

Chapter 2

Principles of Quantum Statistics

In this chapter we will study one of the most important assumptions of the quantum theory, the symmetrization postulate, and its consequence for the statistical properties of an ensemble of particles at thermal equilibrium. The three representative distribution functions, Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac distributions, are introduced here. Then, we will describe the other important assumption of the quantum theory, the non-commutability of conjugate observables, and its consequence for the uncertainty product in determining a certain pair of observables. The discussions in this chapter provide the foundation of thermal noise and quantum noise. Most of the discussions in this chapter follow the excellent texts on statistical mechanics by F. Rief [1] and on quantum mechanics by C. Cohen-Tannoudji et al. [2].

2.1 Symmetrization Postulate of Quantum Mechanics

2.1.1 Quantum indistinguishability

Let us consider a following thought experiment. Two identical quantum particles are incident upon a 50%–50% particle beam splitter and we measure the output by two particle counters.

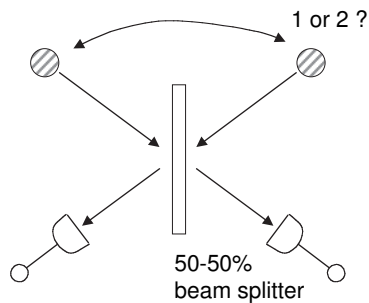


Figure 2.1: Collision of two identical particles.

To analyze this problem, we label the two particles as particle 1 and particle 2 based on

the click event in the detectors. One possible input state is

$$|1, R; 2, L\rangle \cdots \quad \begin{array}{l} \text{particle 1 is in the right input port and} \\ \text{particle 2 is in the left input port.} \end{array}$$

Since identical quantum particles are “indistinguishable”, the following input state is equally possible :

$$|1, L; 2, R\rangle \cdots \quad \begin{array}{l} \text{particle 1 is in the left input port and} \\ \text{particle 2 is in the right input port.} \end{array}$$

Most general input state is thus constructed as the linear superposition of the two :

$$\begin{aligned} & c_0|1, R; 2, L\rangle + c_1|1, L; 2, R\rangle \\ & (|c_0|^2 + |c_1|^2 = 1 \quad \text{if the two states are orthogonal.}) \end{aligned} \tag{2.1}$$

As shown below, an experimental result is dependent on the choice of the two c -numbers c_0 and c_1 . Therefore, the above mathematical state has an inherent ambiguity in predicting an experimental result and we need a fundamental assumption of the theory, “symmetrization postulate” [2].

2.1.2 Statement of the postulate

A physical state which represents a real system consisting of identical quantum particles is either symmetric or anti-symmetric with respect to the permutation of any two particles. A particle which obeys the former is called a boson and a particle which obeys the latter is called a fermion. For instance, the quantum states of two identical bosons and fermions are

$$\begin{aligned} \text{Boson :} & \quad \frac{1}{\sqrt{2}}[|1, R; 2, L\rangle + |1, L; 2, R\rangle], \\ \text{Fermion :} & \quad \frac{1}{\sqrt{2}}[|1, R; 2, L\rangle - |1, L; 2, R\rangle], \end{aligned} \tag{2.2}$$

if the two states are orthogonal. To demonstrate the important consequence of this new postulate, next let us calculate the probability of finding the two particles in the same output port (L). This probability consists of two possibilities.

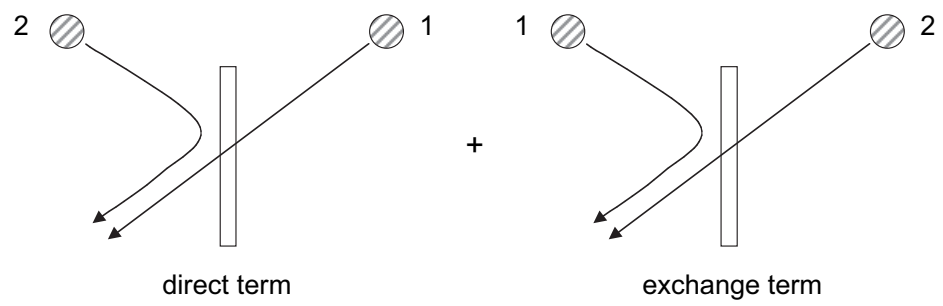


Figure 2.2: Two possibilities for an output state $|1, L; 2, L\rangle$.

The beam splitter scattering matrix is $\hat{U} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}$ in the basis of the two transmission modes $\begin{bmatrix} |k_{R \rightarrow L}\rangle \\ |k_{L \rightarrow R}\rangle \end{bmatrix}$. Therefore, the probability is

$$\begin{aligned}
 \underbrace{\langle 1, L; 2, L |}_{\text{final state}} \underbrace{\hat{U}}_{\text{scattering matrix}} \frac{1}{\sqrt{2}} \underbrace{[|1, R; 2, L\rangle \pm |1, L; 2, R\rangle]}_{\text{initial state}} &= \left| \frac{1}{\sqrt{2}} \left(\frac{1}{\sqrt{2}} \times \frac{1}{\sqrt{2}} \right) \pm \frac{1}{\sqrt{2}} \left(\frac{1}{\sqrt{2}} \times \frac{1}{\sqrt{2}} \right) \right|^2 \\
 &= \begin{cases} \frac{1}{2} : \text{boson} \leftarrow \text{constructive interference} \\ 0 : \text{fermion} \leftarrow \text{destructive interference} \end{cases}
 \end{aligned}
 \tag{2.3}$$

The probability for obtaining $|1, R; 2, R\rangle$ state is identical to (2.3). We can calculate the probability of finding one particle in each output port. The probability of obtaining $|1, L; 2, R\rangle$ state consists of two possibilities:

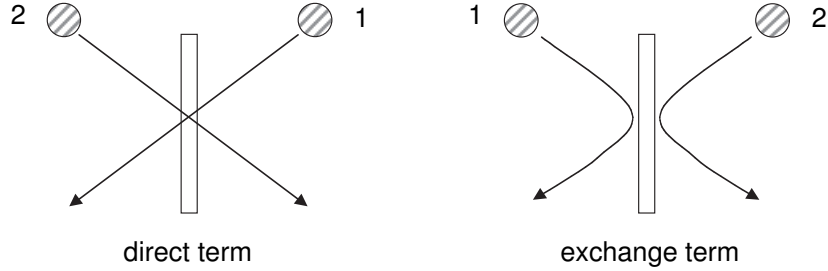


Figure 2.3: Two possibilities for an output state $|1, L; 2, R\rangle$.

$$\begin{aligned}
 \underbrace{\langle 1, L; 2, R |}_{\text{final state}} \underbrace{\hat{U}}_{\text{scattering matrix}} \frac{1}{\sqrt{2}} \underbrace{[|1, R; 2, L\rangle \pm |1, L; 2, R\rangle]}_{\text{initial state}} &= \left| \frac{1}{\sqrt{2}} \left(\frac{1}{\sqrt{2}} \times \frac{1}{\sqrt{2}} \right) \pm \frac{1}{\sqrt{2}} \left(\frac{1}{\sqrt{2}} \times \frac{-1}{\sqrt{2}} \right) \right|^2 \\
 &= \begin{cases} 0 : \text{boson} \leftarrow \text{destructive interference} \\ \frac{1}{2} : \text{fermion} \leftarrow \text{constructive interference} \end{cases}
 \end{aligned}
 \tag{2.4}$$

The probability for obtaining $|1, R; 2, L\rangle$ state is identical to (2.4). The scattering patterns of identical bosons and fermions are shown in Fig. 2.4.

