Notes on Selected topics to accompany Sakurai's "Modern Quantum Mechanics"

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Wien's displacement law

Wien's displacement law is an empirical law given by

$$\lambda_{\rm max} T \approx 2.9 \times 10^{-3} mK.$$

This law can be derived from the Planck's law of radiation. Let us start with

$$u(\lambda, T) = \frac{8\pi hc}{\lambda^5} \frac{1}{e^{hc/\lambda k_{\rm B} T} - 1}.$$

The wavelength corresponding to maximum energy density is obtained by solving the equation

$$\begin{aligned}
\frac{du(\lambda,T)}{d\lambda} &= 0 \\
\Rightarrow \frac{d}{d\lambda}\left(\frac{8\pi hc}{\lambda^5}\frac{1}{e^{hc/\lambda k_{\rm B}T}-1}\right) &= 0 \\
\Rightarrow 8\pi hc \frac{d}{d\lambda}\left(\frac{1}{\lambda^5}\frac{1}{e^{hc/\lambda k_{\rm B}T}-1}\right) &= 0 \\
\Rightarrow \left[\frac{1}{\lambda^5}\left\{-\frac{1}{\left(e^{hc/\lambda k_{\rm B}T}-1\right)^2} e^{hc/\lambda k_{\rm B}T}\left(-\frac{hc}{\lambda^2 k_{\rm B}T}\right)\right\} + \frac{1}{e^{hc/\lambda k_{\rm B}T}-1}\left(-\frac{5}{\lambda^6}\right)\right] &= 0 \\
\Rightarrow \left[\frac{hc}{\lambda^7 k_{\rm B}T}\frac{e^{hc/\lambda k_{\rm B}T}}{\left(e^{hc/\lambda k_{\rm B}T}-1\right)^2} - \left(\frac{5}{\lambda^6}\right)\frac{1}{e^{hc/\lambda k_{\rm B}T}-1}\right] &= 0 \\
\Rightarrow \frac{hc}{\lambda k_{\rm B}T}\frac{e^{hc/\lambda k_{\rm B}T}}{e^{hc/\lambda k_{\rm B}T}-1} - 5 &= 0
\end{aligned}$$

We can substitute the variable

$$x = \frac{hc}{\lambda k_{\rm B} T}$$

to get

$$\begin{aligned}
x\frac{e^x}{e^x-1} - 5 &= 0 \\
\Rightarrow xe^x - 5e^x + 5 &= 0
\end{aligned}$$

which is a transcendental equation. In the following, we will see how to solve this equation

1. graphically
2. numerically, and
3. analytically using the Lambert-W technique

Graphical Solution

A first approximation for the solution of $xe^x - 5e^x + 5 = 0$ can be obtained by simply listing the values of the function $f(x) = xe^x - 5e^x + 5$ for various values of x.

x	$f(x)$
-5.00	4.93
-4.00	4.84
-3.00	4.60
-2.00	4.05
-1.00	2.79
0.00	0.00
1.00	-5.87
2.00	-17.17
3.00	-35.17
4.00	-49.60
5.00	5.00

Table 1: Tabulation of x and $f(x) = xe^x - 5e^x + 5$.

From Table 1 one notes a trivial solution of $x = 0$ at which $f(x) = 0$ and a non-trivial solution in the range 4 to 5 where $f(x)$ changes sign. A more accurate value of the solution can be estimated graphically as shown in Fig. 1 where one clearly notes that $f(5) \approx 0$.

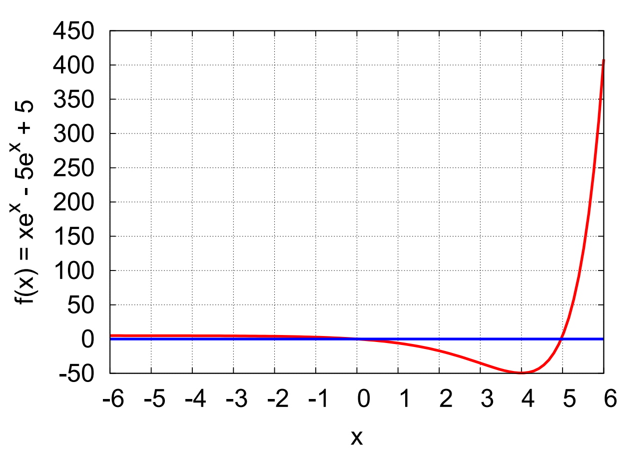

Figure 1: Graphical solution of $xe^x - 5e^x + 5 = 0$.

Method of Iteration

In the method of iteration, an equation is rearranged to the form $x = f(x)$. Starting with an initial value x_0 a better approximation of the solution x_1 is given by $f(x_0)$.

$$x_{i+1} = f(x_i).$$

The equation to be solved is

$$\begin{aligned} e^x(x-5)+5 &= 0 \\ \Rightarrow e^x(x-5) &= -5 \\ \Rightarrow (x-5) &= -5e^{-x} \\ \Rightarrow x &= 5+-5e^{-x} = f(x). \end{aligned}$$

We can start with the initial guess $x_0 = 4.0$, and compute the exact root in a few iterations. The convergence towards the exact root of $x = 4.965$ is shown the following table.

iter.	x_i	$x_{i+1} = f(x_i)$
0	4.00000000	4.90842181
1	4.90842181	4.96307934
2	4.96307934	4.96504317
3	4.96504317	4.96511175
4	4.96511175	4.96511415
5	4.96511415	4.96511423
6	4.96511423	4.96511423

Table 2: Iterative solution of $xe^x - 5e^x + 5 = 0$ or $x = 5 + -5e^{-x}$.

Analytic solution using the Lambert W function

The solution of the transcendental equation $Y = Xe^X$ can be written as the Lambert W function

$$X = W(Y) = \sum_{i=1}^{\infty} \frac{(-1)^{i-1} i^{i-2}}{(i-1)!} Y^i.$$

For the first few terms, the series is given by

$$W(Y) = Y - Y^2 + \frac{3}{2}Y^3 - \frac{8}{3}Y^4 \ldots$$

If $|Y| \geq 0.34$, the series oscillates between large positive and negative values. Now we have to rearrange the original equation to be solved to arrive at the form $Y = Xe^X$.

$$\begin{aligned} (x-5)e^x+5 &= 0 \\ \Rightarrow (x-5)e^x &= -5 \\ \Rightarrow (x-5)e^{(x-5)} &= -5e^{-5} \\ \Rightarrow Xe^X &= Y \end{aligned}$$

From which we get

$$\begin{aligned} x - 5 &= W(-5e^{-5}) \\ x &= W(-5e^{-5}) + 5. \end{aligned}$$

i	x
1	4.96631027
2	4.96517527
3	4.96511791
4	4.96511447
5	4.96511425
6	4.96511423
7	4.96511423

Table 3: Analytic solution of $xe^x - 5e^x + 5 = 0$ using Lambert W Function.

The value of $|Y|$ here is 0.033690. So the Lambert series will not oscillate and will converge monotonously to the exact root. The convergence as a function of number of terms in the Lambert series is shown in the following table. From Table 3 one notes that an accuracy up to 3 decimal places can be reached using the simple approximate expression of $W(x) = x - x^2$ where $x = -5e^{-5}$

$$\begin{aligned} x &\approx W^{\text{first two terms}}(-5e^{-5}) + 5 \\ &= (-5e^{-5}) - (-5e^{-5})^2 + 5 \\ &= 4.96517527 \end{aligned}$$

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