Contents

1 Quantum Statistical Mechanics

this section, statistical mechanics of N identical quanticles will be formulated. For simplicity, a gas of eracting N particles is considered. Since the particle in-interacting, the Hamiltonian of the system is just of N In this section, statistical mechanics of N identical quantum particles will be formulated. For simplicity, a gas of noninteracting N particles is considered. Since the particles are non-interacting, the Hamiltonian of the system is just the sum of N individual Hamiltonian and it is given by

$$
\hat{\mathcal{H}}(\mathbf{q}, \mathbf{p}) = \sum_{i=1}^{N} \hat{\mathcal{H}}_i(q_i, p_i)
$$
(1.1)

where (q_i, p_i) are the coordinate and momentum of the *i* th particle, $\hat{\mathcal{H}}_i$ is the Hamiltonian operator.

A stationary system of N particles in a volume V then can be in any one of the quantum states determined by the solutions of the time independent Schrödinger equation

$$
\hat{\mathcal{H}}\psi_E(\mathbf{q}) = E\psi_E(\mathbf{q})\tag{1.2}
$$

where E is the eigenvalue of the Hamiltonian and ψ_E is the corresponding eigenfunction. The solution of the above

Schrödinger equation of N non-interacting particles can be written as

$$
\psi_E(\mathbf{q}) = \prod_{i=1}^N \phi_{\epsilon_i}(q_i), \quad \text{with} \quad E = \sum_{i=1}^N \epsilon_i \qquad (1.3)
$$

and

$$
\hat{\mathcal{H}}_i \phi_{\epsilon_i} (q_i) = \epsilon_i \phi_{\epsilon_i} (q_i) \qquad (1.4)
$$

 $\psi_{E}(\mathbf{q})=\prod_{i=1}^{N}\phi_{\epsilon_{i}}\left(q_{i}\right),\quad\text{ with }\quad E=\sum_{i=1}^{N}\epsilon_{i}$ and $\hat{\mathcal{H}}_{i}\phi_{\epsilon_{i}}\left(q_{i}\right)=\epsilon_{i}\phi_{\epsilon_{i}}\left(q_{i}\right)$ ere ϕ_{i} is the eigenfunction of the single particle Han n $\hat{\mathcal{H}}_{i}$ with eigenvalue $\epsilon_{i}.$ Each s where ϕ_i is the eigenfunction of the single particle Hamiltonian $\hat{\mathcal{H}}_i$ with eigenvalue ϵ_i . Each single particle wave function ϕ_i is always a linear combination of a set of orthonormal basis functions $\{\varphi_j\}$, $\phi_i = \sum_j c_{ij} \varphi_j$. If there are n_i particles in an eigenstate ϵ_i , then the distribution should satisfy

$$
\sum_{i} n_{i} = N \quad \text{and} \quad \sum_{i} n_{i} \epsilon_{i} = E \tag{1.5}
$$

2 Symmetry of wave functions and particle statistics:

particle statistics:
 Complicity, first consider a two-particle system described $\psi(a, b)$. If the particle *a* described by ϕ_n^a when it is in that a of energy E_n and the particle *b* described be n it is in the For simplicity, first consider a two-particle system described by $\psi(a, b)$. If the particle a described by ϕ_n^a when it is in the n th state of energy E_n and the particle b described by ϕ_k^b k when it is in the k th state of energy E_k , then the wave function for the combined two particle system is given by

$$
\psi(a, b) = \phi_n^a \phi_k^b \quad \text{ with } \quad E = E_n + E_k
$$

where E is the energy of the system. If the two particles are exchanged so that a in the k th state and b in the n th state, the corresponding wave function is

$$
\psi(a, b) = \phi_n^b \phi_k^a \quad \text{ with } \quad E = E_n + E_k
$$

since both the states corresponds to the same energy value, the states are then degenerate. The most general wave function is the linear combinations of these two wave functions. There are two possible combinations and they are given by

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$$
(i)\psi(a,b) = \frac{1}{\sqrt{2!}} \left[\phi_n^a \phi_k^b + \phi_n^b \phi_k^a \right] \quad \text{Symmetric} \tag{2.1}
$$

and

$$
(ii)\psi(a,b) = \frac{1}{\sqrt{2!}} \left[\phi_n^a \phi_k^b - \phi_n^b \phi_k^a \right]
$$

=
$$
\frac{1}{\sqrt{2!}} \begin{vmatrix} \phi_n^a & \phi_n^b \\ \phi_k^a & \phi_k^b \end{vmatrix}
$$
 Anti-symmetric (2.2)

