4.1 Classical Physics

Classical physics is based on the two postulates:

1. **State space postulate:** Any closed system is associated with even dimensional space called the phase space. The state is described by a single point (or vector) in the phase space. The state is specified by $N$ position (usually denoted by $q_i$’s) and $N$ momentum (usually denoted by $p_i$’s) coordinates:

   \[(q_1, q_2, ..., q_N, p_1, p_2, ..., p_N)\]  (4.1)

   What is the dimensionality of the phase space of a simple harmonic oscillator? What is the dimensionality of the phase space of a single particle in a box? How many real numbers needed to specify a state of the harmonic oscillator and how many needed to specify a single particle?

2. **Evolution postulate:** Evolution of any closed system is described by function on the phase space. The function is called Hamiltonian and denoted by $H(q_1, q_2, ..., q_N, p_1, p_2, ..., p_N)$ and the evolution is described by the following equations

   \[
   \dot{q}_i = \frac{\partial H}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial H}{\partial q_i}.
   \]  (4.2)
For a simple harmonic oscillator the Hamiltonian is

\[ H(q, p) = \frac{p^2}{2m} + \frac{kq^2}{2}. \]  \hspace{1cm} (4.3)

and the corresponding equations of motion are

\[ \dot{p} = -kq \]
\[ \dot{q} = \frac{p}{m} \] \hspace{1cm} (4.4)

or equivalently

\[ \ddot{q} = \frac{\dot{p}}{m} = \frac{-kq}{m}. \] \hspace{1cm} (4.5)

### 4.2 Quantum Physics

In contrast the quantum physics is based on three postulates. We will first state the postulates and then introduce the necessary mathematical formalism that goes with it.

1. **State space postulate:** Any closed system is associated with a Hilbert space. The state of the system is described by a single point (or ket-vector) in the Hilbert space

\[ |\psi\rangle \] \hspace{1cm} (4.6)

with unit length

\[ \langle \psi | \cdot |\psi\rangle \equiv \langle \psi |\psi\rangle = 1 \] \hspace{1cm} (4.7)

where \( |\psi\rangle \) is a bra-vector. Ket- and bra- vectors are usually represented by either finite dimensional vectors or by wave-functions.

2. **Evolution postulate:** Evolution of any closed system is described by a unitary operator, i.e.

\[ |\psi(t_2)\rangle = \hat{U}(t_2 - t_1) |\psi(t_1)\rangle \] \hspace{1cm} (4.8)

where

\[ \hat{U}(t_2 - t_1) = e^{-i\hat{H}(t_2 - t_1)H}. \] \hspace{1cm} (4.9)

and \( \hat{H} \) is a Hermitian operator known as Hamiltonian operator. As we will see shortly this postulate can be recast in the form of Schrodinger equation.
3. **Measurement postulate:** A measurement is described by a collection of measurement operators \( \{ \hat{M}_m \} \) with probability of an outcome \( m \) given by

\[
p(m) = \langle \psi | \hat{M}_m^\dagger \hat{M}_m | \psi \rangle
\]

(4.10)

where \( \hat{M}_m^\dagger \) is the Hermitian conjugate of \( \hat{M}_m \) and the state after measurement

\[
\frac{\hat{M}_m | \psi \rangle}{\sqrt{p(m)}}.
\]

(4.11)

Then one can construct an operator (called observable)

\[
\hat{M} \equiv \sum_m m \hat{P}_m \equiv \sum_m m \hat{M}_m^\dagger \hat{M}_m
\]

where projection operator \( \hat{P}_m \) is defined as a projector on eigenspace of \( \hat{M}_m \) with eigenvalue \( m \). If there is a continuum of measurement of operators, then summation is replace with integral. For example,

\[
\hat{X} = \int x |x \rangle \langle x | dx
\]

(4.12)

or

\[
\hat{P} = \int p |p \rangle \langle p | dp.
\]

(4.13)

### 4.3 Schrodinger Picture

One can show that all normal operators have a diagonal representation,

\[
\hat{A} = \sum_{i=1}^n \lambda_i |i \rangle \langle i |.
\]

(4.14)

