The Quantum Distribution Functions

April 26, 2021

Expected number of particles in state s

$$\langle n_s \rangle = \sum_R n_s P(n_s)$$

$$\langle n_s \rangle = \frac{\sum_R n_s e^{-\beta E_R}}{\sum_R e^{-\beta E_R}}$$

Example: Harmonic Oscillator

3 particles distributed among 4 states

R/s	n=0	n=1	n=2	n=3	E_R
1	3	0	0	0	$\frac{3}{2}\hbar\omega$
2	0	3	0	0	$\frac{9}{2}\hbar\omega$
3	0	0	3	0	$\frac{15}{2}\hbar\omega$
4	0	0	0	3	$\frac{21}{2}\hbar\omega$
5	2	1	0	0	$\frac{5}{2}\hbar\omega$
6	2	0	1	0	$\frac{7}{2}\hbar\omega$
7	2	0	0	1	$\frac{9}{2}\hbar\omega$
8	0	2	1	0	$\frac{11}{2}\hbar\omega$
9	0	2	0	1	$\frac{13}{2}\hbar\omega$
10	1	2	0	0	$\frac{7}{2}\hbar\omega$

Example: Harmonic Oscillator

(continued...)

R/s	n=0	n=1	n=2	n=3	E_R
11	0	0	2	1	$\frac{17}{2}\hbar\omega$
12	1	0	2	0	$\frac{11}{2}\hbar\omega$
13	0	1	2	0	$\frac{13}{2}\hbar\omega$
14	1	0	0	2	$\frac{15}{2}\hbar\omega$
15	0	1	0	2	$\frac{17}{2}\hbar\omega$
16	0	0	1	2	$\frac{19}{2}\hbar\omega$
17	1	1	1	0	$\frac{9}{2}\hbar\omega$
18	0	1	1	1	$\frac{15}{2}\hbar\omega$
19	1	0	1	1	$\frac{13}{2}\hbar\omega$
20	1	1	0	1	$\frac{11}{2}\hbar\omega$

Example: Harmonic Oscillator

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1	3	0	0	0	$\frac{3}{2}\hbar\omega$
2	0	3	0	0	$\frac{9}{2}\hbar\omega$
3	0	0	3	0	$\frac{15}{2}\hbar\omega$
4	0	0	0	3	$\frac{21}{2}\hbar\omega$
5	2	1	0	0	$\frac{5}{2}\hbar\omega$
6	2	0	1	0	$\frac{7}{2}\hbar\omega$
7	2	0	0	1	$\frac{9}{2}\hbar\omega$
8	0	2	1	0	$\frac{11}{2}\hbar\omega$
9	0	2	0	1	$\frac{13}{2}\hbar\omega$
10	1	2	0	0	$\frac{7}{2}\hbar\omega$

$$\sum_R n_2 e^{-\beta E_R} =$$
$$0 \cdot e^{-\frac{3}{2}\beta\hbar\omega} +$$
$$0 \cdot e^{-\frac{9}{2}\beta\hbar\omega} +$$
$$3 \cdot e^{-\frac{15}{2}\beta\hbar\omega} +$$
$$0 \cdot e^{-\frac{21}{2}\beta\hbar\omega} +$$
$$0 \cdot e^{-\frac{5}{2}\beta\hbar\omega} +$$
$$1 \cdot e^{-\frac{7}{2}\beta\hbar\omega} +$$
$$0 \cdot e^{-\frac{9}{2}\beta\hbar\omega} +$$
$$1 \cdot e^{-\frac{11}{2}\beta\hbar\omega} +$$
$$0 \cdot e^{-\frac{13}{2}\beta\hbar\omega} +$$
$$0 \cdot e^{-\frac{7}{2}\beta\hbar\omega} + \cdots$$

Expected number of particles in state s

$$\langle n_s \rangle = \frac{\sum_R n_s e^{-\beta E_R}}{\sum_R e^{-\beta E_R}} = \frac{\sum_R n_s e^{-\beta(n_1\epsilon_1 + n_2\epsilon_2 + \cdots + n_s\epsilon_s + \cdots)}}{\sum_R e^{-\beta(n_1\epsilon_1 + n_2\epsilon_2 + \cdots + n_s\epsilon_s + \cdots)}}$$

$$= \frac{\sum_R n_s e^{\beta n_s \epsilon_s} e^{-\beta(n_1\epsilon_1 + n_2\epsilon_2 + \cdots + n_{s-1}\epsilon_{s-1} + \cdots)}}{\sum_R e^{-\beta n_s \epsilon_s} e^{-\beta(n_1\epsilon_1 + n_2\epsilon_2 + \cdots + n_{s-1}\epsilon_{s-1} + \cdots)}}$$

