Exercise Sheet 6

(1) Particle-Number distribution in the grand-canonical ensemble

The grand-canonical distribution of a many-body system is defined by the statistical operator

$$\mathbf{R} = \frac{1}{Z}\exp(-\beta\mathbf{H} - \alpha\mathbf{N}), \quad Z(\beta,\alpha) = \mathrm{Tr}\exp(-\beta\mathbf{H} - \alpha\mathbf{N}). \tag{1}$$

For an ideal gas of fermions or bosons one obtains in the limit of a non-degenerate gas, i.e., where the average occupation number for the single-particle states is small compared to 1, one obtains the Maxwell"=Boltzmann approximation for the phase-space distribution function,

$$f(\vec{p}) = \exp(-\alpha)\exp(-\beta E_p), \quad E_p = \sqrt{m^2 + \vec{p}^2} = \sqrt{m^2 + p^2}. \tag{2}$$

The corresponding phase-space distribution for the particles is then

$$\frac{\mathrm{d}N}{\mathrm{d}^3\vec{x}\,\mathrm{d}^3\vec{p}} = \frac{gV}{(2\pi)^3} f(\vec{p}), \tag{3}$$

where g is the degeneracy factor for the particles under consideration due to spin, isospin etc. In this approximation the partition sum (or rather its logarithm!) is given by

$$\ln Z = \frac{gV}{(2\pi)^3}\int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\, f(\vec{p}). \tag{4}$$

(a) Show with help of (1) that

$$\langle N\rangle = -\partial_\alpha \ln Z = \ln Z. \tag{5}$$

Solution:

$$\langle N\rangle = \mathrm{Tr}(\mathbf{N}\mathbf{R}) = \frac{1}{Z}\mathrm{Tr}[\mathbf{N}\exp(-\beta\mathbf{H} - \mu\mathbf{N})] = -\frac{1}{Z}\partial_\alpha Z = -\partial_\alpha \ln Z. \tag{6}$$

According to (4) with (2) for the phase-space distribution function, we get

$$\ln Z = \frac{gV}{(2\pi)^3}\exp(-\alpha)\int_{\mathbb{R}^3}\mathrm{d}^3\vec{p}\exp(-\beta E_p). \tag{7}$$

From this (5) follows immediately by (6).

(b) According to (1) the probability that the gas contains exactly $\tilde{N}$ particles, is given by

$$P(\tilde{N}) = \mathrm{Tr}[\mathbf{R}\delta(\mathbf{N} - \tilde{N})] = \frac{1}{2\pi}\int_{-\pi}^{\pi}\mathrm{d}\phi\,\mathrm{Tr}\{\mathbf{R}\exp[\mathrm{i}\phi(\mathbf{N} - \tilde{N})]\}. \tag{8}$$

Show that

$$P(\tilde{N}) = \frac{1}{2\pi Z}\int_{-\pi}^{\pi}\mathrm{d}\phi Z(\beta, \alpha - \mathrm{i}\phi)\exp(-\mathrm{i}\phi\tilde{N}). \tag{9}$$

Solution: With (1) we find

$$\mathrm{Tr}\{\mathbf{R}\exp[\mathrm{i}\phi(\mathbf{N} - \tilde{N})]\} = \frac{\exp(-\mathrm{i}\phi\tilde{N})}{Z(\beta,\alpha)}\mathrm{Tr}\{\exp[-\beta\mathbf{H} - (\alpha - \mathrm{i}\phi)]\} = \frac{\exp(-\mathrm{i}\phi\tilde{N})}{Z(\beta,\alpha)} Z(\beta, \alpha - \mathrm{i}\phi). \tag{10}$$

(c) Evaluate the integral to prove that the number distribution is given by the Poisson distribution,

$$P(\tilde{N}) = \frac{\langle N \rangle^{\tilde{N}}}{\tilde{N}!} \exp(-\langle N \rangle). \tag{11}$$

Solution: Now with (7) we get

$$\ln Z(\beta, \alpha - \mathrm{i}\phi) = \ln Z(\beta, \alpha) \exp(\mathrm{i}\phi) \stackrel{(5)}{=} \langle N \rangle \exp(\mathrm{i}\phi) \tag{12}$$

and thus

$$Z(\beta, \alpha - \mathrm{i}\phi) = \exp[\langle N \rangle \exp(\mathrm{i}\phi)] = \sum_{k=0}^{\infty} \frac{\langle N \rangle^k}{k!} \exp(\mathrm{i}k\phi). \tag{13}$$

Plugging this into (9), using

$$\int_{-\pi}^{\pi} \mathrm{d}\phi \exp[\mathrm{i}(k - \tilde{N})\phi] = 2\pi \delta_{k,\tilde{N}} \tag{14}$$

indeed leads to (11).

