Part II Principles of Quantum Mechanics
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Contents

BOOKS

- E. Merzbacher *Quantum Mechanics, 3rd edition.* Wiley 1998 (various prices)
- B.H. Bransden and C.J. Joachain *Quantum Mechanics, 2nd edition.* Pearson 2000 (£50-60 on Amazon)
- J. Binney and D. Skinner *The Physics of Quantum Mechanics, 3rd edition.* Cappella Archive 2013 (£23.71)
- P.A.M. Dirac *The Principles of Quantum Mechanics.* Oxford University Press 1967 reprinted 1999 (£23.99).
- C.J. Isham *Lectures on Quantum Theory: Mathematical and Structural Foundations.* Imperial College Press 1995 (around £18)
- S. Gasiorowicz *Quantum Physics, 3rd edition.* Wiley International 2003 £48.71

Mot of these books are expensive new and there are a lot of pedagogic books on quantum mechanics, so it's good to look at those in the library since many books are good in one area but poor in another. Other books may be recommeneded through the course.

1 Introduction

★ Recall features of elementary (IB) quantum mechanics:

- **wave-particle duality.** Waves behaving like particles – e.g., light quanta, photons and vice-versa; interference of electrons passing through crystal grating and electron microscope. To make this more precise need:
- **wavefunction** $\psi(x)$ for particle. Probability density $|\psi(x)|^2$; probability is intrinsic to the theory.
- **0bservables become (hermitian) operators on wavefunctions**. Lack of commutation limits simultaneous measurement – leads to precise version of uncertainty principle.
- **Schrödinger's equation** specifies dynamics (evolution in time) and determines energy levels.

This is enough to understand e.g., the hydrogen atom and transcends classical physics.

★ Aim of this course:

- reformulate QM in a more powerful, abstract, flexible and useful form: **Dirac formalism**. This allows a simpler analysis of known problems such as the harmonic oscillator and is also the clearest way to understand lots of more novel properties, for example:
- the spin of particles;
- symmetries (e.g., translations and rotations) and conservation laws;
- identical particles;
- it provides the framework for quantizing other, more general, systems e.g., EM field, and ultimately other forces leading to the 'Standard Model' of elementary particles.

★ Will not dwell on applications in any detail, but will keep track of what the mathematical formalism is for.

★ Assume IB QM and IA Dynamics but no electromagnetism beyond Coulomb's law and intuitive ideas about magnetism.

Plan:

1. Dirac formalism.
2. Harmonic oscillator.
3. Pictures of quantization.
4. Composite systems and identical particles.
5. Perturbation theory.
6. Angular momentum.
7. Transformations and symmetries.
8. Time-dependent perturbation theory.
9. Quantum basics.

2 Dirac Formalism

2.1 States and Operators

A quantum state is described at each instant by a **state** $|\psi\rangle$ which belongs to a complex vector apace V. Then

$$|\psi\rangle,\ |\phi\rangle\ \in\ V\ \Longrightarrow\ \alpha|\psi\rangle+\beta|\phi\rangle\ \in\ V\ \ \forall\,\alpha,\beta\ \in\ \mathbb{C}. \tag{2.1.1}$$

Physically this is the superposition principle leading to wave-like behaviour (interference). However, these states are not wavefunctions but we will see that they carry all the quantum information that describes the **state** of the system concerned in a very general way.

There are also **dual** or conjugate states $\langle\phi|$ which belong to the dual space $V^\dagger$. By definition, states and duals can be combined/paired to give a complex number:

$$\underbrace{\langle\phi|}_{\text{'bra'}}\ ,\ \underbrace{|\psi\rangle}_{\text{'ket'}}\ \mapsto\ \underbrace{\langle\phi|\psi\rangle}_{\text{'bra(c)ket'}}\qquad\text{or formally}\quad V^\dagger\times V\ \to\ \mathbb{C}\,, \tag{2.1.2}$$

with

$$\begin{aligned}\langle\phi|\Big(\alpha_1|\psi_1\rangle\ +\ \alpha_2|\psi_2\rangle\Big)\ &=\ \alpha_1\langle\phi|\psi_1\rangle\ +\ \alpha_2\langle\phi|\psi_2\rangle\,,\\ \Big(\beta_1\langle\phi_1|\ +\ \beta_2\langle\phi_2|\Big)|\psi\rangle\ &=\ \beta_1\langle\phi_1|\psi\rangle\ +\ \beta_2\langle\phi_2|\psi\rangle\,,\end{aligned} \tag{2.1.3}$$

$\alpha,\beta\in\mathbb{C}$. This is the definition of the dual as a vector space.

The space of states V and the dual $V^\dagger$ come with an inner-product which can be described as a one-to-one correspondence between states and duals:

$$\begin{array}{lrcl} & V & \longleftrightarrow & V^\dagger \\ \text{with} & |\psi\rangle & \longleftrightarrow & \langle\psi|=(\ |\psi\rangle)^\dagger\ \ \text{(use same label for corresponding states)} \\ \text{and} & \alpha|\psi\rangle+\beta|\phi\rangle & \longleftrightarrow & \alpha^*\langle\psi|\ +\ \beta^*\langle\phi|\,. \end{array} \tag{2.1.4}$$

The inner product is

$$\begin{aligned} V\times V\ &\to\ \mathbb{C}\\ |\phi\rangle,|\psi\rangle\ &\mapsto\ \langle\phi|\psi\rangle\ =\ (|\phi\rangle)^\dagger|\psi\rangle\,, \end{aligned} \tag{2.1.5}$$

and is assumed to obey

$$\begin{array}{rrcll} & \langle\phi|\psi\rangle & = & \langle\psi|\phi\rangle^* & \text{hermitian} \\ & \||\psi\rangle\|^2 & = & \langle\psi|\psi\rangle\ \ \geq\ 0 & \text{(real from above)} \\ \text{with} & \||\psi\rangle\|^2 & = & 0\qquad \text{iffi} & |\psi\rangle=0. \end{array} \tag{2.1.6}$$

This means that the inner product is **positive semidefinite**. Note that knowing $\langle\phi|\psi\rangle$ for all $\langle\phi|$ determines $|\psi\rangle$ uniquely and vice-versa.

The physical content of any state is unaltered by changing $|\psi\rangle\to\alpha|\psi\rangle$ ($\alpha\neq0$). We shall usually normalize states by $\||\psi\rangle\|^2=1$ but still have the freedom to change $|\psi\rangle\to e^{i\theta}|\psi\rangle$. The absolute phase of a single state never has any physical significance,

but relative phases in combination such as $\alpha|\phi\rangle + \beta|\psi\rangle$ can be significant; for example, for interference phenomena.

The space V is complete; we assume appropriate sequences or series converge. A complete inner product space of this kind is a **Hilbert space** and this term is often used for the space V in QM. V can be either finite or infinite dimensional and we shall see examples of both.

