

Statistical and Low Temperature Physics (PHYS393)

# 4. Phonons and Photons

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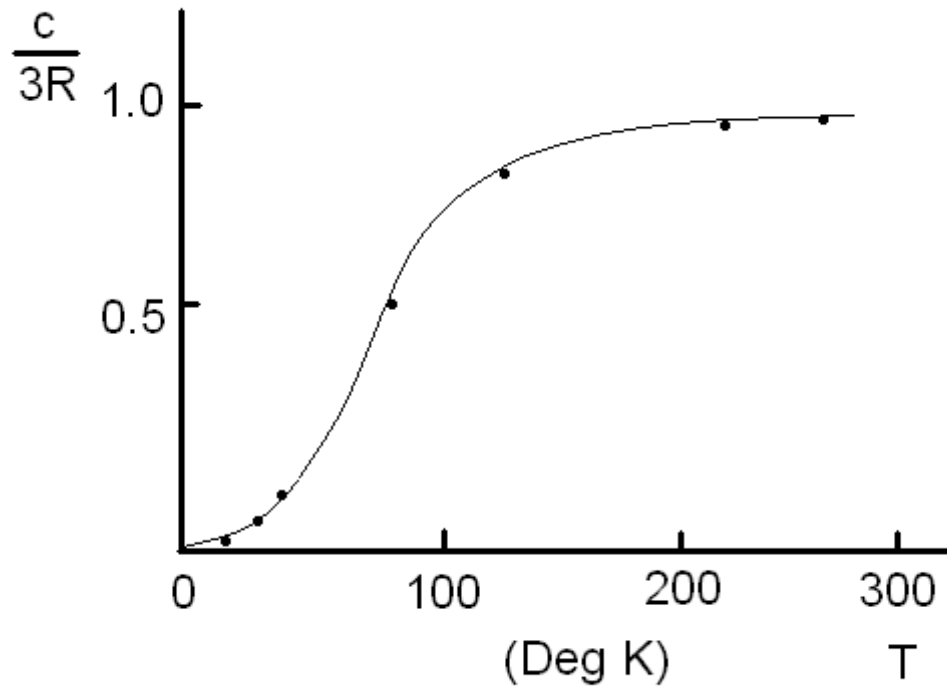
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# Phonons

## Specific heat capacities of solids

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In 1912, Peter Debye, a Dutch physicist working in Germany, produced a theory which predicts the heat capacity of a solid correctly at high and low temperatures.

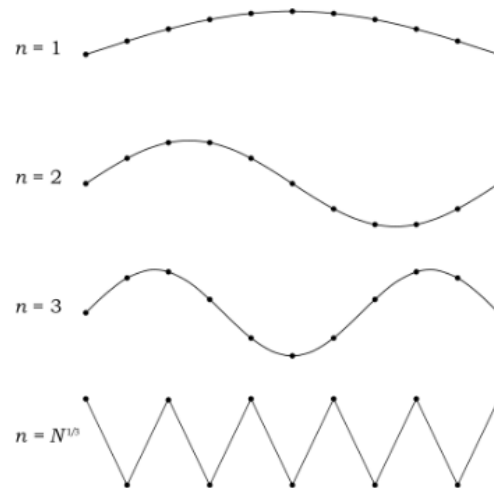


## Atoms vibrating in a solid

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In Debye's model, we think of the atoms in a solid as connected by springs. They vibrate in 3D in a complicated way.

The problem can be simplified by treating the vibration as a superposition of waves of different frequencies.



If we suppose that the atoms are fixed at the edge of the solid, the frequency would be quantised. A quantum of this vibration energy is called a phonon.

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## Quantised thermal waves

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We can count the number of states for the phonons, like we did for atoms in an ideal gas, or electrons in a metal.

Unlike electrons, however, the exclusion principle does not apply to phonons.

So each energy state can be occupied by any number of phonons.

This means that we need yet another way to find the macrostate. This was worked out by Bose and Einstein in the 1920s.

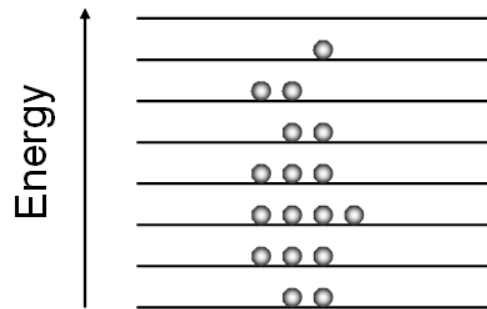
## Bose-Einstein Statistics

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The method is similar to what we have used for the ideal gas.

There, we have made the assumption that there are many more energy levels than there are particles. This has meant that it is unlikely for two gas atoms to occupy the same state.

We do not make this assumption now, since we would be particularly interested in the low temperature behaviour.



Since the exclusion principle does not apply to phonons, more than one phonons can occupy the same state.

## Bose-Einstein Statistics

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Suppose, in the energy bundle  $i$ , that there are  $g_i$  levels and  $n_i$  phonons. The phonons are now completely free to arrange themselves among the energy levels.

This means that we have  $n_i + g_i$  objects altogether in the bundle. There are  $n_i$  of one type, and  $g_i$  of the other type. The number of possible arrangements would be

$$\Omega_i = \frac{(n_i + g_i)!}{n_i!g_i!}$$

The total number of arrangements for all bundles would be obtained by multiplication of the number for every bundle:

$$\Omega = \prod_i \frac{(n_i + g_i)!}{n_i!g_i!}.$$

## Bose-Einstein Distribution

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Then we need to maximise  $\ln \Omega$  using the Lagrange multiplier method.

Using the same constraints as before on the number of particles  $N$  and the total energy  $U$ , the method would give the following answer:

$$\frac{n_i}{g_i} = \frac{1}{\exp(-\lambda_1 - \lambda_2 \varepsilon_i) - 1}.$$

where  $\lambda_1$  and  $\lambda_2$  are the Lagrange multipliers.

This has almost the same form as Fermi-Dirac distribution, except that it is -1 instead of +1 in the denominator.