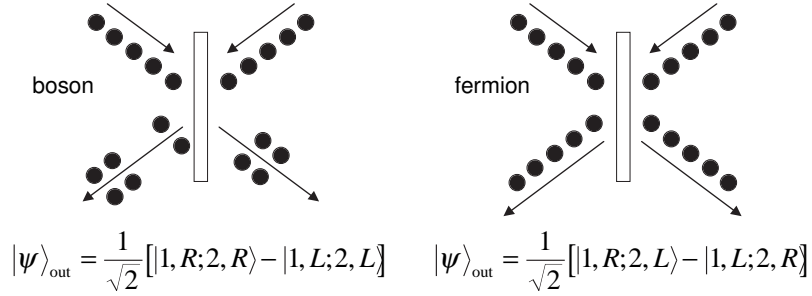


Figure 2.4: The scattering behaviours of two identical bosons and fermions at 50-50% beam splitter.

Comments :

1. The (2, 0) and (0, 2) output characteristics of bosons are called a “bunching” effect. The constructive interference enhances the probability of finding two particles in the same state. This is the ultimate origin of final state stimulation in lasers, Bose Einstein condensation and superconductivity.
2. The deterministic (1, 1) output characteristics of fermions are called “anti-bunching” effect. The destructive interference between the direct and exchange terms suppresses the probability of finding more than two particles in the same state. This is the manifestation of Pauli’s exclusion principle.

2.1.3 Symmetrization postulate for spin $-\frac{1}{2}$ particles

Next let us consider a following thought experiment. Two spin $-\frac{1}{2}$ particles are incident upon a 50%-50% beam splitter. The scattering matrix of a beam splitter is assumed to be spin-independent. If the two particles are in spin triplet states (symmetric spin states), the orbital states are symmetric for bosons and anti-symmetric for fermions to satisfy the symmetrization postulate for overall states :

$$\begin{aligned}
 \text{Boson : } & \frac{1}{\sqrt{2}} [|R\rangle_1 |L\rangle_2 + |L\rangle_1 |R\rangle_2] \otimes \begin{cases} |\uparrow\rangle_1 |\uparrow\rangle_2 \\ |\downarrow\rangle_1 |\downarrow\rangle_2 \\ \frac{1}{\sqrt{2}} [|\uparrow\rangle_1 |\downarrow\rangle_2 + |\downarrow\rangle_1 |\uparrow\rangle_2] \end{cases} \\
 \text{Fermion : } & \frac{1}{\sqrt{2}} [|R\rangle_1 |L\rangle_2 - |L\rangle_1 |R\rangle_2] \otimes \begin{cases} |\uparrow\rangle_1 |\uparrow\rangle_2 \\ |\downarrow\rangle_1 |\downarrow\rangle_2 \\ \frac{1}{\sqrt{2}} [|\uparrow\rangle_1 |\downarrow\rangle_2 + |\downarrow\rangle_1 |\uparrow\rangle_2] \end{cases} \quad (2.5)
 \end{aligned}$$

Their collision characteristics are the same as those for spin-less particles mentioned above. However, if the two particles are in a spin singlet state (anti-symmetric spin state), the orbital states are anti-symmetric for bosons and symmetric for fermions to satisfy the symmetrization postulate for overall states :

$$\begin{aligned}
\text{Boson :} & \quad \frac{1}{\sqrt{2}}[|R\rangle_1|L\rangle_2 - |L\rangle_1|R\rangle_2] \otimes \frac{1}{\sqrt{2}}[|\uparrow\rangle_1|\downarrow\rangle_2 - |\downarrow\rangle_1|\uparrow\rangle_2] \\
\text{Fermion :} & \quad \frac{1}{\sqrt{2}}[|R\rangle_1|L\rangle_2 + |L\rangle_1|R\rangle_2] \otimes \frac{1}{\sqrt{2}}[|\uparrow\rangle_1|\downarrow\rangle_2 - |\downarrow\rangle_1|\uparrow\rangle_2]
\end{aligned} \tag{2.6}$$

Now, the bosons feature a fermionic collision, i.e. (1, 1) output, and the fermions feature a bosonic collision, i.e. (2, 0) or (0, 2) output. This example illustrates a very important nature of two spin $-\frac{1}{2}$ fermions which can occupy the same state. Conversely if two identical fermions occupy the same orbital state, their spin state is always a spin singlet state.

$$\Gamma|x\rangle_1|x\rangle_2 \otimes \frac{1}{\sqrt{2}}[|\uparrow\rangle_1|\downarrow\rangle_2 - |\downarrow\rangle_1|\uparrow\rangle_2] \tag{2.7}$$



same orbital state

2.2 Thermodynamic Partition Functions

2.2.1 A small system in contact with a large heat reservoir

Let us consider an ideal gas of non-interacting identical particles in a volume V and at a temperature T . We assume the total number of particles, $\sum_r n_r = N$, is constant, where r designates a microscopic state and n_r is the number of particles in that state. The total energy of such an ideal gas system is

$$E_R = \sum_r \varepsilon_r n_r \quad , \tag{2.8}$$

where ε_r is the kinetic energy of a microscopic state r and R designates a macroscopic state represented by the occupation number of each microscopic state, $\{n_1, n_2, \dots, n_r, \dots\}$. The thermodynamic partition function Z is defined by

$$Z = \sum_R e^{-\beta E_R} \quad , \tag{2.9}$$

where \sum_R stands for summation over all possible macroscopic states, $\beta = 1/k_B T$ is a temperature parameter and k_B is a Boltzmann constant.

Next let us obtain the probability of finding a particular macroscopic state R . For this purpose we assume that our system is a small system A in thermal contact to a large heat reservoir A' . We also assume the interaction between A and A' is extremely small, so that their energies are additive. The energy of A is not fixed and depends on the specific

macroscopic state R . It is the total energy of the combined system A and A' which has a constant value E_T . This constant total energy is split into those of A and A' :

$$E_T = E_R + E' \quad , \quad (2.10)$$

where E' is the energy of A' .

