

Exercise 1. Ideal bosons in a harmonic trap.

In this exercise we consider an ideal gas of bosons confined in a three-dimensional harmonic potential. Observe the differences to the cases of classical and fermionic particles in the same harmonic potential, which we discussed in Sheet 2, Exercise 3 and in Sheet 5, Exercise 1, respectively.

The energy states of the bosons are given by

$$E_{\mathbf{a}} = \hbar\omega(3/2 + a_x + a_y + a_z), \quad (1)$$

including the zero point energy of $E_0 = 3\hbar\omega/2$. The occupation numbers of the oscillator modes of the state with energy $E_{\mathbf{a}}$ is given by $\mathbf{a} = (a_x, a_y, a_z)$ with $a_i \in \{0, 1, 2, \dots\}$.

- (a) Consider the high-temperature, low-density limit ($z \ll 1$). Derive the grand canonical partition function for the phonons, \mathcal{Z}_b , and compute the grand potential Ω_b . Take into account also the zero-point energy of the harmonic oscillators. Show that

$$\Omega_b \propto g_4 \left(ze^{-\beta E_0} \right), \quad (2)$$

where the function $g_s(z)$ is defined as

$$g_s(z) = \sum_{l=1}^{\infty} \frac{z^l}{l^s}. \quad (3)$$

Solution. We begin with the general definition of the grand canonical partition function within the occupation number formalism (section 2.5 of the lecture notes) and find

$$\mathcal{Z}_b = \prod_{\mathbf{a}} \sum_{n_{\mathbf{a}}=0}^{\infty} \left(ze^{-\beta E_{\mathbf{a}}} \right)^{n_{\mathbf{a}}} = \prod_{\mathbf{a}} (1 - ze^{-\beta E_{\mathbf{a}}})^{-1} \quad (S.1)$$

In order to compute the grand potential $\Omega = -1/\beta \log \mathcal{Z}$, we use the series expansion

$$\log(1+x) = - \sum_{\ell=1}^{\infty} \frac{(-x)^\ell}{\ell} \quad \text{for } -1 < x \leq 1. \quad (S.2)$$

This expansion is applicable for the logarithm of the partition function in (S.1) as $0 < ze^{-\beta E_{\mathbf{a}}} \leq 1$ (as $\mu \leq E_{\min}$).

With this replacement we can exactly calculate $\log(\mathcal{Z}_b)$ in the high-temperature limit ($\beta \rightarrow 0$):

$$\begin{aligned} \log \mathcal{Z}_b &= - \sum_{\mathbf{a}} \log(1 - ze^{-\beta E_{\mathbf{a}}}) = \sum_{\mathbf{a}} \sum_{\ell=1}^{\infty} \frac{z^\ell}{\ell} e^{-\ell\beta E_{\mathbf{a}}} = \sum_{\ell=1}^{\infty} \frac{z^\ell}{\ell} \left(\sum_{\mathbf{a}=0}^{\infty} e^{-\ell\beta\hbar\omega/2} e^{-\ell\beta\hbar\omega a} \right)^3 \\ &= \sum_{\ell=1}^{\infty} \frac{z^\ell}{\ell} \left(\frac{e^{-\ell\beta\hbar\omega/2}}{1 - e^{-\ell\beta\hbar\omega}} \right)^3 \stackrel{\beta \rightarrow 0}{\approx} \sum_{\ell=1}^{\infty} \frac{(ze^{-\beta E_0})^\ell}{\ell} \frac{1}{(\ell\beta\hbar\omega)^3} = \frac{1}{(\beta\hbar\omega)^3} g_4 \left(ze^{-\beta E_0} \right) \end{aligned} \quad (S.3)$$

The grand potential is then given by

$$\Omega_b = - \frac{1}{\beta} \frac{1}{(\beta\hbar\omega)^3} g_4 \left(ze^{-\beta E_0} \right). \quad (S.4)$$

Notice that, even though the zero-point energy E_0 shows up in the expression for Ω_b explicitly, it has no physical consequences. It merely leads to a shift of the chemical potential by E_0 .

