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Quantum Mechanics

Lecture Notes - 2024

These notes are based on Atsushi Higuchi's Quantum Mechanics 2, as well as Matthew Pusey's Quantum Mechanics 1. The latter set was in turn based on notes by Daniel Siemssen and Stefan Weigert.

Contents

1 *Preliminaries*

1.1 INTRODUCTION

Quantum mechanics emerged in the early twentieth century to explain certain experimental observations that could not be justified within the classical framework (i.e. Newtonian mechanics). These phenomena include the discrete frequencies found in the spectrum of hydrogen, the photoelectric effect, the black-body radiation spectrum and the results of the double-slit experiment when carried out with electrons. Intuitions such as the quantisation of energy and the wave-like behaviour of particles provided the conceptual groundwork for the development of the theory.

The experimental success of quantum theory comes at a price: all of its predictions are inherently statistical. The quantum world is one of randomness, where uncertainties regarding properties of individual systems are fundamental, hence unavoidable. This contrasts with the 'classical' notion of uncertainty, tied to a subjective lack of knowledge, which can (at least in principle) be eliminated.

In these lectures, we will explore the mathematical foundations of quantum mechanics and develop our understanding of a number of topics regarding the theory.

In quantum mechanics, the possible *states* of a system correspond to elements of an abstract mathematical space, called a *Hilbert space*. The dynamical and observable properties of these systems are described by specific classes of linear operators acting on such spaces. In the module "Quantum Theory & Quantum Information", you have worked with Hilbert spaces of finite dimensions, which are sufficient to describe fundamental features of quantum theory, as well as applications in Quantum Information science. However, in order to describe, say, quantum particles moving in a potential, or to account for measurements of position or momentum - whose outcomes can be any real number! - we must shift our attention to infinite-dimensional Hibert spaces.

Infinite-dimensional Hilbert spaces can be very tricky things. We will discuss some of the technicalities concerning them, but we will not provide a complete analysis, which would take up too much of our time.

1.2 INNER PRODUCT SPACES

Most of the content in this chapter should hopefully be familiar from the module Quantum Theory & Information (QT&I). To ease fruition, we omit proofs of results that can be found in the QT&I lecture notes.

To define Hilbert spaces, we must start with the notion of a vector space.

DEFINITION 1.1. A *vector space* (over $\mathbb{C}$) is a triple $(\mathcal{V}, +, \cdot)$, where

1. $\mathcal{V}$ is a set,
2. $+ : \mathcal{V} \times \mathcal{V} \to \mathcal{V}$, $(u, v) \mapsto u + v$ (addition),
3. $\cdot : \mathbb{C} \times \mathcal{V} \to \mathcal{V}$, $(\alpha, u) \mapsto \alpha \cdot u$ (scalar multiplication)

satisfying:

1. $u + v = v + u$ for all $u, v \in \mathcal{V}$ (commutativity of $+$),
2. $(u + v) + w = u + (v + w)$ for all $u, v, w \in \mathcal{V}$ (associativity of $+$),
3. there exists $0 \in \mathcal{V}$ such that $0 + v = v$ for all $v \in \mathcal{V}$ (additive identity),
4. given any $v \in \mathcal{V}$ there exists $(-v) \in \mathcal{V}$ with $(-v) + v = 0$ (additive inverse),
5. $\alpha \cdot (\beta \cdot v) = (\alpha\beta) \cdot v$ for all $\alpha, \beta \in \mathbb{C}$ and $v \in \mathcal{V}$ (compatibility of scalar multiplication and multiplication in $\mathbb{C}$),
6. $\alpha \cdot (u + v) = \alpha \cdot u + \alpha \cdot v$ for all $\alpha \in \mathbb{C}$ and $u, v \in \mathcal{V}$ (distributivity of scalar multiplication with respect to vector addition),
7. $(\alpha + \beta) \cdot v = \alpha \cdot v + \beta \cdot v$ for all $\alpha, \beta \in \mathbb{C}$ and $v \in \mathcal{V}$ (distributivity of scalar multiplication with respect to addition in $\mathbb{C}$),
8. $1 \cdot v = v$ for all $v \in \mathcal{V}$ (identity of scalar multiplication).

EXAMPLE 1.2. Consider the set of complex n-tuples $\mathbb{C}^n$ with the usual rules of addition and scalar multiplication. That is, for $u = (u_1, \ldots, u_n) \in \mathbb{C}^n$, $v = (v_1, \ldots, v_n) \in \mathbb{C}^n$ and $\alpha \in \mathbb{C}$, define

$$u + v = (u_1 + v_1, \ldots, u_n + v_n) \quad \text{and} \quad \alpha \cdot v = (\alpha v_1, \ldots, \alpha v_n).$$

$(\mathbb{C}^n, +, \cdot)$ is a vector space (for each n). ◇

EXAMPLE 1.3. Consider the set of n-times continuously differentiable function on the interval $(a, b) \subset \mathbb{R}$ (and with values in $\mathbb{C}$),

$$C^n(a, b) = \{f : (a, b) \to \mathbb{C} \mid \text{the } i\text{-th derivative } f^{(i)} \text{ is continuous for all } i \leq n\}.$$

We define addition and scalar multiplication of functions pointwise:

1. For $f, g \in C^n(a, b)$, define $f + g$ by $(f + g)(x) = f(x) + g(x)$ for all $x \in (a, b)$,

2. For $f \in C^n(a,b)$ and $\alpha \in \mathbb{C}$, define $\alpha \cdot f$ by $(\alpha \cdot f)(x) = \alpha f(x)$ for all $x \in (a,b)$,

$(C^n(a,b), +, \cdot)$ is a vector space (for each n). ◇

DEFINITION 1.4. A *(Hermitian) inner product* on a vector space $\mathcal{V}$ is a map

$$\langle \cdot\,, \cdot \rangle : \mathcal{V} \times \mathcal{V} \to \mathbb{C}$$

satisfying

1. $\overline{\langle v,u \rangle} = \langle u,v \rangle$ for all $u, v \in \mathcal{V}$, where $\overline{(.)}$ is the complex conjugation,
2. $\langle u, v+w \rangle = \langle u,v \rangle + \langle u,w \rangle$ for all $u, v, w \in \mathcal{V}$,
3. $\langle u, \alpha v \rangle = \alpha \langle u,v \rangle$ for all $u, v \in \mathcal{V}$ and $\alpha \in \mathbb{C}$,
4. $\langle v,v \rangle \geq 0$ for all $v \in \mathcal{V}$ with equality if and only if $v = 0$.

A vector space with an inner product is called a *(Hermitian) inner product space*. We denote by $\|\cdot\|$ the *norm* on $\mathcal{V}$ defined by $\|v\| := \sqrt{\langle v,v \rangle}$ for all $v \in \mathcal{V}$. ◇

EXAMPLE 1.5. We define on $\mathbb{C}^n$ the usual Euclidean inner product by

$$\langle u,v \rangle = u^* v = \overline{u}^{\mathrm{T}} v.$$ ◇

EXAMPLE 1.6. Consider again the vector space $C^n(a,b)$ from Example 1.3. The following defines an inner product on it:

$$\langle f,g \rangle = \int_a^b \overline{f(x)} g(x)\, \mathrm{d}x, \quad f, g \in C^n(a,b). \tag{1.1}$$

◇

DEFINITION 1.7. Let $\mathcal{V}$ be an inner product space.

1. $v \in \mathcal{V}$ is called *normalized* if $\langle v,v \rangle = 1$.
2. $u, v \in \mathcal{V}$ are called *orthogonal* if $\langle u,v \rangle = 0$.
3. $u, v \in \mathcal{V}$ are called *orthonormal* if they are orthogonal and normalized.

◇

Some important inequalities for inner product spaces: for all $u, v \in \mathcal{V}$,

– Cauchy–Schwarz: $|\langle u,v \rangle| \leq \|u\| \|v\|$
– triangle inequality: $|\|u\| - \|v\|| \leq \|u+v\| \leq \|u\| + \|v\|$

REMARK 1.8. Note that all concepts defined here carry over to the real setting with very few modifications. For example, the set of real n-tuples $\mathbb{R}^n$ with the usual addition and multiplication by a (real) scalar, and endowed with the inner product

$$\langle u,v \rangle = u^{\mathrm{T}} v$$

is an example of a *real* inner product space. ◇

1.3 HILBERT SPACES

In finite dimensions, the notions of Hilbert space and inner product space coincide. In infinite dimensions, this is no longer true. One must further impose the condition of completeness.

DEFINITION 1.9. A *Hilbert space*, often denoted by $\mathcal{H}$, is a complete inner product space. ◇

REMARK 1.10. Note that a Hilbert space $\mathcal{H}$ is infinite dimensional if, for any positive integer d, there exists an orthogonal set of d vectors. ◇

DEFINITION 1.11. A vector space $\mathcal{V}$ with a norm $\|\cdot\|$ is called *complete* if for every sequence $(v_n)_{n\in\mathbb{N}}$, $v_n \in \mathcal{V}$, such that

$$\lim_{n,m\to\infty} \|v_n - v_m\| = 0$$

there exists a $v \in \mathcal{V}$, called the limit of the sequence $(v_n)_{n\in\mathbb{N}}$, such that

$$\lim_{n\to\infty} \|v - v_n\| = 0$$ ◇

In other words, a complete vector space is one in which every Cauchy sequence converges. For inner product spaces, completeness is equivalent to the requirement that *every absolutely convergent series is convergent* (a series $\sum_{n=1}^{\infty} v_n$ is called absolutely convergent if $\sum_{n=1}^{\infty} \|v_n\| < \infty$).

Although it plays an important role behind the scenes, we will not use the completeness of Hilbert spaces directly. Completeness has several useful consequences, which make Hilbert spaces much easier to deal with than general inner product spaces. One consequence is the existence of *basis expansions*. An orthonormal basis for a Hilbert space $\mathcal{H}$ is a *maximal* orthonormal set; this means that there is no other orthonormal set containing it as a proper subset. A useful criterion for the maximality of an orthonormal set $X \subset \mathcal{H}$ is the following: if ψ is orthogonal to all vectors in X then $\psi = 0$. It can be shown that every Hilbert space has an orthonormal basis and, moreover, that all orthonormal bases of a given Hilbert space have the same cardinality.

EXAMPLE 1.12. $\mathbb{C}^n$ with the Euclidean inner product is a Hilbert space. ◇

This is actually the prototypical finite-dimensional Hilbert space as the following result shows (proof can be found in QT&I lecture notes):

THEOREM 1.13. *Every n-dimensional inner product space $\mathcal{V}$ is 'equivalent' (isometric) to $\mathbb{C}^n$ with the Euclidean inner product. In particular, $\mathcal{V}$ is complete and thus a Hilbert space.*

REMARK 1.14. It is *not* true that every infinite-dimensional inner product space is complete. For example, $C^n(a, b)$ with the inner product (1.1) is not complete. ◇

The Hilbert space we are most interested in for the purposes of this module is that of square integrable functions.

THEOREM 1.15. *The set of* square-integrable functions *(over* $\mathbb{R}$ *and with values in* $\mathbb{C}$*),*

$$L^2(\mathbb{R}) = \Big\{\psi : \mathbb{R} \to \mathbb{C} \;\Big|\; \int_{-\infty}^{\infty} |\psi(x)|^2 \,\mathrm{d}x < \infty\Big\},$$

endowed with pointwise addition and scalar multiplication, and the inner product

$$\langle \varphi, \psi \rangle = \int_{-\infty}^{\infty} \overline{\varphi(x)}\psi(x)\,\mathrm{d}x, \quad \varphi, \psi \in L^2(\mathbb{R}).$$

is an infinite-dimensional Hilbert space.

REMARK 1.16. If you look closely, you will notice that many non-negative functions have a vanishing integral. For this reason it seems that the inner product defined above is not actually positive definite! We can circumvent this problem by identifying all non-negative functions that have a vanishing integral with the zero function, that is, one should actually look at equivalence classes of functions and change the definition of $L^2(\mathbb{R})$ above. ◇

A normalised vector (or *unit vector*) in $L^2(\mathbb{R})$ is hence a function $\psi : \mathbb{R} \to \mathbb{C}$ satisfying $\int_{-\infty}^{\infty} |\psi(x)|^2 \,\mathrm{d}x = 1$. Unit vectors on $L^2(\mathbb{R})$ are a natural choice to represent states of quantum systems moving in one spatial dimension.[1]

[1] We will see later on that it is convenient to consider states even some *improper* vectors, which cannot be normalised and thus do not belong in $L^2(\mathbb{R})$.

EXAMPLE 1.17. Consider the Hilbert space $L^2(\mathbb{R})$ and, for some $x_0 \in \mathbb{R}$, $l > 0$ the state

$$\psi(x) = \frac{1}{\sqrt{l\sqrt{\pi}}} \exp\left(-\frac{(x-x_0)^2}{2l^2}\right).$$

This is normalized because

$$\langle \psi, \psi \rangle = \frac{1}{l\sqrt{\pi}} \int_{-\infty}^{\infty} \exp\left(-\frac{(x-x_0)^2}{l^2}\right) \mathrm{d}x = 1\,,$$

where we used the Gaussian integral $\int_{-\infty}^{\infty} \exp(-\alpha x^2)\,\mathrm{d}x = (\pi/\alpha)^{1/2}$, which holds for $\alpha > 0$. ◇

1.4 OPERATORS ON HILBERT SPACES

1.4.1 Linear operators

Let $\mathcal{H}$ and $\mathcal{K}$ be Hilbert spaces.

DEFINITION 1.18. The map $A : \mathcal{H} \to \mathcal{K}$ is called a *(linear) operator* (also linear transformation or linear map) from $\mathcal{H}$ to $\mathcal{K}$ if the following holds:

1. $A(u+v) = A(u) + A(v)$ for all $u, v \in \mathcal{H}$,
2. $A(\alpha v) = \alpha A(v)$ for all $v \in \mathcal{H}$ and $\alpha \in \mathbb{C}$.

If $\mathcal{H} = \mathcal{K}$, we say that A is a (linear) operator on $\mathcal{H}$. ◇

In this module we will only consider linear operators (as opposed to non-linear operators) and thus will drop the qualifier "linear".

DEFINITION 1.19. An operator $T : \mathcal{H} \to \mathcal{K}$ is *bounded* if there exists a number $t \geq 0$ such that

$$\|Tv\| \leq t\|v\| \quad \text{for all } v \in \mathcal{H}\,. \qquad \diamond$$

A bounded operator $A : \mathcal{H} \to \mathcal{K}$ is fully characterised by its action on a basis of $\mathcal{H}$. Equivalently, it is characterised by the inner products $\langle e_i, Af_j\rangle$ (called *matrix elements*) where $\{f_j\}$ is a basis of $\mathcal{H}$ and $\{e_i\}$ a basis of $\mathcal{K}$.

In finite dimensional Hilbert spaces, all linear operators are bounded. This is no longer true in infinite dimensions.

EXAMPLE 1.20. For each $\psi \in L^2(\mathbb{R})$, define the operator X by the formula

$$(X\psi)(x) = x\psi(x)\,.$$

Let

$$\psi(x) = \begin{cases} 0 & \text{if } x \leq 1, \\ 1/x & \text{if } x > 1 \end{cases}$$

Then $\psi \in L^2(\mathbb{R})$, since $\int_{-\infty}^{\infty} |\psi(x)|^2 \,\mathrm{d}x = 1$ but $X\psi \notin L^2(\mathbb{R})$, since

$$\int_{-\infty}^{\infty} |x\psi(x)|^2 \,\mathrm{d}x = \infty\,. \qquad \diamond$$

REMARK 1.21. Many operators that one encounters in quantum mechanics are unbounded - for example, the operator X of Example 1.21. When working with these operators, we generally restrict them to 'sufficiently nice' functions. Formally, we consider the *domain* of an operator A to be the (usually dense) subset

$$D(A) = \{\psi \in L^2(\mathbb{R}) : A\psi \in L^2(\mathbb{R})\}$$

of $L^2(\mathbb{R})$. We say the (unbounded) operator A is a linear mapping from $D(A)$ to $L^2(\mathbb{R})$. ◇

1.4.2 Adjoint operator

Let $\mathcal{H}$ and $\mathcal{K}$ be Hilbert spaces. For any bounded operator $A : \mathcal{H} \to \mathcal{K}$ there is a unique operator $A^* : \mathcal{K} \to \mathcal{H}$ such that

$$\langle \varphi, A\psi\rangle_{\mathcal{K}} = \langle A^*\varphi, \psi\rangle_{\mathcal{H}} \quad \text{or, equivalently,} \quad \langle \psi, A^*\varphi\rangle_{\mathcal{H}} = \langle A\psi, \varphi\rangle_{\mathcal{K}} \qquad (1.2)$$

for all $\psi \in \mathcal{H}$ and $\varphi \in \mathcal{K}$, where $\langle\cdot,\cdot\rangle_{\mathcal{H}}$ is the inner product on $\mathcal{H}$ and $\langle\cdot,\cdot\rangle_{\mathcal{K}}$ is the inner product on $\mathcal{K}$.

DEFINITION 1.22. The unique operator A^* satisfying (1.2) for all $\psi \in \mathcal{H}$ and $\varphi \in \mathcal{K}$ is called the *adjoint* of A. ◇

TERMINOLOGY & NOTATION. In the physics literature, the adjoint is also often denoted by a dagger '†', that is, the notation $A^\dagger$ (instead of A^*) is used for the adjoint of A. In this module we will primarily use A^*. ◇

EXAMPLE 1.24. Consider the Hilbert spaces $\mathbb{C}^n$ and $\mathbb{C}^m$ (with the Euclidean inner product). Recall that every operator from $\mathbb{C}^n$ to $\mathbb{C}^m$ is given by a matrix $A \in M_{m\times n}(\mathbb{C})$. For any $u \in \mathbb{C}^m$ and $v \in \mathbb{C}^n$ we have

$$\langle u, Av\rangle_{\mathbb{C}^m} = \overline{u}^{\mathrm{T}} A v = (A^{\mathrm{T}}\overline{u})^{\mathrm{T}} v = \overline{(\overline{A}^{\mathrm{T}} u)}^{\mathrm{T}} v = \langle \overline{A}^{\mathrm{T}} u, v\rangle_{\mathbb{C}^n}.$$

Therefore the adjoint is just the conjugate transpose, that is, $A^* = \overline{A}^{\mathrm{T}}$. ◇

What follows now are useful properties of the adjoint operator. Proofs can be found in the lecture notes for QT&I.

PROPOSITION 1.25. *Let A, B be operators on $\mathcal{H}$ and $\alpha \in \mathbb{C}$. We have the properties:*

1. $(\alpha A)^* = \overline{\alpha} A^*$,
2. $(A + B)^* = A^* + B^*$,
3. $(AB)^* = B^* A^*$,
4. $A^{**} = (A^*)^* = A$,
5. $A^*A \geq 0$, *viz.*, $\langle \psi, A^*A\psi\rangle \geq 0$ *for all* $\psi \in \mathcal{H}$.

For unbounded operators, we generally have to restrict ϕ, ψ in Def. 1.22 to their domain. In particular, the expression $\langle \varphi, A\psi\rangle$ only makes sense when $\psi \in D(A)$. The domain $D(A^*)$ of the adjoint A^* will thus be the subset of $\mathcal{K}$ where the functional $\varphi \mapsto \langle \varphi, A\psi\rangle$ is bounded, meaning that there is some $t \geq 0$ such that $|\langle \varphi, A\psi\rangle| \leq t\|\psi\|$ for all $\psi \in D(A)$. On this domain, A^* is defined by the usual requirement $\langle \varphi, A\psi\rangle = \langle A^*\varphi, \psi\rangle$.

REMARK 1.26. The domain $D(A)$ of A and the domain $D(A^*)$ of its adjoint A^* do not necessarily coincide. ◇

1.4.3 Dirac notation

In this module, we will employ the *Dirac* (or *bra-ket*) notation for Hilbert spaces, which is commonly used in the quantum community. For any vector $\psi \in \mathcal{H}$, there is an associated *ket* $|\psi\rangle$ which is a linear map from $\mathbb{C}$ to $\mathcal{H}$ such that for $a \in \mathbb{C}$, $|\psi\rangle : a \mapsto a\psi$. A ket is just a different way of thinking of a vector.[2] The adjoint of $|\psi\rangle$ is called a *bra* and denoted $\langle\psi|$. It is a linear map from $\mathcal{H}$ to $\mathbb{C}$ defined such that for $\phi \in \mathcal{H}$, $\langle\psi| : \phi \mapsto \langle\psi, \phi\rangle$. We can think of $\langle\psi||\phi\rangle = \langle\psi|\phi\rangle$ as the concatenation of the map $|\phi\rangle : \mathbb{C} \to \mathcal{H}$ and $\langle\psi| : \mathcal{H} \to \mathbb{C}$, which overall is a map from $\mathbb{C}$ to $\mathbb{C}$. It is equal to the inner product between ψ and ϕ.

We can use the Dirac notation to represent linear operators, e.g. $|\psi\rangle\langle\phi|$ maps $\mathcal{H}$ to itself. Any linear operator $A : \mathcal{H} \to \mathcal{H}$ (for the purpose of this

[2] In these lectures, elements of a Hilbert space $\mathcal{H}$ will be denoted by both $|\psi\rangle \in \mathcal{H}$ and $\psi \in \mathcal{H}$, depending a bit on the circumstances.

section, $\mathcal{H}$ is finite-dimensional) can be written in the form $A = \sum_i |\psi_i\rangle\langle\phi_i|$. If $\{x_i\}$ forms an orthonormal basis, we can find complex coefficients c_{ij} such that $A = \sum_{ij} c_{ij} |x_i\rangle\langle x_j|$. Then, the adjoint A^* of A can be written as $A^* = \sum_{ij} \overline{c_{ij}} |x_j\rangle\langle x_x|$.

Moreover, for any orthonormal basis $\{x_i\}$,

$$\sum_i |x_i\rangle\langle x_i| = \mathbb{1} \tag{1.3}$$

where $\mathbb{1}$ is the identity on $\mathcal{H}$, i.e. $\mathbb{1} : |\psi\rangle \mapsto |\psi\rangle$ for all $|\psi\rangle$. Eq. (1.3) is called the *completeness relation*, or *resolution of the identity*.

Note that $|\psi\rangle = \mathbb{1}|\psi\rangle = \sum_i |x_i\rangle\langle x_i|\psi\rangle = \sum_i c_i |x_i\rangle$, where $c_i = \langle x_i|\psi\rangle$. The complex coefficients $\{c_i\}$ can be thought as the representation of $|\psi\rangle$ in the $\{|x_i\rangle\}$ basis.

Throughout the module, we will work with the equivalent of Eq. (1.3) in infinite dimensions, e.g.

$$\int_{-\infty}^{\infty} \mathrm{d}x\, |x\rangle\langle x| = \mathbb{1}\,,$$

where $\{|x\rangle, x \in \mathbb{R}\}$ forms a basis of $\mathcal{H} = L^2(\mathbb{R})$.

1.4.4 Symmetric and self-adjoint operators

DEFINITION 1.27. An operator $A : D(A) \to \mathcal{H}$ is said to be *symmetric* if $\langle\varphi|A\psi\rangle = \langle A\varphi|\psi\rangle$ for all $|\psi\rangle, |\varphi\rangle \in D(A)$. ◇

DEFINITION 1.28. An operator $A : D(A) \to \mathcal{H}$ is said to be *self-adjoint* if $A^* = A$. If $A^* = -A$, it is said to be *anti-self-adjoint*. ◇

For bounded operators, the notion of self-adjoint and symmetric operators coincide. Especially in the physics community, bounded self-adjoint operators are also called *Hermitian*.

Proofs of the following results on Hermitian operators in a finite-dimensional $\mathcal{H}$ were shown in QT&I.

THEOREM 1.29. *If A is a self-adjoint operator on $\mathcal{H}$, it holds that*

1. *the eigenvalues λ_i of A are real,*
2. *$\langle\psi_1|\psi_2\rangle = 0$ for all eigenvectors $|\psi_1\rangle, |\psi_2\rangle \in \mathcal{H}$ with distinct eigenvalues.*

DEFINITION 1.30. The set $\{\lambda_1, \lambda_2, \dots\}$ of eigenvalues of A is called the *spectrum* of A. The subspace $\mathcal{H}_{\lambda_i} = \{|\varphi\rangle \in \mathcal{H} : A|\varphi\rangle = \lambda_i |\varphi\rangle\}$ is called the *eigenspace* for the eigenvalue λ_i of A. The multiplicity of the eigenvalue λ_i is the dimension of $\mathcal{H}_{\lambda_i}$, and the eigenvalue λ_i is said to be *degenerate* if $\dim(\mathcal{H}_{\lambda_i}) \geq 2$ and *non-degenerate* if $\dim(\mathcal{H}_{\lambda_i}) = 1$. ◇

Having real eigenvalues makes self-adjoint operators a good candidate to represent observable quantities of quantum systems - after all, we don't measure an imaginary position, or energy!

THEOREM 1.31 (SPECTRAL THEOREM). *Let A be a Hermitian (self-adjoint) operator on a d-dimensional Hilbert space $\mathcal{H}$. Then there exists an orthonormal basis $\{|e_i\rangle\}_{i=1}^d$ of $\mathcal{H}$ consisting of eigenvectors of A. Furthermore, A can be written as*

$$A = \sum_{i=1}^{d} \lambda_i |e_i\rangle\langle e_i|, \tag{1.4}$$

where λ_i are the eigenvalues of A, that is, $A|e_i\rangle = \lambda_i |e_i\rangle$.

The spectral theorem describes the relation between Hermitian operators and projectors.

DEFINITION 1.32. A self-adjoint operator $P : \mathcal{H} \to \mathcal{H}$ is an *orthogonal projection* if $P^2 = P$. ◇

EXAMPLE 1.33. For each (normalised) $|\psi\rangle \in \mathcal{H} = \mathbb{C}^d$, $P_\psi = |\psi\rangle\langle\psi|$ is an orthogonal projection. We often say that "P_ψ projects onto $|\psi\rangle$", because $P_\psi |\phi\rangle$ is proportional to $|\psi\rangle$ for all $|\phi\rangle \in \mathbb{C}^d$. ◇

The self-adjoint operator A of Eq. (1.4) can thus be rewritten as $A = \sum_{i=1}^d \lambda_i P_{e_i}$, where P_{e_i} projects onto the eigenspace $\mathcal{H}_{\lambda_i}$. In particular, the orthogonality of the eigenvectors implies that $P_{e_i} P_{e_j} = 0$ whenever $i \neq j$.

EXAMPLE 1.34. The identity operator $\mathbb{1}$ on $\mathcal{H} = \mathbb{C}^d$ is Hermitian, with all of its d eigenvalues equal 1, and any vector $|\psi\rangle \in \mathcal{H}$ is an eigenvector. Therefore, for any orthonormal basis $\{|x_i\rangle\}_{i=1}^d$ the completeness relation (1.3) can be written as

$$\mathbb{1} = \sum_{i=1}^{d} P_{x_i}. \qquad \diamond$$

REMARK 1.35. If $|e_i\rangle$ is an eigenvector of A with eigenvalue λ_i, then

$$A^2 |e_i\rangle = \lambda_i^2 |e_i\rangle .$$

In general, for any $n \in \mathbb{N}$ we have

$$A^n |e_i\rangle = \lambda_i^n |e_i\rangle . \qquad \diamond$$

The above remark motivates the following definition.

DEFINITION 1.36. For any $f : \mathbb{R} \to \mathbb{C}$ and a self-adjoint operator A, the operator $f(A)$ is defined by

$$f(A) |e_i\rangle = f(\lambda_i) |e_i\rangle ,$$

where $|e_i\rangle$ is any eigenvector of A with eigenvalue λ_i. ◇

This definition indeed defines the operator $f(A)$ on the whole Hilbert space.

PROPOSITION 1.37. *If A is a self-adjoint operator with eigenvalues λ_i, $i = 1, 2, \ldots, d$, then*

$$f(A) = \sum_{i=1}^{d} f(\lambda_i) P_{e_i} .$$

PROOF. Write $|\psi\rangle = \mathbb{1}\,|\psi\rangle = \sum_i P_{e_i}\,|\psi\rangle$, where $|\psi\rangle$ is an arbitrary vector. Then $f(A)\,|\psi\rangle = \sum_i f(A) P_{e_i}\,|\psi\rangle$. But $P_{e_i}\,|\psi\rangle = c_i\,|e_i\rangle$ for some $c_i \in \mathbb{C}$, hence $f(A)\,|\psi\rangle = \sum_i c_i f(A)\,|e_i\rangle$. We apply the above definition to find $f(A)\,|\psi\rangle = \sum_i f(\lambda_i) c_i\,|e_i\rangle = \sum_i f(\lambda_i) P_{e_i}\,|\psi\rangle$. Therefore, $f(A) = \sum_i f(\lambda_i) P_{e_i}$. □

In infinite dimensional Hilbert spaces, Hermitianity and self-adjointness are separate concepts. The latter, in fact, can be defined for unbounded operators as well, provided we restrict our attention to 'sufficiently nice' subsets of $\mathcal{H}$, i.e. the domain of A, which we assume to be dense. Formally, an operator A is self-adjoint, i.e. $A = A^*$, if

(i) A is symmetric;

(ii) $D(A) = D(A^*)$.

One can then show that the spectrum of unbounded self-adjoint operators must be a subset of $\mathbb{R}$.

The *position operator* X, defined by

$$(X\psi)(x) = x\psi(x)$$

(we encountered this operator in Example 1.21) and the *momentum operator* P, defined by

$$(P\psi)(x) = -i\hbar\psi'(x) = -i\hbar \frac{d}{dx}\psi(x)$$

are two examples of unbounded self-adjoint operators on $L^2(\mathbb{R})$. We will discuss these operators more carefully in following lectures.[3]

[3] In the definition of P, $\hbar$ is called *Planck's constant*. Its concrete value depends on the system of units employed and will be of little relevance to us.

EXAMPLE 1.38. For all (sufficiently nice) functions $\varphi(x), \psi(x) \in L^2(\mathbb{R})$ we have

$$\langle\varphi|X\psi\rangle = \int_{-\infty}^{\infty} \overline{\varphi(x)} x\psi(x)\,\mathrm{d}x = \int_{-\infty}^{\infty} \overline{x\varphi(x)}\psi(x)\,\mathrm{d}x = \langle X\varphi|\psi\rangle.$$

It follows that the position operator is self-adjoint: $X^* = X$. ◇

EXAMPLE 1.39. For all (sufficiently nice) $\varphi, \psi \in L^2(\mathbb{R})$ we have

$$\begin{aligned}
\langle\varphi|P\psi\rangle &= \int_{-\infty}^{\infty} \overline{\varphi(x)}(-\mathrm{i}\hbar)\psi'(x)\,\mathrm{d}x \\
&= (-\mathrm{i}\hbar)\Big[\overline{\varphi(x)}\psi(x)\Big]_{x\to-\infty}^{x\to+\infty} - (-\mathrm{i}\hbar)\int_{-\infty}^{\infty} \overline{\varphi'(x)}\psi(x)\,\mathrm{d}x \\
&= \int_{-\infty}^{\infty} \overline{(-\mathrm{i}\hbar)\varphi'(x)}\psi(x)\,\mathrm{d}x,
\end{aligned}$$

where we assumed that 'sufficiently nice' implies that $\lim_{x\to\pm\infty} \overline{\varphi(x)}\psi(x) = 0$ (that is, $\varphi(x)$ and/or $\psi(x)$ go to zero at infinity) so that the first term in the second line drops out. It also follows that the momentum operator is self-adjoint: $P^* = P$. ◇

1.4.5 Unitary operators

DEFINITION 1.40. The operator $U : \mathcal{H} \to \mathcal{H}$ is said to be unitary if $UU^* = \mathbb{1}$ and $U^*U = \mathbb{1}$. ◇

In finite-dimensional $\mathcal{H}$, the existence of a left inverse implies the existence of a right inverse, hence one condition in Def. 1.40 implies the other. This is not true in infinite-dimensional $\mathcal{H}$, where both requirements are needed.

Unitary operators can be equivalently characterised in the following way.

THEOREM 1.41. *The unitary operators on $\mathcal{H}$ are exactly the inner-product preserving bijections.*

PROOF. The unitary operator U is a bijection because $U^{-1} = U^*$ exists. Furthermore, U preserves the inner product. To see this, define $|\psi_U\rangle := U|\psi\rangle$, $|\varphi_U\rangle := U|\varphi\rangle$. Then $\langle\psi_U| = \langle\psi|U^*$, and $\langle\psi_U|\varphi_U\rangle = \langle\psi|U^*U|\varphi\rangle = \langle\psi|\varphi\rangle$, i.e. $\langle\psi_U|\varphi_U\rangle = \langle\psi|\varphi\rangle$.