Following the same procedure that is used for Fermi-Dirac distribution, we write the above result as

$$\frac{n_i}{g_i} = \frac{1}{\exp((\varepsilon_i - \mu)/k_B T) - 1}.$$



## Bose-Einstein Distribution

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This is called the Bose-Einstein distribution function. It looks almost the same as the Fermi-Dirac distribution function, except that it has  $-1$  in the denominator instead of  $+1$ .

When we apply this to phonon, however, we need to make some changes.

## Bose-Einstein Distribution

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Phonons are not real particles like atoms or electrons. The number of phonons is related to the vibration energy. The number would increase when the temperature increases. At 0 Kelvin, there is no vibration, so there would be no phonons.

Because of this, there would be no constraint on the number  $N$ . We really only have one constraint - that of constant energy  $U$ .

The Lagrange function is  $\ln \Omega + \lambda U$ .  $N$  does not appear. Maximising this function, we get

$$\frac{n_i}{g_i} = \frac{1}{\exp(-\lambda \epsilon_i) - 1}.$$

With the help of entropy as before, we would find

$$\lambda = -\frac{1}{k_B T}.$$

## Phonon occupation number

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Maximising Lagrange function, we have obtained

$$\frac{n_i}{g_i} = \frac{1}{\exp(\varepsilon_i/k_B T) - 1}.$$

Following the same notations that we have used for ideal gas and electrons, we rewrite:

$$\begin{aligned} n_i &\text{ as } n(\varepsilon)d\varepsilon \text{ and} \\ g_i &\text{ as } g(\varepsilon)d\varepsilon. \end{aligned}$$

This gives

$$n(\varepsilon)d\varepsilon = \frac{g(\varepsilon)d\varepsilon}{\exp(\varepsilon/k_B T) - 1}$$

Next, we need a formula for the density of states  $g(\varepsilon)$ .

Note that although we have previously used the same symbol  $g(\varepsilon)$  for the particle in a 3-D box, the phonon density of states would have a different formula.

## density of states for phonons

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The vibrations in a solid is described by the wave equation

$$\frac{\partial^2 \xi}{\partial x^2} + \frac{\partial^2 \xi}{\partial y^2} + \frac{\partial^2 \xi}{\partial z^2} = \frac{1}{v^2} \frac{\partial^2 \xi}{\partial t^2}$$

where  $\xi$  is related to the displacement of the atoms.

[http://en.wikipedia.org/wiki/Wave\\_equation](http://en.wikipedia.org/wiki/Wave_equation)

The solution has a similar form to the wave function for the particle in a box:

$$\xi = e^{i\omega t} \sin k_x x \sin k_y y \sin k_z z$$

where  $\omega$  is the angular frequency.

Substituting the solution for  $\xi$  into the wave equation above, we would get

$$k_x^2 + k_y^2 + k_z^2 = \frac{\omega^2}{v^2}.$$

Substituting into the wave equation would be easier if we work out each of the partial derivatives first. For example, differentiating twice with respect to  $x$ , we would get

$$\frac{\partial^2 \xi}{\partial x^2} = e^{i\omega t} (-k_x^2 \sin k_x x) \sin k_y y \sin k_z z = -k_x^2 \xi.$$

Likewise with respect to  $y$  and  $z$ . Differentiating twice with respect to  $t$ , we would get

$$\frac{\partial^2 \xi}{\partial t^2} = (-\omega^2 e^{i\omega t}) \sin k_x x \sin k_y y \sin k_z z = -\omega^2 \xi.$$

Now we can see that substituting into the wave equation gives

$$-k_x^2 \xi - k_y^2 \xi - k_z^2 \xi = \frac{1}{v^2} (-\omega^2 \xi),$$

which is

$$k_x^2 + k_y^2 + k_z^2 = \frac{\omega^2}{v^2}.$$

## density of states for phonons

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Defining  $k$  as the magnitude of the wave vector, we have

$$k^2 = k_x^2 + k_y^2 + k_z^2$$

and

$$k^2 = \frac{\omega^2}{v^2}.$$

The boundary condition requires  $\xi$  to be zero at the walls. Therefore, in the same way as the particle in the box, the wavevector would be quantised:

$$k_x = \frac{n_x \pi}{a}, \quad k_y = \frac{n_y \pi}{a} \quad \text{and} \quad k_z = \frac{n_z \pi}{a}.$$

Substituting these into

$$k^2 = k_x^2 + k_y^2 + k_z^2$$

gives

$$k^2 = \frac{\pi^2}{a^2} (n_x^2 + n_y^2 + n_z^2)$$

## density of states for phonons

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Rearranging,

$$\frac{k^2 a^2}{\pi^2} = n_x^2 + n_y^2 + n_z^2.$$

We have also obtained above the dispersion relation

$$k = \frac{\omega}{v}.$$

Substituting,

$$\frac{\omega^2 a^2}{v^2 \pi^2} = n_x^2 + n_y^2 + n_z^2.$$

We may now follow the same method that we have used for ideal gas to count the states. Comparing with the equation for a sphere

$$R^2 = n_x^2 + n_y^2 + n_z^2$$

the total number of states with frequency less than  $\omega$  is given by the octant of the sphere:

$$G(\omega) = \frac{1}{8} \left( \frac{4\pi}{3} R^3 \right) = \frac{\pi}{6} \left( \frac{\omega a}{v\pi} \right)^3$$

Differentiating the number of states,

$$G(\omega) = \frac{\pi}{6} \left( \frac{\omega a}{v\pi} \right)^3$$

we get the density of states:

$$g(\omega) = \frac{V\omega^2}{2\pi^2v^3}$$

where  $V$  is the volume  $a^3$ .



## About polarisation

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Actually, we are not quite there yet.

There reason is that each state correspond to a wave, and a wave in a solid can have 2 transverse polarisations, and 1 longitudinal polarisation.

Previously, we have only counted the states in terms of the possible wavevector  $(n_x, n_y, n_z)$ . In the case of solids, the 3 different directions of vibrations are in fact different states with the same wavevector  $(n_x, n_y, n_z)$ .