- (b) Derive an expression for the internal energy U and the average particle number $\langle N \rangle$. Follow the same approach as in Sheet 5, Exercise 1 in order to obtain U in terms of N .

Solution. First, we compute the internal energy of the system,

$$U_b = \left. \frac{\partial(\beta \Omega_b)}{\partial \beta} \right|_z, \quad (\text{S.5})$$

where the derivative has to be taken at constant fugacity $z = e^{\beta \mu}$. Starting from (S.4) we find

$$U_b = \frac{3}{\beta} \frac{1}{(\beta \hbar \omega)^3} g_4 \left(z e^{-\beta E_0} \right) + \frac{E_0}{(\beta \hbar \omega)^3} g_3 \left(z e^{-\beta E_0} \right), \quad (\text{S.6})$$

which shows that the internal energy is proportional to the grand potential plus a term representing the zero-point energy of the harmonic oscillators.

The average particle number can be computed in a similar way,

$$\langle N_b \rangle = z \frac{\partial}{\partial z} \log \mathcal{Z}_b. \quad (\text{S.7})$$

We have

$$\langle N_b \rangle = z \frac{\partial}{\partial z} \frac{1}{(\beta \hbar \omega)^3} g_4 \left(z e^{-\beta E_0} \right) = \frac{1}{(\beta \hbar \omega)^3} g_3 \left(z e^{-\beta E_0} \right), \quad (\text{S.8})$$

where we used

$$z \frac{\partial}{\partial z} g_4(z) = g_3(z). \quad (\text{S.9})$$

We immediately see, that the second term in equation (S.6) is just given by $\langle N_b \rangle E_0$.

In order to simplify the following calculation, we define a renormalized fugacity

$$\tilde{z} = z e^{-\beta E_0} \quad (\text{S.10})$$

Now we want to relate the internal energy to the particle number and start with the high-temperature expansion of the particle number equation,

$$\langle N_b \rangle = \frac{1}{(\beta \hbar \omega)^3} g_3(\tilde{z}) \approx \frac{1}{(\beta \hbar \omega)^3} \left(\tilde{z} + \frac{\tilde{z}^2}{8} \right). \quad (\text{S.11})$$

The parameter ρ is given by

$$\rho \equiv \left(\frac{\hbar \omega N^{1/3}}{k_B T} \right)^3. \quad (\text{S.12})$$

The condition $z \ll 1$ also implies $\rho \ll 1$. Expanding in ρ allows us to deal with the particle number instead of the chemical potential. Inverting the series $\rho = z + z^2/8$, we find

$$\tilde{z} = \rho - \frac{\rho^2}{8}. \quad (\text{S.13})$$

To interpret the condition $\rho \ll 1$ we note that $\hbar \omega$ is the characteristic energy scale for a particle in the harmonic potential. Since every particle can carry energy in three degrees of freedom (one for each quantum number describing the state) the characteristic average energy scale for the N particles is $\hbar \omega N^{1/3}$.¹ Therefore, the condition $\rho \ll 1$ requires that the characteristic energy scale of the system is much smaller than the thermal energy $k_B T$ (*high-temperature* limit). This means that we consider temperatures at which the average occupation of the states is much smaller than one (*low-density* limit).

We write the internal energy up to second order in ρ as

$$\begin{aligned} \tilde{U} := U - N E_0 &= \frac{3}{\beta} \frac{1}{(\beta \hbar \omega)^3} g_4(\tilde{z}) = \frac{3}{\beta} \frac{1}{(\beta \hbar \omega)^3} \left(\tilde{z} + \frac{\tilde{z}^2}{16} \right) \\ &= \frac{3}{\beta} \frac{1}{(\beta \hbar \omega)^3} \left(\rho - \frac{\rho^2}{8} \right) \\ &= \frac{3}{\beta} \left(N - N^2 (\beta \hbar \omega)^3 \frac{1}{16} \right) = 3 N k_B T \left(1 - N \left(\frac{\hbar \omega}{k_B T} \right)^3 \frac{1}{16} \right), \end{aligned} \quad (\text{S.14})$$

where we recover the equipartition law in leading order and the (negative) first order quantum corrections $\propto N (\hbar \omega / k_B T)^3 \ll 1$ distinguishing the bosons from the ideal classical gas.