Therefore all positive definite operators as well as Hermitian operators have diagonal representations. Then one can define a function of Hermitian operators as

\[
f(\hat{A}) \equiv \sum_{i=1}^n f(\lambda_i) |i \rangle \langle i |
\]

(4.15)

for an arbitrary function \( f \). This can be applied to Eq. (4.8) since the Hamiltonian operator \( \hat{H} \) must be Hermitian and thus has a spectral decomposition

\[
\hat{H} = \sum E_n |\psi_n \rangle \langle \psi_n |
\]

(4.16)
where $E_n$ and $|\psi_n\rangle$ are the eigenvalues and corresponding eigenstates of Hamiltonian operators, i.e.

$$\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle$$  \hfill (4.17)

The energy eigenstate $|\psi_n\rangle$ with the lowest energy eigenvalue $E_n$ is called the ground state.

Moreover, by expanding both sides of Eq. (4.8) we get

$$|\psi(t_1)\rangle + (t_2 - t_1) \frac{d}{dt} |\psi(t_1)\rangle = \left( 1 - (t_2 - t_1) \frac{i}{\hbar} \hat{H} \right) |\psi(t_1)\rangle$$  \hfill (4.18)

which is the famous time-dependent Schrödinger equation

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle$$ \hfill (4.19)

in contrast to the time-independent Schrödinger equation (4.17). Using (4.8), (4.9), (4.15) and (4.16) one can find the most general solution of the time-dependent Schrödinger equation

$$|\varphi\rangle(t) = \sum_n e^{-iE_n t/\hbar} [\langle \psi_n | \varphi \rangle(0)] |\psi_n\rangle$$  \hfill (4.20)

which is expressed as a linear sum over solutions of the time-independent Schrödinger equation. Note that each solution of the time-independent Schrödinger equation gives rise to a simple solution of the time-dependent Schrödinger equation

$$|\varphi\rangle(t) = e^{-iE_n t/\hbar} |\psi_n\rangle.$$  \hfill (4.21)

### 4.4 The simplest example

Consider a Hamiltonian operator in matrix representation given by

$$\hat{H} = \frac{\hbar \omega}{2} \sigma_3 = \begin{pmatrix} \frac{\hbar \omega}{2} & 0 \\ 0 & -\frac{\hbar \omega}{2} \end{pmatrix},$$ \hfill (4.22)

It can describe, for example, a stationary electron subject to external magnetic field in $z$ direction.

Clearly the energy (or Hamiltonian) eigenvectors (or eigenkets) are given by

$$\hat{H}|+\rangle = \begin{pmatrix} \frac{\hbar \omega}{2} & 0 \\ 0 & -\frac{\hbar \omega}{2} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{\hbar \omega}{2} |z+\rangle$$

$$\hat{H}|+\rangle = \begin{pmatrix} \frac{\hbar \omega}{2} & 0 \\ 0 & -\frac{\hbar \omega}{2} \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = -\frac{\hbar \omega}{2} |z-\rangle$$ \hfill (4.23)
and then an arbitrary initial state
\[ |\psi\rangle = \psi_+ |z+\rangle + \psi_- |z-\rangle \]  
would evolve according to 4.20 as
\[ |\psi(t)\rangle = \psi_+ \exp\left(-i\frac{\omega t}{2}\right) |z+\rangle + \psi_- \exp\left(+i\frac{\omega t}{2}\right) |z-\rangle. \]  

Now consider (normalized) eigenstates of operator
\[ \frac{\hbar}{2} \hat{\sigma}_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \]  
or
\[ |x\rangle = \frac{1}{\sqrt{2}} (|z+\rangle \pm |z-\rangle). \]  
I we start with a state
\[ |\psi\rangle = |x+\rangle = \frac{1}{\sqrt{2}} |z+\rangle + \frac{1}{\sqrt{2}} |z-\rangle \]  
at time \( t = 0 \), then at some later time the state is
\[ |\psi(t)\rangle = \frac{1}{\sqrt{2}} \exp\left(-i\frac{\omega t}{2}\right) |z+\rangle + \frac{1}{\sqrt{2}} \exp\left(+i\frac{\omega t}{2}\right) |z-\rangle. \]  