So we have to multiply by 3 to get the correct density of state:

$$g(\omega)d\omega = 3 \times \frac{V\omega^2 d\omega}{2\pi^2 v^3}$$

## The Debye Frequency

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There is one more practical point to note. In a solid, there is a limit to the highest phonon frequency.

This is related to the fact that the wavelength cannot possibly be shorter than the distance between atoms.

Let this highest frequency be  $\omega_D$ .

In a solid with  $N$  identical atoms, there are  $3N$  energy states, or normal modes. This is when we count every possible frequency, and every possible "direction of vibration" for each frequency.

This can be proven mathematically, but we shall skip that. We can find  $\omega_D$  by integrating the density of states:

$$\int_0^{\omega_D} g(\omega) d\omega = \int_0^{\omega_D} \frac{3V\omega^2 d\omega}{2\pi^2 v^3} = 3N$$

## The Debye Frequency

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This equation

$$\int_0^{\omega_D} g(\omega) d\omega = \int_0^{\omega_D} \frac{3V\omega^2 d\omega}{2\pi^2 v^3} = 3N$$

can then be solved to find the Debye frequency. Integrating gives

$$\frac{V\omega_D^3}{2\pi^2 v^3} = 3N$$

Solving for  $\omega_D$  gives the Debye frequency:

$$\omega_D = \left( \frac{6N\pi^2 v^3}{V} \right)^{1/3}$$

## The phonon distribution

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As we have shown earlier, the distribution of phonons is given by

$$n(\varepsilon)d\varepsilon = \frac{g(\varepsilon)d\varepsilon}{\exp(\varepsilon/k_B T) - 1}$$

We shall express this in terms of frequency  $\omega$  as well. The phonon energy  $\varepsilon$  is given by

$$\varepsilon = \hbar\omega.$$

This is a result of the phonon mode

$$\xi = e^{i\omega t} \sin k_x x \sin k_y y \sin k_z z$$

behaving as a simple harmonic oscillator. The phonon mode is simply vibration of the atoms co-ordinated in a particular way.

## The phonon distribution

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So the energy must take the form

$$E_n = \left( n + \frac{1}{2} \right) \hbar\omega.$$

Each step or quantum is  $\hbar\omega$ , which would be interpreted as a phonon particle in our statistical treatment. The relation

$$\varepsilon = \hbar\omega$$

would be justified by the fact that its predictions agree with experiments.

In terms of the frequency  $\omega$ , the phonon distribution is then given by

$$n(\omega)d\omega = \frac{g(\omega)d\omega}{\exp(\hbar\omega/k_B T) - 1}.$$

## Debye's theory for Heat capacity of solid

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The phonon distribution is given by

$$n(\omega)d\omega = \frac{g(\omega)d\omega}{\exp(\hbar\omega/k_B T) - 1}.$$

We can multiply by  $\hbar\omega$  to get the energy at this frequency interval:

$$\hbar\omega n(\omega)d\omega = \frac{g(\omega)d\omega}{\exp(\hbar\omega/k_B T) - 1}.$$

The total energy is then

$$U = \int_0^{\omega_D} \hbar\omega n(\omega)d\omega = \int_0^{\omega_D} \frac{\hbar\omega g(\omega)d\omega}{\exp(\hbar\omega/k_B T) - 1}.$$

We have found earlier that the density of states is:

$$g(\omega) = 3 \times \frac{V\omega^2}{2\pi^2 v^3}.$$

Substituting into the integral for the total energy above ...

## Debye's theory for Heat capacity of solid

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We get:

$$U = \frac{3V\hbar}{2\pi^2v^3} \int_0^{\omega_D} \frac{\omega^3 d\omega}{\exp(\hbar\omega/k_B T) - 1}$$

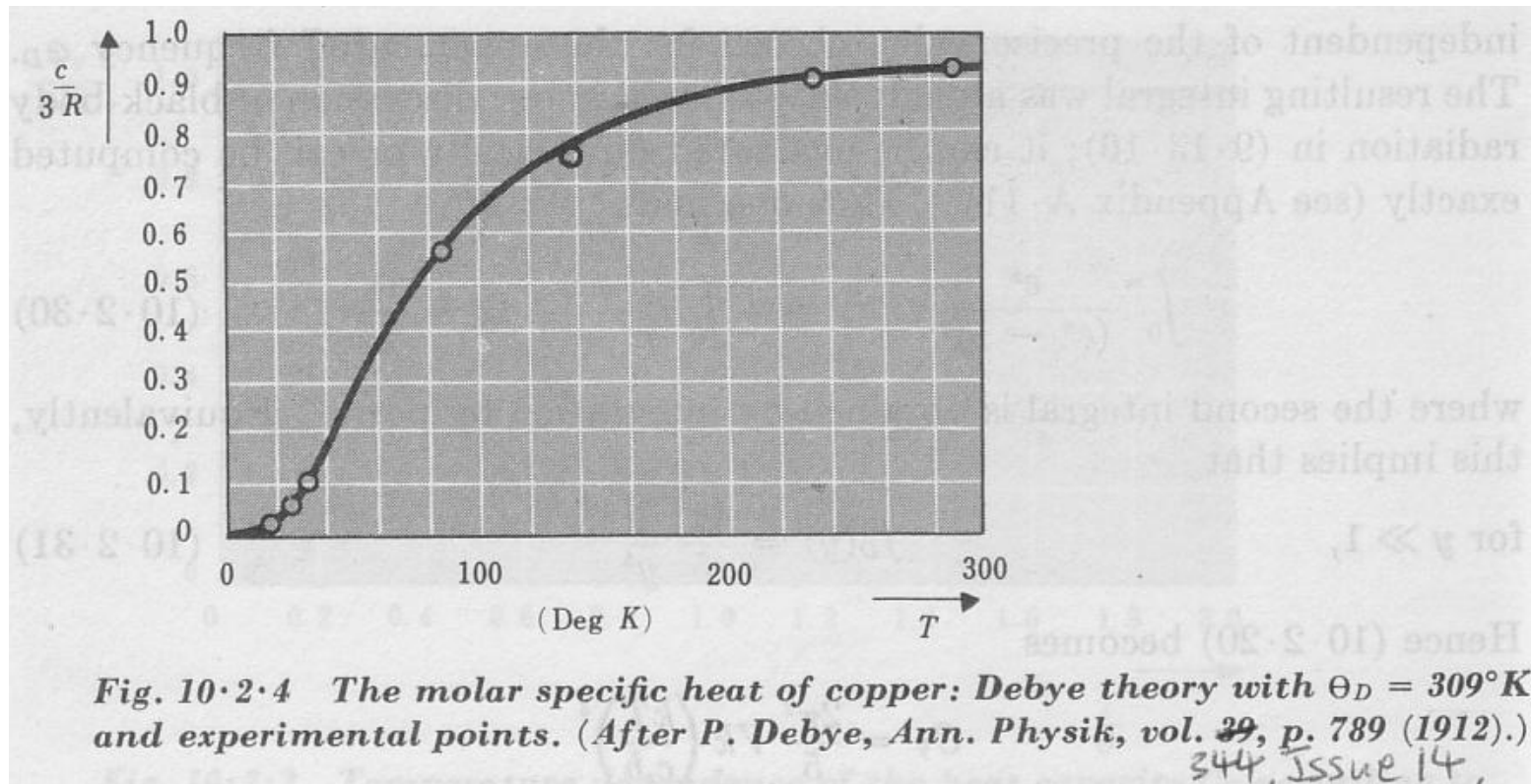
At low temperature, it can be shown that this is proportional to  $T^4$ . This would imply that the heat capacity  $C$  is proportional to  $T^3$ . (This has been mentioned in the topic on the specific heat of electrons in metal.)

