

1 Microstates and macrostates

3 distinguishable particles can occupy 4 states. Find all macrostates and the numbers of microstates realizing each macrostate. Put results into the table. Which macrostate has the highest statistical weight? What is the total number of microstates that can be found immediately? Is the sum of the microstates realizing each macrostate equal to this expected total number?

Macrostates			Numbers of microstates
3	0	0	1
?	?	?	?

Solution: The table is below

Macrostates			Numbers of microstates
3	0	0	1
0	3	0	1
0	0	3	1
2	1	0	3
2	0	1	3
1	2	0	3
1	0	2	3
0	2	1	3
0	1	2	3
1	1	1	6

The total number of microstates is $3^3 = 27$.

2 Method of lagrange multipliers

Find the area of the largest rectangle that can be inscribed into the ellipse

$$\frac{x^2}{a^2} + \frac{y^2}{b^2} = 1.$$

Use the method of Lagrange multipliers: to minimize a function $F(x, y)$ with a constraint $\phi(x, y) = 0$, minimize

$$\Phi(x, y) \equiv F(x, y) - \lambda\phi(x, y)$$

with respect to x , y , and λ .

Solution: Using the method of Lagrange multipliers, we minimize

$$\Phi(x, y) = xy - \lambda \left(\frac{x^2}{a^2} + \frac{y^2}{b^2} - 1 \right).$$

The equations for the extrema are

$$\begin{aligned} 0 &= \frac{\partial \Phi}{\partial x} = y - 2\lambda x/a^2 \\ 0 &= \frac{\partial \Phi}{\partial y} = x - 2\lambda y/b^2 \\ 0 &= \frac{\partial \Phi}{\partial \lambda} = \frac{x^2}{a^2} + \frac{y^2}{b^2} - 1. \end{aligned}$$

Expressing

$$y = 2\lambda x/a^2$$

from the first equation and inserting the result into the second equation, one obtains

$$0 = x - 4\lambda^2 x/(ab)^2,$$

that is,

$$\lambda = ab/2.$$

Then one obtains

$$y = x \frac{b}{a}.$$

Inserting this into the third extrema equation, one obtains

$$0 = \frac{x^2}{a^2} + \frac{x^2}{a^2} - 1$$

and

$$x = a/\sqrt{2}, \quad y = b/\sqrt{2}.$$

The maximal area is now

$$A_{\max} = xy = \frac{ab}{2}.$$

A-posteriori, one can see that with the smart choice of variables

$$\tilde{x} \equiv x/a, \quad \tilde{y} \equiv y/b$$

one could achieve a more elegant and probably completely symmetric solution of the equations.

3 Thermodynamics of particles in a rigid box in the quantum limit

Calculate the partition function, the internal energy, and the heat capacity of an ensemble of non-interacting particles in a cubic box $L_x = L_y = L_z = L$ at low temperatures (quantum limit), assuming Boltzmann statistics. Define the crossover temperature between the quantum and classical limits.

Solution. The quantum energy levels of the particle in a cubic box are given by

$$\varepsilon_{\nu_x, \nu_y, \nu_z} = \frac{\pi^2 \hbar^2}{2mL^2} (\nu_x^2 + \nu_y^2 + \nu_z^2), \quad \nu_\alpha = 1, 2, 3, \dots \quad (1)$$

The energy of the ground state $(\nu_x, \nu_y, \nu_z) = (1, 1, 1)$ is

$$\varepsilon_{111} = \frac{3\pi^2 \hbar^2}{2mL^2}. \quad (2)$$

The energy of the triple-degenerate first excited states $(2, 1, 1)$, $(1, 2, 1)$, $(1, 1, 2)$ is

$$\varepsilon_{211} = \varepsilon_{121} = \varepsilon_{112} = \frac{6\pi^2 \hbar^2}{2mL^2}.$$

The partition function is given by

$$\mathcal{Z} = \exp\left(-\beta \frac{3\pi^2 \hbar^2}{2mL^2}\right) + 3 \exp\left(-\beta \frac{6\pi^2 \hbar^2}{2mL^2}\right) + \dots$$

or

$$\mathcal{Z} = \exp\left(-\beta \frac{3\pi^2 \hbar^2}{2mL^2}\right) \left[1 + 3 \exp\left(-\beta \frac{3\pi^2 \hbar^2}{2mL^2}\right) + \dots\right].$$

The terms denoted by \dots are contributions of the higher levels. In the low-temperature range

$$k_B T \ll k_B T_0 \equiv U_0 \equiv \frac{3\pi^2 \hbar^2}{2mL^2},$$

the ground state makes the dominant contribution to the partition function while the contributions of the excited states are exponentially small. To obtain the temperature-dependent part of the thermodynamic quantities, it is sufficient to keep the contribution of the first excited states, because those from higher excited states are much smaller. From the expression above, one obtains

$$\ln \mathcal{Z} = -\beta U_0 + \ln [1 + 3 \exp(-\beta U_0) + \dots] \cong -\beta U_0 + 3 \exp(-\beta U_0).$$

