

Moderne Theoretische Physik III SS 2014

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Klausur, 100 Punkte

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1. Kurzfragen

(5 + 10 + 10 + 10 + 5 + 10 = 50 Punkte)

- (a) Second law of thermodynamics. Not all heat can be converted into work, i.e. there is no heat engine that can convert all the heat into work.
- (b) Fermi and Bose distribution functions. The Fermi distribution function is given by

$$n_F = \frac{1}{1 + e^{\beta(\epsilon_k - \mu)}} \quad (1)$$

and the Bose function by

$$n_B = \frac{1}{1 - e^{\beta(\epsilon_k - \mu)}}, \quad (2)$$

here ϵ_k is the energy dispersion, $\beta = 1/(kT)$ and $\mu = \mu(T)$ is the chemical potential. In the limit $T \rightarrow \infty$, both n_B and n_F reduce to Maxwell-Boltzmann distribution $n_{MB} = e^{\beta(\epsilon_k - \mu)}$.

The temperature variation of the chemical potential can be seen in the figure below. For bosons: the chemical potential is equal to zero for $T < T_c$, where T_c is the temperature of Bose-Einstein condensation, for $T > T_c$ chemical potential becomes negative. For fermions, at zero temperature the chemical potential is equal to the Fermi energy, and then it drops down as the temperature is increased. Eventually, for high temperatures it becomes negative (as Fermi and Bose statistics both reduce to the Maxwell-Boltzmann).

- (c) Free energy of a classical ideal gas. We start from the partition function

$$\begin{aligned} Z &= \prod_{i=1}^N \int \frac{d^3 p_i d^3 x_i}{h^3} e^{-\beta \frac{p_i^2}{2m}} \\ &= \prod_{i=1}^N \int \frac{d^3 p_i}{h^3} e^{-\beta \frac{p_i^2}{2m}} \\ &= \left(\frac{V}{\lambda^3} \right)^N \end{aligned} \quad (3)$$

where $\lambda = \sqrt{\frac{\beta h^2}{2\pi m}}$ is the deBroglie wavelength at temperature T . We have used that $\int dx e^{-\alpha x^2} = \sqrt{\frac{\pi}{\alpha}}$.

$$F = -kT \ln Z = -NkT \ln \frac{V}{\lambda^3} \quad (4)$$

Quantum effects become important when the inter-particle distance becomes smaller than the thermal de Broglie wavelength. The inter-particle distance a is given by $a = (N/V)^{-3} = n^{-3}$. For $n^{-3} < \sqrt{\frac{\beta h^2}{2\pi m}}$ quantum statistics should be used.

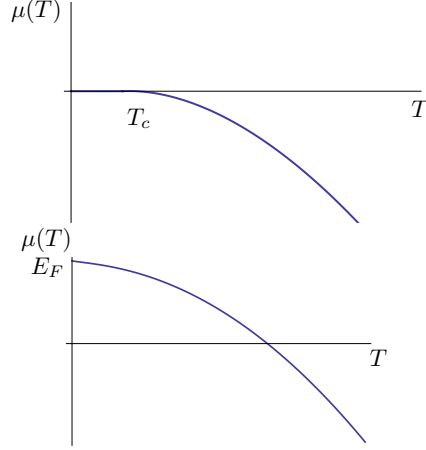


Abbildung 1: Chemical potential as a function of temperature for bosons (above) and fermions (below)

- (d) Grand-canonical function for fermions. This is given by

$$\Omega_F = -kT \sum_p \ln \left(1 + e^{-\beta(\epsilon_p - \mu)} \right) \quad (5)$$

For $T \rightarrow 0$, $\beta \rightarrow \infty$, and at $T = 0$, $\mu = E_F$. Therefore for ϵ_p such that $\epsilon_p < E_F$, we have that $\ln(1 + e^{-\beta(\epsilon_p - \mu)}) \approx \beta(\epsilon_p - E_F)$, while the states with $\epsilon_p > E_F$ will give zero contribution. Then $\omega_F = \sum_{p < p_F} (\epsilon_p - E_F)$, i.e. is related to the total energy of the system which can also be rewritten in terms of an integral over density of states.

