:

$$\psi(x,t) = \sqrt{\frac{2}{L}}\sum_{n=1}^{\infty} c_n\ e^{-in^2\pi^2\hbar t/2mL^2}\sin(\frac{n\pi x}{L})$$

$$c_n = \sqrt{\frac{2}{L}}\int_0^L dx\ \sin(\frac{n\pi x}{L})\psi(x,0)$$

4.1.2. Expectation Values and Uncertainties

Choose simple initial conditions: $c_n = \delta_{n\ell}$

$$\psi(x,t) = e^{-iE_\ell t/\hbar}\phi_\ell(x) \qquad \phi_\ell(x) = \sqrt{\frac{2}{L}}\sin(\frac{\pi\ell x}{L}) \qquad E_\ell = \frac{\ell^2\pi^2\hbar^2}{2mL^2}$$

(so $H\psi = E_\ell\psi$ for all t)

- Position:

$$\begin{aligned}
\langle x\rangle &= \int_0^L dx\ \psi^* x\psi = \frac{2}{L}\int_0^L dx\ x\sin^2(\frac{\pi\ell x}{L}) = \frac{1}{L}\int_0^L dx\ x\left\{1-\cos(\frac{2\pi\ell x}{L})\right\} \\
&= \frac{1}{2}L - \frac{1}{L}\int_0^L dx\ x\cos(\frac{2\pi\ell x}{L}) \\
&= \frac{1}{2}L - \frac{1}{L}\left\{\frac{Lx}{2\pi\ell}\sin(\frac{2\pi\ell x}{L})\Big|_0^L - \frac{L}{2\pi\ell}\int_0^L dx\ \sin(\frac{2\pi\ell x}{L})\right\} \\
&= \frac{1}{2}L - \frac{1}{L}\left\{0 - 0 + \frac{L^2}{4\pi^2\ell^2}\cos(\frac{2\pi\ell x}{L})\Big|_0^L\right\} = \frac{1}{2}L
\end{aligned}$$

$$\begin{aligned}
\langle x^2\rangle &= \int_0^L dx\ \psi^* x^2\psi = \frac{2}{L}\int_0^L dx\ x^2\sin^2(\frac{\pi\ell x}{L}) = \frac{1}{L}\int_0^L dx\ x^2\left\{1-\cos(\frac{2\pi\ell x}{L})\right\} \\
&= \frac{1}{3}L^2 - \frac{1}{L}\int_0^L dx\ x^2\cos(\frac{2\pi\ell x}{L}) = \frac{1}{3}L^2 + \frac{1}{L}\lim_{y\to 2\pi\ell/L}\frac{d^2}{dy^2}\int_0^L dx\ \cos(yx) \\
&= \frac{1}{3}L^2 + \frac{1}{L}\lim_{y\to 2\pi\ell/L}\frac{d^2}{dy^2}\left[y^{-1}\sin(yx)\right]_0^L = \frac{1}{3}L^2 + \frac{1}{L}\lim_{y\to 2\pi\ell/L}\frac{d^2}{dy^2}\left(y^{-1}\sin(yL)\right) \\
&= \frac{1}{3}L^2 + \frac{1}{L}\lim_{y\to 2\pi\ell/L}\left(\frac{2}{y^3}\sin(yL) - \frac{2L}{y^2}\cos(yL) - \frac{L^2}{y}\sin(yL)\right) \\
&= \frac{1}{3}L^2 - \frac{L^2}{2\pi^2\ell^2}
\end{aligned}$$

$$\Delta x = \sqrt{\langle x^2\rangle - \langle x\rangle^2} = L\sqrt{1/12 - 1/2\pi^2\ell^2}$$

- Momentum:

$$\begin{aligned}
\langle p\rangle &= -i\hbar\int_0^L dx\ \psi^*\frac{\partial}{\partial x}\psi = -\frac{2i\hbar}{L}\int_0^L dx\ \sin(\frac{\pi\ell x}{L})\frac{\partial}{\partial x}\sin(\frac{\pi\ell x}{L}) \\
&= -\frac{2i\hbar}{L}\frac{\pi\ell}{L}\int_0^L dx\ \sin(\frac{\pi\ell x}{L})\cos(\frac{\pi\ell x}{L}) = -\frac{i\pi\ell\hbar}{L^2}\int_0^L dx\ \sin(\frac{2\pi\ell x}{L}) \\
&= \frac{i\pi\ell\hbar}{L^2}\frac{L}{2\pi\ell}\cos(\frac{2\pi\ell x}{L})\Big|_0^L = \frac{i\hbar}{2L}\left(\cos(2\pi\ell) - \cos(0)\right) = 0
\end{aligned}$$

$$\langle p^2\rangle = 2m\langle H\rangle = 2mE_\ell = \ell^2\pi^2\hbar^2/L^2$$

$$\Delta p = \sqrt{\langle p^2\rangle - \langle p\rangle^2} = \sqrt{\ell^2\pi^2\hbar^2/L^2} = \ell\pi\hbar/L$$

- Energy:

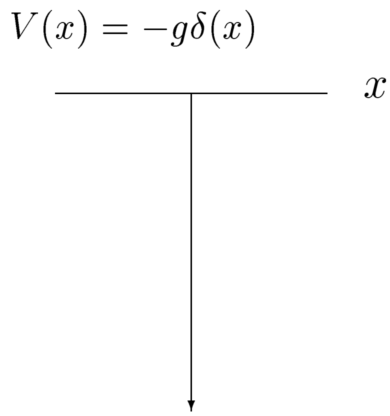
$$\begin{aligned}\langle H\rangle &= E_\ell = \ell^2\pi^2\hbar^2/2mL^2\\ \langle H^2\rangle &= E_\ell^2 = (\ell^2\pi^2\hbar^2/2mL^2)^2\\ \Delta H &= \sqrt{\langle H^2\rangle - \langle H\rangle^2} = \sqrt{0} = 0\end{aligned}$$

Note:

$$\Delta x.\Delta p = \pi\ell\hbar\sqrt{\frac{1}{12} - \frac{1}{2\pi^2\ell^2}} = \frac{1}{2}\hbar\sqrt{\frac{1}{3}\pi^2\ell^2 - 2}$$

$$\ell = 1: \qquad \Delta x.\Delta p = \frac{1}{2}\hbar\sqrt{\frac{1}{3}\pi^2 - 2} \qquad (\sqrt{\frac{1}{3}\pi^2 - 2} \approx 1.136)$$

4.2. Particle in Attractive δ-potential



4.2.1. Solution of the Schrödinger Equation

- Solution of SE by separation of variables:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\phi(x) - g\delta(x)\phi(x) = E\phi(x)$$
$$\psi(x,t) = \sum_n c_n e^{-iE_n t/\hbar}\phi_n(x)$$

To be solved in regions $(-\infty, 0)\bigcup(0, \infty)$:
$\phi''(x) + k^2\phi(x) = 0$, with $k^2 = 2mE/\hbar^2$

$$x < 0: \quad \phi(x) = A_k^- e^{ikx} + B_k^- e^{-ikx}, \qquad A_k^-, B_k^- \in \mathbb{C}$$
$$x > 0: \quad \phi(x) = A_k^+ e^{ikx} + B_k^+ e^{-ikx}, \qquad A_k^+, B_k^+ \in \mathbb{C}$$

- Boundary conditions, $\phi(\infty) = \phi(-\infty) = 0$:

$$\lim_{x\to-\infty}\left[A_k^- e^{ikx} + B_k^- e^{-ikx}\right] = 0 \quad \Rightarrow \quad k = iy, \quad y \in \mathbb{R}^+, \quad A_k^- = 0$$
$$\lim_{x\to\infty}\left[A_k^+ e^{ikx} + B_k^+ e^{-ikx}\right] = 0 \quad \Rightarrow \quad k = iy, \quad y \in \mathbb{R}^+, \quad B_k^+ = 0$$

Hence, upon putting $y \to k$:

$$x < 0: \quad \phi_k(x) = B_k e^{kx}, \qquad B_k \in \mathbb{C}$$
$$x > 0: \quad \phi_k(x) = A_k e^{-kx}, \qquad A_k \in \mathbb{C}$$

with $k > 0$ and $E_k = -\hbar^2 k^2/2m$

- Solution *continuous* at $x = 0$, i.e. $\lim_{x\downarrow 0}\phi(x) = \lim_{x\uparrow 0}\phi(x)$: $B_k = A_k$

$$x \neq 0: \quad \phi_k(x) = e^{-k|x|}, \qquad k > 0, \quad E_k = -\frac{\hbar^2 k^2}{2m}$$

- Connection between $x > 0$ and $x < 0$ regions:
integrate time-independent SE around location of δ-peak ($\epsilon > 0$)

$$\lim_{\epsilon\to 0}\int_{-\epsilon}^{\epsilon} dx \ \left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\phi(x) - g\delta(x)\phi(x)\right] = E\lim_{\epsilon\to 0}\int_{-\epsilon}^{\epsilon} dx \ \phi(x)$$

$$-\frac{\hbar^2}{2m}\lim_{\epsilon\to 0}[\phi'(\epsilon) - \phi'(-\epsilon)] - g\phi(0) = E\lim_{\epsilon\to 0}\int_{-\epsilon}^{\epsilon} dx \ \phi(x)$$

$$\lim_{x\downarrow 0}\phi'(x) - \lim_{x\uparrow 0}\phi'(x) = -\frac{2mg}{\hbar^2}\phi(0)$$

Present solution: $\phi'(x > 0) = -ke^{-kx}$, $\phi'(x < 0) = ke^{kx}$, $\phi(0) = 1$, so
$-k - k = -2mg/\hbar^2$, so $k = mg/\hbar^2$

- Normalize ϕ: $\phi \to Ae^{-k|x|}$

$$1 = |A|^2 \int_{-\infty}^{\infty} dx\ e^{-2k|x|} = 2|A|^2 \int_0^{\infty} dx\ e^{-2kx} = -\frac{2|A|^2}{2k}\ e^{-2kx}\Big|_0^{\infty} = \frac{|A|^2}{k}$$

Thus $A = \sqrt{k} = \sqrt{mg}/\hbar$

$$\phi(x) = \frac{\sqrt{mg}}{\hbar}\ e^{-mg|x|/\hbar^2} \qquad E = -\frac{mg^2}{2\hbar^2}$$

- Solution of full SE:

$$\psi(x,t) = C\frac{\sqrt{mg}}{\hbar}\ e^{img^2t/2\hbar^3 - mg|x|/\hbar^2}, \qquad |C| = 1$$

4.2.2. Expectation Values and Uncertainties

Note: $H\psi = E\psi$ for all t, with $E = -mg^2/2\hbar^2$
Note: $\frac{d}{dx}\ \mathrm{sgn}(x) = 2\delta(x)$

- Position:

$$\langle x \rangle = \int_{-\infty}^{\infty} dx\ \psi^* x \psi k \int_{-\infty}^{\infty} dx\ xe^{-2k|x|} = 0$$

$$\begin{aligned}\langle x^2 \rangle &= \int_{-\infty}^{\infty} dx\ \psi^* x^2 \psi = k\int_{-\infty}^{\infty} dx\ x^2 e^{-2k|x|} = 2k\int_0^{\infty} dx\ x^2 e^{-2kx} \\ &= \frac{k}{2}\frac{d^2}{dk^2}\int_0^{\infty} dx\ e^{-2kx} = \frac{k}{2}\frac{d^2}{dk^2}\left[-\frac{1}{2k}e^{-2kx}\right]_0^{\infty} = \frac{k}{4}\frac{d^2}{dk^2}\frac{1}{k} = \frac{1}{2k^2} = \frac{\hbar^4}{2m^2g^2}\end{aligned}$$

$$\Delta x = \sqrt{\langle x^2\rangle - \langle x\rangle^2} = \hbar^2/mg\sqrt{2}$$

- Momentum:

$$\begin{aligned}\langle p \rangle &= -i\hbar\int_{-\infty}^{\infty} dx\ \psi^* \frac{\partial}{\partial x}\psi = -i\hbar k\int_{-\infty}^{\infty} dx\ e^{-k|x|}\frac{\partial}{\partial x}e^{-k|x|} \\ &= i\hbar k^2\int_{-\infty}^{\infty} dx\ \ \mathrm{sgn}(x)e^{-2k|x|} = 0\end{aligned}$$

$$\begin{aligned}\langle p^2 \rangle &= -\hbar^2\int_{-\infty}^{\infty} dx\ \psi^* \frac{\partial^2}{\partial x^2}\psi = -\hbar^2 k\int_{-\infty}^{\infty} dx\ e^{-k|x|}\frac{\partial^2}{\partial x^2}e^{-k|x|} \\ &= \hbar^2k^2\int_{-\infty}^{\infty} dx\ e^{-k|x|}\frac{\partial}{\partial x}[\ \mathrm{sgn}(x)e^{-k|x|}] \\ &= \hbar^2k^2\int_{-\infty}^{\infty} dx\ e^{-k|x|}\frac{\partial}{\partial x}[2\delta(x)e^{-k|x|} - ke^{-k|x|}] \\ &= 2\hbar^2k^2\int_{-\infty}^{\infty} dx\ e^{-2k|x|}\delta(x) - \hbar^2k^3\int_{-\infty}^{\infty} dx\ e^{-2k|x|} \\ &= 2\hbar^2k^2 - \hbar^2k^3k^{-1} = \hbar^2k^2 = m^2g^2/\hbar^2\end{aligned}$$

$$\Delta p = \sqrt{\langle p^2\rangle - \langle p\rangle^2} = mg/\hbar$$

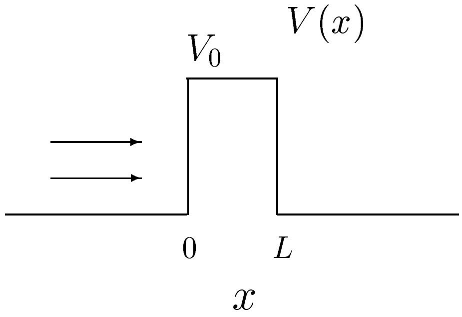
- Energy:

$$\begin{aligned}
\langle H \rangle &= E = -mg^2/2\hbar^2 \\
\langle H^2 \rangle &= E^2 = (-mg^2/2\hbar^2)^2 \\
\Delta H &= \sqrt{\langle H^2 \rangle - \langle H \rangle^2} = \sqrt{0} = 0
\end{aligned}$$

Note:

$$\Delta x . \Delta p = (\hbar^2/mg\sqrt{2}).(mg/\hbar) = \frac{1}{2}\sqrt{2}\ \hbar$$

4.3. Potential Barriers, Tunneling



4.3.1. Solution of the Schrödinger Equation

Note: no normalizable solutions to be expected !
(scattering of incoming waves if $V_0 > 0$)

- Construct solution of time-independent SE:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\phi(x) + V(x)\phi(x) = E\phi(x)$$

To be solved:

$$x \in (-\infty, 0): \quad \phi_{\rm I}''(x) + k^2\phi_{\rm I}(x) = 0 \quad \Rightarrow \quad \phi_{\rm I}(x) = Ae^{ikx} + Be^{-ikx}$$
$$x \in (0, L): \quad \phi_{\rm II}''(x) + k_0^2\phi_{\rm II}(x) = 0 \quad \Rightarrow \quad \phi_{\rm II}(x) = Fe^{ik_0x} + Ge^{-ik_0x}$$
$$x \in (L, \infty): \quad \phi_{\rm III}''(x) + k^2\phi_{\rm III}(x) = 0 \quad \Rightarrow \quad \phi_{\rm III}(x) = Ce^{ikx} + De^{-ikx}$$

with $k^2 = 2mE/\hbar^2$, $k_0^2 = 2m(E-V_0)/\hbar^2$ $(k \in \mathbb{R})$

- Continuity conditions:

$$\phi_{\rm I}(0) = \phi_{\rm II}(0): \quad A + B = F + G$$
$$\phi_{\rm I}'(0) = \phi_{\rm II}'(0): \quad k(A-B) = k_0(F-G)$$
$$\phi_{\rm II}(L) = \phi_{\rm III}(L): \quad Ce^{ikL} + De^{-ikL} = Fe^{ik_0L} + Ge^{-ik_0L}$$
$$\phi_{\rm II}'(L) = \phi_{\rm III}'(L): \quad k(Ce^{ikL} - De^{-ikL}) = k_0(Fe^{ik_0L} - Ge^{-ik_0L})$$

Boundary conditions:
consider incoming (and possibly reflected) waves from the left: $D = 0$

$$x = 0: \quad \frac{A+B}{k(A-B)} = \frac{F+G}{k_0(F-G)} \quad \Rightarrow \quad \frac{1+B/A}{1-B/A} = \frac{k}{k_0}\frac{1+G/F}{1-G/F}$$

$$x = L: \quad \frac{1}{k} = \frac{Fe^{ik_0L} + Ge^{-ik_0L}}{k_0(Fe^{ik_0L} - Ge^{-ik_0L})} \quad \Rightarrow \quad \frac{k_0}{k} = \frac{e^{2ik_0L} + G/F}{e^{2ik_0L} - G/F}$$

$$\Rightarrow \quad e^{2ik_0L}[\frac{k_0}{k} - 1] = \frac{G}{F}[\frac{k_0}{k} + 1] \quad \Rightarrow \quad \frac{G}{F} = e^{2ik_0L}\frac{k_0-k}{k_0+k}$$

