4261 HW 1

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1a

The partition function given corresponds to

$$Z(\beta) = \frac{1}{(2\pi h)^3} \int \exp\left(-\beta \frac{\vec{p}^2}{2m}\right) d\vec{p} \int \exp\left(-\beta k \frac{\vec{x}^2}{2}\right) d\vec{x}$$

The integral in one dimension

$$I = \int_{-\infty}^{\infty} e^{-ax^2} dx$$

may be calculated by first squaring the integral:

$$I^2 = \int_{-\infty}^{\infty} e^{-ax^2} dx \int_{-\infty}^{\infty} e^{-ay^2} dy = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-a(x^2+y^2)} dxdy$$

Transforming to polar coordinates, the Jacobian determinant of which you'll recall is $rdrd\theta$, the above becomes

$$I^2 = \int_0^{2\pi} \int_0^{\infty} re^{-ar^2} drd\theta$$

This can be solved trivially by a u-substitution $u = r^2$, $du = 2rdr$:

$$I^2 = 2\pi \left(\frac{1}{2} \int_0^{\infty} e^{-au} du\right) = \pi \left(-\frac{e^{-au}}{a}\bigg|_0^{\infty}\right) = \frac{\pi}{a}$$

Therefore, the integral is equal to $\sqrt{\frac{\pi}{a}}$.

The integral terms of the partition function are then a product of three such integrals with $a = \frac{\beta}{2m}$ for the three scalar variables of momentum and a product of three such integrals with $a = \frac{\beta k}{2}$ for the three scalar variables of position, i.e.

$$Z(\beta) = \frac{1}{(2\pi h)^3} \left(\sqrt{\frac{\pi}{\beta/2m}}\right)^3 \left(\sqrt{\frac{\pi}{\beta k/2}}\right)^3 = \frac{m^{3/2}}{h^3 \beta^3 k^{3/2}}$$

1b

The expectation of the energy based on the partition function is

$$\langle E\rangle = -\frac{1}{Z}\frac{\partial Z}{\partial \beta} = \frac{h^3\beta^3 k^{3/2}}{m^{3/2}}\frac{3m^{3/2}}{h^3\beta^4 k^{3/2}} = \frac{3}{\beta} = 3k_B T$$

Differentiating to find the heat capacity,

$$C = \frac{\partial\langle E\rangle}{\partial T} = 3k_B$$

as desired.

2a

The energies of the eigenstates of a one-dimensional harmonic oscillator are $E_{n1D} = \hbar\omega(n+\frac{1}{2})$, so the energies of the eigenstates in the three-dimensional case are

$$E_n = E_x + E_y + E_z = \hbar\omega\left(n_x + n_y + n_z + \frac{3}{2}\right)$$

implying the partition function is

$$Z(\beta) = \sum_{n_x,n_y,n_z\geq 0} e^{-\beta\hbar\omega(n_x+n_y+n_z+3/2)} = e^{-3\beta\hbar\omega/2}\sum_{n_x} e^{-\beta\hbar\omega n_x}\sum_{n_y} e^{-\beta\hbar\omega n_y}\sum_{n_z} e^{-\beta\hbar\omega n_z}$$

$$= e^{-3\beta\hbar\omega/2}\left(\frac{1}{1-e^{-\beta\hbar\omega}}\right)^3$$

The Bose occupation factor is the negative of the term in the cube;

$$n_B(x) = \frac{1}{e^x - 1}$$

Functions with this behavior appear in descriptions of the collective behavior of any particles for which multiple may occupy the same quantum state (so-called bosons).

2b

The general expression for the expectation value of the energy is

$$\langle E\rangle = -\frac{1}{Z}\frac{\partial Z}{\partial \beta} = -e^{3\beta\hbar\omega/2}\left(1-e^{-\beta\hbar\omega}\right)^3\left(e^{-3\beta\hbar\omega/2}\left[-3\hbar\omega e^{-\beta\hbar\omega}\left(\frac{1}{1-e^{-\beta\hbar\omega}}\right)^4\right] - \frac{3}{2}\hbar\omega e^{-3\beta\hbar\omega/2}\left(\frac{1}{1-e^{-\beta\hbar\omega}}\right)^3\right)$$

$$= \frac{-3\hbar\omega e^{-\beta\hbar\omega}}{e^{-\beta\hbar\omega}-1} + \frac{3}{2}\hbar\omega = 3\hbar\omega\left(\frac{1}{e^{\beta\hbar\omega}-1}+\frac{1}{2}\right)$$

The heat capacity is

$$C = \frac{\partial\langle E\rangle}{\partial T} = 3\hbar\omega\left(-\frac{\hbar\omega}{k_B T^2}e^{\beta\hbar\omega}\frac{1}{(e^{\beta\hbar\omega}-1)^2}\right) = 3k_B\left(\beta\hbar\omega\right)^2\frac{e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega}-1)^2}$$