To show the converse, suppose a map $U : \mathcal{H} \to \mathcal{H}$ is a bijection preserving the inner product. Then, from the inner-product preserving, by defining $|\psi_U\rangle$ and $|\varphi_U\rangle$ as above, we find $\langle\psi|\varphi\rangle = \langle\psi_U|\varphi_U\rangle = \langle\psi|U^*U|\varphi\rangle$ for all $|\psi\rangle, |\varphi\rangle \in \mathcal{H}$. Hence, $U^*U = \mathbb{1}$. Since U is a bijection, U^{-1} exists and $U^{-1} = U^*$. Then $UU^* = \mathbb{1}$ as well. Therefore an inner-product preserving bijection U is unitary. □

1.4.6 Commutator

DEFINITION 1.42. The *commutator* of two operators A, B (on the same vector space) is

$$[A, B] = AB - BA.$$

If $[A, B] = 0$, we say that A and B *commute*. ◇

EXAMPLE 1.43. Consider the vector space $\mathbb{C}^2$ and the operators (that is, matrices)

$$A = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \text{and} \quad B = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

Their commutator is

$$\begin{aligned}[A, B] &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \\ &= \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} - \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 2 \\ -2 & 0 \end{pmatrix}.\end{aligned}$$ ◇

THEOREM 1.44. *The position operator X and momentum operator P on $L^2(\mathbb{R})$ satisfy the* commutation relation

$$[X, P] = \mathrm{i}\hbar\mathbb{1}. \tag{1.5}$$

(This is also called a canonical commutation relation*.)*

PROOF. Suppose that $\psi \in L^2(\mathbb{R})$ is sufficiently nice (e.g., such that $XP\psi, PX\psi \in L^2(\mathbb{R})$). We calculate

$$\begin{aligned}([X,P]\psi)(x) &= (XP\psi)(x) - (PX\psi)(x)\\ &= x(-\mathrm{i}\hbar)\frac{\mathrm{d}}{\mathrm{d}x}\psi(x) - (-\mathrm{i}\hbar)\frac{\mathrm{d}}{\mathrm{d}x}(x\psi(x))\\ &= -\mathrm{i}\hbar(x\psi'(x) - \psi(x) - x\psi'(x)) = \mathrm{i}\hbar\psi(x).\end{aligned}$$ □

PROPOSITION 1.45. *Let A, B, C be operators on a vector space $\mathcal{V}$ and $\alpha \in \mathbb{C}$. The commutator has the properties:*

1. $[A, \mathbb{1}] = 0$,
2. $[A, B] = -[B, A]$ *(in particular, $[A, A] = 0$)*,
3. $[A + B, C] = [A, C] + [B, C]$,
4. $[\alpha A, B] = \alpha[A, B]$,
5. $[A, BC] = [A, B]C + B[A, C]$,
6. $[AB, C] = A[B, C] + [A, C]B$,
7. $(A - B)(A + B) = A^2 - B^2 + [A, B]$.

PROOF. Let $v \in \mathcal{V}$ be arbitrary.

1. $[A, \mathbb{1}]v = A(\mathbb{1}v) - \mathbb{1}(Av) = Av - Av = 0$
2. $[A, B] = AB - BA = -(BA - AB) = -[B, A]$
3. $\begin{aligned}[A + B, C] &= (A + B)C - C(A + B) = AC + BC - CA + CB\\ &= [A, C] + [B, C]\end{aligned}$
4. $[\alpha A, B] = (\alpha A)B - B(\alpha A) = \alpha(AB - BA) = \alpha[A, B]$
5. $\begin{aligned}[A, B]C + B[A, C] &= (AB - BA)C + B(AC - CA)\\ &= ABC - BCA = [A, BC]\end{aligned}$
6. Similar to 5.
7. $(A - B)(A + B) = A^2 + AB - BA + B^2 = A^2 - B^2 + [A, B]$ □

1.5 CLASSICAL VS QUANTUM

In this section, we draw a comparison between the Hamiltonian formalism of classical mechanics and the standard postulates of quantum mechanics.

1.5.1 Hamiltonian mechanics

Hamiltonian mechanics, a reformulation of Lagrangian mechanics, describes the dynamics of *classical* objects and particles. In particular, it accounts for conservative dynamics and cannot describe generic dissipative interactions like friction (which nevertheless is the result of the interaction of a very large number of particles). Note that a complete analysis of Hamiltonian mechanics is beyond the scope of this module.

For simplicity, we will consider a system with a single degree of freedom, for example a particle moving in one spatial dimension, i.e. along a straight line modelled by $\mathbb{R}$. In classical mechanics:

1. **States**. The state of the particle at any given time is given by two variables $x(t)$ and $p(t)$, respectively its *position* and *momentum*. In other words, the state corresponds to a single point in a two-dimensional phase space $(x(t), p(t)) \in \mathbb{R}^2$.

2. **Observables**. Every dynamical variable ω, that we can observe by performing measurements on the system, is a function of x and p: $\omega = \omega(x, p)$.

3. **Measurements**. A measurement of ω will yield the the value $\omega(x, p)$ if at that time the system is in the state (x, p). Moreover, measurements in classical mechanics are non-disturbing, meaning that the state of the system immediately after the measurement remains (x, p).

4. **Time evolution**. The state changes continuously in time according to *Hamilton's equations*:

$$\dot{x} = \frac{\partial \mathscr{H}}{\partial p}; \qquad \dot{p} = -\frac{\partial \mathscr{H}}{\partial x} \tag{1.6}$$

   where

$$\mathscr{H}(x, p) = \text{kinetic energy} + \text{potential energy} = \frac{p^2}{2m} + V(x) \tag{1.7}$$

   is called the *Hamiltonian*, which is interpreted as the total energy of the system. The Hamiltonian determines the motion of the system.

EXAMPLE 1.46. For a simple harmonic oscillator, $V(x) = kx^2/2$. Hence the Hamiltonian is given by

$$\mathscr{H} = \frac{p^2}{2m} + \frac{kx^2}{2}$$

The equation of motion are

$$\frac{\partial \mathscr{H}}{\partial p} = \dot{x} \to \frac{p}{m} = \dot{x}$$
$$-\frac{\partial \mathscr{H}}{\partial x} = \dot{p} \to -kx = \dot{p}$$

These can be integrated with respect to time, given the initial conditions $x(0)$ and $p(0)$. By differentiating the first equation with respect to time and substituting in the second, we get

$$m\ddot{x} + kx = 0\,,$$

which is Newton's Second Law for the harmonic oscillator. ◇

DEFINITION 1.47. Given two observables $\omega(x,p)$ and $\lambda(x,p)$, their *Poisson bracket* is defined as

$$\{\omega,\lambda\} = \frac{\partial\omega}{\partial x}\frac{\partial\lambda}{\partial p} - \frac{\partial\omega}{\partial p}\frac{\partial\lambda}{\partial x}\,. \qquad \diamond$$

PROPOSITION 1.48. *An observable ω is a constant of motion if its Poisson bracket with $\mathscr{H}$ vanishes.*

PROOF. We write

$$\begin{aligned}\frac{d\omega}{dt} =& \frac{\partial\omega}{\partial x}\dot{x} + \frac{\partial\omega}{\partial p}\dot{p}\\ =& \frac{\partial\omega}{\partial x}\frac{\partial\mathscr{H}}{\partial p} - \frac{\partial\omega}{\partial p}\frac{\partial\mathscr{H}}{\partial x}\\ =& \{\omega,\mathscr{H}\}\,.\end{aligned}$$

Hence, $d\omega/dt = 0$ when $\{\omega,\mathscr{H}\} = 0$. □

1.5.2 The postulates of quantum mechanics

We now compare the framework for classical systems described in Sec. 1.5.1 with the standard postulates of quantum mechanics, which should (at least in part) be familiar from the module QT&I. For simplicity, we formulate them in terms of a particle moving in one spatial dimension, i.e. along a straight line modelled by $\mathbb{R}$.

- **Postulate 1 (States)**. The state of the particle at any given time is given by a unit vector $|\psi(t)\rangle$ in $\mathcal{H} = L^2(\mathbb{R})$.
- **Postulate 2 (Observables)**. The observable quantities, which we can measure, are represented by self-adjoint operators on $\mathcal{H}$. The independent variables x and p of classical mechanics are represented by operators X and P with the following matrix elements in the (generalised) eigenbasis of X:

$$\langle x'|X\,|x\rangle = x\delta(x-x'); \quad \langle x'|P\,|x\rangle = -i\hbar\delta(x-x')\frac{d}{dx'}\,, \tag{1.8}$$

where $\delta(x)$ is the *Dirac delta function*.[4] The operators corresponding to the dependent variables $\omega(x,p)$ are given by the self-adjoint operators $\Omega(X,P) = \omega(x\to X, p\to P)$.[5]

[4] cf. Sec. 1.6 below.

[5] This 'recipe' is ambiguous; for instance, $\omega = xp = px$, but $XP \neq PX$. In such cases, we use the symmetric sum, $\Omega = (XP+PX)/2$. Also, this 'recipe' fails when Ω lacks a classical analogue, e.g., 'spin' angular momentum.

- **Postulate 3 (Measurements)**. A measurement of an observable Ω performed on a system in state $|\psi\rangle$ will yield one of the eigenvalues ω of Ω with probability given by the *Born rule*:

$$\text{Prob}(\Omega = \omega \mid \psi) = |\langle\omega|\psi\rangle|^2 .$$

  Immediately after the measurement, the system will reside in the eigenvector $|\omega\rangle$ corresponding to the observed outcome.

- **Postulate 4 (Time evolution)**. In absence of measurements, the state of the system evolves continuously in time according to the *time-dependent Schrödinger equation* (TDSE):

$$i\hbar\frac{d}{dt}|\psi(t)\rangle = H|\psi(t)\rangle , \tag{1.9}$$

  where $H(X,P) = \mathscr{H}(x \to X, p \to P)$ is the quantum Hamiltonian operator and $\mathscr{H}$ is the Hamiltonian for the corresponding classical problem.

In quantum theory, probabilities play a fundamental role. The quantum state only tells us the probabilities of observing a particular eigenvalue of an observable Ω. Furthermore, measurements are inherently disturbing, and in addition to the *deterministic* time evolution given by (1.9), we must also account for the *probabilistic* and seemingly instantaneous *collapse* of the state upon measurements.

We will see in future lectures that, in analogy with classical mechanics, conserved quantities in quantum mechanics are represented by self-adjoint operators Ω that commute with the Hamiltonian operator, $[\Omega, H] = 0$. Moreover, we will show that the momentum operator P is the generator of spatial translations, which are represented by unitary maps. An analogous relation holds between the angular momentum operator and rotations.

REMARK 1.49. The postulates P1-4 focus on the case of non-degenerate observables Ω. It may happen, however, that $\omega_1 = \omega_2 = \omega$. How do we compute the probabilities in this case? We select some orthonormal basis $\{|\omega,1\rangle, |\omega,2\rangle\}$ of the eigenspace of Ω with eigenvalue ω and construct the corresponding orthogonal projector:

$$P_\omega = |\omega,1\rangle\langle\omega,1| + |\omega,2\rangle\langle\omega,2|$$

Then, the probability of observing outcome ω becomes

$$\text{Prob}(\omega) = \langle\psi|P_\omega|\psi\rangle$$

and the post-measurement state will be

$$|\psi\rangle \propto P_\omega|\psi\rangle . \qquad \diamond$$

REMARK 1.50. What do we do when the eigenvalue spectrum of Ω is continuous? In this case, we use the resolution of the identity

$$\mathbb{1} = \int |\omega\rangle\langle\omega| \, \mathrm{d}\omega$$

to expand $|\psi\rangle$ in the Ω basis,

$$|\psi\rangle = \mathbb{1}\,|\psi\rangle = \int |\omega\rangle\langle\omega|\psi\rangle \, \mathrm{d}\omega \,. \tag{1.10}$$

We expect that as ω varies continuously, so will $\langle\omega|\psi\rangle$, i.e. we expect $\langle\omega|\psi\rangle$ to be a smooth function $\psi(\omega)$. We call $\psi(\omega) = \langle\omega|\psi\rangle$ the *wave function (corresponding to $|\psi\rangle$) in the Ω basis*. The wave function is also called the *probability amplitude* for finding the particle with $\Omega = \omega$. The probability of obtaining a result between ω and $\omega + \mathrm{d}\omega$ is given by $|\psi(\omega)|^2 \, \mathrm{d}\omega$, where $|\psi(\omega)|^2$ is called the *probability density* at ω. ◇

1.6 DIRAC'S DELTA

Dirac's delta function $\delta(x)$ has the following properties:

- $\delta(x) = 0$ if $x \neq 0$, and it is infinite at $x = 0$.
- $\int_{-\infty}^{\infty} \delta(x) \, \mathrm{d}x = 1$.

It is not a function, but should be considered as the limit of some one-parameter family of functions. For example, let $\epsilon > 0$ and define

$$\delta_\epsilon(x) := \frac{\epsilon}{\pi(x^2 + \epsilon^2)} \,,$$

i.e. a Lorentzian function with width $\sim \epsilon$. Then $\delta(x)$ may be thought of as the limit of $\delta_\epsilon(x)$ as $\epsilon \to 0$.

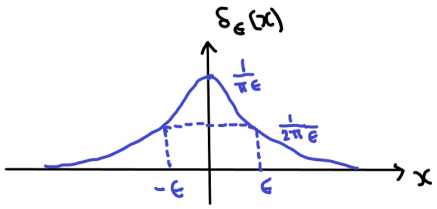

FIGURE 1.1. Sketch of $\delta_\epsilon(x)$.

In fact,

$$\text{If } x \neq 0, \quad \lim_{\epsilon\to 0} \delta_\epsilon(x) = \lim_{\epsilon\to 0} \frac{\epsilon}{\pi(x^2 + \epsilon^2)} = \frac{0}{\pi(x^2 + 0^2)} = 0,$$

$$\text{If } x = 0, \quad \lim_{\epsilon\to 0} \delta_\epsilon(0) = \lim_{\epsilon\to 0} \frac{1}{\pi\epsilon} = \infty.$$

Moreover, one can show that

$$\int_{-\infty}^{\infty} \delta_\epsilon(x)\,\mathrm{d}x = 1$$

for all $\epsilon > 0$ [left as an exercise].

Since $\delta(x) = 0$ unless $x = 0$, we have that $f(x)\delta(x) = f(0)\delta(x)$ for any continuous function $f : \mathbb{R} \to \mathbb{C}$.

PROPOSITION 1.51. *If $f : \mathbb{R} \to \mathbb{C}$ is continuous, then*

$$\int_{-\infty}^{\infty} f(x)\delta(x)\,\mathrm{d}x = f(0). \tag{1.11}$$

"Sketch Proof": Since $f(x)\delta(x) = f(0)\delta(x)$,

$$\int_{-\infty}^{\infty} f(x)\delta(x)\,\mathrm{d}x = \int_{-\infty}^{\infty} f(0)\delta(x)\,\mathrm{d}x = f(0)\int_{-\infty}^{\infty} \delta(x)\,\mathrm{d}x = f(0).$$

This equality for all continuous function f is equivalent to our original definition. So, we may define $\delta(x)$ as the object satisfying Eq. (1.11) for all continuous functions f. From (1.11), it follows that

$$\int_{-\infty}^{\infty} f(x')\delta(x - x')\,\mathrm{d}x' = f(x)\,. \tag{1.12}$$

Notice that this equation corresponds to $\sum_{n'} c_{n'}\delta_{nn'} = c_n$, with the following correspondence:

$$\sum_{n'} \leftrightarrow \int_{-\infty}^{\infty} \mathrm{d}x', \quad n' \leftrightarrow x', \quad n \leftrightarrow x, \quad c \leftrightarrow f, \quad \delta_{nn'} \leftrightarrow \delta(x - x').$$

The Lorentzian function $\delta_\epsilon(x)$ can be written in terms of the following integral [left as an exercise]

$$\delta_\epsilon(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}kx - \epsilon|k|}\mathrm{d}k.$$

Considering the $\epsilon \to 0$ limit of it, we may write

$$\delta(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}kx}\,\mathrm{d}k\,. \tag{1.13}$$

This representation of $\delta(x)$ will be useful when we will discuss the momentum eigenstates.

2 *Position and momentum*

2.1 POSITION EIGENSTATES

Consider candidates $|x\rangle$ for eigenstates of the position operator X, satisfying

$$X\,|x\rangle = x\,|x\rangle\,, \qquad x \in \mathbb{R}\,. \tag{2.1}$$

One can think of $|x\rangle$ as describing a particle that is located exactly at the point $X = x$. Applying the bra $\langle x'|$ to (2.1), we find $\langle x'|X\,|x\rangle = x\langle x'|x\rangle$. The postulates tell us that $\langle x'|X\,|x\rangle = x\delta(x-x')$, hence these vectors satisfy a generalised version of the orthonormality condition,

$$\langle x'|x\rangle = \delta(x-x')\,, \qquad x, x' \in \mathbb{R}\,. \tag{2.2}$$

This means that, while different elements of $\{|x\rangle, x \in \mathbb{R}\}$ are orthogonal, these vectors are *not* square-integrable. They are not *proper* eigenvectors of the operator X on $L^2(\mathbb{R})$, which, a fortiori, has no (proper) eigenvalues. Vectors which do not belong in $L^2(\mathbb{R})$ but that can be 'delta-normalised' are said to be *improper*. The set $\{|x\rangle, x \in \mathbb{R}\}$ constitutes the (improper or generalised) *position basis* of $\mathcal{H} = L^2(\mathbb{R})$. Improper vectors should not be regarded as representing 'physical' states but only as an idealisation. Strictly speaking, we cannot realistically prepare a particle located at a single point $x \in \mathbb{R}$ with infinite precision. Nevertheless, we will continue to use the (generalised) eigenkets $|x\rangle$ as basis vectors because these are convenient to handle mathematically, and their use can be justified rigorously.

For a (proper) state $|\psi\rangle \in L^2(\mathbb{R})$, let $\psi(x) = \langle x|\psi\rangle$. Then

$$\langle x'|\left(\int_{-\infty}^{\infty} \mathrm{d}x\; |x\rangle\langle x|\right)|\psi\rangle = \int_{-\infty}^{\infty} \langle x'|x\rangle\langle x|\psi\rangle\,\mathrm{d}x = \\ = \int_{-\infty}^{\infty} \delta(x-x')\psi(x)\,\mathrm{d}x = \psi(x') = \langle x'|\psi\rangle$$

implies that the position basis of $\mathcal{H}$ satisfies the completeness relation

$$\mathbb{1} = \int_{-\infty}^{\infty} \mathrm{d}x\; |x\rangle\langle x|\,.$$

This resolution of the identity allows us to represent elements $|\psi\rangle$ of the Hilbert space $\mathcal{H} = L^2(\mathbb{R})$. Writing

$$|\psi\rangle = \mathbb{1}\,|\psi\rangle = \int_{-\infty}^{\infty} \mathrm{d}x\; |x\rangle\langle x|\psi\rangle = \int_{-\infty}^{\infty} \mathrm{d}x\,\psi(x)\,|x\rangle\,, \tag{2.3}$$

the expansion coefficients $\psi(x) = \langle x|\psi\rangle$ define a square-integrable function, known as the *wave function* (of $|\psi\rangle$) *in the position basis*, or *position representation* of $|\psi\rangle$.

We may ask: what is the action of the position operator X on arbitrary states of the particle? We start from $X|\psi\rangle = |\widetilde{\psi}\rangle$. Then

$$\begin{aligned}\langle x|X|\psi\rangle &= \int_{-\infty}^{\infty} \langle x|X|x'\rangle\langle x'|\psi\rangle \,\mathrm{d}x' = \int_{-\infty}^{\infty} \delta(x-x')x'\psi(x')\,\mathrm{d}x' \\ &= x\psi(x) = \langle x|\widetilde{\psi}\rangle = \widetilde{\psi}(x)\end{aligned}$$

Hence, the action of X amounts to multiplying each 'entry' $\psi(x)$ by x,

$$X : \psi(x) \mapsto x\psi(x)\,.$$

This should not come as a surprise, as we already dealt with the position operator X in Examples 1.21 and 1.38.

2.2 MOMENTUM EIGENSTATES

Similar arguments apply for the (generalised) momentum eigenstates $|p\rangle$. The eigenvalue relation reads

$$P|p\rangle = |p\rangle\,, \qquad p \in \mathbb{R}\,,$$

which defines the *momentum basis* $\{|p\rangle, p \in \mathbb{R}\}$ of $\mathcal{H} = L^2(\mathbb{R})$. As for X, the operator P has no proper eigenvalues and the vectors $|p\rangle$ are improper. To see this, let us derive the position representation of the momentum eigenstates, i.e. $\psi_p(x) = \langle x|p\rangle$.

We start by representing the action of P in position basis. Let $P|\psi\rangle = |\widetilde{\psi}\rangle$, then

$$\begin{aligned}\langle x|P|\psi\rangle &= \int_{-\infty}^{\infty} \langle x|P|x'\rangle\langle x'|\psi\rangle \,\mathrm{d}x' = \int_{-\infty}^{\infty} -i\hbar\delta(x-x')\frac{\partial\psi(x')}{\partial x'}\,\mathrm{d}x' \\ &= -i\hbar\frac{\partial\psi(x)}{\partial x} = \langle x|\widetilde{\psi}\rangle = \widetilde{\psi}(x)\,,\end{aligned}$$

where we used $\langle x|P|x'\rangle = -i\hbar\delta(x-x')\partial/\partial x'$, as stipulated by the postulates. Hence,

$$P : \psi(x) \mapsto -i\hbar\frac{\partial\psi(x)}{\partial x}\,.$$

Next, we let $|\psi\rangle = |p\rangle$, hence $\langle x|P|p\rangle = p\langle x|p\rangle = p\psi_p(x)$. The eigenvalue equation becomes

$$-i\hbar\frac{\partial\psi_p(x)}{\partial x} = p\psi_p(x)\,.$$

The solutions of this first-order ODEs are *plane waves*,

$$\langle x|p\rangle = \psi_p(x) = Ae^{i\frac{p}{\hbar}x} = Ae^{ikx}\,. \tag{2.4}$$

where we define the *wave number* k by $k = p/\hbar$. These functions are not square-integrable, but they can be 'delta-normalised' by a suitable choice of

the free parameter A. Let $A = (2\pi\hbar)^{-1/2}$, then

$$\begin{aligned}\langle p'|p\rangle =& \int_{-\infty}^{\infty} \langle p'|x\rangle\langle x|p\rangle \,\mathrm{d}x = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} e^{i(k-k')x}\,\mathrm{d}x \\ =& \frac{2\pi}{2\pi\hbar}\delta(k-k') = \frac{1}{\hbar}\delta((p-p')/\hbar) \\ =& \delta(p-p')\,,\end{aligned}$$

where we used Eq. (1.13) and the *scaling property* of the Dirac delta, i.e. $\delta(\alpha x) = \delta(x)/|\alpha|$ for a non-zero scalar α (proof left as exercise). We conclude that momentum eigenstates $|p\rangle$ are improper vectors, satisfying a generalised orthonormality condition. In analogy with position eigenstates, we can write the completeness relation

$$\int_{-\infty}^{\infty} dp\ |p\rangle\langle p| = \mathbb{1}\,, \tag{2.5}$$

which provides another way to represent elements of the Hilbert space,

$$|\psi\rangle = \mathbb{1}\,|\psi\rangle = \int_{-\infty}^{\infty} \mathrm{d}p\ |p\rangle\langle p|\psi\rangle = \int_{-\infty}^{\infty} \mathrm{d}p\,\psi(p)\,|p\rangle\,. \tag{2.6}$$

The expansion coefficients $\psi(p) = \langle p|\psi\rangle$ define the *wave function* (of $|\psi\rangle$) *in momentum basis*, or *momentum representation* of $|\psi\rangle$.

REMARK 2.1. The quantum state of a particle must give relative probabilities for all measurement outcomes. For a position measurement, this information is contained in the components of $|\psi\rangle$ in the X basis, $\psi(x) = \langle x|\psi\rangle$. For a momentum measurement, one does not need a new vector: *the same ket* $|\psi\rangle$ when expanded in terms of the P basis provides information about the probabilities of yielding different outcomes. ◇

It follows from Eq. (2.4) that the probability density function describing the likelihood of finding a particle with precise momentum p at position $X = x$ is uniform over all space,

$$|\psi_p(x)|^2 = \frac{1}{2\pi\hbar}e^{-ipx/\hbar}e^{ipx/\hbar} = \frac{1}{2\pi\hbar}\,.$$

Technically, since $\psi_p(x)$ cannot be normalised, we may interpret $|\psi_p(x)|^2$ as the *relative probability density*. Then, the *absolute* probability of finding the particle with precise momentum p in any finite region $I = [a, b]$ is zero, $\int_a^b |\psi_p(x)|^2\,\mathrm{d}x / \int_{-\infty}^{\infty} |\psi_p(x)|^2\,\mathrm{d}x = 0$. Therefore, regardless of the value of p, the particle can be found anywhere in the Universe equally (un)likely. Recall that this is an idealised, unphysical scenario. In the real world, any particle that we are interested in will definitely be known to exist in some (perhaps large) region of space.

Unsurprisingly, the same result holds for momentum measurements on position eigenstates. We have that $\psi_x(p) = \langle p|x\rangle = \overline{\langle x|p\rangle}$, thus the relative probability density is $|\psi_x(p)|^2 = 1/(2\pi\hbar)$. A particle with definite position does not possess a definite momentum, to the point that a momentum measurement can yield any outcome with same probability.

Generally, the position representation $\psi(x)$ and the momentum representation $\psi(p)$ of the same state $|\psi\rangle$ are related to each other by *Fourier Transform*[6]

$$\begin{aligned}\psi(p) &= \langle p| \int_{-\infty}^{\infty} \mathrm{d}x\, |x\rangle\langle x|\psi\rangle \\ &= \int_{-\infty}^{\infty} \mathrm{d}x \langle p|x\rangle\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \mathrm{d}x e^{-ipx/\hbar}\psi(x)\,.\end{aligned}$$

[6] The transforms may differ from what you've seen before due to the (inconsequential) presence of the constant $\hbar$.

The *inverse* Fourier transform arises when "going in the other direction":

$$\begin{aligned}\psi(x) = \langle x|\psi\rangle &= \langle x| \int_{-\infty}^{\infty} \mathrm{d}p\, |p\rangle\langle p|\psi\rangle \\ &= \int_{-\infty}^{\infty} \mathrm{d}p \langle x|p\rangle\psi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \mathrm{d}p e^{ipx/\hbar}\psi(p)\,.\end{aligned}$$

REMARK 2.2. Momentum eigenstates can be equivalently characterised by k rather than p. The wave function in position basis would read $\psi_k(x) = (2\pi)^{-1/2}\exp(ikx)$, where we dropped the $\hbar$ in the normalisation factor to ensure that $\langle k'|k\rangle = \delta(k-k')$. ◇

DEFINITION 2.3. If for large negative values of x, a wave function $\psi(x)$ of a quantum state $|\psi\rangle$ takes the form $\psi(x) \simeq \mathrm{e}^{\mathrm{i}kx}$ with $k > 0$, we call it a wave *incident from the left*.

If for large positive values of x, a wave function $\psi(x)$ takes the form $\psi(x) \simeq \mathrm{e}^{-\mathrm{i}kx}$ with $k > 0$, we call it a wave *incident from the right*. ◇

2.3 THREE DIMENSIONS

So far our main example of a Hilbert space has been $L^2(\mathbb{R})$, representing a particle moving in one dimension x. (Notice that the number of spatial dimensions, which was 1, is not the same as the dimension of the Hilbert space, which was already infinite.) When considering a particle moving in three spatial dimensions, the relevant Hilbert space is $L^2(\mathbb{R}^3)$, i.e. the vectors are functions $\psi : \mathbb{R}^3 \to \mathbb{C}$ satisfying

$$\int_{\mathbb{R}^3} |\psi(\mathbf{x})|^2\, \mathrm{d}\mathbf{x} < \infty. \tag{2.7}$$

Here we will use Cartesian co-ordinates, writing $\mathbf{x} = (x_1, x_2, x_3)$ or $\mathbf{x} = (x, y, z)$, so that (2.7) becomes

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} |\psi(x,y,z)|^2\, \mathrm{d}x\, \mathrm{d}y\, \mathrm{d}z < \infty, \tag{2.8}$$

although in cases of spherical symmetry it is often useful to adopt spherical coordinates (r, θ, ϕ), in which case we have

$$\int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} |\psi(r,\theta,\phi)|^2\, r^2 \sin\theta\, \mathrm{d}r\, \mathrm{d}\theta\, \mathrm{d}\phi < \infty. \tag{2.9}$$

Instead of a single position operator X, there are now three operators X_1, X_2, X_3, defined by

$$(X_i\psi)(x_1, x_2, x_3) = x_i\psi(x_1, x_2, x_3). \tag{2.10}$$

Similarly there are three momentum operators P_1, P_2, P_3 defined by

$$(P_i\psi)(x_1, x_2, x_3) = (-i\hbar)\frac{\partial}{\partial x_i}\psi(x_1, x_2, x_3). \tag{2.11}$$

All of these operators are self-adjoint by similar reasoning to the 1-dimensional case (Examples 1.38 and 1.39). Their commutators are as follows:

PROPOSITION 2.4. *For $i, j \in \{1, 2, 3\}$, the three-dimensional position and momentum operators satisfy*

$$[X_i, X_j] = 0\,, \quad [P_i, P_j] = 0\,, \quad [X_i, P_j] = \mathrm{i}\hbar\delta_{ij}\mathbb{1}. \tag{2.12}$$

PROOF. Consider some (sufficiently nice) $\psi \in L^2(\mathbb{R}^3)$. We find

$$([X_i, X_j]\psi)(\mathbf{x}) = (X_iX_j\psi)(\mathbf{x}) - (X_jX_i\psi)(\mathbf{x}) = x_ix_j\psi(\mathbf{x}) - x_jx_i\psi(\mathbf{x}) = 0.$$

Similarly

$$([P_i, P_j]\psi)(\mathbf{x}) = (-i\hbar)^2\left(\frac{\partial^2}{\partial x_i\partial x_j}\psi(\mathbf{x}) - \frac{\partial^2}{\partial x_j\partial x_i}\psi(\mathbf{x})\right) = 0,$$

where (for $i \neq j$) we have assumed ψ has continuous second partial derivatives so that we can exchange the order of differentation. Finally,

$$([X_i, P_j]\psi)(\mathbf{x}) = (-i\hbar)\left(x_i\frac{\partial}{\partial x_j}\psi(\mathbf{x}) - \frac{\partial}{\partial x_j}x_i\psi(\mathbf{x})\right) = \mathrm{i}\hbar\delta_{ij}\psi(\mathbf{x}),$$

since the product rule gives $\frac{\partial}{\partial x_j}(x_i\psi(\mathbf{x})) = \frac{\partial x_i}{\partial x_j}\psi(\mathbf{x}) + x_i\frac{\partial}{\partial x_j}\psi(\mathbf{x})$ and we have $\partial x_i/\partial x_j = \delta_{ij}$. □

3 *Quantum measurements*

3.1 DISCRETE MEASUREMENTS

Consider the self-adjoint operator M acting on a finite-dimensional Hilbert space $\mathcal{H}$, with eigenvalues m_k, $k = 0, \ldots, N$. By the spectral theorem 1.31, we can write

$$M = \sum_{k=1}^{N} m_k P_{m_k}$$

where P_{m_k} is the projector onto the (not necessarily one-dimensional) eigenspace of M with eignvalue m_k. In particular, $\sum_{k=1}^{N} P_{m_k} = \mathbb{1}$.

Given a system residing in $|\psi\rangle$, the postulates of quantum mechanics say that the probability of outcome m_k is given by

$$\text{Prob}(M = m_k \mid \psi) = \| P_{m_k} |\psi\rangle \|^2$$

If m_k is non-degenerate, then $P_{m_k} = |m_k\rangle\langle m_k|$ and $\text{Prob}(M = m_k \mid \psi) = |\langle m_k|\psi\rangle|^2$.

As we already mentioned, this interpretation is only consistent if the probabilities add up to unity. Thanks to the normalization condition for quantum states, they do indeed:

$$\begin{aligned}\sum_{k=1}^{N} \text{Prob}(M = m_k \mid \psi) &= \sum_{k=1}^{N} \| P_{m_k} |\psi\rangle \|^2 \\ &= \sum_{k=1}^{N} \langle\psi| P_{m_k} |\psi\rangle \\ &= \langle\psi| \sum_{k=1}^{N} P_{m_k} |\psi\rangle = \langle\psi|\psi\rangle = 1\,.\end{aligned}$$

Note that all probabilities remain unchanged if we replace the state $|\psi\rangle$ by $\alpha|\psi\rangle$, with a phase factor $\alpha \in \mathbb{C}$ with $|\alpha| = 1$,

$$\text{Prob}(M = m_k \mid \alpha\psi) = \| P_{m_k} \alpha |\psi\rangle \|^2 = \| \alpha P_{m_k} |\psi\rangle \|^2 = \| P_{m_k} |\psi\rangle \|^2\,.$$

We refer to such a factor $a \in \mathbb{C}$ as a *global phase*, and we consider $|\psi\rangle$ and $\alpha|\psi\rangle$ to represent the same state.

Immediately after the measurement, the state will have collapsed to

$$|\psi_{m_k}\rangle = \frac{P_{m_k} |\psi\rangle}{\| P_{m_k} |\psi\rangle \|}$$

where we have divided by $\| P_{m_k} |\psi\rangle \|$ to keep the state normalised.

