33-765 Homework 11

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40. The Black Body Spectrum, and How We See It

1. Recall that $j_\omega(T) = \frac{\hbar}{(2\pi c)^2}\frac{\omega^3}{e^{\beta\hbar\omega}-1}$ is the frequency-resolved power radiated by a black body at temperature T per unit area. Express this function in its alternative wavelength-resolved form, $j_\lambda(T)$. Also, calculate $j(T) = \int_0^\infty \mathrm{d}\lambda\, j_\lambda(T)$.

We begin by noting that $\lambda = \frac{2\pi c}{\omega}$. The transformation theorem tells us that

$$j_\lambda(T) = \frac{\hbar}{(2\pi c)^2}\int \mathrm{d}\omega\,\frac{\omega^3}{e^{\beta\hbar\omega}-1}\delta(\lambda - 2\pi c/\omega)$$

Using the substitution $u = \frac{2\pi c}{\omega}$, $\mathrm{d}u = -\frac{2\pi c}{\omega^2}\,\mathrm{d}\omega$, we find that

$$\begin{aligned} j_\lambda(T) &= \frac{\hbar}{(2\pi c)^2}\int_\infty^0 \mathrm{d}u\,\delta(\lambda - u)\frac{(2\pi c)^4}{(e^{\beta\hbar 2\pi c/\lambda}-1)u^5} \\ &= \frac{(2\pi c)^2\hbar}{\lambda^5}\frac{1}{e^{\beta 2\pi\hbar c/\lambda}-1} \\ &= \frac{2\pi c^2 h}{\lambda^5}\frac{1}{e^{\beta hc/\lambda}-1} \end{aligned}$$

The integral is

$$\int_0^\infty j_\lambda(T)\,\mathrm{d}\lambda = \frac{\pi^2}{60c^2\beta^4\hbar^3}$$

2. Find the values $\omega^* = 2\pi f^*$ and λ^* where j_ω and j_λ have their maximum. Now calculate $\lambda^* f^*$. Does the result surprise you?

The derivatives are messy, but I'll write them out:

$$\partial_\omega j_\omega(T) = \frac{3\omega^2\hbar}{(2\pi c)^2(e^{\beta\hbar\omega}-1)} - \frac{\beta\hbar(\omega^2\hbar)e^{\beta\hbar\omega}}{(2\pi c)^2(e^{\beta\hbar\omega}-1)^2} = 0$$

$$\omega^* = \frac{3 + \mathrm{ProductLog}\left[-\frac{3}{e^3}\right]}{\beta\hbar}$$

(I used Mathematica to solve this, the ProductLog[z] function is the principal numerical solution for w in $z = we^w$.)

Repeating for λ, I found

$$\partial_\lambda j_\lambda(T) = \frac{(2\pi c)^3 e^{2\pi\hbar c\beta/\lambda}\beta h^2}{\lambda^7\left(e^{2\pi\hbar c\beta/\lambda}-1\right)^2} - \frac{5(2\pi c)^2\hbar}{\lambda^6(e^{2\pi\hbar c\beta/\lambda}-1)} = 0$$

so

$$\lambda^* = \frac{2c\pi\beta\hbar}{5+\text{ProductLog}\left[-\frac{5}{e^5}\right]}$$

This is interesting because it makes $f^*\lambda^* \approx 1.75978c$ instead of exactly c. As a fun fact, the approximation of that number as $\frac{4-\ln(3)}{\sqrt{e}}$ is accurate to eight decimal places.

3. We get the perceived brightness of light by multiplying its power with the luminous efficiency function $V(\lambda)$ of the human eye. The luminous flux density $\mathcal{F}(T)$ is then

$$\mathcal{F}(T) = 683\frac{\text{lm}}{\text{W}} \times \int_0^\infty \mathrm{d}\lambda\, j_\lambda(T)V(\lambda)$$

with $V(\lambda) \approx e^{-(\lambda-\lambda_{\text{max}})^2/2\delta_\lambda^2}$ and $\lambda_{\text{max}} = 555\text{nm}$ and $\delta_\lambda = 43\text{nm}$. Plot the overall luminous efficacy, $\mathcal{E}(T) = \mathcal{F}(T)/j(T)$ as a function of T!

See the attached plot from Mathematica.