Here we factor terms depending on state s from the sum

Expected number of particles in state s

$$\langle n_s \rangle = \frac{\sum_R n_s e^{\beta n_s \epsilon_s} e^{-\beta(n_1\epsilon_1 + n_2\epsilon_2 + \cdots + n_{s-1}\epsilon_{s-1} + \cdots)}}{\sum_R e^{-\beta n_s \epsilon_s} e^{-\beta(n_1\epsilon_1 + n_2\epsilon_2 + \cdots + n_{s-1}\epsilon_{s-1} + \cdots)}}$$

$$= \frac{\sum_{n_s} n_s e^{-\beta n_s \epsilon_s} \sum_{R^{(s)}} e^{-\beta(n_1\epsilon_1 + n_2\epsilon_2 + \cdots + n_{s-1}\epsilon_{s-1} + \cdots)}}{\sum_{n_s} e^{-\beta n_s \epsilon_s} \sum_{R^{(s)}} e^{-\beta(n_1\epsilon_1 + n_2\epsilon_2 + \cdots + n_{s-1}\epsilon_{s-1} + \cdots)}}$$

And we can sum over system s separately

Expected number of particles in state s

$$\langle n_s \rangle = \frac{\sum_R n_s e^{-\beta n_s \epsilon_s} e^{-\beta(n_1\epsilon_1 + n_2\epsilon_2 + \cdots + n_{s-1}\epsilon_{s-1} + \cdots)}}{\sum_R e^{-\beta n_s \epsilon_s} e^{-\beta(n_1\epsilon_1 + n_2\epsilon_2 + \cdots + n_{s-1}\epsilon_{s-1} + \cdots)}}$$

$$= \frac{\sum_{n_s} n_s e^{-\beta n_s \epsilon_s} \sum_{R^{(s)}} e^{-\beta(n_1\epsilon_1 + n_2\epsilon_2 + \cdots + n_{s-1}\epsilon_{s-1} + \cdots)}}{\sum_{n_s} e^{-\beta n_s \epsilon_s} \sum_{R^{(s)}} e^{-\beta(n_1\epsilon_1 + n_2\epsilon_2 + \cdots + n_{s-1}\epsilon_{s-1} + \cdots)}}$$

$\sum_{R^{(s)}} \rightarrow$sum over all microstates of the subsystem excluding state s (subject to the constraint that $n_s + \sum_{i, i \neq s} n_i = N$)

Example

If $N = 3$, and there are 4 single particle states

$$\sum_{n_s} n_s e^{-\beta n_s \epsilon_s} \sum_{R^{(s)}} e^{-\beta\left(n_1\epsilon_1 + n_2\epsilon_2 + \cdots + n_{s-1}\epsilon_{s-1} + \cdots\right)} =$$

$$0 \cdot e^{-\beta\cdot 0\cdot\epsilon_2}\left(e^{-\beta(3\cdot\epsilon_1+0\cdot\epsilon_3+0\cdot\epsilon_4)} + e^{-\beta(0\cdot\epsilon_1+3\cdot\epsilon_3+0\cdot\epsilon_4)} + e^{-\beta(0\cdot\epsilon_1+0\cdot\epsilon_3+3\cdot\epsilon_4)} + \cdots\right) +$$

$$1 \cdot e^{-\beta\cdot 1\cdot\epsilon_2}\left(e^{-\beta(2\cdot\epsilon_1+0\cdot\epsilon_3+0\cdot\epsilon_4)} + e^{-\beta(0\cdot\epsilon_1+2\cdot\epsilon_3+0\cdot\epsilon_4)} + e^{-\beta(0\cdot\epsilon_1+0\cdot\epsilon_3+2\cdot\epsilon_4)} + \cdots\right) +$$

$$2 \cdot e^{-\beta\cdot 2\cdot\epsilon_2}\left(e^{-\beta(1\cdot\epsilon_1+0\cdot\epsilon_3+0\cdot\epsilon_4)} + e^{-\beta(0\cdot\epsilon_1+1\cdot\epsilon_3+0\cdot\epsilon_4)} + e^{-\beta(0\cdot\epsilon_1+0\cdot\epsilon_3+1\cdot\epsilon_4)}\right) +$$

$$3 \cdot e^{-\beta\cdot 3\epsilon_2}\left(e^{-\beta(0\cdot\epsilon_1+0\cdot\epsilon_3+0\cdot\epsilon_4)}\right)$$

Expected number of particles in state s

Note that

$$\sum_R e^{-\beta(n_1\epsilon_1+n_2\epsilon_2+\cdots+n_s\epsilon_s+\cdots)}$$

Is just the partition function of the entire system.