EXAMPLE 3.1. Suppose that we measure the observable

$$S_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

on a two-dimensional quantum system residing in the state $|+\rangle = (1,1)^{\mathrm{T}}/\sqrt{2} \in \mathbb{C}^2$.[7] To determine the possible outcomes and the post-measurement state, we need to know the eigenvalues and eigenvectors of S_z. They are $+\hbar/2$ with eigenvector $|\uparrow\rangle = (1,0)^{\mathrm{T}}$ and $-\hbar/2$ with eigenvector $|\downarrow\rangle = (0,1)^{\mathrm{T}}$. (Clearly, S_z is a non-degenerate observable). Since

$$|\langle\uparrow|+\rangle|^2 = \frac{1}{2} \quad \text{and} \quad |\langle\downarrow|+\rangle|^2 = \frac{1}{2},$$

we conclude that the probability of observing outcome $+\hbar/2$ is 50%, just like the probability of observing outcome $-\hbar/2$.

In the case that the outcome $+\hbar/2$ has obtained in a specific run, the state after the measurement will be $|\uparrow\rangle$ corresponding to an update of the initial state,

$$|+\rangle \overset{\hbar/2}{\to} \frac{P_\uparrow |+\rangle}{\|P_\uparrow |+\rangle\|} = \frac{|\uparrow\rangle\langle\uparrow|+\rangle}{\langle\uparrow|+\rangle} = |\uparrow\rangle\,,$$

and similarly for the other outcome. ◇

[7] We will see that this scenario corresponds to a measurement of the *spin* of an electron (residing in $|+\rangle$) along the z axis.

We know from probability theory that important aspects of a distribution are characterized by the mean (or expectation) value and the variance of a quantity.

PROPOSITION 3.2. *Let M be a observable (sef-adjoint operator) on a Hilbert space $\mathcal{H}$. Then*

1. *The* expectation value of M *in the state $|\psi\rangle$ is defined as*

$$\langle M\rangle_\psi \equiv \langle\psi|M\psi\rangle\,. \tag{3.1}$$

2. *The* variance of M *in the state $|\psi\rangle$ is defined as*

$$(\Delta_\psi M)^2 = \langle M^2\rangle_\psi - \langle M\rangle_\psi^2\,; \tag{3.2}$$

the square root $\Delta_\psi M$ of the variance is called the uncertainty of M *in the state $|\psi\rangle$.*

PROOF. An expectation value is the probability-weighted sum of the possible outcomes, i.e.

$$\langle M\rangle_\psi = \sum_{k=1}^{N} m_k \,\mathrm{Prob}(M = m_k \mid \psi).$$

Plugging in the expression for the probabilities, we obtain

$$\begin{aligned}\langle M\rangle_\psi =& \sum_{k=1}^{N} m_k \|P_{m_k}|\psi\rangle\|^2 = \sum_{k=1}^{N} m_k \langle\psi|P_{m_k}|\psi\rangle \\ =& \langle\psi|\left(\sum_{k=1}^{N} m_k P_{m_k}\right)|\psi\rangle = \langle\psi|M|\psi\rangle = \langle\psi|M\psi\rangle\,.\end{aligned}$$

The formula for the variance can be shown in a similar way using the identity

$$M^2 = \sum_{k=1}^{N} m_k^2 P_{m_k} \,.$$

□

REMARK 3.3. In Proposition 3.2, we assumed that $|\psi\rangle$ was normalised. If, however, $\langle\psi|\psi\rangle \neq 1$, the formula for the expectation value becomes

$$\langle M\rangle_\psi \equiv \frac{\langle\psi|M\psi\rangle}{\langle\psi|\psi\rangle}\,,$$

which amounts to first normalising the state, $|\psi\rangle \to |\psi\rangle/\sqrt{\langle\psi|\psi\rangle}$, and then computing the expectation value via Eq. (3.1). ◇

EXAMPLE 3.4. We continue Example 3.1. The expectation value of S_z in the state $|+\rangle$ is

$$\langle S_z\rangle_{|+\rangle} = \langle +|S_z|+\rangle = \frac{\hbar}{2}\begin{pmatrix}1 & 1\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}1\\ 1\end{pmatrix} = 0.$$

To find the variance $\langle S_z^2\rangle_{|+\rangle}$, we need to calculate the square of the operator S_z first,

$$S_z^2 = \frac{\hbar^2}{4}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} = \frac{\hbar^2}{4}\mathbb{1}\,,$$

resulting in the variance

$$\langle S_z^2\rangle_{|+\rangle} = \langle +|S_z^2\,|+\rangle - \langle +|S_z|+\rangle^2 = \frac{\hbar^2}{4}\,.$$

◇

3.2 CONTINUOUS MEASUREMENTS

Suppose that we wish to measure a physical quantity represented by a self-adjoint operator A which has a continuous spectrum, such as the position or momentum of a quantum particle with Hilbert space $L^2(\mathbb{R})$. The set of possible outcomes of a measurement of position is the entire real line for both the observables X and P.

Following Sec. 1.5.2, for a (normalised) state $|\psi\rangle$ of the system, the probability that a measurement of, say, X returns a value $x \in [a,b] \subset \mathbb{R}$ is computed as follows,

$$\text{Prob}(X = x \in [a,b] \mid \psi) = \int_a^b |\psi(x)|^2\,\mathrm{d}x\,,$$

where $|\psi(x)|^2$ is the probability density at x.

In analogy to the discrete case, the probability distribution for the measurement outcomes is such that

$$\langle A\rangle_\psi = \langle\psi|A\,|\psi\rangle = \langle\psi|A\psi\rangle\,;$$

This number will also be called the *expectation (value)* of the observable A in the state $|\psi\rangle$. Note that, if $|\psi\rangle$ is *not* normalised, then $\langle A\rangle_\psi = \langle\psi|A\psi\rangle/\langle\psi|\psi\rangle$. For position X, we can write

$$\langle X\rangle_\psi = \langle\psi|X\psi\rangle = \int_{-\infty}^{\infty} \overline{\psi(x)}x\psi(x)\,\mathrm{d}x = \int_{-\infty}^{\infty} x|\psi(x)|^2\,\mathrm{d}x\,.$$

The integral has a simple interpretation: it corresponds to averaging the values of $x \in \mathbb{R}$ occurring in a small interval dx about x with probability $|\psi(x)|^2 dx$. This observation links the wave function $\psi(x)$ associated with a quantum state $|\psi\rangle \in L^2(\mathbb{R})$ to experimentally observable probabilities.

Similarly, the *variance* for the measurement of A in the state $|\psi\rangle$ is given by

$$(\Delta_\psi A)^2 = \langle A^2\rangle_\psi - \langle A\rangle_\psi^2\,,$$

and its square root $\Delta_\psi A$, is called the *uncertainty of* A in the state $|\psi\rangle$.

EXAMPLE 3.5. The variance of position X in state $|\psi\rangle$ is given explicitly by the expression

$$\langle X^2\rangle_\psi = \langle\psi|X^2\psi\rangle - \langle X\rangle_\psi^2\,.$$

Let us consider a state $|\psi_0\rangle$ with the Gaussian wave function

$$\psi_0(x) = (\sqrt{\pi}l)^{-\frac{1}{2}} \exp\left(-\frac{x^2}{2\ell^2}\right), \tag{3.3}$$

for some $\ell > 0$. It is obvious that the expectation of position vanishes in this state,

$$\langle X\rangle_{\psi_0} = \int_{-\infty}^{\infty} x|\psi_0(x)|^2\,\mathrm{d}x\, = 0\,,$$

since the integrand is odd. The variance, however, does not vanish,

$$(\Delta_{\psi_0} X)^2 = \langle X^2\rangle_{\psi_0} = \int_{-\infty}^{\infty} x^2|\psi_0(x)|^2\,\mathrm{d}x = \frac{\ell^2}{2}\,, \tag{3.4}$$

where we used the Gaussian integral $\int_{-\infty}^{\infty} x^2\exp(-\alpha x^2)\,\mathrm{d}x = \sqrt{\pi}/(2\alpha^{3/2})$, for $\alpha > 0$. ◇

EXAMPLE 3.6. Consider now the momentum operator P on $L^2(\mathbb{R})$. In the position representation, its expectation value in a state $|\psi\rangle$ is defined as

$$\langle P\rangle_\psi = \langle\psi|P\psi\rangle = -\mathrm{i}\hbar\int_{-\infty}^{\infty} \overline{\psi(x)}\psi'(x)\,\mathrm{d}x.$$

Its variance is defined as

$$(\Delta_\psi P)^2 = \langle P^2\rangle_\psi - \langle P\rangle_\psi^2 = \langle\psi|P^2\psi\rangle - \langle\psi|P\psi\rangle^2\,.$$

It is convenient to use $\langle\psi|P^2\psi\rangle = \langle P\psi|P\psi\rangle$, which is a consequence of P being a self-adjoint operator, leading to

$$(\Delta_\psi P)^2 = \hbar^2\int_{-\infty}^{\infty} |\psi'(x)|^2\,\mathrm{d}x + \hbar^2\left(\int_{-\infty}^{\infty} \overline{\psi(x)}\psi'(x)\,\mathrm{d}x\right)^2. \qquad \diamond$$

We will later use variances to quantify the incompatibility between pairs of observables through Heisenberg's uncertainty relation.

3.3 THE DOUBLE SLIT EXPERIMENT

We now discuss in qualitative terms the quantum version of the iconic double slit experiment. It highlights the self-interference of the wave function of a *single* particle, thus showing that quantum systems may exhibit wave-like properties. It also serves as a compelling example of the behaviour of quantum measurements, which irreversibly disturb the observed system.

In this experiment (see Fig. 3.1) a source emits single particles (e.g. electrons) towards a wall with two slits (which we can choose to keep open or closed). Behind the wall is a screen/detector which records the arrival point x of the particle. Only a single electron is shot and detected in each run of the experiment. Upon repeating the process (infinitely) many times, a distribution $P(x)$ emerges, describing the likelihood of an electron hitting the screen at point x.

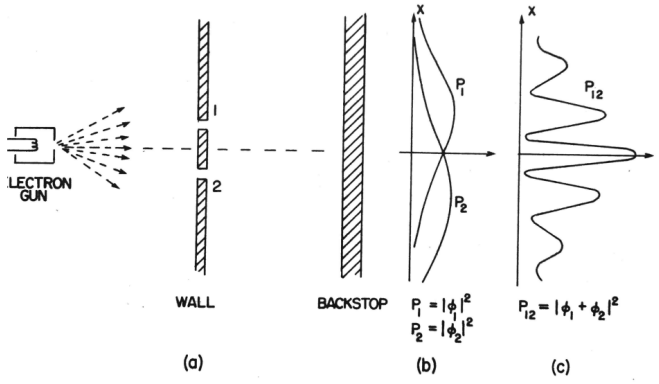

FIGURE 3.1. A double-slit experiment with electrons [R. P. Feynmann. *Lectures on Physics (vol 3)*. Addison Wesley, New York.]

In quantum theory, a single particle is described by a wave function. When only slit 1 is open, the electron is described by a wave function $\phi_1(x)$, leading to the probability density $P_1(x) = |\phi_1(x)|^2$. Similarly, with only slit 2 open, the electron is described by a (different) wave function $\phi_2(x)$ and the distribution $P_2(x) = |\phi_2(x)|^2$ is observed. In particular, $P_i(x)$ will peak in correspondence of slit i and decrease gradually on both sides (see Fig. 3.1). This agrees with our classical expectations: there is a higher chance for the particle to impact the screen directly behind the open slit.

Now consider the scenario where both slits are open. In classical mechanics, each particle travels along a definite trajectory that passes *either* via the first *or* the second slit (and then hits the screen at some point x). In particular, to a particle headed for the first slit, it is immaterial whether the second slit is open or closed. Being localised in space, it has no way of 'knowing' if the other slit is open or not, thus cannot respond to it in any way. Therefore, the total probability density of a classical particle reaching point x on the screen is simply $P_{12}(x) = P_1(x) + P_2(x)$.

However, in quantum mechanics, the state of the *single* electron will be the *superposition* $\phi_{12}(x) = \phi_1(x) + \phi_2(x)$. This means that the new

probability density is

$$P_{12}(x) = |\phi_{12}(x)|^2 = |\phi_1(x) + \phi_2(x)|^2 = P_1(x) + P_2(x) + 2\,\mathrm{Re}(\overline{\phi_1(x)}\phi_2(x))\,.$$

Clearly, $P_{12}(x) \neq P_1(x) + P_2(x)$. The term $2\,\mathrm{Re}(\overline{\phi_1(x)}\phi_2(x))$ is the *interference* term.

Indeed, when the experiment was conducted (with both slits open), an interference pattern like that in Fig. 3.1 is observed, with bands of high and low probability of hitting the screen corresponding to areas of constructive and destructive interference, respectively. These results indicate how the behaviour of a *single* electron may more closely resemble that of a wave (which diffracts and interferes) rather than that of a classical particle. The presence of an interference pattern suggests that electrons cannot be thought of as moving along definite trajectories. In some strange way, each electron passes through both slits.

We may attempt to outsmart the electron by inserting a detector near each slit, so we can know which slit the electron *actually* goes through. However, it turns out that any such additional measurement inevitably disturbs the state of the particle, to the point that the interference pattern disappears. For example, if the detector near slit 1 clicks, then the wave function collapses to

$$\phi_{12}(x) \to \phi_1(x)$$

so the probability density at point x on the screen is $P_1(x)$. A similar argument holds when the other detector clicks. After many runs of the experiment, the observed distribution will converge to $P_1(x)+P_2(x)$. Notably, the same results are obtained when only one detector is placed outside either of the slits. Therefore, it appears that by acquiring information about the trajectory of the electron via measurements, we induce it to behave like a classical particle, instead of a wave.

4 The energy operator

In quantum mechanics, energy is defined in terms of the energy operator H, also called the Hamiltonian operator. Knowing the energy eigenstates of a system is especially useful for computing the time evolution of arbitrary states of a system and gaining insights into its nonclassical properties.

The eigenvalue problem

$$H\,|\psi\rangle = E\,|\psi\rangle\,, \tag{4.1}$$

with $E \in \mathbb{R}$, is commonly referred to as the *time-independent Schrödinger equation* (TISE). Vectors satisfying the TISE correspond to states with a well-defined energy E.

In this section, we will delve into several one-dimensional problems and identify the energy eigenstates. While these scenarios may seem somewhat artificial, they contain most of the features of three dimensional quantum mechanics but little of its complexity.

4.1 FREE PARTICLE

A '*free*' particle is one on which no force acts, hence the potential V vanishes. In classical mechanics, the Hamiltonian coincides with the kinetic energy, $\mathscr{H} = \mathscr{H}_0 = p^2/2m$. In the corresponding quantum problem, the Hamiltonian operator is

$$H_0 = \frac{1}{2m}P^2$$

where P is the momentum operator. Clearly, the (generalised) momentum eigenstates $|p\rangle$ are also eigenstates of H_0,

$$H_0\,|p\rangle = \frac{1}{2m}P^2\,|p\rangle = \frac{p}{2m}P\,|p\rangle = \frac{p^2}{2m}\,|p\rangle$$

with energy $E = p^2/2m$. In particular, $|p\rangle$ and $|-p\rangle$ are eigenvectors of H_0 with the same eigenvalue. Each non-zero eigenvalue E is in fact *twice degenerate*, as to each E there corresponds a two-dimensional eigenspace spanned by the orthogonal vectors $|\pm p\rangle = |\pm\sqrt{2mE}\rangle$

We can reach the same conclusion by going into a specific basis and solving the time-independent Schrödinger equation. For example, in position representation, Eq. (4.1) reads

$$\frac{-i\hbar}{2m}\frac{d}{dx}\left(-i\hbar\frac{d}{dx}\psi(x)\right) = E\psi(x)\,.$$

Rearranging the terms gives

$$\psi''(x) + \frac{2mE}{\hbar^2}\psi(x) = 0\,. \tag{4.2}$$

For every $E > 0$, the general solution is

$$\psi(x) = A\psi_p(x) + B\psi_{-p}(x), \quad p = \sqrt{2mE}, \tag{4.3}$$

where $A, B \in \mathbb{C}$ and $\psi_p(x) = \exp(ipx/\hbar)$ is the position representation of $|p\rangle$ (up to a normalisation factor). As for the momentum operator, the Hamiltonian operator H_0 on $L^2(\mathbb{R})$ for a free particle has no proper eigenvalues.

Eq. (4.3) already encodes a departure from classical mechanics. Classically, a free particle with energy E can *either* be moving to the right *or* to the left with momentum $|p| = \sqrt{2mE}$. Only two options are available. In quantum mechanics, there are infinitely many *superpositions* of $|p\rangle$ and $|-p\rangle$ that are eigenstates of energy. When $A, B \neq 0$, we are describing a *single* particle with energy E which, in a way, is moving to the right *and* to the left at the same time (although when a measurement of P is carried out, only one option is realised).

4.2 PARTICLE IN A BOX

We now explore the scenario where a free particle is constrained within a region of size L, i.e. a one-dimensional '*box*'. We can examine this situation by introducing the following potential

$$V(x) = \begin{cases} 0 & 0 < x < L\,, \\ \infty & \text{otherwise}\,. \end{cases}$$

The Hamiltonian operator becomes $H = P^2/(2m) + V(X)$. It is convenient to split the space into three regions $(x < 0, 0 < x < L, x > L)$ (see Fig. 4.1) and solve the eigenvalue problem for each individually.

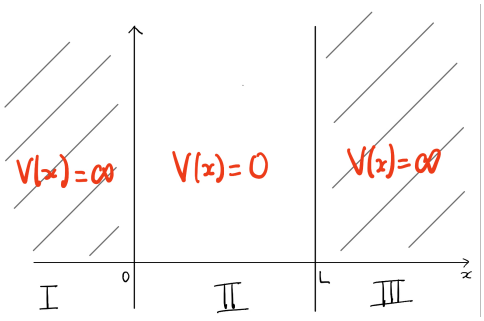

FIGURE 4.1. The potential $V(x)$ for a particle in a box.

Consider region 1: it is useful to first suppose that V is not infinite but equal to some $V_0 > E$. Now, the time-independent Schrödinger equation in

the X basis becomes

$$\frac{d^2\psi_1}{dx} - \frac{2m}{\hbar^2}(V_0 - E)\psi_1 = 0\,.$$

This is solved by

$$\psi_1(x) = Ae^{-\kappa x} + Be^{\kappa x}$$

where $\kappa = \sqrt{2m(V_0 - E)/\hbar^2}$. Since $Ae^{-\kappa x}$ blows up exponentially as $x \to -\infty$, we must set $A = 0$ to keep the solution square-integrable. Then, by letting $V_0 \to \infty$, we have that $\psi_1(x) = 0$ (since $x < 0$). We can apply a similar argument for region 3 and get that $\psi_3(x) = 0$. Therefore, unsurprisingly, the particle cannot be found outside the box. In region 2, we have $V = 0$ hence the solutions are those of a free particle,

$$\psi_2(x) = Ae^{ikx} + Be^{-ikx}, \qquad k = \sqrt{2mE/\hbar^2}\,.$$

We must also require that ψ_2 goes continuously into into its counterparts $\psi_1(x)$ and $\psi_3(x)$ as we cross regions. In other words, we require that

$$\psi_2(0) = 0 \implies A + B = 0 \implies \psi_2(x) = 2iA\sin(kx)$$

but also that

$$\psi_2(L) = 0 \implies \sin(kL) = 0 \implies k = \frac{n\pi}{L}$$

where $n = \pm 1, \pm 2, \ldots$ (we neglect $n = 0$ as it gives $\psi(x) = 0$ everywhere). Therefore, the position representation of the (normalised) energy eigenstates of a particle in a box are

$$\psi_n(x) = \begin{cases} \sqrt{\frac{2}{L}}\sin\left(\frac{\pi n x}{L}\right), & 0 < x < L \\ 0 \quad \text{otherwise} \end{cases} \,. \tag{4.4}$$

We can safely restrict n to $\mathbb{N}$, as negative integers lead to the same vectors with a minus sign (which does not affect the probability density). The first few eigenstates are shown in Fig. 4.2. The corresponding eigenvalues are

$$E_n = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2\pi^2}{2mL^2}n^2, \quad n = 1, 2, 3, \ldots \tag{4.5}$$

Surprisingly, we find that the energy is quantised! The variables encountered so far, X and P, had a continuous spectrum of eigenvalues, which coincided with the allowed values in classical mechanics. The same held true for the energy spectrum of a free particle. The particle in a box is the simplest example of a situation in which Schrödinger equation, combined with appropriate boundary conditions, leads to the quantisation of energy.

4.3 POTENTIAL BARRIER

In this section we will study the behaviour of a particle of mass $m > 0$ in the presence of a *rectangular potential barrier*. Concretely, we will solve the Schrödinger equation for the Hamiltonian

$$H = \frac{1}{2m}P^2 + V(X)\,, \tag{4.6}$$

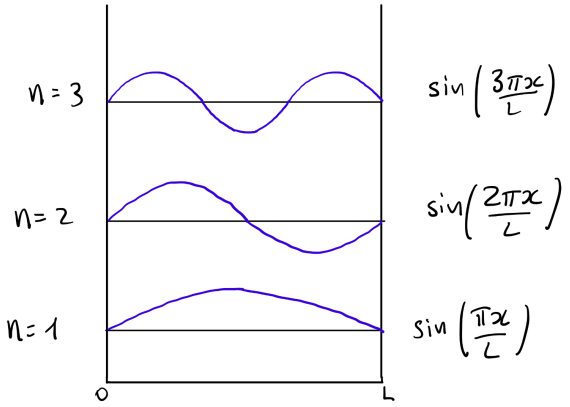

FIGURE 4.2. The first three energy eigenstates for a particle in a box (note that $\psi_n(x) = 0$ outside the box).

where

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

for some $V_0 > 0$.

The eigenvalue equation for the Hamiltonian (4.6) can be written as

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi(x) + V(x)\psi(x) = E\psi(x),$$

and rearranging the terms gives

$$\psi''(x) + \frac{2m}{\hbar^2}(E - V(x))\psi(x) = 0\,.$$

As we did for the particle in a box, it is convenient to split the space into three regions ($x \leq 0$, $0 < x < L$, $x \geq L$) and solve the Schrödinger equation for each one separately. In regions 1 ($x \leq 0$) and 3 ($x \geq L$), the eigenvalue equation reduces to that of a free particle, hence the general solutions are

$$\begin{aligned} \psi_1(x) =& Ae^{ikx} + Be^{-ikx}\,, \\ \psi_3(x) =& Fe^{ikx} + Ge^{-ikx}\,, \end{aligned}$$

where

$$k = \frac{\sqrt{2mE}}{\hbar}\,.$$

In region 2 ($0 < x < L$), the equation becomes

$$\psi_2''(x) + \frac{2m}{\hbar^2}(E - V_0)\psi_2(x) = 0\,, \tag{4.7}$$

which is solved by

$$\psi_2(x) = Ce^{ik'x} + De^{-ik'x}\,, \tag{4.8}$$

where

$$k' = \frac{\sqrt{2m(E - V_0)}}{\hbar}\,.$$

REMARK 4.1. To continue at this point, we will need to make the additional assumption that wave functions in quantum mechanics are *continuously differentiable*. By doing so, we are able to identify appropriate coefficients A, B, C, D, F, G which allow us to join the solutions ψ_1, ψ_2 and ψ_3, to indeed produce continuously differentiable overall solutions. ◇

We will consider two scenarios. In one, the particle's energy E is higher than the barrier's height V_0. In the other, it is lower (the special case of $E = V_0$ is left as an exercise). Throughout the calculation, we will assume that the particle is *incident from the left*. In other words, we remove the possibility of the particle approaching the barrier from the right, i.e. we set $G = 0$.

4.3.1 Case 1: $E > V_0$ (scattering)

For this scenario, classical mechanics predicts that the particle, incoming from the left with some kinetic energy E, slows down in region 2 (kinetic energy $= E - V_0$), then resumes its free motion to the right in region 3 with kinetic energy E. Importantly, the particle is *never reflected* by the barrier.

Let us see what quantum mechanics predicts instead. If $E > V_0$, then $k' \in \mathbb{R}$. The continuity of the wave function at $x = 0$ and $x = L$ imply

$$A + B = C + D\,, \tag{4.9a}$$
$$Ce^{ik'L} + De^{-ik'L} = Fe^{ikL}\,. \tag{4.9b}$$

Moreover, continuity of the derivative at $x = 0, L$ leads to

$$ik(A - B) = ik'(C - D)\,, \tag{4.10a}$$
$$ik'(Ce^{ik'L} - De^{-ik'L}) = ikFe^{ikL} \tag{4.10b}$$

We divide (4.10a) by ik, then add to (4.9a) to find

$$2A = C\left(1 + \frac{k'}{k}\right) + D\left(1 - \frac{k'}{k}\right) \tag{4.11}$$

Similarly, we divide (4.10b) by ik', then add and subtract to (4.9b) to find

$$2Ce^{ik'L} = Fe^{ikL}\left(1 + \frac{k}{k'}\right) \tag{4.12a}$$
$$2De^{-ik'L} = Fe^{ikL}\left(1 - \frac{k}{k'}\right) \tag{4.12b}$$

Combining (4.11), (4.12a) and (4.12b) leads, after a short calculation, to

$$\frac{A}{F}e^{-ikL} = \frac{4kk'\cos(k'L) - 2i\sin(k'L)(k'^2 + k^2)}{4kk'}\,. \tag{4.13}$$

DEFINITION 4.2. Consider a wave incident from the left, that is, $G = 0$, then the reflection and transmission coefficients are

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

PROPOSITION 4.3. *The sum of the reflection and transmission coefficients is* 1.

PROOF. This proof is left as an exercise. □

After rearranging (4.13) (and using the trig identity $\sin^2 + \cos^2 = 1$), we obtain the following formula for the transmission coefficient,

$$T = \left[1 + \frac{(k'^2 - k^2)^2 \sin^2(k'L)}{4k^2k'^2}\right]^{-1} \tag{4.14a}$$

$$= \left[1 + \sin^2(\sqrt{2m(E-V_0)}L/\hbar)\frac{V_0^2}{4E(E-V_0)}\right]^{-1}. \tag{4.14b}$$

The reflection coefficient is then

$$R = 1 - T = \left[1 + \frac{4E(E-V_0)}{V_0^2 \sin^2(\sqrt{2m(E-V_0)}L/\hbar)}\right]^{-1}.$$

We conclude that particle has non-zero probability of being scattered off of the potential barrier, despite having higher energy. The classical result of $R = 0$ is obtained when $E \gg V_0$, but also when $\sin(\sqrt{2m(E-V_0)}L/\hbar) = 0$, i.e. when the energy difference $E - V_0$ and the barrier width L satisfy $(E - V_0) = n^2\frac{\pi^2\hbar^2}{2mL^2}$, where $n \in \mathbb{Z}$.[8]

[8] Formally, you would need to consider these special cases separately.

4.3.2 Case 1: $E < V_0$ (tunnelling)

We now consider a particle with energy lower than the potential barrier. According to classical mechanics, the particle (incoming from the left) incident on the barrier should *always get reflected*. However, in quantum mechanics, there will be a non-zero probability of it 'tunnelling' through the barrier into region 3.

Since we assume that $E - V_0 < 0$, we have that

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

The solution of the eigenvalue equation for region 2 is then

$$\psi_2(x) = Ce^{-\kappa x} + De^{\kappa x}$$

The transmission coefficient can be obtained by substituting $k' = i\kappa$ into Eq. (4.14a), knowing that $\sin(ix) = i\sinh(x)$:

$$T = \left[1 + \frac{(k^2 + \kappa^2)^2}{4\kappa^2k^2}\sinh^2(\kappa L)\right]^{-1}$$

$$= \left[1 + \frac{V_0^2}{4E(V_0 - E)}\sinh^2(\frac{L}{\hbar}\sqrt{2m(V_0 - E)})\right]^{-1}.$$

The phenomenon for which a quantum particle can be transmitted through a potential barrier, despite not having sufficient energy, is called *quantum tunnelling*. Notice that the transmission coefficient T is lower for lower values of E or for higher L. For very wide ($L \gg 0$) or high ($V_0 \gg E$) barriers, the sinh term goes to ∞, hence T approaches 0.

4.4 HARMONIC OSCILLATOR

The goal of this section is to find the eigenvalues and the eigenvectors for the *Hamiltonian of the harmonic oscillator*, which is the operator defined by

$$H_{\text{osc}} = \frac{1}{2m}P^2 + \frac{m\omega^2}{2}X^2 = \frac{1}{2m}\left(P^2 + (m\omega X)^2\right);$$

here m and ω are positive numbers corresponding to the mass of the quantum particle and the frequency characterizing the potential $V(x) = m\omega^2 x^2/2$.

Using the postion-representation of the position and momentum operators, the time-independent Schrödinger equation (4.1) reads explicitly

$$-\frac{\hbar^2}{2m}\psi''(x) + \frac{m\omega^2 x^2}{2}\psi(x) = E\psi(x).$$

A rather lengthy (but completely standard) computation reveals two facts:

1. For square-integrable solutions $\psi(x)$ to exist, the numbers E on the right-hand-side are limited to a discrete set values, namely

   $$E_n = \hbar\omega\left(n + \frac{1}{2}\right), \qquad n \in \mathbb{N}_0.$$

   The set of numbers $\{E_n, n \in \mathbb{N}_0\}$ forms the (discrete) spectrum of eigenvalues of the oscillator Hamiltonian H_{osc}.

2. To each eigenvalue E_n corresponds an eigenvector (or eigenstate) $\psi_n(x) \in L^2(\mathbb{R})$, given (up to a constant) by a product of a Hermite polynomial and a Gaussian (cf. below).

Here, we will determine the eigenstates and eigenvalues of the oscillator Hamiltonian H_{osc} using *algebraic techniques* instead. Our strategy will be to rewrite the Hamiltonian in terms of other operators and to exploit their properties.

4.4.1 Ladder operators

DEFINITION 4.4. The *annihilation* and *creation operators* (also called *lowering* and *raising operators*), denoted by a and a^*, respectively, are given by

$$a = \frac{1}{\sqrt{2\hbar m\omega}}(m\omega X + \mathrm{i}P),$$
$$a^* = \frac{1}{\sqrt{2\hbar m\omega}}(m\omega X - \mathrm{i}P).$$

They are adjoints of each other[9] and together they are called *ladder operators* of the harmonic oscillator. ◇

[9] X and P are self-adjoint, and the adjoint turns i into $-$i.

PROPOSITION 4.5. *The ladder operators satisfy the commutation relation*

$$[a, a^*] = \mathbb{1}. \tag{4.15}$$

PROOF. Recall that $[X, P] = \mathrm{i}\hbar\mathbb{1}$. From this we find

$$\begin{aligned}[a, a^*] &= \frac{1}{2\hbar m\omega}[m\omega X + \mathrm{i}P, m\omega X - \mathrm{i}P] \\ &= \frac{1}{2\hbar m\omega}([m\omega X, -\mathrm{i}P] + [\mathrm{i}P, m\omega X]) \\ &= \frac{1}{\mathrm{i}\hbar}[X, P] = \mathbb{1}.\end{aligned}$$

□

PROPOSITION 4.6. *The* number operator

$$N = a^* a$$

is self-adjoint and has non-negative eigenvalues only.

PROOF. N is self-adjoint,

$$N^* = (a^* a)^* = a^*(a^*)^* = a^* a = N\,,$$

implying that its eigenvalues are real.

To confirm the non-negativity, we consider an eigenvector of N eigenvalue $\nu \in \mathbb{R}$, i.e. $N\,|\psi\rangle = \nu\,|\psi\rangle$, and calculate

$$\nu = \nu\langle\psi|\psi\rangle = \langle\psi|N\,|\psi\rangle = \langle\psi|N\psi\rangle = \langle\psi|a^* a\psi\rangle = \langle a\psi|a\psi\rangle \geq 0\,,$$

using that $|\psi\rangle$ is a unit vector and the last property of Prop. 1.25. □

PROPOSITION 4.7. *The Hamiltonian of the harmonic oscillator can be expressed in terms of the number operator N,*

$$H_{\mathrm{osc}} = \hbar\omega\left(a^* a + \frac{1}{2}\mathbb{1}\right) = \hbar\omega\left(N + \frac{1}{2}\mathbb{1}\right). \tag{4.16}$$

The oparator H_{osc} is self-adjoint and has positive eigenvalues.