Combine:

$$\frac{1+B/A}{1-B/A} = \frac{k}{k_0}\frac{1 + e^{2ik_0L}\frac{k_0-k}{k_0+k}}{1 - e^{2ik_0L}\frac{k_0-k}{k_0+k}} = \frac{k}{k_0}\,\frac{k_0 + k + e^{2ik_0L}(k_0-k)}{k_0 + k - e^{2ik_0L}(k_0-k)}$$

$$= \frac{k}{k_0}\,\frac{(k_0+k)e^{-ik_0L} + e^{ik_0L}(k_0-k)}{(k_0+k)e^{-ik_0L} - e^{ik_0L}(k_0-k)} = \frac{k}{k_0}\,\frac{k_0\cos(k_0L) - ik\sin(k_0L)}{k\cos(k_0L) - ik_0\sin(k_0L)}$$

$$= \frac{1 - i(k/k_0)\tan(k_0L)}{1 - i(k_0/k)\tan(k_0L)}$$

Hence

$$(1+B/A)[1-i(k_0/k)\tan(k_0L)] = [1-i(k/k_0)\tan(k_0L)](1-B/A)$$

$$i\tan(k_0L)\frac{k^2-k_0^2}{kk_0} = \frac{B}{A}\left[i\tan(k_0L)\frac{k^2+k_0^2}{kk_0}-2\right]$$

$$\frac{B}{A} = \frac{(k^2-k_0^2)\tan(k_0L)}{(k^2+k_0^2)\tan(k_0L)+2ikk_0}$$

4.3.2. Interpretation: Reflection and Transmission

- Calculate the probability current $j(x)$

$$j(x) = -\frac{i\hbar}{2m}[\phi^*\frac{\partial\phi}{\partial x}-\phi\frac{\partial\phi^*}{\partial x}]$$

$$j_{\rm I}(x) = -\frac{i\hbar}{2m}ik\left[(A^*e^{-ikx}+B^*e^{ikx})(Ae^{ikx}-Be^{-ikx})+(Ae^{ikx}+Be^{-ikx})(A^*e^{-ikx}-B^*e^{ikx})\right]$$

$$= \frac{\hbar k}{2m}\,2\mathrm{Re}\left[|A|^2-A^*Be^{-2ikx}+B^*Ae^{2ikx}-|B|^2\right] = \frac{\hbar k}{m}\left[|A|^2-|B|^2\right]$$

Other regions similar, hence:

region I : $\quad j(x) = \frac{\hbar k}{m}\left[|A|^2-|B|^2\right]$

region II : $\quad$ if $k_0 \in \mathbb{R}$: $\quad j(x) = \frac{\hbar k}{m}\left[|F|^2-|G|^2\right] \qquad$ (different if $k_0 \notin \mathbb{R}$)

region III : $\quad j(x) = \frac{\hbar k}{m}|C|^2$

Note: $\hbar k/m = p/m = v$ (velocity of a plane wave), so

$(\hbar k/m)|A|^2$ = strength of *incoming* wave
$(\hbar k/m)|B|^2$ = strength of *reflected* wave
$(\hbar k/m)|C|^2$ = strength of *transmitted* wave

Note also: general equation $\frac{d}{dt}|\psi|^2+\boldsymbol{\nabla}\cdot\boldsymbol{j}=0$ reduces here to $\frac{\partial}{\partial x}j(x)=0$
Hence $j(x)$ is independent of x
Hence: $|A|^2-|B|^2 = |C|^2$

- Define reflection and transmission coefficients:
(note: k_0 is either real, for $E > V_0$, or purely imaginary, for $E < V_0$)

$$\mathrm{R} = \frac{(\hbar k/m)|B|^2}{(\hbar k/m)|A|^2} = \frac{|B|^2}{|A|^2} = \left|\frac{(k^2-k_0^2)\tan(k_0L)}{(k^2+k_0^2)\tan(k_0L)+2ikk_0}\right|^2$$

$$= \left|\frac{(k^2+k_0^2)\tan(k_0L)+2ikk_0}{(k^2-k_0^2)\tan(k_0L)}\right|^{-2} = \left[\frac{(k^2+k_0^2)^2\tan^2(k_0L)+4k^2k_0^2}{(k^2-k_0^2)^2\tan^2(k_0L)}\right]^{-1}$$

$$= \; = \left[1+\frac{4k^2k_0^2\tan^2(k_0L)+4k^2k_0^2}{(k^2-k_0^2)^2\tan^2(k_0L)}\right]^{-1} = \left[1+\frac{4k^2k_0^2}{(k^2-k_0^2)^2\sin^2(k_0L)}\right]^{-1}$$

$$\mathrm{T} = \frac{(\hbar k/m)|C|^2}{(\hbar k/m)|A|^2} = \frac{|C|^2}{|A|^2} = \frac{|A|^2 - |B|^2}{|A|^2} = 1 - \mathrm{R}$$

Note: $k^2 = 2mE/\hbar^2$, $k_0^2 = 2m(E - V_0)/\hbar^2$
$E < V_0$: $k_0 = i\hbar^{-1}\sqrt{2m(V_0 - E)}$
$E \geq V_0$: $k_0 = \hbar^{-1}\sqrt{2m(E - V_0)}$
(in former case: use $\sin^2(iq) = [\frac{1}{2i}(e^{-q} - e^{q})]^2 = -\sinh^2(q)$)

- Classical result:

$$E < V_0: \quad \mathrm{T} = 0$$
$$E > V_0: \quad \mathrm{T} = 1$$

QM result :

$$E < V_0: \quad \mathrm{T} = 1 - \left[1 - \frac{4(E/V_0)(E/V_0 - 1)}{\sinh^2(\sqrt{2m(V_0 - E)}L/\hbar)}\right]^{-1}$$
$$E \geq V_0: \quad \mathrm{T} = 1 - \left[1 + \frac{4(E/V_0)(E/V_0 - 1)}{\sin^2(\sqrt{2m(E - V_0)}L/\hbar)}\right]^{-1}$$

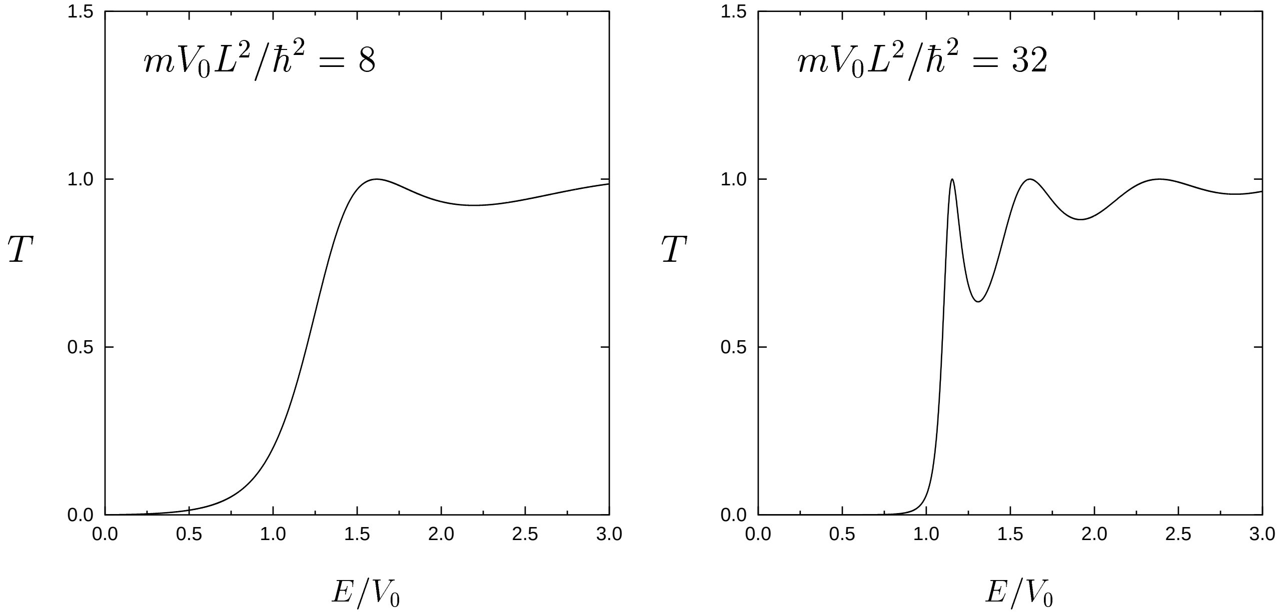
 - $\mathrm{T} > 0$ *even when* $E < V_0$ ('tunneling')
   QM particle can be found in classically forbidden regions

 - $\lim_{E/V_0 \to 0} \mathrm{T} = 0$

 - $\lim_{E/V_0 \to \infty} \mathrm{T} = 1$

 - $\lim_{E/V_0 \to 1} \mathrm{T} = [1 + mV_0L^2/2\hbar^2]^{-1}$

 - $\mathrm{T} = 1$ for $\sin(\sqrt{2m(E - V_0)}L/\hbar) = 0$ $(E > V_0)$,
   i.e. for $\sqrt{2m(E - V_0)}L/\hbar = n\pi$ with $n \in \{1, 2, 3, \ldots\}$)
   i.e. for $E = V_0 + n^2\pi^2\hbar^2/2mL^2$ (Ramsauer-Townsend effect)



$mV_0L^2/\hbar^2 = 8$
T
E/V_0
0.0
0.5
1.0
1.5
2.0
2.5
3.0
$mV_0L^2/\hbar^2 = 32$
T
E/V_0

4.4. The Harmonic Oscillator

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2$$

Note: in 1900 Planck triggered QM by just *assuming* that $E_n = n.\hbar\omega$ in order to get the elusive blackbody radiation law right ...

4.4.1. Solution of Schrödinger Equation

- Solve SE in $(-\infty, \infty)$ by separation of variables:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\phi(x) + \frac{1}{2}m\omega^2 x^2\phi(x) = E\phi(x)$$
$$\psi(x,t) = \sum_n c_n e^{-iE_n t/\hbar}\phi_n(x)$$

  (or integral, dependent on spectrum $\{E_n\}$)
  Note: since we know that $\langle p^2\rangle \geq 0$ and $\langle V\rangle \geq 0$ (for any state ψ): $E \geq 0$

  We define $u = x\sqrt{m\omega/\hbar}$, so $d^2/dx^2 = (m\omega/\hbar)(d^2/du^2)$
  To be solved:

$$-\frac{\hbar^2}{2m}\frac{m\omega}{\hbar}\frac{d^2}{du^2}\phi + \frac{1}{2}m\frac{\hbar}{m\omega}\omega^2 u^2\phi = E\phi$$
$$\text{so :}\qquad \frac{d^2}{du^2}\phi - u^2\phi = -\frac{2E}{\hbar\omega}\phi$$

- Behaviour for $u \to \pm\infty$:

$$\lim_{u\to\pm\infty}\frac{1}{u^2\phi}\frac{d^2}{du^2}\phi = 1$$

  Put $\phi = e^{\chi}$:

$$\lim_{u\to\pm\infty}\frac{1}{u^2}e^{-\chi}\frac{d}{du}\left[e^{\chi}\frac{d}{du}\chi\right] = 1$$
$$\lim_{u\to\pm\infty}\frac{1}{u^2}e^{-\chi}\left[e^{\chi}\left(\frac{d}{du}\chi\right)^2 + e^{\chi}\frac{d^2}{du^2}\chi\right] = 1$$
$$\lim_{u\to\pm\infty}\frac{1}{u^2}\left[\left(\frac{d}{du}\chi\right)^2 + \frac{d^2}{du^2}\chi\right] = 1$$

  Two independent solutions: $\chi = \pm\frac{1}{2}u^2$, i.e. $\phi = e^{\pm\frac{1}{2}u^2}$ $(u \to \pm\infty)$
  Demand normalization: $\phi \to e^{-\frac{1}{2}u^2}$ as $|u| \to \infty$

- Transformation suggested by asymptotic behaviour: $\phi = e^{-\frac{1}{2}u^2}H(u)$
  Eqn for $H(u)$:

$$\frac{d^2}{du^2}\left[e^{-\frac{1}{2}u^2}H(u)\right] - u^2 e^{-\frac{1}{2}u^2}H(u) = -\frac{2E}{\hbar\omega}e^{-\frac{1}{2}u^2}H(u)$$

$$e^{\frac{1}{2}u^2}\frac{d^2}{du^2}\left[e^{-\frac{1}{2}u^2}H(u)\right] - u^2H(u) = -\frac{2E}{\hbar\omega}H(u)$$
$$e^{\frac{1}{2}u^2}\frac{d}{du}\left[e^{-\frac{1}{2}u^2}H'(u) - ue^{-\frac{1}{2}u^2}H(u)\right] - u^2H(u) = -\frac{2E}{\hbar\omega}H(u)$$
$$e^{\frac{1}{2}u^2}\left[e^{-\frac{1}{2}u^2}H''(u) - 2ue^{-\frac{1}{2}u^2}H'(u) + (u^2-1)e^{-\frac{1}{2}u^2}H(u)\right] - u^2H(u) = -\frac{2E}{\hbar\omega}H(u)$$
$$\text{thus :} \qquad H''(u) - 2uH'(u) = [1 - \frac{2E}{\hbar\omega}]H(u)$$

- Assume $H(u)$ is analytic
construct solutions in the form of power series: $H(u) = \sum_{\ell=0}^{\infty} a_\ell u^\ell$
Substitute into eqn:

$$(\forall u \in \mathbb{R}): \qquad \sum_{\ell=2}^{\infty} a_\ell \ell(\ell-1)u^{\ell-2} - 2\sum_{\ell=0}^{\infty} a_\ell \ell u^\ell = [1-\frac{2E}{\hbar\omega}]\sum_{\ell=0}^{\infty} a_\ell u^\ell$$
$$(\forall u \in \mathbb{R}): \qquad \sum_{\ell=0}^{\infty} a_{\ell+2}(\ell+2)(\ell+1)u^\ell - 2\sum_{\ell=0}^{\infty} a_\ell \ell u^\ell = [1-\frac{2E}{\hbar\omega}]\sum_{\ell=0}^{\infty} a_\ell u^\ell$$
$$(\forall u \in \mathbb{R}): \qquad \sum_{\ell=0}^{\infty}\left\{a_{\ell+2}(\ell+2)(\ell+1)u^\ell - \left[2\ell + [1-\frac{2E}{\hbar\omega}]\right]a_\ell\right\}u^\ell = 0$$

Conclusion:

$$(\forall \ell \geq 0 :) \qquad a_{\ell+2} = \frac{2a_\ell}{(\ell+2)(\ell+1)}\left[\ell + (\frac{1}{2} - \frac{E}{\hbar\omega})\right]$$

Two types of solutions:

$$\text{truncating series :} \quad \frac{E}{\hbar\omega} - \frac{1}{2} = n \quad \text{for some } n \in \mathbb{N}$$
$$\text{infinite series :} \quad \frac{E}{\hbar\omega} - \frac{1}{2} \notin \mathbb{N}$$

We show that, if they converge, the non-truncating series give non-normalizable solutions:
(note: even and odd powers give two *independent* solutions)

$$\lim_{\ell\to\infty}\frac{\ell a_{\ell+2}}{a_\ell} = \lim_{\ell\to\infty}\frac{2\ell}{(\ell+2)(\ell+1)}\left[\ell + (\frac{1}{2} - \frac{E}{\hbar\omega})\right] = 2$$
$$\text{hence for } \ell \to \infty : \qquad a_{\ell+2} \sim a_\ell/\ell$$

Asymptotic solutions:
$a_\ell = 1/(\ell/2)!$ for $\ell \to \infty$ even, $a_\ell = 1/(\ell/2 - 1/2)!$ for $\ell \to \infty$ odd
verification:

$$\ell \text{ even :} \quad \lim_{\ell\to\infty}\frac{\ell a_{\ell+2}}{a_\ell} = \lim_{\ell\to\infty}\frac{\ell(\ell/2)!}{(\ell/2+1)!} = \lim_{\ell\to\infty}\frac{\ell}{\ell/2+1} = 2$$
$$\ell \text{ odd :} \quad \lim_{\ell\to\infty}\frac{\ell a_{\ell+2}}{a_\ell} = \lim_{\ell\to\infty}\frac{\ell(\ell/2-1/2)!}{(\ell/2+1/2)!} = \lim_{\ell\to\infty}\frac{\ell}{\ell/2+1/2} = 2$$

We conclude for the non-truncating series:

$$\text{even}: \quad H^+(u) \;\to\; \sum_{\ell\geq 0,\ \text{even}} \frac{u^\ell}{(\ell/2)!} = \sum_{k=0}^{\infty} \frac{u^{2k}}{k!} = e^{u^2} \qquad (|u|\to\infty)$$

$$\text{odd}: \quad H^-(u) \;\to\; \sum_{\ell\geq 1,\ \text{odd}} \frac{u^\ell}{(\ell/2-1/2)!} = \sum_{k=0}^{\infty} \frac{u^{2k+1}}{k!} = ue^{u^2} \qquad (|u|\to\infty)$$

This leads to the two asymptotic solutions $\phi^+ = e^{\frac{1}{2}u^2}$ and $\phi^- = ue^{\frac{1}{2}u^2}$
both are not normalizable