According to the fundamental postulate of statistical mechanics, the probability of finding A in a specific macroscopic state R is proportioned to the number of states $\Omega'(E_T - E_R)$ accessible to A' when its energy lies in a range δE near $E' = E_T - E_R$. Hence

$$P_R = C' \Omega'(E_T - E_R) \quad , \quad (2.11)$$

where C' is a constant independent of R and determined by the normalization condition $\sum_R p_R = 1$.

Since A is a much smaller system than A' , $E_R \ll E_T$ and (2.11) can be approximated by expanding the logarithm of $\Omega'(E_T - E_R)$ about $E' = E_T$:

$$\ln \Omega'(E_T - E_R) \simeq \ln \Omega'(E_T) - \left[\frac{\partial}{\partial E'} \ln \Omega'(E') \right]_{E_T} \cdot E_R \quad . \quad (2.12)$$

The derivative in (2.12) is the definition of the temperature parameter of the heat reservoir according to the statistical mechanics [1],

$$\left[\frac{\partial}{\partial E'} \ln \Omega'(E') \right]_{E_T} \equiv \beta = 1/k_B T \quad . \quad (2.13)$$

The above result means that the heat reservoir A' is much larger than A so that its temperature T remains unchanged by such a small amount of energy it gives to A . Thus, we obtain

$$\Omega'(E_T - E_R) = \Omega'(E_T) e^{-\beta E_R} \quad . \quad (2.14)$$

since $\Omega'(E_T)$ is a constant independent of R , (2.11) becomes

$$P_R = C e^{-\beta E_R} \quad , \quad (2.15)$$

where $C = C' \Omega'(E_T)$ can be determined by the above mentioned normalization condition $\sum_R p_R = 1$.

The probability of finding the gas in a specific macroscopic state $R = \{n_1, n_2, \dots, n_r, \dots\}$ is finally given by

$$P_R = \frac{e^{-\beta E_R}}{\sum_{R'} e^{-\beta E_{R'}}} = \frac{e^{-\beta E_R}}{Z} \quad . \quad (2.16)$$

If the above is true, such a system is called a canonical ensemble[1, 3].

Mean and variance of particle number and total energy

Once we know the thermodynamic function Z , various physical quantities can be evaluated from Z . As a simple example, let us calculate the statistical values for a particle number n_s of a specific state and a total energy E .

A. Mean of particle number

$$\begin{aligned}
\langle n_s \rangle &= \frac{\sum_R n_s P_R}{\sum_R n_s e^{-\beta(\varepsilon_1 n_1 + \varepsilon_2 n_2 + \dots)}} \\
&= \frac{Z}{Z} \\
&= -\frac{1}{\beta Z} \frac{\partial}{\partial \varepsilon_s} Z \\
&= -\frac{1}{\beta} \frac{\partial}{\partial \varepsilon_s} \log Z
\end{aligned} \tag{2.17}$$

B. Mean-square of particle number

$$\begin{aligned}
\langle n_s^2 \rangle &= \frac{\sum_R n_s^2 P_R}{\sum_R n_s^2 e^{-\beta(\varepsilon_1 n_1 + \varepsilon_2 n_2 + \dots)}} \\
&= \frac{Z}{Z} \\
&= \frac{1}{\beta^2 Z} \frac{\partial^2}{\partial \varepsilon_s^2} Z
\end{aligned} \tag{2.18}$$

C. Variance of particle number

$$\begin{aligned}
\sigma_{n_s}^2 &= \langle n_s^2 \rangle - \langle n_s \rangle^2 \\
&= \frac{1}{\beta^2 Z} \frac{\partial^2}{\partial \varepsilon_s^2} Z - \left(\frac{1}{\beta Z} \right)^2 \left(\frac{\partial}{\partial \varepsilon_s} Z \right)^2 \\
&= \frac{1}{\beta^2} \left[\frac{\partial}{\partial \varepsilon_s} \left(\frac{1}{Z} \frac{\partial Z}{\partial \varepsilon_s} \right) + \frac{1}{Z^2} \left(\frac{\partial Z}{\partial \varepsilon_s} \right)^2 \right] - \frac{1}{\beta^2 Z^2} \left(\frac{\partial Z}{\partial \varepsilon_s} \right)^2 \\
&= \frac{1}{\beta^2} \frac{\partial^2}{\partial \varepsilon_s^2} \log Z \quad .
\end{aligned} \tag{2.19}$$

D. Mean energy

$$\begin{aligned}
\langle E \rangle &= \frac{\sum_R E_R P_R}{\sum_R E_R e^{-\beta E_R}} \\
&= -\frac{1}{Z} \frac{\partial}{\partial \beta} Z \\
&= -\frac{\partial}{\partial \beta} \log Z \quad .
\end{aligned} \tag{2.20}$$

E. Mean square of energy

$$\begin{aligned}
\langle E^2 \rangle &= \frac{\sum_R E_R^2 P_R}{\sum_R E_R^2 e^{-\beta E_R}} \\
&= \frac{1}{Z} \frac{\partial^2}{\partial \beta^2} Z \quad .
\end{aligned} \tag{2.21}$$

F. Variance of energy

$$\begin{aligned}
\sigma_E^2 &= \langle E^2 \rangle - \langle E \rangle^2 \\
&= \frac{1}{Z} \frac{\partial^2}{\partial \beta^2} Z - \left(\frac{1}{Z} \frac{\partial}{\partial \beta} Z \right)^2 \\
&= \frac{\partial}{\partial \beta} \left(\frac{1}{Z} \frac{\partial}{\partial \beta} Z \right) \\
&= \frac{\partial^2}{\partial \beta^2} \log Z \quad .
\end{aligned} \tag{2.22}$$

2.3 Various Distribution Functions

If an ensemble of identical particles is at thermal equilibrium, there are certain probability distributions of finding n particles in a specific state s with an energy ε_s . We will derive the four representative probability distribution functions in this section.

2.3.1 Maxwell-Boltzmann statistics

Let us consider an ensemble of “hypothetical” identical particles which can be individually identified. Since it does not obey the principle of quantum indistinguishability, it is often referred to as classical particles.

