1.2 Heisenberg mechanics

1.2.1 Commutation relations

Operators corresponding to independent degrees of freedom commute with each other

$$[\hat{q}_\alpha, \hat{q}_\beta] = 0 \quad (1.2.1)$$
$$[\hat{p}_\alpha, \hat{p}_\beta] = 0 \quad (1.2.2)$$

but degrees of freedom and their conjugate momenta[1] satisfy non-trivial commutation relations

$$[\hat{q}_\alpha, \hat{p}_\beta] = i\hbar\delta_{\alpha\beta} \quad (1.2.3)$$

where

$$\delta_{\alpha\beta} = \begin{cases} 1 & \text{if} \quad \alpha = \beta \\ 0 & \text{if} \quad \alpha \neq \beta \end{cases} \quad (1.2.4)$$

Using Homework Q1.4, we see from Eq. (1.2.3) that, for example, a particle can not have a definite position *and* a definite momentum. However, in the classical limit, $\hbar \to 0$, $\hat{q}$ and $\hat{p}$ commute and so a classical particle can have a definite position and a definite momentum.

1.2.2 Equations of motion

In classical mechanics, the Lagrangian or Hamiltonian determine the dynamics via Lagrange's or Hamilton's equations, see Physics I, Section 2.3. In quantum mechanics, the degrees of freedom, momenta, Lagrangian and Hamiltonian become operators, but otherwise things are much the same. In addition to using the operator versions of Lagrange's or Hamilton's equations, one can also use **Heisenberg's equation**

$$\frac{d\hat{A}}{dt} = \frac{i}{\hbar}\left[\hat{H}, \hat{A}\right] + \frac{\partial \hat{A}}{\partial t} \quad (1.2.5)$$

which avoids the need to take derivatives with respect to operators.

1.2.3 Free non-relativistic particle

The quantum physics of a free non-relativistic particle is specified by its Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2m} \quad (1.2.6)$$

Hamilton's equations, or Heisenberg's equation, give

$$\frac{d\hat{x}}{dt} = \frac{\hat{p}}{m} \quad (1.2.7)$$
$$\frac{d\hat{p}}{dt} = 0 \quad (1.2.8)$$

[1] See Physics I, Eq. (2.3.3).

or, in Lagrange's equation form,

$$\frac{d^2\hat{x}}{dt} = 0 \tag{1.2.9}$$

which have solution

$$\hat{x}(t) = \hat{x}_0 + \frac{\hat{p}_0}{m}t \tag{1.2.10}$$

$$\hat{p}(t) = \hat{p}_0 \tag{1.2.11}$$

Note that the constants of motion, $\hat{x}_0$ and $\hat{p}_0$, are operators.

We can decompose the state vector $|\psi\rangle$ into momentum eigenstates [2]

$$|\psi\rangle = \sum_p |\psi_p\rangle \tag{1.2.12}$$

with

$$\hat{p}\,|\psi_p\rangle = p\,|\psi_p\rangle \tag{1.2.13}$$

and

$$\hat{H}\,|\psi_p\rangle = \frac{p^2}{2m}\,|\psi_p\rangle \tag{1.2.14}$$

1.2.4 Simple harmonic oscillator

The Hamiltonian of the simple harmonic oscillator is

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2\hat{x}^2}{2} \tag{1.2.15}$$

Hamilton's equations, or Heisenberg's equation, give

$$\frac{d\hat{x}}{dt} = \frac{\hat{p}}{m} \tag{1.2.16}$$

$$\frac{d\hat{p}}{dt} = -m\omega^2\hat{x} \tag{1.2.17}$$

or

$$\frac{d^2\hat{x}}{dt^2} = -\omega^2\hat{x} \tag{1.2.18}$$

which has the general solution [3]

$$\hat{x}(t) = \hat{A}e^{-i\omega t} + \hat{B}e^{i\omega t} \tag{1.2.19}$$

$\hat{x}$ is Hermitian, therefore

$$\hat{x}(t) = \hat{x}^\dagger(t) = \hat{A}^\dagger e^{i\omega t} + \hat{B}^\dagger e^{-i\omega t} \tag{1.2.20}$$

[2] Or $\int dp\,|\psi(p)\rangle$ for a continuous range of p.

[3] The solution can be obtained by, for example, factorizing Eq. (1.2.18): $\left(\frac{d}{dt} + i\omega\right)\left(\frac{d}{dt} - i\omega\right)\hat{x} = 0$.

and comparing with Eq. (1.2.19) gives

$$\hat{B} = \hat{A}^\dagger \tag{1.2.21}$$

Therefore

$$\begin{aligned} \hat{x}(t) &= \hat{A}e^{-i\omega t} + \hat{A}^\dagger e^{i\omega t} && (1.2.22) \\ \hat{p}(t) &= -im\omega\hat{A}e^{-i\omega t} + im\omega\hat{A}^\dagger e^{i\omega t} && (1.2.23) \end{aligned}$$

