MATHCHAPTER D

Series and Limits

Frequently, we need to investigate the behavior of an equation for small values (or perhaps large values) of one of the variables in the equation. For example, in Chapter 1 we derived the low-frequency behavior of the Planck blackbody distribution law (Equation 1.2):

$$\rho_\nu(T)d\nu = \frac{8\pi h}{c^3}\frac{\nu^3 d\nu}{e^{\beta h\nu} - 1} \tag{D.1}$$

To do this, we used the fact that e^x can be written as the infinite series (i.e., a series containing an unending number of terms)

$$e^x = \sum_{n=0}^{\infty}\frac{x^n}{n!} = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots \tag{D.2}$$

and then realized if x is small, then x^2, x^3, etc., are even smaller. We can express this result by writing

$$e^x = 1 + x + O(x^2)$$

where $O(x^2)$ is a bookkeeping device that reminds us we are neglecting terms involving x^2 and higher powers of x. If we apply this result to Equation D.1, we have

$$\begin{aligned}
\rho_\nu(T)d\nu &= \frac{8\pi h}{c^3}\frac{\nu^3 d\nu}{1 + \beta h\nu + O[(\beta h\nu)^2] - 1} \\
&\approx \frac{8\pi h}{c^3}\frac{\nu^3 d\nu}{\beta h\nu} \\
&= \frac{8\pi k_B T}{c^3}\nu^2 d\nu
\end{aligned}$$

Thus, we see that $\rho_\nu(T)$ goes as ν^2 for small values of ν. In this MathChapter, we will review some useful series and apply them to some physical problems.

One of the most useful series we will use is the geometric series:

$$\frac{1}{1-x} = \sum_{n=0}^{\infty} x^n = 1 + x + x^2 + x^3 + \cdots \qquad |x| < 1 \tag{D.3}$$

This result can be derived by algebraically dividing 1 by $1 - x$, or by the following trick. Consider the finite series (i.e., a series with a finite number of terms)

$$S_N = 1 + x + x^2 + \cdots + x^N$$

Now multiply S_N by x:

$$xS_N = x + x^2 + \cdots + x^{N+1}$$

Now notice that

$$S_N - xS_N = 1 - x^{N+1}$$

or that

$$S_N = \frac{1 - x^{N+1}}{1 - x} \tag{D.4}$$

If $|x| < 1$, then $x^{N+1} \to 0$ as $N \to \infty$, so we recover Equation D.3.

Recovering Equation D.3 from Equation D.4 brings us to an important point regarding infinite series: Equation D.3 is valid only if $|x| < 1$. It makes no sense at all if $|x| \geq 1$. We say that the infinite series in Equation D.3 converges for $|x| < 1$ and diverges for $|x| \geq 1$. How can we tell whether a given infinite series converges or diverges? There are a number of so-called convergence tests, but one simple and useful one is the *ratio test*. To apply the ratio test, we form the ratio of the $(n + 1)$th term, u_{n+1}, to the nth term, u_n, and then let n become very large:

$$r = \lim_{n\to\infty} \left| \frac{u_{n+1}}{u_n} \right| \tag{D.5}$$

If $r < 1$, the series converges; if $r > 1$, the series diverges; and if $r = 1$, the test is inconclusive. Let's apply this test to the geometric series (Equation D.3):

$$r = \lim_{n\to\infty} \left| \frac{x^{n+1}}{x^n} \right| = |x|$$

Thus, we see that the series converges if $|x| < 1$ and diverges if $|x| > 1$. It actually diverges at $x = 1$, but the ratio test does not tell us that. We would have to use a more sophisticated convergence test to determine the behavior at $x = 1$.

For the exponential series (Equation D.2), we have

$$r = \lim_{n\to\infty}\left|\frac{x^{n+1}/(n+1)!}{x^n/n!}\right| = \lim_{n\to\infty}\left|\frac{x}{n+1}\right|$$

Thus, we conclude that the exponential series converges for all values of x.

In Chapter 5, we encounter the summation

$$S = \sum_{n=0}^{\infty} e^{-nh\nu/k_{\mathrm{B}}T} \tag{D.6}$$

where ν represents the vibrational frequency of a diatomic molecule and the other symbols have their usual meanings. We can sum this series by letting

$$x = e^{-h\nu/k_{\mathrm{B}}T}$$

in which case we have

$$S = \sum_{n=0}^{\infty} x^n \qquad |x| < 1$$

According to Equation D.3, $S = 1/(1-x)$, or

$$S = \frac{1}{1 - e^{-h\nu/k_{\mathrm{B}}T}} \tag{D.7}$$

We say that S has been evaluated in closed form because its numerical evaluation requires only a finite number of steps, in contrast to Equation D.6, which would require an infinite number of steps.