PROOF. The second equality holds by definition of the number operator N. For the first equality we calculate, using Proposition 1.45 and (1.5),

$$\begin{aligned}a^* a &= \frac{1}{2\hbar m\omega}(m\omega X - \mathrm{i}P)(m\omega X + \mathrm{i}P) \\ &= \frac{1}{2\hbar m\omega}(P^2 + (m\omega X)^2 + [m\omega X, \mathrm{i}P]) \\ &= \frac{1}{2\hbar m\omega}(P^2 + (m\omega X)^2) - \frac{1}{2}\mathbb{1}\,,\end{aligned}$$

and solving for H_{osc}. The second statement follows from the fact that N has non-negative eigenvalues. □

4.4.2 Eigenvalues

REMARK 4.8. The identity (4.16) implies an equivalence between the eigenvectors and eigenvalues of the Hamiltonian H_{osc} and those of the number operator N:

$$N|\psi\rangle = \nu|\psi\rangle \quad \Longleftrightarrow \quad H_{\text{osc}}|\psi\rangle = \hbar\omega\left(\nu + \frac{1}{2}\right)|\psi\rangle.$$

Therefore it will be sufficient to study the eigenvalues and the eigenvectors of the number operator to find those of the harmonic oscillator. We already know that the eigenvalues of the operator N are non-negative. ◇

PROPOSITION 4.9. *The commutation relation of the creation- and annihilation operators with the number operator are given by*

$$[N, a] = -a \quad \textit{and} \quad [N, a^*] = a^*. \tag{4.17}$$

PROOF. This follows from an application of Proposition 1.45 together with (4.15):

$$\begin{aligned}[N, a] &= [a^*a, a] = a^*[a, a] + [a^*, a]a = -a,\\ [N, a^*] &= [a^*a, a^*] = a^*[a, a^*] + [a^*, a^*]a = a^*.\end{aligned}$$ □

PROPOSITION 4.10. *Suppose that $|\psi\rangle$ is an eigenvector of N with the eigenvalue ν. Then*

$$Na|\psi\rangle = (\nu - 1)a|\psi\rangle \quad \textit{and} \quad Na^*|\psi\rangle = (\nu + 1)a^*|\psi\rangle.$$

PROOF. Using the commutator identities (4.17), we find

$$\begin{aligned}Na|\psi\rangle &= (aN + [N, a])|\psi\rangle = (aN - a)|\psi\rangle = (\nu - 1)a|\psi\rangle,\\ Na^*|\psi\rangle &= (a^*N + [N, a^*])|\psi\rangle = (a^*N + a^*)|\psi\rangle = (\nu + 1)a^*|\psi\rangle.\end{aligned}$$ □

In other words, if $|\psi\rangle$ is an eigenstate of N with eigenvalue ν, then $a|\psi\rangle = |a\psi\rangle$ is either an eigenstate of N with eigenvalue $\nu - 1$, or the zero vector. Similarly for the vector $a^*|\psi\rangle$.

The next result shows that the eigenvalues ν of N are actually non-negative *integers*, and that a annihilates the eigenstate of N with lowest eigenvalue, i.e. $\nu = 0$.

THEOREM 4.11. *Suppose that $|\psi\rangle$ is an eigenvector for N with eigenvalue ν, i.e. $N|\psi\rangle = \nu|\psi\rangle$. Then ν is a non-negative integer $n \in \mathbb{N}_0$ and there exists an eigenvector $|\psi'\rangle = a^\nu|\psi\rangle$ of N with eigenvalue 0 which is annihilated by a, i.e. $a|\psi'\rangle = 0$.*

PROOF. Applying Proposition 4.10 repeatedly, we find

$$Na^k|\psi\rangle = (\nu - k)a^k|\psi\rangle, \quad k \in \mathbb{N}.$$

Yet the eigenvalues of N are non-negative. Hence there must exist $n \in \mathbb{N}_0$ such that $a^n |\psi\rangle \neq 0$ and $a^{n+1} |\psi\rangle = 0$; we set $|\psi'\rangle = a^n |\psi\rangle$. Since $a |\psi'\rangle = 0$, we have

$$0 = a^* a |\psi'\rangle = N |\psi'\rangle = N a^n |\psi\rangle = (\nu - n) a^n |\psi\rangle.$$

Therefore $|\psi'\rangle$ is an eigenvector of N with eigenvalue 0 and $\nu = n$. □

REMARK 4.12. The operator N is called the *number operator* because it counts the number of 'quanta' in the harmonic oscillator. As we see from Proposition 4.10, the annihilation operator a *decreases* the number of quanta by one while the creation operator a^* *increases* the number of quanta by one. This observation will be underlined by a change in notation introduced in the next section. ◇

4.4.3 Eigenvectors

In this section, we reserve the name $|n\rangle$, $n \in \mathbb{N}_0$, for the eigenvectors of N (hence of H_{osc} too). That is, $N |n\rangle = n |n\rangle$. These states can be constructed from the lowest energy eigenstate by repeated applications of a^*.

THEOREM 4.13. *Suppose that $|0\rangle$ is normalized and satisfies $a|0\rangle = 0$. Then the vectors*

$$|n\rangle = \frac{1}{\sqrt{n!}} (a^*)^n |0\rangle, \quad n \in \mathbb{N}_0, \tag{4.18}$$

satisfy for $n, m \in \mathbb{N}_0$ the relations

1. $a^* |n\rangle = \sqrt{n+1}\, |n+1\rangle$,
2. $N |n\rangle = n |n\rangle$,
3. $a |n+1\rangle = \sqrt{n+1}\, |n\rangle$,
4. *the vectors $|n\rangle$ are orthonormal:* $\langle m|n\rangle = \delta_{mn} = \begin{cases} 1 & if \quad n = m\,, \\ 0 & if \quad n \neq m\,. \end{cases}$

PROOF.

1. Follows directly from the definition of $|n+1\rangle$:

$$\sqrt{n+1}\, |n+1\rangle = \frac{1}{\sqrt{n!}} (a^*)^{n+1} |0\rangle = a^* |n\rangle.$$

2. Using $N a^* = a^* N + a^*$ repeatedly to move the operator N to the right, we find

$$\begin{aligned} N |n\rangle &= \frac{1}{\sqrt{n!}} N (a^*)^n |0\rangle = \frac{1}{\sqrt{n!}} a^* N (a^*)^{n-1} |0\rangle + |n\rangle \\ &= \frac{1}{\sqrt{n!}} (a^*)^2 N (a^*)^{n-2} |0\rangle + 2 |n\rangle = \ldots = n |n\rangle\,, \end{aligned}$$

finally using the fact that $N |0\rangle = a^* a |0\rangle = 0$.

3. Using 1) and 2), we calculate

$$a\,|n+1\rangle = \frac{1}{\sqrt{n+1}} aa^*\,|n\rangle = \frac{1}{\sqrt{n+1}}(N+\mathbb{1})\,|n\rangle = \sqrt{n+1}\;|n\rangle.$$

4. Eigenvectors to different eigenvalues are orthogonal (Theorem 1.29) thus we only need to check that $|n\rangle$ is normalized. We proceed by induction. First note that $|0\rangle$ is normalized. Suppose now that $|n\rangle$ is normalized. Then

$$\begin{aligned}(n+1)\langle n+1|n+1\rangle &= (a^*\,|n\rangle)^*\, a^*\,|n\rangle = (\langle n|a)\, a^*\,|n\rangle = \langle n|aa^*\,|n\rangle \\ &= \langle n|(N+\mathbb{1})\,|n\rangle = (n+1)\langle n|n\rangle\,. \end{aligned}$$ □

This is essentially as far as we can go using the algebraic methods based on the commutation relations for the ladder operators.

To complete the discussion of the harmonic oscillator, we need to prove that the assumption of the previous theorem—the existence of a vector $|0\rangle$ which is normalized and satisfies $a\,|0\rangle = 0$—is actually satisfied for the harmonic oscillator. For this purpose, we will work with the ladder operators a^* and a in the position representation, for which we know the action of the position and momentum operators. As a side benefit, we will obtain explicit expressions for the square-integrable functions associated with the vectors $|n\rangle$.

THEOREM 4.14. *The normalized square-integrable function (a Gaussian)*

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \exp\left(-\frac{m\omega}{2\hbar}x^2\right) \tag{4.19}$$

satisfies $a\psi_0(x) = 0$. All other functions φ_0 which satisfy this conditions are given by $\varphi_0(x) = \alpha\psi_0(x)$ for some $\alpha \in \mathbb{C}$.

PROOF. To simplify our proof, it is useful to hide the constants $\hbar$, m and ω inside a natural length scale; set

$$\ell = \sqrt{\frac{\hbar}{m\omega}}.$$

Then we rescale the position variable x to

$$\tilde{x} = \frac{x}{\ell} \quad \text{so that} \quad \frac{\mathrm{d}}{\mathrm{d}\tilde{x}} = \ell\frac{\mathrm{d}}{\mathrm{d}x}.$$

Therefore, for all (sufficiently nice) $|\psi\rangle \in L^2(\mathbb{R})$

$$(a\psi)(x) = \frac{1}{\sqrt{2}}\left(\frac{x}{\ell} + \mathrm{i}\frac{\ell}{\hbar}\left(-\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}x}\right)\right)\psi(x) = \frac{1}{\sqrt{2}}\left(\tilde{x} + \frac{\mathrm{d}}{\mathrm{d}\tilde{x}}\right)\psi(x).$$

The condition $a\psi_0 = 0$ can thus be written as

$$\frac{1}{\sqrt{2}}\left(\tilde{x} + \frac{\mathrm{d}}{\mathrm{d}\tilde{x}}\right)\psi_0(x) = 0.$$

The general solution[10] to this first-order ordinary differential equation is

$$\psi_0(x) = \alpha \mathrm{e}^{-\frac{1}{2}\tilde{x}^2}$$

with $\alpha \in \mathbb{C}$. The normalization condition

$$1 = \langle 0|0\rangle = \int_{-\infty}^{\infty} |\psi_0(x)|^2 \,\mathrm{d}x = \int_{-\infty}^{\infty} |\psi_0(x)|^2 \,\ell \,\mathrm{d}\tilde{x} = \sqrt{\pi}\ell\,|\alpha|^2$$

puts a constraint on the modulus of the parameter α, namely

$$|\alpha| = \frac{1}{\sqrt{\sqrt{\pi}\ell}} = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4},$$

finally resulting in

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \exp\left(-\frac{m\omega}{2\hbar}x^2\right).$$

All other normalized solutions differ from this one by a constant multiplicative factor with unit modulus only, that is, a phase factor $\mathrm{e}^{\mathrm{i}\phi}$, $\phi \in \mathbb{R}$. □

[10] This first-order differential equation can be solved using the separation of variables, for example.

Terminology & Notation. We call $\psi_0(x)$ given by (4.19) the *ground state* of the harmonic oscillator. It is the eigenvector with the smallest possible eigenvalue of the operator H_{osc}. The vectors $\psi_n(x)$ associated with $\psi_0(x)$ by (4.18) are the *excited states* of the harmonic oscillator. They can be obtained from the ground state by repeatedly acting with the creation operator a^* on it, thereby 'adding quanta'. ◇

Theorem 4.16. *The states $\psi_n(x) \sim |n\rangle, n \in \mathbb{N}_0$, are the only*[11] *eigenvectors of the number operator N and, a fortiori, the Hamiltonian H_{osc}. The excited states are given by the square-integrable functions*

$$\psi_n(x) = \frac{1}{\sqrt{2^n n!}} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right)\psi_0(x),$$

where H_n are the Hermite polynomials

$$H_n(x) = (-1)^n \mathrm{e}^{x^2} \frac{\mathrm{d}^n}{\mathrm{d}x^n} \mathrm{e}^{-x^2},$$

i.e. $H_0(x) = 1$, $H_1(x) = 2x$, $H_2(x) = 4x^2 - 2$, etc.

[11] Of course we mean uniqueness up to a constant multiplicative factor.

Proof. In the previous Theorem 4.14, we already established that the ground state $\psi_0(x)$ is unique. The uniqueness of the excited states $\psi_n(x)$ follows from the fact that it is connected to the ground state by (4.18).

The second part of the proof will be omitted. □

Remark 4.17. The set of eigenstates $\{|n\rangle\}_{n\in\mathbb{N}_0}$ of the number operator N (as well as the oscillator Hamiltonian H_{osc}) form an orthonormal basis, so we have a corresponding resolution of the identity,

$$\sum_{n=0}^{\infty} |n\rangle\langle n| = \mathbb{1}.$$

◇

Let us summarize the results of this chapter: We have found that, upon introducing the creation and annihilation operators a^* and a, the Hamiltonian of the harmonic oscillator can be expressed in terms of the number operator $N = a^*a$. The commutation relations of these three operators were sufficient to determine the eigenvalues the Hamiltonian. In this way, we confirmed that the Hamiltonian $H_{\text{osc}} = \hbar\omega(N + 1/2)$ of the harmonic oscillator has a discrete spectrum of eigenvalues

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right), \quad n \in \mathbb{N}_0\,,$$

while its eigenvectors $\psi_n(x)$ are given (up to a constant) by a product of a Hermite polynomial and a Gaussian.

5 *Angular momentum*

In this section, we will discuss angular momentum in quantum mechanics. In analogy with classical mechanics, *orbital* angular momentum describes rotational motion. We will also introduce *spin* angular momentum, an intrinsic property of elementary particles that has no classical counterpart.

5.1 DEFINITION AND THE EIGENVALUES

We consider a particle moving in three-dimensional space. Denote by $\Psi(x,y,z) \in L^2(\mathbb{R}^3)$ the wave function of the particle in position representation. We will use x, y, z instead of $1, 2, 3$ to denote the axes (as it was done in Sec. 2.3). The position, linear and angular momentum operators will be denoted by bold-face letters: $\mathbf{X} = (X, Y, Z)$, $\mathbf{P} = (P_x, P_y, P_z)$ and $\mathbf{L} = (L_x, L_y, L_z)$, respectively.

DEFINITION 5.1. The orbital angular momentum operator $L = (L_x, L_y, L_z)$ is defined by

$$\begin{aligned}(L_x, L_y, L_z) &= \mathbf{L} \\ &:= \mathbf{X} \times \mathbf{P} \\ &= (YP_z - ZP_y, ZP_x - XP_z, XP_y - YP_x)\,.\end{aligned}$$

That is,

$$L_x = YP_z - ZP_y\,, \quad L_y = ZP_x - XP_z\,, \quad L_z = XP_y - YP_x\,. \qquad \diamond$$

Note that L_y and L_z can be found by cyclic permutations $x \to y \to z \to x$ from L_x.

In position representation, L_z is expressed as

$$\begin{aligned}L_z &= XP_y - YP_x \\ &= x\left(-\mathrm{i}\hbar\frac{\partial}{\partial y}\right) - y\left(-\mathrm{i}\hbar\frac{\partial}{\partial x}\right) \\ &= -\mathrm{i}\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)\,.\end{aligned}$$

Its eigenvalues can be readily found using spherical polar coordinates (r, θ, ϕ):

$$\begin{aligned}x &= r\sin\theta\cos\phi\,, \\ y &= r\sin\theta\sin\phi\,, \\ z &= r\cos\theta,\,.\end{aligned}$$

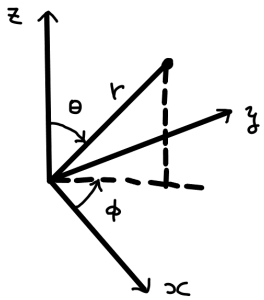

FIGURE 5.1. Spherical polar coordinates

By the chain rule

$$\begin{aligned}\frac{\partial}{\partial\phi}\Psi &= \left(\frac{\partial x}{\partial\phi}\frac{\partial}{\partial x} + \frac{\partial y}{\partial\phi}\frac{\partial}{\partial y} + \frac{\partial z}{\partial\phi}\frac{\partial}{\partial z}\right)\Psi \\ &= \left(-r\sin\theta\sin\phi\frac{\partial}{\partial x} + r\sin\theta\cos\phi\frac{\partial}{\partial y}\right)\Psi \\ &= \left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)\Psi\,.\end{aligned}$$

By comparing this equation with Eq. (5.1) above, we find

$$L_z = -\mathrm{i}\hbar\frac{\partial}{\partial\phi}\,. \tag{5.1}$$

More correctly, this is written as

$$(L_z\Psi)(r,\theta,\phi) = -\mathrm{i}\hbar\frac{\partial\Psi}{\partial\phi}(r,\theta,\phi)\,.$$

The eigenvalue equation reads

$$L_z\Psi = -\mathrm{i}\hbar\frac{\partial\Psi}{\partial\phi} = \lambda\Psi\,,$$

That is,

$$\frac{\partial\Psi}{\partial\phi} = \frac{\mathrm{i}\lambda}{\hbar}\Psi\,.$$

Thus, an eigenfunction is of the form

$$\Psi(r,\theta,\phi) = f(r,\theta)\exp\left(\frac{\mathrm{i}\lambda}{\hbar}\phi\right)\,. \tag{5.2}$$

Since the angle ϕ is the azimuthal angle about the z-axis, the wave function Ψ must satisfy

$$\Psi(r,\theta,\phi+2\pi) = \Psi(r,\theta,\phi)\,.$$

By applying this condition to the eigenfunction of L_z in Eq. (5.2) we find

$$\exp\left(\frac{\mathrm{i}\lambda}{\hbar}\phi + \frac{2\pi\mathrm{i}\lambda}{\hbar}\right) = \exp\left(\frac{\mathrm{i}\lambda}{\hbar}\phi\right)\,.$$

Thus,

$$\frac{\lambda}{\hbar} = m \in \mathbb{Z}$$

i.e.

$$\lambda = m\hbar\,, \quad m \in \mathbb{Z}\,.$$

Thus, *the eigenvalues of L_z are integer multiples of $\hbar$.* That is, unlike linear momentum, angular momentum of a quantum particle is quantised!

The corresponding eigenfunctions can be found by substituting $\lambda = m\hbar$ into (5.2) as

$$\Psi(r, \theta\, \phi) = f(r, \theta) e^{\mathrm{i}m\phi}.$$

By symmetry, the eigenvalues of L_x and L_y must also be integer multiples of $\hbar$. However, if a state is an eigenstate of both L_x and L_z, say, then it must be an eigenstate of all L_i, $i = x, y, z$, with eigenvalue 0 [left as an exercise].

5.2 COMMUTATORS OF ANGULAR MOMENTUM OPERATORS

In analogy with our treatment of the harmonic oscillator, we shall see that the action of the angular momentum operators on their eigenstates can be derived from their commutation relations. We will use the known commutator relations satisfied by the three-dimensional position and momentum operators shown in Sec. 2.3.

REMARK 5.2. The operators L_x, L_y and L_z are self-adjoint: $L_z^* = (XP_y - YP_x)^* = P_yX - P_xY = XP_y - YP_x = L_z$. ◇

THEOREM 5.3. $[L_y, L_z] = \mathrm{i}\hbar L_x$, $[L_z, L_x] = \mathrm{i}\hbar L_y$, $[L_x, L_y] = \mathrm{i}\hbar L_z$.

PROOF. We find

$$\begin{aligned}[L_y, L_z] &= [ZP_x - XP_z, XP_y - YP_x] \\ &= [ZP_x, XP_y] - [ZP_x, YP_x] - [XP_z, XP_y] + [XP_z, YP_x].\end{aligned}$$

Now, $ZP_xYP_x = YP_xZP_x$ and $XP_zXP_y = XP_yXP_z$. Hence

$$[L_y, L_z] = [ZP_x, XP_y] + [XP_z, YP_x].$$

Since Z and P_y commute with all operators in the first commutator and that P_z and Y commute with all opertors in the second commutator, we can treat them as if they were numbers. Hence they can be moved out of the commutator:

$$\begin{aligned}[L_y, L_z] &= ZP_y[P_x, X] + P_zY[X, P_x] \\ &= -\mathrm{i}\hbar ZP_y + \mathrm{i}\hbar YP_z \\ &= \mathrm{i}\hbar(YP_z - ZP_y) \\ &= \mathrm{i}\hbar L_x.\end{aligned}$$

The other commutators can be found in exactly the same way (or by cyclic permutations). □

We want to study the eigenstates of operators satisfying the commutation relations given in Theorem 5.3. It turns out that there are other observables in quantum mechanics that satisfy the same commutation relations. For this reason, we use the notations $J_x, \dots$ instead of $L_x, \dots$ below. Thus,

> $\mathbf{J} = (J_x, J_y, J_z)$ is a self-adjoint operator satisfying $[J_y, J_z] = \mathrm{i}\hbar J_x$, $[J_z, J_x] = \mathrm{i}\hbar J_y$ and $[J_x, J_y] = \mathrm{i}\hbar J_z$.

The operator $\mathbf{J}$ has dimensions of $\hbar$ because, if the dimensions of X is denoted by $[X]$, then their commutators imply $[\mathbf{J}]^2 = [\hbar][\mathbf{J}]$ and $[\mathbf{J}] = [\hbar]$.

DEFINITION 5.4. Define $\mathbf{J}^2 := J_x^2 + J_y^2 + J_z^2$. ◇

THEOREM 5.5. *Suppose that the self-adjoint operators J_x, J_y and J_z satisfy $[J_y, J_z] = \mathrm{i}\hbar J_x$, $[J_z, J_x] = \mathrm{i}\hbar J_y$ and and $[J_x, J_y] = \mathrm{i}\hbar J_z$. $[\mathbf{J}^2, J_x] = [\mathbf{J}^2, J_y] = [\mathbf{J}^2, J_z] = 0$. That is, $\mathbf{J}^2$ commutes with J_x, J_y and J_z.*

PROOF. Proof is left as an exercise. □

We notice that the eigenvalues of $\mathbf{J}^2$ are non-negative.

PROPOSITION 5.6. *The eigenvalues of $\mathbf{J}^2$ are non-negative.*

PROOF. Let $\mathbf{J}^2|\psi\rangle = \lambda|\psi\rangle$ where $\langle\psi|\psi\rangle = 1$. Then

$$\begin{aligned}\lambda &= \langle\psi|\mathbf{J}^2|\psi\rangle \\ &= \langle\psi|J_x^2|\psi\rangle + \langle\psi|J_y^2|\psi\rangle + \langle\psi|J_z^2|\psi\rangle \\ &= \langle J_x\psi|J_x\psi\rangle + \langle J_y\psi|J_y\psi\rangle + \langle J_z\psi|J_z\psi\rangle \\ &= \|J_x|\psi\rangle\|^2 + \|J_y|\psi\rangle\|^2 + \|J_z|\psi\rangle\|^2 \\ &\geq 0\,,\end{aligned}$$

as required. □

REMARK 5.7. Any non-negative number λ with the dimensions of $\hbar^2$ can be expressed as $\lambda = j(j+1)\hbar^2$ with $j \geq 0$. (Given $\lambda \geq 0$, solve the quadratic equation for j and let $j = (\sqrt{1 + 4\lambda/\hbar^2} - 1)/2$.) This means that we are free to write the eigenvalues of $\mathbf{J}^2$ as $j(j+1)\hbar^2$. ◇

REMARK 5.8. If self-adjoint operators A and B acting on a Hilbert space $\mathcal{H}$ commute, i.e, if $[A, B] = 0$, then there is a basis of $\mathcal{H}$ such that all basis states are eigenstates of A *and* B. (We will prove this result in a future lecture.) ◇

This fact allows us to consider a state $|j, m\rangle$ which is an eigenstate of the two operators $\mathbf{J}^2$ and J_z satisfying

$$\mathbf{J}^2|j,m\rangle = j(j+1)\hbar^2|j,m\rangle\,, \quad J_z|j,m\rangle = m\hbar|j,m\rangle\,,$$

where $j, m \in \mathbb{R}$ and $j \geq 0$.[12]

[12] We are not assuming that $J_z = L_z$, so at the moment we can only say that $m \in \mathbb{R}$, which follows from J_z being self-adjoint.

Now,

$$\begin{aligned} j(j+1)\hbar^2 &= \langle j,m|\mathbf{J}^2|j,m\rangle \\ &= \|J_x|j,m\rangle\|^2 + \|J_y|j,m\rangle\|^2 + \|J_z|j,m\rangle\|^2 \\ &= \|J_x|j,m\rangle\|^2 + \|J_y|j,m\rangle\|^2 + m^2\hbar^2\,. \end{aligned}$$

Hence

$$|m| \leq \sqrt{j(j+1)} < j+1\,,\ \text{(classically } |J_z| \leq \sqrt{\mathbf{J}^2}\text{)}$$

and

$$-(j+1) < m < j+1\,. \tag{5.3}$$

That is, from the commutation relations alone, we are able to show that the eigenvalues of $\mathbf{J}^2$ put a constraint to the eigenvalues of J_z.

But we can do more. In the following, we will show that j can only take integer or half-odd-integer values, $j = 0, 1/2, 1, 3/2, 2, \ldots$, and that m can only go from $-j$ to j in integer steps, $m = -j, -j+1, \ldots, j-1, j$ (in agreement with Eq. (5.3)).

To show this, we introduce the operators $J_\pm$.

DEFINITION 5.9. $J_\pm := J_x \pm \mathrm{i}J_y$. ◇

Clearly, they are the adjoints of each other,

$$J_\pm^* = (J_x \pm \mathrm{i}J_y)^* = J_x \mp \mathrm{i}J_y = J_\mp\,.$$

and they obey the following commutator relations (proof left as an exercise),

$$[J_z, J_\pm] = \pm\hbar J_\pm, \quad [J_+, J_-] = 2\hbar J_z\,, \quad [\mathbf{J}^2, J_\pm] = 0\,.$$

The result below provides the reason we introduced the operators $J_\pm$.

PROPOSITION 5.10. $J_z J_\pm|j,m\rangle = (m \pm 1)\hbar J_\pm|j,m\rangle$.

PROOF. By definition, $J_z|j,m\rangle = m\hbar|j,m\rangle$. Then

$$\begin{aligned} J_z J_\pm|j,m\rangle &= (J_z J_\pm - J_\pm J_z)|j,m\rangle + J_\pm J_z|j,m\rangle \\ &= [J_z, J_\pm]|j,m\rangle + J_\pm J_z|j,m\rangle \\ &= \pm\hbar J_\pm|j,m\rangle + m\hbar J_\pm|j,m\rangle \\ &= (m \pm 1)\hbar J_\pm|j,m\rangle, \end{aligned}$$

as required. □

In other words, the operator J_+ (J_-) raises (lowers) the eigenvalue of J_z by one 'quantum' $\hbar$ or annihilates the state (i.e. sends $|j,m\rangle$ to the zero vector). Notice the close analogy with the raising (lowering) operator a^* (a) for the harmonic oscillator (Sec. 4.4) which increases (decreases) the energy eigenvalue.

We also have that the operators $J_\pm$ do *not* affect the eigenvalue of $\mathbf{J}^2$, *provided that* $J_\pm\,|j,m\rangle \neq 0$,

$$\mathbf{J}^2 J_\pm|j,m\rangle = J_\pm\mathbf{J}^2|j,m\rangle = j(j+1)\hbar^2 J_\pm|j,m\rangle\,.$$

Therefore, we may write $J_\pm|j,m\rangle = C_\pm|j,m\pm1\rangle$, i.e. j remains the same, while m is increased/decreased by 1, where $C_\pm$ is a normalisation constant such that $\langle j,m\pm1|j,m\pm1\rangle = 1$ provided that $J_\pm|j,m\rangle \neq 0$. We can let

$$|j,m\pm1\rangle = \frac{J_\pm|j,m\rangle}{\|J_\pm|j,m\rangle\|}\,, \quad C_\pm = \|J_\pm|j,m\rangle\|\,.$$

Starting from $|j,m\rangle$, we can apply $J_\pm$ and normalise the resulting state to construct a chain of normalised eigenstates of J_z, which are all eigenstates of $\mathbf{J}^2$ with same eigenvalue $j(j+1)\hbar^2$:

$$\cdots \xleftarrow{J_-} |j,m-2\rangle \xleftarrow{J_-} |j,m-1\rangle \xleftarrow{J_-} |j,m\rangle \xrightarrow{J_+} |j,m+1\rangle \xrightarrow{J_+} |j,m+2\rangle \xrightarrow{J_+} \cdots$$

Recall that (5.3) restricts the values of m (for given j), hence this process cannot go on forever. The sequence must therefore look like

$$0 \xleftarrow{J_-} |j,m^{(-)}\rangle \xleftarrow{J_-} \cdots \xleftarrow{J_-} |j,m-1\rangle \xleftarrow{J_-} |j,m\rangle \xrightarrow{J_+} |j,m+1\rangle \xrightarrow{J_+} \cdots \xrightarrow{J_+} |j,m^{(+)}\rangle \xrightarrow{J_+} 0\,.$$

In other words, there must be some $m^{(\pm)}$, where $-(j+1) < m^{(-)} \leq m^{(+)} < j+1$, and such that $J_-|j,m^{(-)}\rangle = 0$ and $J_+|j,m^{(+)}\rangle = 0$. To find these values, the following identity is useful (proof left as an exercise).

LEMMA 5.11. $J_\mp J_\pm = \mathbf{J}^2 - J_z^2 \mp \hbar J_z$.

REMARK 5.12. Note that the classical counterpart is $j_\mp j_\pm = (j_x \mp \mathrm{i}j_y)(j_x \pm \mathrm{i}j_y) = j_x^2 + j_y^2 = \mathbf{j}^2 - j_z^2$ (which is obtained from the above identity by setting $\hbar \to 0$). ◇

Now,

$$\begin{aligned} J_-J_+|j,m\rangle &= (\mathbf{J}^2 - J_z^2 - \hbar J_z)|j,m\rangle \\ &= [j(j+1)\hbar^2 - m^2\hbar^2 - m\hbar^2]|j,m\rangle \\ &= [j(j+1) - m(m+1)]\hbar^2|j,m\rangle \\ &= (j-m)(j+m+1)\hbar^2|j,m\rangle\,. \end{aligned} \tag{5.4}$$

We require that $J_+|j,m^{(+)}\rangle = 0$. Since $j + m^{(+)} + 1 > 0$, we must have $m^{(+)} = j$. Similarly, we can show that the requirement $J_-|j,m^{(-)}\rangle = 0$ leads to $m^{(-)} = -j$. (Exercise)

Thus, we must have

$$0 \xleftarrow{J_-} |j,-j\rangle \xleftarrow{J_-} \cdots \xleftarrow{J_-} |j,m-1\rangle \xleftarrow{J_-} |j,m\rangle \xrightarrow{J_+} |j,m+1\rangle \xrightarrow{J_+} \cdots \xrightarrow{J_+} |j,j\rangle \xrightarrow{J_+} 0\,.$$

The maximum and minimum eigenvalues of J_z for this sequence are therefore j and $-j$, respectively. Moreover, the difference $j-(-j) = 2j$ must be a integer. Therefore, we can conclude that

> The possible values of j are $j = 0, \frac{1}{2}, 1, \frac{3}{2}, \cdots$, and $m = -j, -j+1, \ldots j-1, j$.

It remains to find the the normalisation factor $C_\pm$, after which we can summarise our results. From Eq. (5.4) we find

$$\langle j,m|J_-J_+|j,m\rangle = (j-m)(j+m+1)\hbar^2\,,$$

because $\langle j,m|j,m\rangle = 1$. Since

$$\langle j,m|J_-J_+|j,m\rangle = \langle j,m|J_+^*J_+|j,m\rangle = \|J_+|j,m\rangle\|^2\,,$$

we have

$$\|J_+|j,m\rangle\| = \sqrt{(j-m)(j+m+1)}\,\hbar\,.$$

Thus, if we write $J_+|j,m\rangle = C_+|j,m{+}1\rangle$, we can choose $C_+ = \sqrt{(j-m)(j+m+1)}\,\hbar$. Then

$$J_+|j,m\rangle = \sqrt{(j-m)(j+m+1)}\,\hbar|j,m+1\rangle\,.$$

We can apply a similar argument for C_- and show that

$$J_-|j,m\rangle = \sqrt{(j+m)(j-m+1)}\,\hbar|j,m-1\rangle\,.$$

The results we have derived can be summarised as follows.

THEOREM 5.13. *Suppose J_x, J_y and J_z are self-adjoint operators satisfying $[J_y,J_z] = \mathrm{i}\hbar J_x$, $[J_z,J_x] = \mathrm{i}\hbar J_y$ and $[J_x,J_y] = \mathrm{i}\hbar J_z$. Define $J_\pm := J_x \pm \mathrm{i}J_y$. Then:*

1. *The possible eigenvalues of $\mathbf{J}^2$ are $j(j+1)\hbar^2$, where $j = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots$;*

2. *The eigenstates of J_z that are eigenstates of $\mathbf{J}^2$ with eigenvalue $j(j{+}1)\hbar^2$ occur in a multiplet of $2j+1$ normalised states, $|j,m\rangle$, $m = -j, -j+1, \ldots, j-1, j$, satisfying*

$$\begin{aligned}
\mathbf{J}^2|j,m\rangle &= j(j+1)\hbar^2|j,m\rangle,\\
J_z|j,m\rangle &= m\hbar|j,m\rangle,\\
J_+|j,m\rangle &= \sqrt{(j-m)(j+m+1)}\hbar|j,m+1\rangle,\\
J_-|j,m\rangle &= \sqrt{(j+m)(j-m+1)}\hbar|j,m-1\rangle,\\
J_+|j,j\rangle &= 0,\\
J_-|j,-j\rangle &= 0.
\end{aligned}$$

Therefore, j can be $1/2, 3/2, \ldots$ as well as $0, 1, 2, \ldots$. As a result, the eigenvalues of J_z can be half-odd-integer multiples of $\hbar$ as well as integer multiples of $\hbar$. For orbital angular momentum, i.e. $J_i = L_i$, these results imply that the number j must be an integer, since we proved that the eigenvalues of L_z are integer multiples of $\hbar$. The half-odd-integer cases occur, for example, for the *spin* of the electron, for which $j = 1/2$ and $m = -1/2, 1/2$ (see Sec. 5.4).

5.3 THE SPHERICAL HARMONICS

The goal of this section is to construct the eigenstates of $\mathbf{L}^2$ and L_z, $|\ell, m\rangle$, ($|j, m\rangle$ in Theorem 5.13 with $j = \ell$) as functions of θ and ϕ. They are called the *spherical harmonics* and denoted by $Y_\ell^m(\theta, \phi)$ (rather than by the usual Ψ).