(d) Evaluate its generating function,

$$g(x) = \sum_{\tilde{N}=0}^{\infty} x^{\tilde{N}} P(\tilde{N}). \tag{15}$$

Solution:

$$g(x) = \exp(-\langle N \rangle) \sum_{\tilde{N}=0}^{\infty} \frac{(x \langle N \rangle)^{\tilde{N}}}{\tilde{N}!} = \exp(-\langle N \rangle) \exp(x \langle N \rangle) = \exp[\langle N \rangle (x-1)]. \tag{16}$$

(e) Determine $\langle N \rangle$ and $\left\langle N^2 \right\rangle$ using

$$g'(1) = \langle N \rangle, \quad g''(1) = \langle N(N-1) \rangle = \left\langle N^2 \right\rangle - \langle N \rangle. \tag{17}$$

Solution: Obviously with (14) we get

$$\begin{aligned} &g'(x) = \langle N \rangle \exp[\langle N \rangle (x-1)], \quad g''(x) = \langle N \rangle^2 \exp[\langle N \rangle (x-1)] \\ \Rightarrow &g'(1) = \langle N \rangle, \quad g''(1) = \langle N \rangle^2 = \left\langle N^2 \right\rangle - \langle N \rangle. \end{aligned} \tag{18}$$

From this we get

$$\left\langle N^2 \right\rangle = \langle N \rangle^2 + \langle N \rangle \;\; \Delta N^2 = \left\langle (N - \langle N \rangle)^2 \right\rangle = \left\langle N^2 \right\rangle - \langle N \rangle^2 = \langle N \rangle, \tag{19}$$

i.e., for the Poisson distribution

$$\frac{\Delta N}{\langle N \rangle} = \frac{1}{\sqrt{\langle N \rangle}}, \tag{20}$$

i.e., for $\langle N \rangle \gg 1$ the fluctutions of N become negligible, and $\left\langle N^2 \right\rangle \approx \langle N \rangle^2$.

(f) Why are the equations (17) valid?

Solution: From (15) one has for an arbitrary pobability distribution $P(\tilde{N})$

$$g'(x) = \sum_{\tilde{N}=0}^{\infty} \tilde{N} x^{\tilde{N}-1} P(\tilde{N}), \quad g''(x) = \sum_{\tilde{N}=0}^{\infty} \tilde{N}(\tilde{N}-1) x^{\tilde{N}-2} P(\tilde{N}), \tag{21}$$

and setting $x = 1$ gives indeed (17).

(g) What is the k^{th} derivative, $g^{(k)}(1)$, for a generating function of an arbitrary distribution function?

Solution: As in the previous item, with (17) we get

$$g^{(k)}(x) = \sum_{\tilde{N}=0}^{\infty} \tilde{N}(\tilde{N}-1)\cdots(\tilde{N}-k+1)x^{\tilde{N}-k}P(\tilde{N}) = \sum_{\tilde{N}=0}^{\infty} \frac{\tilde{N}!}{(\tilde{N}-k)!} x^{\tilde{N}-k} P(\tilde{N}). \tag{22}$$

Setting $x = 1$ finally gives

$$g^{(k)}(1) = \left\langle \frac{N!}{(N-k)!} \right\rangle. \tag{23}$$

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(2) Rate equation for grand-canonical ($\langle N_s \rangle \gg 1$) and "ultra-canonical" treatment ($\langle N_s \rangle \ll 1$)

In the lecture we have derived the master equation for the generating function $g(\tau, x)$ in the general case, where the time evolution for a single event is described with the exact number of $s\bar{s}$ pairs,

$$\partial_\tau g = \frac{L}{V}(1-x)(x\partial_x^2 g + \partial_x g - \epsilon g), \tag{24}$$

where $\epsilon = G\langle N_A \rangle \langle N_B \rangle / L$, with $\langle N_{A,B} \rangle$ the grand-canonical expectation values for the Numbers of the "light particles" in the reaction $A + B \longleftrightarrow s + \bar{s}$, underlying the Boltzmann collision term.

The master equation for the approximation, where also the strange particles are treated in the grand-canonical approximation, which is valid in the limit $\langle N_s \rangle = \langle N_{\bar{s}} \rangle \gg 1$, i.e., when $\langle N^2 \rangle \simeq \langle N \rangle^2$,

$$\partial_\tau g_{gc} = \frac{L}{V}\sqrt{\epsilon}(1-x)(\partial_x g_{gc} - \sqrt{\epsilon} g_{gc}). \tag{25}$$

(a) Use (24) and (25) to derive the rate equations for the time evolution of the average number $\langle N \rangle(\tau)$ of $s\bar{s}$ by making use of $\partial_x g(\tau, 1) = N(\tau)$ in the exact case

$$\frac{d}{d\tau}\langle N \rangle = \frac{L}{V}(\epsilon - \langle N^2 \rangle) \tag{26}$$

and in the case where the strange particles are treated by the grand-canonical approximation in the "single event",

$$\frac{d}{d\tau}\langle N \rangle_{gc} = \frac{L}{V}\sqrt{\epsilon}(\sqrt{\epsilon} - \langle N \rangle_{gc}). \tag{27}$$

Note that (27) is a closed differential equation for $\langle N \rangle_{gc}$, while (27) is not closed, because on the right-hand side one has $\langle N^2 \rangle$. One can use (24) to prove that one obtains an "infinite tower" of equations for all moments $\langle N^k \rangle$, $k \in \mathbb{N}$, whose solution would be equivalent to solve (24) itself.