The internal energy is given by

$$U = -N \frac{\partial \ln \mathcal{Z}}{\partial \beta} = NU_0 + 3NU_0 \exp(-\beta U_0) = NU_0 [1 + 3 \exp(-\beta U_0)].$$

The first term is just the ground-state energy. The second term is the exponentially small thermal energy. The heat capacity is entirely due to the latter:

$$C = \frac{dU}{dT} = 3NU_0 \left[\frac{\partial}{\partial \beta} \exp(-\beta U_0) \right] \frac{\partial \beta}{\partial T} = 3NU_0 [-U_0 \exp(-\beta U_0)] \left(-\frac{1}{k_B T^2} \right) = 3Nk_B \left(\frac{U_0}{k_B T} \right)^2 \exp\left(-\frac{U_0}{k_B T}\right). \quad (3)$$

or

$$C = 3Nk_B \left(\frac{T_0}{T} \right)^2 \exp \left(-\frac{T_0}{T} \right) \ll Nk_B.$$

The temperature T_0 defined above is the crossover temperature between the quantum and classical regimes. For $T \gtrsim T_0$, many excited levels make a contribution to the partition function, and one has to perform a numerical summation to compute \mathcal{Z} . For $T \gg T_0$, the highly excited states are dominating, and one can replace summation by integration and calculate the partition function analytically.

4 Density of states of particles in the rigid box in 1d and 2d

The density of states of quantum particles in a rigid 3d box has been calculated in the lectures. Generalize these results for one and two dimensions.

Solution: In one dimension, the energy levels are given by

$$\varepsilon_n = \frac{\hbar^2 k_\nu^2}{2m}, \quad k_\nu = \frac{\pi}{L} \nu, \quad \nu = 1, 2, 3, \dots \quad (4)$$

To calculate the density of states defined by

$$dn_\varepsilon = \rho(\varepsilon) d\varepsilon, \quad (5)$$

start with

$$dn_\nu = d\nu, \quad (6)$$

as the number of states (energy levels) in the interval $d\nu$ of the quantum number ν . Using the expression for the quantized wave vector in Eq. (4), one can rewrite Eq. (6) in terms of k as

$$dn_k = \frac{L}{\pi} dk.$$

Using now the relation between the wave vector and the energy,

$$k = \sqrt{\frac{2m\varepsilon}{\hbar^2}}, \quad (7)$$

one obtains

$$dn_\varepsilon = \frac{L}{\pi} \frac{dk}{d\varepsilon} d\varepsilon = \frac{L}{2\pi} \left(\frac{2m}{\hbar^2} \right)^{1/2} \frac{d\varepsilon}{\sqrt{\varepsilon}}.$$

thus the density of states is given by

$$\rho(\varepsilon) = \frac{L}{2\pi} \left(\frac{2m}{\hbar^2} \right)^{1/2} \frac{1}{\sqrt{\varepsilon}}$$

In two dimensions, instead of Eq. (6) we use

$$dn_{\nu_x \nu_y} = d\nu_x d\nu_y \quad (8)$$

that in terms of k becomes

$$dn_{k_x k_y} = \frac{L_x L_y}{\pi^2} dk_x dk_y. \quad (9)$$

Now we go over to the number of states within the circular shell $k, k + dk$ taking into account that both k_x and k_y are positive and thus there is only one quarter of the circular shell. One obtains

$$dn_k = \frac{L_x L_y}{\pi^2} \frac{2\pi}{4} k dk.$$

Further with the help of Eq. (7) follows

$$dn_\varepsilon = \frac{S}{2\pi} \sqrt{\frac{2m\varepsilon}{\hbar^2}} \left(\frac{2m}{\hbar^2} \right)^{1/2} \frac{d\varepsilon}{\sqrt{\varepsilon}} = \frac{S}{2\pi} \frac{2m}{\hbar^2} d\varepsilon$$

and thus

$$\rho(\varepsilon) = \frac{S}{2\pi} \frac{2m}{\hbar^2},$$

where $S = L_x L_y$ is the area of the rigid box. Note that in 2d particle's density of states is a constant.

5 Density of states of phonons in $1d$ and $2d$

The density of states of phonons in $3d$ has been calculated in the lectures. Generalize these results for one and two dimensions.

Solution: In $1d$, we use the density of states with respect to the wave vector k that is the same for particles and lattice vibrations,

$$dn_k = \frac{L}{\pi} dk.$$

Here we change from k to ω using the phonon dispersion law $\omega = vk$ to obtain the density of states

$$\rho(\omega) = \frac{L}{\pi v}$$

that is a constant.

In $2d$ one can start, again, with the DOS in terms of k

$$dn_k = \frac{S}{2\pi} k dk,$$

as for the particles above. Here $S = L_x L_y$ is the area of the system. Changing to ω , one obtains the phonon DOS

$$\rho(\omega) = \frac{S\omega}{2\pi v^2}.$$