We have seen already that, in coordinate basis,

$$L_z = -\mathrm{i}\hbar \frac{\partial}{\partial \phi},$$

if the wave function is expressed in spherical polar coordinates, $(x, y, z) = (r\sin\theta\cos\phi, r\sin\theta\sin\phi, \cos\theta)$. Similarly [proofs left as exercises],

$$\begin{aligned} L_\pm &:= L_x \pm \mathrm{i}L_y \\ &= \hbar \mathrm{e}^{\pm\mathrm{i}\phi}\left(\pm\frac{\partial}{\partial\theta} + \mathrm{i}\cot\theta\frac{\partial}{\partial\phi}\right), \\ \mathbf{L}^2 &:= L_x^2 + L_y^2 + L_z^2 \\ &= -\hbar^2\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right), \end{aligned}$$

where the differential operators act on all factors to the right.

The angular-momentum operators in spherical polar coordinates do not involve r, so the r-dependence of the wave function is not relevant to angular momentum (this justifies why Y_ℓ^m does not depend on r). We can thus write

$$L_z Y_\ell^m(\theta,\phi) = -\mathrm{i}\hbar\frac{\partial}{\partial\phi}Y_\ell^m(\theta,\phi) = m\hbar Y_\ell^m(\theta,\phi), \tag{5.5}$$

$$\mathbf{L}^2 Y_\ell^m(\theta,\phi) = \ell(\ell+1)\hbar^2 Y_\ell^m(\theta,\phi), \tag{5.6}$$

$$L_+ Y_\ell^m(\theta,\phi) = \sqrt{(\ell-m)(\ell+m+1)}\,\hbar\, Y_\ell^{m+1}(\theta,\phi), \tag{5.7}$$

$$L_- Y_\ell^{-\ell}(\theta,\phi) = 0. \tag{5.8}$$

From our calculations of Sec. 5.1 and Theorem 5.13, we know that

$$Y_\ell^m(\theta,\phi) = f_\ell^m(\theta)\mathrm{e}^{\mathrm{i}m\phi}, \quad -\ell \le m \le \ell,$$

where the *quantum numbers* ℓ and m take integer values. It thus remains to find $f_\ell^m(\theta)$. We start with Eq. (5.8)

$$\hbar\mathrm{e}^{-\mathrm{i}\phi}\left(-\frac{\partial}{\partial\theta} + \mathrm{i}\cot\theta\frac{\partial}{\partial\phi}\right)Y_\ell^{-\ell}(\theta,\phi) = 0.$$

Since we defined $Y_\ell^{-\ell}(\theta,\phi) = f_\ell^{-\ell}(\theta)\mathrm{e}^{-\mathrm{i}\ell\phi}$, we have

$$\left(-\frac{\mathrm{d}}{\mathrm{d}\theta} + \ell\cot\theta\right)f_\ell^{-\ell}(\theta) = 0,$$

which can be solved as

$$f_\ell^{-\ell}(\theta) = A(\sin\theta)^\ell.$$

Thus, $Y_\ell^{-\ell}(\theta,\phi) = A(\sin\theta)^\ell\mathrm{e}^{-\mathrm{i}\ell\phi}$.

We determine A via the normalisation condition

$$\begin{aligned} 1 &= \int_0^{2\pi} \mathrm{d}\phi \int_0^{\pi} \mathrm{d}\theta \, \sin\theta |Y_\ell^{-\ell}(\theta,\phi)|^2 \\ &= 2\pi |A|^2 \int_0^{\pi} \mathrm{d}\theta \, (\sin\theta)^{2\ell+1} \\ &= 2\pi |A|^2 \cdot \frac{2(2^\ell \ell!)^2}{(2\ell+1)!}. \qquad \text{(Exercise).} \end{aligned}$$

Notice we are integrating over the surface of the unit sphere (since we do not care about r), and the surface element is $\sin\theta \mathrm{d}\theta \mathrm{d}\phi$. We find that

$$A = \left[\frac{(2\ell+1)!}{4\pi}\right]^{1/2} \frac{1}{2^\ell \ell!},$$

therefore

$$f_\ell^{-\ell}(\theta) = \left[\frac{(2\ell+1)!}{4\pi}\right]^{1/2} \frac{1}{2^\ell \ell!} (\sin\theta)^\ell. \tag{5.9}$$

To find the spherical harmonics $Y_\ell^m(\theta,\phi)$ with higher m's, we use Eq. (5.7)

$$L_+ Y_\ell^m(\theta,\phi) = \sqrt{(\ell-m)(\ell+m+1)}\, Y_\ell^{m+1} \hbar(\theta,\phi),$$

i.e. we apply L_+ to raise the value of m. This gives $Y_\ell^{m+1}(\theta,\phi)$ in terms of $Y_\ell^m(\theta,\phi)$:

$$Y_\ell^{m+1}(\theta,\phi) = \frac{\mathrm{e}^{\mathrm{i}\phi}}{\sqrt{(\ell-m)(\ell+m+1)}} \left(\frac{\partial}{\partial\theta} + \mathrm{i}\cot\theta \frac{\partial}{\partial\phi}\right) Y_\ell^m(\theta,\phi).$$

Writing $Y_\ell^m(\theta,\phi) = f_\ell^m(\theta)\mathrm{e}^{\mathrm{i}m\phi}$, we have

$$f_\ell^{m+1}(\theta) = \frac{1}{\sqrt{(\ell-m)(\ell+m+1)}} \left(\frac{\mathrm{d}}{\mathrm{d}\theta} - m\cot\theta\right) f_\ell^m(\theta). \tag{5.10}$$

Starting from $f_\ell^{-\ell}(\theta)$ given above, we can use Eq. (5.10) repeatedly to obtain $f_\ell^m(\theta)$, hence $Y_\ell^m(\theta,\phi)$, for all $m = -\ell, -\ell+1, \ldots, \ell-1, \ell$.

EXAMPLE 5.14. We now compute the explicit formulae for the spherical harmonics for $\ell = 0, 1$.

- For $\ell = 0$, we have only $m = 0$ because $-\ell \le m \le \ell$. We have by (5.9)

$$f_0^0(\theta) = \left[\frac{1!}{4\pi}\right]^{1/2} \frac{1}{2^0 0!} (\sin\theta)^0 = \frac{1}{\sqrt{4\pi}}.$$

  Hence

$$Y_0^0(\theta,\phi) = \frac{1}{\sqrt{4\pi}} \mathrm{e}^{\mathrm{i}0\phi} = \frac{1}{\sqrt{4\pi}}.$$

- For $\ell = 1$, Eq. (5.9) gives

$$f_1^{-1}(\theta) = \left[\frac{3!}{4\pi}\right]^{1/2} \frac{1}{2^1 1!} \sin\theta = \sqrt{\frac{3}{8\pi}} \sin\theta.$$

Then by (5.10) with $m = -1$ and $\ell = 1$ we find

$$f_1^0(\theta) = \frac{1}{\sqrt{2}}\left(\frac{\mathrm{d}}{\mathrm{d}\theta} + \cot\theta\right)\sqrt{\frac{3}{8\pi}}\sin\theta$$
$$= \sqrt{\frac{3}{4\pi}}\cos\theta\,.$$

Then, by (5.10) with $m = 0$ and $\ell = 1$ we find

$$f_1^1(\theta) = \frac{1}{\sqrt{2}}\frac{\mathrm{d}}{\mathrm{d}\theta}\sqrt{\frac{3}{4\pi}}\cos\theta$$
$$= -\sqrt{\frac{3}{8\pi}}\sin\theta\,.$$

Then,

$$Y_1^{-1}(\theta,\phi) = \sqrt{\frac{3}{8\pi}}\sin\theta\,\mathrm{e}^{-\mathrm{i}\phi} = \sqrt{\frac{3}{8\pi}}\frac{x-\mathrm{i}y}{r}\,,$$
$$Y_1^{0}(\theta,\phi) = \sqrt{\frac{3}{4\pi}}\cos\theta = \sqrt{\frac{3}{4\pi}}\frac{z}{r}\,,$$
$$Y_1^{1}(\theta,\phi) = -\sqrt{\frac{3}{8\pi}}\sin\theta\,\mathrm{e}^{\mathrm{i}\phi} = -\sqrt{\frac{3}{8\pi}}\frac{x+\mathrm{i}y}{r}\,,$$

since $(x, y, z) = (r\sin\theta\cos\phi, r\sin\theta\sin\phi, r\cos\theta)$. ◇

5.4 SPIN ANGULAR MOMENTUM

The case with $j = 1/2$ in Theorem 5.13 is not realised by the orbital angular momentum $\mathbf{X}\times\mathbf{P}$. It is realised by the '*spin angular momentum*', an intrinsic angular momentum of elementary particles.

TERMINOLOGY & NOTATION. We will denote spin angular momentum with $\mathbf{S} = (S_x, S_y, S_z)$; that is, we set $J = S$, $j = s$, $m = m_s$ in the results obtained in the previous sections. ◇

To describe the spin degree of freedom of the electron, we set $s = 1/2$, hence have $m_s = -1/2, 1/2$. Therefore, there are two states $|\frac{1}{2}, \pm\frac{1}{2}\rangle$. These satisfy

$$\mathbf{S}^2|\tfrac{1}{2},\pm\tfrac{1}{2}\rangle = \tfrac{3}{4}\hbar^2|\tfrac{1}{2},\pm\tfrac{1}{2}\rangle\,,$$
$$S_z|\tfrac{1}{2},\pm\tfrac{1}{2}\rangle = \pm\tfrac{1}{2}\hbar|\tfrac{1}{2},\pm\tfrac{1}{2}\rangle\,,$$
$$S_+|\tfrac{1}{2},-\tfrac{1}{2}\rangle = \hbar|\tfrac{1}{2},\tfrac{1}{2}\rangle\,,$$
$$S_+|\tfrac{1}{2},\tfrac{1}{2}\rangle = 0\,,$$
$$S_-|\tfrac{1}{2},\tfrac{1}{2}\rangle = \hbar|\tfrac{1}{2},-\tfrac{1}{2}\rangle\,,$$
$$S_-|\tfrac{1}{2},-\tfrac{1}{2}\rangle = 0\,.$$

We construct a matrix representation of S_i, with $|\frac{1}{2},\frac{1}{2}\rangle(=|\uparrow\rangle)$ represented by $\begin{pmatrix}1\\0\end{pmatrix}$ and $|\frac{1}{2},-\frac{1}{2}\rangle(=|\downarrow\rangle)$ by $\begin{pmatrix}0\\1\end{pmatrix}$. Now,

$$S_z\begin{pmatrix}1\\0\end{pmatrix} = \tfrac{1}{2}\hbar\begin{pmatrix}1\\0\end{pmatrix}\,,\quad S_z\begin{pmatrix}0\\1\end{pmatrix} = -\tfrac{1}{2}\hbar\begin{pmatrix}0\\1\end{pmatrix}\,.$$

This implies that

$$S_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} .$$

Next we have

$$S_+ \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \hbar \begin{pmatrix} 0 \\ 0 \end{pmatrix} , \quad S_+ \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \hbar \begin{pmatrix} 1 \\ 0 \end{pmatrix} .$$

This implies

$$S_+ = \hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} .$$

We have $S_- = S_+^*$, i.e., the matrix S_- is the adjoint of S_+: $S_- = \overline{S_+}^T$. Thus,

$$S_- = \hbar \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} .$$

Now, $S_\pm = S_x \pm \mathrm{i} S_y$. Hence

$$S_x = \frac{1}{2}(S_+ + S_-) = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} ,$$
$$S_y = -\frac{\mathrm{i}}{2}(S_+ - S_-) = \frac{\hbar}{2}\begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix} .$$

The Pauli spin matrices are defined by

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} , \quad \sigma_y = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix} , \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} .$$

Then,

$$S_i = \frac{\hbar}{2}\sigma_i \, , i = x, y, z \, .$$

6 *Incompatible observables and uncertainty relations*

6.1 COMPATIBLE AND INCOMPATIBLE OBSERVABLES

DEFINITION 6.1. Observables A and B acting on a Hilbert space $\mathcal{H}$ are said to be *compatible* if $[A, B] = 0$. They are said to be *incompatible* if $[A, B] \neq 0$. ◇

EXAMPLE 6.2. $[\mathbf{J}^2, J_z] = 0$, where J_x, J_y and J_z are the three components of the angular momentum and where $\mathbf{J}^2 := J_x^2 + J_y^2 + J_z^2$. So $\mathbf{J}^2$ and J_z are compatible. (In fact $\mathbf{J}^2$ and J_x are compatible and $\mathbf{J}^2$ and J_y are also compatible.) ◇

We consider two self-adjoint operators A and B acting on a finite-dimensional Hilbert space. Let their eigenvalues be λ_k, $k = 1, 2, \ldots, M$ with the corresponding orthogonal projectors $P^{(A)}_{\lambda_k}$, and μ_ℓ, $\ell = 1, 2, \ldots, M'$, with the corresponding orthogonal projectors $P^{(B)}_{\mu_\ell}$, respectively.

THEOREM 6.3. $[A, B] = 0 \Leftrightarrow [P^{(A)}_{\lambda_k}, P^{(B)}_{\mu_\ell}] = 0$ *for all* k *and* ℓ.

PROOF. *Proof of* "$\Leftarrow$". Suppose $[P^{(A)}_{\lambda_k}, P^{(B)}_{\mu_\ell}] = 0$ for all k and ℓ. Then, we find

$$\begin{aligned}[A, B] &= \left[\sum_{k=1}^{M} \lambda_k P^{(A)}_{\lambda_k}, \sum_{\ell=1}^{M'} \mu_\ell P^{(B)}_{\lambda_\ell}\right] \\ &= \sum_{k=1}^{M}\sum_{\ell=1}^{M'} \lambda_k \mu_\ell [P^{(A)}_{\lambda_k}, P^{(B)}_{\mu_\ell}] = 0,\end{aligned}$$

as required.

Proof of "$\Rightarrow$". If $[A, B] = 0$, then $B|\Psi^{(A)}_{\lambda_{k'}}\rangle$ is an eigenvector of A with eigenvalue $\lambda_{k'}$: $AB|\Psi^{(A)}_{\lambda_{k'}}\rangle = BA|\Psi^{(A)}_{\lambda_{k'}}\rangle = \lambda_{k'} B|\Psi^{(A)}_{\lambda_{k'}}\rangle$. Therefore

$$P^{(A)}_{\lambda_k} B|\Psi^{(A)}_{\lambda_{k'}}\rangle = \delta_{kk'} B|\Psi^{(A)}_{\lambda_{k'}}\rangle.$$

We also have that $P^{(A)}_{\lambda_k}|\Psi^{(A)}_{\lambda_{k'}}\rangle = \delta_{kk'}|\Psi^{(A)}_{\lambda_{k'}}\rangle$, hence

$$B P^{(A)}_{\lambda_k}|\Psi^{(A)}_{\lambda_{k'}}\rangle = \delta_{kk'} B|\Psi^{(A)}_{\lambda_{k'}}\rangle.$$

It follows that $[P^{(A)}_{\lambda_k}, B]|\Psi^{(A)}_{\lambda_{k'}}\rangle = 0$ for all k and k'. But since any state can be expanded in terms of the eigenstates $|\Psi^{(A)}_{\lambda_{k'}}\rangle$ of A, this implies that $[P^{(A)}_{\lambda_k}, B] = 0$ for all k.

Now, recall that $B = \sum_{\ell=1}^{M'} \mu_\ell P^{(B)}_{\mu_\ell}$. In the paragraph above, we proved that $[A, B] = 0 \Rightarrow [P^{(A)}_{\lambda_k}, B] = 0$. Applying the same result, but with $A \to B$ and $B \to C$ leads to $[B, C] = 0 \Rightarrow [P^{(B)}_{\mu_\ell}, C] = 0$. Letting $C = P^{(A)}_{\lambda_k}$, we conclude that $[P^{(A)}_{\lambda_k}, P^{(B)}_{\mu_\ell}] = 0$ for all k and ℓ. □

COROLLARY 6.4. *For any $f, g : \mathbb{R} \to \mathbb{C}$, if A and B are self-adjoint operators and if $[A, B] = 0$, then $[f(A), g(B)] = 0$.*

PROOF. If $[A, B] = 0$, then by Theorem 6.3 we have $[P^{(A)}_{\lambda_k}, P^{(B)}_{\mu_\ell}] = 0$ for all (k, ℓ). Now, by definition

$$f(A) = \sum_{k=1}^{M} f(\lambda_k) P^{(A)}_{\lambda_k}, \quad g(B) = \sum_{\ell=1}^{M'} g(\mu_\ell) P^{(B)}_{\mu_\ell}.$$

Hence

$$\begin{aligned}
[f(A), g(B)] &= \left[\sum_{k=1}^{M} f(\lambda_k) P^{(A)}_{\lambda_k}, \sum_{\ell=1}^{M'} g(\mu_\ell) P^{(B)}_{\mu_\ell} \right] \\
&= \sum_{k=1}^{M} \sum_{\ell=1}^{M'} f(\lambda_k) g(\mu_\ell) [P^{(A)}_{\lambda_k}, P^{(B)}_{\ell}] \\
&= 0,
\end{aligned}$$

as required. □

We now justify our definition of observable (in)compatibility of by looking at the implications for sequential measurements, i.e. measurements carried out at different times on the same system.

PROPOSITION 6.5. *Suppose a quantum system described by $\mathcal{H}$ is in the state $|\psi\rangle$. If the observable B is measured and then the observable A is measured immediately after,[13] then the probability of observing outcome μ_ℓ for B and outcome λ_k for A is given by*

$$\text{Prob}(\, B = \mu_\ell \to A = \lambda_k | \psi) = \| P^{(A)}_{\lambda_k} P^{(B)}_{\mu_\ell} \, |\psi\rangle |^2.$$

[13] i.e. the state does not time-evolve between the two measurements.

Here, we do not assume that A and B are compatible or incompatible.

PROOF. The probability for the outcome μ_ℓ in the measurement of B is $\| P^{(B)}_{\mu_\ell} |\psi\rangle \|^2$, and the state after the measurement is

$$|\phi_{\mu_\ell}\rangle := \frac{P^{(B)}_{\mu_\ell} |\psi\rangle}{\| P^{(B)}_{\mu_\ell} |\psi\rangle \|}.$$

The probability of the outcome λ_k in the subsequent measurement of A is

$$\begin{aligned}\|P^{(A)}_{\lambda_k}|\phi_{\mu_\ell}\rangle\|^2 &= \left\| \frac{P^{(A)}_{\lambda_k} P^{(B)}_{\mu_\ell}|\psi\rangle}{\|P^{(B)}_{\mu_\ell}|\psi\rangle\|} \right\|^2 \\ &= \frac{1}{\|P^{(B)}_{\mu_\ell}|\psi\rangle\|^2} \|P^{(A)}_{\lambda_k} P^{(B)}_{\mu_\ell}|\psi\rangle\|^2.\end{aligned}$$

Hence, the probability of the outcome that the observable B is measured to be μ_ℓ and then the observable A is measured to be λ_k is

$$\begin{aligned}\text{Prob}(B = \mu_\ell \to A = \lambda_k|\psi) &= \|P^{(B)}_{\mu_\ell}|\psi\rangle\|^2 \times \frac{1}{\|P^{(B)}_{\mu_\ell}|\psi\rangle\|^2} \|P^{(A)}_{\lambda_k} P^{(B)}_{\mu_\ell}|\psi\rangle\|^2 \\ &= \|P^{(A)}_{\lambda_k} P^{(B)}_{\mu_\ell}|\psi\rangle\|^2,\end{aligned}$$

as required. □

If $[A, B] \neq 0$, then $[P^{(A)}_{\lambda_k}, P^{(B)}_{\mu_\ell}] \neq 0$ for some (k, ℓ). Hence, $\text{Prob}(B = \mu_\ell \to A = \lambda_k|\psi)$ may not equal $\text{Prob}(A = \lambda_k \to B = \mu_\ell|\psi)$ for some (k, ℓ).

COROLLARY 6.6. *If A and B are compatible, then*

$$\text{Prob}(B = \mu_\ell \to A = \lambda_k|\psi) = \text{Prob}(A = \lambda_k \to B = \mu_\ell|\psi) \quad \textit{for all} \quad (k, \ell).$$

PROOF. Let $[A, B] = 0$. Then, $P^{(A)}_{\lambda_k} P^{(B)}_{\mu_\ell} = P^{(B)}_{\mu_\ell} P^{(A)}_{\lambda_k}$ for all (k, ℓ) by Theorem 6.3. Hence

$$\begin{aligned}\text{Prob}(B = \mu_\ell \to A = \lambda_k|\psi) &= \|P^{(A)}_{\lambda_k} P^{(B)}_{\mu_\ell}|\psi\rangle\|^2 \\ &= \|P^{(B)}_{\mu_\ell} P^{(A)}_{\lambda_k}|\psi\rangle\|^2 \\ &= \text{Prob}(A = \lambda_k \to B = \mu_\ell|\psi),\end{aligned}$$

as required. □

Therefore, if A and B are compatible, then the probability for the outcome λ_k in the measurement of A *and* the outcome μ_ℓ in the measurement of B is $\|P^{(A)}_{\lambda_k} P^{(B)}_{\mu_\ell}|\psi\rangle\|^2$ regardless of the order in which A and B are measured. If they are incompatible, then the order of implementation generally matters, as the measurement of the first observable has interfered with the measurement of the second observable.

An equivalent definition for the compatibility of A and B relies on the existence of a basis of $\mathcal{H}$ composed entirely of eigenstates of both A and B.

THEOREM 6.7. *The observables A and B acting on a Hilbert space $\mathcal{H}$ are compatible if and only if there is an orthonormal basis of $\mathcal{H}$ such that all basis states are eigenstates of both A and B.*

PROOF. *Proof of the "if" part.* Suppose the orthonormal basis $\{|\varphi_{\lambda_k,\mu_\ell,i}\rangle\}_{k,\ell,i}$, where $k = 1, \ldots, M$, $\ell = 1, \ldots M'$ and $i = 1, \ldots, m(\lambda_k, \mu_\ell)$,[14] satisfies $A|\varphi_{\lambda_k,\mu_\ell,i}\rangle = \lambda_k|\varphi_{\lambda_k,\mu_\ell,i}\rangle$ and $B|\varphi_{\lambda_k,\mu_\ell,i}\rangle = \mu_\ell|\varphi_{\lambda_k,\mu_\ell,i}\rangle$. That is, it is composed entirely by common eigenstates of A and B. Since all vectors in $\mathcal{H}$ are

[14] The index i accounts for degenerate eigenspaces. We will discuss its relevance only at the end of the proof.

linear combinations of $|\varphi_{\lambda_k,\mu_\ell,i}\rangle$, all we need to show to prove that $[A,B]=0$ is $[A,B]|\varphi_{\lambda_k,\mu_\ell,i}\rangle = 0$. We can show the latter as

$$\begin{aligned}[A,B]|\varphi_{\lambda_k,\mu_\ell,i}\rangle &= AB|\varphi_{\lambda_k,\mu_\ell,i}\rangle - BA|\varphi_{\lambda_k,\mu_\ell,i}\rangle \\ &= \mu_\ell A|\varphi_{\lambda_k,\mu_\ell,i}\rangle - \lambda_k B|\varphi_{\lambda_k,\mu_\ell,i}\rangle \\ &= \mu_\ell\lambda_k|\varphi_{\lambda_k,\mu_\ell,i}\rangle - \lambda_k\mu_\ell|\varphi_{\lambda_k,\mu_\ell,i}\rangle \\ &= 0,\end{aligned}$$

as required.

Proof of the "only if" part. Since $\sum_{k=1}^{M} P_{\lambda_k}^{(A)} = \sum_{\ell=1}^{M'} P_{\mu_\ell}^{(B)} = \mathbb{1}$, any $|\psi\rangle \in \mathcal{H}$ can be expressed as

$$|\psi\rangle = \left(\sum_{k=1}^{M} P_{\lambda_k}^{(A)}\right)\left(\sum_{\ell=1}^{M'} P_{\mu_\ell}^{(B)}\right)|\psi\rangle = \sum_{k=1}^{M}\sum_{\ell=1}^{M'} P_{\lambda_k}^{(A)} P_{\mu_\ell}^{(B)}|\psi\rangle.$$

Now, $AP_{\lambda_k}^{(A)}P_{\mu_\ell}^{(B)}|\psi\rangle = \lambda_k P_{\lambda_k}^{(A)}P_{\mu_\ell}^{(B)}|\psi\rangle$ and $BP_{\lambda_k}^{(A)}P_{\mu_\ell}^{(B)}|\psi\rangle = BP_{\mu_\ell}^{(B)}P_{\lambda_k}^{(A)}|\psi\rangle = \mu_\ell P_{\lambda_k}^{(A)}P_{\mu_\ell}^{(B)}|\psi\rangle$, where for the last result we used the fact that $[P_{\lambda_k}^{(A)}, P_{\mu_\ell}^{(B)}] = 0$ if $[A,B]=0$ (Theorem 6.3). Hence

$$P_{\lambda_k}^{(A)}P_{\mu_\ell}^{(B)}|\psi\rangle \in \mathcal{H}_{\lambda_k,\mu_\ell}^{(A,B)},$$

where

$$\mathcal{H}_{\lambda_k,\mu_\ell}^{(A,B)} = \{|\phi\rangle \in \mathcal{H} : A|\phi\rangle = \lambda_k|\phi\rangle,\ B|\phi\rangle = \mu_\ell|\phi\rangle\}.$$

Therefore, any state in $\mathcal{H}$ can be written as the sum of common eigenstates of A and B, i.e.

$$\mathcal{H} = \bigoplus_{k=1}^{M}\bigoplus_{\ell=1}^{M'} \mathcal{H}_{\lambda_k,\mu_\ell}^{(A,B)},$$

Note that some subspaces $\mathcal{H}_{\lambda_k,\mu_\ell}^{(A,B)}$ may only contain the zero vector, i.e. $\dim\mathcal{H}_{\lambda_k,\mu_\ell}^{(A,B)} = 0$ for some (k,ℓ). Similarly, it might be that they are degenerate, $\dim\mathcal{H}_{\lambda_k,\mu_\ell}^{(A,B)} > 1$. In any case, we can set $m(\lambda_k,\mu_\ell) := \dim\mathcal{H}_{\lambda_k,\mu_\ell}^{(A,B)}$ and choose an orthonormal basis $\{|\varphi_{\lambda_k,\mu_\ell,i}\rangle\}_{i=1,\ldots,m(\lambda_k,\mu_\ell)}$ of $\mathcal{H}_{\lambda_k,\mu_\ell}^{(A,B)}$. Then, the set $\{|\varphi_{\lambda_k,\mu_\ell,i}\rangle\}_{k=1,\ldots,M;\ell=1,\ldots,M';i=1,\ldots,m(\lambda_k,\mu_\ell)}$ is an orthonormal basis of the whole space $\mathcal{H}$, such that $A|\varphi_{\lambda_k,\mu_\ell,i}\rangle = \lambda_k|\varphi_{\lambda_k,\mu_\ell,i}\rangle$ and $B|\varphi_{\lambda_k,\mu_\ell,i}\rangle = \mu_\ell|\varphi_{\lambda_k,\mu_\ell,i}\rangle$. □

6.2 HEISENBERG'S UNCERTAINTY RELATION

Recall that the *variance* for the measurement of A in the state $|\psi\rangle$ is given by

$$(\Delta_\psi A)^2 = \langle A^2\rangle_\psi - \langle A\rangle_\psi^2\,,$$

and its square root $\Delta_\psi A$, is called the *uncertainty of* A in the state $|\psi\rangle$.

THEOREM 6.8 (HEISENBERG'S UNCERTAINTY RELATION). *Let $|\psi\rangle \in L^2(\mathbb{R})$ be a (sufficiently nice) state. Then we have the inequality*

$$\Delta_\psi X \; \Delta_\psi P \geq \frac{\hbar}{2}. \tag{6.1}$$

REMARK 6.9. Heisenberg's uncertainty relation states that it is impossible to prepare a quantum particle in a state $|\psi\rangle \in L^2(\mathbb{R})$ in such a way that the product of its position and momentum uncertainties (the square roots of the variances) would take arbitrarily small values. There is a lower bound for the value of their product which cannot be undercut.

In other words, the uncertainty in the position of the particle is inversely proportional to the uncertainty in the momentum: any attempt to narrow down the spread of values obtained from position measurements will lead to a broader distribution of values when measuring the momentum of the particle.

This property is in stark contrast to the case of a classical particle. In principle, it is possible to specify the values of its position and momentum with arbitrary precision meaning that the product of the classical uncertainties Δx and Δp can be made arbitrarily small,

$$(\Delta x \Delta p)_{\text{class}} \geq 0\,.$$

From a conceptual point of view, we are able to simultaneously assign *precise* values to both the position and the momentum, x_0 and p_0, say, of a classical particle, corresponding to a *point* in phase space. Perfect position and momentum measurements would then reveal these values with no spread whatsoever, implying vanishing variances (and hence uncertainties). ◇

For a proof of the theorem, we will need two lemmata.

LEMMA 6.10. *For every (sufficiently nice) state $\psi \in L^2(\mathbb{R})$ we have the inequality*

$$\langle X^2\rangle_\psi \; \langle P^2\rangle_\psi \geq \frac{\hbar^2}{4}. \tag{6.2}$$

PROOF. To begin, we use the Cauchy–Schwarz inequality to find a first bound on the product of the variances,

$$\langle X^2\rangle_\psi \langle P^2\rangle_\psi = \langle X\psi|X\psi\rangle\langle P\psi|P\psi\rangle = \|X\psi\|^2\|P\psi\|^2 \geq |\langle X\psi|P\psi\rangle|^2$$

Next, we use the simple fact that the squared modulus of a complex number $z = x + iy$, $x, y \in \mathbb{R}$, must be at least as large as the square of it imaginary part,

$$|z|^2 = x^2 + y^2 \geq y^2\,.$$

Thus, for the complex number $z = \langle X\psi|P\psi\rangle$, we have

$$|\langle X\psi|P\psi\rangle|^2 \geq \left(\operatorname{Im}\langle X\psi|P\psi\rangle\right)^2.$$

The exact value of the right-hand-side of this inequality can be found from—crucially—using the fundamental commutation relation $[X, P] = \mathrm{i}\hbar\mathbb{1}$ and the self-adjointness of the operators associated with position and momentum,

$$\begin{aligned}\operatorname{Im}\langle X\psi|P\psi\rangle &= \frac{1}{2\mathrm{i}}\big(\langle X\psi|P\psi\rangle - \overline{\langle X\psi|P\psi\rangle}\big) = \frac{1}{2\mathrm{i}}\big(\langle X\psi|P\psi\rangle - \langle P\psi|X\psi\rangle\big)\\ &= \frac{1}{2\mathrm{i}}\big(\langle\psi|XP\psi\rangle - \langle\psi|PX\psi\rangle\big) = \frac{1}{2\mathrm{i}}\big(\langle\psi|[X,P]\psi\rangle\big)\\ &= \frac{\hbar}{2}\langle\psi|\psi\rangle = \frac{\hbar}{2},\end{aligned}$$

Combining these three results leaves us with the Eq. (6.2) which corresponds to Heisenberg's relation for states with vanishing mean values of position and momentum. □

LEMMA 6.11. *The operators*

$$\tilde{X} = X - \langle X\rangle_\psi\mathbb{1} \qquad \text{and } \tilde{P} = P - \langle P\rangle_\psi\mathbb{1}\,,$$

satisfy the same commutation relations as X and P,

$$[\tilde{X}, \tilde{P}] = i\hbar\mathbb{1},$$

while their expectations in the state $|\psi\rangle \in L^2(\mathbb{R})$ vanish,

$$\langle\tilde{X}\rangle_\psi = 0, \qquad \text{and} \qquad \langle\tilde{P}\rangle_\psi = 0\,,$$

and we also have

$$\langle\tilde{X}^2\rangle_\psi = (\Delta_\psi X)^2 \qquad \text{and } \langle\tilde{P}^2\rangle_\psi = (\Delta_\psi P)^2\,.$$

PROOF. Denoting the expectations of X and P by $\langle X\rangle_\psi = x_0$ and $\langle P\rangle_\psi = p_0$, respectively, we have

$$[\tilde{X}, \tilde{P}] = [X - x_0\mathbb{1}, P - p_0\mathbb{1}] = [X, P] = i\hbar\mathbb{1}\,,$$

since the identity operator $\mathbb{1}$ commutes with every other operator. The expectations of the new operators vanish by construction, e.g.

$$\langle\tilde{X}\rangle_\psi = \langle X\rangle_\psi - \langle X\rangle_\psi\langle\mathbb{1}\rangle_\psi = 0\,.$$

To establish the remaining relations, we use the definition of the new operators to calculate

$$\langle\tilde{X}^2\rangle_\psi = \langle X^2\rangle_\psi - 2x_0\langle X\rangle_\psi + x_0^2 = \langle X^2\rangle_\psi - \langle X\rangle_\psi^2 \equiv (\Delta_\psi X)^2\,,$$

and similarly for momentum. □

In a final step, we combine these results to to conclude the proof of Theorem 6.8.