An operator Q is a linear map on states, $V \to V$:

$$|\psi\rangle \mapsto Q|\psi\rangle, \tag{2.1.7}$$

and, by definition

$$Q\Big(\alpha|\phi\rangle + \beta|\psi\rangle\Big) = \alpha Q|\phi\rangle + \beta Q|\psi\rangle \ . \tag{2.1.8}$$

The same operator can be regarded as acting 'to the left' on dual states, $V^\dagger \to V^\dagger$:

$$\langle\phi| \mapsto \langle\phi|Q \ , \tag{2.1.9}$$

$$\begin{aligned} \Big(\langle\phi|Q\Big)|\psi\rangle &= \langle\phi|\Big(Q|\psi\rangle\Big) \quad \forall \quad |\psi\rangle \\ \text{or simply} \qquad &= \langle\phi|Q|\psi\rangle \ . \end{aligned} \tag{2.1.10}$$

For any Q the **hermitian conjugate** or **adjoint** is an operator $Q^\dagger$ defined by

$$\langle\phi|Q^\dagger = \Big(Q|\phi\rangle\Big)^\dagger \ , \tag{2.1.11}$$

or, equivalently,

$$\begin{aligned} \langle\phi|Q^\dagger|\psi\rangle &= \Big(Q|\phi\rangle\Big)^\dagger|\psi\rangle \\ &= \langle\psi|Q|\phi\rangle^* \quad \forall \quad |\psi\rangle,\ |\phi\rangle \ . \end{aligned} \tag{2.1.12}$$

Simple consequences are

$$\begin{aligned} \Big(\alpha A + \beta B\Big)^\dagger &= \alpha^* A^\dagger + \beta^* B^\dagger \ , \\ \Big(AB\Big)^\dagger &= B^\dagger A^\dagger \ , \end{aligned} \tag{2.1.13}$$

for any A, B.[1]

[1]

$$\begin{aligned} \langle\psi|(AB)^\dagger|\phi\rangle &= \Big((AB)|\psi\rangle\Big)^\dagger|\phi\rangle && \text{defn of } (AB)^\dagger \\ &= \Big(A|\psi'\rangle\Big)^\dagger|\phi\rangle && |\psi'\rangle \equiv B|\psi\rangle \\ &= \langle\psi'|A^\dagger|\phi\rangle && \text{defn of } A^\dagger \\ &= \Big(B|\psi\rangle\Big)^\dagger\Big(A^\dagger|\phi\rangle\Big) \\ &= \langle\psi|B^\dagger A^\dagger|\phi\rangle && \text{defn of } B^\dagger \ . \end{aligned} \tag{2.1.14}$$

True for all $|\psi\rangle, |\phi\rangle$ and result follows.

For any operator Q call $|\psi\rangle$ ($\neq 0$) an **eigenstate** of Q with eigenvalue λ if

$$Q|\psi\rangle \;=\; \lambda|\psi\rangle \;. \tag{2.1.15}$$

Equivalently (taking † of this)

$$\langle\psi|Q^\dagger \;=\; \lambda^*\langle\psi| \;. \tag{2.1.16}$$

For general Q, λ can be complex.
Of particular importance are commutators of operators

$$[A,B] \;=\; AB - BA \;=\; -\,[B,A] \;. \tag{2.1.17}$$

We have the identities

$$\begin{array}{rcl} [\alpha_1 A_1 + \alpha_2 A_2, B] & = & \alpha_1[A_1,B] \;+\; \alpha_2[A_2,B] \\ [A, \beta_1 B_1 + \beta_2 B_2] & = & \beta_1[A,B_1] \;+\; \beta_2[A,B_2] \end{array} \qquad \text{linearity} \tag{2.1.18}$$

$$\begin{array}{rcl} [A,B_1B_2] & = & [A,B_1]B_2 \;+\; B_1[A,B_2] \\ [A_1A_2,B] & = & [A_1,B]A_2 \;+\; A_1[A_2,B] \end{array} \qquad \text{Leibnitz properties} \tag{2.1.19}$$

$$[A,[B,C]] \;+[B,[C,A]] \;+\; [C,[A,B]] \;=0 \qquad \text{Jacobi identity} \tag{2.1.20}$$

2.2 Observables and measurements

An operator Q is **hermitian** or **self-adjoint** if

$$Q^\dagger \;=\; Q \;. \tag{2.2.1}$$

Such operators are called **observables** because they correspond to physical, measurable, quantities e.g., position, momentum, energy, angular momentum. Key results for any hermitian Q:

(i) All eigenvalues are real.
(ii) Eigenstates with distinct eigenvalues are orthogonal.
(iii) The eigenstates form a complete basis for V (and their duals for $V^\dagger$). So any state can be expanded in terms of (written as a linear combination of) the eigenstates.

We prove (i) and (ii) and assume (iii).

(i)

$$\begin{array}{lrcll} & Q|\psi\rangle & = & \lambda|\psi\rangle & \\ \text{and} & \langle\psi|Q^\dagger & = & \lambda^*\langle\psi| & \\ \Rightarrow & \langle\psi|Q & = & \lambda^*\langle\psi| & \text{since } Q \text{ is hermitian} \\ \Rightarrow & \langle\psi|Q|\psi\rangle & = & \lambda\langle\psi|\psi\rangle \;=\; \lambda^*\langle\psi|\psi\rangle \;. & \end{array} \tag{2.2.2}$$

But $\||\psi\rangle\|^2 = \langle\psi|\psi\rangle \neq 0$ ($|\psi\rangle \neq 0$) and so deduce

$$\lambda \;= \lambda^* \;. \tag{2.2.3}$$

(ii) Let $|n\rangle$ be eigenstates of Q with eigenvalues $\lambda = q_n$ real, with n a discrete label possibly of infinite range.

$$\begin{array}{lrcl} & Q|n\rangle & = & q_n|n\rangle \\ \text{and} & Q|m\rangle & = & q_m|m\rangle \\ \text{or} & \langle m|Q & = & q_m\langle m| \\ \Rightarrow & \langle m|Q|n\rangle & = & q_n\langle m|n\rangle \;=\; q_m\langle m|n\rangle \,. \end{array} \tag{2.2.4}$$

So $q_n \neq q_m \;\Rightarrow\; \langle m|n\rangle = 0$.

Combining these three properties we have

★ For any observable Q there is an orthonormal **basis** of eigenstates $\{|n\rangle\}$ for the space of states V with

$$\begin{aligned} Q|n\rangle &= q_n|n\rangle \,, \\ \langle m|n\rangle &= \delta_{mn} \,. \end{aligned} \tag{2.2.5}$$

We speak of **diagonalizing** Q by choosing the basis to be the eigenstates $|n\rangle$ of Q. This means that a general state $|\psi\rangle$ can be expanded as

$$|\psi\rangle \;=\; \sum_n \alpha_n|n\rangle \,, \tag{2.2.6}$$

where $\alpha_n = \langle n|\psi\rangle$.

For the state to be properly normalized

$$\begin{array}{rcl} \||\psi\rangle\|^2 \;=\; \langle\psi|\psi\rangle & = & 1 \\ \Longleftrightarrow \qquad \Big(\sum_m \alpha_m^*\langle m|\Big)\Big(\sum_n \alpha_n|n\rangle\Big) & = & \sum_n |\alpha_n|^2 \;=\; 1 \,. \end{array} \tag{2.2.7}$$

There might be several states with the same eigenvalue λ. Define the **eigenspace** for a given eigenvalue by

$$V_\lambda \;=\; \{|\psi\rangle :\; Q|\psi\rangle = \lambda|\psi\rangle\} \,, \tag{2.2.8}$$

which has the basis $\{|n\rangle :\; q_n = \lambda\}$.

The **degeneracy** of λ is the number of states in this basis, or $\dim V_\lambda$. We say that λ is **non-degenerate** if the degeneracy is 1.

⌈ Note that passing from our three key results to the conclusion (★) is achieved by choosing an orthonormal basis for each V_λ:

(ii) ensures that these spaces are mutually orthogonal;

(iii) implies that the sum of all the eigenspaces is V, the entire space of states. ⌋

Consider a measurement of Q when the system is in state $|\psi\rangle$ immediately before. Then

- The result is an eigenvalue, λ, say.

- This value is obtained with the probability

$$p(\lambda) \;=\; \sum_{n:q_n=\lambda} |\alpha_n|^2. \tag{2.2.9}$$

- Immediately after the measurement the state is

$$|\phi\rangle \;=\; c \sum_{n:q_n=\lambda} \alpha_n |n\rangle \;, \tag{2.2.10}$$

  where c is a normalization constant chosen so that $\langle\phi|\phi\rangle = 1$.

So measurement **projects** the system into the eigenspace V_λ.