4. White LEDs reach luminous efficacies in excess of $100\frac{\text{lm}}{\text{W}}$. How much more energy efficient are such LEDs compared to a typical incandescent light bulb operating at 2900K?

Plugging in $T = 2900\text{K}$ into our equation for $\mathcal{E}(T)$, I found that $\mathcal{E}(T) \approx 17.2456\frac{\text{lm}}{\text{W}}$, so LEDs are at least 5.8 times more efficient.

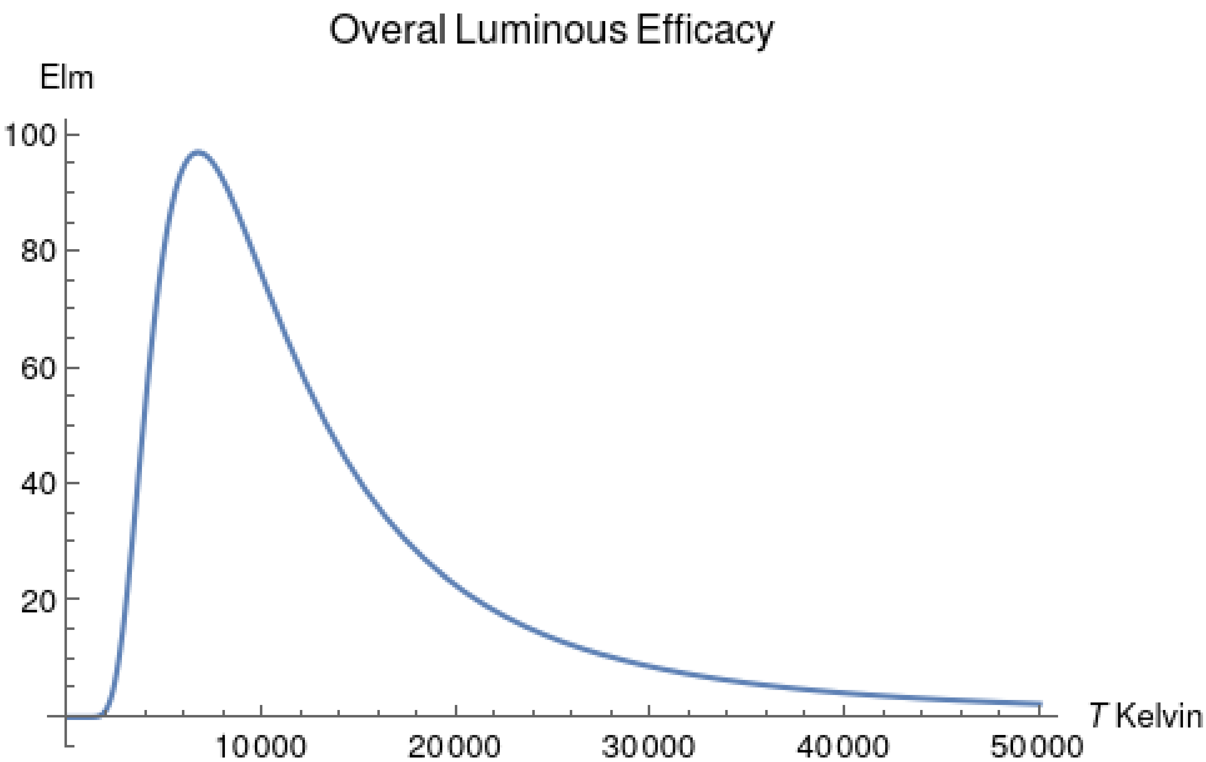

Figure 0.1: Problem 40.3: Plot of Efficacy vs. Temperature

41. The Simple and the Not-Quite-So-Simple Rigid Rotator

A simple rigid rotator has only rotational energy, and its Hamiltonian is give by $H = \frac{1}{2I}L^2$ where L is the operator of angular momentum and I is the moment of inertia.

1. What are the eigenvalues of L, and what are their degeneracies?

The eigenvalues of L are $\hbar^2 l(l+1)$ and the degeneracies are $g(l) \equiv 2l+1$.