The thermodynamic partition function for distinguishable particles should be modified from Eq. (2.9) since all particles are “different” or have “unique labels” in an ensemble of distinguishable particles,

$$\begin{aligned}
Z &= \sum_{\{n_1, n_2, \dots\}} \left(\frac{N!}{n_1! n_2! \dots} \right) e^{-\beta(\varepsilon_1 n_1 + \varepsilon_2 n_2 + \dots)} \\
&= \left(e^{-\beta \varepsilon_1} + e^{-\beta \varepsilon_2} + \dots \right)^N \quad ,
\end{aligned} \tag{2.23}$$

$$\log Z = N \log \left(\sum_r e^{-\beta \varepsilon_r} \right) \quad . \tag{2.24}$$

Using Eq. (2.23) in Eq. (2.17), we obtain the mean particle number in a specific state,

$$\begin{aligned}
\langle n_s \rangle &= -\frac{1}{\beta} \frac{\partial}{\partial \varepsilon_s} \log Z \\
&= N \times \frac{e^{-\beta \varepsilon_s}}{\sum_r e^{-\beta \varepsilon_r}} \quad .
\end{aligned} \tag{2.25}$$

This is a Maxwell-Boltzmann distribution. The variance of the particle number is calculated using Eq. (2.19),

$$\begin{aligned}
\langle \Delta n_s^2 \rangle &= -\frac{1}{\beta} \frac{\partial}{\partial \varepsilon_s} \langle n_s \rangle \\
&= \langle n_s \rangle \left(1 - \frac{\langle n_s \rangle}{N} \right) \\
&\simeq \langle n_s \rangle \quad .
\end{aligned} \tag{2.26}$$

The above result suggests that the probability of finding n_s particles in a specific state in the Maxwell-Boltzmann distribution obeys a Poisson distribution.

2.3.2 Bose-Einstein statistics

If an ensemble of identical bosonic particles is at thermal equilibrium, it is enough to specify how many particles are in each state $\{n_1, n_2, \dots\}$. Therefore, the mean particle number in a microscopic state s is

$$\begin{aligned} \langle n_s \rangle &= \frac{\sum_{\{n_1, n_2, \dots\}} n_s e^{-\beta(\varepsilon_1 n_1 + \varepsilon_2 n_2 + \dots)}}{\sum_{\{n_1, n_2, \dots\}} e^{-\beta(\varepsilon_1 n_1 + \varepsilon_2 n_2 + \dots)}} \\ &= \frac{\sum_{n_s} n_s e^{-\beta \varepsilon_s n_s} \cdot \sum^{(s)} e^{-\beta(\varepsilon_1 n_1 + \varepsilon_2 n_2 + \dots)}}{\sum_{n_s} e^{-\beta \varepsilon_s n_s} \cdot \sum^{(s)} e^{-\beta(\varepsilon_1 n_1 + \varepsilon_2 n_2 + \dots)}} \quad . \end{aligned} \quad (2.27)$$

Here $\sum^{(s)}$ stands for the summation over $\{n_1, n_2, \dots\}$ except for the particular microscopic state s .

If the particular microscopic state s does not have a particle, i.e. $n_s = 0$, N particles must be distributed over the states other than s ,

$$\begin{aligned} Z_s(N) &= \sum^{(s)} e^{-\beta(\varepsilon_1 n_1 + \varepsilon_2 n_2 + \dots)} \\ \sum_r^{(s)} n_r &= N \quad . \end{aligned} \quad (2.28)$$

If the particular state s has one particle, i.e. $n_s = 1$, the remaining $N - 1$ particles must be distributed over the states other than s ,

$$\begin{aligned} Z_s(N - 1) &= \sum^{(s)} e^{-\beta(\varepsilon_1 n_1 + \varepsilon_2 n_2 + \dots)} \\ \sum_r^{(s)} n_r &= N - 1 \quad . \end{aligned} \quad (2.29)$$

Using these notations, Eq. (2.27) can be rewritten as

$$\langle n_s \rangle = \frac{0 \times Z_s(N) + e^{-\beta \varepsilon_s} Z_s(N - 1) + 2e^{-2\beta \varepsilon_s} Z_s(N - 2) + \dots}{Z_s(N) + e^{-\beta \varepsilon_s} Z_s(N - 1) + e^{-2\beta \varepsilon_s} Z_s(N - 2) + \dots} \quad . \quad (2.30)$$

In order to proceed the evaluation of Eq. (2.30), we introduce a new parameter α by

$$\begin{aligned} \log Z_s(N - \Delta N) &\simeq \log Z_s(N) + \left[\frac{\partial}{\partial N} \log Z_s(N) \right] (-\Delta N) \\ &= \log Z_s(N) - \alpha_s \Delta N \quad , \end{aligned} \quad (2.31)$$

where

$$\alpha_s = \frac{\partial}{\partial N} \log Z_s(N) \simeq \frac{\partial}{\partial N} \log Z(N) = \alpha \quad . \quad (2.32)$$

Eq.(2.32) holds by the following reason. Since $Z_s(N)$ is a summation over very many states, variation of its logarithm with respect to the total number of particles should be insensitive as to which particular state s is omitted. Using Eq. (2.32) in Eq. (2.31), we obtain

$$Z_s(N - \Delta N) = Z_s(N) e^{-\alpha \Delta N} \quad , \quad (2.33)$$

$$\begin{aligned} \langle n_s \rangle &= \frac{Z_s(N) \left[0 + e^{-\beta \varepsilon_s - \alpha} + 2e^{-2\beta \varepsilon_s - 2\alpha} + \dots \right]}{Z_s(N) \left[1 + e^{-\beta \varepsilon_s - \alpha} + e^{-2\beta \varepsilon_s - 2\alpha} + \dots \right]} \\ &= \frac{\sum_{n_s} n_s e^{-n_s(\beta \varepsilon_s + \alpha)}}{\sum_{n_s} e^{-n_s(\beta \varepsilon_s + \alpha)}} \\ &= -\frac{1}{\beta} \frac{\partial}{\partial \varepsilon_s} \log \left(\sum_{n_s} e^{-n_s(\beta \varepsilon_s + \alpha)} \right) \\ &= -\frac{1}{\beta} \frac{\partial}{\partial \varepsilon_s} \log \left[\frac{1}{1 - e^{-(\beta \varepsilon_s + \alpha)}} \right] \\ &= \frac{1}{e^{\beta \varepsilon_s + \alpha} - 1} \quad . \end{aligned} \quad (2.34)$$

The parameter α is determined by the total number of particles,

$$N = \sum_r \langle n_r \rangle = \sum_r \frac{1}{e^{\beta \varepsilon_r + \alpha} - 1} \quad . \quad (2.35)$$

Rewriting α in terms of $\mu = -\frac{\alpha}{\beta} = -k_B T \alpha$, Eq. (2.34) is reduced to

$$\langle n_s \rangle = \frac{1}{e^{\beta(\varepsilon_s - \mu)} - 1} \quad . \quad (2.36)$$

This is a Bose-Einstein distribution and μ is called a chemical potential. Note that the chemical potential μ must be always smaller than the minimum energy $\varepsilon_{s,\min}$ of the system to conserve the particle number.