A practical question that arises is how we find the infinite series that corresponds to a given function. For example, how do we derive Equation D.2? First, assume that the function $f(x)$ can be expressed as a power series (i.e., a series in powers of x):

$$f(x) = c_0 + c_1x + c_2x^2 + c_3x^3 + \cdots$$

where the c_j are to be determined. Then let $x = 0$ and find that $c_0 = f(0)$. Now differentiate once with respect to x,

$$\frac{df}{dx} = c_1 + 2c_2x + 3c_3x_2 + \cdots$$

and let $x = 0$ to find that $c_1 = (df/dx)_{x=0}$. Differentiate again,

$$\frac{d^2f}{dx^2} = 2c_2 + 3\cdot 2c_3x + \cdots$$

and let $x = 0$ to get $c_2 = (d^2 f/dx^2)_{x=0}/2$. Differentiate once more,

$$\frac{d^3 f}{dx^3} = 3 \cdot 2c_3 + 4 \cdot 3 \cdot 2x + \cdots$$

and let $x = 0$ to get $c_3 = (d^3 f/dx^3)_{x=0}/3!$. The general result is

$$c_n = \frac{1}{n!}\left(\frac{d^n f}{dx^n}\right)_{x=0} \tag{D.8}$$

so we can write

$$f(x) = f(0) + \left(\frac{df}{dx}\right)_{x=0} x + \frac{1}{2!}\left(\frac{d^2 f}{dx^2}\right)_{x=0} x^2 + \frac{1}{3!}\left(\frac{d^3 f}{dx^3}\right)_{x=0} x^3 + \cdots \tag{D.9}$$

Equation D.9 is called the Maclaurin series of $f(x)$. If we apply Equation D.9 to $f(x) = e^x$, we find that

$$\left(\frac{d^n e^x}{dx^n}\right)_{x=0} = 1$$

so

$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots$$

Some other important Maclaurin series, which can be obtained from a straightforward application of Equation D.9 (Problem D–13) are

$$\sin x = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + \cdots \tag{D.10}$$

$$\cos x = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \frac{x^6}{6!} + \cdots \tag{D.11}$$

$$\ln(1 + x) = x - \frac{x^2}{2} + \frac{x^3}{3} - \frac{x^4}{4} + \cdots \qquad -1 < x \leq 1 \tag{D.12}$$

and

$$(1 + x)^n = 1 + nx + \frac{n(n-1)}{2!}x^2 + \frac{n(n-1)(n-2)}{3!}x^3 + \cdots \qquad x^2 < 1 \tag{D.13}$$

Series D.10 and D.11 converge for all values of x, but as indicated, Series D.12 converges only for $-1 < x \leq 1$ and Series D.13 converges only for $x^2 < 1$. Note that if n is a positive integer in Series D.13, the series truncates. For example, if $n = 2$ or 3, we have

$$(1 + x)^2 = 1 + 2x + x^2$$

and

$$(1+x)^3 = 1 + 3x + 3x^2 + x^3$$

Equation D.13 for a positive integer is called the binomial expansion. If n is not a positive integer, the series continues indefinitely, and Equation D.13 is called the binomial series. For example,

$$(1+x)^{1/2} = 1 + \frac{x}{2} - \frac{1}{8}x^2 + O(x^3) \tag{D.14}$$

$$(1+x)^{-1/2} = 1 - \frac{x}{2} + \frac{3}{8}x^2 + O(x^3) \tag{D.15}$$

Any handbook of mathematical tables will have the Maclaurin series for many functions. Problem D–20 discusses a Taylor series, which is an extension of a Maclaurin series.

We can use the series presented here to derive a number of results used throughout the book. For example, the limit

$$\lim_{x\to 0} \frac{\sin x}{x}$$

occurs several times. Because this limit gives 0/0, we could use l'Hôpital's rule, which tells us that

$$\lim_{x\to 0} \frac{\sin x}{x} = \lim_{x\to 0} \frac{\dfrac{d \sin x}{dx}}{\dfrac{dx}{dx}} = \lim_{x\to 0} \cos x = 1$$

We could derive the same result by dividing Equation D.10 by x and then letting $x \to 0$. (These two methods are really equivalent. See Problem D–21.)

We will do one final example involving series and limits. Einstein's theory of the temperature dependence of the molar heat capacity of a crystal is given by

$$\overline{C}_V = 3R\left(\frac{\Theta_E}{T}\right)^2 \frac{e^{-\Theta_E/T}}{(1-e^{-\Theta_E/T})^2} \tag{D.16}$$

where R is the molar gas constant and Θ_E is a constant, called the Einstein constant, that is characteristic of the solid (cf. Section 1.4). We'll now show that this equation gives the Dulong and Petit limit ($\overline{C}_V \to 3R$) at high temperatures. First let $x = \Theta_E/T$ in Equation D.16 to obtain

$$\overline{C}_V = 3Rx^2 \frac{e^{-x}}{(1-e^{-x})^2} \tag{D.17}$$

When T is large, x is small, and so we shall use

$$e^{-x} = 1 - x + O(x^2)$$

Equation D.17 becomes

$$\overline{C}_V = 3Rx^2 \frac{1 - x + O(x^2)}{(x + O(x^2))^2} \longrightarrow 3R$$

as $x \to 0$ ($T \to \infty$). This result is called the law of Dulong and Petit; the molar heat capacity of a crystal becomes $3R = 24.9\ \mathrm{J \cdot K^{-1} \cdot mol^{-1}}$ for a monatomic crystal at high temperatures. By "high temperatures" we actually mean that $T \gg \Theta_E$, which for many substances is less than 1000 K.