 $(i)\psi(a, b) = \frac{1}{\sqrt{2!}} \left[\phi_n^a \phi_k^b + \phi_n^b \phi_k^a \right]$ Symmetric

 $(ii)\psi(a, b) = \frac{1}{\sqrt{2!}} \left[\phi_n^a \phi_k^b - \phi_n^b \phi_k^a \right]$
 $= \frac{1}{\sqrt{2!}} \left| \phi_k^a \phi_k^b \right|$ Anti-symmetric

If a and b are interchanged, (i) remains unchanged
 If a and b are interchanged, (i) remains unchanged and it is called symmetric wave function, (ii) the absolute vale remains unchanged but reverses the sign and it is called anti-symmetric wave function. However, the wave functions ϕ_n^a $_{n}^{a}\phi _{k}^{b}$ $\frac{b}{k}$ and ϕ_n^b $_{n}^{b}\phi _{k}^{a}$ $\frac{a}{k}$ individually are neither symmetric nor antisymmetric. The interchange of the particles leads to different microstates which means the particles are distinguishable as classical particles.

Now, one could write the wave functions for N particles $\{a_1, a_2, \cdots, a_N\}$ with a_i particle in the n_i th state. The corresponding wave functions are

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$$
\psi(a_1, a_2, \dots, a_N) = \prod_{i=1}^N \phi_{n_i}^{a_i}
$$
 Product (2.3)

$$
\psi(a_1, a_2, \dots, a_N) = \frac{1}{\sqrt{N!}} \sum \prod_{i=1}^N \phi_{n_i}^{a_i}
$$
 Symmetric (2.4)

$$
\psi(a_1, a_2, \dots, a_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_{n_1}^{a_1} & \phi_{n_1}^{a_2} & \cdots & \phi_{n_1}^{a_N} \\ \phi_{n_2}^{a_1} & \phi_{n_2}^{a_2} & \cdots & \phi_{n_2}^{a_N} \\ \vdots & \vdots & \ddots & \vdots \\ \phi_{n_N}^{a_1} & \phi_{n_N}^{a_2} & \cdots & \phi_{n_N}^{a_N} \end{vmatrix}
$$
 (2.5)
Anti-symmetric
The particles described by these three wave functions
ney different statistics.
(i) The particles described by the product function cor-
spond to different microstate by interchanging particles

The particles described by these three wave functions obey different statistics.

(i) The particles described by the product function correspond to different microstate by interchanging particles between states. These are then distinguishable particles and obey Maxwell-Boltzmann statistics.

(ii) In the case of symmetric wave functions, interchanging of particles does not generate a new microstate. Thus, the particles are indistinguishable. Also, all the particles in a single state corresponds to a nonvanishing wave function. That means accumulation of all the particles in a single state is possible. These particles obey Bose-Einstein statistics and are called bosons.

of particles does not generate a new microstate. To particles are indistinguishable. Also, all the paralle state corresponds to a nonvanishing wave in. That means accumulation of all the particles gle state is possible. Th (iii) For the anti-symmetric wave function, if the two particles are exchanged, the two columns of the determinant are exchanged and leads to the same wave function with a different sign. Thus, the particles are again indistinguishable. However, if any two particles are in one state then the corresponding rows of the determinant are the same and the wave function vanishes. This means that a state cannot be occupied by more than one particle. This is known as Pauli principle. These particles obey Fermi-Dirac statistics and they are called fermions.

3 Quantum distribution functions from grand canonical ensemble

Consider an ideal gas of N identical particles. Let s represents the single particle state and S denotes the state of the whole system. At the state S , the total energy E_S and the number of particles N are given by

$$
E_S = \sum_s n_s \epsilon_s \quad \text{and} \quad N = \sum_s n_s
$$

The distribution functions can be calculated by obtaining the appropriate partition function.

3.1 MB statistics

from grand canonical ensemb

nsider an ideal gas of N identical particles. Let s r

ts the single particle state and S denotes the state c

ole system. At the state S, the total energy E_S and

mber of particles N are We consider the particles are distinguishable in formulation of MB statistics. If they are indistinguishable like classical ideal gas molecules then we divide the partition function by N!. The canonical partition function is given by

$$
Z = \sum_{S} e^{-\beta E_{S}} = \sum_{S} e^{-\beta \sum_{s} n_{s} \epsilon_{s}} \tag{3.1}
$$

where the sum is all states S. All states is the collection of states with all possible values of n_s . This, the partition function can be written as

$$
Z = \sum_{\{s_i\}} e^{-\beta \left(\epsilon_{s_1} + \epsilon_{s_2} + \dots + \epsilon_{s_N}\right)} \tag{3.2}
$$

where the sum is now over the all possible states of individual particles. The summation in the partition function can be carried out in the following manner.