¹The reason for this is that in three-dimensional (configuration-)space the radius of a ball grows with the volume as $V^{1/3}$. Think of N as the volume.

- (c) Compute the specific heat C_N for constant particle number.

Compute the thermal expansion coefficient α . Use the average square displacement of the harmonic oscillator $r_{\text{eff}}^2 = x_0^2 \langle a_x + a_y + a_z \rangle$ in order to define an effective volume $V_{\text{eff}} = 4\pi/3 r_{\text{eff}}^3$. Give an interpretation of V_{eff} .

Solution. Since our system does not really have a volume as thermodynamic variable we have to compute the specific heat C_N by fixing the number of particles. Hence, as a starting point we use the expression (S.14) for the internal energy, where we can keep N fixed:

$$C_N = \left(\frac{\partial U}{\partial T} \right)_N = 3Nk_B \left(1 + \frac{1}{8} N \left(\frac{\hbar\omega}{k_B T} \right)^3 \right). \quad (\text{S.15})$$

Finally, we compute the thermal expansion coefficient $\alpha = V^{-1} (\partial V / \partial T)$ at fixed N . For this we have to define an effective volume of the system by introducing an effective radius $r_{\text{eff}}^2 \equiv \langle r^2 \rangle$. From basic quantum mechanics we know that $r_{\text{eff}}^2 = x_0^2 \langle a_x + a_y + a_z \rangle$, where x_0 represents the characteristic length scale which we fix to unity. Hence, we can relate r_{eff}^2 to the internal energy of the system via

$$\hbar\omega r_{\text{eff}}^2 N = \tilde{U}. \quad (\text{S.16})$$

Therefore, we find

$$V_{\text{eff}} \equiv \frac{4\pi}{3} r_{\text{eff}}^3 = \frac{4\pi}{3} \left(\frac{\tilde{U}}{\hbar\omega N} \right)^{3/2}. \quad (\text{S.17})$$

For the thermal expansion coefficient we obtain

$$\begin{aligned} \alpha &= \tilde{U}^{-3/2} \left(\frac{\partial \tilde{U}^{3/2}}{\partial T} \right)_N = \frac{3}{2} \tilde{U}^{-1} C_N \\ &= \frac{3}{2} \tilde{U}^{-1} 3k_B N \left(1 + \frac{1}{8} N \left(\frac{\hbar\omega}{k_B T} \right)^3 \right) \\ &= \frac{3}{2} \frac{1}{T} \frac{1 + \frac{\rho}{8}}{1 - \frac{\rho}{16}} = \frac{3}{2} \frac{1}{T} \left(1 + \frac{3}{16} \rho \right), \end{aligned} \quad (\text{S.18})$$

which agrees (in leading order) with the result for a classical gas in the harmonic trap ($\alpha = 3/(2T)$).

- (d) Plot your results for U , C , and α for the classical, the fermionic, and the bosonic case and note the differences.

Solution. In summary, in Sheet 5, Exercise 1 and in this exercise we have found up to first order in ρ :

$$U = 3Nk_B T \left(1 \pm N \left(\frac{\hbar\omega}{k_B T} \right)^3 \frac{1}{16} \right), \quad (\text{S.19})$$

$$C_N = 3Nk_B \left(1 \mp \frac{1}{8} N \left(\frac{\hbar\omega}{k_B T} \right)^3 \right), \quad (\text{S.20})$$

$$\alpha = \frac{3}{2} \frac{1}{T} \left(1 \mp \frac{3}{16} N \left(\frac{\hbar\omega}{k_B T} \right)^3 \right), \quad (\text{S.21})$$

where the upper and lower sign corresponds to fermions and bosons, respectively. For the classical case, the corrections to 1 vanish for all three formulas.

