Task 1

Consider a system with two single-particle energy levels, $\epsilon_1 = \epsilon$ and $\epsilon_2 = 2\epsilon$. Because they are fermionic levels, each can be occupied by $n_i \in \{0,1\}$. The grand canonical partition function is defined as:

$$\Xi = \sum_{n_1=0}^{1} \sum_{n_2=0}^{1} \exp[\beta \mu (n_1 + n_2)] \exp[-\beta (\epsilon n_1 + 2\epsilon n_2)].$$

Factor out the terms associated with each level:

$$\Xi = \left(\sum_{n_1=0}^{1} \exp[\beta \mu \, n_1 - \beta \, \epsilon \, n_1] \right) \left(\sum_{n_2=0}^{1} \exp[\beta \mu \, n_2 - 2\beta \, \epsilon \, n_2] \right).$$

Let $z \equiv e^{\beta\mu}$. Note that for each level i, the sum over $n_i = 0, 1$ is:

$$\sum_{n_i=0}^{1} \left(z e^{-\beta \epsilon_i} \right)^{n_i} = 1 + z e^{-\beta \epsilon_i}.$$

Hence, for our 2-level system:

$$\Xi \ = \ \left(1 + z\,e^{-\beta\epsilon}\right) \left(1 + z\,e^{-2\beta\epsilon}\right).$$

Task 2

 \mathbf{a}

In the two level BEC case, each pair of n_0 and n_1 is considered to be a microstate, where n_0 represents the number of particle in the ground state and n_0 for first excited state.

b

We have two single-particle energy levels:

Ground state energy: $E_0 = 0$, First excited state: $E_1 = \epsilon$.

We assume there are N particles and, in a classical (Maxwell–Boltzmann) treatment, the particles are effectively distinguishable for counting microstates.

Let n_1 be the number of particles in the excited state (with energy ϵ), so the total energy is

$$E(n_1) = n_1 \epsilon.$$

Since $n_0 + n_1 = N$, we have $n_0 = N - n_1$ in the ground state (energy 0).

Even though the particles are identical bosons physically, in the classical (MB) counting we introduce a degeneracy factor for which n_1 of the N particles occupy the excited state. This factor is given by the binomial coefficient

$$\binom{N}{n_1} = \frac{N!}{n_1! (N - n_1)!}.$$

It counts the number of ways of choosing which n_1 of the N distinguishable particles are in the excited state.

In the canonical ensemble, the classical partition function Z_C is the sum over all possible $n_1 = 0, 1, 2, ..., N$ of the Boltzmann factor times the degeneracy:

$$Z_C = \sum_{n_1=0}^{N} {N \choose n_1} e^{-\beta E(n_1)} = \sum_{n_1=0}^{N} {N \choose n_1} e^{-\beta n_1 \epsilon},$$

where $\beta = \frac{1}{k_B T}$. This sum is a straightforward binomial expansion:

$$Z_C = \left(1 + e^{-\beta \epsilon}\right)^N.$$

The probability of finding exactly n_1 particles in the excited state (and $n_0 = N - n_1$ in the ground state) is

$$P(n_1) = \frac{\binom{N}{n_1} e^{-\beta n_1 \epsilon}}{Z_C} = \frac{\binom{N}{n_1} e^{-\beta n_1 \epsilon}}{\left(1 + e^{-\beta \epsilon}\right)^N}.$$

 \mathbf{c}

We have a 2-level system with:

Ground state energy: 0,

Excited state energy: ϵ .

There are N bosons, and in a classical (Maxwell–Boltzmann) approach, the canonical partition function is

$$Z_C = (1 + e^{-\beta \epsilon})^N$$
, where $\beta = \frac{1}{k_B T}$.

If we let n_1 be the number of particles in the excited state, then $n_0 = N - n_1$ is the number of particles in the ground state.

The probability of having $n_1 = k$ particles in the excited state is

$$P(n_1 = k) = \frac{\binom{N}{k} \left(e^{-\beta \epsilon}\right)^k}{\left(1 + e^{-\beta \epsilon}\right)^N}.$$

(a) Average number in the excited state, $\langle n_{\epsilon} \rangle_C$ We define $n_{\epsilon} \equiv n_1$. Then

$$\langle n_{\epsilon} \rangle_C = \sum_{k=0}^{N} k P(n_1 = k).$$

Recognizing the binomial expansion identity $\sum_{k=0}^{N} k {N \choose k} x^k = N x (1+x)^{N-1}$, we set $x = e^{-\beta \epsilon}$. Therefore,

$$\langle n_{\epsilon} \rangle_C = \frac{1}{(1+x)^N} \sum_{k=0}^N k \binom{N}{k} x^k = \frac{N x (1+x)^{N-1}}{(1+x)^N} = \frac{N x}{1+x},$$

where $x = e^{-\beta \epsilon}$. Hence

(b) Average number in the ground state, $\langle n_0 \rangle_C$ Since $n_0 = N - n_1$, we have

$$\langle n_0 \rangle_C = N - \langle n_\epsilon \rangle_C = N - \frac{N e^{-\beta \epsilon}}{1 + e^{-\beta \epsilon}} = \frac{N}{1 + e^{-\beta \epsilon}}.$$

Hence

$$\langle n_0 \rangle_C = \frac{N}{1 + e^{-\beta \epsilon}}.$$

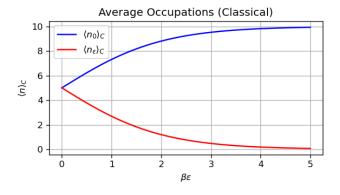


Figure 1: Schematic plot of $\langle n_0 \rangle_C$ and $\langle n_\epsilon \rangle_C$ vs. temperature (or equivalently vs. β). As $T \to 0$, $\langle n_0 \rangle_C \to N$ and $\langle n_\epsilon \rangle_C \to 0$. As $T \to \infty$, both approach N/2.