At high temperatures, the heat capacity tends to  $3Nk_B$ .

Is verified at high temperature

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In 1912, Debye measured the high temperature behaviour of copper.



He showed that the heat capacity did tend to  $3Nk_B$ , as he had predicted.

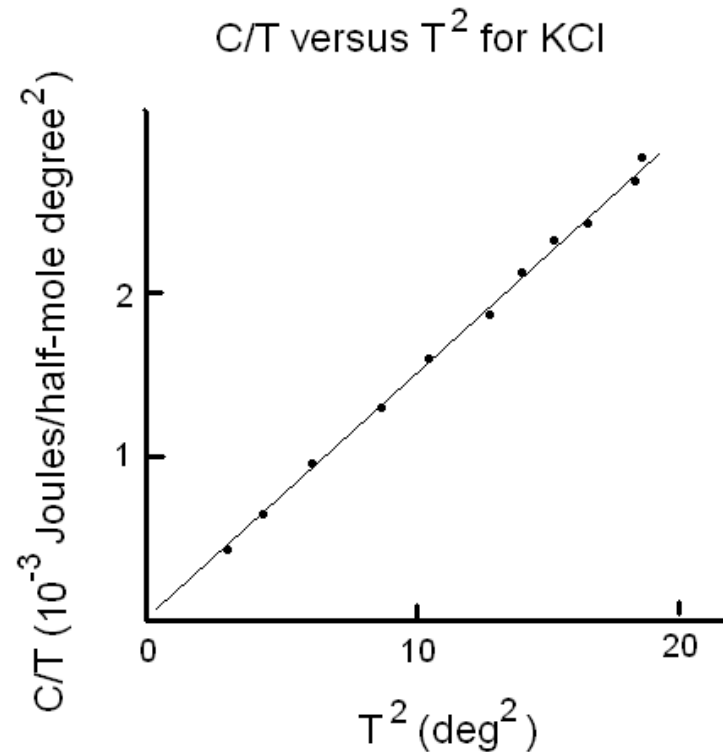
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## And verified at low temperature

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In 1953, at Purdue University, Keesom and Pearlman measured the low temperature behaviour of potassium chloride. This picture is a sketch of the results.



As predicted by Debye, the heat capacity was indeed proportional to  $T^3$ .

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# Photons

## Radiation from a very hot object

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When an object gets very hot, it can give out light.

The temperature of a volcano lava flow can be estimated by observing its color. The result agrees well with the measured temperatures of lava flows at about 1,000 to 1,200 deg C.



[http://en.wikipedia.org/wiki/Black\\_body](http://en.wikipedia.org/wiki/Black_body)

## An ideal black body

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The amount of radiation emitted depends on the nature of the object - its colour, whether it is smooth or rough, etc.

An ideal black body is one that absorbs all the radiation that falls on it.

No real material can do this. Soot is about the best, absorbing all but 3%.

In 1859 Kirchhoff had a good idea: "a small hole in the side of a large box is an excellent absorber, since any radiation that goes through the hole bounces around inside, a lot getting absorbed on each bounce, and has little chance of ever getting out again."

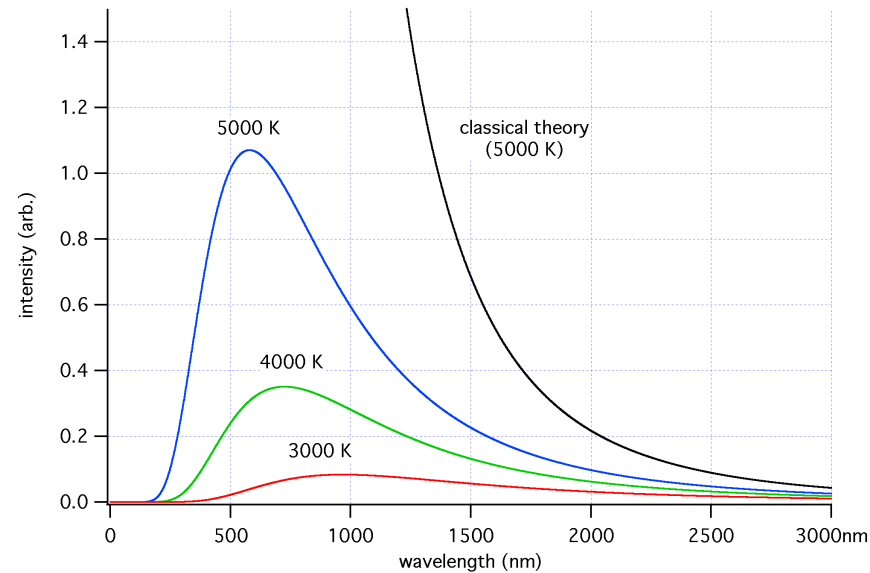
[http://galileo.phys.virginia.edu/classes/252/black\\_body\\_radiation.html](http://galileo.phys.virginia.edu/classes/252/black_body_radiation.html)

The energy of the absorbed radiation reaches equilibrium among different frequencies in the cavity. This results in a characteristic spectrum that would be emitted again through the hole.