These results as a function of temperature are plotted in Fig. 1; each for the classical, the fermionic, and the bosonic case. Note that our expansions up to first order in ρ are only valid for $\rho \ll 1$. We can still plot these expansions for larger values of ρ (that is, lower temperatures) to observe the trends, keeping in mind that these results are not exactly valid.

We see that

- In zeroth order in ρ the results for the classical (Boltzmann) gas in a harmonic trap are recovered.

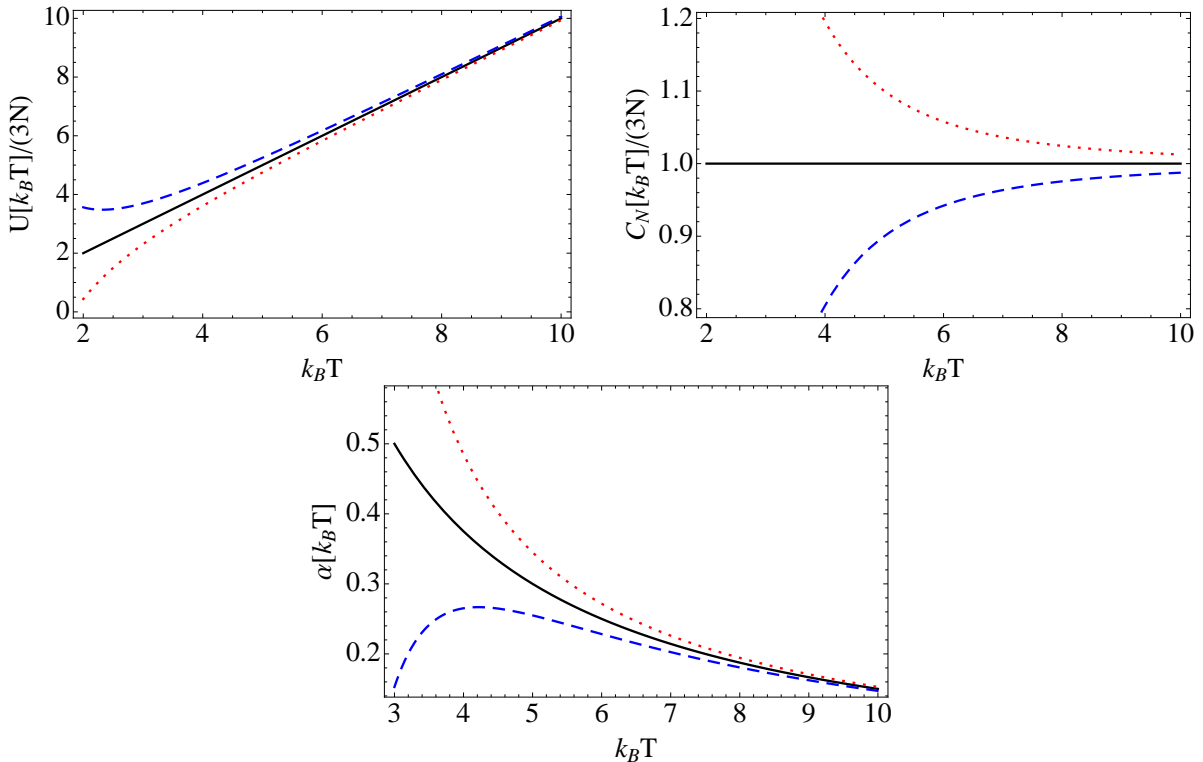


Figure 1: Thermodynamics of fermionic and bosonic gases compared to the classical gas. Note that these quantities are computed within the high-temperature, low-density approximation and are therefore not exact results. Still, they can be used to observe trends. The dashed (blue) line is for the fermions, the dotted (red) line for the bosons, and the continuous (black) line for the classical gas. We set $N\hbar\omega = 100$.