Then if we decide to measure the system using
\[ \hat{S}_x \equiv \frac{\hbar}{2} \hat{\sigma}_x + \frac{\hbar}{2} \hat{\sigma}_x - \]  
and expectation value of observable operator
\[ \langle S_x \rangle = \left(\frac{\hbar}{2}\right) \cos(\omega t) \]
Similarly one can show that

\[ \langle S_y \rangle = \left( \frac{\hbar}{2} \right) \sin(\omega t) \]  

(4.34)

which can be interpreted as precession of spin (to be defined precisely later on). A similar phenomena gives rise to, for example, neutrino oscillations.

### 4.5 Heisenberg Picture

A framework where the state vectors evolves with time, but the operators remain constant is a Schrodinger picture. There is also a Heisenberg picture where the operators change with time, and the state vectors remain constant. Consider a time independent Hermitian operator \( \hat{A}_S \) in the Schrodinger picture then

\[ \langle \hat{A}_S \rangle(t) = \langle \psi_S(t) | \hat{A}_S | \psi_S(t) \rangle. \]  

(4.35)

The time evolution is described by a Schrodinger equation whose solution is

\[ |\psi_S(t)\rangle = e^{-\frac{i}{\hbar}Ht} |\psi_S(0)\rangle. \]  

(4.36)

From (4.35) and (4.36) we obtain

\[ \langle \hat{A}_S \rangle(t) = \langle \psi_S(0) | e^{\frac{i}{\hbar}Ht} \hat{A}_S e^{-\frac{i}{\hbar}Ht} | \psi_S(0) \rangle \]

\[ = \langle \psi_H | \hat{A}_H(t) | \psi_H \rangle \]

\[ = \langle \hat{A}_H(t) \rangle \]  

(4.37)

where

\[ \hat{A}_H(t) = e^{\frac{i}{\hbar}Ht} \hat{A}_S e^{-\frac{i}{\hbar}Ht} \]  

(4.38)

\[ |\psi_H\rangle \equiv |\psi_S(0)\rangle. \]  

(4.39)

It is easy to calculate the time evolution of operators in Heisenberg picture,

\[ \frac{d\hat{A}_H(t)}{dt} = \frac{d}{dt} e^{\frac{i}{\hbar}Ht} \hat{A}_S e^{-\frac{i}{\hbar}Ht} + e^{\frac{i}{\hbar}Ht} \hat{A}_S \frac{d}{dt} e^{-\frac{i}{\hbar}Ht} \]

\[ = \frac{i}{\hbar} \hat{H} e^{\frac{i}{\hbar}Ht} \hat{A}_S e^{-\frac{i}{\hbar}Ht} - e^{\frac{i}{\hbar}Ht} \hat{A}_S \frac{i}{\hbar} \hat{H} e^{-\frac{i}{\hbar}Ht} \]

\[ = \frac{i}{\hbar} \left( \hat{H} \hat{A}_H(t) - \hat{A}_H(t) \hat{H} \right) \]

\[ = \frac{i}{\hbar} [\hat{H}, \hat{A}_H(t)] \]  

(4.40)
where the commutator is defined as
\[
[\hat{A}, \hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A}.
\] (4.41)

Expression (4.40) is known as the Heisenberg equations. It reduces to the Hamiltonian equations of motion in classical mechanics with the identification we described above
\[-\frac{i}{\hbar} \{\cdot, \cdot\} \rightarrow \{\cdot, \cdot\} \equiv \frac{\partial}{\partial q} \frac{\partial}{\partial p} - \frac{\partial}{\partial p} \frac{\partial}{\partial q}
\] (4.42)
i.e. commutators replaced by Poisson brackets,
\[
\frac{dp}{dt} = \{p, H\} = -\frac{\partial H}{\partial q}
\] (4.43)
\[
\frac{dq}{dt} = \{q, H\} = \frac{\partial H}{\partial p}
\] (4.44)

Once again (4.40) is related to (2.56) through identification (4.42).