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# Black Body Spectrum

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[http://en.wikipedia.org/wiki/Black\\_body](http://en.wikipedia.org/wiki/Black_body)

As the temperature decreases, the peak of the black-body radiation curve moves to lower intensities and longer wavelengths. The black-body radiation graph is also compared with the classical model of Rayleigh and Jeans.

## Photons in a box

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We can derive a formula for the black body radiation by considering the energies of photons in a box (like a idea black body).

This follows steps very similar to the Debye theory for phonons.

The wave equation for photons is derived from Maxwell's equation:

$$\frac{\partial^2 \mathbf{E}}{\partial x^2} + \frac{\partial^2 \mathbf{E}}{\partial y^2} + \frac{\partial^2 \mathbf{E}}{\partial z^2} = \frac{1}{c^2} \frac{\partial^2 \mathbf{E}}{\partial t^2}$$

It has the same form as the wave equation for vibration of atoms, except that the speed is now that of light instead of sound.

So we would expect that the same formula for the density of states can be used.

## Photons in a box

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Like phonons, the photon number is not fixed. We get few photons when the box is cold, and more photons when it is hot.

Unlike phonons, there is no upper limit to the frequency (no Debye frequency). The wavelength in a solid cannot be shorter than the distance between atoms. The electromagnetic wave in a box has no such limit.

Finally, phonons in a solid can have 3 polarisations: 2 transverse and 1 longitudinal (like sound). Photons can only have 2: both transverse (e.g. light).

## Counting photon states

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Recall that for phonons, the density of states is give by:

$$g(\omega)d\omega = 3 \times \frac{V\omega^2 d\omega}{2\pi^2 v^3}$$

where the factor of 3 comes from the 3 polarisations of a phonon, 2 transverse and 1 longitudinal.

Since photons only have 2 polarisations, both transverse, the 3 should be replaced by a 2:

$$g(\omega)d\omega = 2 \times \frac{V\omega^2 d\omega}{2\pi^2 c^3}$$

where the sound speed  $v$  is replaced by light speed  $c$ .



## Distribution of photon number

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Like phonons, each energy state can be occupied by any number of photons.

So it obeys Bose-Einstein statistics.

The number density is therefore given by the same formula:

$$n(\epsilon)d\epsilon = \frac{g(\epsilon)d\epsilon}{\exp(\epsilon/k_B T) - 1}$$

So the number of photons in a given frequency interval is

$$n(\omega)d\omega = 2 \times \frac{V\omega^2 d\omega}{2\pi^2 c^3} \times \frac{d\omega}{\exp(\hbar\omega/k_B T) - 1}$$

## Distribution of photon energy

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The energy of a photon is  $\hbar\omega$ . The energy in the frequency interval  $d\omega$  is then

$$\hbar\omega n(\omega)d\omega = 2 \times \hbar\omega \times \frac{V\omega^2 d\omega}{2\pi^2 c^3} \times \frac{d\omega}{\exp(\hbar\omega/k_B T) - 1}$$

The energy density is given by:

$$u(\omega) = \hbar\omega n(\omega) = \frac{V\hbar\omega^3}{\pi^2 c^3} \frac{1}{\exp(\hbar\omega/k_B T) - 1}.$$

This is essentially Planck's law for black body radiation. Integrating gives the total energy:

$$U = \frac{\pi^2 V k_B^4}{15 \hbar^3 c^3} T^4$$

It can be shown that this leads to Stefan's law of radiation:

$$\eta = \sigma T^4$$

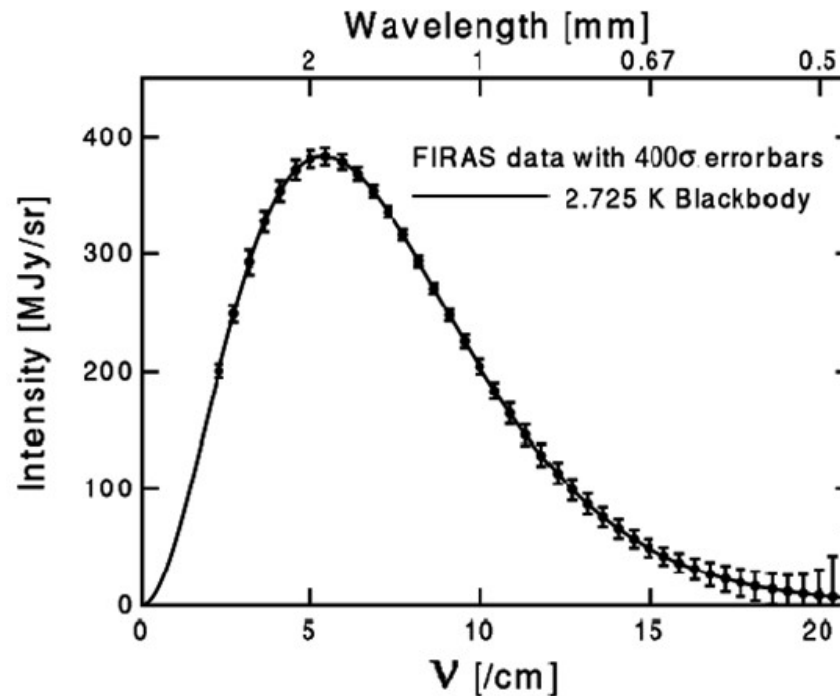
for radiation emitted by an object at a temperature  $T$ .

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## Example

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The cosmic microwave background is an example of blackbody radiation. The spectrum has been measured. Planck's radiation formula is then fitted to the spectrum.