- Conclusion: normalizable solutions correspond to

$$E_n = [n+\frac{1}{2}]\hbar\omega \qquad n\in\{0,1,2,3,\ldots\}$$

$$\phi_n(x) = e^{-\frac{1}{2}m\omega x^2/\hbar} H_n(x\sqrt{m\omega/\hbar}), \qquad H_n(u): \ \text{Hermite polynomials}$$

Properties of $H_n(u)$:

- solutions of: $H''(u) - 2uH'(u) + 2nH_n(u) = 0$
- $\frac{d}{du}H_n(u) = 2nH_{n-1}(u)$
- $H_n(u) = (-1)^n e^{u^2}(d^n e^{-u^2}/du^n)$
- examples: $H_0(u)=1$, $H_1(u)=2u$, $H_2(u)=-2+4u^2$, $H_3(u)=-12u+8u^3$, …
- orthogonality: $\int du H_n(u)H_m(u)e^{-u^2} = 2^n n!\sqrt{\pi}\delta_{mn}$

Now also $\{\phi_n\}$ orthogonal:

$$\int dx\ \phi_n^*(x)\phi_m(x) = \int dx\ e^{-m\omega x^2/\hbar} H_n(x\sqrt{m\omega/\hbar})H_m(x\sqrt{m\omega/\hbar})$$

$$= \sqrt{\frac{\hbar}{m\omega}}\int du\ e^{-u^2}H_n(u)H_m(u) = \sqrt{\frac{\hbar}{m\omega}}2^n n!\sqrt{\pi}\ \delta_{mn}$$

One can prove: $\{\phi_n\}$ are also *complete* in $L^2(\mathbb{R})$

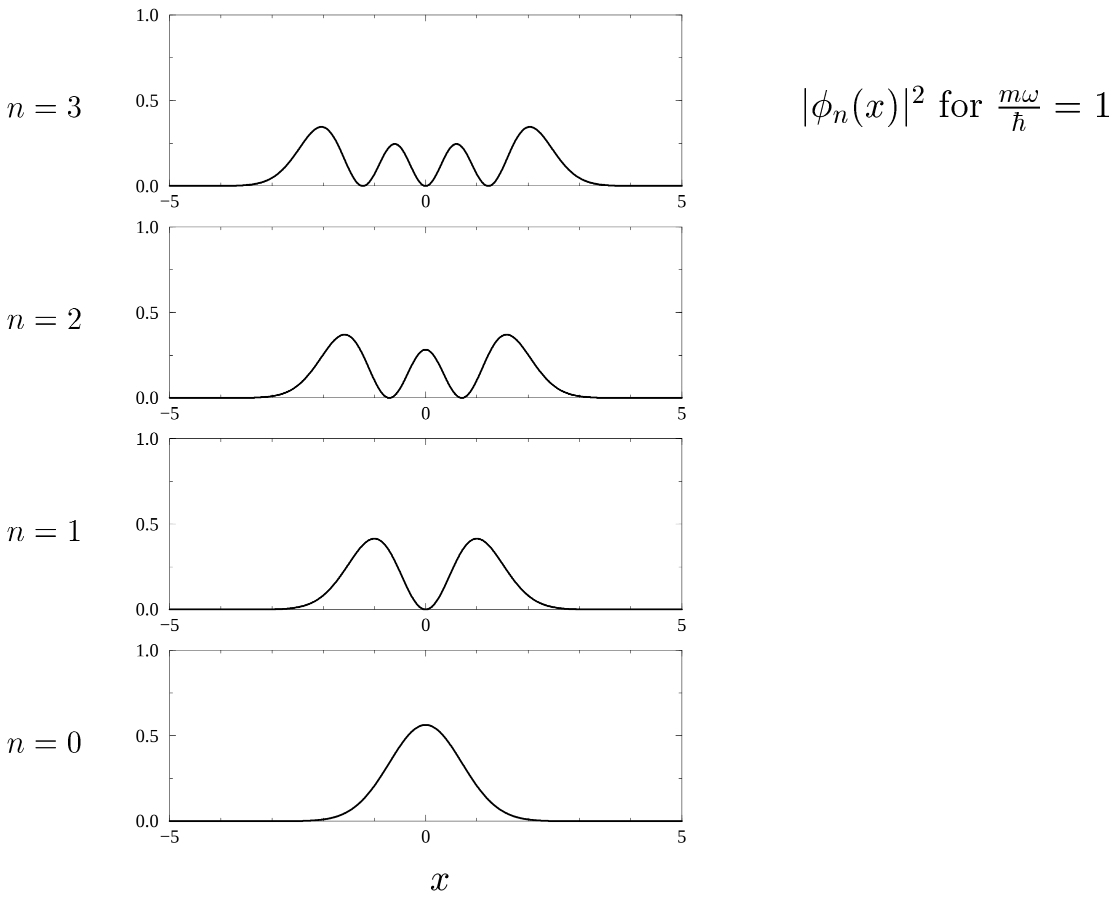
- Normalize ϕ_n:
$\phi_n \to C_n e^{-\frac{1}{2}m\omega x^2/\hbar}H_n(x\sqrt{m\omega/\hbar})$

$$|\phi_n|^2 = |C_n|^2\sqrt{\frac{\hbar}{m\omega}}2^n n!\sqrt{\pi} \qquad \Rightarrow \qquad C_n = \left[\frac{\sqrt{m\omega}}{2^n n!\sqrt{\hbar\pi}}\right]^{\frac{1}{2}}$$

$$\phi_n(x) = \left[\frac{\sqrt{m\omega}}{2^n n!\sqrt{\hbar\pi}}\right]^{\frac{1}{2}} e^{-\frac{1}{2}m\omega x^2/\hbar}H_n(x\sqrt{m\omega/\hbar})$$

General solution of SE:

$$\psi(x,t) = \sum_{n=0}^{\infty} c_n e^{-i(n+\frac{1}{2})\omega t}\phi_n(x) \qquad c_n = \int_{-\infty}^{\infty} dx\ \phi_n(x)\psi(x,0)$$



4.4.2. Expectation Values and Uncertainties

Choose simple initial conditions: $c_n = \delta_{n\ell}$

$$\psi(x,t) = e^{-iE_\ell t/\hbar}\phi_\ell(x) \qquad \phi_\ell(x) = C_\ell \; e^{-\frac{1}{2}m\omega x^2/\hbar} H_\ell(x\sqrt{m\omega/\hbar})$$

$$C_\ell = \left[\frac{\sqrt{m\omega}}{2^\ell \ell! \sqrt{\hbar\pi}}\right]^{\frac{1}{2}} \qquad E_\ell = (\ell + \frac{1}{2})\hbar\omega$$

(so $H\psi = E_\ell\psi$ for all t)

- Position:

$$\langle x \rangle = \int_{-\infty}^{\infty} dx \; \psi^* x \psi = C_\ell^2 \int_{-\infty}^{\infty} dx \; x e^{-m\omega x^2/\hbar} H_\ell^2(x\sqrt{m\omega/\hbar}) = 0$$

(integration of an odd function over $(-\infty, \infty)$!)

- Momentum:

$$\langle p \rangle = -i\hbar \int_{-\infty}^{\infty} dx \; \psi^* \frac{\partial}{\partial x}\psi$$

$$\begin{aligned} &= -i\hbar C_\ell^2 \int_{-\infty}^{\infty} dx\ e^{-\frac{1}{2}m\omega x^2/\hbar} H_\ell(x\sqrt{m\omega/\hbar}) \frac{\partial}{\partial x}\left\{e^{-\frac{1}{2}m\omega x^2/\hbar} H_\ell(x\sqrt{m\omega/\hbar})\right\} \\ &= -i\hbar C_\ell^2 \int_{-\infty}^{\infty} dx\ e^{-\frac{1}{2}m\omega x^2/\hbar} H_\ell(x\sqrt{m\omega/\hbar}) \left\{\sqrt{\frac{m\omega}{\hbar}} e^{-\frac{1}{2}m\omega x^2/\hbar} H'_\ell(x\sqrt{m\omega/\hbar}) \right. \\ &\qquad \left. - \frac{m\omega x}{\hbar} e^{-\frac{1}{2}m\omega x^2/\hbar} H_\ell(x\sqrt{m\omega/\hbar})\right\} \\ &= -iC_\ell^2\sqrt{m\hbar\omega} \int_{-\infty}^{\infty} dx\ e^{-m\omega x^2/\hbar} H_\ell(x\sqrt{m\omega/\hbar}).2\ell H'_{\ell-1}(x\sqrt{m\omega/\hbar}) \\ &\qquad + iC_\ell^2 m\omega \int_{-\infty}^{\infty} dx\ x e^{-m\omega x^2/\hbar} H_\ell^2(x\sqrt{m\omega/\hbar}) = 0 \end{aligned}$$

(integration of odd functions over $(-\infty,\infty)$)

- Calculate $\langle x^2\rangle$ and $\langle p^2\rangle$ using the Virial Theorem (proof given in exercise 9):

$$\frac{d}{dt}\langle xp\rangle = \frac{1}{m}\langle p^2\rangle - \langle x\frac{dV}{dx}\rangle$$

$$-i\hbar\frac{d}{dt}\int dx\ \psi^*(x,t)\left[x\frac{\partial}{\partial x}\right]\psi(x,t) = \frac{1}{m}\langle p^2\rangle - m\omega^2\langle x^2\rangle$$

$$-i\hbar\frac{d}{dt}\int dx\ \phi_\ell(x)\left[x\frac{\partial}{\partial x}\right]\phi_\ell(x) = \frac{1}{m}\langle p^2\rangle - m\omega^2\langle x^2\rangle$$

$$\frac{1}{m}\langle p^2\rangle - m\omega^2\langle x^2\rangle = 0 \qquad \Rightarrow \qquad \langle p^2\rangle = (m\omega)^2\langle x^2\rangle$$

Combine with $E_\ell = (\ell+\frac{1}{2})\hbar\omega = \langle p^2\rangle/2m + \frac{1}{2}m\omega^2\langle x^2\rangle$:

$$\langle x^2\rangle = (\ell+\frac{1}{2})\frac{\hbar}{m\omega} \qquad \langle p^2\rangle = (\ell+\frac{1}{2})\hbar m\omega$$

Uncertainties:

$$\Delta x = \sqrt{\langle x^2\rangle - \langle x\rangle^2} = \sqrt{(\ell+\frac{1}{2})\frac{\hbar}{m\omega}}$$

$$\Delta p = \sqrt{\langle p^2\rangle - \langle p\rangle^2} = \sqrt{(\ell+\frac{1}{2})\hbar m\omega}$$

- Energy:

$$\begin{aligned} \langle H\rangle &= E_\ell = (\ell+\frac{1}{2})\hbar\omega \\ \langle H^2\rangle &= E_\ell^2 = (\ell+\frac{1}{2})^2\hbar^2\omega^2 \\ \Delta H &= \sqrt{\langle H^2\rangle - \langle H\rangle^2} = \sqrt{0} = 0 \end{aligned}$$

Note:

$$\Delta x.\Delta p = \sqrt{(\ell+\frac{1}{2})\frac{\hbar}{m\omega}}.\sqrt{(\ell+\frac{1}{2})\hbar m\omega} = \frac{1}{2}\hbar(1+2\ell)$$

4.4.3. Algebraic Solution of SE for Harmonic Oscillator

As an alternative to the previous analysis at the level of functions and differential equations, we now turn to solution at the operator level. This will turn out to be much simpler.

Define:

$$\text{annihilation operator :} \quad a = \left[\frac{m\omega}{2\hbar}\right]^{\frac{1}{2}}[x + \frac{ip}{m\omega}]$$

$$\text{creation operator :} \quad a^\dagger = \left[\frac{m\omega}{2\hbar}\right]^{\frac{1}{2}}[x - \frac{ip}{m\omega}]$$

$$\text{number operator :} \quad N = a^\dagger a$$

- Fact: $H = \hbar\omega(N + \frac{1}{2})$
  Proof (use $[x, p] = i\hbar$):

$$\hbar\omega N = \hbar\omega a^\dagger a = \frac{1}{2}m\omega^2[x - \frac{ip}{m\omega}][x + \frac{ip}{m\omega}] = \frac{1}{2}m\omega^2\left[x^2 + \frac{i}{m\omega}[x,p] + \frac{p^2}{m^2\omega^2}\right]$$
$$= \frac{1}{2}m\omega^2x^2 - \frac{1}{2}\hbar\omega + \frac{p^2}{2m} = H - \frac{1}{2}\hbar\omega$$

  Hence, solving the time-independent SE $\Leftrightarrow$ finding eigenfunctions of $N = a^\dagger a$
  Note: if $H\phi_n = E_n\phi_n$, then $E_n \geq \frac{1}{2}\hbar\omega$ (follows from $H = \hbar\omega(N + \frac{1}{2})$ and $N = a^\dagger a$)
- Theorem 1: $(\forall n \in \mathbb{N}, \geq 1)$: $[a, a^{\dagger n}] = na^{\dagger\ n-1}$
  Proof by induction:

$$n = 1: \quad [a, a^\dagger] = \frac{m\omega}{2\hbar}[x + \frac{ip}{m\omega}, x - \frac{ip}{m\omega}] = -\frac{i}{2\hbar}.2[x,p] = 1 \qquad \text{OK}$$
$$n \to n+1: \quad [a, a^{\dagger\ n+1}] = a^\dagger[a, a^{\dagger n}] + [a, a^\dagger]a^{\dagger\ n} = a^\dagger.na^{\dagger\ n-1} + 1.a^{\dagger\ n}$$
$$= (n+1)a^{\dagger n} \qquad \text{OK}$$

- Theorem 2: $(\forall n \in \mathbb{N}, \geq 1)$: $[H, a^{\dagger n}] = \hbar\omega na^{\dagger n}$
  Proof (use theorem 1):

$$[H, a^{\dagger n}] = \hbar\omega[a^\dagger a, a^{\dagger n}] = \hbar\omega\left\{a^\dagger[a, a^{\dagger n}] + [a^\dagger, a^{\dagger n}]a\right\} = \hbar\omega\left\{a^\dagger.na^{\dagger\ n-1} + 0\right\}$$
$$= \hbar\omega na^{\dagger n}$$

- Define $E_0 = \min_n\{E_n\}$, with eigenfunction $H\phi_0 = E_0\phi_0$
  Define $\phi_n = a^{\dagger n}\phi_0$, and use theorem 2:

$$0 = [H, a^{\dagger n}]\phi_0 - \hbar\omega na^{\dagger n}\phi_0 = Ha^{\dagger n}\phi_0 - a^{\dagger n}H\phi_0 - \hbar\omega na^{\dagger n}\phi_0$$
$$= H\phi_n - E_0\phi_n - \hbar\omega n\phi_n$$

  Hence: $H\phi_n = (E_0 + n\hbar\omega)\phi_n$, with $E_0 \geq \frac{1}{2}\hbar\omega$
- Finding E_0: determine properties of ϕ_0, use $[a, a^\dagger] = 1$

$$Na\phi_0 = (a^\dagger a)a\phi_0 = (aa^\dagger - 1)a\phi_0 = a(a^\dagger a - 1)\phi_0 = a(N-1)\phi_0$$

$$H a\phi_0 = \hbar\omega(N+\frac{1}{2})a\phi_0 = \hbar\omega(aN - a + \frac{1}{2}a)\phi_0 = \hbar\omega a(N-\frac{1}{2})\phi_0$$
$$= a(H-\hbar\omega)\phi_0 = a(E_0-\hbar\omega)\phi_0 = (E_0-\hbar\omega)a\phi_0$$

Conflict with our assumption that E_0 is smallest eigenvalue, unless: $a\phi_0 = 0$

$$a\phi_0 = 0 \quad \text{and} \quad \hbar\omega(a^\dagger a + \frac{1}{2})\phi_0 = E_0\phi_0 : \qquad E_0 = \frac{1}{2}\hbar\omega$$

Corresponding function:

$$[x + \frac{ip}{m\omega}]\phi_0 = 0 : \quad \frac{\hbar}{m\omega}\frac{d}{dx}\phi_0 = -\frac{m\omega x}{\hbar}\phi_0 \quad \Rightarrow \quad \phi_0(x) = e^{-m\omega x^2/2\hbar}$$

- We now have $H\phi_n = \hbar\omega(n+\frac{1}{2})\hbar\omega\phi_n$ and $N\phi_n = n\phi_n$
- Normalization of ϕ_n: $\phi_n = C_n a^{\dagger n}\phi_0$ (hence $C_0 = 1$ if ϕ_0 normalized)
  Use $[a, a^\dagger] = 1$ and demand $|\phi_n| = 1$:

$$1 = |C_n|^2\langle a^{\dagger n}\phi_0|a^{\dagger n}\phi_0\rangle = \langle a^{\dagger\ n-1}\phi_0|(aa^\dagger)a^{\dagger\ n-1}\phi_0\rangle = \langle a^{\dagger\ n-1}\phi_0|(aa^\dagger)a^{\dagger\ n-1}\phi_0\rangle$$
$$= \langle a^{\dagger\ n-1}\phi_0|(N+1)a^{\dagger\ n-1}\phi_0\rangle = \frac{|C_n|^2}{|C_{n-1}|^2}\langle\phi_{n-1}|(N+1)\phi_{n-1}\rangle = \frac{|C_n|^2}{|C_{n-1}|^2}n$$

$$\text{Hence}: \quad |C_n|^2 = \frac{|C_n|^2}{n} \quad \Rightarrow \quad C_n = \frac{C_0}{\sqrt{n!}} = \frac{1}{\sqrt{n!}} \quad \Rightarrow \quad \phi_n = \frac{1}{\sqrt{n!}}a^{\dagger n}\phi_0$$