states with all possible values of
$$
n_s
$$
. Thus, the partition
\naction can be written as
\n
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Z = \sum_{\{s_i\}} e^{-\beta(\epsilon_{s_1} + \epsilon_{s_2} + \cdots + \epsilon_{s_N})}
$$
\n(3.2)
\nere the sum is now over the all possible states of individual-
\nparticles. The summation in the partition function can
\ncarried out in the following manner.
\n
$$
Z = \sum_{s_1, s_2, \ldots, s_N} e^{-\beta \epsilon_{s_1}} e^{-\beta \epsilon_{s_2} \ldots e^{-\beta \epsilon_{s_N}}}
$$
\n
$$
= \left[\sum_{s_1} e^{-\beta \epsilon_{s_1}} \right] \left[\sum_{s_2} e^{-\beta \epsilon_{s_2}} \right] \cdots \left[\sum_{s_N} e^{-\beta \epsilon_{s_N}} \right]
$$
\n(3.3)
\n
$$
= \left[\sum_{s_i} e^{-\beta \epsilon_{s_i}} \right]^N
$$
\nand
\n
$$
\ln Z = N \ln \left(\sum_{s_i} e^{-\beta \epsilon_{s_i}} \right)
$$
\n(3.4)

The mean number of particles in state s is then given by

$$
\langle n_s \rangle_{MB} = -\frac{1}{\beta} \frac{\partial \ln Z}{\partial \epsilon_s} = \frac{N e^{-\beta \epsilon_s}}{\sum_s e^{-\beta \epsilon_s}} \tag{3.5}
$$

This is the Maxwell-Boltzmann distribution as already obtained classical statistical mechanics.

3.2 BE statistics:

The grand canonical partition function $\mathcal Z$ of N indistinguishable bosons is given by

$$
\mathcal{Z} = \sum_{s} e^{-\beta(n_1 \epsilon_1 + n_2 \epsilon_2 + \cdots) + \mu \beta(n_1 + n_2 + \cdots)}
$$
 (3.6)

 $\langle n_s \rangle_{MB} = -\frac{1}{\beta} \frac{\partial}{\partial \epsilon_s} = \frac{1}{\sum_s e^{-\beta \epsilon_s}}$
This is the Maxwell-Boltzmann distribution as alreained classical statistical mechanics.
2 **BE statistics:**
 ϵ grand canonical partition function Z of N indishable boson where the sum is over all possible single particle states s. The number of particles n_i in each state i could be $0, 1, 2, \cdots$ subject to the condition $\sum n_i = N$. Therefore,

$$
\mathcal{Z} = \left(\sum_{n_1} e^{-\beta(\epsilon_1 - \mu)n_1}\right) \left(\sum_{n_2} e^{-\beta(\epsilon_2 - \mu)n_2}\right) \cdots \qquad (3.7)
$$

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Now since (geometric progression)

$$
\sum_{n=0}^{\infty} e^{-\beta(\epsilon_1 - \mu)n} = \frac{1}{1 - e^{-\beta(\epsilon - \mu)}}\tag{3.8}
$$

so the partition function then can be written as

$$
\mathcal{Z} = \left(\frac{1}{1 - e^{-\beta(\epsilon_1 - \mu)}}\right) \left(\frac{1}{1 - e^{-\beta(\epsilon_2 - \mu)}}\right) \cdots \tag{3.9}
$$

and so

$$
\ln \mathcal{Z} = -\sum_{s} \ln \left(1 - e^{-\beta (\epsilon_s - \mu)} \right) \tag{3.10}
$$

The number of particles in an grand canonical ensemble is given by

$$
\sum_{n=0}^{\infty} e^{-\beta(\epsilon_1 - \mu)n} = \frac{1}{1 - e^{-\beta(\epsilon - \mu)}} \quad (3.8)
$$
\nso the partition function then can be written as

\n
$$
\mathcal{Z} = \left(\frac{1}{1 - e^{-\beta(\epsilon_1 - \mu)}}\right) \left(\frac{1}{1 - e^{-\beta(\epsilon_2 - \mu)}}\right) \cdots \quad (3.9)
$$
\nand so

\n
$$
\ln \mathcal{Z} = -\sum_{s} \ln \left(1 - e^{-\beta(\epsilon_s - \mu)}\right) \quad (3.10)
$$
\nThe number of particles in an grand canonical ensemble is given by