- (e) Equipartition theorem: Every quadratic degree of freedom in the Hamiltonian contributes $kT/2$ to the internal energy. For a molecule of two atoms in $d = 3$, there is a vibrational mode that contributes $2 \frac{kT}{2}$ to the internal energy and $3 \frac{kT}{2}$ from the translation. Rotational degrees of freedom contribute $2 \frac{kT}{2}$ to the internal energy. Therefore $U = \frac{7}{2} NkT$, and hence $c = \frac{dU}{dT} = \frac{7}{2} Nk$.
- (f) Bose Einstein condensation and critical temperature in $d = 3$. Bose Einstein condensation: for temperatures below some critical temperature T_c , there is a macroscopic occupation of the lowest energy state in the spectrum ($p = 0$, for quadratic dispersion $\epsilon_p = \frac{p^2}{2m}$). At $T = 0$ all bosons condensed into the ground state. Critical temperature. For this purpose we can set $\mu \approx 0$. The number of bosons in the excited $k \neq 0$ states is

$$\begin{aligned} N_e &= \frac{V}{(2\pi)^3} \int d^3k \frac{1}{\exp\left(\beta \frac{\hbar^2 k^2}{2m}\right) - 1} \\ &= \frac{V}{(2\pi)^3} \left(\frac{2mkT}{\hbar^2} \right)^{3/2} \underbrace{2\pi \int_0^\infty dx \frac{\sqrt{x}}{e^x - 1}}_{\frac{\sqrt{\pi}}{2} \zeta(3/2)} \\ &= \zeta(3/2) \frac{V}{\lambda^3} \end{aligned} \quad (6)$$

where

$$\lambda = \sqrt{\frac{\beta \hbar^2}{2\pi m}} \quad (7)$$

and we have used the substitution $x = \beta \frac{\hbar^2 k^2}{2m}$. When $N_e = N$, we get the critical temperature T_c . This leads to

$$T_c = \frac{\hbar^2}{2mk\pi} \left(\frac{(2\pi)^3 N}{V\zeta(3/2)} \right)^{2/3}. \quad (8)$$

2. Elektronen in Kohlenstoffnanoröhrchen (5 + 5 + 5 + 10 = 25 Punkte)

(a) Fermi energy. The number of particles is given by

$$N = g_s \int g(k) dk = 2 \int_0^{k_F} \frac{2dk}{\frac{2\pi}{L}} = \frac{2}{\pi} k_F L \quad (9)$$

where $g_s = 2$ is the spin degeneracy, and $g(k)$ is the density of states in the momentum space. From this it follows that

$$\begin{aligned} k_F &= \frac{N \pi}{L 2} \\ \epsilon_F = vk_F &= v \frac{N \pi}{L 2} \end{aligned} \quad (10)$$

(b) The internal energy at $T = 0$. This is given by

$$E_{T=0} = 2 \int g(k) vk dk = \frac{L}{\pi} vk_F^2 = \frac{N^2 \pi v}{4L} \quad (11)$$

(c) Grand-canonical potential, its relation with energy E , and the pressure p . We start from

$$\begin{aligned} \Omega &= -kTg_s \int g(k) dk \ln(1 + \exp(-\beta(\epsilon_k - \mu))) \\ &= -2kT \frac{L}{\pi} \int_0^\infty dk \ln(1 + \exp(-\beta(vk - \mu))) \end{aligned} \quad (12)$$

After integrating by parts, we get that

$$\begin{aligned} \Omega &= -kTg_s \int g(k) dk \ln(1 + \exp(-\beta(\epsilon_k - \mu))) \\ &= -2kT \frac{L}{\pi} \left\{ [k \ln(1 + \exp(-\beta(\epsilon_k - \mu)))]_0^\infty + \beta v \int dk k \frac{1}{1 + e^{\beta(vk - \mu)}} \right\} \\ &= -\frac{Lv}{\pi} \int dk k \frac{1}{1 + e^{\beta(vk - \mu)}} \end{aligned} \quad (13)$$

The internal energy E_T of a gas of fermions at temperature T is given by

$$\begin{aligned}
E_T &= g_s \int dk g(k) \epsilon_k n_F(\epsilon_k, T) \\
&= 2 \frac{L}{\pi} \int dk vk \frac{1}{1 + e^{\beta(vk - \mu)}} \\
&= -\Omega
\end{aligned} \tag{14}$$

where we have compared this with (13) to obtain the equality in the last line.

(d) Adiabatic process.

We can start from the Gibbs - Dunham relation, according to which $\Omega = -pL$. In the previous part of the question, we have proved that in $d = 1$, $\Omega = -E$. Then it follows that $E = pL$. Differentiating this expression we get that

$$\delta E = p\delta L + L\delta p \tag{15}$$

For the adiabatic process, it holds that $\delta E = \delta Q - p\delta L = -p\delta L$, since there is no heat exchanged with the environment. Using this in conjunction with (15) we get that

$$-p\delta L = p\delta L + L\delta p \tag{16}$$

From this it follows that $pL^2 = \text{const}$. From (13) we see that we can rewrite the grand-canonical potential in the form of

$$\Omega = T^2 L f(\mu/T) \tag{17}$$

The entropy per unit length is given by

$$\begin{aligned}
S/L &= -1/L \left(\frac{\partial \Omega}{\partial T} \right)_{L, \mu} \\
&= 2T f(\mu/T) - \mu f'(\mu/T)
\end{aligned} \tag{18}$$