Expected number of particles in state s

Note that

$$\sum_R e^{-\beta(n_1\epsilon_1+n_2\epsilon_2+\cdots+n_s\epsilon_s+\cdots)}$$

So we interpret the quantity

$$\sum_{R^{(s)}} e^{-\beta(n_1\epsilon_1+n_2\epsilon_2+\cdots+n_{s-1}\epsilon_{s-1}+\cdots)}$$

As the partition function of the subsystem consisting of:

- All system states *except* s
- All N system particles *except* n_s

Expected number of particles in state s

And we introduce the following definition:

$$Z_s(N - n_s) \equiv \sum_{R^{(s)}} e^{-\beta(n_1\epsilon_1 + n_2\epsilon_2 + \cdots + n_{s-1}\epsilon_{s-1} + \cdots)}$$

Expected number of particles in state s

$$\langle n_s \rangle = \frac{\sum_{n_s} n_s e^{-\beta n_s \epsilon_s} Z_s(N - n_s)}{\sum_{n_s} e^{-\beta n_s \epsilon_s} Z_s(N - n_s)}$$

$\langle n_s \rangle$ for fermions

$$\langle n_s \rangle = \frac{\sum_{n_s} n_s e^{-\beta n_s \epsilon_s} Z_s(N - n_s)}{\sum_{n_s} e^{-\beta n_s \epsilon_s} Z_s(N - n_s)}$$

For **fermions** $\sum_{n_s}$ is simple:

- n_s can only be 0 or 1

$\langle n_s \rangle$ for fermions

$$\langle n_s \rangle = \frac{\sum_{n_s} n_s e^{-\beta n_s \epsilon_s} Z_s(N - n_s)}{\sum_{n_s} e^{-\beta n_s \epsilon_s} Z_s(N - n_s)}$$

$$= \frac{0 \cdot e^{-\beta \cdot 0 \cdot \epsilon_s} Z_s(N) + 1 \cdot e^{-\beta \cdot 1 \cdot \epsilon_s} Z_s(N-1)}{e^{-\beta \cdot 0 \cdot \epsilon_s} Z_s(N) + e^{-\beta \cdot 1 \cdot \epsilon_s} Z_s(N-1)}$$

$$= \frac{e^{-\beta \epsilon_s} Z_s(N-1)}{Z_s(N) + e^{-\beta \epsilon_s} Z_s(N-1)}$$

$\langle n_s \rangle$ for fermions

$$\langle n_s \rangle = \frac{e^{-\beta\epsilon_s} Z_s(N-1)}{Z_s(N) + e^{-\beta\epsilon_s} Z_s(N-1)}$$

$$= \frac{1}{\frac{Z_s(N)}{Z_s(N-1)} e^{-\beta\epsilon_s} + 1}$$

$\langle n_s \rangle$ for fermions

$$\langle n_s \rangle = \frac{1}{\frac{Z_s(N)}{Z_s(N-1)} e^{\beta \epsilon_s} + 1}$$

$\langle n_s \rangle$ for fermions

Now we use a Taylor expansion to relate $Z_s(N)$ to $Z_s(N-1)$ (since $N >> 1$)

$$\ln Z_s(N-1) \approx \ln Z_s(N) - 1 \cdot \frac{\partial}{\partial N} \ln Z_s(N)$$

$\langle n_s \rangle$ for fermions

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$$\ln Z_s(N-1) \approx \ln Z_s(N) - 1 \cdot \frac{\partial}{\partial N} \ln Z_s(N)$$

Recall that:

$$F = -kT \ln Z_s(N)$$

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So:

$$\frac{\partial}{\partial N} \ln Z_s(N) = -\frac{1}{kT} \frac{\partial F}{\partial N} = -\beta \frac{\partial F}{\partial N}$$

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$$\frac{\partial}{\partial N} \ln Z_s(N) = -\frac{1}{kT} \frac{\partial F}{\partial N} = -\beta \frac{\partial F}{\partial N}$$