Example. Consider a system with three orthonormal states: $|1\rangle, |2\rangle, |3\rangle$ on which Q has eigenvalues $q_1 = q_2 = 0,\ q_3 = 1$. Let the state of the system be

$$|\psi\rangle \;=\; \frac{1}{\sqrt{6}}(2|1\rangle + |2\rangle + |3\rangle) \;. \tag{2.2.11}$$

Then

$$\text{Probability of measuring} \begin{cases} 1 & \left|\frac{1}{\sqrt{6}}\right|^2 \;=\; \frac{1}{6} & |3\rangle \\ 0 & \left|\frac{2}{\sqrt{6}}\right|^2 + \left|\frac{1}{\sqrt{6}}\right|^2 \;=\; \frac{5}{6} & \frac{1}{\sqrt{5}}(2|1\rangle + |2\rangle) \\ & & \uparrow \\ & & \text{final states} \end{cases} \tag{2.2.12}$$

In this example we had degeneracy: two states with eigenvalue 0. However, often have the case with λ non-degenerate with eigenstate $|n\rangle$ unique up to a phase. Then

- $p(\lambda) \;=\; |\alpha_n|^2 \;=\; |\langle n|\psi\rangle|^2$.
- $\alpha_n \;=\; \langle n|\psi\rangle$ is called the **amplitude**.
- The state after measurement is $|n\rangle$.

In general,

$$\sum_\lambda p(\lambda) = \sum_n |\alpha_n|^2 = 1 \;, \tag{2.2.13}$$

as required for a probability distribution.

The **expectation value** (mean) of Q in state $|\psi\rangle$ is

$$\langle Q\rangle_\psi \;=\; \langle\psi|Q|\psi\rangle \;=\; \sum_\lambda \lambda p(\lambda) \;=\; \sum_n q_n |\alpha_n|^2 \;, \tag{2.2.14}$$

and the **uncertainty** (spread or variance) is

$$(\Delta Q)^2_\psi \;=\; \langle (Q - \langle Q\rangle_\psi)^2\rangle_\psi \;=\; \langle Q^2\rangle_\psi - \langle Q\rangle^2_\psi \;. \tag{2.2.15}$$

In thinking about many repeated measurements we must be careful to prepare the system in the same state each time.

In the case that $|\psi\rangle$ is an eigenstate of Q with eigenvalue λ, say, then

$$\langle Q\rangle_\psi \;=\; \lambda\,, \quad \text{and} \quad (\Delta Q)_\psi \;=\; 0\,. \tag{2.2.16}$$

⌈ The process of measurement is still a source of some deep questions about the interpretation of QM ⌋.

Quantum mechanical behaviour arises from the fact that observables do not commute in general. In any state $|\psi\rangle$

$$\langle \Delta A\rangle_\psi \langle \Delta B\rangle_\psi \;\geq\; \frac{1}{2}|\langle [A,B]\rangle_\psi|\,, \tag{2.2.17}$$

so $[A,B]\neq 0$ means we cannot expect to measure exact values for A and B simultaneously. This generalized **Uncertainty Principle** follows from

$$\|(A+i\lambda B)|\psi\rangle\|^2 \;\geq\; 0 \quad \forall \quad \text{real} \;\; \lambda\,. \tag{2.2.18}$$

The LHS is a quadratic in λ and the condition implies that the discriminant is ≤ 0; the stated Uncertainty Principle then follows.

Paradigm example: position, $\hat{x}$, and momentum, $\hat{p}$, in one dimension obey

$$\begin{aligned} [\hat{x},\hat{p}] \;&=\; i\hbar \\ \Rightarrow \qquad \Delta x\,\Delta p \;&\geq\; \frac{\hbar}{2}\,. \end{aligned} \tag{2.2.19}$$

In $D=3$, $\hat{x}_i$ and $\hat{p}_i$ obey

$$[\hat{x}_i,\hat{p}_j] \;=\; i\hbar\delta_{ij}\,, \tag{2.2.20}$$

and so the uncertainty principle applies to components of position and momentum which are not orthogonal.

2.3 Time evolution and the Schrödinger Equation

So far our discussion of quantum states has been at a fixed time, even measurement is assumed to be an instantaneous change of state. The evolution of states $|\psi(t)\rangle$ in time is governed by the Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle \;=\; H|\psi(t)\rangle\,, \tag{2.3.1}$$

where $H=H^\dagger$ is the Hamiltonian. Equivalently,

$$-i\hbar\frac{\partial}{\partial t}\langle\psi(t)| \;=\; \langle\psi(t)|H\,. \tag{2.3.2}$$

Note that these equations imply

$$\frac{\partial}{\partial t}\Big(\langle\psi(t)|\psi(t)\rangle\Big) \;=\; 0\,, \tag{2.3.3}$$

so that the normalization of $|\psi(t)\rangle$, and hence the probabilistic interpretation, is preserved in time.

H is an observable: the energy. Consider the eigenstates

$$H|n\rangle \;=\; E_n|n\rangle \;. \tag{2.3.4}$$

Then the states

$$e^{-iE_nt/\hbar}|n\rangle \tag{2.3.5}$$

are **stationary state** solutions of the Schrödinger Equation.

The Schrödinger Equation is first-order in t and linear in $|\psi(t)\rangle$ and so for an initial state at $t = 0$,

$$|\psi(0)\rangle \;=\; \sum_n \alpha_n|n\rangle \;, \tag{2.3.6}$$

we have the unique solution

$$|\psi(t)\rangle \;=\; \sum_n \alpha_n e^{-iE_nt/\hbar}|n\rangle \;. \tag{2.3.7}$$

Example. Consider system with two energy eigenstates $|1\rangle, |2\rangle$ with energy eigenvalues E_1, E_2, respectively. We are interested in measuring Q defined by

$$Q|1\rangle \;=\; |2\rangle, \quad Q|2\rangle \;=\; |1\rangle \quad \Rightarrow \quad [Q, H] \;\neq\; 0 \;. \tag{2.3.8}$$

The eigenstates of Q are easily found to be

$$|\pm\rangle \;=\; \frac{1}{\sqrt{2}}\Big(|1\rangle \pm |2\rangle\Big) \quad \text{with eigenvalues} \quad q_\pm = \pm 1 \;. \tag{2.3.9}$$

Let the initial state, the state at $t = 0$, be $|\psi(0)\rangle = |+\rangle$. Then have

$$|\psi(t)\rangle \;=\; \frac{1}{\sqrt{2}}\Big(e^{-iE_1t/\hbar}|1\rangle + e^{-iE_2t/\hbar}|2\rangle\Big) \;. \tag{2.3.10}$$

The probability of measuring Q at time t and getting ± 1 is

$$\begin{aligned} |\langle\pm|\psi(t)\rangle|^2 \;&=\; \left|\frac{1}{2}\Big(\langle 1| \pm \langle 2|\Big)\Big(e^{-iE_1t/\hbar}|1\rangle + e^{-iE_2t/\hbar}|2\rangle\Big)\right|^2 \\ &=\; \left|\frac{1}{2}\Big(e^{-iE_1t/\hbar} \pm e^{-iE_2t/\hbar}\Big)\right|^2 \\ &=\; \begin{cases} \cos^2\left(\frac{(E_1-E_2)t}{2\hbar}\right) \\ \\ \sin^2\left(\frac{(E_1-E_2)t}{2\hbar}\right) \end{cases} \end{aligned} \tag{2.3.11}$$

Note that we are assuming **no** time-dependence in H. This would become a much more complex situation.