PROOF. Using the lemma just shown and subsequently applying the first lemma to the operators $\tilde{X}$ and $\tilde{P}$ instead of X and P we find

$$\Delta_\psi X \; \Delta_\psi P = \sqrt{\langle \tilde{X}^2 \rangle_\psi \langle \tilde{P}^2 \rangle_\psi} \geq \frac{\hbar}{2}$$

as required. □

EXAMPLE 6.12. It is interesting question to ask whether there are states $|\psi\rangle \in L^2(\mathbb{R})$ for which the inequality is *saturated*, $\Delta_\psi X \; \Delta_\psi P = \hbar/2$, *i.e.* the uncertainty relation holds as an equality. We now show that at least one such a state exists.

If we consider a state $|\psi_0\rangle$ with the Gaussian wave function (cf. Example 3.5)

$$\psi_0(x) = (\sqrt{\pi} l)^{-\frac{1}{2}} \exp\left(-\frac{x^2}{2\ell^2}\right),$$

for some $\ell > 0$, we find

$$\langle X \rangle_{\psi_0} = \int_{-\infty}^{\infty} x |\psi_0(x)|^2 \, \mathrm{d}x \; = 0 \,,$$

as the integrand is odd. The variance, however, does not vanish,

$$(\Delta_{\psi_0} X)^2 = \langle X^2 \rangle_{\psi_0} = \int_{-\infty}^{\infty} x^2 |\psi_0(x)|^2 \, \mathrm{d}x = \ell^2/2 \,, \tag{6.3}$$

which clearly is a measure for the width of the Gaussian distribution $|\psi_0(x)|^2$.

For the state with wave function $\psi_0(x)$ defined above, we also need to calculate the variance of position. The expectation value of momentum vanishes,

$$\langle P \rangle_{\psi_0} = \frac{\mathrm{i}\hbar}{\sqrt{\pi}\ell^3} \int_{-\infty}^{\infty} x \exp\left(-\frac{x^2}{\ell^2}\right) \mathrm{d}x = 0 \,, \tag{6.4}$$

which leaves a single integral to evaluate for the variance

$$(\Delta_{\psi_0} P)^2 = \frac{\hbar^2}{\sqrt{\pi}\ell^5} \int_{-\infty}^{\infty} x^2 \exp\left(-\frac{x^2}{\ell^2}\right) \mathrm{d}x = \frac{\hbar^2}{2\ell^2} \,.$$

Combined with $(\Delta_{\psi_0} X)^2 = \ell^2/2$, calculated in Eq. (6.3), we find indeed

$$\Delta_{\psi_0} X \; \Delta_{\psi_0} P = \frac{\hbar}{2} \,.$$ ◇

REMARK 6.13. Heisenberg's uncertainty relation can be generalized to arbitrary pairs of self-adjoint operators. Namely, if A and B are observables acting on a Hilbert space $\mathcal{H}$, and if $|\psi\rangle \in \mathcal{H}$ is a state, then

$$\Delta_\psi A \Delta_\psi B \geq \left| \langle \psi | \tfrac{1}{2\mathrm{i}} [A, B] \, |\psi\rangle \right| . \tag{6.5}$$

This generalisation of Eq. (6.1) is due to Robertson (1929). ◇

7 Time evolution

7.1 TIME-DEPENDENT SCHRÖDINGER EQUATION

In the absence of measurements, quantum states evolve continuously in time according to the *time-dependent Schrödinger equation*:

$$\mathrm{i}\hbar\frac{d}{dt}\left|\psi(t)\right\rangle = H\left|\psi(t)\right\rangle, \tag{7.1}$$

where H is the Hamiltonian operator and $|\psi(t)\rangle$ is the state of the system at time t. A solution of this equation is a function $t \mapsto |\psi(t)\rangle$, associating to every time t a state $|\psi(t)\rangle$ in the Hilbert space.

For a particle of mass m moving in a single spatial dimension under the a potential $V(x)$ (which we assume does not depends on t explicitly), Eq. (7.1) in position representation reads

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x)\psi(x,t), \tag{7.2}$$

where $\psi(x,t) = \langle x|\psi(t)\rangle$. We attempt to solve it by reducing it to a pair of ordinary differential equations in one variable. We write

$$\psi(x,t) = T(t)\phi(x)$$

which leads to

$$i\hbar\phi(x)\frac{dT(t)}{dt} = \left[-\frac{\hbar^2}{2m}\frac{d^2\phi(x)}{dx^2} + V(x)\phi(x)\right]T(t).$$

Dividing by $T(t)\phi(x)$ we find

$$i\hbar\frac{dT(t)/dt}{T(t)} = \frac{1}{\phi(x)}\left[-\frac{\hbar^2}{2m}\frac{d^2\phi(x)}{dx^2} + V(x)\phi(x)\right]$$

The LHS is a function of t only, whereas the RHS depends only on x. For the equality to hold, both sides must be equal to the same constant which, as will be obvious shortly, we call E. Then, the solution of

$$i\hbar\frac{dT(t)}{dt} = ET(t)$$

is $T(t) = Ce^{-iEt/\hbar}$, where C is a constant. The other equation is

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

which is our friend the time-independent Schrödinger equation (4.1) which characterises the energy eigenstates.

For an Hamiltonian with eigenvalues E_n and eigenvectors $|\phi_n\rangle$, where $n = 1, 2, \ldots$ (this is a case where energy is quantised, like that of a particle in a box), any linear combination

$$\psi(x,t) = \sum_n c_n \psi_n(x,t) = \sum_n c_n T_n(t)\phi_n(x) = \sum_n c_n e^{-iE_n t/\hbar}\phi_n(x)\,, \quad c_n \in \mathbb{C}$$

is a solution of Eq. (7.2) (note that for a valid wave function we would need the additional normalisation condition $\sum_n |c_n|^2 = 1$). In terms of kets, the solution of the Schrödinger equation reads

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

where $|\psi(0)\rangle = \sum_n c_n\,|\phi_n\rangle$ is the state of the system at time $t = 0$.

The above calculation provides a 'recipe' for computing the time-evolution of *any* quantum state. Suppose at $t = 0$ our system resides in some known state $|\psi(0)\rangle$.

- *Step 1:* solve the time-independent Schrödinger equation, hence find the eigenvalues E_n of H and the corresponding eigenvectors $|\phi_n\rangle$;
- *Step 2:* express $|\psi(0)\rangle$ in a basis of $\mathcal{H}$ composed of energy eigenstates, e.g.
$$|\psi(0)\rangle = \sum_n c_n\,|\phi_n\rangle, \tag{7.3}$$
where $c_n = \langle\phi_n|\psi(0)\rangle$ and $\sum_n |c_n|^2 = 1$;[15]
- *Step 3:* multiply each coefficient in the sum by the phase factor $e^{-iE_n t/\hbar}$ to find the state $|\psi(t)\rangle$ at some later time t,
$$|\psi(t)\rangle = \sum_n c_n e^{-iE_n t/\hbar}\,|\phi_n\rangle.$$

[15] Here we assume that H is non-degenerate.

EXAMPLE 7.1. Consider the Schrödinger equation

$$\mathrm{i}\hbar\frac{d}{dt}\,|\psi(t)\rangle = \omega S_z\,|\psi(t)\rangle\,, \qquad \omega > 0.$$

Clearly, the (non-degenerate) eigenvalues of $H = \omega S_z$ are $\pm\hbar\omega/2$. If the initial state at $t = 0$ is given by

$$|\psi(0)\rangle = |+\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix},$$

then the solution of the Schrödinger equation tells us that the time-evolved state is

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}}\big(\mathrm{e}^{-\frac{1}{2}\mathrm{i}\omega t}\,|\uparrow\rangle + \mathrm{e}^{+\frac{1}{2}\mathrm{i}\omega t}\,|\downarrow\rangle\big) = \frac{1}{\sqrt{2}}\begin{pmatrix}\mathrm{e}^{-\frac{1}{2}\mathrm{i}\omega t}\\ \mathrm{e}^{+\frac{1}{2}\mathrm{i}\omega t}\end{pmatrix}.$$

The probability that a measurement of S_x returns, say, spin 'up'(i.e. the eigenvalue $S_x = +1$ with associated eigenvector $|+\rangle$) changes with time:

$$\mathrm{Prob}(S_x = \frac{\hbar}{2}\mid \psi(t)) = |\langle +|\psi(t)\rangle|^2 = \cos^2(\omega t/2)\,.$$

◇

REMARK 7.2. Energy eigenstates are aso called *stationary states*. If $|\psi(0)\rangle = |\psi_n\rangle$, then the time-evolved state will be $|\psi(t)\rangle = e^{-iE_nt/\hbar}|\psi_n\rangle$. That is, the vector only picks up an irrelevant *global* phase factor, i.e. $|\psi(t)\rangle = |\psi(0)\rangle$. ◇

7.2 THE TIME-EVOLUTION OPERATOR

The time-evolution of the state of a quantum system can be described in terms of the action of a *time-evolution operator* $U(t)$, such that $U(t)\,|\psi(0)\rangle = |\psi(t)\rangle$.

PROPOSITION 7.3. *The time-evolution operator $U(t)$ is unitary and given by the expression*

$$U(t) = \exp\left(-\frac{i}{\hbar}Ht\right)$$

PROOF. We must show that $|\psi(t)\rangle = U(t)\,|\psi(0)\rangle$ solves the time-dependent Schrödinger equation (7.1). The exponential of an operator such as H is defined by the power series

$$\exp\left(-\frac{i}{\hbar}Ht\right) = \sum_{k=0}^{\infty}\left(-\frac{\mathrm{i}t}{\hbar}\right)^k\frac{H^k}{k!}\,, \tag{7.4}$$

which allows us to work out the time derivative on left-hand-side of Eq. (7.1),

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle &= \frac{\mathrm{d}}{\mathrm{d}t}\left(\sum_{k=0}^{\infty}\left(-\frac{\mathrm{i}t}{\hbar}\right)^k\frac{H^k}{k!}\right)|\psi(0)\rangle = -\frac{\mathrm{i}}{\hbar}\left(\sum_{k=0}^{\infty}k\left(-\frac{\mathrm{i}t}{\hbar}\right)^{k-1}\frac{H^k}{k!}\right)|\psi(0)\rangle\\
&= -\frac{\mathrm{i}}{\hbar}H\left(\sum_{k=1}^{\infty}\left(-\frac{\mathrm{i}t}{\hbar}\right)^{k-1}\frac{H^{k-1}}{(k-1)!}\right)|\psi(0)\rangle\\
&= -\frac{\mathrm{i}}{\hbar}H\left(\sum_{k=0}^{\infty}\left(-\frac{\mathrm{i}t}{\hbar}\right)^k\frac{H^k}{k!}\right)|\psi(0)\rangle = -\frac{\mathrm{i}}{\hbar}H\exp\left(-\frac{\mathrm{i}}{\hbar}Ht\right)|\psi(0)\rangle\\
&= -\frac{\mathrm{i}}{\hbar}H\,|\psi(t)\rangle\,,
\end{aligned}$$

producing to the desired result. Moreover, from Eq. (7.4) we have that

$$(U(t))^* = \exp\left(\frac{i}{\hbar}Ht\right)\,.$$

The action of $U(t)$ on an eigenstate of H is

$$\begin{aligned}
\exp\left(-\frac{\mathrm{i}}{\hbar}Ht\right)|\phi_n\rangle &= \sum_{k=0}^{\infty}\left(-\frac{\mathrm{i}t}{\hbar}\right)^k\frac{H^k}{k!}\,|\phi_n\rangle\\
&= \sum_{k=0}^{\infty}\left(-\frac{\mathrm{i}t}{\hbar}\right)^k\frac{E_n^k}{k!}\,|\phi_n\rangle = \exp\left(-\frac{\mathrm{i}}{\hbar}E_nt\right)|\phi_n\rangle\,,
\end{aligned}$$

hence we have

$$\begin{aligned}
(U(t))^*U(t)\,|\phi_n\rangle &= \exp\left(\frac{i}{\hbar}E_nt\right)\exp\left(-\frac{i}{\hbar}E_nt\right)|\phi_n\rangle = |\phi_n\rangle\,,\\
U(t)(U(t))^*\,|\phi_n\rangle &= \exp\left(-\frac{i}{\hbar}E_nt\right)\exp\left(\frac{i}{\hbar}E_nt\right)|\phi_n\rangle = |\phi_n\rangle\,.
\end{aligned}$$

Since the eigenstates of H form a basis of $\mathcal{H}$, we conclude that

$$\mathrm{e}^{-\mathrm{i}Ht/\hbar}(\mathrm{e}^{-\mathrm{i}Ht/\hbar})^* = (\mathrm{e}^{-\mathrm{i}Ht/\hbar})^*\mathrm{e}^{-\mathrm{i}Ht/\hbar} = \mathbb{1}$$

that is, $U(t)$ is unitary. □

REMARK 7.4. Note that the family $\{U(t)\}_{t\in\mathbb{R}}$ is in fact a *group*, $U(t)U(s) = U(t+s)$ and $U(0) = \mathbb{1}$, and thus $U(t)$ can be understood as the (unique) map which sends the state $\psi(s)$ at time s to the state $\psi(t+s)$ at time $t+s$. ◇

7.3 DYNAMICS OF A FREE PARTICLE

For a free particle, energy is not a quantised variable, c.f. Sec. 4.1. Nevertheless, the 'recipe' for evolving quantum states still applies.

Suppose at $t = 0$ a quantum particle is described by some known wave function $\psi(x, 0)$.

- *Step 1.* Find the eigenstates of $H = H_0$: in position representation, these are plane waves[16] $\langle x|k\rangle = (2\pi)^{-1/2}e^{ikx}$ with eigenvalue $E_k = \hbar^2k^2/(2m) = \hbar\omega_k$, where we let $\omega_k = \hbar k^2/(2m)$.

- *Step 2.* Express the wave function in the momentum basis. That is, calculate the expansion coefficients

$$\psi(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\psi(x,0)e^{-ikx}\,\mathrm{d}x$$

  and use them in

$$\psi(x,0) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\psi(k)e^{ikx}\,\mathrm{d}k\,.$$

- *Step 3.* Multiply each coefficient $\psi(k)$ by the phase factor $e^{-iE_kt/\hbar} = e^{-i\omega_kt}$ to find the wave function at some later time t,

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\psi(k)e^{i(kx-\omega_kt)}\,\mathrm{d}k\,.$$

  Then solve the integral to obtain the probability amplitude at point x and time t.

[16] Notice we denote here momentum eigenstates by the wave number k, instead of $p = \hbar k$.

We now apply this to the case of a Gaussian wavepacket. In Example 6.12, we saw that the wave function

$$\psi_0(x) = (\sqrt{\pi}l)^{-\frac{1}{2}}\exp\left(-\frac{x^2}{2\ell^2}\right),$$

saturates Heisenberg's uncertainty relation (6.1). It describes a localised particle with mean position $\langle X\rangle_{\psi_0} = 0$, mean momentum $\langle P\rangle_{\psi_0} = 0$, but with non-zero width for their distributions, i.e. $(\Delta_{\psi_0}X)^2 = \ell^2/2$ and $(\Delta_{\psi_0}P)^2 =$

$\hbar^2/(2\ell^2)$, respectively. Setting $\psi(x,0) = \psi_0(x)$, to obtain the wave function at some later time t, we first apply a Fourier transform:

$$\begin{aligned}\psi(k) =& \frac{1}{\sqrt{2\pi}}(\sqrt{\pi}l)^{-\frac{1}{2}} \int_{-\infty}^{\infty} e^{-\frac{x^2}{2\ell^2} - ikx}\,\mathrm{d}x \\ =& \sqrt{\frac{\ell}{\sqrt{\pi}}} e^{-\frac{k^2\ell^2}{2}}\,,\end{aligned}$$

where we used the Gaussian integral solution

$$\int_{-\infty}^{\infty} \exp(-\alpha x^2 + \beta x)\,\mathrm{d}x = \sqrt{\frac{\pi}{\alpha}} \exp\left(\frac{\beta^2}{4\alpha}\right)$$

holding for all $\alpha, \beta \in \mathbb{C}$, provided $\mathrm{Re}(\alpha) > 0$. We then write $\psi(x,0)$ in momentum basis:

$$\psi(x,0) = \frac{\sqrt{\ell}}{\sqrt{2\pi\sqrt{\pi}}} \int_{-\infty}^{\infty} \exp\left(-\frac{\ell^2}{2}k^2 + ikx\right)\mathrm{d}k\,.$$

To find $\psi(x,t)$ we multiply the integrand by $\exp(-iE_k t/\hbar) = \exp[(-i\hbar k^2 t)/(2m)]$,

$$\psi(x,t) = \frac{\sqrt{\ell}}{\sqrt{2\pi\sqrt{\pi}}} \int_{-\infty}^{\infty} \exp\left[-\left(\frac{\ell^2}{2} + i\frac{\hbar t}{2m}\right)k^2 + ikx\right]\mathrm{d}k\,.$$

The solution of the Gaussian integral [exercise!] is another Gaussian,

$$\psi(x,t) = \left[\sqrt{\pi}\left(\ell + \frac{i\hbar t}{m\ell}\right)\right]^{-1/2} \exp\left[-\frac{x^2}{2\ell^2\left(1 + \frac{i\hbar t}{m\ell^2}\right)}\right]\,.$$

We can now compute the probability density

$$|\psi(x,t)|^2 = \left[\sqrt{\pi}\left(\ell^2 + \frac{\hbar^2 t^2}{m^2\ell^2}\right)^{1/2}\right]^{-1} \exp\left[-\frac{x^2}{\ell^2\left(1 + \frac{\hbar^2 t^2}{m^2\ell^4}\right)}\right]\,.$$

The mean position remains zero, $\langle X\rangle_{\psi(t)} = 0$ but the uncertainty in position (i.e. the width of the wavepacket) grows linearly in time according to

$$\Delta_{\psi(t)}X = \frac{\ell}{\sqrt{2}}\left(1 + \frac{\hbar^2 t^2}{m^2\ell^4}\right)^{1/2}\,.$$

The increasing uncertainty in position is a consequence of the fact that any uncertainty in the initial momentum (velocity) will be reflected with passing time as a growing uncertainty in position. The fact that the initial spread in momentum ($\Delta_{\psi(0)}P$) is unavoidable (by Heinseberg's uncertainty relation, if we want to know the initial position to an accuracy ℓ) makes this increment a purely quantum mechanical feature.

7.4 EHRENFEST'S THEOREM

It is anything but obvious how our everyday world, where physical phenomena can generally be accurately described using classical physics such as Newton's laws, emerges from the quantum realm following the (at least at first glance) unintuitive laws of quantum physics. A very rudimentary link between quantum physics and Newtonian physics is given by Ehrenfest's theorem which we discuss in this section.

THEOREM 7.5. *Consider a state $|\psi(t)\rangle \in \mathcal{H}$ solving the Schrödinger equation*

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = H|\psi(t)\rangle$$

for the Hamiltonian H. Then, for any self-adjoint operator A such that $|A\psi(t)\rangle \in \mathcal{H}$,

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\langle A\rangle_{\psi(t)} = \langle [A,H]\rangle_{\psi(t)}. \tag{7.5}$$

PROOF. We show this by a direct calculation:

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\langle A\rangle_{\psi(t)} &= \frac{\mathrm{d}}{\mathrm{d}t}\langle\psi(t)|A\psi(t)\rangle = \Big\langle\frac{\mathrm{d}}{\mathrm{d}t}\psi(t)\Big|A\psi(t)\Big\rangle + \Big\langle\psi(t)\Big|A\frac{\mathrm{d}}{\mathrm{d}t}\psi(t)\Big\rangle \\
&= \frac{1}{\mathrm{i}\hbar}\big(-\langle H\psi(t)|A\psi(t)\rangle + \langle\psi(t)|AH\psi(t)\rangle\big) \\
&= \frac{1}{\mathrm{i}\hbar}\big(-\langle\psi(t)|HA\psi(t)\rangle + \langle\psi(t)|AH\psi(t)\rangle\big) \\
&= \frac{1}{\mathrm{i}\hbar}\langle\psi(t)|[A,H]\psi(t)\rangle = \frac{1}{\mathrm{i}\hbar}\langle[A,H]\rangle_{\psi(t)}.
\end{aligned}$$

□

LEMMA 7.6. *Let $V : \mathbb{R} \to \mathbb{R}$ be a (sufficiently nice) function. Then we have*

$$[X, V(X)] = 0\,, \qquad \textit{and} \qquad [P, V(X)] = -\mathrm{i}\hbar V'(X).$$

PROOF. This proof is left as an exercise. □

THEOREM 7.7 (EHRENFEST'S THEOREM). *Consider a state $|\psi(t)\rangle \in L^2(\mathbb{R})$ solving the Schrödinger equation*

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = H|\psi(t)\rangle \quad \textit{for} \quad H = \frac{1}{2m}P^2 + V(X).$$

Then

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle X\rangle_{\psi(t)} = \frac{1}{m}\langle P\rangle_{\psi(t)} \tag{7.6a}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle P\rangle_{\psi(t)} = -\langle V'(X)\rangle_{\psi(t)} \tag{7.6b}$$

and thus

$$m\frac{\mathrm{d}^2}{\mathrm{d}t^2}\langle X\rangle_{\psi(t)} = -\langle V'(X)\rangle_{\psi(t)}. \tag{7.6c}$$

PROOF. This is an application of Theorem 7.5 using Lemma 7.6:

$$\begin{aligned} \mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\langle X\rangle_{\psi(t)} &= \langle[X,H]\rangle_{\psi(t)} = \frac{1}{2m}\langle[X,P^2]\rangle_{\psi(t)} + \langle[X,V(X)]\rangle_{\psi(t)} \\ &= \frac{\mathrm{i}\hbar}{m}\langle P\rangle_{\psi(t)}, \end{aligned}$$

where we used that $[X,P^2] = [X,P]P + P[X,P] = 2\mathrm{i}\hbar P$, and

$$\begin{aligned} \mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\langle P\rangle_{\psi(t)} &= \langle[P,H]\rangle_{\psi(t)} = \frac{1}{2m}\langle[P,P^2]\rangle_{\psi(t)} + \langle[P,V(X)]\rangle_{\psi(t)} \\ &= -\mathrm{i}\hbar\langle V'(X)\rangle_{\psi(t)}. \end{aligned}$$

□

REMARK 7.8. Taking another look at Ehrenfest's theorem, we see that expectation values for X and P are related in the same way as the classical position and momentum. However, the expectation value of the position, $\langle X\rangle_{\psi(t)}$, does not quite satisfy Newton's second law because, in general,

$$m\frac{\mathrm{d}^2}{\mathrm{d}x^2}\langle X\rangle_{\psi(t)} = -\langle V'(X)\rangle_{\psi(t)} \neq -V'(\langle X\rangle_{\psi(t)}).$$

However, the classical equation does hold for $\langle X\rangle_{\psi(t)}$ in some special cases that we will discuss in the following examples. ◇

EXAMPLE 7.9. For a free particle, that is, $V = 0$, we have

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle P\rangle_{\psi(t)} = 0$$

so that $\langle P\rangle_{\psi(t)} = \langle P\rangle_{\psi(0)}$ is time-independent. An integration of (7.6a) thus yields

$$\langle X\rangle_{\psi(t)} = \frac{t}{m}\langle P\rangle_{\psi(0)} + \langle X\rangle_{\psi(0)}. \tag{7.7}$$

◇

PROPOSITION 7.10. *Consider Theorem 7.5 for a free particle, that is, for the Hamiltonian $H = H_0$. Then, besides (7.7), we have*

$$\langle X^2\rangle_{\psi(t)} = \langle X^2\rangle_{\psi(0)} + \frac{t}{m}\langle XP+PX\rangle_{\psi(0)} + \frac{t^2}{m^2}\langle P^2\rangle_{\psi(0)}$$

and thus the spread of the wave function in time is described by

$$(\Delta_{\psi(t)}X)^2 = (\Delta_{\psi(0)}X)^2 + \frac{t}{m}\big(\langle XP+PX\rangle_{\psi(0)} - 2\langle X\rangle_{\psi(0)}\langle P\rangle_{\psi(0)}\big) + \frac{t^2}{m^2}(\Delta_{\psi(0)}P)^2. \tag{7.8}$$

PROOF. By an application of Theorem 7.5 we find

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\langle X^2\rangle_{\psi(t)} = \frac{1}{2m}\langle[X^2,P^2]\rangle_{\psi(t)} = \frac{\mathrm{i}\hbar}{m}\langle XP+PX\rangle_{\psi(t)},$$

where we used

$$\begin{aligned} [X^2,P^2] &= [X^2,P]P + P[X^2,P] \\ &= X[X,P]P + [X,P]XP + PX[X,P] + P[X,P]X = 2\mathrm{i}\hbar(XP+PX). \end{aligned}$$

Another application of Theorem 7.5 yields

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\langle XP+PX\rangle_{\psi(t)} = \frac{1}{2m}\langle[XP+PX,P^2]\rangle_{\psi(t)} = \frac{2\mathrm{i}\hbar}{m}\langle P^2\rangle_{\psi(t)},$$

where we used

$$[XP+PX,P^2] = [XP,P^2]+[PX,P^2] = [X,P^2]P+P[X,P^2] = 4\mathrm{i}\hbar P^2.$$

All together we thus find

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}\langle X^2\rangle_{\psi(t)} = \frac{2}{m^2}\langle P^2\rangle_{\psi(t)} = \frac{2}{m^2}\langle P^2\rangle_{\psi(0)}.$$

The last step can be seen, e.g., from the fact that the probability density for the momentum operator for a free particle is time-independent. Integrating these equations, we obtain the desired result for $\langle X^2\rangle_{\psi(t)}$. The equation for $(\Delta_{\psi(t)}X)^2$ can now be obtained by direct calculation. □

EXAMPLE 7.11. Consider the time evolution of a Gaussian wavepacket

$$\psi(x,0) = (\sqrt{\pi}l)^{-\frac{1}{2}}\exp\left(-\frac{x^2}{2\ell^2}\right).$$

We can extrapolate useful information about the dynamics without actually computing the wave function at later time, $\psi(x,t)$, as we did in Sec. 7.3. In fact, we can substitute $\langle X\rangle_{\psi_0}=0$ and $\langle P\rangle_{\psi_0}=0$ into (7.7) to deduce that $\langle X\rangle_{\psi(t)}=0$, i.e. the expectation value of position remains zero for all $t>0$. Moreover, we can use Eq. (7.8) to compute the spread of the wave function. We know that $(\Delta_{\psi(0)}X)^2=\ell^2/2$ and $(\Delta_{\psi(0)}P)^2=\hbar^2/(2\ell^2)$. Besides, we can show that

$$\begin{aligned}\langle XP+PX\rangle_{\psi(0)} =& 2\langle XP\rangle_{\psi(0)} - i\hbar\langle\mathbb{1}\rangle_{\psi(0)}\\ =& 2\frac{i\hbar}{2} - i\hbar = 0\end{aligned}$$

thus Eq. (7.8) returns

$$(\Delta_{\psi(t)}X)^2 = \frac{\ell^2}{2}\left(1+\frac{\hbar^2t^2}{m^2\ell^4}\right),$$

which agrees with our result of Eq. (7.3) ◇

7.5 THE HEISENBERG PICTURE

Let $|\varphi(0)\rangle$ be a state at time $t=0$, then $|\varphi(t)\rangle = U(t)\,|\varphi(0)\rangle = e^{-iHt/\hbar}\,|\varphi(0)\rangle$. This implies that $\langle\varphi(t)| = \langle\varphi(0)|e^{iHt/\hbar}$, hence

$$\langle\varphi(t)|A|\psi(t)\rangle = \langle\varphi(0)|e^{iHt/\hbar}Ae^{-iHt/\hbar}|\psi(0)\rangle. \tag{7.9}$$

All experimental predictions are determined by numbers of the form $\langle\varphi(t)|A|\psi(t)\rangle$, "matrix elements" of self-adjoint operators between two states.

The same matrix element is obtained if we adopt $A_H(t) := e^{iHt/\hbar}Ae^{-iHt/\hbar}$ as the operator and $|\psi_H\rangle := |\psi(0)\rangle$ as the state. Thus,

$$\langle\varphi(t)|A|\psi(t)\rangle = \langle\varphi_H|A_H(t)|\psi_H\rangle.$$

We call $A_H(t)$ the *Heisenberg operator* corresponding to A. We define the *Heisenberg state* by $|\psi_H\rangle := |\psi(0)\rangle$. Thus a Heisenberg state is time independent. When we contrast the operator A with the Heisenberg operator, we call it the *Schrödinger operator*. Similarly, we call the state $|\psi(t)\rangle$ the *Schrödinger state*. In the Heisenberg picture, the time evolution is attributed to operators. Hence we need an equation describing the time evolution of $A_H(t)$.

In deriving the time-evolution equation for $A_H(t)$ it is useful to note that differentiation of an operator $f(A,t)$ with respect to t has to be done "locally". We illustrate this in an example.

EXAMPLE 7.12. Suppose $[A,B] \neq 0$ and $[A,C] \neq 0$. Then,

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(Be^{At}C\right) = BAe^{At}C = Be^{At}AC.$$

This derivative is not equal to $ABe^{At}C$ or $Be^{At}CA$ in general. ◇

An important fact to note is the following,

$$H_H(t) = e^{iHt/\hbar}He^{-iHt/\hbar} = e^{iHt/\hbar}e^{-iHt/\hbar}H = H$$

where the second step follows immediately if we substitute the power series expansion (7.4), whereas the last step follows by unitarity.

THEOREM 7.13 (THE HEISENBERG EQUATION OF MOTION). *If the operator A in the Schrödinger picture is time-independent, then the corresponding Heisenberg operator $A_H(t)$ satisfies*

$$\frac{\mathrm{d}A_H(t)}{\mathrm{d}t} = \frac{1}{i\hbar}\left[A_H(t), H_H(t)\right].$$

PROOF. We have

$$\begin{aligned}
i\hbar\frac{\mathrm{d}}{\mathrm{d}t}A_H(t) &= i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\left(e^{iHt/\hbar}Ae^{-iHt/\hbar}\right)\\
&= i\hbar\left\{\frac{i}{\hbar}He^{iHt/\hbar}Ae^{-iHt/\hbar} + e^{iHt/\hbar}Ae^{-iHt/\hbar}\left(-\frac{i}{\hbar}H\right)\right\}\\
&= -HA_H(t) + A_H(t)H\\
&= [A_H(t), H]\\
&= \left[A_H(t), H_H(t)\right],
\end{aligned}$$

where we have used the equality $H = H_H(t)$ in the last line. The equation to be proved is obtained by dividing this by $i\hbar$. □

In applying the Heisenberg equation of motion we use the fact that operator relations in the Schrödinger picture are valid in the Heisenberg picture. Let us show this fact. Let $U_t := e^{-iHt/\hbar}$, we have $\Omega_H(t) = U_t^*\Omega U_t$

1. If $A = A^*$, then $A_H^*(t) = (U_t^* A U_t)^* = U_t^* A^* U_t^{**} = U_t^* A U_t = A_H(t)$. Thus, if A is self-adjoint, so is $A_H(t)$.

2. If $A = A^*$, then $(f(A))_H(t) = U_t^* f(A) U_t = f(U_t^* A U_t) = f(A_H(t))$ (proof of the second equality left as an exercise, see Problem Set 4).

3. $(AB)_H(t) = A_H(t)B_H(t)$ because $A_H(t)B_H(t) = U_t^* A U_t U_t^* B U_t = U_t^* A B U_t = (AB)_H(t)$ because $U_t U_t^* = \mathbb{1}$. This implies that

$$[A, B] = C \Rightarrow [A_H, B_H] = C_H.$$

Thus, commutation relations are the same in the Schrödinger and Heisenberg pictures.

8 *Symmetries in quantum mechanics*

We start by discussing the relation between space translations for a quantum particle and the momentum operator, as well as the relation between rotations and the angular momentum operator. Then, we will discuss symmetries in quantum mechanics.

8.1 SPACE TRANSLATIONS AND THE MOMENTUM OPERATOR

We consider a quantum particle on a line with wave function $\psi(x)$. The translation operator $T(a) : L^2(\mathbb{R}) \to L^2(\mathbb{R})$, which translates ψ by a, is defined by

$$(T(a)\psi)(x) = \psi(x-a).$$

The operator $T(a)$ maps a function ψ to a function $T(a)\psi$.

PROPOSITION 8.1. *The operator $T(a)$, $a \in \mathbb{R}$, is unitary.*

PROOF. It is a bijection, i.e. its inverse exists: $T^{-1}(a) = T(-a)$. Also, the inner product is preserved:

$$\begin{aligned}\langle T(a)\psi | T(a)\varphi\rangle &= \int_{-\infty}^{\infty} \overline{(T(a)\psi)(x)}(T(a)\varphi)(x)\,\mathrm{d}x \\ &= \int_{-\infty}^{\infty} \overline{\psi(x-a)}\varphi(x-a)\,\mathrm{d}x \\ &= \int_{-\infty}^{\infty} \overline{\psi(y)}\varphi(y)\,\mathrm{d}y \qquad (y = x-a) \\ &= \langle\psi|\varphi\rangle.\end{aligned}$$

Hence $T(a)$ is an inner-product preserving bijection, i.e. a unitary. □

Now, the definition of the momentum operator $P = -i\hbar\dfrac{d}{dx}$ implies $\dfrac{d}{dx} = iP/\hbar$. Using this and the Taylor expansion, we can relate the translation operator $T(a)$ with the momentum operator P.

THEOREM 8.2. $T(a) = e^{-iaP/\hbar}$.