And:

$$\frac{\partial F}{\partial N} = \mu$$

$\langle n_s \rangle$ for fermions

So:

$$\frac{\partial}{\partial N} \ln Z_s(N) = -\beta\mu$$

And:

$$\ln Z_s(N-1) \approx \ln Z_s(N) - 1 \cdot \frac{\partial}{\partial N} \ln Z_s(N)$$

$$= \ln Z_s(N) + \mu\beta$$

$\langle n_s \rangle$ for fermions

$$\ln Z_s(N-1) \approx \ln Z_s(N) + \mu\beta$$

So:

$$Z_s(N-1) \approx Z_s(N) e^{\mu\beta}$$

And:

$$\frac{Z_s(N)}{Z_s(N-1)} \approx e^{-\mu\beta}$$

$\langle n_s \rangle$ for fermions

$$\frac{Z_s(N)}{Z_s(N-1)} \approx e^{-\mu\beta}$$

And:

$$\langle n_s \rangle = \frac{1}{\frac{Z_s(N)}{Z_s(N-1)} e^{\beta\epsilon_s} + 1}$$

So:

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

$\langle n_s \rangle$ for fermions

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

$\langle n_s \rangle$ for *bosons*

$$\langle n_s \rangle = \frac{\sum_{n_s} n_s e^{-\beta n_s \epsilon_s} Z_s(N - n_s)}{\sum_{n_s} e^{-\beta n_s \epsilon_s} Z_s(N - n_s)}$$

$\langle n_s \rangle$ for *bosons*

$$\langle n_s \rangle = \frac{\sum_{n_s} n_s e^{-\beta n_s \epsilon_s} Z_s(N - n_s)}{\sum_{n_s} e^{-\beta n_s \epsilon_s} Z_s(N - n_s)}$$

For **bosons**, $\sum_{n_s}$ ranges from $n_s = 0$ up to $n_s = N$

$\langle n_s \rangle$ for *bosons*

$$\langle n_s \rangle = \frac{\sum_{n_s} n_s e^{-\beta n_s \epsilon_s} Z_s(N - n_s)}{\sum_{n_s} e^{-\beta n_s \epsilon_s} Z_s(N - n_s)}$$

$$= \frac{0 \cdot e^{\beta \cdot 0 \cdot \epsilon_s} \cdot Z_s(N) + 1 \cdot e^{-\beta \cdot \epsilon_s} \cdot Z_s(N-1) + 2 \cdot e^{-\beta \cdot 2 \cdot \epsilon_s} \cdot Z_s(N-2) + 3 \cdot e^{-\beta \cdot 3 \cdot \epsilon_s} \cdot Z_s(N-3) + \cdots}{e^{\beta \cdot 0 \cdot \epsilon_s} \cdot Z_s(N) + e^{-\beta \cdot \epsilon_s} \cdot Z_s(N-1) + e^{-\beta \cdot 2 \cdot \epsilon_s} \cdot Z_s(N-2) + e^{-\beta \cdot 3 \cdot \epsilon_s} \cdot Z_s(N-3) + \cdots}$$

$\langle n_s \rangle$ for bosons

Again using a Taylor expansion:

$$\ln Z_s(N - \Delta N) \approx \ln Z_s(N) - \Delta N \cdot \frac{\partial}{\partial N} \ln Z_s(N)$$

$\langle n_s \rangle$ for bosons

Again using a Taylor expansion:

$$\ln Z_s(N - \Delta N) \approx \ln Z_s(N) - \Delta N \cdot \frac{\partial}{\partial N} \ln Z_s(N)$$

And recalling that:

$$\frac{\partial}{\partial N} \ln Z_s(N) = \beta \frac{\partial F}{\partial N} = -\beta\mu$$

$\langle n_s \rangle$ for bosons

Again using a Taylor expansion:

$$\ln Z_s(N - \Delta N) \approx \ln Z_s(N) - \Delta N \cdot \frac{\partial}{\partial N} \ln Z_s(N)$$

And recalling that:

$$\frac{\partial}{\partial N} \ln Z_s(N) = \beta \frac{\partial F}{\partial N} = -\beta\mu$$