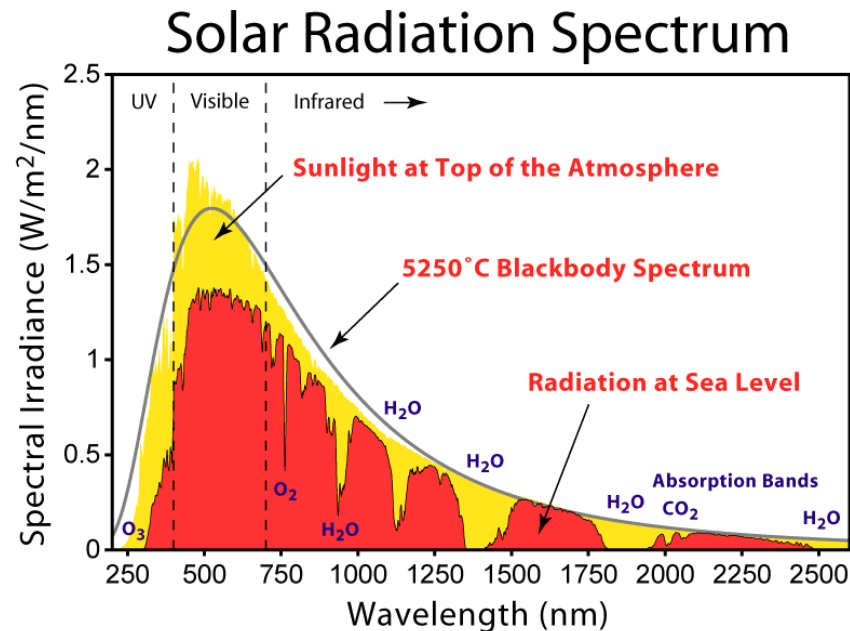
Using a temperature value of 2.74 K in the formula was found to fit the measurement well. This tells us that deep space has a temperature of 2.74 K.

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## Example

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In the same way, Planck's formula may be fitted to the sun's spectrum.



(<http://en.wikipedia.org/wiki/Sunlight>)

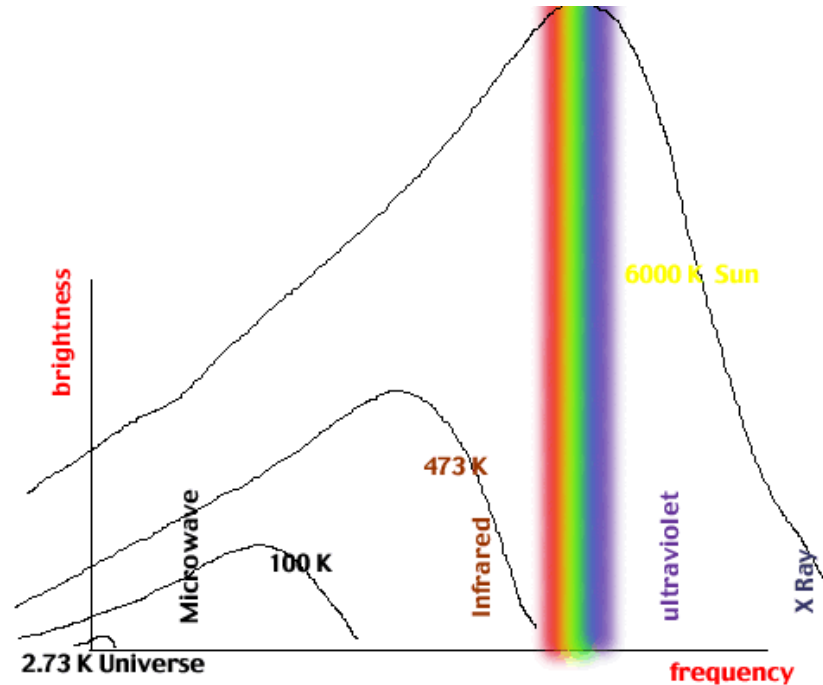
A 5800 K temperature gives a reasonable fit. However, part of the fitted curve deviates from measured data. This could be due to absorption by atmosphere, or emission from other sources.

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## Example

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The radiation spectrum of a higher temperature object peak at higher frequency.



(<http://www.launc.tased.edu.au/online/sciences/physics/blackbody1.html>)

For example, human emit radiation with the peak in the infrared wavelength  $9.3 \mu\text{m}$ . A hot plate at  $400^\circ\text{C}$  has a peak at  $4.3 \mu\text{m}$ , with a bit in visible red. That is why it looks red hot.

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## Worked Examples

### Example 1

Sketch the density of states as a function of frequency for 1, 2 and 3-D solids in the Debye approximation. Consider a 2-D solid. Show according to the Debye theory that the heat capacity varies as  $T^2$  at low temperature. In graphite it is found that  $C_V \propto T^{2.4}$  at low temperature. Explain this behaviour.

## Example

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Recall the steps leading to the density of states of a phonon in a 3-D solid. First, we obtain the quantised energy states:

$$\frac{\omega^2 a^2}{v^2 \pi^2} = n_x^2 + n_y^2 + n_z^2.$$

Then we compare with the equation for a sphere

$$R^2 = n_x^2 + n_y^2 + n_z^2$$

For positive integers  $(n_x, n_y, n_z)$ , the total number of states with frequency less than  $\omega$  is given by the octant of the sphere:

$$G(\omega) = \frac{1}{8} \left( \frac{4\pi}{3} R^3 \right) = \frac{\pi}{6} \left( \frac{\omega a}{v\pi} \right)^3$$

Differentiating, we get the density of states:

$$g(\omega) = 3 \times \frac{V \omega^2}{2\pi^2 v^3}$$

where  $V$  is the volume  $a^3$ . There is an extra factor of 3 because in 3-D, there can be 3 modes for each phonon frequency: 2 transverse and 1 longitudinal.