Inverting Eqs. (1.2.22) and (1.2.23) gives

$$\begin{aligned} \hat{A} &= \frac{1}{2}\left(\hat{x} + \frac{i\hat{p}}{m\omega}\right) e^{i\omega t} && (1.2.24) \\ \hat{A}^\dagger &= \frac{1}{2}\left(\hat{x} - \frac{i\hat{p}}{m\omega}\right) e^{-i\omega t} && (1.2.25) \end{aligned}$$

and the commutation relation Eq. (1.2.3) gives

$$\left[\hat{A}, \hat{A}^\dagger\right] = \frac{\hbar}{2m\omega} \tag{1.2.26}$$

Defining the dimensionless operators

$$\begin{aligned} \hat{a} &= \sqrt{\frac{2m\omega}{\hbar}}\,\hat{A} && (1.2.27) \\ \hat{a}^\dagger &= \sqrt{\frac{2m\omega}{\hbar}}\,\hat{A}^\dagger && (1.2.28) \end{aligned}$$

we get the commutation relation

$$\left[\hat{a}, \hat{a}^\dagger\right] = 1 \tag{1.2.29}$$

Since $\hat{a}$ is not normal it cannot be interpreted as a quantity with values, but only as an operator that transforms one state into another.

The Hamiltonian, Eq. (1.2.15), can be expressed in terms of $\hat{a}$ and $\hat{a}^\dagger$ using Eqs. (1.2.22), (1.2.23), (1.2.27) and (1.2.28)

$$\hat{H} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right) \tag{1.2.30}$$

The operator

$$\hat{N} = \hat{a}^\dagger\hat{a} \tag{1.2.31}$$

is Hermitian and so has a complete set of eigenvectors [4]

$$\hat{N}\,|n\rangle = n\,|n\rangle \tag{1.2.32}$$

and

$$\hat{H}\,|n\rangle = \hbar\omega\left(n + \frac{1}{2}\right)|n\rangle \tag{1.2.33}$$

[4] For simplicity, we assume the eigenspaces are one dimensional.

To determine the effect of $\hat{a}$ and $\hat{a}^\dagger$ on these eigenvectors, and hence on any vector, we calculate the commutators of $\hat{a}$ and $\hat{a}^\dagger$ with $\hat{N}$. Eqs. (1.2.31) and (1.2.29) give

$$\left[\hat{N}, \hat{a}\right] = \hat{a}^\dagger \hat{a} \hat{a} - \hat{a} \hat{a}^\dagger \hat{a} = \left[\hat{a}^\dagger, \hat{a}\right] \hat{a} = -\hat{a} \tag{1.2.34}$$

and

$$\left[\hat{N}, \hat{a}^\dagger\right] = -\left[\hat{N}, \hat{a}\right]^\dagger = \hat{a}^\dagger \tag{1.2.35}$$

Therefore

$$\hat{N}\hat{a} = \hat{a}\left(\hat{N} - 1\right) \tag{1.2.36}$$

$$\hat{N}\hat{a}^\dagger = \hat{a}^\dagger\left(\hat{N} + 1\right) \tag{1.2.37}$$

and so, using Eq. (1.2.32),

$$\hat{N}\hat{a}\left|n\right\rangle = (n-1)\,\hat{a}\left|n\right\rangle \tag{1.2.38}$$

$$\hat{N}\hat{a}^\dagger\left|n\right\rangle = (n+1)\,\hat{a}^\dagger\left|n\right\rangle \tag{1.2.39}$$

and hence

$$\hat{a}\left|n\right\rangle \propto \left|n-1\right\rangle \tag{1.2.40}$$

$$\hat{a}^\dagger\left|n\right\rangle \propto \left|n+1\right\rangle \tag{1.2.41}$$

Thus, using Eq. (1.2.33), we see that $\hat{a}^\dagger$ and $\hat{a}$ create and destroy the energy quanta $\hbar\omega$ and so we interpret them as **creation** and **annihilation operators**, respectively.

To determine the eigenvalues n of $\hat{N}$, and hence the physical states, we use the above properties of $\hat{N}$, $\hat{a}$ and $\hat{a}^\dagger$. Using Eqs. (1.2.32) and (1.2.31),

$$n\left\langle n|n\right\rangle = \left\langle n\right|\hat{N}\left|n\right\rangle = \left|\hat{a}\left|n\right\rangle\right|^2 \geq 0 \tag{1.2.42}$$

therefore

$$n \geq 0 \tag{1.2.43}$$

with

$$\hat{a}\left|n\right\rangle = 0 \iff n = 0 \tag{1.2.44}$$

Eqs. (1.2.40), (1.2.43) and (1.2.44) imply $n \in \{0, 1, 2, \ldots\}$ since otherwise Eq. (1.2.40) would allow us to generate eigenvectors with negative eigenvalues in contradiction with Eq. (1.2.43). Also, using Eqs. (1.2.29) and (1.2.43),

$$\left|\hat{a}^\dagger\left|n\right\rangle\right|^2 = \left\langle n\right|\hat{a}\hat{a}^\dagger\left|n\right\rangle = \left\langle n\right|\left(\hat{N} + 1\right)\left|n\right\rangle = (n+1)\left\langle n|n\right\rangle > 0 \tag{1.2.45}$$

and hence

$$a^\dagger\left|n\right\rangle \neq 0 \tag{1.2.46}$$

Therefore, starting with an eigenvector with a non-negative integer eigenvalue, we can use Eqs. (1.2.40) and (1.2.41) to generate eigenvectors with any other non-negative integer eigenvalue. Therefore $\hat{N}$ has eigenvalues

$$n = 0, 1, 2, \ldots \tag{1.2.47}$$