The variance in the particle number is

$$\begin{aligned} \langle \Delta n_s^2 \rangle &= -\frac{1}{\beta} \frac{\partial}{\partial \varepsilon_s} \langle n_s \rangle \\ &= \frac{1}{\beta} \cdot \frac{e^{\beta(\varepsilon_s - \mu)}}{[e^{\beta(\varepsilon_s - \mu)} - 1]^2} \cdot \beta \left(1 - \frac{\partial \mu}{\partial \varepsilon_s} \right) \\ &= \langle n_s \rangle (1 + \langle n_s \rangle) \left(1 - \frac{\partial \mu}{\partial \varepsilon_s} \right) \quad . \end{aligned} \quad (2.37)$$

Unless a temperature is so low that only a very few states are occupied, a small change of ε_s leaves μ unchanged and we have $\frac{\partial \mu}{\partial \varepsilon_s} = 0$. In this case, we have the two limiting cases:

$$\langle \Delta n_s^2 \rangle = \begin{cases} \langle n_s \rangle^2 & : \quad \varepsilon_s - \mu \ll k_B T \quad (\text{quantumdegenerategas}) \\ \langle n_s \rangle & : \quad \varepsilon_s - \mu \gg k_B T \quad (\text{non - degenerategas}) \end{cases} \quad . \quad (2.38)$$

If a temperature is very low, most of the particles are at the lowest energy ground state or nearly degenerate low-energy state, which satisfy $\varepsilon_s - \mu \ll k_B T$. Such a situation is called Bose-Einstein condensation.

2.3.3 Photon statistics

There is another type of bosonic particles, which are photons and phonons. Those particles are quantized electromagnetic fields and lattice vibrations. Such elementary excitations do not have any constraint on the total number of particles when a temperature is varied. Thus we cannot determine a chemical potential μ through the relation Eq. (2.35). We set the chemical potential μ to be zero for this case.

The mean particle number is

$$\begin{aligned}
 \langle n_s \rangle &= \frac{\sum_{n_s} n_s e^{-\beta \varepsilon_s n_s}}{\sum_{n_s} e^{-\beta \varepsilon_s n_s}} \\
 &= -\frac{1}{\beta} \frac{\partial}{\partial \varepsilon_s} \log \left(\sum_{n_s} e^{-\beta \varepsilon_s n_s} \right) \\
 &= -\frac{1}{\beta} \frac{\partial}{\partial \varepsilon_s} \log \left[\frac{1}{1 - e^{-\beta \varepsilon_s}} \right] \\
 &= \frac{1}{e^{\beta \varepsilon_s} - 1} .
 \end{aligned} \tag{2.39}$$

Here $\varepsilon_s = \hbar \omega_s$ is an energy of photon or phonon, which is uniquely determined by the oscillation frequency ω_s . This is called a Planck distribution. The variance in the particle number is

$$\begin{aligned}
 \langle \Delta n_s^2 \rangle &= -\frac{1}{\beta} \frac{\partial}{\partial \varepsilon_s} \langle n_s \rangle \\
 &= \langle n_s \rangle (1 + \langle n_s \rangle) \\
 &= \begin{cases} \langle n_s \rangle^2 & : \varepsilon_s \ll k_B T \\ \langle n_s \rangle & : \varepsilon_s \gg k_B T \end{cases} .
 \end{aligned} \tag{2.40}$$

2.3.4 Fermi-Dirac statistics

Due to the Pauli exclusion principle, each state has the occupation number, either 0 or 1, for an ensemble of identical Fermionic particles. Thus, the mean particle number is

$$\begin{aligned}
 \langle n_s \rangle &= \frac{\sum_{n_s} n_s e^{-\beta \varepsilon_s n_s} \cdot \sum^{(s)} e^{-\beta(\varepsilon_1 n_1 + \varepsilon_2 n_2 + \dots)}}{\sum_{n_s} e^{-\beta \varepsilon_s n_s} \cdot \sum^{(s)} e^{-\beta(\varepsilon_1 n_1 + \varepsilon_2 n_2 + \dots)}} \\
 &= \frac{0 \times Z_s(N) + e^{-\beta \varepsilon_s} Z_s(N-1)}{Z_s(N) + e^{-\beta \varepsilon_s} Z_s(N-1)}
 \end{aligned}$$

$$\begin{aligned}
&= \frac{1}{e^{\beta\varepsilon_s + \alpha} + 1} \\
&= \frac{1}{e^{\beta(\varepsilon_s - \mu)} + 1} \quad , \tag{2.41}
\end{aligned}$$

where $Z_s(N-1) = Z_s(N)e^{-\alpha}$ and $\mu = -\frac{\alpha}{\beta}$ are used. Note that there is no constraint for a chemical potential μ with respect to ε_s in this case. The chemical potential can be much smaller or much larger than the minimum energy $\varepsilon_{s,\min}$. The variance in the particle number is

$$\begin{aligned}
\langle \Delta n_s^2 \rangle &= -\frac{1}{\beta} \frac{\partial}{\partial \varepsilon_s} \langle n_s \rangle \\
&= \langle n_s \rangle (1 - \langle n_s \rangle) \left(1 - \frac{\partial \mu}{\partial \varepsilon_s} \right) \\
&\simeq \langle n_s \rangle (1 - \langle n_s \rangle) \quad . \tag{2.42}
\end{aligned}$$

The maximum variance is $\langle \Delta n_s^2 \rangle = \frac{1}{4}$ at $\varepsilon_s = \mu$ (at Fermi energy) and the variance disappears at $\varepsilon_s \ll \mu$ due to constant and full occupation of $n_s = 1$. If a temperature is very low, most of the particles are under this full occupation and there are very few particles near the chemical potential and subject to a finite variance $\langle \Delta n_s^2 \rangle$. Such a gas is called Fermi degeneracy.


It is interesting to note that the quantum statistics play an important role in the particle distribution when a temperature is very low and only a few states are occupied. When a temperature is very high and the particles are distributed over very many states the Bose-Einstein distribution and the Fermi-Dirac distribution become indistinguishable from the (classical) Maxwell-Boltzmann distribution because the mean particle number per state is much smaller than one at such a high temperature limit. However, for photon statistics, the mean particle number can be much greater than one whenever $\varepsilon_s \ll k_B T$ and so the photon statistics can never be reduced to the (classical) Maxwell-Boltzmann statistics no matter how high a temperature is.

2.4 Equipartition Theorem of Statistical Mechanics

Let us derive here the equipartition theorem mentioned in the previous chapter. Statement of the theorem: If a total system energy is given by the independent sum of quadratic terms of each degree of freedom (DOF), the thermal equilibrium energy per DOF is equal to $\frac{1}{2}k_B\theta$.