\n
$$
N = \frac{1}{\beta} \frac{\partial \ln \mathcal{Z}}{\partial \mu} = -\frac{1}{\beta} \frac{\partial}{\partial \mu} \left\{ \sum_{s} \ln \left(1 - e^{-\beta(\epsilon_s - \mu)}\right) \right\} = \sum_{s} \langle n_s \rangle \quad (3.11)
$$
\nThus the average number of molecules in the *s* level is

\n
$$
\langle n_s \rangle_{BE} = -\frac{1}{\beta} \frac{\partial}{\partial \mu} \left\{ \ln \left(1 - e^{-\beta(\epsilon_s - \mu)}\right) \right\}
$$
\n
$$
= \frac{e^{-\beta(\epsilon_s - \mu)}}{1 - e^{-\beta(\epsilon_s - \mu)}} = \frac{1}{e^{\beta(\epsilon_s - \mu)} - 1} \quad (3.12)
$$

Thus the average number of molecules in the s level is

$$
\langle n_s \rangle_{BE} = -\frac{1}{\beta} \frac{\partial}{\partial \mu} \left\{ \ln \left(1 - e^{-\beta(\epsilon_s - \mu)} \right) \right\}
$$

$$
= \frac{e^{-\beta(\epsilon_s - \mu)}}{1 - e^{-\beta(\epsilon_s - \mu)}} = \frac{1}{e^{\beta(\epsilon_s - \mu)} - 1}
$$
(3.12)

This is Bose-Einstein distribution where always $\mu < \epsilon_s$, otherwise $\langle n_s \rangle$ could be negative.

3.3 FD statistics:

e fermions have only two states, $n_s = 0$ or 1. Thus, it

and canonical partition function for N indistinguish

mions
 $\mathcal{Z} = \left(\sum_{n_1} e^{-\beta(e_1 - \mu)n_1}\right) \left(\sum_{n_2} e^{-\beta(e_2 - \mu)n_2}\right) \cdots$

(re will be only two particles in each The fermions have only two states, $n_s = 0$ or 1. Thus, in the grand canonical partition function for N indistinguishable fermions

$$
\mathcal{Z} = \left(\sum_{n_1} e^{-\beta(\epsilon_1 - \mu)n_1}\right) \left(\sum_{n_2} e^{-\beta(\epsilon_2 - \mu)n_2}\right) \cdots \qquad (3.13)
$$

there will be only two particles in each sum $n_s = 0$ or 1.

So

$$
\mathcal{Z} = \left(1 + e^{\beta(\mu - \epsilon_1)}\right) \left(1 + e^{\beta(\mu - \epsilon_2)}\right) \cdots \tag{3.14}
$$

and

$$
\ln \mathcal{Z} = \sum_{s} \ln \left(1 + e^{\beta(\mu - \epsilon_s)} \right) \tag{3.15}
$$

The number of particles is given by

$$
N = \frac{1}{\beta} \frac{\partial \ln \mathcal{Z}}{\partial \mu} = \sum_{s} \frac{e^{\beta(\mu - \epsilon_s)}}{1 + e^{\beta(\mu - \epsilon_s)}} = \sum_{s} \langle n_s \rangle \tag{3.16}
$$

Thus the average number of molecules in the s level is

$$
\langle n_s \rangle_{FD} = \frac{1}{e^{\beta(\epsilon_s - \mu)} + 1} \tag{3.17}
$$

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3.4 Boltzmann limit of Boson and Fermion gasses:

The Bose-Einstein (BE) and Fermi-Dirac (FD) distributions are given by

$$
\langle n_s \rangle = \frac{1}{e^{\beta(\epsilon_s - \mu)} \pm 1}
$$

where + corresponds to FD and - corresponds to BE distribution. Suppose that,

$$
e^{-\beta\mu} \gg 1
$$
 that is $e^{\beta(\epsilon_s - \mu)} \gg 1$

In this case,

$$
\langle n_s \rangle \approx \frac{1}{e^{\beta(\epsilon_s - \mu)}} = e^{\beta \mu_e - \beta \epsilon_s}
$$

and

gasses:
\ne Bose-Einstein (BE) and Fermi-Dirac (FD) distribut
\ngiven by
\n
$$
\langle n_s \rangle = \frac{1}{e^{\beta(\epsilon_s - \mu)} \pm 1}
$$
\nere + corresponds to FD and - corresponds to BE dis-
\ntion. Suppose that,
\n
$$
e^{-\beta \mu} \gg 1 \quad \text{that is} \quad e^{\beta(\epsilon_s - \mu)} \gg 1
$$
\nIn this case,
\n
$$
\langle n_s \rangle \approx \frac{1}{e^{\beta(\epsilon_s - \mu)}} = e^{\beta \mu_e - \beta \epsilon_s}
$$
\n
$$
\sum \langle n_s \rangle = N = e^{\beta \mu} \sum_s e^{-\beta \epsilon_s} \quad \text{or} \quad e^{\beta \mu} = \frac{N}{\sum_s e^{-\beta \epsilon_s}}
$$
\nThus the distribution becomes