2.4 Bases and Representations

Another use of a basis is that we can choose to reduce all states and operators to, possibility infinite, column/row vectors and to matrices as follows

$$\begin{aligned} |\psi\rangle &= \sum_n \alpha_n |n\rangle \quad \Leftrightarrow \quad \alpha_n = \langle n|\psi\rangle \\ |\phi\rangle &= \sum_n \beta_n |n\rangle \quad \Leftrightarrow \quad \beta_n = \langle n|\phi\rangle \ . \end{aligned} \tag{2.4.1}$$

The inner product is then

$$\langle\phi|\psi\rangle = \sum_n \beta_n^* \alpha_n \ . \tag{2.4.2}$$

The operation of operator A can be written as

$$A|n\rangle = \sum_m |m\rangle A_{mn} \ , \tag{2.4.3}$$

where $A_{mn} = \langle m|A|n\rangle$ are the **matrix elements** of the **complex** matrix **representing** the operator A in this basis. Note that the entries in this matrix depend on the basis; a familiar result in linear algebra for any linear map. In contrast, the result of operating with A on any state is **independent** of the basis. Check this result

$$\underbrace{|\phi\rangle = A|\psi\rangle}_{\text{basis-independent}} \quad \Leftrightarrow \quad \underbrace{\beta_m = \sum_n A_{mn}\alpha_n}_{\text{basis-dependent}} \ . \tag{2.4.4}$$

Clearly, this representation is multiplication of a vector by a matrix: $\boldsymbol{\beta} = \boldsymbol{A}\boldsymbol{\alpha}$. Also, have that the Hermitian conjugate has the familiar matrix form:

$$(A^\dagger)_{mn} = A^*_{nm} \ . \tag{2.4.5}$$

If B is another operator with matrix $\boldsymbol{B}$ then

$$(AB)_{mn} = \sum_p A_{mp} B_{pn} \ . \tag{2.4.6}$$

I.e., as expected the usual rules of matrix multiplication apply.

This, by now familiar, way of representing linear maps on a vector space by the linear algebra of matrices gives the matrix representation of Quantum Mechanics. It is most useful when the number of basis states is finite, but can also be useful for an ∞ dimensional basis as well (does need care).

We are often interested in a function $f(Q)$ of an operator Q. How should this be defined? The answer may be obvious if f is a polynomial or a series:

$$Q + \frac{Q^3}{3} \ , \quad e^Q \ , \quad \sin(Q) \qquad \text{assuming convergence} \ . \tag{2.4.7}$$

But what about $1/Q$ or $\log(Q)$?

For Q an observable and $|n\rangle$ an eigenbasis for Q:

$$Q|n\rangle \;=\; q_n|n\rangle \qquad \langle n|m\rangle \;=\; \delta_{mn}\;, \tag{2.4.8}$$

setting

$$f(Q)|n\rangle \;=\; f(q_n)|n\rangle \tag{2.4.9}$$

defines $f(Q)$ provided $f(q_n)$ is defined for all n; $f(Q)$ is defined on a basis and so is defined on any state. This is certainly true if f is a polynomial or a power series that converges for all q_n. If $q_n \neq 0 \;\; \forall \;\; n$ then can define

$$Q^{-1}|n\rangle \;=\; \frac{1}{q_n}|n\rangle\;, \tag{2.4.10}$$

and likewise $\log(Q)$ is defined if $0 < q_n < \infty$.

A useful way to express that $\{|n\rangle\}$ is an orthonormal basis is the **completeness relation** or **resolution of the identity**:

$$\sum_n\; |n\rangle\langle n| \;=\; \mathbb{I}\;, \qquad \text{the identity operator.} \tag{2.4.11}$$

The notation is

$$\Big(\; \underbrace{|n\rangle\langle m|}_{\text{operator}} \;\Big)\; \underbrace{|\psi\rangle}_{\text{state}} \;=\; \underbrace{|n\rangle}_{\text{state}} \Big(\; \underbrace{\langle m|\psi\rangle}_{\text{number}} \;\Big)\;. \tag{2.4.12}$$

This is confirmed by applying each side to an arbitrary state

$$\sum_n\; |n\rangle\langle n|\psi\rangle \;=\; |\psi\rangle \;=\; \mathbb{I}|\psi\rangle\;. \tag{2.4.13}$$

In the same way can resolve any operator in a similar fashion:

$$\begin{aligned} Q \;&=\; \sum_n\; q_n|n\rangle\langle n|\;, \\ f(Q) \;&=\; \sum_n\; f(q_n)|n\rangle\langle n|\;. \end{aligned} \tag{2.4.14}$$

In the case where the eigenvalues are degenerate then we can define a projection operator onto the subspace of eigenstates with eigenvalue λ by

$$P_\lambda \;=\; \sum_{n:\; q_n=\lambda}\; |n\rangle\langle n|\;. \tag{2.4.15}$$

The bases considered so far may be infinite but have been assumed **discrete** which includes countably infinite bases. However, we can extend the index n to be continuous. This requires some modifications in all relevant formulas:

$$\begin{aligned} \sum_n \;\;&\to\;\; \int dn \qquad \left\{ \begin{array}{rcl} |\psi\rangle &=& \int dn\; \alpha_n|n\rangle \\ \mathbb{I} &=& \int dn\; |n\rangle\langle n| \\ Q &=& \int dn\; q(n)|n\rangle\langle n| \end{array} \right. \\ \langle n|m\rangle \;&=\; \delta_{nm} \;\;\to\;\; \delta(n-m) \end{aligned} \tag{2.4.16}$$

with $|\alpha_n|^2 \;=\; |\langle n|\psi\rangle|^2$. There is no longer a probability for discrete outcomes but a **probability density** for the continuous range of n. We will see this below for position and momentum operators.

2.5 Position and momentum basis – wavefunctions

Consider particle motion in one dimension. Position and momentum operators $\hat{x}, \hat{p}$ obey

$$[\hat{x}, \hat{p}] \;=\; i\hbar\,. \tag{2.5.1}$$

Let $|x\rangle$ be position eigenstates

$$\hat{x}|x\rangle \;=\; x|x\rangle\,, \tag{2.5.2}$$

with continuous eigenvalue x and normalization

$$\langle x|x'\rangle \;=\; \delta(x-x')\,, \qquad \int dx\;|x\rangle\langle x| \;=\; \mathbb{I}\,. \tag{2.5.3}$$

In this basis, any state can be expanded as

$$\begin{aligned} |\psi\rangle \;&=\; \int dx\;\psi(x)|x\rangle \\ \text{with}\quad \psi(x) \;&=\; \langle x|\psi\rangle \qquad \text{a complex function}\,. \end{aligned} \tag{2.5.4}$$

$\psi(x)$ is just the usual position wavefunction and the standard interpretation is the obvious extension of the measurement postulates in section 2.2 to continuous eigenvalues:

$$|\psi(x)|^2 \;\text{ is the probability density for measuring position.} \tag{2.5.5}$$

The inner product in terms of wavefunctions becomes

$$\begin{aligned} \langle\phi|\psi\rangle \;&=\; \left(\int dx\;\phi(x)^*\langle x|\right)\left(\int dx'\;\psi(x')|x'\rangle\right) \\ &=\; \int dx \int dx' \phi(x)^*\psi(x')\;\underbrace{\langle x|x'\rangle}_{\delta(x-x')} \\ &=\; \int dx \phi(x)^*\psi(x)\,. \end{aligned} \tag{2.5.6}$$

So, in particular,

$$\||\psi\rangle\|^2 \;=\; \langle\psi|\psi\rangle \;=\; \int dx\;|\psi(x)|^2 \;=\; 1 \tag{2.5.7}$$

for a normalized state.