### 4.6 Density matrix

If the exact knowledge of the quantum microstate is not available, the system is said to be in a not pure, but mixed state. Such states are not specified by a unique vector in Hilbert space, but by a collection of vector \{\ket{\varphi_\alpha}\} with relative probabilities \{p_\alpha\}, such that
\[
\sum_\alpha p_\alpha = 1.
\] (4.45)
And the entropy of a mixed state is defined as
\[
S \equiv \sum_\alpha p_\alpha \log p_\alpha.
\] (4.46)

Then, the ensemble average of a given operator \(\hat{O}\) is given by
\[
\langle \hat{O} \rangle = \sum_\alpha p_\alpha \langle \varphi_\alpha | \hat{O} | \varphi_\alpha \rangle.
\] (4.47)
In a given set of orthonormal basis, $|\psi_n\rangle$, the above expression takes the following form

$$\langle \hat{O} \rangle = \sum_{\alpha,n,m} p_\alpha \langle \varphi_\alpha | \psi_n \rangle \langle \psi_n | \varphi_\alpha \rangle =$$

$$= \sum_{n,m} \left( \sum_\alpha p_\alpha \langle \psi_m | \varphi_\alpha \rangle \langle \varphi_\alpha | \psi_n \rangle \right) \langle \psi_n | \varphi_\alpha \rangle =$$

$$= \sum_{n,m} \langle \psi_m | \hat{\rho} | \psi_n \rangle \langle \varphi_\alpha | \psi_m \rangle =$$

$$= \sum_{n,m} \langle \psi_m | \hat{\rho} \varphi_\alpha \rangle | \psi_m \rangle =$$

$$= \text{Tr}(\hat{\rho} \hat{O}) \quad (4.48)$$

where the so-called density matrix is defined as

$$\hat{\rho} \equiv \sum_\alpha p_\alpha | \varphi_\alpha \rangle \langle \varphi_\alpha |. \quad (4.49)$$

This is the Hermitian operator which replaces the probability distribution function in classical phase space.

Let $|\psi_n\rangle$ be the energy eigenstates, then

$$\langle \psi_n | i\hbar \frac{\partial}{\partial t} \hat{\rho}(t) | \psi_m \rangle = i\hbar \frac{\partial}{\partial t} \sum_\alpha p_\alpha \langle \psi_n | \varphi_\alpha(t) \rangle \langle \varphi_\alpha(t) | \psi_m \rangle =$$

$$= \sum_\alpha p_\alpha \left( \langle \psi_n | i\hbar \frac{\partial}{\partial t} | \varphi_\alpha \rangle \langle \varphi_\alpha | \psi_m \rangle + \langle \psi_n | \varphi_\alpha \rangle i\hbar \frac{\partial}{\partial t} \langle \varphi_\alpha | \psi_m \rangle \right)$$

$$= \sum_\alpha p_\alpha \left( \langle \psi_n | \hat{H} | \varphi_\alpha \rangle \langle \varphi_\alpha | \psi_m \rangle + \langle \psi_n | \varphi_\alpha \rangle \left( -i\hbar \frac{\partial}{\partial t} \langle \varphi_\alpha | \varphi_\alpha \rangle \right) \right)$$

$$= \sum_\alpha p_\alpha \left( (E_n \langle \psi_n | \varphi_\alpha \rangle \langle \varphi_\alpha | \psi_m \rangle - E_m \langle \psi_n | \varphi_\alpha \rangle \langle \psi_m | \varphi_\alpha \rangle) \right)$$

$$= \langle \psi_n | \hat{\rho} (E_n - E_m) | \psi_m \rangle$$

$$= \langle \psi_n | \hat{H} \hat{\rho} - \hat{\rho} \hat{H} | \psi_m \rangle \quad (4.50)$$

Thus, independently of basis we get the Von Neumann equation:

$$i\hbar \frac{\partial}{\partial t} \hat{\rho}(t) = [\hat{H}, \hat{\rho}], \quad (4.51)$$

which is a quantum version of Liouville’s equation obtained (once again) by a formal substitution of Poisson brackets with commutator, i.e. $\{,\} \rightarrow -\frac{i}{\hbar} [\cdot]$. 

\[CH. 4. \ POSTULATES \ OF \ QUANTUM \ MECHANICS\]