Thus the distribution becomes

$$
\langle n_s \rangle = \frac{N e^{-\beta \epsilon_s}}{\sum_s e^{-\beta \epsilon_s}}
$$

as that of classical Maxwell-Boltzmann distribution. Thus the quantum statistics will behave like a classical statistics in the limit of

$$
e^{-\beta\mu}\gg 1
$$

equantum statistics will behave like a classical stat

the limit of
 $e^{-\beta\mu} \gg 1$

where μ is chemical potential of an ideal gas of N mo

a volume V at temperature T, since the partition

in of an ideal gas of N molec where μ is chemical potential of an ideal gas of N molecules in a volume V at temperature T . since the partition function of an ideal gas of N molecules in a volume V at temperature T is given by

$$
Z(N, V, T) = \frac{1}{N!} \left[\frac{V}{h^3} (2m\pi k_B T)^{3/2} \right]^N
$$

and correspondingly the free energy will be

$$
F = -k_B T \ln Z = -Nk_B T \ln \frac{V}{N} \left(\frac{2m\pi k_B T}{h^2}\right)^{3/2} - Nk_B T
$$

The chemical potential of the ideal gas is then given by

$$
\mu = \left(\frac{\partial F}{\partial N}\right)_{V,T} = -k_B T \ln \left[\left(\frac{2\pi m k_B T}{h^2}\right)^{3/2} \frac{V}{N} \right]
$$

Thus one has,

$$
\left(\frac{2\pi mk_BT}{h^2}\right)^{3/2}\frac{V}{N} \gg 1 \quad \Longrightarrow \quad \frac{1}{\lambda^3}\frac{V}{N} \gg 1 \tag{3.18}
$$

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where $\lambda = h/\sqrt{2\pi mk_BT}$ is the thermal wavelength. The above condition will be then satisfied only for the values of the physical parameters $T \to \infty$ and $\rho \to 0$. This is known as the classical limit of the quantum gas.

3.5 Equation of state of a quantum Ideal Gas

Consider a gas of N non-interacting identical quantum particles enclosed in a volume V . The distribution function for the particles of the gas is given by

$$
\langle n \rangle = \frac{1}{e^{\beta(\epsilon-\mu)}\pm 1}
$$

by condition will be then satisfied only for the value
physical parameters $T \to \infty$ and $\rho \to 0$. This is known the classical limit of the quantum gas.
Equation of state of a quantum Ic
Gas
msider a gas of N non-inter where $+$ sign corresponds to FD and $-$ sign corresponds to BE distribution. In order to obtain the equation of state, one needs to establish a relationship between the pressure P, volume V and energy E . The mean energy E of the system is given by

$$
E = \int_0^\infty \epsilon g(\epsilon) \langle n \rangle d\epsilon \tag{3.19}
$$

where $g(\epsilon)$ is the density of states between energy ϵ and $\epsilon+d\epsilon$. The number of states $g(p)$ between momentum p and $p + dp$ is

$$
g(p)dp = \frac{1}{h^3}d^3qd^3p = \frac{V}{h^3}d^3p = \frac{V}{h^3}4\pi p^2 dp \qquad (3.20)
$$

since $p^2 = 2m\epsilon$, the number of states $g(\epsilon)$ between energy ϵ and $\epsilon + d\epsilon$ is then

$$
g(\epsilon)d\epsilon = \frac{2\pi V}{h^3} (2m)^{3/2} \epsilon^{1/2} d\epsilon \qquad (3.21)
$$

de. The number of states $g(p)$ between momentum p
 dp is
 $g(p)dp = \frac{1}{h^3}d^3qd^3p = \frac{V}{h^3}d^3p = \frac{V}{h^3}4\pi p^2dp$ (

since $p^2 = 2m\epsilon$, the number of states $g(\epsilon)$ between en
 $g(\epsilon) d\epsilon = \frac{2\pi V}{h^3}(2m)^{3/2}\epsilon^{1/2}d\epsilon$ (
 If the particles have spin we must multiply the spin degeneracy with the number of states. We will discuss more on DOS in the next section.