Define similarly momentum eigenstates $|p\rangle$ with

$$\hat{p}|p\rangle \;=\; p|p\rangle\,, \tag{2.5.8}$$

and with

$$\langle p|p'\rangle \;=\; \delta(p-p')\,, \qquad \int dp\;|p\rangle\langle p| \;=\; \mathbb{I}\,. \tag{2.5.9}$$

It is very important that the eigenstates of $\hat{x}$ and $\hat{p}$ can be chosen so that they are related by

$$\langle x|p\rangle \;=\; \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}\,, \tag{2.5.10}$$

$$\Rightarrow \qquad \langle p|x\rangle \;=\; \frac{1}{\sqrt{2\pi\hbar}} e^{-ipx/\hbar}\,. \tag{2.5.11}$$

We justify this later after deducing some consequences. First find action of $\hat{x}$ and $\hat{p}$ in terms of position wavefunctions:

$$\begin{aligned}
\hat{x}|\psi\rangle \quad \text{wavefunction}: \quad & \langle x|\hat{x}|\psi\rangle \;=\; x\langle x|\psi\rangle \;=\; x\psi(x) \\
\hat{p}|\psi\rangle \quad \text{wavefunction}: \quad & \langle x|\hat{p}|\psi\rangle \\
&= \int dp\, \langle x|\hat{p}|p\rangle\langle p|\psi\rangle \qquad \text{[resolution of identity using p-states]} \\
&= \int dp\, p\langle x|p\rangle\langle p|\psi\rangle \\
&= \int dp\; -i\hbar\frac{\partial}{\partial x}\Big(\langle x|p\rangle\Big)\langle p|\psi\rangle \\
&= -i\hbar\frac{\partial}{\partial x}\int dp\, \langle x|p\rangle\langle p|\psi\rangle \\
&= -i\hbar\frac{\partial}{\partial x}\langle x|\psi\rangle \;=\; -i\hbar\frac{\partial}{\partial x}\psi(x)\,, \qquad (2.5.12)
\end{aligned}$$

and so recover familiar results. However, also have new possibility. Can expand states in momentum basis instead:

$$\begin{aligned}
|\psi\rangle &= \int dp\, \tilde{\psi}(p)|p\rangle\,, \\
\text{with} \qquad \tilde{\psi}(p) &= \langle p|\psi\rangle\,, \qquad (2.5.13)
\end{aligned}$$

which is the momentum space wavefunction where $|\tilde{\psi}(p)|^2$ is the probability density for measurements of momentum. Then have

$$\||\psi\rangle\|^2 \;=\; \int dp\, \langle\psi|p\rangle\langle p|\psi\rangle \;=\; \int dp\, |\tilde{\psi}(p)|^2 \;=\; 1\,. \qquad (2.5.14)$$

As before, but with $x \leftrightarrow p$:

$$\left.\begin{array}{lcl} \hat{p}|\psi\rangle & \longrightarrow & p\tilde{\psi}(p) \\ \hat{x}|\psi\rangle & \longrightarrow & i\hbar\dfrac{\partial}{\partial p}\tilde{\psi}(p) \end{array}\right\} \quad \begin{array}{l}\text{momentum space} \\ \text{wavefunctions}\end{array} \qquad (2.5.15)$$

The relationship between the wavefunctions follows from Eq. (2.5.10):

$$\begin{aligned}
\tilde{\psi}(p) &= \langle p|\psi\rangle \;=\; \int dx\, \langle p|x\rangle\langle x|\psi\rangle \\
&= \frac{1}{\sqrt{2\pi\hbar}}\int dx\, e^{-ipx/\hbar}\,\psi(x) \qquad \text{Fourier transform,} \\
\text{and} \quad \psi(x) &= \frac{1}{\sqrt{2\pi\hbar}}\int dp\, e^{ipx/\hbar}\,\tilde{\psi}(p) \qquad \text{inverse FT.} \qquad (2.5.16)
\end{aligned}$$

Think of these as two different **representations** of states $|\psi\rangle$ and the operators on them:

$$\begin{array}{ccc|ccc} & \psi(x) & & & \tilde{\psi}(p) & \\ \hat{x} & \longrightarrow & x & \hat{x} & \longrightarrow & i\hbar\dfrac{\partial}{\partial p} \\ \hat{p} & \longrightarrow & -i\hbar\dfrac{\partial}{\partial x} & \hat{p} & \longrightarrow & p \end{array} \qquad (2.5.17)$$

⌈ The transforms between x and p space are familiar but here we are deriving all the results, including the transform inversion theorem, on the assumption that $\{|x\rangle\}$ and $\{|p\rangle\}$ are bases. ⌋

The corresponding **representations** of the Hamiltonian

$$H(\hat{x},\hat{p}) \;=\; \frac{\hat{p}^2}{2m} \;+\; V(\hat{x}) \tag{2.5.18}$$

are

$$\begin{aligned} \text{on} \quad \psi(x): \qquad H \;&\longrightarrow\; -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} \;+\; V(x)\;, \\ \text{on} \quad \tilde{\psi}(p): \qquad H \;&\longrightarrow\; -\frac{p^2}{2m} \;+\; V\left(i\hbar\frac{\partial}{\partial p}\right)\;. \end{aligned} \tag{2.5.19}$$

It may be easy to interpret the potential term in momentum space. E.g., $V(x) = \lambda x^n \;\Rightarrow$

$$V\left(i\hbar\frac{\partial}{\partial p}\right) \;=\; \lambda(i\hbar)^n\frac{\partial^n}{\partial p^n}\;, \tag{2.5.20}$$

but more generally need to use first principles.

$$\begin{aligned} \langle p|V(\hat{x})|\psi\rangle \;&=\; \int dx\;\langle p|V(\hat{x})|x\rangle\langle x|\psi\rangle \\ &=\; \int dx\;V(x)\langle p|x\rangle\int dp'\langle x|p'\rangle\langle p'|\psi\rangle \\ &=\; \int dp'\;\left(\frac{1}{2\pi\hbar}\int dx\;V(x)\;e^{-i(p-p')x/\hbar}\right)\tilde{\psi}(p') \\ &=\; \frac{1}{\sqrt{2\pi\hbar}}\int dp'\;\tilde{V}(p-p')\tilde{\psi}(p')\;. \end{aligned} \tag{2.5.21}$$

Thus $H|\psi\rangle = E|\psi\rangle$ becomes

$$\begin{aligned} -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\;\psi(x) \;&=\; E\;\psi(x) \qquad\qquad \text{in position space}\;, \\ \frac{p^2}{2m}\tilde{\psi}(p) + \frac{1}{\sqrt{2\pi\hbar}}\int dp'\;\tilde{V}(p-p')\;\tilde{\psi}(p') \;&=\; E\;\tilde{\psi}(p) \qquad\qquad \text{in momentum space}\;. \end{aligned} \tag{2.5.22}$$

⌈ Note that the convolution theorem derived here. ⌋

Now return to the key condition in Eq. (2.5.10) and justify it:

$$\langle x|p\rangle \;=\; \frac{1}{\sqrt{2\pi\hbar}}e^{ipx/\hbar}\;. \tag{2.5.23}$$

The point is that eigenstates are only ever unique up to a phase, even if normalized, so we need to show there is a way to choose $|x\rangle$ and $|p\rangle$ which makes this result true. Doing this will involve an approach to translations to which we return later. Claim that

$$|x_0 + a\rangle \;=\; e^{-ia\hat{p}/\hbar}|x_0\rangle\;, \tag{2.5.24}$$

which involves the operator

$$U(a) \equiv e^{-ia\hat{p}/\hbar} = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{-ia}{\hbar} \right)^n \hat{p}^n , \tag{2.5.25}$$

defines position eigenstates $|x\rangle \ \forall \ x$ given one with $x = x_0$. To check this first note that

$$[\hat{x}, \hat{p}] = i\hbar \ \Rightarrow \ [\hat{x}, \hat{p}^n] = i\hbar n \, \hat{p}^{n-1} . \tag{2.5.26}$$

⌈ Note that $\hat{x}$ acts like " $i\hbar \, d/d\hat{p}$ " inside a commutator. ⌋ Thus find

$$[\hat{x}, U(a)] = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{-ia}{\hbar} \right)^n n \, \hat{p}^{n-1} = aU(a) . \tag{2.5.27}$$

So

$$\begin{aligned} \hat{x} \, U(a)|x_0\rangle &= ([\hat{x}, U(a)] + U(a)\hat{x})|x_0\rangle \\ &= (aU(a) + U(a)x_0)|x_0\rangle \\ &= (x_0 + a)U(a)|x_0\rangle \qquad \text{as required.} \end{aligned} \tag{2.5.28}$$

Similarly,

$$|p_0 + b\rangle = e^{ib\hat{x}/\hbar}|p_0\rangle , \tag{2.5.29}$$

defines momentum eigenstates $|p\rangle \ \forall \ p$ given one with $p = p_0$. But then

$$\begin{aligned} \langle x_0 + a|p_0 + b\rangle &= \langle x_0| \, e^{ia\hat{p}/\hbar}|p_0 + b\rangle \\ &= e^{ia(p_0+b)/\hbar}\langle x_0|e^{ib\hat{x}/\hbar}|p_0\rangle \\ &= e^{i(ab+ap_0+bx_0)/\hbar}\langle x_0|p_0\rangle . \end{aligned} \tag{2.5.30}$$

Choosing $\langle x_0|p_0\rangle = 1/\sqrt{2\pi\hbar}$ for reference values $x_0 = p_0 = 0$, then gives (relabelling a, b as x, p, repectively)

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar} . \tag{2.5.31}$$

Actually, need justification for this last step.