From above we conclude that $\frac{S}{L}(\alpha\mu, \alpha T) = \alpha \frac{S}{L}(\mu, T)$, i.e. $\frac{S}{L}$ is a homogeneous function of μ, T of degree 1. Similarly we get that

$$\begin{aligned}
N/L &= -1/L \left(\frac{\partial \Omega}{\partial \mu} \right)_{T, \mu} \\
&= -T f'(\mu/T)
\end{aligned} \tag{19}$$

From above we conclude that $\frac{N}{L}(\alpha\mu, \alpha T) = \alpha \frac{N}{L}(\mu, T)$, i.e. $\frac{N}{L}$ is a homogeneous function of μ, T of degree 1.

Therefore, it follows that $\frac{S(\mu, T)}{N(\mu, T)} = \frac{S(\alpha\mu, \alpha T)}{N(\alpha\mu, \alpha T)}$ is homogeneous function of degree 0. Since in adiabatic process S is constant, and N is constant, it must follow that $\frac{\mu}{T}$ is constant in adiabatic process. From (19), it follows that $TL = \text{const}$. To find the $pT^{-\delta} = \text{const}$ exponent, we use that $pL^2 = \text{const}$ and $T^2 L^2 = \text{const}$. Dividing these leads to $pT^{-2} = \text{const}$. Hence $\delta = 2$.

3. Brownsche Bewegung

(5 + 5 + 5 + 5 + 5 = 25 Punkte)

The Langevin equation is given by

$$m\ddot{x}(t) + m\gamma\dot{x}(t) + m\omega_0^2 x(t) = \xi(t).$$

- (a) We only need to solve the homogeneous equation (since we are given the Green's function)

$$m\ddot{x}(t) + m\gamma\dot{x}(t) + m\omega_0^2x(t) = 0$$

This is a standard damped harmonic oscillator equation with the solution of the form $x_h(t) \simeq e^{i\omega t}$. After substituting this in the Langevin equation, we obtain the equation for ω :

$$-\omega^2 + i\omega\gamma + \omega_0^2 = 0 \quad (20)$$

which leads to the solutions of the form

$$\omega = \frac{i\gamma}{2} \pm \underbrace{\sqrt{\omega_0^2 - \frac{\gamma^2}{4}}}_{\Omega} \quad (21)$$

and

$$x_h(t) = e^{-\frac{\gamma}{2}t} (A \cos(\Omega t) + B \sin(\Omega t)) \quad (22)$$

the constant A and B can be determined from the initial conditions. From $x(0) = x_0$ we get $A = x_0$ and similarly from $\dot{x}(0) = v_0$ it follows that $B = \frac{v_0 + \frac{\gamma}{2}x_0}{\Omega}$. The final solution is then given by

$$x(t) = e^{-\frac{\gamma}{2}t} \left(x_0 \cos(\Omega t) + \frac{v_0 + \frac{\gamma}{2}x_0}{\Omega} \sin(\Omega t) \right) + \int_0^t dt' e^{-\gamma\frac{t-t'}{2}} \sin(\Omega(t-t'))/\Omega \quad (23)$$

- (b) Bearing in mind that $\langle \xi(t) \rangle_\xi = 0$, and using the result of part a) for $x(t)$, we have that

$$\langle x(t) \rangle_\xi = e^{-\frac{\gamma}{2}t} \left(x_0 \cos(\Omega t) + \frac{v_0 + \frac{\gamma}{2}x_0}{\Omega} \sin(\Omega t) \right), \quad (24)$$

this is damped harmonic motion as expected, and in the limit of large t , $\langle x(t) \rangle_\xi \rightarrow 0$.

- (c) Calculating $\langle x(t)x(t') \rangle_\xi$ for $t > t'$. We substitute $x(t)$, as given by (23). In calculating $\langle x(t)x(t') \rangle_\xi$, only the cross terms that contain no ξ terms, or two ξ terms will survive after taking the averages (since $\langle \xi(t) \rangle_\xi = 0$). Therefore, we have that

$$\begin{aligned} \langle x(t)x(t') \rangle_\xi &= e^{-\frac{\gamma}{2}(t+t')} \left(x_0 \cos(\Omega t) + \frac{v_0 + \frac{\gamma}{2}x_0}{\Omega} \sin(\Omega t) \right) \left(x_0 \cos(\Omega t') + \frac{v_0 + \frac{\gamma}{2}x_0}{\Omega} \sin(\Omega t') \right) \\ &+ \frac{1}{(m\Omega)^2} e^{-\frac{\gamma}{2}(t+t')} \int_0^t dt_1 \sin(\Omega(t-t_1)) \int_0^{t'} ds \sin(\Omega(t'-s)) \underbrace{\langle \xi(t_1)\xi(s) \rangle_\xi}_{2m\gamma k_B T \delta(t_1-s)} \\ &= e^{-\frac{\gamma}{2}(t+t')} \left(x_0 \cos(\Omega t) + \frac{v_0 + \frac{\gamma}{2}x_0}{\Omega} \sin(\Omega t) \right) \left(x_0 \cos(\Omega t') + \frac{v_0 + \frac{\gamma}{2}x_0}{\Omega} \sin(\Omega t') \right) \\ &+ e^{-\frac{\gamma}{2}(t+t')} \frac{2\gamma k_B T}{m\Omega^2} \int_0^{t'} ds e^{\gamma s} \sin[\Omega(t-s)] \sin[\Omega(t'-s)] \end{aligned} \quad (25)$$