2. Write down the canonical quantum partition function Z of the rigid rotator, as well as its free energy F, energy U, and specific heat c. Substitute $T_{\text{rot}} = \frac{\hbar^2}{2Ik_B}$.

$$Z = \text{Tr}\big[e^{-\beta H}\big] = \sum_{l=0}^{\infty} g(l)e^{-\beta l(l+1)\frac{\hbar^2}{2I}} = \sum_{l=0}^{\infty} g(l)e^{-\beta l(l+1)k_B T_{\text{rot}}}$$

For convenience, I'll define $\epsilon(l) \equiv l(l+1)k_B T_{\text{rot}}$.

$$F = -k_B T \log[Z] = -k_B T \log[\sum_{l=0}^{\infty} g(l)e^{-\beta\epsilon(l)}]$$

$$U = -\frac{\partial}{\partial\beta}\log[Z] = \frac{\sum_{l=0}^{\infty} g(l)\epsilon(l)e^{-\beta\epsilon(l)}}{Z}$$

$$\begin{aligned} c_V &= \frac{\partial}{\partial T}U = -\frac{\partial}{\partial T}\frac{\partial}{\partial\beta}\log[Z] = \frac{(\partial_T Z)(\partial_\beta Z)}{Z^2} - \frac{\partial_T\partial_\beta Z}{Z} \\ &= \frac{(\sum_{l=0}^{\infty} -g(l)\epsilon(l)e^{-\beta\epsilon(l)})(\sum_{l=0}^{\infty} k_B^{-1}T^{-2}g(l)\epsilon(l)e^{-\beta\epsilon(l)})}{Z^2} - \frac{\sum_{l=0}^{\infty} k_B^{-1}T^{-2}\epsilon(l)^2 g(l)e^{-\beta\epsilon(l)}}{Z} \end{aligned}$$

3. Plot $c(T)/k_B$ as a function of T/T_{rot} for $0 \le T/T_{\text{rot}} \le 3$. Give an analytical explanation for the limit $T \to \infty$.

All the plots are located at the end of this document. I did a partial sum up to about 40 because after that point, $e^{l(l+1)}$ for $l > 40$ evaluates to basically zero in Mathematica, so I figured that around that order of magnitude would cancel out the other terms. Analytically, for large T, all of the exponentials go to $e^0 = 1$, so we get

$$Z = \sum g(l)$$

and

$$c_V = \frac{(\sum -g(l)\epsilon(l))(\sum k_B^{-1}T^{-2}g(l)\epsilon(l))}{(\sum g(l))^2} - \frac{\sum k_B^{-1}T^{-2}\epsilon(l)^2 g(l)}{\sum g(l)} \to 0$$

The factors of T^{-2} also go to 0, so in the end we just have a bunch of zeros, so I must have done something wrong when I calculated the derivatives, but I cant figure out what it would be (since the Mathematica answer makes it seem like it approaches 1).

4. Repeat with parahydrogen.

I would rather not write everything out again, since, in my notation, all of the equations will be identical. Instead, I'll just explain that for parahydrogen, we are looking at the singlet state which must have l be even, so I can substitute $l \to 2l$ in the equations for $\epsilon(l)$ and $g(l)$ above.

5. Repeat for orthohydrogen.

Again, I won't write it out. There are three degenerate states which must have l odd, so $g(l) \to 3g(2l+1)$ and $\epsilon(l) \to \epsilon(2l+1)$.

6. Repeat for the equilibrium state.

Here, we just want to include both ortho- and parahydrogen in the summations. Note that $\frac{1+(-1)^l}{2} = \begin{cases} 1 & l \text{ even} \\ 0 & l \text{ odd} \end{cases}$ acts as an indicator function for the parity of l. With some simple manipulation, I can turn this into $p(l) \equiv 2 - (-1)^l$, which gives the desired degeneracy of 1 for parahydrogen and 3 for orthohydrogen, but only at those specific parities. The partition function then becomes

$$Z = \sum_{l=0}^{\infty} p(l) g(l) e^{-\beta\epsilon(l)}$$

and the other equations are identical with a multiplication of $p(l)$ after each sum.

7. Repeat for normal hydrogen.

Normal hydrogen can be treated as two distinct gasses in a fixed ratio. The new heat capacity is

$$c_{\text{normal}} = \frac{1}{4} c_{\text{para}} + \frac{3}{4} c_{\text{ortho}}$$

8. Plot the four theoretically calculated rotational specific heats for $0 \leq T/T_{\text{rot}} \leq 3.5$. By a careful comparison with the experimentally measured rotational specific heat, determine the length of the hydrogen-hydrogen bond.