- We have proven generally that $\langle\phi_n|\phi_m\rangle = 0$ if $E_n \neq E_n$ (for any QM system !) so we do not need to verify orthogonality of the $\{\phi_n\}$. Let us check for fun. First assume $m > n > 0$:

$$\sqrt{m!n!}\langle\phi_m|\phi_n\rangle = \langle a^{\dagger m}\phi_0|a^{\dagger n}\phi_0\rangle = \langle a^{\dagger m-n}\phi_0|a^n a^{\dagger n}\phi_0\rangle = \langle a^{\dagger m-n}\phi_0|a^{n-1}(aa^\dagger)a^{\dagger n-1}\phi_0\rangle$$
$$= \langle a^{\dagger m-n}\phi_0|a^{n-1}(N+1)a^{\dagger n-1}\phi_0\rangle = n\langle a^{\dagger m-n}\phi_0|a^{n-1}a^{\dagger n-1}\phi_0\rangle$$

Repeat argument until all a in right-hand side of the inner product have vanished:

$$\sqrt{m!n!}\langle\phi_m|\phi_n\rangle = n!\langle a^{\dagger m-n}\phi_0|\phi_0\rangle$$

Note: this statement is also true when $m > n = 0$. Finally, since $m > n$ we can move over one more $a^\dagger$ from left to right, and use $a\phi_0 = 0$:

$$\sqrt{m!n!}\langle\phi_m|\phi_n\rangle = n!\langle a^{\dagger m-n-1}\phi_0|a\phi_0\rangle = 0 \qquad \text{hence} \qquad \langle\phi_m|\phi_n\rangle = 0$$

Summary of results (with $n = 0, 1, 2, 3, \ldots$):

$$\phi_0(x) = \left[\frac{m\omega}{\hbar\sqrt{\pi}}\right]^{\frac{1}{2}} e^{-\frac{1}{2}m\omega x^2/\hbar} \qquad \phi_n = \frac{1}{\sqrt{n!}}a^{\dagger n}\phi_0 \qquad E_n = \hbar\omega(n+\frac{1}{2})$$

$$\langle\phi_n|\phi_m\rangle = \delta_{nm} \qquad a^\dagger\phi_n = \sqrt{n+1}\phi_{n+1} \qquad a\phi_n = \sqrt{n}\phi_{n-1} \qquad N\phi_n = n\phi_n$$

$$x = \left[\frac{\hbar}{2m\omega}\right]^{\frac{1}{2}}(a^\dagger + a) \qquad p = i\left[\frac{\hbar m\omega}{2}\right]^{\frac{1}{2}}(a^\dagger - a)$$

Let us now calculate expectation values with these tools:
(note: $\langle\phi_n|a^\ell\phi_n\rangle = \langle\phi_n|a^{\dagger\ell}\phi_n\rangle = 0$ for all $\ell \in \{1, 2, 3, \ldots\}$)

- Position:

$$\begin{aligned}\langle\phi_n|x\phi_n\rangle &= \left[\frac{\hbar}{2m\omega}\right]^{\frac{1}{2}}\langle\phi_n|(a^\dagger+a)\phi_n\rangle = 0\\ \langle\phi_n|x^2\phi_n\rangle &= \frac{\hbar}{2m\omega}\langle\phi_n|(a^\dagger+a)^2\phi_n\rangle = \frac{\hbar}{2m\omega}\langle\phi_n|(a^\dagger a+aa^\dagger)\phi_n\rangle\\ &= \frac{\hbar}{2m\omega}\langle\phi_n|(2N+1)\phi_n\rangle = (n+\frac{1}{2})\frac{\hbar}{m\omega}\end{aligned}$$

- Momentum:

$$\begin{aligned}\langle\phi_n|p\phi_n\rangle &= i\left[\frac{\hbar m\omega}{2}\right]^{\frac{1}{2}}\langle\phi_n|(a^\dagger-a)\phi_n\rangle = 0\\ \langle\phi_n|p^2\phi_n\rangle &= -\frac{1}{2}\hbar m\omega\langle\phi_n|(a^\dagger-a)^2\phi_n\rangle = -\frac{1}{2}\hbar m\omega\langle\phi_n|(-a^\dagger a-aa^\dagger)\phi_n\rangle\\ &= \frac{1}{2}\hbar m\omega\langle\phi_n|(2N+1)\phi_n\rangle = (n+\frac{1}{2})\hbar m\omega\end{aligned}$$

5. Simultaneous Measurement and Uncertainty

5.1. Simultaneous Diagonalization of Operators

5.1.1. Operator Commutation and Existence of Common Eigenfunctions

Let A and B denote Hermitian operators, acting on Hilbert space $\mathcal{H}$,
and let A have a complete set of eigenfunctions $\{\phi_n\}$ in $\mathcal{H}$

Fact: A and B have complete set of *common* eigenfunctions in $\mathcal{H}$ if and only if $[A, B] = 0$

- PROOF (first part): *complete set of common e.f. implies* $[A, B] = 0$

  Assume: $\{\phi_n\}$ complete in $\mathcal{H}$, $(\forall n) : A\phi_n = a_n\phi_n$ and $B\phi_n = b_n\phi_n$

  $$(\forall n) : \quad [A, B]\phi_n = AB\phi_n - BA\phi_n = a_n b_n\phi_n - b_n a_n\phi_n = 0$$

  Each $\phi \in \mathcal{H}$ is a linear combination of $\{\phi_n\}$ (completeness), so: $(\forall\psi \in \mathcal{H}) : \ [A, B]\psi = 0$

- PROOF (second part): $[A, B] = 0$ *implies complete set of common e.f.*

  (i) Suppose eigenvalue a_n non-degenerate:

  $$0 = [A, B]\phi_n = AB\phi_n - BA\phi_n = A(B\phi_n) - a_n(B\phi_n)$$

  Since a_n non-degenerate: $B\phi_n = b_n\phi_n$, so ϕ_n is also eigenfunction of B, QED.

  (ii) Suppose eigenvalue a_n m-fold degenerate, i.e. $A\phi_{n\mu} = a_n\phi_{n\mu}$ for $\mu = 1, \ldots, m$:
  Call the degenerate eigenspace: $S_n \subset \mathcal{H}$
  One can always choose $\{\phi_{n\mu}\}$ orthonormal (Gram-Schmidt) in S_n
  Proceed as before:

  $$0 = [A, B]\phi_{n\mu} = AB\phi_{n\mu} - BA\phi_{n\mu} = A(B\phi_{n_\mu}) - a_n(B\phi_{n\mu})$$

  Hence: $B\phi_{n\mu}$ is in *same degenerate eigenspace*, so $(\exists D_{\mu\nu} \in \mathbb{C}) : \ B\phi_{n\mu} = \sum_{\nu=1}^m D_{\mu\nu}\phi_{n\nu}$
  Inner product with $\phi_{n\lambda}$: $\langle\phi_{n\lambda}|B\phi_{n\mu}\rangle = \sum_{\nu=1}^m D_{\mu\nu}\langle\phi_{n\lambda}|\phi_{n\nu}\rangle = D_{\mu\lambda}$

  Note: $\{D_{\mu\nu}\}$ is a complex $m \times m$ matrix, with $D_{\mu\nu} = D^*_{\nu\mu}$
  $\Rightarrow$ D^* is self-adjoint in vector space $\mathbb{C}^m$, with inner product $\boldsymbol{x} \cdot \boldsymbol{y} = \sum_{\mu=1}^m x^*_\mu y_\mu$
  $\Rightarrow$ D^* has m linearly independent eigenvectors $\boldsymbol{x}^\ell \in \mathbb{C}^m$, where $\ell = 1, \ldots, m$
  for all $\ell \in \{1, \ldots, m\}$: $\quad \sum_{\nu=1}^m D_{\nu\mu}x^\ell_\nu = d_\ell x^\ell_\mu$
  one can always choose $\{\boldsymbol{x}_\ell\}$ orthonormal (Gram-Schmidt) in $\mathbb{C}^m$

  Construct m new functions $\psi_{n\mu} \in S_n$: $\psi_{n\rho} = \sum_{\mu=1}^m x^\rho_\mu\phi_{n\mu}, \quad \rho = 1, \ldots, m$

  $$\langle\psi_{n\rho}|B\psi_{n\rho'}\rangle = \sum_{\mu,\nu=1}^m x^\rho_\mu x^{\rho'}_\nu \langle\phi_{n\mu}|B\phi_{n\nu}\rangle = \sum_{\mu,\nu=1}^m x^\rho_\mu x^{\rho'}_\nu D_{\nu\mu}$$

  $$= \sum_{\mu=1}^m x^\rho_\mu \sum_{\nu=1}^m D^*_{\mu\nu}x^{\rho'}_\nu = \sum_{\mu=1}^m x^\rho_\mu d_{\rho'} x^{\rho'}_\mu = d_\rho\delta_{\rho\rho'}$$

Note also: $\langle\psi_{n\rho}|\psi_{n\rho'}\rangle = \sum_{\mu,\nu=1}^{m} x_\mu^\rho x_\nu^{\rho'} \delta_{\mu\nu} = \delta_{\rho\rho'}$
We conclude: $\{\psi_{n\rho}\}$ are a *complete orthonormal basis* in S_n, such that $A\psi_{n\rho} = a_n\psi_{n\rho}$ and $B\psi_{n\rho} = d_n\psi_{n\rho}$, QED.

5.1.2. Example: Parity

Consider time-indep SE in one dimension, with $H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$

- Define *parity operator* P: $[P\psi](x) = \psi(-x)$
  Properties:
  (i) $P^\dagger = P$, since for any two functions ϕ and ψ:
  $$\langle\phi|P\psi\rangle - \langle\psi|P\phi\rangle^* = \int dx\, \{\phi^*(x)\psi(-x) - [\psi^*(x)\phi(-x)]^*\} = 0$$
  (ii) $P^2 = 1$, since for any function ψ: $[P^2\psi](x) = [P\psi](-x) = \psi(x)$
  (iii) Eigenvalues: $\lambda = \pm 1$. Proof: use $P^2 = 1$
  $$P\phi = \lambda\phi: \quad P^2\phi = \lambda^2\phi \quad \Rightarrow \quad \phi = \lambda^2\phi \quad \Rightarrow \quad \lambda^2 = 1$$
  (iv) Eigenfunctions:
  $$\lambda = 1: \quad P\phi = \phi \quad \Rightarrow \quad \phi(-x) = \phi(x) \quad \text{for all } x \in \mathbb{R}$$
  $$\lambda = -1: \quad P\phi = -\phi \quad \Rightarrow \quad \phi(-x) = -\phi(x) \quad \text{for all } x \in \mathbb{R}$$
  Eigenspace of $\lambda = 1$: all *even* functions of x
  Eigenspace of $\lambda = -1$: all *odd* functions of x
- Fact: $[P, H] = 0$ if $V(x) = V(-x)$ for all $x \in \mathbb{R}$
  Proof: consider arbitrary $\psi(x)$ and calculate $[P, H]\psi$. Define $\tilde{\psi}(x) = \psi(-x)$:
  $$\begin{aligned}([P,H]\psi)(x) &= (PH\psi)(x) - (HP\psi)(x) \\ &= (P[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi + V\psi])(x) - ([-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\tilde{\psi} + V\tilde{\psi}])(x) \\ &= -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\tilde{\psi}(x) + V(-x)\tilde{\psi}(x) + \frac{\hbar^2}{2m}\frac{d^2}{dx^2}\tilde{\psi}(x) - V(x)\tilde{\psi}(x) \\ &= [V(-x) - V(x)]\psi(-x) = 0\end{aligned}$$
- Hence: if $V(x) = V(-x)$ for all $x \in \mathbb{R}$ then
  H and P have a complete set of *common* eigenfunctions in $L^2(\mathbb{R})$
- Verify the validity for the normalizable solutions in the examples worked out so far:
  (i) Free particle in a box, zero boundaries:
  all eigenfunctions $\phi_n(x) = \sqrt{2/L}\sin(n\pi x/L)$ are odd
  (ii) Attractive δ-potential: eigenfunction $\phi(x) = (\sqrt{mg}/\hbar)e^{-mg|x|/\hbar^2}$ is even
  (iii) Harmonic oscillator: all eigenfunctions pf H are eigenfunctions of P
  Even functions: $\phi_n(x) = C_e^{-\frac{1}{2}m\omega x^2/\hbar} H_n(x\sqrt{m\omega}/\hbar)$ with n even
  Odd functions: $\phi_n(x) = C_e^{-\frac{1}{2}m\omega x^2/\hbar} H_n(x\sqrt{m\omega}/\hbar)$ with n odd

5.2. The Heisenberg Uncertainty Relations

5.2.1. Derivation and Consequences of Uncertainty Relations

- Definition:
  Heisenberg uncertainty relation for arbitrary Hermitian operators A and B acting in Hilbert space $\mathcal{H}$

$$\Delta A.\Delta B \geq \frac{1}{2}|\langle [A,B]\rangle|$$

Proof:
Consider an Hermitian operator $F : \mathcal{H} \to \mathcal{H}$ and a quantum system in state ψ. Note that

$$\begin{aligned}(\Delta F)^2 &= \langle (F-\langle F\rangle)^2\rangle = \langle \psi|(F-\langle F\rangle)^2\psi\rangle = \langle (F-\langle F\rangle)\psi|(F-\langle F\rangle)\psi\rangle \\ &= |(F-\langle F\rangle)\psi|^2\end{aligned}$$

Hence:

$$\begin{aligned}\Delta A.\Delta B &= |(A-\langle A\rangle)\psi||(B-\langle B\rangle)\psi| \geq |\langle (A-\langle A\rangle)\psi|(B-\langle B\rangle)\psi\rangle| \quad \text{(Schwartz)} \\ &= |\langle \psi|(A-\langle A\rangle)(B-\langle B\rangle)\psi\rangle|\end{aligned}$$

Now split the operator $G \equiv (A-\langle A\rangle)(B-\langle B\rangle)$ into Hermitian part $\frac{1}{2}(G+G^\dagger) \equiv \frac{1}{2}S$ and anti-Hermitian part $\frac{1}{2}(G-G^\dagger) \equiv \frac{1}{2}iC$. Thus $G = \frac{1}{2}S + \frac{1}{2}iC$, with $S^\dagger = S$ and $C^\dagger = C$:

$$\begin{aligned}S &= (A-\langle A\rangle)(B-\langle B\rangle) + (B-\langle B\rangle)(A-\langle A\rangle) \\ C &= \frac{1}{i}\left\{(A-\langle A\rangle)(B-\langle B\rangle) - (B-\langle B\rangle)(A-\langle A\rangle)\right\} \\ &= -i[A-\langle A\rangle, B-\langle B\rangle] = -i[A,B]\end{aligned}$$

Since $\langle S\rangle \in \mathbb{R}$ and $\langle C\rangle \in \mathbb{R}$:

$$\begin{aligned}\Delta A.\Delta B &= |\langle \psi|G\psi\rangle| = \frac{1}{2}|\langle \psi|(S+iC)\psi\rangle| = \frac{1}{2}|\langle S\rangle + i\langle C\rangle| = \frac{1}{2}\sqrt{\langle S\rangle^2 + \langle C\rangle^2} \\ &\geq \frac{1}{2}|\langle C\rangle| = \frac{1}{2}|\langle -i[A,B]\rangle| = \frac{1}{2}|\langle [A,B]\rangle| \qquad \text{QED}\end{aligned}$$

- Consequence:
  if two physical observables correspond to the quantum operators A and B, we can only know the values of these observables to unlimited accuracy *simultaneously* if $[A,B]=0$

  (conversely, if $[A,B]=0$ we know that A and B are simultaneously diagonalizable, and therefore also simultaneously measurable to arbitrary accuracy)

5.2.2. Examples & Applications

- Position and momentum: $[x_i, p_j] = i\hbar\delta_{ij}$

$$\Delta x_i.\Delta p_j \geq \frac{1}{2}|\langle [x_i,p_j]\rangle| = \frac{1}{2}\hbar\delta_{ij}$$

(confirm for the explicit solutions worked out earlier !)