The energy E of the system is then given by

$$
E = \frac{2\pi V}{h^3} (2m)^{3/2} \int_0^\infty \frac{\epsilon^{3/2}}{e^{\beta(\epsilon - \mu)} \pm 1} d\epsilon \qquad (3.22)
$$

The grand canonical partition function of the gas is given by

$$
q = \ln \mathcal{Z} = \int_0^\infty \ln \left(1 \pm e^{-\beta(\epsilon - \mu)} \right)^{\pm 1} g(\epsilon) d\epsilon \qquad (3.23)
$$

 $q = \ln \mathcal{Z} = \int_0^\infty \ln \left(1 \pm e^{-\beta(\epsilon - \mu)} \right)^{\pm 1} g(\epsilon) d\epsilon$
where + sign corresponds to FD and - sign corresp
BE distribution as before. The pressure P of the g
n
 $P = k_B T q / V = \frac{k_B T}{V} \int_0^\infty \ln \left(1 \pm e^{-\beta(\epsilon - \mu)} \right)^{\pm 1} g(\epsilon) d\epsilon$
 P where $+$ sign corresponds to FD and $-$ sign corresponds to BE distribution as before. The pressure P of the gas is then

$$
P = k_B T q/V = \frac{k_B T}{V} \int_0^\infty \ln \left(1 \pm e^{-\beta(\epsilon - \mu)} \right)^{\pm 1} g(\epsilon) d\epsilon
$$

or

$$
P = k_B T \frac{2\pi}{h^3} (2m)^{3/2} \int_0^\infty \ln\left(1 \pm e^{-\beta(\epsilon - \mu)}\right)^{\pm 1} \epsilon^{1/2} d\epsilon
$$

Integrating by parts, you can get the pressure as

$$
P = \frac{2}{3V} \left(\frac{2\pi V}{h^3} (2m)^{3/2} \int_0^\infty \frac{\epsilon^{3/2}}{e^{\beta(\epsilon - \mu)} \pm 1} d\epsilon \right) = \frac{2}{3} \frac{E}{V} \quad (3.24)
$$

So the equation of state

$$
PV = \frac{2}{3}E\tag{3.25}
$$

You see that the equation of state is then independent of whether the particles follow FD or BE statistics

4 Density matrix and average values

We will learn through problems. Suppose there are N.particles fixed in space. The Hamiltonian of the system is

ues

will learn through problems. Suppose there are N.pa

ed in space. The Hamiltonian of the system is

system is, $H = K \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$

leulate *A*, *S* and *Cv*
 Solution:

(1) We take out th system is, $H = K$ $\sqrt{ }$ $\ddot{}$ 0 1 0 1 0 1 0 1 0 \setminus $\begin{array}{c} \hline \end{array}$

Calculate A, S and Cv

Solution:

(1) We take out the possible energies by calculating the eigenvalues n.

(2) Use that energies to calculate Partition Function.

(3) Calculate required quantities using the Partition Function.

 $H = K$ $\sqrt{2}$ $\overline{\mathcal{L}}$ 0 1 0 1 0 1 0 1 0 \setminus $\bigg)$

Eigan values $= 0, +$ √ $2K, -$ √ $2K$ Single particle and total Partition function is then

$$
Z_1 = e^{-\beta \cdot 0} + e^{-\beta \sqrt{2}k} + e^{\beta \sqrt{2}k}
$$

= 1 + e^{-\beta \sqrt{2}k} + e^{\beta \sqrt{2}k}

$$
Z = Z_1^N
$$

Calculate the asked quantities.

Now

Given another obsovable,
$$
A = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 3 \\ 0 & 3 & 4 \end{pmatrix}
$$

Find $\langle A \rangle$ in the same basis. (in which the Hamiltonian is diagonalized)

Solution:

$$
Z_1 = e^{-\beta \cdot 0} + e^{-\beta \sqrt{2}k} + e^{\beta \sqrt{2}k}
$$

\n
$$
= 1 + e^{-\beta \sqrt{2}k} + e^{\beta \sqrt{2}k}
$$

\n
$$
Z = Z_1^N
$$

\nCalculate the asked quantities.
\nNow
\n
$$
Given another obsovable, A = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 3 \\ 0 & 3 & 4 \end{pmatrix}
$$

\nFind $\langle A \rangle$ in the same basis. (in which the Hamiltonian
\ndiagonalized)
\nSolution:
\n
$$
Avg. Quantities: -\langle f(\epsilon) \rangle = \frac{\int f(\epsilon)e^{-\beta \epsilon}d\epsilon}{\int e^{-\beta \epsilon}d\epsilon} : Continuous
$$