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## density of states for phonons

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Now we repeat the steps for 2-D. First, we obtain the quantised energy states (no  $n_z$ ):

$$\frac{\omega^2 a^2}{v^2 \pi^2} = n_x^2 + n_y^2.$$

Then we compare with the equation for a circle (not sphere)

$$R^2 = n_x^2 + n_y^2$$

For positive integers  $(n_x, n_y)$ , the total number of states with frequency less than  $\omega$  is given by the quadrant of the circle (not octant):

$$G(\omega) = \frac{1}{4}(\pi R^2) = \frac{\pi}{4} \left( \frac{\omega a}{v \pi} \right)^2$$

Differentiating, we get the density of states:

$$g(\omega) = 2 \times \frac{A\omega}{2\pi v^2}$$

where  $A$  is the area  $a^2$  (not volume). There is an extra factor of 2 because in 2-D, there can be 2 modes for each phonon frequency: 1 transverse and 1 longitudinal.

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## Example

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Finally we repeat the steps for 1-D. First, we obtain the quantised energy states (no  $n_y$ ):

$$\frac{\omega^2 a^2}{v^2 \pi^2} = n_x^2.$$

Then we compare with the equation for a line (not circle)

$$R^2 = n_x^2$$

For positive integers  $n_x$ , the total number of states with frequency less than  $\omega$  is given by half of the line (not quadrant):

$$G(\omega) = \frac{1}{2}(2R) = \frac{\omega a}{v\pi}$$

Differentiating, we get the density of states:

$$g(\omega) = 1 \times \frac{L}{\pi v}$$

where  $L$  is the length  $a$  (not area). There is no additional factor because in 1-D, there can be only be 1 mode for each phonon frequency: the longitudinal.

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## Example

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Summarising, we have obtained the following results for the density of states:

$$\begin{aligned} \text{1-D:} & \quad g(\omega) = \text{constant} \\ \text{2-D:} & \quad g(\omega) \propto \omega \\ \text{3-D:} & \quad g(\omega) \propto \omega^2 \end{aligned}$$

The internal energy is given by:

$$U = \int_0^{\omega_D} \frac{\hbar\omega g(\omega) d\omega}{\exp(\hbar\omega/k_B T) - 1}.$$

In 2-D,

$$g(\omega) \propto \omega.$$

So

$$U \propto \int_0^{\omega_D} \frac{\omega^2 d\omega}{\exp(\hbar\omega/k_B T) - 1}.$$

## Example

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We have obtained

$$U \propto \int_0^{\omega_D} \frac{\omega^2 d\omega}{\exp(\hbar\omega/k_B T) - 1}.$$

Let

$$x = \frac{\hbar\omega}{k_B T}.$$

At low temperature,  $T \rightarrow 0$  and  $x \rightarrow \infty$ . The integral for  $U$  can be written as

$$U \propto T^3 \int_0^{\infty} \frac{x^2 dx}{e^x - 1}.$$

The factor of  $T^3$  appears because of the factor of  $T$  in the substitution for  $\omega$ :

$$\omega = \frac{k_B T}{\hbar} x.$$

## Example

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Since the definite integral here

$$U \propto T^3 \int_0^\infty \frac{x^2 dx}{e^x - 1}.$$

is a constant, we have

$$U \propto T^3.$$

Differentiating, the heat capacity is

$$C_V \propto T^2.$$

Graphite has a layered structure. Each layer consists of carbon atoms strongly bonded, with weak forces between layers.

Vibration (like sound) would propagate much faster along the layer than across the layers. So it can be thought of as intermediate between 2-D and 3-D.

This explains why the heat capacity of graphite is

$$C_V \propto T^{2.4}.$$

### Example 2

According to Debye's theory, the total energy of phonons in a solid is given by

$$U = \frac{3V\hbar}{2\pi^2v^3} \int_0^{\omega_D} \frac{\omega^3 d\omega}{\exp(\hbar\omega/k_B T) - 1}.$$

Show that at low temperatures, i.e.  $T \ll \hbar\omega_D/k_B$ , Debye's theory predicts that the heat capacity of a solid is proportional to  $T^3$ .

[ You are given that

$$\int_0^{\infty} \frac{x^3}{e^x - 1} dx = \frac{\pi^4}{15}.$$

]

## Exercises

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To use the formula given, let the argument of the exponential function be  $x$ :

$$x = \frac{\hbar\omega}{k_B T}.$$

Make frequency the subject:

$$\omega = \frac{k_B T}{\hbar} x.$$

Then substitute into the integral for the energy:

$$U = \frac{3V\hbar}{2\pi^2\nu^3} \left(\frac{k_B T}{\hbar}\right)^4 \int_0^{x_D} \frac{x^3 dx}{e^x - 1}$$

where the new limit is related to the old one by the substitution formula:

$$x_D = \frac{\hbar\omega_D}{k_B T}.$$

## Example

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The condition given is  $T \ll \hbar\omega_D/k_B$ . Rearranging, we have

$$1 \ll \frac{\hbar\omega_D}{k_B T}.$$

The right hand side is just  $x_D$ , so

$$1 \ll x_D.$$

This means  $x_D$  is large. We may approximate the integral by replacing the limit by infinity:

$$U \approx \frac{3V\hbar}{2\pi^2 v^3} \left(\frac{k_B T}{\hbar}\right)^4 \int_0^\infty \frac{x^3 dx}{e^x - 1}.$$

Then using the formula given,

$$U = \frac{3V\hbar}{2\pi^2 v^3} \left(\frac{k_B T}{\hbar}\right)^4 \frac{\pi^4}{15}.$$



## Example

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We have found the total energy.

$$U = \frac{V\pi^2 k_B^4 T^4}{10\hbar^3 v^3}$$

Note that this is proportional to  $T^4$ . To get the heat capacity, we differentiate with respect to temperature  $T$ :

$$C = \frac{2V\pi^2 k_B^4 T^3}{5\hbar^3 v^3}$$

which is proportional to  $T^3$ .

This answers the question.

## Example

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Some remarks:

Going back to our approximation, how large must  $x_D$  be for the approximation

$$\int_0^{x_D} \frac{x^3 dx}{e^x - 1} \approx \int_0^{\infty} \frac{x^3 dx}{e^x - 1}$$

to be valid? We can get some idea if we carry out the integration numerically:

$x_D$	$\int \frac{x^3 dx}{e^x - 1}$	error
1	0.225	96%
10	6.432	1%
100	6.494	$10^{-18}$
$\infty$	$\pi^4/15$	0

As long as  $x_D$  is more than 10, the approximation would be better than 1%.