We use that (given in the question)

$$\begin{aligned}
& \frac{2\gamma k_B T}{m\Omega^2} \int_0^{t'} ds e^{\gamma s} \sin[\Omega(t-s)] \sin[\Omega(t'-s)] \\
&= -\frac{k_B T}{m\omega_0^2} \cos(\Omega t) \cos(\Omega t') - \frac{\gamma k_B T}{2m\omega_0^2 \Omega} \sin[\Omega(t+t')] - \frac{k_B T(4\omega_0^2 + \gamma^2)}{4m\omega_0^2 \Omega^2} \sin(\Omega t) \sin(\Omega t') \\
& \quad + \frac{k_B T}{m\omega_0^2} e^{\gamma t'} \left(\cos[\Omega(t-t')] + \frac{\gamma}{2\Omega} \sin[\Omega(t-t')] \right)
\end{aligned}$$

Then:

$$\begin{aligned}
\langle x(t)x(t') \rangle_\xi &= e^{-\frac{\gamma}{2}(t+t')} \left\langle \left(x_0 \cos(\Omega t) + \frac{v_0 + \frac{\gamma}{2}x_0}{\Omega} \sin(\Omega t) \right) \left(x_0 \cos(\Omega t') + \frac{v_0 + \frac{\gamma}{2}x_0}{\Omega} \sin(\Omega t') \right) \right\rangle \\
& - e^{-\frac{\gamma}{2}(t+t')} \frac{k_B T}{m\omega_0^2} \cos(\Omega t) \cos(\Omega t') - e^{-\frac{\gamma}{2}(t+t')} \frac{\gamma k_B T}{2m\omega_0^2 \Omega} \sin[\Omega(t+t')] \\
& - e^{-\frac{\gamma}{2}(t+t')} \frac{k_B T(4\omega_0^2 + \gamma^2)}{4m\omega_0^2 \Omega^2} \sin(\Omega t) \sin(\Omega t') \\
& + \frac{k_B T}{m\omega_0^2} e^{-\frac{\gamma}{2}(t+t')} e^{\gamma t'} \left(\cos[\Omega(t-t')] + \frac{\gamma}{2\Omega} \sin[\Omega(t-t')] \right) \tag{26}
\end{aligned}$$

- (d) $\langle x(t)x(t') \rangle_\xi$ in the regime $t \gg \gamma^{-1}$ and $t' \gg \gamma^{-1}$. In this limit $e^{-\frac{\gamma}{2}(t+t')} \rightarrow 0$, and the only term that doesn't disappear in (26) is given by

$$\langle x(t)x(t') \rangle_\xi = \frac{k_B T}{m\omega_0^2} e^{-\frac{\gamma}{2}(t-t')} \left(\cos[\Omega(t-t')] + \frac{\gamma}{2\Omega} \sin[\Omega(t-t')] \right) \tag{27}$$

Then $\langle x(t)x(t') \rangle_{|t-t'| \rightarrow 0} = \frac{k_B T}{m\omega_0^2}$, i.e. $\langle x^2(t) \rangle = \frac{k_B T}{m\omega_0^2}$ (equipartition theorem). Similarly, in the other limit $\langle x(t)x(t') \rangle_{|t-t'| \rightarrow \infty} = 0$, i.e. after long time equilibrium is reached.

- (e) In thermal equilibrium we have that $m\omega \langle x_0^2 \rangle_\xi / 2 = k_B T / 2$ and $m \langle v_0^2 \rangle_\xi / 2 = k_B T / 2$, as well as $\langle x_0 v_0 \rangle_\xi = 0$. If we substitute this in correlator (26), it is easy to show that all terms that come with a prefactor $e^{-\frac{\gamma}{2}(t+t')}$ add up to zero. Then

$$\langle x(t)x(t') \rangle_\xi = \frac{k_B T}{m\omega_0^2} e^{-\frac{\gamma}{2}(t-t')} \left(\cos[\Omega(t-t')] + \frac{\gamma}{2\Omega} \sin[\Omega(t-t')] \right) \tag{28}$$