- Due to quantum corrections the internal energy U for fermions (bosons) is higher (lower) than the ideal classical gas.

This can be understood by taking quantum statistics into account. Fermions are not allowed to occupy the same state (Pauli) while bosons tend to gather in the same quantum state. Lowering the temperature, the system tends to occupy low energy states with growing probability. While the classical system is not influenced at all by double occupancy, in the fermionic system the double occupancy is forbidden and occupation of low-energy states is thus reduced, increasing the internal energy U_b compared to the classical gas. In the bosonic case, the opposite happens: the probability of occupying low energy states is enhanced, reducing the internal energy U_b .

- The thermal expansion coefficient is lowered (enhanced) for fermions (bosons) compared to classical gas. This feature represents the fact that with decreasing temperature the bosons tend to occupy more low energy states than the fermions, thus reducing the effective volume V_{eff} more strongly with temperature which enhances the thermal expansion coefficient.

- (e) Find the critical temperature T_c at which Bose-Einstein condensation occurs. How can this be reconciled with the high-temperature, low-density limit?

Hint. The chemical potential can not be larger than the lowest energy level of the particles.

Solution. We now analyse the number equation (S.8) for the bosonic system in detail. If we decrease the temperature, in order to keep the particle number constant, the function $g_3(z)$ has to increase. For a bosonic system, the chemical potential must always be smaller than the state with lowest energy. In this case, this corresponds to

$$z \leq e^{3\beta\hbar\omega/2} . \quad (\text{S.22})$$

The maximum of the monotonically increasing function $g_3(\tilde{z})$ (see Fig. 2) is taken when $z = e^{3\beta\hbar\omega/2}$.

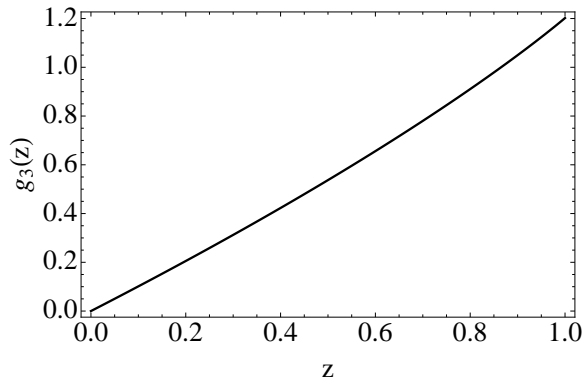


Figure 2: Plot of the function $g_3(z)$ for values of z between 0 and 1.

Hence, the number equation cannot hold for arbitrary small temperature. There exists a critical temperature T_c at which the chemical potential is equal to the ground-state energy, $\mu = E_0$, and thus $ze^{-\beta E_0} = 1$. This temperature can easily be computed as

$$T_c = \frac{\hbar\omega N^{1/3}}{k_B} (g_3(1))^{-1/3}. \quad (\text{S.23})$$

The physical interpretation of this critical point is simple: For the derivation of the number equation, the zero energy state has been neglected. For temperatures above T_c this is a negligible error, but for temperatures below T_c it becomes energetically favorable to occupy this single state with a macroscopically large particle number. Hence, the approximation to neglect the occupation of the zero energy state becomes bad for temperatures below T_c . Macroscopically large occupation of a single quantum state, or equivalently a density matrix where a single eigenvalue is by far the dominant one, is a definition of a condensate. Hence, T_c represents the critical temperature for the bosonic gas to form a Bose-Einstein condensate.

With equation (S.23) we show that our high temperature approximation holds even until T_c if the number of particles N is large: when we compress enough particles, they will condense at a high temperature and we can use the instability of this approximation to find our T_c . Of course, at T_c itself the approximation breaks down.