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## Example

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Recall that  $x_D$  is related to the Debye frequency by

$$x_D = \frac{\hbar\omega_D}{k_B T},$$

This means that for 1% accuracy, we should have

$$\frac{\hbar\omega_D}{k_B T} > 10.$$

Rearranging, we get

$$T < \frac{\theta_D}{10}$$

where

$$\theta_D = \frac{\hbar\omega_D}{k_B}.$$

$\theta_D$  is called the Debye temperature, and can be used as a reference when we want to tell whether a temperature is high or low. Note that in the numerator is  $\hbar\omega_D$ , which is the highest possible phonon energy.

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### Example 3

The energy distribution of a gas of photons in a box given by:

$$u(\omega)d\omega = \frac{V\hbar}{\pi^2c^3}d\omega \frac{\omega^3}{\exp(\hbar\omega/k_B T) - 1}.$$

Wien's displacement law for black body radiation is given by

$$\lambda_{\max} = \frac{b}{T},$$

where  $\lambda_{\max}$  is the wavelength of the peak of the radiation intensity, and  $b$  is  $2.90 \times 10^{-3}$  m.K.

Derive Wien's displacement law from the energy distribution.

## Example

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We must rewrite the distribution in terms of wavelength  $\lambda$ :

$$\omega = 2\pi f = 2\pi \frac{c}{\lambda}$$

Differentiating,

$$d\omega = -\frac{2\pi c}{\lambda^2} d\lambda.$$

Substituting into the energy distribution:

$$u(\lambda)d\lambda = \frac{Vh}{\pi^2 c^2 \lambda^5} \frac{d\lambda}{\exp(hc/\lambda k_B T) - 1}.$$

To find the maximum, we can ignore the constants in  $u(\omega)$  and just focus on the part that depends on  $\omega$ :

$$\frac{1}{\lambda^5} \frac{1}{\exp(hc/\lambda k_B T) - 1}.$$

To find the maximum, differentiate this ...

## Example

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and set to zero:

$$-\frac{5}{\lambda^6} \frac{1}{\exp(hc/\lambda k_B T) - 1} - \frac{1}{\lambda^5} \frac{(-hc/\lambda^2 k_B T) \exp(hc/\lambda k_B T)}{[\exp(hc/\lambda k_B T) - 1]^2} = 0.$$

Multiplying by  $\lambda^6 [\exp(hc/\lambda k_B T) - 1]^2$ ,

$$-5[\exp(hc/\lambda k_B T) - 1] + \frac{hc}{\lambda k_B T} \exp(hc/\lambda k_B T) = 0.$$

We can simplify this by defining

$$x = \frac{hc}{\lambda k_B T}.$$

Substituting, we get

$$-5(e^x - 1) + xe^x = 0.$$

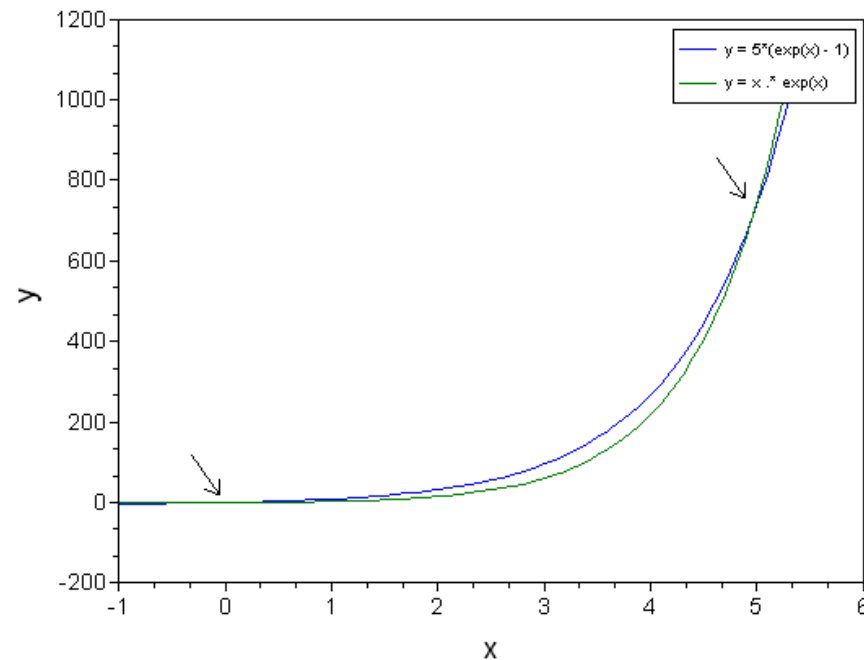
## Example

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If we plot each side of the equation,

$$5(e^x - 1) = xe^x.$$

we see that there are 2 solutions.



We can solve this numerically. The answers are

$$x_1 = 0 \quad \text{and} \quad x_2 = 4.965.$$

## Example

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The nontrivial solution is

$$x_2 = 4.965.$$

Substituting this into the definition for  $x$ ,

$$x = \frac{\hbar}{\lambda k_B T}.$$

or making  $\lambda$  the subject, we get

$$\lambda = \frac{hc}{x_2 k_B T}.$$

Comparing this with the displacement law,

$$\lambda_{\max} = \frac{b}{T},$$

we see that

$$b = \frac{hc}{x_2 k_B}.$$

Substituting the constants and calculating, we get the Wien's displacement constant  $2.90 \times 10^{-3}$  m.K.

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## Useful Integrals

## Useful Integrals

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For Debye model, to find heat capacity at low temperature;  
and for black body radiation, to find Stefan's law:

$$\int_0^{\infty} \frac{x^3}{e^x - 1} dx = \frac{\pi^4}{15}.$$

For liquid helium-4, later in the course:-

to find condensation temperature of Bose Einstein condensate:

$$\int_0^{\infty} \frac{x^{1/2}}{e^x - 1} dx = 2.315$$

to the find heat capacity:

$$\int_0^{\infty} \frac{x^{3/2}}{e^x - 1} dx = 1.783$$