Solution: Taking the derivative of (24) with respect to x and setting $x = 1$ gives

$$\begin{aligned} \frac{d}{d\tau}\langle N \rangle = \partial_\tau \partial_x g|_{x=1} &= -\frac{L}{V}\left[x\partial_x^2 g + \partial_x g - \epsilon g\right]\Big|_{x=1} \\ &\overset{(17)}{=} -\frac{L}{V}\left[\langle N^2 \rangle - \langle N \rangle + \langle N \rangle - \epsilon\right] \\ &= -\frac{L}{V}(\langle N^2 \rangle - \epsilon) \end{aligned} \tag{28}$$

and in the same way, starting from (25)

$$\frac{d}{d\tau}\langle N \rangle_{gc} = -\frac{L}{V}\sqrt{\epsilon}(\langle N \rangle_{gc} - \sqrt{\epsilon}) = -\gamma(\langle N \rangle_{gc} - \sqrt{\epsilon}). \tag{29}$$

(b) Solve (27) and show that for $\tau \to \infty$ one finds for the equilibrium value $\langle N \rangle_{\text{gc,eq}} = \sqrt{\epsilon}$. What is the "relaxation time", i.e., the typical time scale at which $\left\langle N_{\text{gc}} \right\rangle(\tau)$ approaches $\langle N \rangle_{\text{gc,eq}}$.

Solution: Writing $N = \langle N \rangle_{\text{gc}}$ for convenience, separation of variables for (29) gives

$$\int_{N_0}^{N} \mathrm{d}N' \frac{1}{\sqrt{\epsilon} - N'} = \ln\left(\frac{\sqrt{\epsilon} - N_0}{\sqrt{\epsilon} - N} \right) = \gamma \tau \tag{30}$$

Solving for N gives the solution

$$N = \langle N \rangle_{\text{gc}} = N_0 \exp(-\gamma\tau) + \sqrt{\epsilon}[1 - \exp(-\gamma\tau)]. \tag{31}$$

The equilibrium number is $\langle N \rangle_{\text{gc,eq}} = \sqrt{\epsilon}$, and the relaxation-time scale is $\tau_{0,\text{gc}} = 1/\gamma = \frac{V}{L\sqrt{\epsilon}}$.

(c) Now consider the case that $\langle N_{\text{s}} \rangle = \langle N_{\bar{\text{s}}} \rangle \ll 1$. To that end assume that $x \partial_x^2 g \ll \partial_x g$, i.e., one can simply omit this term on the right-hand side of (24).

Solution: Then from (24) we get

$$\partial_\tau g_{\text{uc}} = \frac{L}{V}(1 - x)(\partial_x g_{\text{uc}} - \epsilon\, g_{\text{uc}}). \tag{32}$$

(d) How does the rate equation for the corresponding expectation value $\langle N \rangle$ look like now? What is the equilibrium value, $\langle N \rangle_{\text{eq}}$ and the relaxation time in that case? Is the result consistent with the assumption made to derive the approximate rate equation?

Solution: Then as above, taking the derivative of (32) wrt. x and then setting $x = 1$ leads to

$$\frac{\mathrm{d}}{\mathrm{d}\tau} \langle N \rangle_{\text{uc}} = -\frac{L}{V}(\langle N \rangle_{\text{uc}} - \epsilon). \tag{33}$$

In exactly the same way as the drivation of (31) we find, setting $\gamma_{\text{uc}} = L/V$

$$\langle N \rangle_{\text{uc}} = \langle N_0 \rangle_{\text{uc}} \exp(-\gamma_{\text{uc}}\tau) + \epsilon[1 - \exp(-\gamma_{\text{uc}}\tau)]. \tag{34}$$

Both the equilibrium number $\langle N \rangle_{\text{uc,eq}} = \epsilon$ and the relaxation time $\tau_{0,\text{uc}} = V/L$ are much smaller than the expectation when using the grand-canonical result $\sqrt{\epsilon}$ and $V/(\sqrt{\epsilon}L)$ (for $\epsilon \ll 1$).

The assumption is justified at least in the equilibrium limit. Since then from (32) we get

$$\partial_\tau g_{\text{uc,eq}} = 0 \Rightarrow g'_{\text{uc,eq}}(x) = \epsilon\, g_{\text{uc,eq}}. \tag{35}$$

With the "initial condition" $g_{\text{uc}}(1) = 1$ the unique solution of (35) is

$$g_{\text{uc,eq}} = \exp[\epsilon(x - 1)], \tag{36}$$

which, according to (16) is the generating function for a Poisson distribution with average value, ϵ. If $\epsilon \gg 1$

$$P(\tilde{N}) = P(0)\frac{\epsilon^{\tilde{N}}}{\tilde{N}!}, \tag{37}$$

i.e., in the defining equation of $g_{\text{uc,eq}}$ the terms of of order x^k for $k \geq 2$ are largely suppressed compared to the terms up to linear order.