- Position and energy: $[x_i, H] = [x_i, \boldsymbol{p}^2/2m] = \sum_j [x_i, p_j^2]/2m = \frac{p_i}{2m}[x_i, p_i] + [x_i, p_i]\frac{p_i}{2m} = \frac{i\hbar}{m}p_i$

$$\Delta x_i.\Delta H \geq \frac{1}{2}|\langle [x_i, H]\rangle| = \frac{\hbar}{2m}|\langle p_i\rangle|$$

- Angular momentum: $L_i = \sum_{jk} \epsilon_{ijk} x_j p_k$

  Let us first calculate some commutators:

  (i) $[L_i, L_j] = i\hbar \sum_k \epsilon_{ijk} L_k$

  Proof (see classical case worked out in exercises), use $\sum_i \epsilon_{ijk}\epsilon_{imn} = \delta_{jm}\delta_{kn} - \delta_{jn}\delta_{km}$:

$$\begin{aligned}
[L_i, L_j] &= \sum_{klmn} \epsilon_{ikl}\epsilon_{jmn}[x_k p_l, x_m p_n] = \sum_{klmn} \epsilon_{ikl}\epsilon_{jmn}\{x_k[p_l, x_m p_n] + [x_k, x_m p_n]p_l\} \\
&= \sum_{klmn} \epsilon_{ikl}\epsilon_{jmn}\{x_k x_m[p_l, p_n] + x_k[p_l, x_m]p_n + x_m[x_k, p_n]p_l + [x_k, x_m]p_n p_l\} \\
&= i\hbar \sum_{klmn} \epsilon_{ikl}\epsilon_{jmn}\{-\delta_{lm} x_k p_n + \delta_{kn} x_m p_l\} \\
&= -i\hbar \sum_{lnk} \epsilon_{lik}\epsilon_{lnj} x_k p_n + i\hbar \sum_{klm} \epsilon_{kli}\epsilon_{kjm} x_m p_l \\
&= -i\hbar \sum_{nk} [\delta_{in}\delta_{kj} - \delta_{ij}\delta_{kn}] x_k p_n + i\hbar \sum_{lm} [\delta_{lj}\delta_{im} - \delta_{lm}\delta_{ij}] x_m p_l \\
&= -i\hbar x_j p_i + i\hbar x_i p_j = i\hbar \sum_k \epsilon_{ijk} L_k
\end{aligned}$$

  (ii) $[L_i, \boldsymbol{L}^2] = 0$

  Proof:
$$\begin{aligned}
[L_i, \boldsymbol{L}^2] &= \sum_j [L_i, L_j^2] = \sum_j \{L_j[L_i, L_j] + [L_i, L_j]L_j\} \\
&= i\hbar \sum_{jk} \epsilon_{ijk}\{L_j L_k + L_k L_j\} = 0
\end{aligned}$$

  (since we sum over (j, k) an object which is anti-symmetric under $j \leftrightarrow k$)

  We now conclude the following from the uncertainty relations:

$$\Delta L_1.\Delta L_2 \geq \frac{1}{2}\hbar|\langle L_3\rangle| \qquad \Delta L_2.\Delta L_3 \geq \frac{1}{2}\hbar|\langle L_1\rangle| \qquad \Delta L_1.\Delta L_3 \geq \frac{1}{2}\hbar|\langle L_2\rangle|$$

  Yet, for every given i: L_i and $\boldsymbol{L}^2$ are simultaneously measurable to arbitrary accuracy.

6. Representations in Quantum Theory

6.1. Dirac's Bra-Ket Notation

Primary objective: reduce messy calculations to transparent symbolic manipulation
Secondary objective: generalize quantum formalism to arbitrary Hilbert spaces
Idea: exploit interpretation of inner product with a *fixed* vector as a linear functional on $\mathcal{H}$

$$\text{for given } \phi \in \mathcal{H} : \quad \langle\phi|.\rangle : \ \mathcal{H} \to \mathbb{C}$$

- Bra-vectors and Ket-vectors:
  (i) Write each ordinary element $\psi \in \mathcal{H}$ as a 'ket-vector': $|\psi\rangle$

Write basis elements $\phi_n \in \mathcal{H}$ as:	$|n\rangle$
If $\psi = \sum_n a_n \phi_n$:	$|\psi\rangle = \sum_n a_n |n\rangle$
Ket-vector corresponding to $\lambda\psi$ ($\lambda \in \mathbb{C}$):	$\lambda|\psi\rangle$
Ket-vector corresponding to $A\psi$ ($A : \mathcal{H} \to \mathcal{H}$):	$A|\psi\rangle$

  (ii) Write the linear functional associated with each $|\psi\rangle \in \mathcal{H}$ as a 'bra-vector': $\langle\psi|$

Write the functional associated with a basis element $\phi_n \in \mathcal{H}$ as:	$\langle n|$
If $\psi = \sum_n a_n \phi_n$:	$\langle\psi| = \sum_n a_n^* \langle n|$
Bra-vector corresponding to $\lambda\psi$ ($\lambda \in \mathbb{C}$):	$\lambda^*\langle\psi|$
Bra-vector corresponding to $A\psi$ ($A : \mathcal{H} \to \mathcal{H}$):	$\langle\psi|A^\dagger$

- Simple familiar objects and relations:

$$\begin{aligned}
&\text{inner product :} && \langle\phi|\psi\rangle \\
& && \langle\psi|\phi\rangle = \langle\phi|\psi\rangle^* \\
& && \{\langle\phi|A\}\,|\psi\rangle = \langle\phi|\,\{A|\psi\rangle\} = \langle\phi|A|\psi\rangle \\
&\text{adjoint } A^\dagger \text{ of } A : && \langle\phi|A^\dagger|\psi\rangle = \langle\psi|A|\phi\rangle^* \quad \text{for all } \ |\phi\rangle, |\psi\rangle \in \mathcal{H} \\
&\text{Hermitian } A : && \langle\phi|A|\psi\rangle = \langle\psi|A|\phi\rangle^* \quad \text{for all } \ |\phi\rangle, |\psi\rangle \in \mathcal{H} \\
&\{|n\rangle\} \text{ orthonormal :} && \langle n|m\rangle = \delta_{nm}
\end{aligned}$$

  Note: an object of the form $|\phi\rangle\langle\chi|$, where $|\phi\rangle, |\chi\rangle \in \mathcal{H}$, is an *operator*
  since: $\{|\phi\rangle\langle\chi|\}\,|\psi\rangle = |\phi\rangle\langle\chi|\psi\rangle = (\langle\chi|\psi\rangle)|\phi\rangle \in \mathcal{H}$

- Closure relation:
  If $\{|n\rangle\}$ complete and orthonormal basis, then $\sum_n |n\rangle\langle n| = 1$ (unit operator in $\mathcal{H}$)

  Proof: take any $|\psi\rangle \in \mathcal{H}$

$$\left\{\sum_n |n\rangle\langle n|\right\}|\psi\rangle = \sum_n |n\rangle\langle n|\psi\rangle = \sum_n \langle n|\psi\rangle|n\rangle = |\psi\rangle$$

- Matrix representations of operators:
  If $\{|n\rangle\}$ complete and orthonormal basis and $A : \mathcal{H} \to \mathcal{H}$, then
  $$A = \sum_{n,m} A_{nm}|n\rangle\langle m| \qquad \text{with} \qquad A_{nm} = \langle n|A|m\rangle$$
  Proof:
  Consider an arbitrary $|\phi\rangle \in \mathcal{H}$, $\quad |\phi\rangle = \sum_n c_n|n\rangle$
  Define $|\phi'\rangle = A|\phi\rangle \in \mathcal{H}$, $\qquad |\phi'\rangle = \sum_n d_n|n\rangle$
  $$d_m = \langle m|\phi'\rangle = \langle m|A|\phi\rangle = \sum_n c_n\langle m|A|n\rangle = \sum_n c_n A_{mn}$$
  Hence
  $$|\phi'\rangle = \sum_m d_m|m\rangle = \sum_{n,m} c_n A_{mn}|m\rangle = \sum_{n,m} A_{mn}\langle n|\phi\rangle|m\rangle = \left\{\sum_{n,m} A_{mn}|m\rangle\langle n|\right\}|\phi\rangle$$
- Matrix representation of A in terms of eigenstate basis
  If $\{|n\rangle\}$ complete and orthonormal basis and $A|n\rangle = a_n|n\rangle$ for all n, then
  $$A_{mn} = a_n\delta_{mn} \qquad A = \sum_n a_n|n\rangle\langle n|$$
  Proof: trivial
- If $AB = C$: $\qquad C_{mn} = \sum_k A_{mk}B_{kn}$
  Proof: $C_{mn} = \langle m|AB|n\rangle = \langle m|A\left\{\sum_k |k\rangle\langle k|\right\}B|n\rangle = \sum_k A_{mk}B_{kn}$

  If $B = A^\dagger$: $\qquad B_{mn} = A^*_{nm}$
  Proof: $A^*_{nm} = \langle n|A|m\rangle^* = \langle m|A^\dagger|n\rangle = \langle m|B|n\rangle = B_{mn}$

  If $A^\dagger = A$: $\qquad A_{mn} = A^*_{nm}$
  Proof: follows immediately from previous statement

Note 1: the representation $\{A_{mn}\}$ of an operator $A : \mathcal{H} \to \mathcal{H}$, given the complete orthonormal basis $\{|n\rangle\}$, is *unique*

Note 2: the representation $\{A_{mn}\}$ of an operator $A : \mathcal{H} \to \mathcal{H}$ will, however, depend on which complete orthonormal basis $\{|n\rangle\}$ is used (as with ordinary matrices)

Note 3: since our Hilbert space are generally infinite-dimensional, the representations $\{A_{mn}\}$ of operators $A : \mathcal{H} \to \mathcal{H}$ are generally matrices of *infinite size*

Note 4: for eigenvector bases of operators with a continuous spectrum one finds the above replaced by:

$$\text{closure :} \qquad \int dn\ |n\rangle\langle n| = 1$$
$$\text{operators :} \qquad A = \int dndm\ A_{mn}|m\rangle\langle n|$$

6.2. Representations

Given a complete orthonormal basis $\{|n\rangle\}$ in $\mathcal{H}$, we have for any state $|\psi\rangle \in \mathcal{H}$ and any operator $A : \mathcal{H} \to \mathcal{H}$:

$$|\psi\rangle = \sum_n c_n |n\rangle \qquad A = \sum_{n,m} A_{nm} |n\rangle\langle m|$$

Definition: the choice of basis $\{|n\rangle\}$ is called the *representation*

6.2.1. Representations and Basis Transformations

- Given a representation, $c_n \in \mathbb{C}$ and $A_{mn} \in \mathbb{C}$ are unique: $c_n = \langle n|\psi\rangle$, $A_{mn} = \langle m|A|n\rangle$

  Hence, on basis $\{|n\rangle\}$ states and operators are represented by ∞-dimensional *complex* vectors and matrices:

$$\psi = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \\ \vdots \end{pmatrix} \qquad A = \begin{pmatrix} A_{11} & A_{12} & \dots & A_{1n} & \dots \\ A_{21} & A_{22} & \dots & A_{2n} & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ A_{n1} & A_{n2} & \dots & A_{nn} & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}$$

- If $|\phi\rangle = \sum_n c_n|n\rangle$ and $|\psi\rangle = \sum_n d_n|n\rangle$, then: $\quad \langle\phi|\psi\rangle = \sum_n c_n^* d_n$

  Proof:
$$\langle\phi|\psi\rangle = \sum_{n,m} c_n^* d_m \langle n|m\rangle = \sum_n c_n^* d_n$$

- If $|\psi\rangle = A|\phi\rangle$, with $|\phi\rangle = \sum_n c_n|n\rangle$ and $|\psi\rangle = \sum_n c_n'|n\rangle$, then: $\quad c_k' = \sum_n A_{kn} c_n$

  Proof:
$$\begin{aligned} |\psi = A|\phi\rangle \;\Rightarrow\; & (\forall k):\ \langle k|\psi\rangle = \langle k|A|\phi\rangle \\ & (\forall k):\ \sum_n c_n' \langle k|n\rangle = \sum_n c_n \langle k|A|n\rangle \\ & (\forall k):\ c_k' = \sum_n A_{kn} c_n \end{aligned}$$

- Consider switching from one orthonormal basis $\{|n\rangle\}$ to another $\{|n'\rangle\}$.
  We can write any $|\psi\rangle \in \mathcal{H}$ in two ways: $\quad |\psi\rangle = \sum_n c_n|n\rangle, \quad |\psi\rangle = \sum_m c_m'|m'\rangle$
  Take inner product with $\langle k'|$:

$$c_k' = \sum_n S_{kn} c_n \qquad S_{kn} = \langle k'|n\rangle$$

  Fact: matrices $\{S_{kn}\}$ representing basis transformations are *unitary*, i.e. $S^\dagger S = SS^\dagger = 1$
  Proof: use $(S^\dagger)_{k\ell} = S_{\ell k}^*$ and closure

$$\sum_n S_{kn} S_{n\ell}^\dagger = \sum_n \langle k'|n\rangle\langle \ell'|n\rangle^* = \sum_n \langle k'|n\rangle\langle n|\ell'\rangle = \langle k'| \left\{ \sum_n |n\rangle\langle n| \right\} |\ell'\rangle = \langle k'|\ell'\rangle = \delta_{k\ell}$$

$$\sum_n S_{kn}^\dagger S_{n\ell} = \sum_n \langle n'|k\rangle^* \langle n'|\ell\rangle = \sum_n \langle k|n'\rangle\langle n'|\ell\rangle = \langle k| \left\{ \sum_n |n'\rangle\langle n'| \right\} |\ell\rangle = \langle k|\ell\rangle = \delta_{k\ell}$$

6.2.2. Examples of Representations

(i) *'Number Representation'*:

Representation of eigenstates $\{|n\rangle\}$ of $N = a^\dagger a$ in $\mathcal{H} = L^2(\mathbb{R})$, $n = 0, 1, 2, 3, \ldots$
use: $a|n\rangle = \sqrt{n}|n-1\rangle$, $a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$

$$\begin{aligned}
a_{nm} &= \langle n|a|m\rangle = \sqrt{m}\langle n|m-1\rangle = \sqrt{m}\delta_{n,m-1} \\
a^\dagger_{nm} &= \langle n|a^\dagger|m\rangle = \sqrt{m+1}\langle n|m+1\rangle = \sqrt{m+1}\delta_{n,m+1} \\
x_{nm} &= \left[\frac{\hbar}{2m\omega}\right]^{\frac{1}{2}} \langle n|(a^\dagger + a)|m\rangle = \left[\frac{\hbar}{2m\omega}\right]^{\frac{1}{2}} \left[\sqrt{m+1}\delta_{n,m+1} + \sqrt{m}\delta_{n,m-1}\right] \\
p_{nm} = &= i\left[\frac{\hbar m\omega}{2}\right]^{\frac{1}{2}} \langle n|(a^\dagger - a)|m\rangle = i\left[\frac{\hbar m\omega}{2}\right]^{\frac{1}{2}} \left[\sqrt{m+1}\delta_{n,m+1} - \sqrt{m}\delta_{n,m-1}\right] \\
N_{nm} &= \langle n|N|m\rangle = m\delta_{mn}
\end{aligned}$$

$$a = \begin{pmatrix} 0 & \sqrt{1} & & & \emptyset \\ & 0 & \sqrt{2} & & \\ & & 0 & \sqrt{3} & \\ & & & 0 & \\ & & & & \ddots \\ & \emptyset & & & \end{pmatrix} \qquad a^\dagger = \begin{pmatrix} 0 & & & & \emptyset \\ \sqrt{1} & 0 & & & \\ & \sqrt{2} & 0 & & \\ & & \sqrt{3} & 0 & \\ & & & & \ddots \\ & \emptyset & & & \end{pmatrix} \qquad N = \begin{pmatrix} 0 & & & & \emptyset \\ & 1 & & & \\ & & 2 & & \\ & & & 3 & \\ & & & & \ddots \\ & \emptyset & & & \end{pmatrix}$$

$$x = \sqrt{\frac{\hbar}{2m\omega}} \begin{pmatrix} 0 & \sqrt{1} & & & \emptyset \\ \sqrt{1} & 0 & \sqrt{2} & & \\ & \sqrt{2} & 0 & \sqrt{3} & \\ & & \sqrt{3} & 0 & \\ & & & & \ddots \\ & \emptyset & & & \end{pmatrix} \qquad p = i\sqrt{\frac{\hbar m\omega}{2}} \begin{pmatrix} 0 & -\sqrt{1} & & & \emptyset \\ \sqrt{1} & 0 & -\sqrt{2} & & \\ & \sqrt{2} & 0 & -\sqrt{3} & \\ & & \sqrt{3} & 0 & \\ & & & & \ddots \\ & \emptyset & & & \end{pmatrix}$$

(ii) *'Momentum Representation'*:

Representation of eigenstates $\{|k\rangle\}$ of p in $\mathcal{H} = L^2(\mathbb{R})$, $k \in \mathbb{R}$

$$\phi_k(x) = \frac{1}{\sqrt{2\pi}}e^{ikx} \qquad p|k\rangle = \hbar k|k\rangle \qquad \langle k|k'\rangle = \int_{-\infty}^{\infty} \frac{dx}{2\pi} e^{-ik(k-k')} = \delta(k-k')$$

$$\begin{aligned}
x_{kk'} &= \langle k|x|k'\rangle = \int dx\ \phi^*_k(x) x \phi_{k'}(x) = \int \frac{dx}{2\pi}\ x e^{-ix(k-k')} = i\frac{\partial}{\partial k}\delta(k-k') \\
p_{kk'} &= \langle k|p|k'\rangle = \hbar k'\langle k|k'\rangle = \hbar k\delta(k-k')
\end{aligned}$$

$$x = i\begin{pmatrix} \ddots & & \emptyset \\ & \frac{\partial}{\partial k} & \\ \emptyset & & \ddots \end{pmatrix} \qquad p = \hbar\begin{pmatrix} \ddots & & \emptyset \\ & k & \\ \emptyset & & \ddots \end{pmatrix}$$

(iii) *'Position Representation'*:

Representation of eigenstates $\{|u\rangle\}$ of x in $\mathcal{H} = L^2(\mathbb{R})$, $u \in \mathbb{R}$

$$\phi_u(x) = \delta[x-u] \qquad x|u\rangle = u|u\rangle \qquad \langle u|u'\rangle = \int_{-\infty}^{\infty} dx\ \delta[x-u]\delta[x-u'] = \delta[u-u']$$

$$\begin{aligned} x_{uu'} &= \langle u|x|u'\rangle = u\delta[u-u'] \\ p_{uu'} &= \int dx\ \phi_u^*(x) p \phi_{u'}(x) = -i\hbar \int dx\ \delta[x-u] \frac{\partial}{\partial x}\delta[x-u'] \\ &= i\hbar \frac{\partial}{\partial u'} \int dx\ \delta[x-u]\delta[x-u'] \\ &= i\hbar \frac{\partial}{\partial u'}\delta[u-u'] = -i\hbar\frac{\partial}{\partial u}\delta[u-u'] \end{aligned}$$

$$x = \begin{pmatrix} \ddots & & & & \emptyset \\ & \ddots & & & \\ & & u & & \\ & & & \ddots & \\ \emptyset & & & & \ddots \end{pmatrix} \qquad p = -i\hbar \begin{pmatrix} \ddots & & & & \emptyset \\ & \ddots & & & \\ & & \frac{\partial}{\partial u} & & \\ & & & \ddots & \\ \emptyset & & & & \ddots \end{pmatrix}$$

Note: we have so far always used position representation implicitly
but this is just one of an infinite number of mathematically equivalent representations

6.3. Schrödinger vs Heisenberg Picture

6.3.1. Exponentials of Operators

Definition: $e^A = \sum_{n\geq 0} \frac{A^n}{n!}, \quad A^0 = 1$

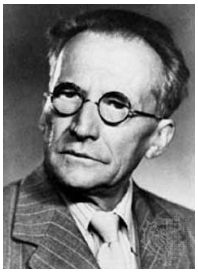
- If $A|n\rangle = a_n|n\rangle$ and $\{|n\rangle\}$ complete: $\quad e^A = \sum_n e^{a_n}|n\rangle\langle n|$
  Proof:
  $$e^A = \sum_{\ell\geq 0}\frac{A^\ell}{\ell!}\sum_n |n\rangle\langle n| = \sum_n\sum_{\ell\geq 0}\frac{a_n^\ell}{\ell!}|n\rangle\langle n| = \sum_n e^{a_n}|n\rangle\langle n|$$
- $e^A.e^{-A} = 1$
  Proof:
  $$e^A.e^{-A} = \sum_{k,\ell\geq 0}\frac{(-1)^\ell A^{k+\ell}}{k!\ell!} = A^0 + \sum_{m>0}\frac{A^m}{m!}\sum_{\ell=0}^{m}\frac{(-1)^\ell m!}{\ell!(m-\ell)!}$$
  $$= 1 + \sum_{m>0}\frac{A^m}{m!}[1+(-1)]^m = 1$$
- $[e^A]^\dagger = \sum_{n\geq 0}\frac{1}{n!}[A^n]^\dagger = \sum_{n\geq 0}\frac{1}{n!}[A^\dagger]^n = e^{A^\dagger}$

- If $A^\dagger = A$, then $U = e^{iA}$ is unitary
  Proof:
  $$U^\dagger U = e^{-iA^\dagger}e^{iA} = e^{-iA}e^{iA} = 1$$
  $$UU^\dagger = e^{iA}e^{-iA^\dagger} = e^{iA}e^{-iA} = 1$$

6.3.2. Summary of Schrödinger Picture

- Schrödinger equation: $i\hbar\frac{d}{dt}|\psi\rangle = H|\psi\rangle$, with $H^\dagger = H$
  Define $U(t)$: $\quad |\psi_t\rangle = U(t)|\psi_0\rangle$
  $$i\hbar\frac{d}{dt}U(t) = HU(t), \qquad U(0) = 1$$
  $$\text{solution}: \quad U(t) = e^{tH/i\hbar}, \qquad \text{so} \qquad |\psi_t\rangle = e^{tH/i\hbar}|\psi_0\rangle$$
- Compare with familiar form of solution:
  use closure, with $H|n\rangle = E_n|n\rangle$ and $c_n = \langle n|\psi_0\rangle$
  $$|\psi_t\rangle = e^{tH/i\hbar}|\psi_0\rangle = e^{tH/i\hbar}\left\{\sum_n |n\rangle\langle n|\right\}|\psi_0\rangle$$
  $$= \sum_n e^{tE_n/i\hbar}|n\rangle\langle n|\psi_0\rangle = \sum_n c_n\, e^{tE_n/i\hbar}|n\rangle$$
- Properties of $U(t)$:
  $$U(t) = e^{tH/i\hbar}: \qquad [U(t),H] = 0 \qquad U^\dagger(t)U(t) = U(t)U^\dagger(t) = 1$$
  $U(t)$ unitary (like basis transformation), but *time-dependent*
- Expectation values of operators:
  $$\langle A(t)\rangle = \langle\psi_t|A(t)|\psi_t\rangle = \langle\psi_0|U^\dagger(t)A(t)U(t)|\psi_0\rangle$$

6.3.3. The Heisenberg Picture



1925

$\frac{d}{dt}\hat{A} = \frac{1}{i\hbar}[\hat{A}, H] + \frac{\partial}{\partial t}\hat{A}$

∞-*dimensional matrices*

1926

$i\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\psi + V(\boldsymbol{x})\psi$

wave functions

- Both pictures: observables represented by linear Hermitian operators

  Schrodinger : time−dependent state vector $|\psi_t\rangle$
  observables generally time−independent, e.g. x, p, V

  Heisenberg : time − independent state vector $|\psi_0\rangle$
  observables generally time−dependent, e.g. $\hat{x}(t)$, $\hat{p}(t)$, $\hat{V}(t)$

- The link: for every Hermitian Schrödinger operator A

  Heisenberg operator : $\hat{A}(t) = U^\dagger(t)AU(t) \qquad U(t) = e^{tH/i\hbar}$

  (i) Expectation values: $\langle A\rangle = \langle\psi_0|\hat{A}(t)|\psi_0\rangle$

  (ii) Heisenberg's equation of motion for operators:

$$\frac{d}{dt}\hat{A}(t) = \frac{1}{i\hbar}[\hat{A}(t), H] + \frac{\partial}{\partial t}\hat{A}(t)$$

  Proof:

$$\begin{aligned}
\frac{d}{dt}\hat{A}(t) &= \frac{d}{dt}\left[U^\dagger(t)A(t)U(t)\right] \\
&= \frac{dU^\dagger(t)}{dt}.A(t)U(t) + U^\dagger(t)A(t)\frac{dU(t)}{dt} + U^\dagger(t)\frac{\partial A(t)}{\partial t}U(t) \\
&= \left[\frac{1}{i\hbar}HU(t)\right]^\dagger A(t)U(t) + U^\dagger(t)A(t)\left[\frac{1}{i\hbar}HU(t)\right] + U^\dagger(t)\frac{\partial A(t)}{\partial t}U(t) \\
&= -\frac{1}{i\hbar}U^\dagger(t)HA(t)U(t) + \frac{1}{i\hbar}U^\dagger(t)A(t)HU(t) + U^\dagger(t)\frac{\partial A(t)}{\partial t}U(t) \\
&= \frac{1}{i\hbar}\left\{\hat{A}(t)H - H\hat{A}(t)\right\} + U^\dagger(t)\frac{\partial A(t)}{\partial t}U(t) = \frac{1}{i\hbar}[\hat{A}(t), H] + \frac{\partial}{\partial t}\hat{A}(t)
\end{aligned}$$

7. Symmetries in QM

7.1. Physical Symmetries

7.1.1. Physical Symmetries and Unitary Operators

- Consider invertible symmetry transformations: $(\forall \boldsymbol{x} \in \mathbb{R}^3):\ \boldsymbol{x} \to \mathrm{T}(\boldsymbol{x})$
  with $\mathrm{Det}|\partial \mathrm{T}_i(\boldsymbol{x})/\partial x_j| = 1$ (rotations, translations, reflections, coordinate permutations)

  Corresponding QM operator S: $(\forall \boldsymbol{x} \in \mathbb{R}^3):\ S|\boldsymbol{x}\rangle = |\mathrm{T}(\boldsymbol{x})\rangle$
  (linear, but generally not Hermitian)

$$S = \int d\boldsymbol{x}d\boldsymbol{x}'\ |\boldsymbol{x}'\rangle\langle \boldsymbol{x}'|S|\boldsymbol{x}\rangle\langle \boldsymbol{x}| = \int d\boldsymbol{x}d\boldsymbol{x}'\ |\boldsymbol{x}'\rangle\langle \boldsymbol{x}'|\mathrm{T}(\boldsymbol{x})\rangle\langle \boldsymbol{x}|$$
$$= \int d\boldsymbol{x}d\boldsymbol{x}'\ \delta[\boldsymbol{x}' - \mathrm{T}(\boldsymbol{x})]|\boldsymbol{x}'\rangle\langle \boldsymbol{x}| = \int d\boldsymbol{x}\ |\mathrm{T}(\boldsymbol{x})\rangle\langle \boldsymbol{x}|$$

- S is unitary:

$$SS^\dagger = \int d\boldsymbol{x}d\boldsymbol{x}'\ |\mathrm{T}(\boldsymbol{x})\rangle\langle \boldsymbol{x}|\boldsymbol{x}'\rangle\langle \mathrm{T}(\boldsymbol{x}')| = \int d\boldsymbol{x}d\boldsymbol{x}'\ \delta[\boldsymbol{x} - \boldsymbol{x}']|\mathrm{T}(\boldsymbol{x})\rangle\langle \mathrm{T}(\boldsymbol{x}')|$$
$$= \int d\boldsymbol{x}\ |\mathrm{T}(\boldsymbol{x})\rangle\langle \mathrm{T}(\boldsymbol{x})| = \int d\boldsymbol{x}\ |\boldsymbol{x}\rangle\langle(\boldsymbol{x})| = 1$$
$$S^\dagger S = \int d\boldsymbol{x}d\boldsymbol{x}'\ |\boldsymbol{x}\rangle\langle \mathrm{T}(\boldsymbol{x})|\mathrm{T}(\boldsymbol{x}')\rangle\langle \boldsymbol{x}'| = \int d\boldsymbol{x}d\boldsymbol{x}'\ \delta[\boldsymbol{x} - \boldsymbol{x}']|T^{-1}(\boldsymbol{x})\rangle\langle T^{-1}(\boldsymbol{x}')|$$
$$= \int d\boldsymbol{x}\ |T^{-1}(\boldsymbol{x})\rangle\langle T^{-1}(\boldsymbol{x})| = \int d\boldsymbol{x}\ |\boldsymbol{x}\rangle\langle(\boldsymbol{x})| = 1$$

7.1.2. Continuous Symmetry Groups

Consider *continuously and analytically parametrized groups* of symmetry transformations $\mathrm{T}_{\boldsymbol{\xi}}(\boldsymbol{x})$ with $\boldsymbol{\xi} \in \mathbb{R}^n$ as above.

$$(\forall \boldsymbol{x} \in \mathbb{R}^3):\ \mathrm{T}_{\boldsymbol{0}}(\boldsymbol{x}) = \boldsymbol{x} \qquad \mathrm{T}_{\boldsymbol{\xi}}\mathrm{T}_{\boldsymbol{\xi}'} = \mathrm{T}_{\boldsymbol{\zeta}(\boldsymbol{\xi},\boldsymbol{\xi}')} \quad \text{for some } \boldsymbol{\zeta}(\boldsymbol{\xi},\boldsymbol{\xi}')$$

We also assume:

$$\mathrm{T}_{\lambda\boldsymbol{\xi}}\mathrm{T}_{\mu\boldsymbol{\xi}} = \mathrm{T}_{(\lambda+\mu)\boldsymbol{\xi}} \quad \text{for all } \lambda,\mu \in \mathbb{R}$$

(e.g. rotations, translations, ...)

- Associated unitary operators:

$$S_{\boldsymbol{0}} = 1, \qquad S_{\boldsymbol{\xi}}S_{\boldsymbol{\xi}'} = S_{\boldsymbol{\zeta}(\boldsymbol{\xi},\boldsymbol{\xi}')}, \qquad S_{\lambda\boldsymbol{\xi}}S_{\mu\boldsymbol{\xi}} = S_{(\lambda+\mu)\boldsymbol{\xi}} \quad \text{for all } \lambda,\mu \in \mathbb{R}$$

  The $\{S_{\boldsymbol{\xi}}\}$ also form a group $\mathcal{G}$:

$$S_{\boldsymbol{\xi}}S_{\boldsymbol{\xi}'} \in \mathcal{G} \qquad (S_{\boldsymbol{\xi}}S_{\boldsymbol{\lambda}})S_{\boldsymbol{\zeta}} = S_{\boldsymbol{\xi}}(S_{\boldsymbol{\lambda}}S_{\boldsymbol{\zeta}}) \qquad 1 \in \mathcal{G} \qquad S_{\boldsymbol{\xi}}S_{-\boldsymbol{\xi}} = S_{-\boldsymbol{\xi}}S_{\boldsymbol{\xi}} = 1$$

  Define *generators* $G_i = i\hbar \lim_{\boldsymbol{\xi}\to\boldsymbol{0}} \frac{\partial}{\partial \xi_i} S_{\boldsymbol{\xi}}$

$$\text{if } \{G_i\} \text{ and } e^{\sum_i \xi_i G_i/i\hbar} \text{ exist}: \qquad S_{\boldsymbol{\xi}} = e^{\sum_i \xi_i G_i/i\hbar} \qquad (\mathcal{G} \text{ is a Lie group})$$

Proof:
$$\frac{1}{\epsilon}\left\{S_{(\lambda+\epsilon)\boldsymbol{\xi}} - S_{\lambda\boldsymbol{\xi}}\right\} = \frac{1}{\epsilon}\left\{S_{\epsilon\boldsymbol{\xi}} - 1\right\} S_{\lambda\boldsymbol{\xi}} = \frac{1}{\epsilon}\left\{S_{\mathbf{0}} + \frac{\epsilon}{i\hbar}\sum_i \xi_i G_i + \mathcal{O}(\epsilon^2) - 1\right\} S_{\lambda\boldsymbol{\xi}}$$
$$= \frac{1}{i\hbar}(\sum_i \xi_i G_i) S_{\lambda\boldsymbol{\xi}} + \mathcal{O}(\epsilon)$$

hence: $\frac{d}{d\lambda}S_{\lambda\boldsymbol{\xi}} = (\frac{1}{i\hbar}\sum_i \xi_i G_i)S_{\lambda\boldsymbol{\xi}}$, so $S_{\lambda\boldsymbol{\xi}} = e^{\frac{\lambda}{i\hbar}\sum_i \xi_i G_i} S_{\mathbf{0}} = e^{\frac{\lambda}{i\hbar}\sum_i \xi_i G_i}$

- If $\mathcal{G}$ is a Lie group:
  - (i) $G_i^\dagger = G_i$ for all i.
    Proof, demand that for all $\boldsymbol{\xi} \in \mathbb{R}^n$:
$$1 = S^\dagger_{\boldsymbol{\xi}} S_{\boldsymbol{\xi}} = e^{-\frac{1}{i\hbar}\sum_i \xi_i G_i^\dagger} e^{\frac{1}{i\hbar}\sum_i \xi_i G_i}$$
$$= \left\{1 - \frac{1}{i\hbar}\sum_i \xi_i G_i^\dagger + \mathcal{O}(\boldsymbol{\xi}^2)\right\}\left\{1 + \frac{1}{i\hbar}\sum_i \xi_i G_i + \mathcal{O}(\boldsymbol{\xi}^2)\right\}$$
$$= \left\{1 + \frac{1}{i\hbar}\sum_i \xi_i (G_i - G_i^\dagger) + \mathcal{O}(\boldsymbol{\xi}^2)\right\} \quad \text{hence} \quad (\forall i): \; G_i^\dagger = G_i$$
  - (ii) $(\exists\{\ell_{ijk} \in \mathbb{R}\}):$ $[G_i, G_j] = i\hbar \sum_k \ell_{ijk} G_k$
    $\{\ell_{ijk}\}$, with $\ell_{ijk} = -\ell_{jik}$: *structure constants*