PROOF. We use a Taylor expansion, assuming that it is convergent for the wave function in question. Recall

$$\psi(x+\Delta x) = \psi(x) + \sum_{n=1}^{\infty} \psi^{(n)}(x)\frac{(\Delta x)^n}{n!}.$$

Using this formula with $\Delta x = -a$ we find

$$\begin{aligned}(T(a)\psi)(x) &= \psi(x-a)\\ &= \psi(x) + \sum_{n=1}^{\infty} \frac{(-a)^n}{n!}\frac{d^n}{dx^n}\psi(x)\\ &= \left[1 + \sum_{n=1}^{\infty} \frac{1}{n!}\left(-a\frac{d}{dx}\right)^n\right]\psi(x).\end{aligned}$$

Now we substitute $\dfrac{d}{dx} = iP/\hbar$ to find

$$\begin{aligned}(T(a)\psi)(x) &= \left[1 + \sum_{n=1}^{\infty} \frac{1}{n!}\left(-iaP/\hbar\right)^n\right]\psi(x)\\ &= (e^{-iaP/\hbar}\psi)(x).\end{aligned}$$

Hence $T(a) = e^{-iaP/\hbar}$. □

8.2 GENERATORS OF UNITARY OPERATORS

The relation between the translation operators $T(a)$ the momentum operator P we established is an example of a self-adjoint operator "generating" a one-parameter family of unitary operators. Note that $\{T(a)\}_{a\in\mathbb{R}}$ is a one-parameter family of unitary operators satisfying $T(a)T(b) = T(a+b)$, for all $a, b \in \mathbb{R}$. We state the following theorem without proof.

THEOREM 8.3 (STONE'S THEOREM). *If a one-parameter family of unitary operators $U(a)$ satisfies $U(a)U(b) = U(a+b)$ for all $a, b \in \mathbb{R}$ (with some further technical conditions), then there is a unique self-adjoint operator A such that $U(a) = e^{-iaA/\hbar}$.*

(The technical conditions are satisfied for the cases we treat in this module.) The operator A in this theorem is called the *generator* of the one-parameter family of unitary operators $\{U(a)\}_{a\in\mathbb{R}}$.

For $U(a) = T(a)$, $A = P$. The momentum operator P is the generator of space translations for the quantum particle on a line. An analogous relation holds in classical mechanics.

8.3 ROTATIONS AND THE ANGULAR MOMENTUM OPERATOR

Consider a quantum particle in three dimensions with wave function $\psi(x, y, z) = \Psi(r, \theta, \phi)$ in spherical polar coordinates: The rotation operator $R(\phi_0\mathbf{e}_3)$,

which rotates the wave functions about the z-axis through an angle ϕ_0, is defined by

$$(R(\phi_0\mathbf{e}_3)\Psi)(r,\theta,\phi) = \Psi(r,\theta,\phi-\phi_0).$$

Here, the vector $\mathbf{e}_3$ is the unit vector in the z-direction. Recall

$$L_3 = L_z = -\mathrm{i}\hbar\frac{\partial}{\partial\phi}\,.$$

Recall also that from

$$(T(a)\psi)(x) = \psi(x-a)\,,$$
$$P = -i\hbar\frac{d}{dx}\,,$$

we found

$$T(a) = e^{-iaP/\hbar}\,.$$

With $x \leftrightarrow \phi$ and $a \leftrightarrow \phi_0$, we have

$$R(\phi_0\mathbf{e}_3) = e^{-i\phi_0 L_3/\hbar} = \mathrm{e}^{-\mathrm{i}\phi_0\mathbf{e}_3\cdot\mathbf{L}}\,,$$

where $\mathbf{L} = (L_1, L_2, L_3)$. By rotational symmetry for the rotation operator $R(\phi_0\mathbf{n})$ for a rotation about the axis parallel to $\mathbf{n} = (n_1, n_2, n_3)$ ($\|\mathbf{n}\| = 1$) through an angle ϕ_0 can be expressed as

$$R(\phi_0\mathbf{n}) = \mathrm{e}^{-\mathrm{i}\phi_0\mathbf{n}\cdot\mathbf{L}/\hbar}\,. \tag{8.1}$$

8.4 PASSIVE TRANSFORMATIONS

To find the change of the system under a unitary transformation U, e.g., space translation, we let

$$|\psi\rangle \mapsto U|\psi\rangle, \quad A \to A. \tag{8.2}$$

Then,

$$\langle\psi|A|\varphi\rangle \mapsto \langle\psi|U^*AU|\varphi\rangle\,. \tag{8.3}$$

The effect of the unitary transformation can be attributed to the operators by letting

$$|\psi\rangle \mapsto |\psi\rangle, \quad A \to U^*AU\,. \tag{8.4}$$

The transformations (8.2) and (8.4) are equivalent in the sense that they both lead to (8.3).

We say that transformation (8.2) is in the *active* transformation picture and transformation (8.4) is in the *passive* transformation picture. The relation between the active and passive transformation pictures is analogous to that between the Schrödinger and Heisenberg pictures.

We now examine how the position operator is transformed under space translation in the passive transformation picture.

PROPOSITION 8.4. $T^*(a)XT(a) = X + a\mathbb{1}$.

PROOF. Define $\Omega(a) := T^*(a)XT(a)$. Recall that $T(a) = e^{-iaP/\hbar}$ and $T^*(a) = e^{iaP/\hbar}$. We are going to use a differential equation satisfied by $\Omega(a)$. First we note

$$\frac{dT(a)}{da} = -\frac{iP}{\hbar}T(a),$$
$$\frac{dT^*(a)}{da} = T^*(a)\frac{iP}{\hbar}.$$

Note that he operators $T(a) = e^{-iaP/\hbar}$ and P commute, so P may be placed before or after $T(a)$. Then we find

$$\begin{aligned}\frac{d}{da}\Omega(a) &= \frac{dT^*(a)}{da}XT(a) + T^*(a)X\frac{dT(a)}{da}\\ &= \frac{i}{\hbar}\left[T^*(a)PXT(a) - T^*(a)XPT(a)\right]\\ &= \frac{i}{\hbar}T^*(a)[P,X]T(a)\\ &= \frac{i}{\hbar}T^*(a)(-i\hbar\mathbb{1})T(a)\\ &= \mathbb{1}\,.\end{aligned}$$

Hence

$$\Omega(a) - \Omega(0) = \int_0^a \mathbb{1}\, da = a\mathbb{1}.$$

Since $\Omega(0) = T^*(0)XT(0) = X$ since $T(0) = T^*(0) = \mathbb{1}$, we find $\Omega(a) = X + a\mathbb{1}$, i.e. $T^*(a)XT(a) = X + a\mathbb{1}$. □

8.5 SYMMETRIES OF THE HAMILTONIAN

DEFINITION 8.5. If the Hamiltonian H is invariant under the transformation by a unitary operator U, i.e. if $U^*HU = H$, then this transformation is said to be a *symmetry* of the Hamiltonian H. ◇

We note that by multiplying the equation $U^*HU = H$ by U from the left, we find $HU = HU$. Thus, if U is a symmetry of H, then $[U, H] = 0$.

PROPOSITION 8.6. *If a one-parameter family of unitary operators $U(a) = e^{-iaA/\hbar}$ is composed of symmetries of H, then its generator A commutes with H.*

PROOF.

$$\frac{d}{da}\left[e^{-iaA/\hbar}, H\right] = \left[-\frac{i}{\hbar}Ae^{-iaA/\hbar}, H\right] = 0\,.$$

Hence, $[Ae^{-iaA/\hbar}, H] = 0$. By letting $a = 0$ we find $[A, H] = 0$. □

This means that if $U(a) = e^{-iaA/\hbar}$, where A is self-adjoint, is a symmetry of H, then A and H are compatible. Then, by Theorem 6.7, there is an orthormal basis of the Hilbert space composed of eigenstates of both H and A. Thus, the energy eigenstates constituting the orthonormal basis of the

Hilbert space can be chosen to be eigenstates of A as well. Moreover, since the expectation value of an arbitrary observable A obeys

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\langle A\rangle_{\psi(t)} = \langle [A,H]\rangle_{\psi(t)}$$

(see Eq. (7.5)), it turns out that observables A commuting with H correspond to *conserved quantities*, $\langle A\rangle_{\psi(t)} = \langle A\rangle_{\psi(0)}$ for all t. Notice the analogy with the classical scenario, wherein the conserved quantities (or constants of motion) correspond to those whose Poisson bracket with the Hamiltonian $\mathscr{H}$ vanishes.

We can see this in the Heisenberg picture as well, we have

$$\frac{d}{dt}A_H = \frac{1}{i\hbar}[A_H, H_H] = 0\,.$$

Thus, the Heisenberg operator A_H will be time-independent and equal to its Schrödinger-picture counterpart $A = A_H(0)$. That implies that that $\langle A(t)\rangle_{\psi_H} = \langle A(0)\rangle_{\psi_H}$ is constant in time.

EXAMPLE 8.7. Consider the Hamiltonian for a quantum particle in three dimensions in the presence of a central potential

$$H = \frac{1}{2m}\mathbf{P}^2 + V(\mathbf{X}),$$

where $V(\mathbf{x})$ depends only on $r = \|\mathbf{x}\|$. This Hamiltonian is invariant under rotations. Hence, the generators of rotations, the angular momentum operator $\mathbf{L}$, commute with H: $[L_1, H] = [L_2, H] = [L_3, H] = 0$. Hence $[\mathbf{L}^2, H] = [L_3, H] = 0$.

An orthonormal basis of the Hilbert space can be chosen in such a way that each basis state is an energy eigenstate that is also an eigenstate of $\mathbf{L}^2$ and L_3. The energy eigenstates are of the form $f_\ell(r)Y_\ell^m(\theta,\phi)$, where $Y_\ell{}^m(\theta,\phi)$ are spherical harmonics. These are eigenstates of $\mathbf{L}^2$ and L_3 with eigenvalues $\ell(\ell+1)\hbar^2$ and $m\hbar$, respectively. In the Heisenberg picture $\mathbf{L}_H$ is time-independent. ◇

8.5.1 Extra: Parity, a discrete symmetry

For wave functions $\psi(x)$ for a quantum particle on a line, the parity operator Π is defined by $(\Pi\psi)(x) = \psi(-x)$. We have $\Pi^{-1} = \Pi^* = \Pi$ and hence Π is unitary. We have that

$$\Pi H\psi(x) = -\frac{\hbar^2}{2m}\Pi\psi''(x) + \Pi V(x)\psi(x) = -\frac{\hbar^2}{2m}\psi''(-x) + V(-x)\psi(-x)\,,$$

whereas

$$H\Pi\psi(x) = -\frac{\hbar^2}{2m}\psi''(-x) + V(x)\psi(-x)\,.$$

Therefore, parity is a symmetry of the Hamiltonian, i.e. $[\Pi, H] = 0$ if $V(x) = V(-x)$, i.e. if $V(x)$ is an even function, e.g. for the harmonic oscillator. In that case, the energy eigenfunctions can be chosen to be

eigenfunctions of Π. Since $\Pi^2 = \mathbb{1}$, the eigenvalues of Π are ± 1. If $\varphi(x)$ is even, then $\Pi\varphi = \varphi$ and if $\varphi(x)$ is odd, then $\Pi\varphi = -\varphi$. For a quantum particle on a line, if the energy spectrum is discrete, all energy levels are known to be non-degenerate. This means that, if $V(x)$ is even, then the energy eigenstates are either even or odd. For example, for the quantum harmonic oscillator with $V(x) = \frac{1}{2}m\omega^2 x^2$, the eigenstate for the energy level $E_n = \hbar\omega(n + \frac{1}{2})$ is even if n is even and odd if n is odd.

8.6 SPIN ROTATIONS

In section 5.4, we found that the spin angular-momentum operators S_1, S_2 and S_3 are represented by 2×2 matrices acting on $\mathbb{C}^2$:

$$S_i = \frac{\hbar}{2}\sigma_i, \quad i = 1, 2, 3, \tag{8.5}$$

where

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The matrices σ_1, σ_2, σ_3 are called the Pauli spin matrices. We readily find

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

We can find the products of other components as well, and find

$$\sigma_1\sigma_2 = \mathrm{i}\sigma_3, \quad \sigma_2\sigma_3 = \mathrm{i}\sigma_1, \quad \sigma_3\sigma_1 = \mathrm{i}\sigma_2,$$
$$\sigma_2\sigma_1 = -\mathrm{i}\sigma_3, \quad \sigma_3\sigma_2 = -\mathrm{i}\sigma_1, \quad \sigma_1\sigma_3 = -\mathrm{i}\sigma_2\,.$$

Then the commutators of these matrices are

$$[\sigma_1, \sigma_2] = 2\mathrm{i}\sigma_3, \quad [\sigma_2, \sigma_3] = 2\mathrm{i}\sigma_1, \quad [\sigma_3, \sigma_1] = \mathrm{i}\sigma_2.$$

Then we can find the commutators for the spin matrices S_i given by Eq. (8.5) above. For example,

$$[S_1, S_2] = \frac{\hbar^2}{4} \cdot 2\mathrm{i}\sigma_3 = \mathrm{i}\hbar \cdot \frac{\hbar}{2}\sigma_3.$$

Thus.

$$[S_1, S_2] = \mathrm{i}\hbar S_3,$$

and similarly,

$$[S_2, S_3] = \mathrm{i}\hbar S_1\,, \quad [S_3, S_1] = \mathrm{i}\hbar S_2\,.$$

The matrix $\mathbf{S} = S_1\mathbf{e}_1 + S_2\mathbf{e}_2 + S_3\mathbf{e}_3$ describes an intrinsic angular momentum, the spin, of an electron, proton, neutron and other particles. It is also easy to verify that

$$\sigma_1^2 = \sigma_2^2 = \sigma_3^2 = \mathbb{1} \quad (2 \times 2 \text{ identity matrix}).$$

Then we find

$$\mathbf{S}^2 = \frac{\hbar^2}{4}(\sigma_1^2 + \sigma_2^2 + \sigma_3^2) = \frac{3\hbar^2}{4}\mathbb{1} = \frac{1}{2}(\frac{1}{2}+1)\hbar^2\mathbb{1}.$$

Hence, any (nonzero) $|\psi\rangle \in \mathbb{C}^2$ is an eigenvector of $\mathbf{S}^2$ with eigenvalue $j(j+1)\hbar^2$ with $j = \frac{1}{2}$.

The spin-rotation operator rotating states about the axis parallel to the unit vector $\mathbf{n}$, $\mathbf{n} = (n_1, n_2, n_3)$ with $n_1^2 + n_2^2 + n_3^2 = 1$, through an angle ϕ can be defined in analogy with the rotation operator as follows:

$$R^{(s)}(\phi\mathbf{n}) = \mathrm{e}^{-\mathrm{i}\phi\mathbf{n}\cdot\mathbf{S}/\hbar}, \quad \mathbf{S} = \frac{\hbar}{2}\boldsymbol{\sigma}.$$

By substituting Eq. (8.5) we find

$$R^{(s)}(\phi\mathbf{n}) = \mathrm{e}^{-\mathrm{i}\phi\mathbf{n}\cdot\boldsymbol{\sigma}/2}.$$

The operators $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ are the rescaled spin operators. We call $\boldsymbol{\sigma}$ the spin operators from now on.

It will be useful to simplify $(\mathbf{n}\cdot\boldsymbol{\sigma})^2$ in order to simplify the expression for $R^{(s)}(\phi\mathbf{n})$. Since

$$\mathbf{n}\cdot\boldsymbol{\sigma} = n_1\sigma_1 + n_2\sigma_2 + n_3\sigma_3,$$

we find

$$(\mathbf{n}\cdot\boldsymbol{\sigma})^2 = (n_1\sigma_1 + n_2\sigma_2 + n_3\sigma_3)(n_1\sigma_1 + n_2\sigma_2 + n_3\sigma_3).$$

Note that the cross terms cancel out: e.g.

$$\begin{aligned} n_1\sigma_1\, n_2\sigma_2 + n_2\sigma_2\, n_1\sigma_1 &= n_1n_2(\sigma_1\sigma_2 + \sigma_2\sigma_1) \\ &= n_1n_2(\mathrm{i}\sigma_3 - \mathrm{i}\sigma_3) \\ &= 0. \end{aligned}$$

Hence

$$\begin{aligned} (\mathbf{n}\cdot\boldsymbol{\sigma})^2 &= n_1^2\sigma_1^2 + n_2^2\sigma_2^2 + n_3^2\sigma_3^2 \\ &= (n_1^2 + n_2^2 + n_3^2)\mathbb{1} \\ &= \mathbb{1}. \end{aligned}$$

Alternatively one can find $(\mathbf{n}\cdot\boldsymbol{\sigma})^2$ by directly computing the square of

$$\mathbf{n}\cdot\boldsymbol{\sigma} = \begin{pmatrix} n_3 & n_1 - \mathrm{i}n_2 \\ n_1 + \mathrm{i}n_2 & -n_3 \end{pmatrix}.$$

Thus,

$$\begin{aligned}
R^{(s)}(\phi\mathbf{n}) &= \mathrm{e}^{-\mathrm{i}\phi\mathbf{n}\cdot\boldsymbol{\sigma}/2} \\
&= \sum_{j=0}^{\infty} \frac{(-\mathrm{i})^j}{j!}(\mathbf{n}\cdot\boldsymbol{\sigma})^j \left(\frac{\phi}{2}\right)^j \\
&= \sum_{k=0}^{\infty} \frac{(-\mathrm{i})^{2k}}{(2k)!}(\mathbf{n}\cdot\boldsymbol{\sigma})^{2k} \left(\frac{\phi}{2}\right)^{2k} + \sum_{k=0}^{\infty} \frac{(-\mathrm{i})^{2k+1}}{(2k+1)!}(\mathbf{n}\cdot\boldsymbol{\sigma})^{2k+1} \left(\frac{\phi}{2}\right)^{2k+1} \\
&= \mathbb{1} \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k)!} \left(\frac{\phi}{2}\right)^{2k} - \mathrm{i}\mathbf{n}\cdot\boldsymbol{\sigma} \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k+1)!} \left(\frac{\phi}{2}\right)^{2k+1} \\
&= \mathbb{1}\cos\frac{\phi}{2} - \mathrm{i}\mathbf{n}\cdot\boldsymbol{\sigma}\sin\frac{\phi}{2}.
\end{aligned}$$

Thus we find that the spin-rotation matrix is given by

$$R^{(s)}(\phi\mathbf{n}) = \mathbb{1}\cos\frac{\phi}{2} - \mathrm{i}\mathbf{n}\cdot\boldsymbol{\sigma}\sin\frac{\phi}{2}. \tag{8.6}$$

We'll find in what sense this matrix rotates spin states. Before doing so, we derive some important facts about spin states.

DEFINITION 8.8. For a given spin state $|\psi\rangle \in \mathbb{C}^2$, we call the the three-dimensional vector

$$\mathbf{m} = \langle\psi|\boldsymbol{\sigma}|\psi\rangle = \left(\langle\psi|\sigma_1|\psi\rangle, \langle\psi|\sigma_2|\psi\rangle, \langle\psi|\sigma_3|\psi\rangle\right).$$

the associated *direction of the spin*. ◇

This is always a unit vector, as per the following lemma.

LEMMA 8.9. $\|\mathbf{m}\| = 1$ *for all* $|\psi\rangle = \begin{pmatrix} a \\ b \end{pmatrix} \in \mathbb{C}^2$ *with* $|a|^2 + |b|^2 = 1$.

PROOF. Proof left as an exercise. □

Equivalently, we can define the spin direction of the state $|\psi\rangle$ to be the unit vector $\mathbf{m}$ such that $\mathbf{m}\cdot\boldsymbol{\sigma}\,|\psi\rangle = |\psi\rangle$, i.e. the direction $\mathbf{m}$ for which $|\psi\rangle$ is the eigenstate of the operator $\mathbf{m}\cdot\boldsymbol{\sigma}$ with eigenvalue $+1$. The following lemma shows the equivalence.

LEMMA 8.10. *Let* $\mathbf{m}$ *be a vector in space of unit length. Then* $\mathbf{m} = \langle\psi|\boldsymbol{\sigma}|\psi\rangle \Leftrightarrow \mathbf{m}\cdot\boldsymbol{\sigma}|\psi\rangle = |\psi\rangle$.

PROOF. We have

$$\mathbf{m}\cdot\boldsymbol{\sigma}|\psi\rangle - |\psi\rangle = \mathbf{0} \Leftrightarrow \|\mathbf{m}\cdot\boldsymbol{\sigma}|\psi\rangle - |\psi\rangle\|^2 = 0\,.$$

We recall that $(\mathbf{m}\cdot\boldsymbol{\sigma})^2 = \mathbb{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ and that the matrices σ_1, σ_2 and σ_3 are Hermitian. Now,

$$\begin{aligned}
\|\mathbf{m}\cdot\boldsymbol{\sigma}|\psi\rangle - |\psi\rangle\|^2 &= (\langle\psi|\mathbf{m}\cdot\boldsymbol{\sigma} - \langle\psi|)(\mathbf{m}\cdot\boldsymbol{\sigma}|\psi\rangle - |\psi\rangle) \\
&= \langle\psi|(\mathbf{m}\cdot\boldsymbol{\sigma})^2|\psi\rangle - 2\langle\psi|\mathbf{m}\cdot\boldsymbol{\sigma}|\psi\rangle + \langle\psi|\psi\rangle \\
&= 2(1 - \langle\psi|\mathbf{m}\cdot\boldsymbol{\sigma}|\psi\rangle)\,.
\end{aligned}$$

Hence,

$$\mathbf{m}\cdot\boldsymbol{\sigma}|\psi\rangle = |\psi\rangle \Leftrightarrow \langle\psi|\mathbf{m}\cdot\boldsymbol{\sigma}|\psi\rangle = 1 \Leftrightarrow \mathbf{m} = \langle\psi|\boldsymbol{\sigma}|\psi\rangle\,,$$

as required. □

EXAMPLE 8.11. The state $|\uparrow\rangle = \begin{pmatrix}1\\0\end{pmatrix}$ is an eigenstate of $\sigma_3 = \begin{pmatrix}1 & 0\\0 & -1\end{pmatrix}$ with eigenvalue 1. $\sigma_3 = \mathbf{m}\cdot\boldsymbol{\sigma}$ with $\mathbf{m} = (0,0,1)$. Thus, the state $|\uparrow\rangle$ has the spin in the z-direction. ◇

We now discuss how spin-rotation matrices operate on spin states.

THEOREM 8.12. *Suppose that the vector* $\mathbf{m}$ *in space is rotated to* $\mathbf{m}'$ *under the rotation about the axis parallel to the unit vector* $\mathbf{n}$ *through angle* ϕ *as shown in Fig. 8.6. If the state* $|\psi\rangle \in \mathbb{C}^2$ *has the spin in the* $\mathbf{m}$*-direction, then the state* $R^{(s)}(\phi\mathbf{n})|\psi\rangle$ *has the spin in the* $\mathbf{m}'$*-direction.*

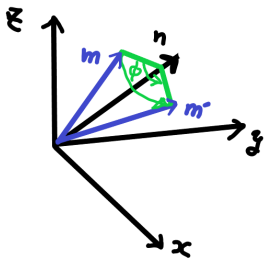

FIGURE 8.1. Sketch of the rotation of the spin direction vector by an angle ϕ about the vector $\mathbf{n}$.

We do not prove this theorem, but we examine an example illustrating it.

EXAMPLE 8.13. Recall $\sigma_1 = \begin{pmatrix}0 & 1\\1 & 0\end{pmatrix}$. The state $|+\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}$ satisfies $\sigma_1|+\rangle = |+\rangle$. Thus the state $|+\rangle$ has the spin in the x-direction. We rotate this state about the z-axis through an angle ϕ. The corresponding spin-rotation matrix is

$$\begin{aligned}
R^{(s)}(\phi\mathbf{e}_3) &= \mathbb{1}\cos\frac{\phi}{2} - \mathrm{i}\mathbf{e}_3\cdot\boldsymbol{\sigma}\sin\frac{\phi}{2}\\
&= \mathbb{1}\cos\frac{\phi}{2} - \mathrm{i}\sigma_3\sin\frac{\phi}{2} \quad \left(\sigma_3 = \begin{pmatrix}1 & 0\\0 & -1\end{pmatrix}\right)\\
&= \begin{pmatrix}\cos\frac{\phi}{2} - \mathrm{i}\sin\frac{\phi}{2} & 0\\ 0 & \cos\frac{\phi}{2} + \mathrm{i}\sin\frac{\phi}{2}\end{pmatrix}\\
&= \begin{pmatrix}\mathrm{e}^{-\mathrm{i}\phi/2} & 0\\ 0 & \mathrm{e}^{\mathrm{i}\phi/2}\end{pmatrix}.
\end{aligned}$$

Then

$$R^{(s)}(\phi\mathbf{e}_3)|+\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} \mathrm{e}^{-\mathrm{i}\phi/2} \\ \mathrm{e}^{\mathrm{i}\phi/2} \end{pmatrix}.$$

Since $\mathbf{m} = (1,0,0) \mapsto \mathbf{m}' = (\cos\phi, \sin\phi, 0)$ under this rotation, the state $R^{(s)}(\phi\mathbf{e}_3)|+\rangle$ should be an eigenstate of $\mathbf{m}' \cdot \boldsymbol{\sigma}$ with $\mathbf{m}' = (\cos\phi, \sin\phi, 0)$. We have

$$\begin{aligned} \mathbf{m}' \cdot \boldsymbol{\sigma} &= \cos\phi \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \sin\phi \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix} \\ &= \begin{pmatrix} 0 & \mathrm{e}^{-\mathrm{i}\phi} \\ \mathrm{e}^{\mathrm{i}\phi} & 0 \end{pmatrix}. \end{aligned}$$

Then, we have indeed

$$\begin{aligned} \mathbf{m}' \cdot \boldsymbol{\sigma} R^{(s)}(\phi\mathbf{e}_3)|+\rangle &= \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & \mathrm{e}^{-\mathrm{i}\phi} \\ \mathrm{e}^{\mathrm{i}\phi} & 0 \end{pmatrix} \begin{pmatrix} \mathrm{e}^{-\mathrm{i}\phi/2} \\ \mathrm{e}^{\mathrm{i}\phi/2} \end{pmatrix} \\ &= \frac{1}{\sqrt{2}} \begin{pmatrix} \mathrm{e}^{-\mathrm{i}\phi/2} \\ \mathrm{e}^{\mathrm{i}\phi/2} \end{pmatrix} = R^{(s)}(\phi\mathbf{e}_3)|+\rangle. \end{aligned}$$

Thus, $R^{(s)}(\phi\mathbf{e}_3)|+\rangle$ is an eigenstate of $\mathbf{m}' \cdot \boldsymbol{\sigma}$ with eigenvalue 1. ◇

8.6.1 Extra: $SO(3)$ and $SU(2)$

In this extra *non-examinable* section, we examine the relation between the spin-rotation matrices and the real 3×3 matrices that rotate three-dimensional vectors.

We saw that the (complex) spin-rotation matrices $R^{(s)}(\phi\mathbf{n})$ are 2×2 unitary matrices. The group of unitary matrices in n dimensions is called the unitary group of degree n and denoted by $U(n)$. Thus, $R^{(s)}(\phi\mathbf{n}) \in U(2)$. It is easy to show that $\det R^{(s)}(\phi\mathbf{n}) = 1$. The subgroup of $U(n)$ with the condition that the determinant is 1 is called the special unitary group of degree n and denoted by $SU(n)$. Thus, $R^{(s)}(\phi\mathbf{n}) \in SU(2)$. It can be shown that all elements of $SU(2)$ is a spin-rotation matrix with some ϕ and $\mathbf{n}$.

Now consider rotations of real three-dimensional vectors. If we represent the three unit vectors along the x- y- and z-axes, as

$$\mathbf{e}_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad \mathbf{e}_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad \mathbf{e}_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix},$$

then, for example, the matrix representing the rotation about the z-axis through an angle ϕ is

$$R^{(v)}(\phi\mathbf{e}_3) = \begin{pmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Let $R^{(v)}(\phi\mathbf{n})$ denote the matrix for the rotation about the axis parallel to $\mathbf{n}$ through and angle ϕ. These matrices form a group.

If $\mathbf{V} = R\mathbf{v}$ and $\mathbf{W} = R\mathbf{w}$, where R is a rotation matrix, then the dot product is conserved, i.e. $\mathbf{V}^T\mathbf{W} = \mathbf{v}^T\mathbf{w}$:

$$\mathbf{V}^T\mathbf{W} = \mathbf{v}^T R^T R\mathbf{w} = \mathbf{v}^T\mathbf{w}\,,$$

for all vectors $\mathbf{v}$ and $\mathbf{w}$. Hence $R^T R = \mathbb{1}$ and hence $R^T = R^{-1}$ since R acts on a finite dimensional Hilbert space.

The group formed by the n-dimensional real matrices R satisfying $R^T R = \mathbb{1}$ is called an orthogonal group of degree n and denoted by $O(n)$. We also note that

$$\det(R^T R) = \det(\mathbb{1}) = 1\,,$$

but $\det(R^T R) = \det(R^T)\det(R) = (\det(R))^2$. Hence $\det(R) = \pm 1$. If $R = R(\phi\mathbf{n})$, then $\det(R(\phi\mathbf{n}))$ must be a continuous function of ϕ, but it is either 1 or -1, and it is 1 for $\phi = 0$. Hence we must have $\det(R) = 1$. The subgroup of $O(n)$ with the condition $\det(R) = 1$ is called the special orthogonal group of degree n and denoted by $SO(n)$. Thus, the rotations in 3 dimensions form the group $SO(3)$.

We ask the question: what is the relation between $SU(2)$ and $SO(3)$? We can define a map $f : SU(2) \to SO(3)$ by

$$R^{(s)}(\phi\mathbf{n}) \mapsto R^{(v)}(\phi\mathbf{n})\,.$$

This map preserves the group multiplication. That is, if $R_1^{(s)} \mapsto R_1^{(v)}$ and $R_2^{(s)} \mapsto R_2^{(v)}$, then $R_1^{(s)} R_2^{(s)} \mapsto R_1^{(v)} R_2^{(v)}$. A map between two groups with this property is called a homomorphism.

An important observation is that in $SU(2)$ the 2π-rotation is not represented by the identity matrix. For any $\mathbf{n}$ we have

$$R^{(s)}(2\pi\mathbf{n}) = \mathbb{1}\cos\pi - \mathrm{i}\mathbf{n}\cdot\boldsymbol{\sigma}\sin\pi = -\mathbb{1}.$$

Thus, in $SU(2)$ the 2π-rotation about any axis is given by $-\mathbb{1}$. Hence

$$R^{(s)}((\phi + 2\pi)\mathbf{n}) = R^{(s)}(2\pi\mathbf{n})R^{(s)}(\phi\mathbf{n}) = -R^{(s)}(\phi\mathbf{n}).$$

In $SO(3)$ we have $R^{(v)}((\phi + 2\pi)\mathbf{n}) = R^{(v)}(\phi\mathbf{n})$. Thus, both $R^{(s)}(\phi\mathbf{n})$ and $R^{(s)}((\phi + 2\pi)\mathbf{n}) = -R^{(s)}(\phi\mathbf{n})$ in $SU(2)$ correspond to $R^{(v)}(\phi\mathbf{n})$ in $SO(3)$. Thus, we have a 2-1 homomorphism from $SU(2)$ to $SO(3)$. This observation is related to the fact that the 2π-rotation cannot be undone but the 4π-rotation can (see https://en.wikipedia.org/wiki/Plate_trick).

9 *Systems of multiple particles*

Up to now, our discussions have centered around *single* systems in quantum mechanics. In this chapter, we shift our focus to *composite* systems. The characterisation of quantum states for composite systems requires a postulate of its own, complementing those outlined in Sec. 1.5.2.

- **Postulate 5 (Composite systems)**. The state of a system composed of N particles, each described by a Hilbert space $\mathcal{H}^{(i)}$, $i = 1 \dots N$, is given by a unit vector in the *tensor product* Hilbert space $\mathcal{H}^{(1)} \otimes \mathcal{H}^{(2)} \otimes \cdots \otimes \mathcal{H}^{(N)}$.

Consider the simplest case of two particles. If $\mathcal{H}^{(1)}$ has an orthonormal basis $\{|\alpha_m^{(1)}\rangle\}$ and $\mathcal{H}^{(2)}$ has an orthonormal basis $\{|\alpha_n^{(2)}\rangle\}$, then the *tensor product* of $\mathcal{H}^{(1)}$ and $\mathcal{H}^{(2)}$, denoted by $\mathcal{H}^{(1)} \otimes \mathcal{H}^{(2)}$, is the space of all (normalisable) states of the form

$$\sum_{m,n} c_{m,n} |\alpha_m^{(1)}\rangle \otimes |\alpha_n^{(2)}\rangle, \quad \sum_{m,n} |c_{m,n}|^2 < \infty.$$

After a brief discussion of bi-partite (i.e. with *two* constituents) composite systems of *distinguishable* particles, we will focus on bi-partite composite systems of *identical* (i.e. indistinguishable) particles, for which not all elements of $\mathcal{H} \otimes \mathcal{H}$ represent valid states. We conclude with a generalisation to systems of N identical particles.