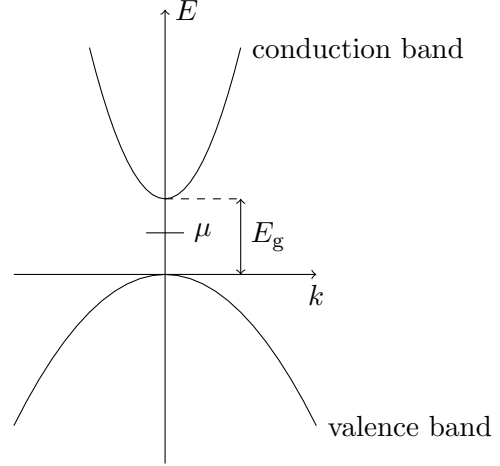
Exercise 2. Behavior of excitations in a semiconductor.

In this exercise we analyze the properties and behavior of electron-excitations of a semiconductor at finite temperature. In solid state theory, electronic states $|\mathbf{k}, \alpha\rangle$ are usually labeled by a *pseudomomentum* $\mathbf{k} = (k_x, k_y, k_z)$ and a band-index $\alpha \in \{1, 2, \dots\}$. For a crystal with lattice constant a , the pseudomomentum takes values in the so-called *Brillouin zone* $\{-\pi/a, \pi/a\}^3$. Assuming a cubic crystal with side-length L there exist $(L/a)^3$ equally distributed \mathbf{k} -vectors in this Brillouin zone. Each of the states is doubly degenerate due to the spin, such that there are in total $2(L/a)^3$ states for each band.

In order to simplify the treatment, we only take into account two bands whose energies are approximated as parabolic,

$$\epsilon_v(\mathbf{k}) = -\frac{\hbar^2 \mathbf{k}^2}{2m_v} \quad \epsilon_c(\mathbf{k}) = E_g + \frac{\hbar^2 \mathbf{k}^2}{2m_c}, \quad (4)$$

as shown in the figure. Here the indices v and c stand for valence and conduction band, respectively. The parameters m_v and m_c which define the curvature of the two bands are called *effective masses* and can in general be different from one another and from the electron mass. The *bandgap*, E_g , is the energy difference between the bottom of the conduction band and the top of the valence band.



Assume for this exercise that the bandgap is much larger than the thermal energy and the chemical potential lies within the gap, $\beta E_g \gg \beta \mu \gg 1$.

- (a) Assume first that the particle number is not fixed and calculate the grand potential Ω of this system.

Hint. For large L , a sum over \mathbf{k} can be approximated by an integral:

$$\sum_{\mathbf{k}} \approx \int_{-\pi/a}^{\pi/a} d^3k \frac{L^3}{8\pi^3} \quad (5)$$

Solution. In the grandcanonical ensemble, each of the states can be either occupied or empty, such that we can write the partition function in the occupation number formalism:

$$\begin{aligned} \mathcal{Z}(\beta, z) &= \left[\prod_{\mathbf{k}} \prod_{\alpha=v,c} \sum_{n_{\mathbf{k},\alpha}=0}^1 \left(z e^{-\beta \epsilon_{\alpha}(\mathbf{k})} \right)^{n_{\mathbf{k},\alpha}} \right]^2 \\ &= \prod_{\mathbf{k}} \left[\left(1 + z e^{\beta \hbar^2 \mathbf{k}^2 / 2m_v} \right) \left(1 + z e^{-\beta (E_g + \hbar^2 \mathbf{k}^2 / 2m_c)} \right) \right]^2 \end{aligned} \quad (S.24)$$

Here the exponent 2 is present due to the spin degeneracy. The grand potential is now given by

$$\Omega(\beta, z) = -1/\beta \log(\mathcal{Z}(\beta, z)) = 2 \sum_{\mathbf{k}} \left[\log \left(1 + z e^{\beta \hbar^2 \mathbf{k}^2 / 2m_v} \right) + \log \left(1 + z e^{-\beta (E_g + \hbar^2 \mathbf{k}^2 / 2m_c)} \right) \right]. \quad (S.25)$$