This is the equipartition theorem. The proof runs as follows[1]. The total energy of a system consisting of f subsystems depends on f generalized coordinates q_k and f generalized momenta $p_k (k = 1, 2, \dots, f)$. Then, this total energy is split into

$$E(q_1 \cdots q_f, p_1 \cdots p_f) = \varepsilon_i(p_i) + E'(q_1 \cdots q_f, p_1 \cdots p_f) \quad , \tag{2.43}$$



does not depend on p_i

where

$$\varepsilon_i(p_i) = bp_i^2 \tag{2.44}$$

The ensemble averaged energy associated with p_i is now evaluated as

$$\begin{aligned}
\langle \varepsilon_i(p_i) \rangle &= \frac{\int_{-\infty}^{\infty} \varepsilon_i(p_i) e^{-\beta E(q_1 \dots q_f, p_1 \dots p_f)} dq_1 \dots dp_f}{\int_{-\infty}^{\infty} e^{-\beta E(q_1 \dots q_f, p_1 \dots p_f)} dq_1 \dots dp_f} \\
&= \frac{\int_{-\infty}^{\infty} \varepsilon_i(p_i) e^{-\beta \varepsilon_i(p_i)} dp_i \times \int_{-\infty}^{\infty} e^{-\beta E'(q_1 \dots p_f)} dq_1 \dots dp_f}{\int_{-\infty}^{\infty} e^{-\beta \varepsilon_i(p_i)} dp_i \times \int_{-\infty}^{\infty} e^{-\beta E'(q_1 \dots p_f)} dq_1 \dots dp_f} \\
&= \frac{\int_{-\infty}^{\infty} \varepsilon_i(p_i) e^{-\beta \varepsilon_i(p_i)} dp_i}{\int_{-\infty}^{\infty} e^{-\beta \varepsilon_i(p_i)} dp_i} \\
&= \frac{\partial}{\partial \beta} \log \left(\int_{-\infty}^{\infty} e^{-\beta \varepsilon_i(p_i)} dp_i \right). \tag{2.45}
\end{aligned}$$

The integral in the logarithmic function is calculated as,

$$\int_{-\infty}^{\infty} e^{-\beta b p_i^2} dp_i = \beta^{-\frac{1}{2}} \int_{-\infty}^{\infty} e^{-b y^2} dy, \tag{2.46}$$

where $y = \beta^{\frac{1}{2}} p_i$. Substitution of (2.46) into (2.45) provides the described result.

$$\begin{aligned}
\langle \varepsilon_i(p_i) \rangle &= -\frac{\partial}{\partial \beta} \left[-\frac{1}{2} \log \beta + \log \left(\int_{-\infty}^{\infty} e^{-b y^2} dy \right) \right] \\
&= \frac{1}{2\beta} \\
&= \frac{1}{2} k_B \theta. \tag{2.47}
\end{aligned}$$

Note that the proof is quite general and thus valid for many situations.

2.5 Non-commutability Postulate of Quantum Mechanics

2.5.1 Heisenberg uncertainty principle

In quantum mechanics, a pair of conjugate observables, such as a position q and a momentum p of a particle, must satisfy the following commutation relation [2]:

$$[q, p] = qp - pq = i\hbar. \tag{2.48}$$

In classical mechanics, q and p commute, i.e. $qp = pq$, but in quantum mechanics, q and p do not commute. This non-commutability is one of the fundamental postulates of the quantum theory, by which the quantum theory departs most profoundly from the classical counterpart.

Let us introduce the fluctuation operators by

$$\Delta q = q - \langle q \rangle, \Delta p = p - \langle p \rangle, \tag{2.49}$$

where $\langle q \rangle$ and $\langle p \rangle$ are the ensemble-averaged values of q and p and real numbers if q and p are a pair of observables (Hermitian operators) such as position and momentum. This

assumption is supported by the fact that whenever we measure a physical quantity, the measurement result is always a real number. Using (2.49) we can rewrite (2.48) as

$$[\Delta q, \Delta p] = i\hbar \quad . \quad (2.50)$$

In order to calculate the uncertainty product for Δq and Δp , we let $|\varphi\rangle = \Delta q|\psi\rangle$ and $|\chi\rangle = \Delta p|\psi\rangle$ and use the Schwartz inequality

$$\langle\varphi|\varphi\rangle\langle\chi|\chi\rangle \geq |\langle\varphi|\chi\rangle|^2 \quad , \quad (2.51)$$

where $|\psi\rangle$ is a ket vector representing a quantum state of a given particle system [2]. In (2.51), the equality holds if and only if $|\varphi\rangle$ and $|\chi\rangle$ represent an identical state:

$$|\varphi\rangle = c_1|\chi\rangle \quad , \quad (2.52)$$

where c_1 is a c -number. The state is uniquely determined by the “direction” of the state vector (its norm is irrelevant) so that (2.52) means $|\varphi\rangle$ and $|\chi\rangle$ represent an identical state. Since q and p are Hermitian operators, it follows that $\Delta q = \Delta q^+$ and $\Delta p = \Delta p^+$. The inequality (2.51) is rewritten as

$$\langle\Delta q^2\rangle\langle\Delta p^2\rangle \geq |\langle\Delta q\Delta p\rangle|^2 \quad , \quad (2.53)$$

where

$$\begin{aligned} \Delta q\Delta p &= \frac{1}{2}(\Delta q\Delta p + \Delta p\Delta q) + \frac{1}{2}(\Delta q\Delta p - \Delta p\Delta q) \\ &= \frac{1}{2}(\Delta q\Delta p + \Delta p\Delta q) + \frac{i}{2}\hbar \quad . \end{aligned} \quad (2.54)$$

From (2.53) and (2.55), we obtain

$$\langle\Delta q^2\rangle\langle\Delta p^2\rangle \geq \frac{1}{4}|\langle\Delta q\Delta p + \Delta p\Delta q\rangle + i\hbar|^2 \quad . \quad (2.55)$$

Here $\langle\Delta q\Delta p + \Delta p\Delta q\rangle$ is a real number since it is an ensemble-averaged value of a Hermitian operator. Accordingly, (2.55) may be further rewritten as

$$\langle\Delta q^2\rangle\langle\Delta p^2\rangle \geq \frac{\hbar^2}{4} \quad . \quad (2.56)$$

This is the Heisenberg uncertainty principle. It places an irreducible lower bound on the product of the uncertainties in the measurements of q and p .