We find:

$$\frac{Z_s(N)}{Z_s(N - \Delta N)} \approx e^{-\Delta N \mu \beta}$$

$\langle n_s \rangle$ for bosons

Using this fact: we can rewrite $\langle n_s \rangle$:

$$\langle n_s \rangle = \frac{0 \cdot e^{\beta \cdot 0 \cdot \epsilon_s} \cdot Z_s(N) + 1 \cdot e^{-\beta \cdot \epsilon_s} \cdot Z_s(N-1) + 2 \cdot e^{-\beta \cdot 2 \cdot \epsilon_s} \cdot Z_s(N-2) + 3 \cdot e^{-\beta \cdot 3 \cdot \epsilon_s} \cdot Z_s(N-3) + \cdots}{e^{\beta \cdot 0 \cdot \epsilon_s} \cdot Z_s(N) + e^{-\beta \cdot \epsilon_s} \cdot Z_s(N-1) + e^{-\beta \cdot 2 \cdot \epsilon_s} \cdot Z_s(N-2) + e^{-\beta \cdot 3 \cdot \epsilon_s} \cdot Z_s(N-3) + \cdots}$$

$$= \frac{Z_s(N)\left(0 + \frac{Z_s(N-1)}{Z_s(N)} e^{-\beta \epsilon_s} + 2\frac{Z_s(N-2)}{Z_s(N)} e^{-2\beta \epsilon_s} + \cdots\right)}{Z_s(N)\left(0 + \frac{Z_s(N-1)}{Z_s(N)} e^{-\beta \epsilon_s} + \frac{Z_s(N-2)}{Z_s(N)} e^{-2\beta \epsilon_s} + \cdots\right)}$$

$\langle n_s \rangle$ for bosons

$$\langle n_s \rangle = \frac{Z_s(N)\left(0 + \frac{Z_s(N-1)}{Z_s(N)} e^{-\beta\epsilon_s} + 2\frac{Z_s(N-2)}{Z_s(N)} e^{-2\beta\epsilon_s} + \cdots\right)}{Z_s(N)\left(0 + \frac{Z_s(N-1)}{Z_s(N)} e^{-\beta\epsilon_s} + \frac{Z_s(N-2)}{Z_s(N)} e^{-2\beta\epsilon_s} + \cdots\right)}$$

And:

$$\frac{Z_s(N - \Delta N)}{Z_s(N)} \approx e^{\Delta N \beta \mu}$$

$\langle n_s \rangle$ for bosons

So:

$$\langle n_s \rangle = \frac{Z_s(N)\left(0 + e^{\beta\mu} e^{-\beta\epsilon_s} + 2e^{2\beta\mu} e^{-2\beta\epsilon_s} + \cdots\right)}{Z_s(N)\left(0 + e^{\beta\mu} e^{-\beta\epsilon_s} + e^{2\beta\mu} e^{-2\beta\epsilon_s} + \cdots\right)}$$

$$= \frac{e^{-\beta(\epsilon_s - \mu)} + 2e^{-2\beta(\epsilon_s - \mu)} + 3e^{-3\beta(\epsilon_s - \mu)} + \cdots}{1 + e^{-\beta(\epsilon_s - \mu)} + e^{-2\beta(\epsilon_s - \mu)} + e^{-3\beta(\epsilon_s - \mu)} + \cdots}$$

$$= \frac{\sum_{n_s} n_s e^{-\beta n_s(\epsilon_s - \mu)}}{\sum_{n_s} e^{-\beta n_s(\epsilon_s - \mu)}}$$

$\langle n_s \rangle$ for bosons

So:

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

$\langle n_s \rangle$ for bosons

So:

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

Which we write as:

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

$$= \frac{-\frac{1}{\beta}\frac{\partial}{\partial \epsilon_s} \sum_{n_s} e^{-\beta n_s(\epsilon_s - \mu)}}{\sum_{n_s} e^{-\beta n_s(\epsilon_s - \mu)}}$$

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

$\langle n_s \rangle$ for bosons

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

$\sum_{n_s} e^{-\beta n_s(\epsilon_s - \mu)}$ is a **geometric series**:

$$S_N = \sum_{n_s}^{N} r^{n_s}$$

Where $r = e^{-\beta(\epsilon_s - \mu)}$

$\langle n_s \rangle$ for bosons

We showed how to solve this series in class:

$$S_N = \sum_{n_s}^{N} r^{n_s} = \frac{1 - r^{N+1}}{1 - r}$$

If $|r| = \left| e^{-\beta(\epsilon_s - \mu)} \right| < 1$, and $N >> 1$:

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

$\langle n_s \rangle$ for bosons

Finally:

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

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

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

$\langle n_s \rangle$ for bosons

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

The quantum *distribution functions*

Fermions (*Fermi-Dirac statistics*)

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

Bosons (*Bose-Einstein statistics*)

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