- The definitions in Eqs. (2.5.24, 2.5.29) ensure

$$\langle x + a|x' + a\rangle = \langle x|x'\rangle \quad \text{and} \quad \langle p + b|p' + b\rangle = \langle p|p'\rangle , \tag{2.5.32}$$

  so that if $|x_0\rangle$ is correctly normalized we will have

$$\langle x|x'\rangle = \delta(x - x') . \tag{2.5.33}$$

- Since $\{|x\rangle\}$ is a basis we cannot have $\langle x|p_0\rangle = 0$ for every x, and then Eq. (2.5.24) implies $\langle x_0|p_0\rangle \neq 0$, the required result, since

$$\begin{aligned} |x_0\rangle &= |x + (x_0 - x)\rangle = e^{-i(x_0-x)\hat{p}/\hbar}|x\rangle \\ \Rightarrow \qquad \langle x_0|p_0\rangle &= e^{i(x_0-x)p_0/\hbar}\langle x|p_0\rangle \neq 0 . \end{aligned} \tag{2.5.34}$$

- Now, the phase of $\langle x_0|p_0\rangle$ is a matter of convention but the modulus must be consistent with

$$\langle p|p'\rangle \;=\; \delta(p-p')\;, \tag{2.5.35}$$

which is the desired normalization for the $\{|p\rangle\}$ basis. To check:

$$\begin{aligned}\langle p|p'\rangle \;&=\; \int dx\;\langle p|x\rangle\langle x|p'\rangle \\ &=\; \int dx\;\frac{1}{2\pi\hbar}e^{i(p'-p)/\hbar} \;=\; \delta(p-p') \qquad \text{as required.}\end{aligned} \tag{2.5.36}$$

Note that the operator $U(a)$ implements translation by a on the position states.

2.6 Simultaneous Measurements and Complete Commuting Sets

Return to idea of labelling basis states by eigenvalues of observables. If this cannot uniquely be done with eigenvalues λ of some observable Q because some eigenvalues are degenerate, then need at least one more observable Q' to distinguish the corresponding degenerate states.

Physically, we must be able to measure Q and Q' **simultaneously** or

- first measure Q with result λ,
- then immediately measure Q' with result λ'.
- This second measurement must not change the value for Q and so still get result λ if it is measured again immediately.

Mathematically, this requires a basis of **joint eigenstates** which **simultaneously diagonalize** Q and Q':

$$\begin{aligned}Q|\lambda,\lambda'\rangle \;&=\; \lambda|\lambda,\lambda'\rangle \\ Q'|\lambda,\lambda'\rangle \;&=\; \lambda'|\lambda,\lambda'\rangle\;,\end{aligned} \tag{2.6.1}$$

which is only possible iffi

$$[Q,Q'] \;=\; 0\;, \tag{2.6.2}$$

as we now show.

- If there is a basis of joint eigenstates as above then

$$QQ'|\lambda,\lambda'\rangle \;=\; Q'Q|\lambda,\lambda'\rangle \;=\; \lambda\lambda'|\lambda,\lambda'\rangle\;, \tag{2.6.3}$$

so $QQ'=Q'Q$ on these basis states and hence on all states since they can be expanded on this basis.

- Conversely, if $[Q,Q']=0$ and $|\psi\rangle$ belongs to the eigenspace V_λ of Q then

$$Q\Big(Q'|\psi\rangle\Big) \;=\; Q'\Big(Q|\psi\rangle\Big) \;=\; \lambda\Big(Q'|\psi\rangle\Big)\;, \tag{2.6.4}$$

and so $Q'|\psi\rangle$ also belongs to V_λ.

- The definition of a hermitian operator that

$$\langle\phi|Q'|\psi\rangle \;=\; \langle\psi|Q'|\phi\rangle^* \quad \forall \quad |\psi\rangle,\ |\phi\rangle \;\in\; V \tag{2.6.5}$$

  holds for the restriction $|\psi\rangle,\ |\phi\rangle \;\in\; V_\lambda$. Hence, $\exists$ a basis for V_λ consisting of eigenstates of Q'. Call these $|\lambda, \lambda'\rangle$.

- Doing this for each V_λ gives a basis of such joint eigenstates for V.

⌈ Note that if dim $V_\lambda = 1$ (no degeneracy) then any state in V_λ is automatically an eigenstate of Q' since Q' maps $V_\lambda \;\to\; V_\lambda$. ⌋

Now can extend to any number of hermitian operators. Observables $\{Q_1, Q_2, Q_3 \ldots\}$ are said to be a **complete commuting set** if any pair commute. Then there is a basis of joint eigenstates with members

$$|\lambda_1, \lambda_2, \lambda_3, \ldots\rangle \;. \tag{2.6.6}$$

An equivalent way to characterize a complete commuting set is as follows. If A is any other observable with $[A, Q_i] = 0 \;\; \forall \;\; Q_i$ then

$$A \;=\; f(Q_1, Q_2, Q_3, \ldots) \tag{2.6.7}$$

for some function f. This means that

$$A|\lambda_1, \lambda_2, \lambda_3, \ldots\rangle \;=\; f(\lambda, \lambda_1, \lambda_2, \ldots)|\lambda_1, \lambda_2, \lambda_3, \ldots\rangle \;. \tag{2.6.8}$$

An example is the generalization from one to three dimensions of the position and momentum operators $(\hat{\boldsymbol{x}}, \hat{\boldsymbol{p}})$. These obey the commutation relations defined in terms of their Cartesian component operators in usual notation

$$[\hat{x}_i, \hat{p}_j] \;=\; i\hbar\delta_{ij} \;. \tag{2.6.9}$$

One complete commuting set is

$$\hat{\boldsymbol{x}} \;=\; (\hat{x}_1, \hat{x}_2, \hat{x}_3) \tag{2.6.10}$$

with joint eigenstates:

$$\begin{array}{lrcl} & \hat{x}_i|\boldsymbol{x}\rangle & = & x_i|\boldsymbol{x}\rangle \\ \text{orthonormality:} & \langle\boldsymbol{x}|\boldsymbol{x}'\rangle & = & \delta^{(3)}(\boldsymbol{x} - \boldsymbol{x}') \\ \text{basis:} & |\psi\rangle & = & \int d^3x\ \psi(\boldsymbol{x})|\boldsymbol{x}\rangle \\ \text{position space wavefunction} & \psi(\boldsymbol{x}) & = & \langle\boldsymbol{x}|\psi\rangle \;. \end{array}$$

An alternative complete commuting set is

$$\hat{\boldsymbol{p}} \;=\; (\hat{p}_1, \hat{p}_2, \hat{p}_3) \tag{2.6.11}$$

with joint eigenstates

$$\hat{p}_i|\boldsymbol{p}\rangle \;=\; p_i|\boldsymbol{p}\rangle \tag{2.6.12}$$

and momentum space wavefunction $\tilde{\psi}(\boldsymbol{p}) = \langle\boldsymbol{p}|\psi\rangle$.