Due to the assumption $\beta E_g \gg \beta \mu \gg 1$ we know that

$$z e^{\beta \hbar^2 \mathbf{k}^2 / 2m_v} \gg 1 \quad \text{and} \quad z e^{-\beta (E_g + \hbar^2 \mathbf{k}^2 / 2m_c)} \ll 1 \quad (S.26)$$

for all \mathbf{k} , leading to the approximations

$$\begin{aligned}\log\left(1+z e^{\beta \hbar^2 k^2 / 2 m_v}\right) &\approx \beta\left(\mu+\frac{\hbar^2 k^2}{2 m_v}\right)+z^{-1} e^{-\beta \hbar^2 k^2 / 2 m_v} \\ \log\left(1+z e^{-\beta\left(E_g+\hbar^2 k^2 / 2 m_c\right)}\right) &\approx z e^{-\beta\left(E_g+\hbar^2 k^2 / 2 m_c\right)} .\end{aligned}\tag{S.27}$$

At this point we can replace the sum over \mathbf{k} in (S.25) by an integral over \mathbf{k} . This leads to

$$\begin{aligned}\Omega &= -\frac{1}{\beta} \int_{-\pi / a}^{\pi / a} d^3 k \frac{L^3}{4 \pi^3}\left[\beta \mu+\frac{\beta \hbar^2 k^2}{2 m_v}+z^{-1} e^{-\beta \hbar^2 k^2 / 2 m_v}+z e^{-\beta\left(E_g+\hbar^2 k^2 / 2 m_c\right)}\right] \\ &\approx -2 \mu(L / a)^3-\frac{(L / a)^3 \hbar^2 \pi^2}{m_v a^2}-\frac{L^3\left(k_B T\right)^{5 / 2}}{\sqrt{2} \pi^{3 / 2} \hbar^3}\left(m_v^{3 / 2} e^{-\beta \mu}+m_c^{3 / 2} e^{\beta\left(\mu-E_g\right)}\right),\end{aligned}\tag{S.28}$$

where we have replaced the integration interval $[-\pi / a, \pi / a]^3$ by \mathbb{R}^3 for the Gaussian integrals (last two terms in the integral).

- (b) In a realistic system, the particle number is fixed, as every atom in the solid contributes a specific number of electrons. We assume here a particle number, such that the lower band is completely filled at zero temperature, i. e. $N=2(L / a)^3$. Calculate the chemical potential $\mu(T)$ at finite temperature.

Solution. In the grandcanonical ensemble the average particle number is given by

$$\langle N\rangle=-\frac{\partial \Omega}{\partial \mu} .\tag{S.29}$$

Here we assumed that $\langle N\rangle=2(L / a)^3$. This leads to the equation

$$2(L / a)^3=2(L / a)^3+\frac{L^3\left(k_B T\right)^{5 / 2}}{\sqrt{2} \pi^{3 / 2} \hbar^3}\left[-\beta m_v^{3 / 2} e^{-\beta \mu}+\beta m_c^{3 / 2} e^{\beta\left(\mu-E_g\right)}\right] .\tag{S.30}$$

This is equivalent to

$$\left(\frac{m_v}{m_c}\right)^{3 / 2}=e^{\beta\left(2 \mu-E_g\right)},\tag{S.31}$$

leading to the result

$$\mu=\frac{E_g}{2}+\frac{3}{4} k_B T \log\left(\frac{m_v}{m_c}\right) .\tag{S.32}$$

- (c) Starting from your result for Ω , calculate the internal energy $U(T, N)-U(T=0, N)$ (for $N=2(L / a)^3$), using a Legendre transform.

