HW [number]

Yourname

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Introduction

Inline math can be included as follows: $f(x) = \alpha x^4$.

Numbered equations can be generated as follows:

$$f(x) = \gamma x^2 \tag{1}$$

and referenced as Eqn 1.

We can reference a figure similarly to an equation: Fig 1.

Figure 1: Figures can be included and referenced in this way.

1 Example homework problem: Simons problem 2.1

1.1 Classical Einstein or "Boltzmann" solid

Problem statement. Consider a three-dimensional simple harmonic oscillator with mass m and spring constant k. The Hamiltonian is given by.

$$H = \frac{\mathbf{p}^2}{2m} + \frac{k}{2}\mathbf{x}^2 \tag{2}$$

1.1.1 Calculate the classical partition function

.

$$Z = \int \frac{dp}{(2\pi\hbar)^3} \int dx e^{-\beta H(p,x)} \tag{3}$$

Solution: Substituting in for H,

$$Z = \int \frac{dp}{(2\pi\hbar)^3} \int dx e^{-\beta\left(\frac{\mathbf{p}^2}{2m} + \frac{k}{2}\mathbf{x}^2\right)}. \tag{4}$$

Since $e^{A+B} = e^A e^B$,

$$Z = \int \frac{dp}{(2\pi\hbar)^3} e^{-\beta\left(\frac{\mathbf{p}^2}{2m}\right)} \int dx e^{-\beta\left(\frac{k}{2}\mathbf{x}^2\right)}. \tag{5}$$

We can evaluate this integral from tables, which we can obtain as

$$\int e^{-\alpha x^2} d^3x = \left(\frac{\pi}{\alpha}\right)^{3/2}. \tag{6}$$

So,

$$Z = \frac{1}{(2\pi\hbar)^3} \left(\frac{2m\pi}{\beta}\frac{2\pi}{k\beta}\right)^{3/2} \equiv C\beta^{-3}, \tag{7}$$

where we have defined C as the constant in front of β.

1.1.2 Calculate the heat capacity and show that it is equal to $3k_B$.

Solution: Since no volume enters into this model, we take the heat capacity to be the constant volume heat capacity,

$$C_V \equiv \frac{\partial U}{\partial T} \tag{8}$$

The average energy is given by

$$U = \frac{1}{Z}\int H(p,x) e^{-\beta H(p,x)} = -\frac{1}{Z}\frac{\partial Z}{\partial \beta} \tag{9}$$

$$= -\frac{1}{C\beta^{-3}}(-3)C\beta^{-4} \tag{10}$$

$$= 3\beta^{-1} = 3k_B T \tag{11}$$

Plugging this back into our expression for C_V, we get $C_V = 3k_B$.

1.1.3 Heat capacity for a solid of N harmonic wells

Conclude that if you can consider a solid to consist of N atoms all in harmonic wells, then the heat capacity should be $3NkB = 3R$.

Solution: For a single harmonic oscillator, we computed the internal energy as $U = 3k_BT$. Since internal energy is extensive, for N harmonic oscillators, the internal energy must be given as $U = 3Nk_BT$. Therefore, $C_V = 3k_BT$, in accordance with the law of Dulong and Petit.

1.2 Quantum Einstein solid

Now consider the same Hamiltonian quantum-mechanically.

1.2.1 Calculate the quantum partition function

Solution: The partition function is

$$Z = \sum_{n_x=0}^{\infty} \sum_{n_y=0}^{\infty} \sum_{n_z=0}^{\infty} e^{-\beta\hbar\omega(n_x+n_y+n_z+3/2)} \tag{12}$$

This is separable into

$$Z = \sum_{n_x=0}^{\infty} e^{-\beta\hbar\omega(n_x+1/2} \left(\sum_{n_y=0}^{\infty} e^{-\beta\hbar\omega(n_y+1/2} \left(\sum_{n_z=0}^{\infty} e^{-\beta\hbar\omega(n_z+1/2} \right) \right) \tag{13}$$

Using the identity

$$\sum_{n_z=0}^{\infty} e^{-\beta\hbar\omega(n_z+1/2} = \left(2\sinh(\beta\hbar\omega/2)\right)^{-1} \tag{14}$$

we obtain

$$Z = \left(2\sinh(\beta\hbar\omega/2)\right)^{-3} \tag{15}$$

1.2.2 Explain the relationship with Bose statistics

Solution: The number of quanta in each mode is the same as the Bose-Einstein distribution.