2.5.2 Minimum uncertainty wavepacket

For the equality to hold in (2.56), the state vector $|\psi\rangle$ must satisfy the following two conditions simultaneously:

$$\Delta q|\psi\rangle = c_1\Delta p|\psi\rangle \quad , \quad (2.57)$$

$$\langle\psi|\Delta q\Delta p + \Delta p\Delta q|\psi\rangle \quad . \quad (2.58)$$

Next let us obtain such a state that satisfies (2.57) and (2.58). If we use (2.57) and its adjoint in (2.58), we have

$$(c_1 + c_1^*) \langle \psi | \Delta p^2 | \psi \rangle = 0 \quad . \quad (2.59)$$

If $|\psi\rangle$ is not an eigenstate of p , $\langle \Delta p^2 \rangle \neq 0$ so that c_a must be a pure imaginary number. If we let $c_1 = -ic_2$, where c_2 is a real number, (2.57) is rewritten as

$$(q - \langle q \rangle) |\psi\rangle = -ic_2 (p - \langle p \rangle) |\psi\rangle \quad . \quad (2.60)$$

If we project an eigen-bra $\langle q' |$ from the left of (2.60), we obtain

$$(q' - \langle q \rangle) \psi(q') = -ic_2 \left(\frac{\hbar}{i} \frac{\partial}{\partial q'} - \langle p \rangle \right) \psi(q') \quad . \quad (2.61)$$

Here $\psi(q') \equiv \langle q' | \psi \rangle$ is the Schrödinger wavefunction of the state $|\psi\rangle$ in q' -representation and we use the identity [2]

$$\langle q' | p | \psi \rangle = \frac{\hbar}{i} \frac{\partial}{\partial q'} \psi(q') \quad . \quad (2.62)$$

The solution of (2.61) is given by

$$\psi(q') = c_3 \exp \left[\frac{i}{\hbar} \langle p \rangle q' - \frac{1}{2\hbar c_2} (q' - \langle q \rangle)^2 \right] \quad , \quad (2.63)$$

where c_3 is a constant of integration. c_2 and c_3 in (2.63) can be determined by the relations:

$$\int_{-\infty}^{\infty} |\psi(q')|^2 dq' = 1 \quad , \quad (2.64)$$

$$\int_{-\infty}^{\infty} (q' - \langle q \rangle)^2 |\psi(q')|^2 dq' = \langle \Delta q^2 \rangle \quad , \quad (2.65)$$

Using (2.63) in (2.64) and (2.65), we find that $c_2 = \frac{2\langle \Delta q^2 \rangle}{\hbar}$ and $|c_3|^2 = \frac{1}{\sqrt{2\pi\langle \Delta q^2 \rangle}}$. Without loss of generality, we can choose c_3 is a real positive number, and then (2.63) becomes

$$\psi(q') = (2\pi\langle \Delta q^2 \rangle)^{-\frac{1}{4}} \exp \left[\frac{i}{\hbar} \langle p \rangle q' - \frac{(q' - \langle q \rangle)^2}{4\langle \Delta q^2 \rangle} \right] \quad , \quad (2.66)$$

This is the Gaussian wavepacket centered at $q' = \langle q \rangle$ with a variance $\langle \Delta q^2 \rangle$.

The Schrödinger wavefunction in p' -representation can be obtained by the Fourier transform of (2.66) [4]:

$$\begin{aligned} \varphi(p') &\equiv \langle p' | \psi \rangle = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \exp \left(-\frac{i}{\hbar} p' q' \right) \psi(q') dq' \\ &= (2\pi\langle \Delta p^2 \rangle)^{-\frac{1}{4}} \exp \left[-\frac{i}{\hbar} \langle q \rangle (p' - \langle p \rangle) - \frac{(p' - \langle p \rangle)^2}{4\langle \Delta p^2 \rangle} \right] \quad , \end{aligned} \quad (2.67)$$

where $\langle \Delta p^2 \rangle = \hbar^2/4\langle \Delta q^2 \rangle$ as expected.

Equation (2.60) can be rewritten as

$$(e^r q + i e^{-r} p) |\psi\rangle = (e^r \langle q \rangle + i e^{-r} \langle p \rangle) |\psi\rangle \quad , \quad (2.68)$$

where a new parameter is defined by $c_2 = e^{-2r}$. The above equation suggests the very important insight: The minimum uncertainty state $|\psi\rangle$ is an eigenstate of a “non-Hermitian” operator $e^r q + i e^{-r} p$ with a c -number eigenvalue $e^r \langle q \rangle + i e^{-r} \langle p \rangle$.

2.5.3 coherent state and squeezed state

If we interpret the previous result for a mechanical harmonic oscillator, in which the Hamiltonian corresponding to the total energy of the system is given by

$$\mathcal{H} = \frac{p^2}{2m} + \frac{1}{2}kq^2 \quad . \quad (2.69)$$

The oscillation frequency is given by $\omega = \sqrt{\frac{k}{m}}$. The minimum uncertainty state of such a mechanical harmonic oscillator is given by the eigenstate of the non-Hermitian operator (2.68). The uncertainties of q and p are respectively given by

$$\langle \Delta q^2 \rangle = \frac{\hbar}{2} e^{-2r} \quad , \quad (2.70)$$

$$\langle \Delta p^2 \rangle = \frac{\hbar}{2} e^{2r} \quad . \quad (2.71)$$

The parameter r determines the noise distribution between q and p under the constraint of (2.56) with equality. Thus, it is called a squeezing parameter.

The position and momentum operators can be replaced by the annihilation and creation operators for an elementary excitation of a harmonic oscillator by the transformation

$$\hat{q} = \sqrt{\frac{\hbar}{2m\omega}} (a + a^+) \quad , \quad (2.72)$$

$$\hat{p} = \frac{1}{i} \sqrt{\frac{\hbar\omega m}{2}} (a - a^+) \quad . \quad (2.73)$$

If the Hamiltonian amplitude operators a_1 and a_2 are introduced by the relation,

$$a_1 = \frac{1}{2} (a + a^+) = \sqrt{\frac{m\omega}{2\hbar}} q \quad , \quad (2.74)$$

$$a_2 = \frac{1}{2i} (a - a^+) = \sqrt{\frac{1}{2\hbar\omega m}} p \quad , \quad (2.75)$$

the new commutator bracket and resulting uncertainty relation are

$$[a_1, a_2] = \frac{i}{2} \quad , \quad (2.76)$$

$$\langle \Delta a_1^2 \rangle \langle \Delta a_2^2 \rangle \geq \frac{1}{16} \quad . \quad (2.77)$$

The minimum uncertainty state is an eigenstate of the non-Hermitian operator, $e^r a_1 + i e^{-r} a_2$, and possesses the following uncertainties

$$\langle \Delta a_1^2 \rangle = \frac{1}{4} e^{-2r} \quad , \quad (2.78)$$

$$\langle \Delta a_2^2 \rangle = \frac{1}{4} e^{2r} \quad . \quad (2.79)$$

When the squeezing parameter is $r = 0$, the non-Hermitian operator is reduced to the annihilation operator \hat{a} and the minimum uncertainty state in this special case is a coherent state [5]. Time evolution of the coherent state with a positive excitation amplitude, is schematically shown in Fig. 2.5(a). When the squeezing parameter r is positive or negative and there is the same excitation amplitude $\langle a_1 \rangle > 0$, oscillation behavior of the state is shown in Fig. 2.5(b) and (c). They are respectively called amplitude squeezed state and phase squeezed state, since the quantum uncertainty is minimum when an amplitude is measured for $r > 0$ and when a phase is measured when $r < 0$. The pulsating uncertainties of the normalized position $\langle \Delta a_1^2 \rangle = \frac{m\omega}{2\hbar} \langle \Delta q^2 \rangle$ are shown in Fig. 2.6 [6].