The relationship between these eigenstates is

$$\begin{aligned}
\langle \boldsymbol{x}|\boldsymbol{p}\rangle &= \frac{1}{(2\pi\hbar)^{3/2}} e^{i\boldsymbol{p}\cdot\boldsymbol{x}/\hbar} \quad \Rightarrow \\
\tilde{\psi}(\boldsymbol{p}) &= \frac{1}{(2\pi\hbar)^{3/2}} \int d^3x \; e^{-i\boldsymbol{p}\cdot\boldsymbol{x}/\hbar} \psi(x) \\
\psi(\boldsymbol{x}) &= \frac{1}{(2\pi\hbar)^{3/2}} \int d^3p \; e^{i\boldsymbol{p}\cdot\boldsymbol{x}/\hbar} \tilde{\psi}(p) \; .
\end{aligned} \tag{2.6.13}$$

There are other possibilities such as $\{\hat{x}_1, \hat{x}_2, \hat{p}_3\}$ leading to mixed position and momentum space wavefunctions.

3 The Harmonic Oscillator

A one-dimensional harmonic oscillator of mass m and frequency ω is defined by the Hamiltonian

$$H \;=\; \frac{1}{2m}\hat{p}^2 \;+\; \frac{1}{2} m\omega^2 \hat{x}^2 \; . \tag{3.1}$$

We will derive the energy levels and construct eigenstates using operator methods and then also see how to find the wavefunctions.

3.1 Analysis using annihilation, creation and number operators

Define

$$\begin{aligned}
a &= \left(\frac{m\omega}{2\hbar}\right)^{1/2} \left(\hat{x} + \frac{i\hat{p}}{m\omega}\right) \; , \\
a^\dagger &= \left(\frac{m\omega}{2\hbar}\right)^{1/2} \left(\hat{x} - \frac{i\hat{p}}{m\omega}\right) \; .
\end{aligned} \tag{3.1.1}$$

Note that these are dimensionless. Equivalently,

$$\begin{aligned}
\hat{x} &= \left(\frac{\hbar}{2m\omega}\right)^{1/2} \left(a + a^\dagger\right) \; , \\
\hat{p} &= \left(\frac{\hbar m\omega}{2}\right)^{1/2} \; i\left(a^\dagger - a\right) \; .
\end{aligned} \tag{3.1.2}$$

It is easy to check that

$$[\hat{x}, \hat{p}] \;=\; i\hbar \quad \Leftrightarrow \quad [a, a^\dagger] \;=\; 1 \; . \tag{3.1.3}$$

Also have

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

and similarly

$$a^\dagger a \;=\; \frac{1}{\hbar\omega}H \;-\; \frac{1}{2} \qquad \text{(opposite sign for commutator)}, \tag{3.1.4}$$

which confirms the commutation relations and also gives

$$H \;=\; \hbar\omega\left(N+\frac{1}{2}\right)\,, \tag{3.1.5}$$

where $N = a^\dagger a$ is the **number operator**. $N^\dagger = N$ and finding its eigenstates and eigenvalues is equivalent to doing this for H:

$$N|\lambda\rangle \;=\; \lambda|\lambda\rangle \quad\Leftrightarrow\quad H|\lambda\rangle \;=\; E|\lambda\rangle \quad \text{with} \quad E \;=\; \hbar\omega\left(\lambda+\frac{1}{2}\right)\,. \tag{3.1.6}$$

Let $|\lambda\rangle$ be **any** such eigenstate normalized s.t. $\||\lambda\rangle\|^2 = 1$. Then

$$\lambda \;=\; \langle\lambda|N|\lambda\rangle \;=\; \langle\lambda|a^\dagger a|\lambda\rangle \;=\; \|a|\lambda\rangle\|^2 \;\geq\; 0\,. \tag{3.1.7}$$

Thus,

$$\begin{aligned} \lambda &\geq 0 && \text{all eigenvalues non-negative} \\ &= 0 && \text{iffi} \quad a|\lambda\rangle \;=\; 0\,. \end{aligned} \tag{3.1.8}$$

Next consider commutators

$$\begin{aligned} [N,a^\dagger] &= [a^\dagger a,a^\dagger] &&= a^\dagger[a,a^\dagger] &&= a^\dagger\,, \\ [N,a] &= [a^\dagger a,a] &&= [a^\dagger,a]a &&= -a\,. \end{aligned} \tag{3.1.9}$$

These relations imply that $a^\dagger$ and a act on eigenstates by respectively raising and lowering the eigenvalues by 1, provided the new states are non-zero and so actually are eigenstates.

$$\begin{aligned} N(a^\dagger|\lambda\rangle) &= ([N,a^\dagger]+a^\dagger N)|\lambda\rangle \\ &= (a^\dagger + a^\dagger\lambda)|\lambda\rangle \\ &= (\lambda+1)(a^\dagger|\lambda\rangle)\,, \end{aligned}$$

$$\begin{aligned} N(a|\lambda\rangle) &= ([N,a]+aN)|\lambda\rangle \\ &= (-a+a\lambda)|\lambda\rangle \\ &= (\lambda-1)(a|\lambda\rangle)\,. \end{aligned} \tag{3.1.10}$$

To find whether the new states are non-zero we compute their norms.

$$\|a|\lambda\rangle\|^2 \;=\; \lambda \qquad \text{(already done above)} \tag{3.1.11}$$

which is only ever zero if $\lambda = 0$.

$$\begin{aligned} \|a^\dagger|\lambda\rangle\|^2 &= \langle\lambda|aa^\dagger|\lambda\rangle \\ &= \langle\lambda|a^\dagger a + 1|\lambda\rangle \\ &= \lambda + 1 \,, \end{aligned} \tag{3.1.12}$$

which is never zero since $\lambda \geq 0$. Because of these properties $a^\dagger$ and a are called, respectively, **creation** and **annihilation** operators.

Suppose there is an eigenstate $|\lambda\rangle$ with λ not an integer. Then

$$\begin{array}{lllll} & a|\lambda\rangle, & a^2|\lambda\rangle, & \ldots, & a^m|\lambda\rangle, \quad \ldots \qquad \text{are } \mathbf{all} \text{ non-zero.} \\ \text{eigenvalues:} & \lambda - 1, & \lambda - 2, & \ldots, & \lambda - m \quad \ldots \,. \end{array} \tag{3.1.13}$$

But for m sufficiently large $\lambda - m < 0$ which is a contradiction since all eigenvalues are non-negative. By contrast if $\lambda = n = 0, 1, 2, \ldots$ then the contradiction is avoided because

$$\begin{array}{lllll} & a|n\rangle, & a^2|n\rangle, & \ldots, & a^n|n\rangle, \qquad \text{are non-zero states} \\ \text{eigenvalues:} & n - 1, & n - 2, & \ldots, & 0 \,, \end{array} \tag{3.1.14}$$

but $a^m|n\rangle = 0,\ m > n$ and so the sequence terminates. Furthermore, have additional eigenstates

$$\begin{array}{lll} & a^\dagger|n\rangle, & (a^\dagger)^2|n\rangle, \quad \ldots, \\ \text{eigenvalues:} & n + 1, & n + 2, \qquad \ldots \qquad . \end{array} \tag{3.1.15}$$

The eigenvalues of N are therefore **precisely** the non-negative integers and the oscillator energy levels are

$$E_n \;=\; \hbar\left(n + \frac{1}{2}\right) \qquad n \;=\; 0, 1, 2, 3, \ldots \,. \tag{3.1.16}$$

From calculations of norms above, we can choose normalized eigenstates $|n\rangle$, $\langle n|n\rangle = 1$ which are then related by

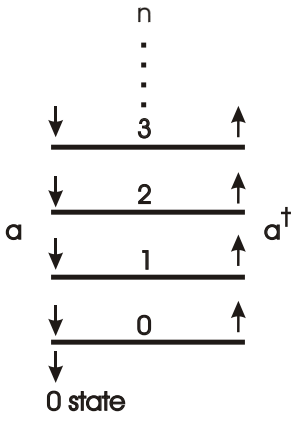
$$\left.\begin{aligned} a^\dagger|n\rangle &= \sqrt{n+1}\,|n+1\rangle \\ a|n\rangle &= \sqrt{n}\,|n-1\rangle \end{aligned}\right\} \qquad \textbf{ladder operators} \tag{3.1.17}$$

Starting from one state reach others by operating with a and $a^\dagger$. In particular, starting from the **ground state**, $|0\rangle$, characterized by

$$a|0\rangle \;=\; 0 \,, \tag{3.1.18}$$

have normalized eigenstates

$$|n\rangle \;=\; \frac{1}{\sqrt{n!}}(a^\dagger)^n|0\rangle \,. \tag{3.1.19}$$



In the absence of any internal structure can take $\{\hat{x}\}$ or $\{\hat{p}\}$ or $\{N\}$ as a complete commuting set. Then the energy levels are non-degenerate (eigenvalues of N label them uniquely) and, in particular, $|0\rangle$ is completely specified by

$$a|0\rangle \;=\; 0\,. \tag{3.1.20}$$

If there **is** some internal structure then all states can carry an additional label i associated with some observable Q (or its eigenvalues) commuting with $\hat{x}, \hat{p}, a, a^\dagger, N$. All energy levels have the same degeneracy with states $|n;i\rangle$ related by $a, a^\dagger$ without affecting i.