Hint. The final result is given by

$$U(T, N)-U(T=0, N)=N\left(\frac{k_B T}{2 \pi \hbar^3}\right)^{3 / 2} e^{-\beta E_g / 2}\left(m_v m_c\right)^{3 / 4}\left(3 k_B T+E_g\right) .\tag{6}$$

Solution. The internal energy is given by

$$U=\Omega+T S+\mu N .\tag{S.33}$$

We already calculated μ as a function of T and N . The entropy is given by the partial derivative

$$S=-\frac{\partial \Omega}{\partial T}=\frac{L^3\left(k_B T\right)^{5 / 2}}{\sqrt{2} \pi^{3 / 2} \hbar^3}\left[\frac{5}{2 T}\left(m_v^{3 / 2} e^{-\beta \mu}+m_c^{3 / 2} e^{\beta\left(\mu-E_g\right)}\right)-\frac{1}{k_B T^2}\left(-\mu m_v^{3 / 2} e^{-\beta \mu}+\left(\mu-E_g\right) m_c^{3 / 2} e^{\beta\left(\mu-E_g\right)}\right)\right]\tag{S.34}$$

where we used $\frac{\partial}{\partial T} = -\frac{1}{k_B T^2} \frac{\partial}{\partial \beta}$. Using equation (S.32), we find

$$\left(m_v^{3/2} e^{-\beta\mu} + m_c^{3/2} e^{\beta(\mu - E_g)} \right) = 2 e^{-\beta E_g/2} (m_v m_c)^{3/4} \quad (\text{S.35a})$$

$$\left(-\mu m_v^{3/2} e^{-\beta\mu} + (\mu - E_g) m_c^{3/2} e^{\beta(\mu - E_g)} \right) = E_g e^{-\beta E_g/2} (m_v m_c)^{3/4} , \quad (\text{S.35b})$$

and with $N = 2(L/a)^3$

$$\frac{L^3 (k_B T)^{5/2}}{\sqrt{2} \pi^{3/2} \hbar^3} = N \left(\frac{a^2 k_B T}{2\pi \hbar^2} \right)^{3/2} k_B T . \quad (\text{S.35c})$$

Inserting equations (S.35) and (S.34) into equation (S.33), we now obtain the result

$$U(T, N) - U(T=0, N) = N \left(\frac{a^2 k_B T}{2\pi \hbar^2} \right)^{3/2} e^{-\beta E_g/2} (m_v m_c)^{3/4} (3k_B T + E_g) . \quad (\text{S.36})$$

The zero-temperature energy

$$U(T=0, N) = -\frac{N \hbar^2 \pi^2}{2m_v a^2} \quad (\text{S.37})$$

that we subtracted is just the energy of the completely filled valence band.

- (d) A picture that is frequently used in solid state theory is that of electrons and *holes*: When an electron is excited to the conduction band, it leaves an empty state in the valence band. This empty state now behaves like a particle itself and is called a *hole*. Therefore an excitation can be regarded as a creation of two particles, similar to the creation of particle-antiparticle pairs in particle physics.

Use this scheme to interpret the calculated internal energy in terms of the equipartition law for an ideal gas. How many electrons are in the conduction band?

Solution. We call N_c the number of electrons in the conduction band. In the particle-hole picture this is also equal to the number of holes in the valence band. Assuming now the behavior of ideal gas particles for both electrons and holes, the internal energy of electrons and holes is given by

$$U_e = \frac{3}{2} N_c k_B T + N_c E_g \quad U_h = \frac{3}{2} N_c k_B T , \quad (\text{S.38})$$

where E_g describes the energy offset of the conduction band. The total internal energy is then

$$U = N_c (3k_B T + E_g) . \quad (\text{S.39})$$

By comparing this with equation (S.36) we find the number of electrons in the conduction band

$$N_c = N \left(\frac{a^2 k_B T}{2\pi \hbar^2} \right)^{3/2} e^{-\beta E_g/2} (m_v m_c)^{3/4} , \quad (\text{S.40})$$

which is exponentially suppressed by the size of the bandgap.