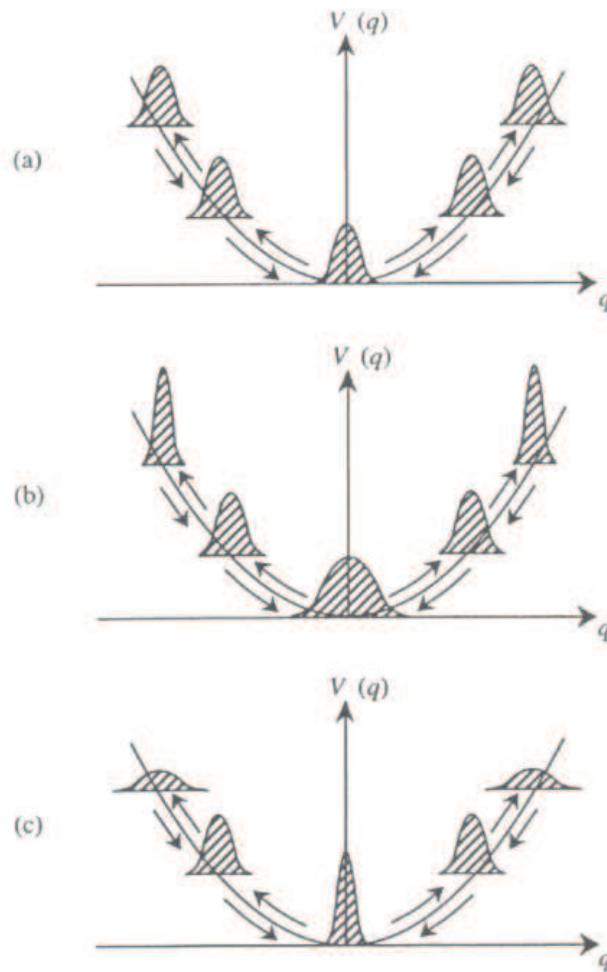


Figure 2.5: The minimum uncertain wavepackets in a harmonic potential $V(q) = \frac{1}{2}kq^2$. (a) coherent state and (b)(c) quadrature amplitude squeezed states.

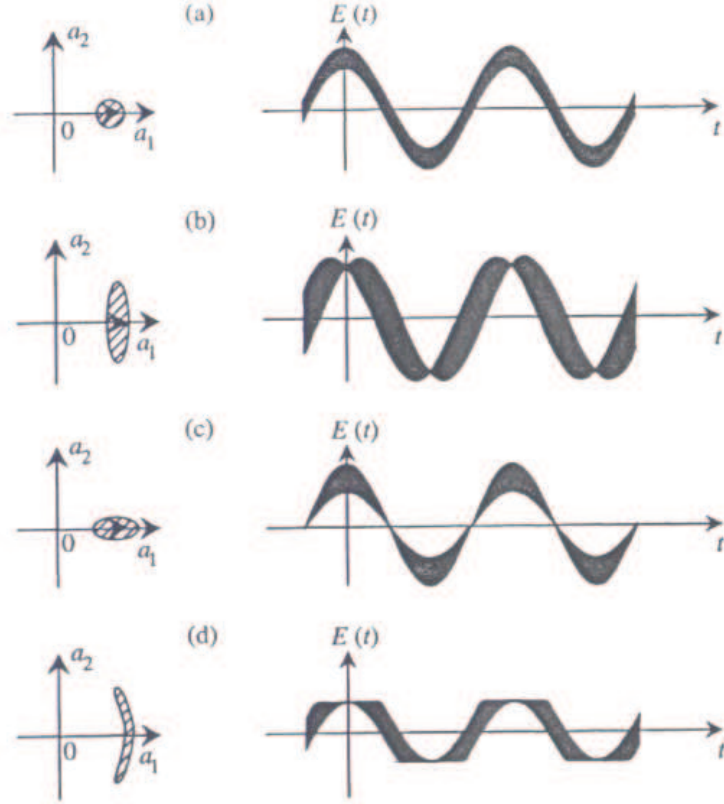


Figure 2.6: (a) A coherent state of light, (b) (amplitude) squeezed state of light, (c) (phase) squeezed state of light, and (d) number-phase squeezed state of light.

2.6 Quantum and thermal noise of a simple harmonic oscillator

When a harmonic oscillator is at thermal equilibrium, the energy associated with the position q and momentum p are independently given by $\frac{1}{2}k_B T$ according to the equipartition theorem of statistical mechanics. If we take into account the quantization effect, that is, the energy of a simple harmonic oscillator is quantized in unit of $\hbar\omega$, the thermal energy is given by

$$E_t = \hbar\omega\bar{n} = \frac{\hbar\omega}{e^{\hbar\omega/k_B T} - 1} \quad , \quad (2.80)$$

where \bar{n} is the equilibrium photon statistics at a temperature T . When $\hbar\omega \ll k_B T$, the quantization effect is not important and (2.80) is reduced to $E_t = k_B T$. This is an expected result since a simple harmonic oscillator energy consists of two degrees of freedom, q and p , and each degree of freedom carries and energy of $\frac{1}{2}k_B T$.

When $\hbar\omega \gg k_B T$ (zero temperature limit), (2.80) is reduced to zero. This is not correct. Even at zero temperature $T = 0$, the uncertainty principle requires the zero-point fluctuation in both position and momentum. The ground state $|0\rangle$ of the simple harmonic oscillator is defined by

$$a|0\rangle = 0 \quad , \quad (2.81)$$

which indicates that the ground state $|0\rangle$ is a coherent state with an eigenvalue of zero. The zero-point energy associated with the ground state is

$$\begin{aligned}
 E_q &= \frac{1}{2m}\langle\Delta p^2\rangle + \frac{1}{2}k\langle\Delta x^2\rangle \\
 &= \hbar\omega\left(\langle\Delta a_1^2\rangle + \langle\Delta a_2^2\rangle\right) \\
 &= \frac{1}{2}\hbar\omega \quad ,
 \end{aligned}
 \tag{2.82}$$

The total energy of a simple harmonic oscillator is thus given by

$$E_T = E_t + E_q = \hbar\omega\left(\frac{1}{e^{\hbar\omega/k_B T} - 1} + \frac{1}{2}\right) \quad .
 \tag{2.83}$$

E_t is referred to as thermal noise while E_q is called quantum noise. The measurement of the position or momentum of a simple harmonic oscillator at equilibrium condition is thus constrained by the quantum mechanical zero-point fluctuation when $\hbar\omega \gg k_B T$ and by the thermal equilibrium noise when $\hbar\omega \ll k_B T$.

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