The analysis above is convenient for finding wavefunctions. In the position representation

$$\begin{aligned}
|0\rangle \qquad &\rightsquigarrow \qquad \psi_0(x) \;=\; \langle x|0\rangle \\
a \;=\; \left(\frac{m\omega}{2\hbar}\right)^{1/2}\left(\hat{x} + \frac{i}{m\omega}\,\hat{p}\right) \qquad &\rightsquigarrow \qquad \left(\frac{m\omega}{2\hbar}\right)^{1/2}\left(x + \frac{\hbar}{m\omega}\,\frac{\partial}{\partial x}\right) \\
a|0\rangle \;=\; 0 \qquad &\rightsquigarrow \qquad \left(x + \frac{\hbar}{m\omega}\,\frac{\partial}{\partial x}\right)\psi_0(x) \;=\; 0 \\
&\Longrightarrow \qquad \psi_0(x) \;=\; N\, e^{-\frac{m\omega x^2}{2\hbar}}
\end{aligned} \tag{3.1.21}$$

with normalization factor $N = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}$.

Can also find wavefunctions for higher energy states by using Eq. (3.1.19). E.g.,

$$\begin{aligned}
|1\rangle \;=\; a^\dagger|0\rangle \qquad \rightsquigarrow \qquad \psi_1(x) \;&=\; \left(\frac{m\omega}{2\hbar}\right)^{1/2}\left(x - \frac{\hbar}{m\omega}\,\frac{\partial}{\partial x}\right)\psi_0(x) \\
&=\; \left(\frac{2m\omega}{\hbar}\right)^{1/2} x\psi_0(x)\,.
\end{aligned} \tag{3.1.22}$$

The correct normalization is guaranteed.

3.2 Importance of the oscillator – applications in outline

"Physics is that subset of human experience that can be reduced to coupled harmonic oscillators."

M. Peskin

- The oscillator is the simplest QM model beyond steps, wells etc. that can be solved exactly; the hydrogen atom with a Coulomb potential is also special in this respect. It is a very useful example to use as test case for new ideas, approaches and techniques.
- More importantly, many physical systems can be described, exactly or approximately, in terms of oscillators.

- Consider a smooth potential $V(x)$ with equilibrium point x_0 ($V'(x_0) = 0$). For displacements x from equilibrium

$$V(x_0 + x) \;=\; V(x_0) + \frac{1}{2}V''(x_0)x^2 + O(x^3)\;, \tag{3.2.1}$$

and so if the displacements are not too large neglecting the $O(x^3)$ contribution may be a good approximation. Indeed, can include the effects of these anharmonic corrections systematically using perturbation theory (see later). The point is that we start with a soluble model. E.g., diatomic molecules where the quantization of vibrational energies is important in understanding the internal energy and hence the heat capacity of the gas – has macroscopic consequences. In other systems this approach can breakdown, though.

- More complicated systems can be analyzed in terms of **normal modes**: each mode is a coherent motion in which all degrees of freedom oscillate with common frequency ω. This is common classically and can now quantize this motion. The general solution for the classical oscillator is

$$x(t) \;=\; A\, e^{-i\omega t} + A^*\, e^{i\omega t} \qquad A \text{ a complex constant.} \tag{3.2.2}$$

Normal modes for a system with variables $x_n,\ n = 1 \ldots N$ are of the form

$$x_n(t) \;=\; Au_n\, e^{-i\omega t} + A^* u_n^*\, e^{i\omega t}\;, \tag{3.2.3}$$

with $u_n,\ n = 1 \ldots N$ a complex vector specific to each allowed **normal frequency** ω. The general solution is a superposition of normal modes. To quantize treat normal modes as **independent** oscillators. E.g.,

- Benzene ring with 6 CH units which oscillate around the "clock face" of the ring. They are treated as if joined by identical springs. Actually, analyzed by discrete group theory based on the symmetries of the ring.

- Crystal with # atoms $\mathcal{N} \sim 10^{23}$. The forces between the atoms are approximately elastic and in 3D there are $N = 3\mathcal{N}$ independent coordinates. Each of the $3\mathcal{N}$ modes is a collective motion of the atoms and if the approximation of elastic forces is good then interaction between normal modes is small. If you excite just a single mode then no other mode starts up – no energy transfer between modes; they are effectively independent oscillators.

- Electromagnetic field – normal mode oscillations of electric and magnetic fields at each point in space

$$\boldsymbol{E}(\boldsymbol{x}, t) \;=\; A\boldsymbol{u}(\boldsymbol{x})\, e^{-i\omega t} \;+\; A^*\boldsymbol{u}(\boldsymbol{x})^*\, e^{i\omega t}\;. \tag{3.2.4}$$

In fact,

$$\boldsymbol{u}(\boldsymbol{x}) \;=\; \boldsymbol{\epsilon}\, e^{i\boldsymbol{k}\cdot\boldsymbol{x}} \quad \text{with polarization} \quad \boldsymbol{\epsilon} \;\perp\; \boldsymbol{k} \quad \text{and} \quad |\boldsymbol{k}| \;=\; \frac{\omega}{c}\;. \tag{3.2.5}$$

This gives a wave solution with behaviour $e^{\pm i(\boldsymbol{k}\cdot\boldsymbol{x} - \omega t)}$. General solution is a linear combination of normal modes for various $\omega, \boldsymbol{\epsilon}, \boldsymbol{k}$ – exact for EM field.

- Quantization of normal modes as independent oscillators. For each normal mode have $a(\omega)$ and $a(\omega)^\dagger$ (ω and other labels as necessary). Then

$$\text{Ground state} \qquad |0\rangle \quad \text{with} \quad a(\omega)|0\rangle \;=\; 0 \quad \forall \text{ modes}\,.$$

$$a^\dagger(\omega)|0\rangle \qquad \begin{cases}\text{state carrying energy but also momentum } \hbar k \text{ – like a particle.}\end{cases}$$

$$\left.\begin{array}{ll} a & \text{destroy} \\ a^\dagger & \text{create}\end{array}\right\} \quad \text{particles} \quad \left\{\begin{array}{l}\textbf{phonons} \text{ in a crystal} \\ \textbf{photons} \text{ in EM field}\,.\end{array}\right. \tag{3.2.6}$$

  Phonon modes with long wavelength are sound waves (see AQM course in Lent). Macroscopic consequences: heat capacity of crystals, blackbody radiation.

- In summary, the EM field, a relativistically invariant theory, can be understood exactly as a collection of oscillators with quantization producing photons.

  The modern view of **all** elementary particles is that they arise by quantizing some field (though not classically observable like the EM field) but also with interactions between the modes causing energy transfer between them. This give rise to particle decay etc. This is the way to build special relativity into QM and allows particles to be created and destroyed by the action of appropriate combinations of a and $a^\dagger$ on the initial state. This give Quantum Field Theory and the Standard Model of quarks, leptons, gluons, photons, $W^\pm$, Z, ...