\n
$$
\langle f(\epsilon) \rangle = \frac{\sum_{i} f_i e^{-\beta \epsilon_i}}{\sum_{i} e^{-\beta \epsilon_i}} : Discrete
$$

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Average value of an observable is

$$
\langle A \rangle = \frac{\text{Tr}\left(Ae^{-\beta H}\right)}{\text{Tr}\left(e^{-\beta H}\right)}\tag{4.1}
$$

√

We know from function of a matrix

$$
\Lambda = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix} \implies e^{A} = \begin{pmatrix} e^{1} & 0 & 0 \\ 0 & e^{2} & 0 \\ 0 & 0 & e^{3} \end{pmatrix}
$$

$$
\langle A \rangle = \frac{\text{Tr}(Ae^{-\beta H})}{\text{Tr}(e^{-\beta H})}
$$

We know from function of a matrix

$$
\Lambda = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix} \implies e^{A} = \begin{pmatrix} e^{1} & 0 & 0 \\ 0 & e^{2} & 0 \\ 0 & 0 & e^{3} \end{pmatrix}
$$

In our problem, $H = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \sqrt{2k} & 0 \\ 0 & 0 & -\sqrt{2k} \end{pmatrix}$

$$
e^{-\beta H} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & e^{-\beta\sqrt{2}k} & 0 \\ 0 & 0 & e^{\beta\sqrt{2}k} \end{pmatrix}
$$

we transform the A matrix by similarity transform.
h the S matrix which diagonalizes the Hamiltonian
(writing the eigenvectors of the H matrix columnw

0 0 e β Now transform the A matrix by similarity transformation with the S matrix which diagonalizes the Hamiltonian (formed my writing the eigenvectors of the H matrix columnwise))

$$
A' = S^{-1}AS
$$

Then calculate the Trace.

5 Density of states calculation

In different dimensions start the DOS calculation with these basic formulas

$$
1D \quad \Longrightarrow \quad \left(\frac{L}{2\pi}\right) \int dk \tag{5.1}
$$

$$
2D \quad \Longrightarrow \quad \left(\frac{L}{2\pi}\right)^2 \int 2\pi k dk \tag{5.2}
$$

$$
3D \implies \left(\frac{L}{2\pi}\right)^3 \int 4\pi k^2 dk \tag{5.3}
$$

d D
$$
\Longrightarrow
$$
 $\left(\frac{L}{2\pi}\right)^d \int \frac{2\pi^{d/2}}{\Gamma(d/2)} k^{d-1} dk$ (5.4)

different dimensions start the DOS calculation with

sic formulas
 $1D \implies \left(\frac{L}{2\pi}\right) \int dk$
 $2D \implies \left(\frac{L}{2\pi}\right)^2 \int 2\pi k dk$
 $3D \implies \left(\frac{L}{2\pi}\right)^3 \int 4\pi k^2 dk$
 $dD \implies \left(\frac{L}{2\pi}\right)^d \int \frac{2\pi^{d/2}}{\Gamma(d/2)} k^{d-1} dk$

There are relati There are relations between energy and momentum $E =$ $E(k)$, which is sometimes also written as $\omega = \omega(k)$. Use these dispersion relations to get the DOS as a function of energy / frequency / momentum.

5.1 DOS of 3D photon gas

Dispersion relation of photon gas

$$
\epsilon = h\nu = \hbar ck \tag{5.5}
$$

Hence DOS

$$
2\left(\frac{L}{2\pi}\right)^3 \int 4\pi \left(\frac{\epsilon}{\hbar c}\right)^2 \frac{d\epsilon}{\hbar c} \tag{5.6}
$$

5.2 DOS of 3D phonon: Debye model

Dispersion relation

$$
\omega = v k \tag{5.7}
$$

spersion relation of photon gas
 $\epsilon = h\nu = \hbar ck$

Hence DOS
 $2\left(\frac{L}{2\pi}\right)^3 \int 4\pi \left(\frac{\epsilon}{\hbar c}\right)^2 \frac{d\epsilon}{\hbar c}$

2 DOS of 3D phonon: Debye model

spersion relation
 $\omega = vk$

ere are three modes - One for longitudinal Two for There are three modes - One for longitudinal Two for transverse. Velocities may be different. Let's say v_l for longitudinal and v_t for transverse. So DOS

$$
\left(\frac{L}{2\pi}\right)^3 \int 4\pi k^2 dk \Rightarrow \left(\frac{L}{2\pi}\right)^3 \int 4\pi \left(\frac{\omega^2}{v_l^2} \frac{d\omega}{v_l} + 2\frac{\omega^2}{v_t^2} \frac{d\omega}{v_t}\right)
$$

$$
= \left(\frac{L}{2\pi}\right)^3 4\pi \left(\frac{1}{v_l^3} + \frac{2}{v_t^3}\right) \int \omega^2 d\omega
$$
(5.8)

