Partition Function

• *One-particle partition function:* For a particle of mass m in a box of volume V at temperature T,

$$Z_1 = \mathrm{tr}\,\mathrm{e}^{-\beta\hat H} = \textstyle\sum_\nu \langle\nu|\mathrm{e}^{-\beta\hat H}|\nu\rangle\ , \quad \text{where} \quad \langle\mathbf{r}|\nu\rangle = \psi_\mathbf{k}(\mathbf{r}) = \frac{1}{\sqrt{V}}\,\mathrm{e}^{\mathrm{i}\,\mathbf{k}\cdot\mathbf{r}}\ ,$$

where, in the case of periodic boundary conditions (easier to handle than other ones, and physically reasonable for $L \gg \lambda$), the allowed values of $\mathbf{k}$ are $k_i = (2\pi n/L_i)$.

• *Two-particle states:* For two identical particles of mass m in a box of volume V at temperature T, a complete set of plane wave states is, for bosons and fermions respectively,

$$\psi_{\mathbf{k}_1,\mathbf{k}_2}(\mathbf{r}_1,\mathbf{r}_2) = \langle\mathbf{r}_1,\mathbf{r}_2 \mid \mathbf{k}_1,\mathbf{k}_2\rangle = \frac{1}{\sqrt2}\,[\psi_{\mathbf{k}_1}(\mathbf{r}_1)\,\psi_{\mathbf{k}_2}(\mathbf{r}_2) \pm \psi_{\mathbf{k}_2}(\mathbf{r}_1)\,\psi_{\mathbf{k}_1}(\mathbf{r}_2)]\ .$$

• *N-particle states:* Generalizing to N identical particles of mass m in a box of volume V at temperature T, we write a complete set of plane wave states, for bosons and fermions respectively, as

$$\psi_{\mathbf{k}_1,\mathbf{k}_2,...,\mathbf{k}_N}(\mathbf{r}_1,\mathbf{r}_2,...,\mathbf{r}_N) = \langle\mathbf{r}_1,\mathbf{r}_2,...,\mathbf{r}_N \mid \mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_N\rangle = \frac{1}{\sqrt{N!}}\sum_\mathcal{P}(\pm1)^{|\mathcal{P}|}\prod_{i=1}^N \psi_{\mathbf{k}_i}(\mathbf{r}_{\mathcal{P}_i})\ ,$$

where $\mathcal{P}$ is a permutation of the first N integers, and $|\mathcal{P}|$ its parity. The $\mathbf{k}_i$ are assumed to be all different (otherwise the combinatorics changes—see Halley).

• *N-particle partition function:* Using a Fock basis for the Hilbert space, one can easily get that, for non-interacting particles (in practice, neutrinos and photons), for which $E = \sum_\nu n_\nu\epsilon_\nu$,

$$Z_\mathrm{g} = \mathrm{tr}\,\mathrm{e}^{-\beta H+\beta\mu N} = \sum_{\{n_\nu\}} \mathrm{e}^{\Sigma_\nu n_\nu(\mu-\epsilon_\nu)\,\beta} = \prod_\nu \begin{cases} [1-\mathrm{e}^{(\mu-\epsilon_\nu)\beta}]^{-1} & \text{(bosons)} \\ 1+\mathrm{e}^{(\mu-\epsilon_\nu)\beta} & \text{(fermions)} \end{cases}.$$

For bosons, we must have $\mathrm{e}^{\beta\mu} > 0$.

Derivation of Thermodynamics

• *Idea:* We will derive, as examples, the mean number of particles $\bar N$ and the entropy S for the above partition function; other thermodynamical quantities can be obtained with the usual equations.

• *Grand potential:* From the general expression in terms of the partition function,

$$\Omega = -k_\mathrm{B}T\,\ln Z_\mathrm{g} = k_\mathrm{B}T\sum_\nu \ln[1 \mp \mathrm{e}^{(\mu-\epsilon_\nu)\beta}]\ .$$

• *Number of particles:* From the general expression in terms of the grand potential,

$$\bar N = -\frac{\partial\Omega}{\partial\mu}\Big|_{T,V} = \sum_\nu \frac{1}{\mathrm{e}^{(\epsilon_\nu-\mu)\beta}\mp1} = \sum_\nu \bar n_\nu\ , \quad \text{where} \quad \bar n_\nu = \frac{1}{\mathrm{e}^{(\epsilon_\nu-\mu)\beta}\mp1}\ .$$

[⋆ For photons, using Z_c with a sum over arbitrarily many particles, one gets an $\bar n_{\mathbf{k},\epsilon}$ which coincides with the $\bar n_\nu$ above except for the absence of μ: Understand precisely in what sense that is equivalent to a Z_g with vanishing μ.] From the last expression we also get that for all ν, $\ln(\bar n_\nu \pm 1) - \ln \bar n_\nu = \beta\,(\epsilon_\nu - \mu)$.

• *Entropy and heat capacity:* Again from the general expressions,

$$S = -\frac{\partial\Omega}{\partial T}\Big|_{V,\mu} = -k_\mathrm{B}\sum_\nu \ln[1\mp\mathrm{e}^{(\mu-\epsilon_\nu)\beta}] + \frac1T\sum_\nu \frac{\mp(\mu-\epsilon_\nu)\,\mathrm{e}^{(\mu-\epsilon_\nu)\beta}}{1\mp\mathrm{e}^{(\mu-\epsilon_\nu)\beta}} = k_\mathrm{B}\sum_\nu \big[(\bar n_\nu\pm1)\ln(1\pm\bar n_\nu) - \bar n_\nu\ln\bar n_\nu\big]\ ,$$

from which

$$\bar E = \Omega + ST + \mu\bar N \qquad \text{or} \qquad \sum_\nu \bar n_\nu\epsilon_\nu = \sum_\nu \frac{\epsilon_\nu}{\mathrm{e}^{(\epsilon_\nu-\mu)\beta}\mp1}\ , \qquad \text{and} \qquad C_V = ...$$

Relevant Sections: PHY 731; Chandler; Halley, Ch 5; Reif; Schwabl.
Related Topics: Other quantum statistics, like anyons in 2D.