9.1 TWO DISTINGUISHABLE PARTICLES

Consider the system of two *distinguishable* particles 1 and 2 described by the Hilbert spaces $\mathcal{H}^{(1)}$ and $\mathcal{H}^{(2)}$, respectively. The composite state with particle 1 in the state $|\psi^{(1)}\rangle \in \mathcal{H}^{(1)}$ and particle 2 in the state $|\psi^{(2)}\rangle \in \mathcal{H}^{(2)}$ is denoted by $|\psi^{(1)}\rangle \otimes |\psi^{(2)}\rangle$, the tensor product of $|\psi^{(1)}\rangle$ and $|\psi^{(2)}\rangle$.

The inner product of $|\Psi\rangle = |\psi^{(1)}\rangle \otimes |\psi^{(2)}\rangle$ and $|\Phi\rangle = |\varphi^{(1)}\rangle \otimes |\varphi^{(2)}\rangle$ is

$$\langle \Psi | \Phi \rangle = \langle \psi^{(1)} | \varphi^{(1)} \rangle \langle \psi^{(2)} | \varphi^{(2)} \rangle.$$

If both particles 1 and 2 were described by the same Hilbert space $\mathcal{H}$ with orthonormal basis $\{|\alpha_n\rangle\}$, then the composite system of particles 1 and 2 would be described by $\mathcal{H} \otimes \mathcal{H}$ consisting of the (normalisable) states of the form

$$\sum_{m,n} c_{m,n} |\alpha_m\rangle \otimes |\alpha_n\rangle.$$

9.2 TWO IDENTICAL PARTICLES

What is the Hilbert space of the system consisting of two *identical* particles, e.g. photons (quanta of electromagnetic waves), each described by the Hilbert space $\mathcal{H}$? Is it $\mathcal{H} \otimes \mathcal{H}$?

DEFINITION 9.1. For a system of identical particles, each described by the Hilbert space $\mathcal{H}$, a state $|\psi\rangle \in \mathcal{H}$ is called a *one-particle state* and the Hilbert space $\mathcal{H}$ is called the *one-particle Hilbert space*. ◇

If the system of two identical particles, each described by the one-particle Hilbert space $\mathcal{H}$, were described by $\mathcal{H} \otimes \mathcal{H}$, then there would be *two* independent two-particle states with one particle in the one-particle state $|\psi\rangle$ and the other particle in a different one-particle state $|\phi\rangle$:

$$|\psi\rangle \otimes |\phi\rangle \text{ and } |\phi\rangle \otimes |\psi\rangle.$$

As we saw in Sec. 9.1, this is fine for distinguishable particles, where the scenario "particle (1) in $|\psi\rangle$ & particle (2) in $|\phi\rangle$" can be distinguished from the scenario "particle (1) in $|\phi\rangle$ & particle (2) in $|\psi\rangle$". But if the particles are identical, we cannot identify which one is in $|\psi\rangle$ and which in $|\phi\rangle$.[17] Therefore, we expect that there should be only *one* independent state describing two identical particles, one in $|\psi\rangle$ and the other in $|\phi\rangle$.

[17] Imagine sealing two identical spheres in an box, shaking the box, and then drawing one sphere. You won't be able to tell if the one you picked was the first or second sphere that was placed in the box.

Let the *exchange operator* $\hat{X}$ (not to be confused with the position operator X) on $\mathcal{H} \otimes \mathcal{H}$ be defined by

$$\hat{X}(|\psi\rangle \otimes |\phi\rangle) = |\phi\rangle \otimes |\psi\rangle.$$

Clearly, $\hat{X}^2 = \mathbb{1}$, hence $\hat{X}$ has eigenvalues ± 1. We define the *symmetric subspace* of $\mathcal{H} \otimes \mathcal{H}$ the eigenspace of $\hat{X}$ with eigenvalue $+1$,

$$(\mathcal{H} \otimes \mathcal{H})_{\text{sym}} := \{|\Psi\rangle \in \mathcal{H} \otimes \mathcal{H} : \hat{X}|\Psi\rangle = |\Psi\rangle\},$$

and the *antisymmetric subspace* of $\mathcal{H} \otimes \mathcal{H}$ the eigenspace of $\hat{X}$ with eigenvalue -1,

$$(\mathcal{H} \otimes \mathcal{H})_{\text{antisym}} := \{|\Psi\rangle \in \mathcal{H} \otimes \mathcal{H} : \hat{X}|\Psi\rangle = -|\Psi\rangle\}.$$

A particle can be one of the following two 'species': a *Bose-Einstein* particle (*boson* in short); or a *Fermi-Dirac* particle (*fermion* in short). Then:

- The system of two identical bosons with one-particle Hilbert space $\mathcal{H}$ is described by $(\mathcal{H} \otimes \mathcal{H})_{\text{sym}}$.
- The system of two identical fermions with one-particle Hilbert space $\mathcal{H}$ is described by $(\mathcal{H} \otimes \mathcal{H})_{\text{antisym}}$.

Photons are bosons whereas electrons, protons and neutrons are fermions.

REMARK 9.2. We often (but not always) denote $|\varphi\rangle \otimes |\psi\rangle$ by $|\varphi, \psi\rangle$ for simplicity. ◇

Let $\{|\varphi_n\rangle\}$ be an orthonormal basis of $\mathcal{H}$.

(*Bosons*) An orthonormal basis for $(\mathcal{H}\otimes\mathcal{H})_{\text{sym}}$, which is the state space of two identical bosons, each described by $\mathcal{H}$ consists of:

- $|\varphi_n,\varphi_n\rangle$: both bosons are in $|\varphi_n\rangle$;
- $\frac{1}{\sqrt{2}}(|\varphi_m,\varphi_n\rangle+|\varphi_n,\varphi_m\rangle)$, $m<n$: one boson is in $|\varphi_m\rangle$ and the other is in $|\varphi_n\rangle$.

(*Fermions*) An orthonormal basis for $(\mathcal{H}\otimes\mathcal{H})_{\text{antisym}}$, which is the state space of two identical fermions, consists of

- $\frac{1}{\sqrt{2}}(|\varphi_m,\varphi_n\rangle-|\varphi_n,\varphi_m\rangle)$, $m<n$: one fermion is in $|\varphi_m\rangle$ and the other is in $|\varphi_n\rangle$.

Note that there is no two-fermion state with both in the same one-particle state. This fact is known as *Pauli's exclusion principle*.

Pauli's exclusion principle. No two identical fermions can occupy the same one-particle state.

9.3 N IDENTICAL PARTICLES

Suppose $\mathcal{H}$ has an orthonormal basis $\{|\varphi_n\rangle\}$. The tensor product $\underbrace{\mathcal{H}\otimes\mathcal{H}\otimes\cdots\otimes\mathcal{H}}_{N}$ is the space of all normalisable linear combinations of vectors of the form $|\varphi_{n_1}\rangle\otimes|\varphi_{n_2}\rangle\otimes\cdots\otimes|\varphi_{n_N}\rangle$, i.e. all vectors of the form

$$\sum_{n_1}\sum_{n_2}\cdots\sum_{n_N}c_{n_1n_2\ldots n_N}|\varphi_{n_1}\rangle\otimes|\varphi_{n_2}\rangle\otimes\cdots\otimes|\varphi_{n_N}\rangle,$$

such that

$$\sum_{n_1}\sum_{n_2}\cdots\sum_{n_N}|c_{n_1n_2\ldots n_N}|^2<\infty.$$

We define the exchange operator $\hat{X}_{pq}$ by

$$\begin{aligned}&\hat{X}_{pq}(|\psi_1\rangle\otimes|\psi_2\rangle\otimes\cdots\otimes|\psi_p\rangle\otimes\cdots\otimes|\psi_q\rangle\otimes\cdots|\psi_N\rangle\\&=|\psi_1\rangle\otimes|\psi_2\rangle\otimes\cdots\otimes|\psi_q\rangle\otimes\cdots\otimes|\psi_p\rangle\otimes\cdots|\psi_N\rangle,\end{aligned}$$

where $|\psi_p\rangle$ and $|\psi_q\rangle$ are in the pth and qth slots, respectively, in the first line and in the qth and pth slots, respectively, in the second line.

We define the *symmetric subspace* of $\underbrace{\mathcal{H}\otimes\mathcal{H}\otimes\cdots\otimes\mathcal{H}}_{N}$ by

$$(\underbrace{\mathcal{H}\otimes\mathcal{H}\otimes\cdots\otimes\mathcal{H}}_{N})_{\text{sym}}:=\{|\Psi\rangle\in\underbrace{\mathcal{H}\otimes\mathcal{H}\otimes\cdots\otimes\mathcal{H}}_{N}:\forall p\forall q\ \ \hat{X}_{pq}|\Psi\rangle=|\Psi\rangle\}$$

We define the *anti-symmetric subspace* of $\underbrace{\mathcal{H}\otimes\mathcal{H}\otimes\cdots\otimes\mathcal{H}}_{N}$ by

$$(\underbrace{\mathcal{H}\otimes\mathcal{H}\otimes\cdots\otimes\mathcal{H}}_{N})_{\text{antisym}}:=\{|\Psi\rangle\in\underbrace{\mathcal{H}\otimes\mathcal{H}\otimes\cdots\otimes\mathcal{H}}_{N}:\forall p\forall q\ \ \hat{X}_{pq}|\Psi\rangle=-|\Psi\rangle\}$$

- The Hilbert space for the system of N identical bosons, each described by $\mathcal{H}$, is $(\underbrace{\mathcal{H}\otimes\mathcal{H}\otimes\cdots\otimes\mathcal{H}}_{N})_{\text{sym}}$.
- The Hilbert space for the system of N identical fermions, each described by $\mathcal{H}$, is $(\underbrace{\mathcal{H}\otimes\mathcal{H}\otimes\cdots\otimes\mathcal{H}}_{N})_{\text{antisym}}$.

Let $\{|\varphi_n\rangle\}$ be an orthonormal basis of $\mathcal{H}$.

(*Fermions*) The space $(\mathcal{H}\otimes\mathcal{H}\otimes\mathcal{H})_{\text{antisym}}$, the Hilbert space for three identical fermions with one-particle Hilbert space $\mathcal{H}$, is spanned by — we use an abbreviation $|\varphi_k,\varphi_m,\varphi_n\rangle := |\varphi_k\rangle\otimes|\varphi_m\rangle\otimes|\varphi_n\rangle$:

$$\frac{1}{\sqrt{6}}(|\varphi_k,\varphi_m,\varphi_n\rangle - |\varphi_k,\varphi_n,\varphi_m\rangle - |\varphi_m,\varphi_k,\varphi_n\rangle + |\varphi_m,\varphi_n,\varphi_k\rangle + |\varphi_n,\varphi_k,\varphi_m\rangle - |\varphi_n,\varphi_m,\varphi_k\rangle),\quad k<m<n.$$

(One fermion occupies each of the one-particle states $|\varphi_k\rangle$, $|\varphi_m\rangle$ and $|\varphi_n\rangle$).

(*Bosons*) The space $(\mathcal{H}\otimes\mathcal{H}\otimes\mathcal{H})_{\text{sym}}$, a Hilbert space for three identical bosons with one-particle Hilbert space $\mathcal{H}$, is spanned by

$$\frac{1}{\sqrt{6}}(|\varphi_k,\varphi_m,\varphi_n\rangle + |\varphi_k,\varphi_n,\varphi_m\rangle + |\varphi_m,\varphi_k,\varphi_n\rangle + |\varphi_m,\varphi_n,\varphi_k\rangle + |\varphi_n,\varphi_k,\varphi_m\rangle + |\varphi_n,\varphi_m,\varphi_k\rangle),\quad k<m<n,$$

(One boson occupies each of the one-particle states $|\varphi_k\rangle$, $|\varphi_m\rangle$ and $|\varphi_n\rangle$);

$$\frac{1}{\sqrt{3}}(|\varphi_m,\varphi_n,\varphi_n\rangle + |\varphi_n,\varphi_m,\varphi_n\rangle + |\varphi_n,\varphi_n,\varphi_m\rangle),\quad m\neq n,$$

(Two bosons occupy the one-particle state $|\varphi_n\rangle$ and one boson occupies the one-particle state $|\varphi_m\rangle$);

$$|\varphi_n,\varphi_n,\varphi_n\rangle.$$

(All three identical bosons occupy the one-particle state $|\varphi_n\rangle$.)

10 Perturbation theory and the variational method

We will first discuss *first-order time-independent* perturbation theory (both the non-degenerate and degenerate cases), after which we will focus on the *variational method* for obtaining approximate energies.

10.1 TIME-INDEPENDENT PERTURBATION THEORY

10.1.1 The non-degenerate case

Suppose we want to solve the time-independent Schrödinger equation

$$H|\varphi\rangle = E|\varphi\rangle,$$

with $H = H^{(0)} + H^{(1)}$. Suppose we know the solution to the eigenvalue equation $H^{(0)}|\varphi^{(0)}\rangle = E^{(0)}|\varphi^{(0)}\rangle$, $\langle\varphi^{(0)}|\varphi^{(0)}\rangle = 1$. Assuming that the effect of $H^{(1)}$ is small, we want to find an approximate solution to $H|\varphi\rangle = E|\varphi\rangle$ with $E = E^{(0)} + E^{(1)}$, $|\varphi\rangle = |\varphi^{(0)}\rangle + |\varphi^{(1)}\rangle$ such that $E^{(1)}$ and $|\varphi^{(1)}\rangle$ are small. In other words, knowing the solution to the eigenvalue problem $H^{(0)}|\varphi^{(0)}\rangle = E^{(0)}|\varphi^{(0)}\rangle$, can we find approximate solutions is we add a small "perturbation" to the Hamiltonian, which now reads $H = H^{(0)} + H^{(1)}$?

We aim to find an approximate value for $E^{(1)}$ to first order in small quantities. That is, we neglect the product of two small quantities such as $E^{(1)}|\varphi^{(1)}\rangle$. We also assume there are no other independent states with the same eigenvalue $E^{(0)}$ of $H^{(0)}$. Thus, the zeroth order energy is non-degenerate.

The equation we want study is

$$(H^{(0)} + H^{(1)})|\varphi\rangle = E|\varphi\rangle. \tag{10.1}$$

By taking the inner product of both sides with $\langle\varphi^{(0)}|$ we find

$$\langle\varphi^{(0)}|H^{(0)}|\varphi\rangle + \langle\varphi^{(0)}|H^{(1)}|\varphi\rangle = E\langle\varphi^{(0)}|\varphi\rangle. \tag{10.2}$$

Now, $H^{(0)}|\varphi^{(0)}\rangle = E^{(0)}|\varphi^{(0)}\rangle$ implies $\langle\varphi^{(0)}|H^{(0)} = E^{(0)}\langle\varphi^{(0)}|$ (note $E^{(0)}$ is a real number). Hence,

$$\langle\varphi^{(0)}|H^{(0)}|\varphi\rangle = E^{(0)}\langle\varphi^{(0)}|\varphi\rangle.$$

By substituting this equation into (10.2) we find

$$(E - E^{(0)})\langle\varphi^{(0)}|\varphi\rangle = \langle\varphi^{(0)}|H^{(1)}|\varphi\rangle.$$

We can let $\langle\varphi^{(0)}|\varphi\rangle = 1$ by redefining $|\varphi\rangle$ by multiplying it by a constant. The resulting state $|\varphi\rangle$ still satisfies Eq. (10.1) Then,

$$E - E^{(0)} = \langle\varphi^{(0)}|H^{(1)}|\varphi\rangle.$$

(Note that we have not introduced any approximation yet.) To find the energy shift $E - E^{(0)}$ to first order in $H^{(1)}$ we can approximate $|\varphi\rangle$ by the zeroth-order eigenstate $|\varphi^{(0)}\rangle$. Then,

$$E - E^{(0)} \approx \langle\varphi^{(0)}|H^{(1)}|\varphi^{(0)}\rangle.$$

Hence, the energy shift $E - E^{(0)} \approx E^{(1)}$ due to $H^{(1)}$ to first order in $H^{(1)}$ is

$$E^{(1)} = \langle\varphi^{(0)}|H^{(1)}|\varphi^{(0)}\rangle\,. \tag{10.3}$$

Note that the "energy shift" $E^{(1)}$ is not exact but just an approximation when the effect of $H^{(1)}$ in the Hamiltonian $H = H^{(0)} + H^{(1)}$ is small.

For a quantum paricle on a line with $\langle x|\varphi^{(0)}\rangle = \varphi^{(0)}(x)$ and $H^{(1)} = V^{(1)}(X)$, we have

$$\begin{aligned} E^{(1)} &= \langle\varphi^{(0)}|V^{(1)}(X)|\varphi^{(0)}\rangle \\ &= \int_{-\infty}^{\infty} \overline{\varphi^{(0)}(x)} V^{(1)}(x)\varphi^{(0)}(x)\,\mathrm{d}x \\ &= \int_{-\infty}^{\infty} V^{(1)}(x)|\varphi^{(0)}(x)|^2\,\mathrm{d}x. \end{aligned}$$

EXAMPLE 10.1. Let $H^{(0)}$ be the standard harmonic-oscillator Hamiltonian,

$$H^{(0)} = \frac{1}{2m}P^2 + \frac{1}{2}m\omega^2 X^2.$$

with the ground-state wave function,

$$\varphi^{(0)}(x) = \frac{\beta^{1/2}}{\pi^{1/4}} \exp\left(-\frac{\beta^2 x^2}{2}\right).$$

where $\beta = (m\omega/\hbar)^{1/2}$. If the potential energy is $\frac{1}{2}m\omega^2x^2 + V_1\beta^4x^4$, i.e. if

$$H^{(1)} = V_1\beta^4 X^4, \quad V_1 = \text{constant},$$

is added to the Hamiltonian, the energy shift at first order in perturbation theory is

$$\begin{aligned} E^{(1)} &= V_1 \frac{\beta^5}{\sqrt{\pi}} \int_{-\infty}^{\infty} x^4 \exp\left(-\beta^2x^2\right)\mathrm{d}x \\ &= \frac{V_1}{\sqrt{\pi}} \int_{-\infty}^{\infty} y^4 \mathrm{e}^{-y^2}\mathrm{d}y \quad (y = \beta x) \\ &= \frac{V_1}{\sqrt{\pi}} \cdot \frac{3}{4}\sqrt{\pi} \\ &= \frac{3}{4}V_1. \end{aligned}$$

The integral

$$I = \int_{-\infty}^{\infty} y^4 \mathrm{e}^{-y^2}\,\mathrm{d}y\,,$$

can be evaluated as follows.

$$\begin{aligned} I &= 2\int_0^{\infty} y^4 \mathrm{e}^{-y^2}\mathrm{d}y \\ &= \int_0^{\infty} t^{3/2}\mathrm{e}^{-t}\,\mathrm{d}t \quad (t = y^2) \\ &= \Gamma\left(\frac{5}{2}\right) \\ &= \frac{3}{2}\cdot\frac{1}{2}\Gamma\left(\frac{1}{2}\right) \\ &= \frac{3}{4}\sqrt{\pi}\,, \end{aligned}$$

where we have used the fact that Euler's Γ-function,

$$\Gamma(x) = \int_0^{\infty} t^{x-1}\mathrm{e}^{-t}\,\mathrm{d}t\,, \quad x > 0\,,$$

satisfies $\Gamma(x+1) = x\Gamma(x)$ because

$$\begin{aligned} \Gamma(x+1) &= \int_0^{\infty} t^x \mathrm{e}^{-t}\,\mathrm{d}t \\ &= \left[-t^x\mathrm{e}^{-t}\right]_{t=0}^{t=\infty} + \int_0^{\infty} x t^{x-1}\,\mathrm{e}^{-t}\,\mathrm{d}t \\ &= x\Gamma(x)\,, \end{aligned}$$

and that

$$\begin{aligned} \Gamma\left(\frac{1}{2}\right) &= \int_0^{\infty} t^{-1/2}\mathrm{e}^{-t}\,\mathrm{d}t \\ &= \int_{-\infty}^{\infty} \mathrm{e}^{-y^2}\,\mathrm{d}y \quad (y^2 = t) \\ &= \sqrt{\pi}\,. \end{aligned}$$

◇

10.1.2 The degenerate case

Suppose the orthonormal states $|\varphi_i^{(0)}\rangle$, $i = 1, 2, \ldots, D$, satisfy $H^{(0)}|\varphi_i^{(0)}\rangle = E^{(0)}|\varphi_i^{(0)}\rangle$ with the same energy $E^{(0)}$. We study

$$(H^{(0)} + H^{(1)})|\varphi_j\rangle = E_j|\varphi_j\rangle,$$

with $|\varphi_j\rangle \approx |\varphi_j^{(0)}\rangle$, $E_j \approx E^{(0)}$, assuming that the effect of $H^{(1)}$ is small. We seek to find $E_j - E^{(0)}$ approximately to first order in $H^{(1)}$.

By taking the inner product of both sides of the above equation with $\langle\varphi_i^{(0)}|$, we find

$$\langle\varphi_i^{(0)}|H^{(0)}|\varphi_j\rangle + \langle\varphi_i^{(0)}|H^{(1)}|\varphi_j\rangle = E_j\langle\varphi_i^{(0)}|\varphi_j\rangle.$$

We find $\langle\varphi_i^{(0)}|H^{(0)} = E^{(0)}\langle\varphi_i^{(0)}|$ as before. Hence

$$E^{(0)}\langle\varphi_i^{(0)}|\varphi_j\rangle + \langle\varphi_i^{(0)}|H^{(1)}|\varphi_j\rangle = E_j\langle\varphi_i^{(0)}|\varphi_j\rangle,$$

then,

$$(E_j - E^{(0)})\langle\varphi_i^{(0)}|\varphi_j\rangle = \langle\varphi_i^{(0)}|H^{(1)}|\varphi_j\rangle.$$

As before, we make the approximation $|\varphi_j\rangle \approx |\varphi_j^{(0)}\rangle$:

$$(E_j - E^{(0)})\langle\varphi_i^{(0)}|\varphi_j^{(0)}\rangle \approx \langle\varphi_i^{(0)}|H^{(1)}|\varphi_j^{(0)}\rangle.$$

The set $\{|\varphi_i^{(0)}\rangle\}_{i=1,2,\ldots,D}$ is orthonormal, i,e, $\langle\varphi_i^{(0)}|\varphi_j^{(0)}\rangle = \delta_{ij}$. Hence

$$(E_j - E^{(0)})\delta_{ij} \approx \langle\varphi_i^{(0)}|H^{(1)}|\varphi_j^{(0)}\rangle.$$

— This equation is consistent only if the matrix whose ij-element is $\langle\varphi_i^{(0)}|H^{(1)}|\varphi_j^{(0)}\rangle$ is diagonal.

— We should have started with an orthonormal basis $\{\varphi_i^{(0)}\rangle\}_{i=1,2,\ldots,D}$ of the space of states with energy $E^{(0)}$ such that the matrix with the ij-element $\langle\varphi_i^{(0)}|H^{(1)}|\varphi_j^{(0)}\rangle$ is diagonal.

If this matrix is diagonal, then $E_j \approx E^{(0)} + E_j^{(1)}$, where the energy shift for the energy eigenstate $|\varphi_j\rangle \approx |\varphi_j^{(0)}\rangle$ to first order in perturbation theory is

$$E_j^{(1)} = \langle\varphi_j^{(0)}|H^{(1)}|\varphi_j^{(0)}\rangle.$$

In practice, we proceed as follows.

Step 1 Compute the matrix whose ij-element is $\langle\varphi_i^{(0)}|H^{(1)}|\varphi_j^{(0)}\rangle$.

Step 2 If the matrix is diagonal, move to Step 3. Otherwise, pick a basis for the space of energy eigenstates with energy $E^{(0)}$ such that the matrix whose ij-element is $\langle\varphi_i^{(0)}|H^{(1)}|\varphi_j^{(0)}\rangle$ is diagonal.

Step 3 Then the approximate energy shift $E_i^{(1)}$ for the energy eigenstate $|\varphi_i\rangle \approx |\varphi_i^{(0)}\rangle$ is given by $E_i^{(1)} = \langle\varphi_i^{(0)}|H^{(1)}|\varphi_i^{(0)}\rangle$.

EXAMPLE 10.2. Consider a quantum particle on a circle of circumference $2\pi a$ with mass m and Hamiltonian

$$H^{(0)} = \frac{1}{2m}P^2.$$

The position wave function $\psi(x)$ of a state $|\psi\rangle$ satisfies $\psi(x + 2\pi a) = \psi(x)$. For any states $|\psi\rangle$ and $|\phi\rangle$, and any operator $V(X)$, where X is the position operator, we define

$$\langle\psi|V(X)\,|\phi\rangle = \int_0^{2\pi a} \overline{\psi(x)}V(x)\phi(x)\,\mathrm{d}x.$$

The first excited (normalised) states $|\psi_A\rangle$ and $|\psi_B\rangle$ have wave functions

$$\psi_A(x) = \frac{1}{\sqrt{2\pi a}} e^{ix/a}, \qquad \psi_B(x) = \frac{1}{\sqrt{2\pi a}} e^{-ix/a},$$

respectively, and have energy $\hbar^2/(2ma^2)$, i.e. this energy level is twofold degenerate. Suppose the system is perturbed with the addition of the term $H^{(1)} = G\cos(2X/a)$ to the Hamiltonian, where G is a small real constant. We have that

$$\langle\psi_A|H^{(1)}\,|\psi_A\rangle = \int_0^{2\pi a} G\cos\frac{2x}{a}|\psi_A(x)|^2\,\mathrm{d}x = \frac{G}{2\pi a}\left[\frac{a}{2}\sin\frac{2x}{a}\right]_0^{2\pi a} = 0$$

and that

$$\langle\psi_B|H^{(1)}\,|\psi_B\rangle = \int_0^{2\pi a} G\cos\frac{2x}{a}|\psi_B(x)|^2\,\mathrm{d}x = 0.$$

What about the non-diagonal entries of the matrix with elements $\langle\psi_i|H^{(1)}\,|\psi_j\rangle$? We find

$$\begin{aligned}\langle\psi_A|H^{(1)}\,|\psi_B\rangle =& \frac{1}{2\pi a}\int_0^{2\pi a} e^{-ix/a} G\cos\frac{2x}{a} e^{-ix/a}\,\mathrm{d}x\\ =& \frac{G}{4\pi a}\int_0^{2\pi a}(1+e^{-4ix/a})\,\mathrm{d}x\\ =& \frac{G}{4\pi a}\left[x - \frac{a}{4i}e^{-4ix/a}\right]_0^{2\pi a}\\ =& G/2,\end{aligned}$$

and also $\langle\psi_B|H^{(1)}\,|\psi_A\rangle = G/2$. Clearly, the matrix is not diagonal, hence we need another basis for the eigenspace of $H^{(0)}$ of first excited states. Consider

$$|\psi_\pm\rangle = \frac{1}{\sqrt{2}}(|\psi_A\rangle \pm |\psi_B\rangle),$$

then we find

$$\langle\psi_\pm|H^{(1)}\,|\psi_\pm\rangle = \frac{1}{2}(\pm\langle\psi_A|H^{(1)}\,|\psi_B\rangle \pm \langle\psi_B|H^{(1)}\,|\psi_A\rangle) = \pm\frac{G}{2}$$

and

$$\langle\psi_\pm|H^{(1)}\,|\psi_\mp\rangle = \frac{1}{2}(\mp\langle\psi_A|H^{(1)}\,|\psi_B\rangle \pm \langle\psi_B|H^{(1)}\,|\psi_A\rangle) = 0.$$

Hence

$$\begin{pmatrix}\langle\psi_+|H^{(1)}\,|\psi_+\rangle & \langle\psi_+|H^{(1)}\,|\psi_-\rangle\\ \langle\psi_-|H^{(1)}\,|\psi_+\rangle & \langle\psi_-|H^{(1)}\,|\psi_-\rangle\end{pmatrix} = \begin{pmatrix}G/2 & 0\\ 0 & -G/2\end{pmatrix},$$

◇

and the approximate eigenstates of $H = H^{(0)} + H^{(1)}$ are $|\psi_\pm\rangle$ and the energy shift for $|\psi_+\rangle$ is $G/2$ whereas that for $|\psi_-\rangle$ is $-G/2$. That is, the perturbation *lifts* the degeneracy and the two states $|\psi_\pm\rangle$ no longer have the same energy.

10.2 THE VARIATIONAL METHOD

Suppose that the Hamiltonian H has orthonormal eigenstates $|\varphi_j\rangle$, $j = 0, 1, 2, \ldots$, satisfying $H|\varphi_j\rangle = E_j|\varphi_j\rangle$. Suppose that the state $|\varphi_0\rangle$ is the only state with the lowest energy E_0. Thus, $E_j > E_0$ for all $j \geq 1$. Any (normalised) state $|\psi\rangle$ can be expanded as

$$|\psi\rangle = \sum_j c_j|\varphi_j\rangle,$$

where $\langle\psi|\psi\rangle = \sum_j |c_j|^2 = 1$. Then

$$H|\psi\rangle = \sum_j c_j E_j|\varphi_j\rangle.$$

and

$$\langle\psi|H|\psi\rangle = \sum_j |c_j|^2 E_j.$$

The expectation value of the energy is

$$\begin{aligned}\langle H\rangle_\psi &= \langle\psi|H|\psi\rangle \\ &= \sum_j |c_j|^2 E_j \\ &\geq \sum_j |c_j|^2 E_0 \\ &\geq E_0 \quad (\text{since } \sum_j |c_j|^2 = 1)\end{aligned}$$

because $E_j \geq E_0$ for all j by assumption.

If the ground-state energy is unknown, we can calculate $\langle H\rangle_\psi$ for some *trial wave functions* with some parameters and take the smallest value of the energy as an approximate ground state energy and the corresponding wave function as an approximate ground state. This way of finding an approximate ground-state energy and wave function is called the variational method.

Thus, in the variational method, for trial states $|\psi_\alpha\rangle$ we compute

$$E(\alpha) = \frac{\langle\psi_\alpha|H|\psi_\alpha\rangle}{\langle\psi_\alpha|\psi_\alpha\rangle},$$

(in case $|\psi_\alpha\rangle$ is not necessarily normalised) and minimise $E(\alpha)$ as a function of α.

EXAMPLE 10.3. The Hamiltonian of the quantum particle in one dimension is given by

$$H = \frac{1}{2m}P^2 + \lambda X^4.$$

We want to find the minimum energy expectation value for the trial wave functions $\psi_\alpha(x) = \mathrm{e}^{-x^2/(2\alpha^2)}$, $\alpha > 0$. (Note that α has the dimensions of length.)

First we find

$$\begin{aligned}\langle\psi_\alpha|\psi_\alpha\rangle &= \int_{-\infty}^{\infty} \mathrm{e}^{-x^2/\alpha^2}\mathrm{d}x \\ &= \sqrt{\pi}\alpha,\end{aligned}$$

hence the functions are not generally normalised. Next we compute $P|\psi_\alpha\rangle$ in the position representation:

$$\begin{aligned}-\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}x}\psi_\alpha(x) &= -\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}x}\mathrm{e}^{-x^2/(2\alpha^2)} \\ &= \frac{\mathrm{i}\hbar x}{\alpha^2}\mathrm{e}^{-x^2/(2\alpha^2)}.\end{aligned}$$

Then,

$$\begin{aligned}\frac{1}{2m}\langle\psi_\alpha|P^2|\psi_\alpha\rangle &= \frac{1}{2m}\left|P|\psi\rangle\right|^2 \\ &= \frac{1}{2m\alpha^4}\int_{-\infty}^{\infty}\hbar^2x^2\mathrm{e}^{-x^2/\alpha^2}\mathrm{d}x \\ &= \frac{\sqrt{\pi}\hbar^2}{4m\alpha},\end{aligned}$$

and

$$\begin{aligned}\lambda\langle\psi_\alpha|X^4|\psi_\alpha\rangle &= \lambda\int_{-\infty}^{\infty}x^4\mathrm{e}^{-x^2/\alpha^2}\mathrm{d}x \\ &= \frac{3\sqrt{\pi}\lambda}{4}\alpha^5.\end{aligned}$$

Then

$$\begin{aligned}E(\alpha) &= \frac{\langle\psi_\alpha|H|\psi_\alpha\rangle}{\langle\psi_\alpha|\psi_\alpha\rangle} \\ &= \frac{\hbar^2}{4m\alpha^2} + \frac{3\lambda}{4}\alpha^4.\end{aligned}$$

The minimum of this function can be found by letting

$$E'(\alpha) = -\frac{\hbar^2}{2m\alpha^3} + 3\lambda\alpha^3 = 0.$$

The solution is $\alpha = \alpha_0$, where

$$\alpha_0 = \left(\frac{\hbar^2}{6\lambda m}\right)^{1/6}.$$

To simplify the calculation a little we define the frequency $\omega > 0$ by

$$\lambda = \frac{m^2\omega^3}{6\hbar},$$

(then λx^4 has the dimensions of energy.) Then

$$\alpha_0 = \sqrt{\frac{\hbar}{m\omega}},$$

and the approximate energy is

$$\begin{aligned} E(\alpha_0) &= \frac{\hbar^2}{4m} \cdot \frac{m\omega}{\hbar} + \frac{3}{4} \cdot \frac{m^2\omega^3}{6\hbar} \cdot \frac{\hbar^2}{m^2\omega^2} \\ &= \frac{3}{8}\hbar\omega. \end{aligned}$$

This is indeed slightly larger than the approximate ground-state energy $0.3675\hbar\omega$ obtained numerically. ◇