2c

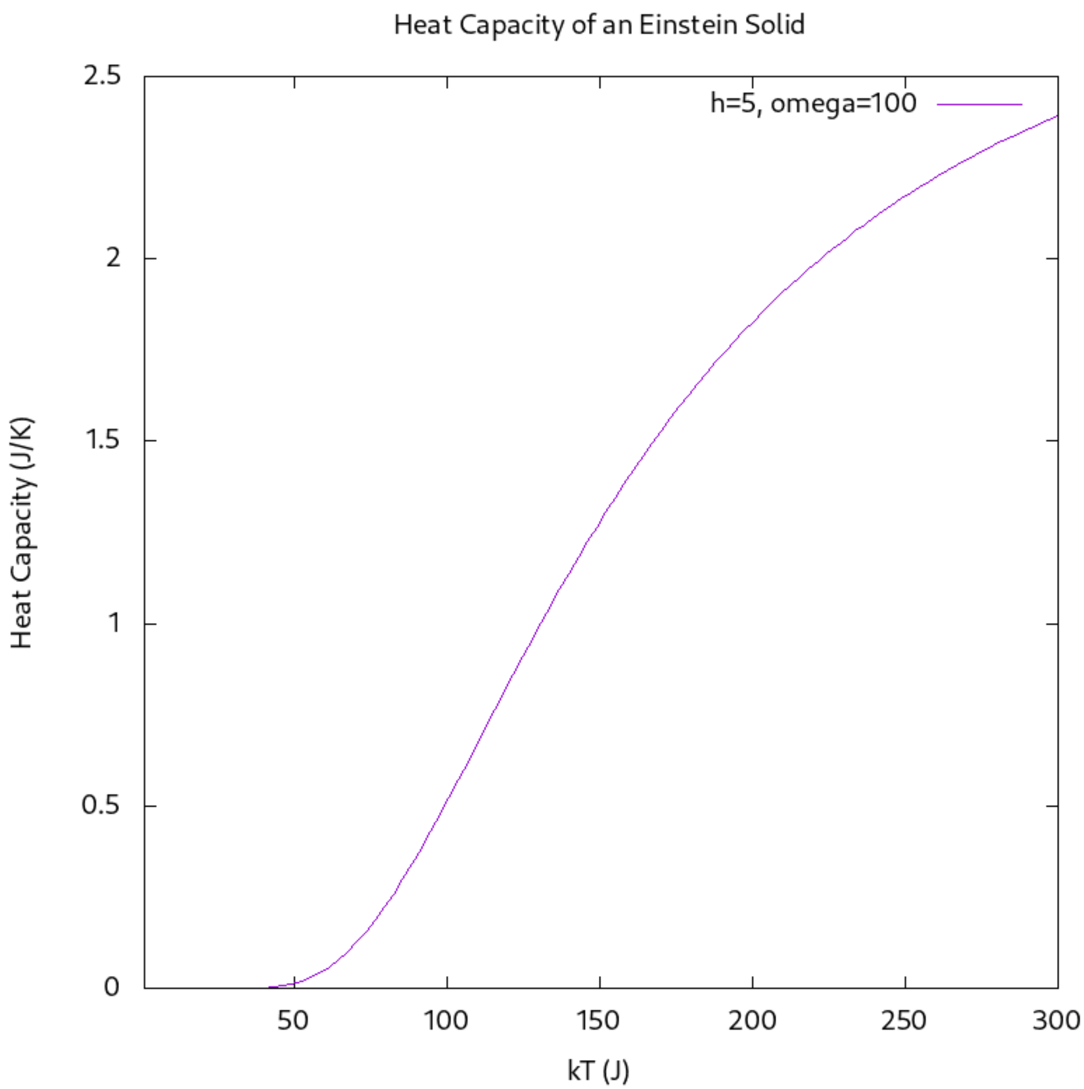
As $\beta \to 0$, and therefore $e^{\beta\hbar\omega} \to 1 + \beta\hbar\omega$, the heat capacity becomes

$$C \to 3k_B(\beta\hbar\omega)^2 \frac{1+\beta\hbar\omega}{(\beta\hbar\omega)^2} = 3k_B + 3k_B\beta\omega\hbar \to 3k_B$$

which confirms the law of Dulong-Petit.

2d

The heat capacity function with nonsense values of h and ω is gnuplotted below.



3a

The Debeye model presumes that heat-capacity-related oscillations behave like sound waves, and are transverse with three polarizations. It then quantizes these waves following Planck, and imposes a maximum frequency cutoff so that the classical $3N$ vibrational degrees of freedom is retained.