The graph is attached. Experimentally (without units) I chose $c = \{0.5, 0.75, 0.8\}$ for $T = \{150\text{K}, 185\text{K}, 200\text{K}\}$ in the experimental plot. On my plot, I found the temperature values corresponding to those values of c: $T' = \{2.054, 9.3725, 9.3728\}$. By averaging, $T_{\text{rot}} = \frac{1}{3} \sum \frac{T}{T'} \approx 38.0249$. Recall that $T_{\text{rot}} = \frac{\hbar^2}{2Ik_B}$ and for a rigid rotator comprised of two fixed masses connected by a massless rod, $I = \frac{mL^2}{2}$, so

$$L = \sqrt{\frac{\hbar^2}{k_B m T_{\text{rot}}}} = 1.12491 \times 10^{-10}\text{m} \neq 74\text{pm}$$

I must have some error in my calculation.

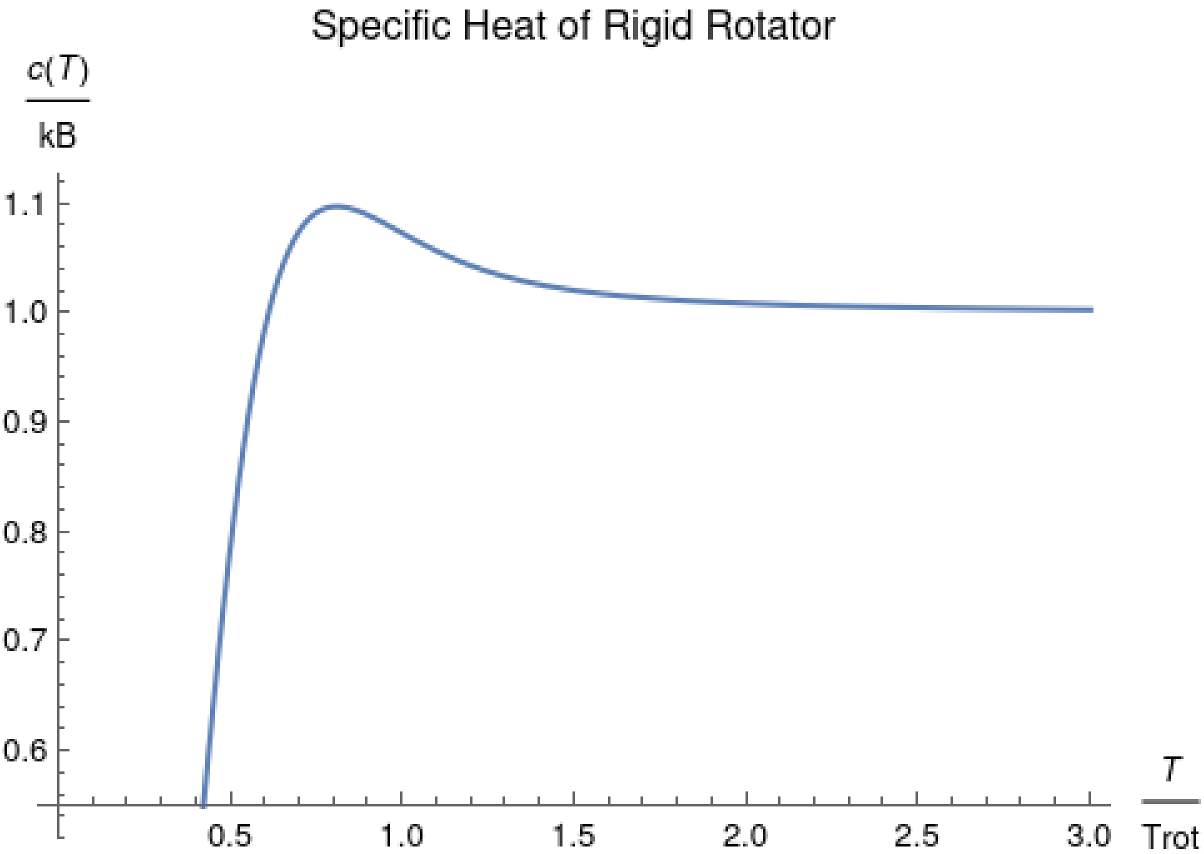

Figure 0.2: Plot for Problem 41.3

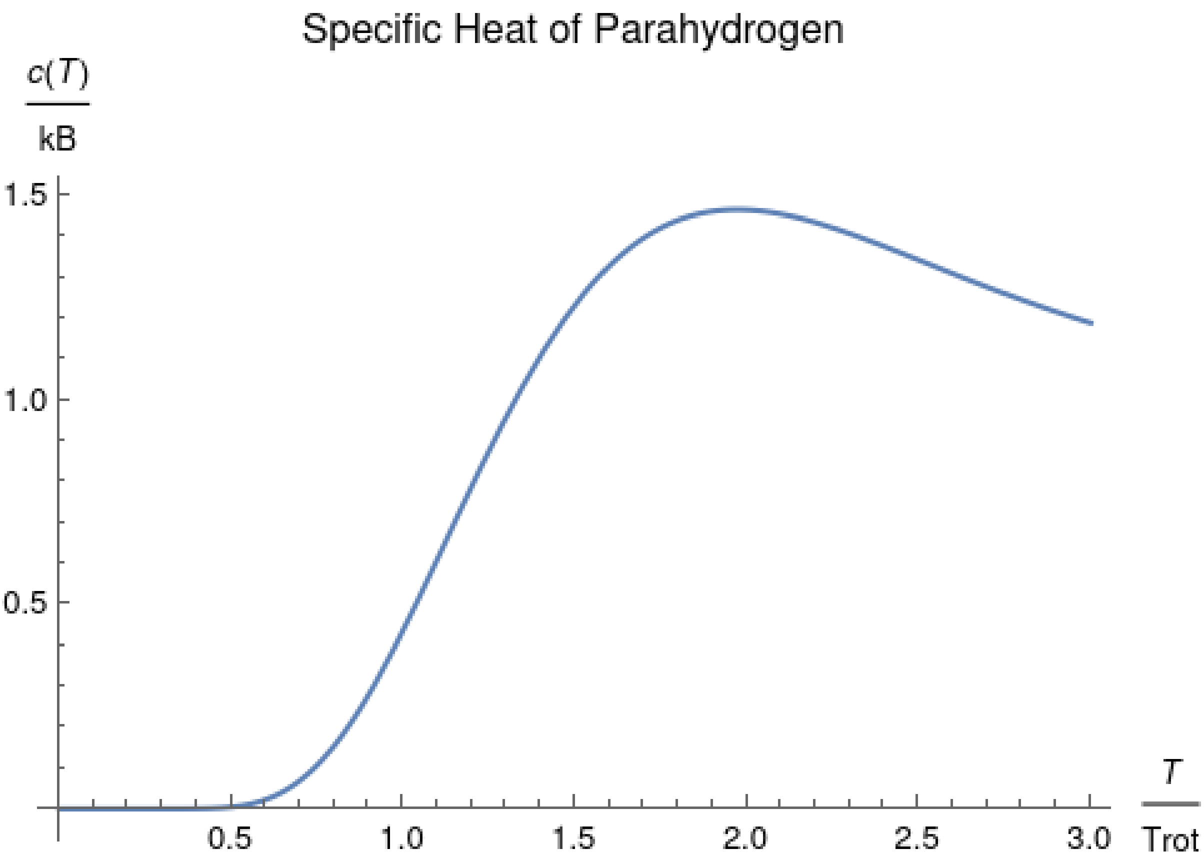

Figure 0.3: Plot for Problem 41.4

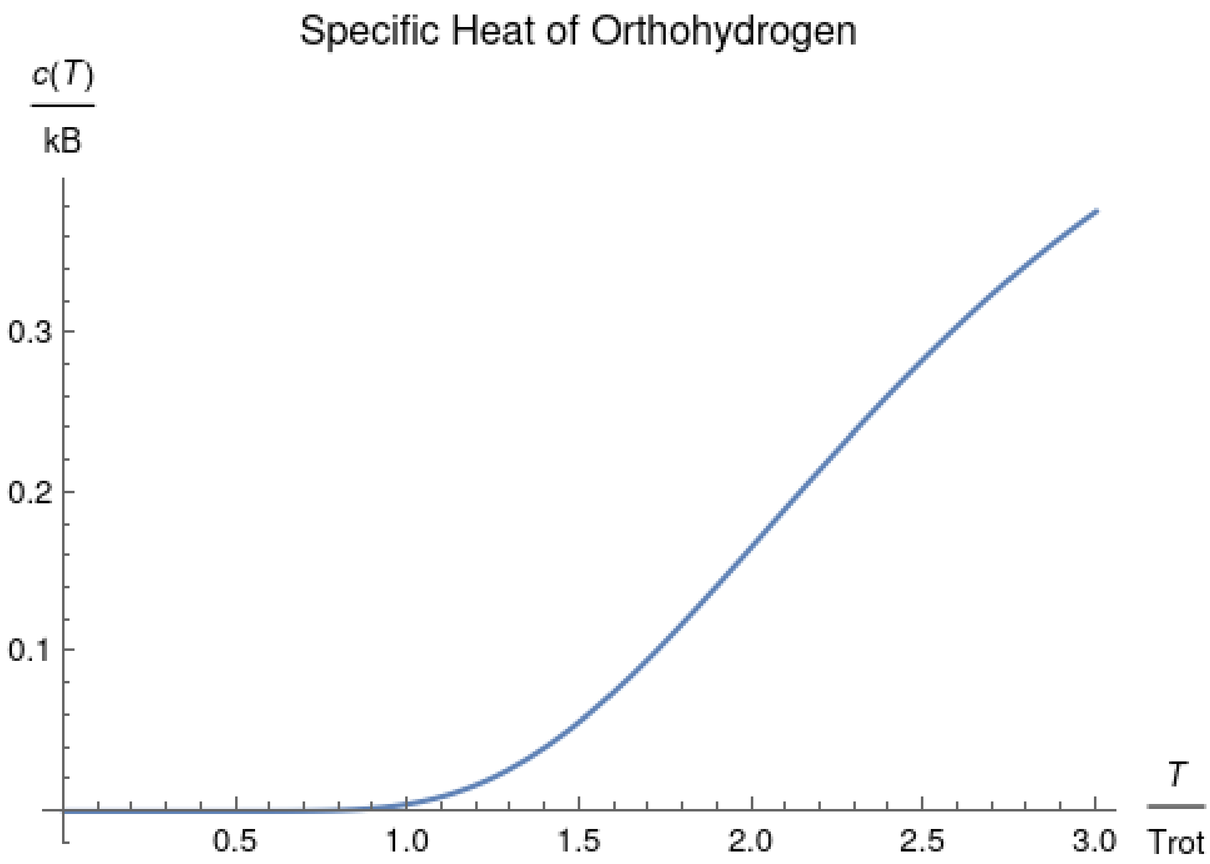

Figure 0.4: Plot for Problem 41.5