\mathbf{d}

For N indistinguishable bosons in a 2-level system (energies 0 and ϵ), the allowed microstates are specified by the occupation numbers (n_0, n_1) such that $n_0 + n_1 = N$. Each distinct pair (n_0, n_1) corresponds to a unique many-body state with energy $E = n_1 \epsilon$.

Partition function Z (no derivation shown):

$$Z = \sum_{n_1=0}^{N} e^{-\beta \, n_1 \, \epsilon} = 1 + e^{-\beta \, \epsilon} + e^{-2\beta \, \epsilon} + \dots + e^{-\beta \, N \, \epsilon} = \frac{1 - e^{-\beta \, (N+1) \, \epsilon}}{1 - e^{-\beta \, \epsilon}}.$$

Probability of microstate with $n_1 = n$ (hence $n_0 = N - n$) is

$$P(n_1 = n) = \frac{e^{-\beta n \epsilon}}{Z}.$$

 \mathbf{e}

For N indistinguishable bosons in a 2-level system with energies 0 and ϵ , the canonical partition function is

$$Z = \sum_{k=0}^{N} e^{-\beta k\epsilon}.$$

The probability of having k particles in the excited state is

$$P(k) = \frac{e^{-\beta k\epsilon}}{Z}.$$

Thus, the average number of particles in the excited state is

$$\langle n_{\epsilon} \rangle = \sum_{k=0}^{N} k \cdot P(k) = \frac{\sum_{k=0}^{N} k e^{-\beta k \epsilon}}{\sum_{k=0}^{N} e^{-\beta k \epsilon}},$$

and

$$\langle n_0 \rangle = N - \langle n_{\epsilon} \rangle.$$

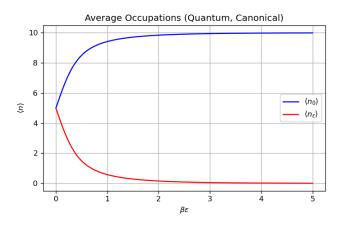


Figure 2: Plot of $langlen_0 rangle$ (blue) and $langlen_{epsilon} rangle$ (red) vs. betaepsilon for N=10.

 \mathbf{f}

For a 2-level bosonic system with single-particle energies 0 and ϵ , the grand partition function Ω_G (sometimes denoted Ξ) is obtained by introducing the chemical potential μ via the fugacity $z = e^{\beta\mu}$. Each level can be occupied by $n = 0, 1, 2, \ldots$ bosons, so:

$$\Omega_G = \underbrace{\sum_{n=0}^{\infty} \left(z e^{-\beta \cdot 0} \right)^n}_{\text{ground state}} \times \underbrace{\sum_{m=0}^{\infty} \left(z e^{-\beta \epsilon} \right)^m}_{\text{excited state}} = \frac{1}{1 - z} \frac{1}{1 - z e^{-\beta \epsilon}}.$$

The condition for the system to be normalizable (i.e. to ensure the sums converge) is that

$$e^{\beta\mu} < 1$$
, which implies $\mu < 0$.

 \mathbf{g}

For a 2-level bosonic system (energies 0 and ϵ) with chemical potential μ , define the fugacity $z \equiv e^{\beta\mu}$. The grand partition function is

$$\Omega_G = \frac{1}{1-z} \frac{1}{1-z e^{-\beta \epsilon}}.$$

The grand potential is $\Phi = -k_B T \ln(\Omega_G)$, and by standard thermodynamic relations, the average total number of particles is

$$\langle N \rangle \; = \; k_B T \, \frac{\partial}{\partial \mu} \, \ln(\Omega_G).$$

Because the ground-state (energy 0) sector contributes a factor $\frac{1}{1-z}$, one finds that the **average** number of particles in the ground state is

$$\left| \langle n_0 \rangle \right| = \left| \frac{z}{1 - z} \right| = \left| \frac{e^{\beta \mu}}{1 - e^{\beta \mu}} \right|,$$

provided $|z| = e^{\beta\mu} < 1$ (i.e. $\mu < 0$ for convergence).

h

From the previous part, for a 2-level bosonic system (energies 0 and ϵ), the average total particle number in the grand canonical ensemble is

$$\langle N \rangle \; = \; \frac{z}{1-z} \; + \; \frac{z \, e^{-\beta \epsilon}}{1-z \, e^{-\beta \epsilon}} \, , \quad \text{where} \quad z = e^{\beta \mu}. \label{eq:energy_equation}$$

We impose $\langle N \rangle = 10^5$.

Final Numeric Example (Dimensionless Units) If we set $k_BT=\epsilon=1$ (i.e. $\beta=1$), then $x=e^{-\beta\epsilon}=e^{-1}\approx 0.3679$. Solving numerically for z such that $\langle N\rangle=10^5$ gives

$$z \approx 0.99999$$
,

and the average ground-state occupation is

$$\langle n_0 \rangle = \frac{z}{1-z} \approx 9.999958 \times 10^4,$$

while the excited state has

$$\langle n_{\epsilon} \rangle \approx 0.42,$$

so they sum to 10^5 as desired.