    Proof:
    use first group property $e^{\frac{1}{i\hbar}\sum_i \xi_i G_i} e^{\frac{1}{i\hbar}\sum_i \xi'_i G_i} = e^{\frac{1}{i\hbar}\sum_i \lambda_i(\boldsymbol{\xi},\boldsymbol{\xi}')G_i}$ for some $\lambda_i(\boldsymbol{\xi},\boldsymbol{\xi}')$
    use expansion to 2nd order: $e^{\frac{1}{i\hbar}\sum_i \xi_i G_i} = 1 + \frac{1}{i\hbar}\sum_i \xi_i G_i - \frac{1}{2\hbar^2}\sum_{ij}\xi_i\xi_j G_i G_j + \ldots$
$$e^{\frac{1}{i\hbar}\sum_i \lambda_i(\boldsymbol{\xi},\boldsymbol{\xi}')G_i} = e^{\frac{1}{i\hbar}\sum_i \xi_i G_i} . e^{\frac{1}{i\hbar}\sum_i \xi'_i G_i} =$$
$$\left\{1 + \frac{1}{i\hbar}\sum_i \xi_i G_i - \frac{1}{2\hbar^2}\sum_{ij}\xi_i\xi_j G_i G_j + \ldots\right\}\left\{1 + \frac{1}{i\hbar}\sum_i \xi'_i G_i - \frac{1}{2\hbar^2}\sum_{ij}\xi'_i\xi'_j G_i G_j + \ldots\right\}$$
$$= 1 + \frac{1}{i\hbar}\sum_i (\xi_i + \xi'_i) G_i - \frac{1}{2\hbar^2}\sum_{ij}(\xi_i\xi_j + \xi'_i\xi'_j + 2\xi_i\xi'_j) G_i G_j + \ldots$$
    Expand left-hand side:
$$e^{\frac{1}{i\hbar}\sum_i \lambda_i(\boldsymbol{\xi},\boldsymbol{\xi}')G_i} = 1 + \frac{1}{i\hbar}\sum_i \lambda_i(\boldsymbol{\xi},\boldsymbol{\xi}')G_i - \frac{1}{2\hbar^2}\sum_{ij}\lambda_j(\boldsymbol{\xi},\boldsymbol{\xi}')\lambda_i(\boldsymbol{\xi},\boldsymbol{\xi}')G_i G_j + \mathcal{O}(\boldsymbol{\lambda}^3)$$
    Require identity in lowest orders: $\lambda_i(\boldsymbol{\xi},\boldsymbol{\xi}') = \xi_i + \xi'_i + \frac{1}{2}\Lambda_i(\boldsymbol{\xi},\boldsymbol{\xi}')$, $\Lambda_i = \mathcal{O}(.^2)$,
    hence also: $\lambda_i(\boldsymbol{\xi},\boldsymbol{\xi}')\lambda_j(\boldsymbol{\xi},\boldsymbol{\xi}') = (\xi_i + \xi'_i)(\xi_j + \xi'_j) + \mathcal{O}(.^3)$
    Now compare second order terms:
$$\frac{1}{2i\hbar}\sum_i \Lambda_i(\boldsymbol{\xi},\boldsymbol{\xi}')G_i - \frac{1}{2\hbar^2}\sum_{ij}(\xi_i + \xi'_i)(\xi_j + \xi'_j)G_i G_j = -\frac{1}{2\hbar^2}\sum_{ij}(\xi_i\xi_j + \xi'_i\xi'_j + 2\xi_i\xi'_j)G_i G_j + \mathcal{O}(.^3)$$
$$-i\hbar\sum_i \Lambda_i(\boldsymbol{\xi},\boldsymbol{\xi}')G_i = \sum_{ij}(\xi_i + \xi'_i)(\xi_j + \xi'_j)G_i G_j - \sum_{ij}(\xi_i\xi_j + \xi'_i\xi'_j + 2\xi_i\xi'_j)G_i G_j + \mathcal{O}(.^3)$$
$$-i\hbar\sum_k \Lambda_k(\boldsymbol{\xi},\boldsymbol{\xi}')G_k = \sum_{ij}(\xi'_i\xi_j - \xi_i\xi'_j)G_i G_j + \mathcal{O}(.^3)$$

$$i\hbar \sum_k \Lambda_k(\boldsymbol{\xi},\boldsymbol{\xi}')G_k = \sum_{ij} \xi_i \xi'_j [G_i, G_j] + \mathcal{O}(.^3)$$

Hence $[G_i, G_j] = i\hbar \sum_k \ell_{ijk} G_k$, and $\Lambda_k(\boldsymbol{\xi},\boldsymbol{\xi}') = \sum_{ij} \xi_i \xi'_j \ell_{ijk} + \mathcal{O}(.^3)$

Proof that $\ell_{ijk} \in \mathbb{R}$: consider adjoint of $[G_i, G_j] = i\hbar \sum_k \ell_{ijk} G_k$

$$[G_i, G_j]^\dagger = -i\hbar \sum_k \ell^*_{ijk} G^\dagger_k \quad \Rightarrow \quad (G_iG_j - G_jG_i)^\dagger = -i\hbar \sum_k \ell^*_{ijk} G_k \quad \Rightarrow$$

$$[G_j, G_i] = -i\hbar \sum_k \ell^*_{ijk} G_k \quad \Rightarrow \quad [G_i, G_j] = i\hbar \sum_k \ell^*_{ijk} G_k \quad \Rightarrow$$

$$(\forall i,j): \qquad \sum_k (\ell_{ijk} - \ell^*_{ijk}) G_k = 0 \qquad \text{so} \ \ \ell_{ijk} \in \mathbb{R}$$

Note: all representations of $\mathcal{G}$ must have generators with the same structure constants

7.1.3. Examples of Continuous Transformations

- Translations: $\mathrm{T}_{\boldsymbol{\xi}}(\boldsymbol{x}) = \boldsymbol{x} + \boldsymbol{\xi}$

  Meet criteria above for continuously symmetry groups !

$$S_{\boldsymbol{\xi}} = \int d\boldsymbol{x}' \ |\mathrm{T}_{\boldsymbol{\xi}'}(\boldsymbol{x}')\rangle\langle \boldsymbol{x}'| = \int d\boldsymbol{x}' \ |\boldsymbol{x}' + \boldsymbol{\xi}\rangle\langle \boldsymbol{x}'|$$

$$\langle \boldsymbol{x}|S_{\boldsymbol{\xi}}\psi\rangle = \int d\boldsymbol{x}' \ \langle \boldsymbol{x}|\boldsymbol{x}' + \boldsymbol{\xi}\rangle\langle \boldsymbol{x}'|\psi\rangle = \int d\boldsymbol{x}' \ \delta[\boldsymbol{x} - \boldsymbol{x}' - \boldsymbol{\xi}]\psi(\boldsymbol{x}') = \psi(\boldsymbol{x} - \boldsymbol{\xi})$$

  Generators:

$$\langle \boldsymbol{x}|G_i\psi\rangle = i\hbar \lim_{\boldsymbol{\xi}\to\boldsymbol{0}} \frac{\partial}{\partial \xi_i}\langle \boldsymbol{x}|S_{\boldsymbol{\xi}}\psi\rangle = i\hbar \lim_{\boldsymbol{\xi}\to\boldsymbol{0}} \frac{\partial}{\partial \xi_i}\psi(\boldsymbol{x} - \boldsymbol{\xi}) = -i\hbar \frac{\partial}{\partial x_i}\psi(\boldsymbol{x}) = [p_i\psi](\boldsymbol{x})$$

  Hence : $\quad \boldsymbol{G} = \boldsymbol{p}, \qquad S_{\boldsymbol{\xi}} = e^{\frac{1}{i\hbar}\boldsymbol{\xi}\cdot\boldsymbol{p}}$

  Note:

  (i) $e^{\boldsymbol{\xi}\cdot\boldsymbol{p}/i\hbar} = \int d\boldsymbol{p} \ e^{\boldsymbol{\xi}\cdot\boldsymbol{p}/i\hbar}|\boldsymbol{p}\rangle\langle\boldsymbol{p}|$ exists

  (ii) $[G_i, G_j] = [p_i, p_j] = 0$ so $\ell_{ijk} = 0$

  (iii) $G^\dagger_i = G_i$ for all i, $e^{\boldsymbol{\xi}\cdot\boldsymbol{p}/i\hbar}$ is unitary

- Rotations:

  First consider rotation around x_3 axis: $\mathrm{T}_\xi(\boldsymbol{x}) = \mathrm{R}_\xi \boldsymbol{x}$

  Meets criteria above for continuously symmetry groups !

$$\mathrm{R}_\xi = \begin{pmatrix} \cos(\xi) & -\sin(\xi) & 0 \\ \sin(\xi) & \cos(\xi) & 0 \\ 0 & 0 & 1 \end{pmatrix} = \mathbb{1} + \begin{pmatrix} 0 & -\xi & 0 \\ \xi & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} + \mathcal{O}(\xi^2)$$

Thus
$$\mathrm{R}_\xi \boldsymbol{x} = \boldsymbol{x} + \xi \begin{pmatrix} -x_2 \\ x_1 \\ 0 \end{pmatrix} + \mathcal{O}(\xi^2) = \boldsymbol{x} + \begin{pmatrix} 0 \\ 0 \\ \xi \end{pmatrix} \times \boldsymbol{x} + \mathcal{O}(\xi^2)$$

Arbitrary rotation axis $\boldsymbol{\xi}/|\boldsymbol{\xi}|$:
$$\mathrm{R}_{\boldsymbol{\xi}} \boldsymbol{x} = \boldsymbol{x} + \boldsymbol{\xi} \times \boldsymbol{x} + \mathcal{O}(\boldsymbol{\xi}^2)$$

Generators:
$$\begin{aligned}
\langle \boldsymbol{x} | G_i \psi \rangle &= i\hbar \lim_{\boldsymbol{\xi}\to\boldsymbol{0}} \frac{\partial}{\partial \xi_i} \langle \boldsymbol{x} | S_{\boldsymbol{\xi}} \psi \rangle = i\hbar \lim_{\boldsymbol{\xi}\to\boldsymbol{0}} \frac{\partial}{\partial \xi_i} \int d\boldsymbol{x}' \langle \boldsymbol{x} | S_{\boldsymbol{\xi}} | \boldsymbol{x}' \rangle \langle \boldsymbol{x}' | \psi \rangle \\
&= i\hbar \lim_{\boldsymbol{\xi}\to\boldsymbol{0}} \frac{\partial}{\partial \xi_i} \int d\boldsymbol{x}' \langle \boldsymbol{x} | \mathrm{R}_{\boldsymbol{\xi}} \boldsymbol{x}' \rangle \psi(\boldsymbol{x}') = i\hbar \lim_{\boldsymbol{\xi}\to\boldsymbol{0}} \frac{\partial}{\partial \xi_i} \int d\boldsymbol{x}' \; \delta[\boldsymbol{x}' - \mathrm{R}_{-\boldsymbol{\xi}} \boldsymbol{x}] \psi(\boldsymbol{x}') \\
&= i\hbar \lim_{\boldsymbol{\xi}\to\boldsymbol{0}} \frac{\partial}{\partial \xi_i} \psi(\mathrm{R}_{-\boldsymbol{\xi}} \boldsymbol{x}) = i\hbar \lim_{\boldsymbol{\xi}\to\boldsymbol{0}} \frac{\partial}{\partial \xi_i} \psi(\boldsymbol{x} - \boldsymbol{\xi} \times \boldsymbol{x} + \mathcal{O}(\boldsymbol{\xi}^2)) \\
&= i\hbar \lim_{\boldsymbol{\xi}\to\boldsymbol{0}} \frac{\partial}{\partial \xi_i} \left\{ \psi(\boldsymbol{x}) - \sum_j (\boldsymbol{\xi} \times \boldsymbol{x})_j \frac{\partial}{\partial x_j} \psi(\boldsymbol{x}) + \mathcal{O}(\boldsymbol{\xi}^2) \right\} \\
&= \sum_{jk\ell=1}^{3} \epsilon_{jk\ell} \frac{\partial}{\partial \xi_i} \xi_j x_\ell [p_j \psi](\boldsymbol{x}) = \sum_{k\ell=1}^{3} \epsilon_{ik\ell} x_\ell [p_j \psi](\boldsymbol{x}) = \langle \boldsymbol{x} | L_i \psi \rangle
\end{aligned}$$

Hence : $\quad \boldsymbol{G} = \boldsymbol{L} \quad (\boldsymbol{L} = \boldsymbol{x} \times \boldsymbol{p}), \qquad S_{\boldsymbol{\xi}} = e^{\frac{1}{i\hbar}\boldsymbol{\xi}\cdot\boldsymbol{L}}$

Note:

(i) $e^{\boldsymbol{\xi}\cdot\boldsymbol{L}/i\hbar}$ exists (but will not give proof here, will come later)

(ii) $[G_i, G_j] = [L_i, L_j] = i\hbar \sum_k \epsilon_{ijk} L_k = 0$ so $\ell_{ijk} = \epsilon_{ijk}$

(iii) $G_i^\dagger = G_i$ for all i, $e^{\boldsymbol{\xi}\cdot\boldsymbol{L}/i\hbar}$ is unitary

7.1.4. Scalar Operators and Vector Operators

- <u>Definitions</u>: A is scalar operator : $[L_i, A] = 0$ for all i
  $\boldsymbol{A}$ is vector operator : $[L_i, A_j] = i\hbar \sum_k \epsilon_{ijk} A_k$ for all i

Examples of vector operators:

$$\begin{aligned}
\boldsymbol{x} : \quad [L_i, x_j] &= \sum_{k\ell} \epsilon_{ik\ell} [x_k p_\ell, x_j] = \sum_{k\ell} \epsilon_{ik\ell} \left\{ x_k [p_\ell, x_j] + [x_k, x_j] p_\ell \right\} \\
&= -i\hbar \sum_{k\ell} \epsilon_{ik\ell} x_k \delta_{\ell j} = -i\hbar \sum_k \epsilon_{ikj} x_k = i\hbar \sum_k \epsilon_{ijk} x_k \\
\boldsymbol{p} : \quad [L_i, p_j] &= \sum_{k\ell} \epsilon_{ik\ell} [x_k p_\ell, p_j] = \sum_{k\ell} \epsilon_{ik\ell} \left\{ x_k [p_\ell, p_j] + [x_k, p_j] p_\ell \right\} \\
&= i\hbar \sum_{k\ell} \epsilon_{ik\ell} \delta_{kj} p_\ell = i\hbar \sum_\ell \epsilon_{ij\ell} p_\ell \\
\boldsymbol{L} : \quad [L_i, L_j] &= i\hbar \sum_k \epsilon_{ijk} L_k
\end{aligned}$$

Examples of scalar operators:

$$\begin{aligned}
\boldsymbol{L}^2: \qquad [L_i, \boldsymbol{L}^2] &= \sum_k [L_i, L_k^2] = \sum_k \{L_k[L_i, L_k] + [L_i, L_k]L_k\} \\
&= i\hbar \sum_{k\ell} \epsilon_{ik\ell} \{L_k L_\ell + L_\ell L_k\} = 0 \\
\boldsymbol{x}\cdot\boldsymbol{p}: \qquad [L_i, \boldsymbol{x}\cdot\boldsymbol{p}] &= \sum_k [L_i, x_k p_k] = \sum_k \{x_k[L_i, p_k] + [L_i, x_k]p_k\} \\
&= i\hbar \sum_{k\ell} \epsilon_{ik\ell} \{x_k p_\ell + x_\ell p_k\} = 0
\end{aligned}$$

- Physical implications:

  let $\mathrm{R}_{\boldsymbol{\xi}}$ denote a rotation in $\mathbb{R}^3$ (axis $\boldsymbol{\xi}/|\boldsymbol{\xi}|$, angle $|\boldsymbol{\xi}|$),
  with corresponding QM transformation $|\psi'\rangle = e^{\boldsymbol{\xi}\cdot\boldsymbol{L}/i\hbar}|\psi\rangle$
  Then:

$$\begin{aligned}
A \text{ is scalar operator}: &\quad \langle\psi'|A|\psi'\rangle = \langle\psi|A|\psi\rangle \\
\boldsymbol{A} \text{ is vector operator}: &\quad \langle\psi'|\boldsymbol{A}|\psi'\rangle = \mathrm{R}_{\boldsymbol{\xi}}\langle\psi|\boldsymbol{A}|\psi\rangle
\end{aligned}$$

  (i.e. expectation values of A and $\boldsymbol{A}$ transform like scalars and vectors, respectively)

  Proof for A:
  Note that $[\boldsymbol{\xi}\cdot\boldsymbol{L}, A] = \sum_i \xi_i [L_i, A] = 0$, hence $[e^{\boldsymbol{\xi}\cdot\boldsymbol{L}/i\hbar}, A] = 0$:

$$\langle\psi'|A|\psi'\rangle = \langle\psi|e^{-\boldsymbol{\xi}\cdot\boldsymbol{L}/i\hbar} A e^{\boldsymbol{\xi}\cdot\boldsymbol{L}/i\hbar}|\psi\rangle = \langle\psi|e^{-\boldsymbol{\xi}\cdot\boldsymbol{L}/i\hbar} e^{\boldsymbol{\xi}\cdot\boldsymbol{L}/i\hbar} A|\psi\rangle = \langle\psi|A|\psi\rangle$$

  Proof for $\boldsymbol{A}$:
  We prove this by showing that LHS and RHS obey an identical first order differential eqn, with identical initial conditions.
  First note that $[\boldsymbol{\xi}\cdot\boldsymbol{L}, \boldsymbol{A}] = -i\hbar(\boldsymbol{\xi}\times\boldsymbol{A})$:

$$[\boldsymbol{\xi}\cdot\boldsymbol{L}, A_j] = \sum_i \xi_i [L_i, A_j] = i\hbar \sum_{ik} \xi_i \epsilon_{ijk} A_k = -i\hbar \sum_{ik} \epsilon_{jik} \xi_i A_k = -i\hbar(\boldsymbol{\xi}\times\boldsymbol{A})_j$$