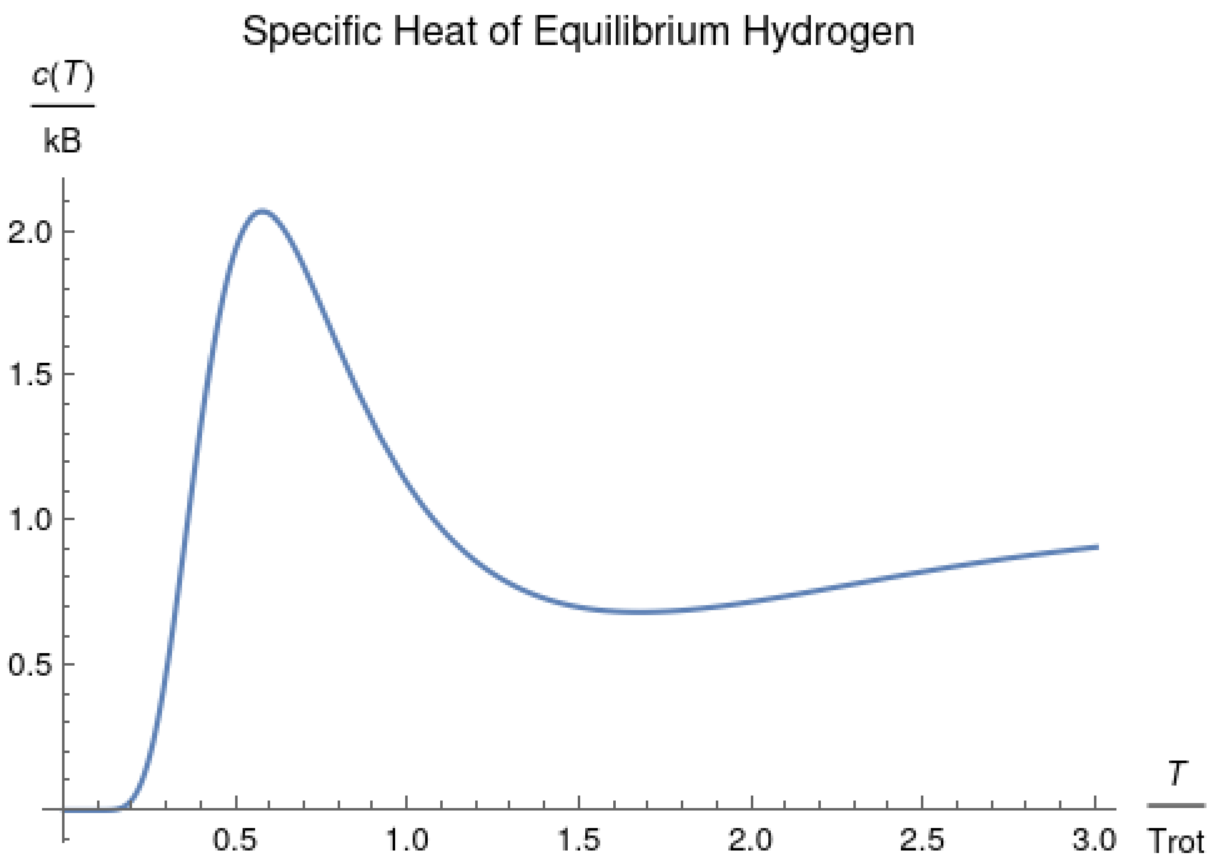

Figure 0.5: Plot for Problem 41.6

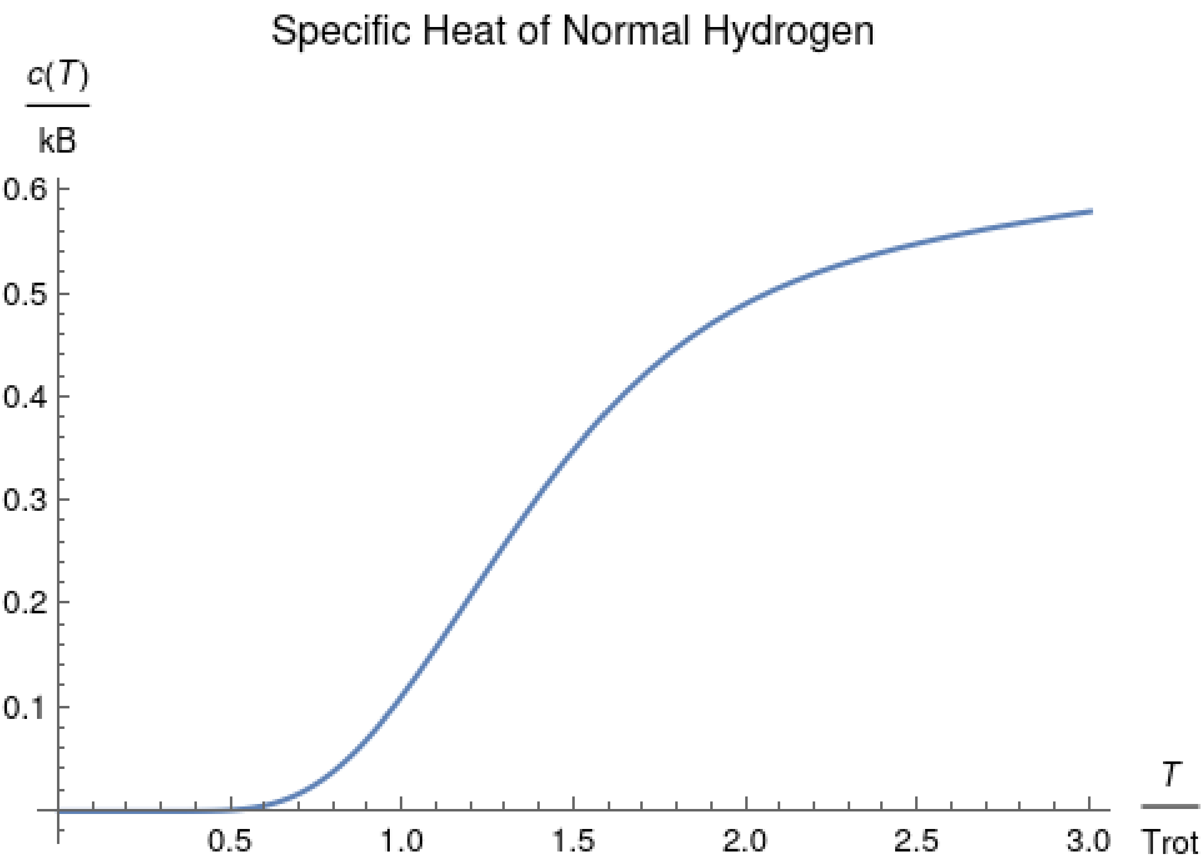

Figure 0.6: Plot for Problem 41.7

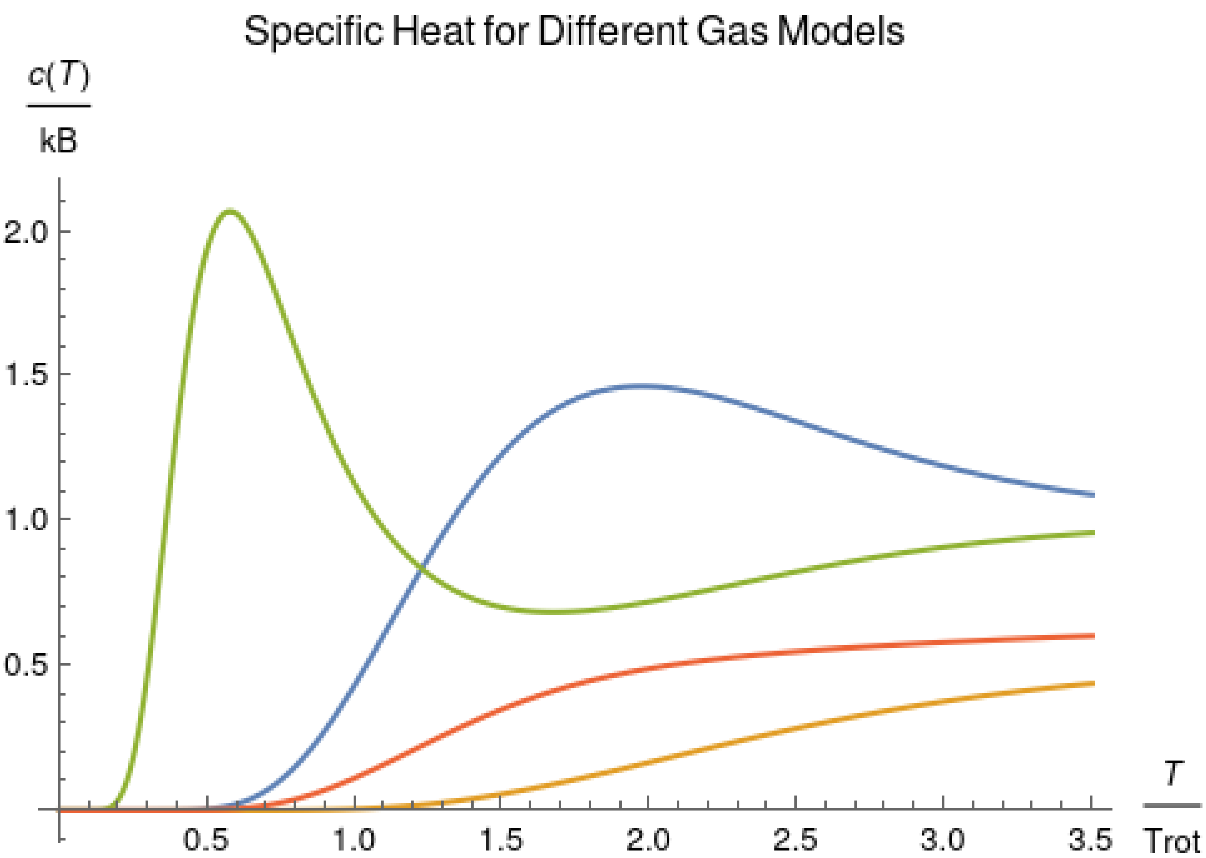

Figure 0.7: Plot for Problem 41.8