5.3 DOS of 3D gas

Dispersion relation

$$
\epsilon = \frac{\hbar^2 k^2}{2m}
$$

(5.9)

Hence

$$
k = \sqrt{\frac{2m\epsilon}{\hbar^2}} \quad \to \quad dk = \frac{\sqrt{2m}}{\hbar} \cdot \epsilon^{-1/2} d\epsilon
$$

So DOS

expression relation

\n
$$
\epsilon = \frac{\hbar^2 k^2}{2m}
$$
\nsince

\n
$$
k = \sqrt{\frac{2m\epsilon}{\hbar^2}} \rightarrow dk = \frac{\sqrt{2m}}{\hbar} \cdot \epsilon^{-1/2} d\epsilon
$$
\nDOS

\n
$$
\left(\frac{L}{2\pi}\right)^3 \int 4\pi k^2 dk
$$
\n
$$
\Rightarrow (2j+1) \cdot \left(\frac{L}{2\pi}\right)^3 \int 4\pi \frac{2m\epsilon}{\hbar^2} \frac{\sqrt{2m}}{\hbar} \cdot \epsilon^{-1/2} d\epsilon
$$
\n(5.10)

\ne multiplication of (2j+1) is because of spin degeneracy.

\ne DOS is simplified as for the electrons $j = 1/2$

\n
$$
\frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \int \epsilon^{1/2} d\epsilon
$$
\n(5.11)

\nDOS of 3D relativistic system

The multiplication of $(2j + 1)$ is because of spin degeneracy. The DOS is simplified as for the electrons $j=1/2$

$$
\frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \int \epsilon^{1/2} d\epsilon \tag{5.11}
$$

5.4 DOS of 3D relativistic system

Energy momentum relation

$$
E = \sqrt{\hbar^2 k^2 c^2 + m^2 c^4} \tag{5.12}
$$

Hence

$$
g(E) = \frac{VE}{2\pi^2\hbar^3 c^3} \sqrt{E^2 - m^2 c^4}
$$
 (5.13)

For massless particles

$$
g(E) = \frac{VE^2}{2\pi^2\hbar^3 c^3} \tag{5.14}
$$

5.5 General DOS for d dimensional system with general dispersion relation: $\epsilon =$ ck^s

Dispersion relation

$$
\epsilon = ck^s \quad \Rightarrow \quad k = \left(\frac{\epsilon}{c}\right)^{1/s} \quad \Rightarrow \quad dk = \frac{1}{s} \left(\frac{\epsilon}{c}\right)^{\frac{1}{s}-1} d\epsilon \tag{5.15}
$$

So DOS

$$
g(E) = \frac{g(E)}{2\pi^2 \hbar^3 c^3} \sqrt{E^2 - m^2 c^4}
$$
\nfor massless particles\n
$$
g(E) = \frac{VE^2}{2\pi^2 \hbar^3 c^3}
$$
\n(5.14)\n6.5 General DOS for *d* dimensional system with general dispersion relation: $\epsilon = ck^s$ \n
$$
\epsilon = ck^s \Rightarrow k = \left(\frac{\epsilon}{c}\right)^{1/s} \Rightarrow dk = \frac{1}{s} \left(\frac{\epsilon}{c}\right)^{\frac{1}{s}-1} de
$$
\n(5.15)\n6 DOS\n
$$
\left(\frac{L}{2\pi}\right)^d \int \frac{2\pi^{d/2}}{\Gamma(d/2)} k^{d-1} dk
$$
\n
$$
\Rightarrow (2j+1) \left(\frac{L}{2\pi}\right)^d \int \frac{2\pi^{d/2}}{\Gamma(d/2)} \left(\frac{\epsilon}{c}\right)^{(d-1)/s} \frac{1}{s} \left(\frac{\epsilon}{c}\right)^{\frac{1}{s}-1} de
$$
\n
$$
= (2j+1)A \int \epsilon^{\frac{d}{s}-1} de
$$
\n(5.16)

Most of the time it is sufficient to remember the parties. Where all the constants has been accomodated under A. Most of the time it is sufficient to remember the power: $\epsilon^{\frac{d}{s}}$ $\frac{d}{s}-1$