1.2.3 Heat Capacity

Solution: As we noted above, we need $\frac{\partial Z}{Z\partial\beta}$. Through multiple applications of the chain rule, we arrive to

$$\begin{aligned} \frac{\partial Z}{\partial \beta} &= -3\left(2\sinh(\beta\hbar\omega/2)\right)^{-4} 2\cosh(\beta\hbar\omega/2)\hbar\omega/2 && (16) \\ &= -3\hbar\omega\left(2\sinh(\beta\hbar\omega/2)\right)^{-4}\cosh(\beta\hbar\omega/2) && (17) \end{aligned}$$

So

$$\begin{aligned} U = -\frac{\partial Z}{Z\partial\beta} &= 3\hbar\omega\left(2\sinh(\beta\hbar\omega/2)\right)^{-1}\cosh(\beta\hbar\omega/2) && (18) \\ &= \frac{3}{2}\hbar\omega\coth(\beta\hbar\omega/2), && (19) \end{aligned}$$

where we used the identity $\coth(x) = \cosh(x)/\sinh(x)$.

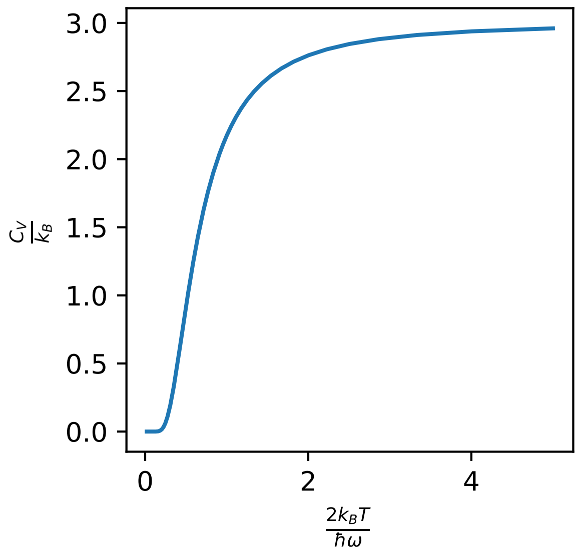

Figure 2: Heat capacity of an Einstein solid as a function of temperature

Now to obtain C_V,

$$\frac{\partial U}{\partial T} = \frac{\partial U}{\partial \beta}\frac{\partial \beta}{\partial T} \tag{20}$$

$$= \frac{3}{2}\hbar\omega\left(1 - \coth^2(\beta\hbar\omega/2)\right)\frac{\hbar\omega}{2}\left(-k_B\beta^2\right) \tag{21}$$

$$= -\frac{3}{4}\hbar^2\omega^2\beta^2 k_B(1 - \coth^2(\beta\hbar\omega/2)) \tag{22}$$

The important energy scale here is $\hbar\omega\beta/2$. Let's define $x = \hbar\omega\beta/2$. Then

$$C_V = -3k_B x^2(1 - \coth^2(x)) \tag{23}$$

1.2.4 Check versus the law of Dulong and Petit

Solution: We know that as $T \to \infty$, then $U \to 3k_BT$. Equivalently, as $\beta \to 0$, then $U \to 3/\beta$.

$$\coth(x) = \frac{e^x + e^{-x}}{e^x - e^{-x}} \tag{24}$$

$$\simeq \frac{2}{2x} = \frac{1}{x} \tag{25}$$

where we used a Taylor expansion at small x. Plugging this into the above formula, we get

$$U \simeq \frac{3}{2}\hbar\omega 2/\beta\hbar\omega = 3/\beta \tag{26}$$

as was anticipated from the large T limit. This is reassuring!

1.2.5 Sketch the heat capacity as a function of temperature.

Solution: The heat capacity is shown in Fig 2. You should write what checks you have done to make sure the plot is reasonable here. At large T, the heat capacity goes to $3k_B$, as expected from the law of Dulong and Petit, and as shown in the previous section. At small values of T, $C_V \to 0$. This actually must happen thermodynamically, since $\Delta S = \int \frac{C_V}{T} dT$ (from PHYS 213!!). Assuming that $S(T=0) = 0$, that means that

$$S(T) = \int_0^T \frac{C_V}{T'} dT' \tag{27}$$

Therefore, $C_V(T)$ must go to zero as $T \to 0$; otherwise the total entropy would be infinite.