  Now inspect $\mathrm{R}_{\lambda\boldsymbol{\xi}}$ and its associated operator $e^{\lambda\boldsymbol{\xi}\cdot\boldsymbol{L}/i\hbar}$:

$$\begin{aligned}
\frac{d}{d\lambda}\langle\psi|e^{-\lambda\boldsymbol{\xi}\cdot\boldsymbol{L}/i\hbar}\boldsymbol{A}e^{\lambda\boldsymbol{\xi}\cdot\boldsymbol{L}/i\hbar}|\psi\rangle &= -\frac{1}{i\hbar}\langle\psi|e^{-\lambda\boldsymbol{\xi}\cdot\boldsymbol{L}/i\hbar}\{(\boldsymbol{\xi}\cdot\boldsymbol{L})\boldsymbol{A} - \boldsymbol{A}(\boldsymbol{\xi}\cdot\boldsymbol{L})\} e^{\lambda\boldsymbol{\xi}\cdot\boldsymbol{L}/i\hbar}|\psi\rangle \\
&= \langle\psi|e^{-\lambda\boldsymbol{\xi}\cdot\boldsymbol{L}/i\hbar}\{\boldsymbol{\xi}\times\boldsymbol{A}\} e^{\lambda\boldsymbol{\xi}\cdot\boldsymbol{L}/i\hbar}|\psi\rangle \\
&= \boldsymbol{\xi}\times\langle\psi|e^{-\lambda\boldsymbol{\xi}\cdot\boldsymbol{L}/i\hbar}\boldsymbol{A}e^{\lambda\boldsymbol{\xi}\cdot\boldsymbol{L}/i\hbar}|\psi\rangle \\
\frac{d}{d\lambda}\left\{\mathrm{R}_{\lambda\boldsymbol{\xi}}\langle\psi|\boldsymbol{A}|\psi\rangle\right\} &= \lim_{\epsilon\to 0}\frac{1}{\epsilon}\left\{\mathrm{R}_{\lambda\boldsymbol{\xi}+\epsilon\boldsymbol{\xi}} - \mathrm{R}_{\lambda\boldsymbol{\xi}}\right\}\langle\psi|\boldsymbol{A}|\psi\rangle \\
&= \lim_{\epsilon\to 0}\frac{1}{\epsilon}\left\{\mathrm{R}_{\epsilon\boldsymbol{\xi}} - \mathbb{1}\right\}\mathrm{R}_{\lambda\boldsymbol{\xi}}\langle\psi|\boldsymbol{A}|\psi\rangle \\
&= \lim_{\epsilon\to 0}\left\{\boldsymbol{\xi}\times\mathrm{R}_{\lambda\boldsymbol{\xi}}\langle\psi|\boldsymbol{A}|\psi\rangle + \mathcal{O}(\epsilon^2)\right\} = \boldsymbol{\xi}\times\mathrm{R}_{\lambda\boldsymbol{\xi}}\langle\psi|\boldsymbol{A}|\psi\rangle
\end{aligned}$$

The vectors $\langle\psi|e^{-\lambda\boldsymbol{\xi}\cdot\boldsymbol{L}/i\hbar}\boldsymbol{A}e^{\lambda\boldsymbol{\xi}\cdot\boldsymbol{L}/i\hbar}|\psi\rangle$ and $\mathrm{R}_{\lambda\boldsymbol{\xi}}\langle\psi|\boldsymbol{A}|\psi\rangle$ are both solutions of

$$\frac{d}{d\lambda}\boldsymbol{k}(\lambda) = \boldsymbol{\xi}\times\boldsymbol{k}(\lambda) \qquad\qquad \boldsymbol{k}(0) = \langle\psi|\boldsymbol{A}|\psi\rangle$$

Solution is unique, hence

$$(\forall\lambda \geq 0): \quad \langle\psi|e^{-\lambda\boldsymbol{\xi}\cdot\boldsymbol{L}/i\hbar}\boldsymbol{A}e^{\lambda\boldsymbol{\xi}\cdot\boldsymbol{L}/i\hbar}|\psi\rangle = \mathrm{R}_{\lambda\boldsymbol{\xi}}\langle\psi|\boldsymbol{A}|\psi\rangle$$

The actual statement we wish to prove follows by putting $\lambda = 1$.

7.2. Intrinsic Angular Momentum: Spin

7.2.1. Angular Momentum Operators

No define angular momentum operators J_i $(i = 1, 2, 3)$ more generally as generators of rotations in arbitrary Hilbert spaces, i.e. *just by the group structure*

$$S = e^{\boldsymbol{\xi}\cdot\boldsymbol{J}/i\hbar} \qquad [J_i, J_j] = i\hbar\sum_k \epsilon_{ijk}J_k \qquad J_i^\dagger = J_i$$

Much can be proved from structure only:

- $[J_i, \boldsymbol{J}^2] = 0$ (we have proved this earlier from commutation relations)
  Hence $\boldsymbol{J}^2$ and J_3 have a common basis of eigenstates.
- One can prove algebraically (similar to the algebraic solution of the harmonic oscillator) that these eigenstates $|j, m\rangle$ and correspond to the following spectrum of eigenvalues (no proof given here, due to lack of time):

$$\boldsymbol{J}^2|j, m\rangle = j(j+1)\hbar^2|j, m\rangle \qquad j \in \{0, \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots\}$$
$$J_3|j, m\rangle = m\hbar|j, m\rangle \qquad m \in \{-j, -j+1, -j+2, \ldots, j-1, j\}$$
$$\langle j, m|j', m'\rangle = \delta_{jj'}\delta_{mm'}$$

  So-called quantum numbers: (j, m)
- One also finds that the effect of rotation over 2π depends on the quantum number j:

$$\begin{aligned} S_{2\pi(0,0,1)}|j, m\rangle &= e^{2\pi J_3/i\hbar}|j, m\rangle = e^{2\pi m}|j, m\rangle \\ &= |j, m\rangle \quad \text{for } j \text{ even} \\ &= -|j, m\rangle \quad \text{for } j \text{ odd} \end{aligned}$$

- Define $\boldsymbol{J}$ as sum of *ordinary* angular momentum and *intrinsic* angular momentum ('spin'): $\boldsymbol{J} = \boldsymbol{L} + \boldsymbol{S}$

$$[L_i, L_j] = i\hbar\sum_k \epsilon_{ijk}L_k \qquad [S_i, S_j] = i\hbar\sum_k \epsilon_{ijk}S_k$$

  Since the standard energy dependence on angular momentum (charged particle moving in magnetic field $\boldsymbol{B}$) takes the form $\Delta H = g\boldsymbol{J}\cdot\boldsymbol{B}$:

$$[H, \boldsymbol{S}^2] = 0 \quad \text{hence} \quad \boldsymbol{S}^2 \quad \text{conserved}$$

  Consequence: if a particle is at $t = 0$ described by an eigenstate of $\boldsymbol{S}^2$, with quantum number s, the state will remain in this eigenspace for *all* times. Intrinsic angular momentum is called 'spin'. We may call the particle a spin-s particle.

7.2.2. Spin-$\frac{1}{2}$ Particles

(very brief)
Inspect particles with only intrinsic angular momentum as degrees of freedom.
Simplest particles: spin-$\frac{1}{2}$

- Two dimensional Hilbert space: spanned by $|\uparrow\rangle = |\frac{1}{2}, \frac{1}{2}\rangle$ and $|\downarrow\rangle = |\frac{1}{2}, -\frac{1}{2}\rangle$
  Operators S_i are represented by 2×2 complex Hermitian matrices
- Transform $S_i = \frac{1}{2}\hbar\sigma_i$: $[\sigma_i, \sigma_j] = 2i\epsilon_{ijk} \sum_k \sigma_k$
  by definition:
  $\sigma_3|\uparrow\rangle = \frac{2}{\hbar} S_3 |\frac{1}{2}, \frac{1}{2}\rangle = |\uparrow\rangle$
  $\sigma_3|\downarrow\rangle = \frac{2}{\hbar} S_3 |\frac{1}{2}, \frac{1}{2}\rangle = |\downarrow\rangle$

  $$\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

  Final objective: find matrices σ_1 and σ_2 such that

  $$[\sigma_1, \sigma_2] = 2i\sigma_3 \qquad [\sigma_2, \sigma_3] = 2i\sigma_1 \qquad [\sigma_1, \sigma_3] = -2i\sigma_2$$

  Solution:

  $$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

  (Pauli matrices)
  Note: $\sigma_i^2 = 1$
- Hamiltonian: $H = g\boldsymbol{B} \cdot \boldsymbol{\sigma} = g \sum_{i=1}^{3} \sigma_i$ (also a 2×2 matrix !)

8. Exercises

(i) Define the Kronecker symbol $\{\delta_{ij}\}$ and the tensor $\{\epsilon_{ijk}\}$ with $i, j, k \in \{1, 2, 3\}$ as follows:

$$\delta_{ij} = 1 \quad \text{if } i = j$$
$$\delta_{ij} = 0 \quad \text{otherwise}$$

$$\epsilon_{ijk} = 1 \quad \text{if } (i, j, k) \text{ is an even permutation of } (1, 2, 3)$$
$$\epsilon_{ijk} = -1 \quad \text{if } (i, j, k) \text{ is an odd permutation of } (1, 2, 3)$$
$$\epsilon_{ijk} = 0 \quad \text{otherwise}$$

- (a) Show, for $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^3$, that $(\boldsymbol{x} \times \boldsymbol{y})_i = \sum_{jk=1}^3 \epsilon_{ijk} x_j y_k$
- (b) Prove the following identity: $\sum_{i=1}^3 \epsilon_{ijk}\epsilon_{imn} = \delta_{jm}\delta_{kn} - \delta_{jn}\delta_{km}$

(ii) Define for a classical particle with $\boldsymbol{x}, \boldsymbol{p} \in \mathbb{R}^3$ the angular momentum vector $\boldsymbol{L} = \boldsymbol{x} \times \boldsymbol{p} \in \mathbb{R}^3$, with components $L_k = \sum_{\ell m=1}^3 \epsilon_{k\ell m} x_\ell p_m$. Let (A, B) denote the Poisson bracket:

$$(A, B) = \sum_{i=1}^{3} \left\{ \frac{\partial A}{\partial x_i}\frac{\partial B}{\partial p_i} - \frac{\partial A}{\partial p_i}\frac{\partial B}{\partial x_i} \right\}$$

- (a) Show that $(L_i, L_j) = \sum_{k=1}^3 \epsilon_{ijk} L_k$
- (b) Use the equation $df/dt = \partial f/\partial t + (f, H)$ to show that angular momentum is conserved for spherically symmetric potentials, i.e. when $V(\boldsymbol{x}) = V(|\boldsymbol{x}|)$.

(iii) Consider the wave function ψ of a QM particle in $\mathbb{R}^3$ moving in a (real-valued) potential $V(\boldsymbol{x})$, described by the Schrödinger equation. Define expectation values of operators as $\langle A \rangle = \int_{\mathbb{R}^3} d\boldsymbol{x}\ \psi^* A \psi$. You may assume that $\lim_{|\boldsymbol{x}|\to\infty} |\boldsymbol{x}|^3 |\psi(\boldsymbol{x}, t)|^2 = 0$.

- (a) Prove that $d\langle \boldsymbol{x} \rangle/dt = \langle \boldsymbol{p} \rangle/m$
- (b) Prove that $d\langle \boldsymbol{p} \rangle/dt = -\langle \boldsymbol{\nabla} V \rangle$

(iv) Let $\langle \phi|\psi \rangle$ denote an inner product on a Hilbert space $\mathcal{H}$, and let $\phi, \psi \in \mathcal{H}$.

- (a) Prove the Schwartz inequality: $|\langle \phi|\psi \rangle| \le |\phi||\psi|$.
  (hint: calculate $|\psi + \lambda\phi|^2|\phi|^2$ with $\lambda \in \mathbb{C}$)
- (b) Prove the triangular inequality: $|\phi - \psi| \le |\phi| + |\psi|$
- (c) Prove that strong convergence of a series $\{\psi_n\}$ in $\mathcal{H}$ implies weak convergence, i.e. that

$$\text{If } \lim_{n\to\infty} |\psi_n - \psi| = 0 \quad \text{then} \quad (\forall \chi \in \mathcal{H}): \quad \lim_{n\to\infty} \langle \psi_n|\chi \rangle = \langle \psi|\chi \rangle$$

(v) Consider the Hilbert space $L^2(0, 1)$. Prove that the following object defines an inner product on $L^2(0, 1)$:

$$\langle \psi|\phi \rangle = \int_0^1 dx\ \psi^*(x)\phi(x)$$

(vi) Find the norm $|f|$ of the function $f(\theta) = \cos(\theta)$ in the Hilbert space $L^2(0, 2\pi)$ with inner product $\langle f|g \rangle = \int_0^{2\pi} d\theta\ f^*(\theta)g(\theta)$.

(vii) Define the functions $\phi_n(\theta) = \sin(n\theta)$ for $n \in \{1, 2, 3, \ldots\}$, in the Hilbert space $L^2(0, \pi)$ with the standard complex inner product. Prove that $\langle \phi_n | \phi_m \rangle = 0$ if $m \neq n$.

(viii) Let $H = \boldsymbol{p}^2/2m + V(\boldsymbol{x})$, with $\boldsymbol{p} = -i\hbar\boldsymbol{\nabla}$. Calculate the two commutators $[x_i, H]$ and $[p_i, H]$.

(ix) Consider the wave function $\psi \in L^2(\mathbb{R}^3)$ of a QM particle in $\mathbb{R}^3$ moving in a (real-valued) potential $V(\boldsymbol{x})$, described by the Schrödinger equation. Define expectation values of operators as $\langle A \rangle = \langle \psi | A\psi \rangle$. Use the Ehrenfest Theorem to prove the following statements:

(a) $d\langle \boldsymbol{x} \rangle/dt = \langle \boldsymbol{p} \rangle/m$
(b) $d\langle \boldsymbol{p} \rangle/dt = -\langle \boldsymbol{\nabla} V \rangle$
(c) If $V(\boldsymbol{x}) = V(|\boldsymbol{x}|)$ then $d\langle \boldsymbol{L} \rangle/dt = \boldsymbol{0}$
(d) Virial Theorem: $d\langle \boldsymbol{x} \cdot \boldsymbol{p} \rangle/dt = m^{-1}\langle \boldsymbol{p}^2 \rangle - \langle \boldsymbol{x} \cdot \boldsymbol{\nabla} V \rangle$

(x) Solve the Schrödinger equation for a free particle in a one-dimensional box (i.e. $x \in [0, L]$), as was done in the lectures, but now with *periodic* boundary conditions. In other words, all eigenfunctions of H are now to satisfy $(\forall x \in [0, L]) : \ \phi_n(x) = \phi_n(x+L)$, rather than $\phi(0) = \phi_n(L) = 0$.

(xi) Solve the Schrödinger equation for a free particle in a two-dimensional box (i.e. $x_i \in [0, L_i]$ for $i = 1, 2$), similar to the lectures, with zero boundary conditions. Hint: use separation of spatial variables in the time-independent Schrödinger equation.

(xii) Calculate the transmission coefficient T for incoming plane waves in one dimension, scattering at a delta-peak of the form $V(x) = g\delta(x)$ (with $g > 0$). Use the following two methods, and verify that the two results which you thereby obtain are identical:

(a) Calculate directly the non-normalizable solutions of the Schrödinger equation, describing an incoming wave from the left, in analogy with the derivation for scattering at a block potential in the lectures. Deal with the singularity using the method described in the lectures for $V(x) = -g\delta(x)$.
(b) Take a suitable limit in the expression for T which was derived for scattering at a block potential in the lectures.

(xiii) Solve the Schrödinger equation for a charged particle in a one-dimensional harmonic oscillator potential, in the presence of an electric field, where

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2 - qx$$

(xiv) We consider the one-dimensional harmonic oscillator, i.e.

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

Define the standard creation and annihilation operators. Use the creation and annihilation operators to calculate $\langle x \rangle$ and $\langle p \rangle$ as functions of time from the general solution of the Schrödinger equation, for *arbitrary* initial states $\psi(x, 0)$. Express $\langle x \rangle$ and $\langle p \rangle$ in terms of $\langle x\rangle_{t=0}$ and $\langle p\rangle_{t=0}$. Verify the correspondence principle, i.e. confirm that your solution satisfies

$$\frac{d}{dt}\langle x\rangle = \langle p\rangle/m \qquad \frac{d}{dt}\langle p\rangle = -\langle\frac{d}{dx}V(x)\rangle = -m\omega^2\langle x\rangle$$

(xv) We consider again the one-dimensional harmonic oscillator. Define the standard creation and annihilation operators. Investigate and compare the following two alternative methods for calculating $\langle x\rangle$ and $\langle p\rangle$ as functions of time, for arbitrary initial states $\psi(x,0)$.

(a) Use the Ehrenfest theorem to derive ordinary differential equations for $\langle x\rangle$ and $\langle p\rangle$, and solve these equations. Verify that the outcome agrees with that of the previous exercise.

(b) Use the Ehrenfest theorem to prove that $\langle a\rangle = e^{-i\omega t}\langle a\rangle_{t=0}$ and $\langle a^\dagger\rangle = e^{i\omega t}\langle a^\dagger\rangle_{t=0}$. Use the result to express $\langle x\rangle$ and $\langle p\rangle$ in terms of $\langle x\rangle_{t=0}$ and $\langle p\rangle_{t=0}$. Verify that the outcome agrees with your earlier results.

(xvi) Verify the validity of the operator identity $[x,p] = i\hbar$ upon writing x and p in each of the following representations (where they take the form of ∞-dimensional matrices or integral operators):

(a) In number representation, i.e. with respect to the basis of eigenstates of $N = a^\dagger a$.

(b) In momentum representation, i.e. with respect to the basis of eigenstates of p.

(c) In position representation, i.e. with respect to the basis of eigenstates of x.

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