Problems

D–1. Calculate the percentage difference between e^x and $1 + x$ for $x = 0.0050, 0.0100, 0.0150, \ldots, 0.1000$.

D–2. Calculate the percentage difference between $\ln(1 + x)$ and x for $x = 0.0050, 0.0100, 0.0150, \ldots, 0.1000$.

D–3. Write out the expansion of $(1 + x)^{1/2}$ through the quadratic term.

D–4. Write out the expansion of $(1 + x)^{-1/2}$ through the quadratic term.

D–5. Show that

$$\frac{1}{(1 - x)^2} = 1 + 2x + 3x^2 + 4x^3 + \cdots$$

D–6. Evaluate the series

$$S = \frac{1}{2} + \frac{1}{4} + \frac{1}{8} + \frac{1}{16} + \cdots$$

D–7. Evaluate the series

$$S = \sum_{n=0}^{\infty} \frac{1}{3^n}$$

D–8. Evaluate the series

$$S = \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{2^n}$$

D–9. Numbers whose decimal formula are recurring decimals such as 0.272 727 . . . are rational numbers, meaning that they can be expressed as the ratio of two numbers (in other words, as a fraction). Show that $0.272\,727\ldots = 27/99$.

D–10. Show that 0.142 857 142 857 142 857 . . . = 1/7. (See the previous problem.)

D–11. Series of the form

$$S(x) = \sum_{n=0}^{\infty} n x^n$$

occur frequently in physical problems. To find a closed expression for $S(x)$, we start with

$$\frac{1}{1-x} = \sum_{n=0}^{\infty} x^n$$

Notice now that $S(x)$ can be expressed as

$$x \frac{d}{dx} \sum_{n=0}^{\infty} x^n = \sum_{n=0}^{\infty} n x^n$$

and show that $S(x) = x/(1-x)^2$.

D–12. Using the method introduced in the previous problem, show that

$$S(x) = \sum_{n=0}^{\infty} n^2 x^n = \frac{x(1+x)}{(1-x)^3}$$

D–13. Use Equation D.9 to derive Equations D.10 and D.11.

D–14. Show that Equations D.2, D.10, and D.11 are consistent with the relation $e^{ix} = \cos x + i \sin x$.

D–15. Use Equation D.2 and the definitions

$$\sinh x = \frac{e^x - e^{-x}}{2} \qquad \text{and} \qquad \cosh x = \frac{e^x + e^{-x}}{2}$$

to show that

$$\sinh x = x + \frac{x^3}{3!} + \frac{x^5}{5!} + \cdots$$

$$\cosh x = 1 + \frac{x^2}{2!} + \frac{x^4}{4!} + \cdots$$

D–16. Show that Equations D.10 and D.11 and the results of the previous problem are consistent with the relations

$$\sin ix = i \sinh x \qquad \cos ix = \cosh x$$

$$\sinh ix = i \sin x \qquad \cosh ix = \cos x$$

D–17. Evaluate the limit of

$$f(x) = \frac{e^{-x}\sin^2 x}{x^2}$$

as $x \to 0$.

D–18. Evaluate the integral

$$I = \int_0^a x^2 e^{-x}\cos^2 x dx$$

for small values of a by expanding I in powers of a through quadratic terms.

D–19. Prove that the series for $\sin x$ converges for all values of x.

D–20. A Maclaurin series is an expansion about the point $x = 0$. A series of the form

$$f(x) = c_0 + c_1(x - x_0) + c_2(x - x_0)^2 + \cdots$$

is an expansion about the point x_0 and is called a Taylor series. First show that $c_0 = f(x_0)$. Now differentiate both sides of the above expansion with respect to x and then let $x = x_0$ to show that $c_1 = (df/dx)_{x=x_0}$. Now show that

$$c_n = \frac{1}{n!}\left(\frac{d^n f}{dx^n}\right)_{x=x_0}$$

and so

$$f(x) = f(x_0) + \left(\frac{df}{dx}\right)_{x=x_0}(x - x_0) + \frac{1}{2}\left(\frac{d^2 f}{dx^2}\right)_{x=x_0}(x - x_0)^2 + \cdots$$

D–21. Show that l'Hôpital's rule amounts to forming a Taylor expansion of both the numerator and the denominator. Evaluate the limit

$$\lim_{x\to 0}\frac{\ln(1+x) - x}{x^2}$$

both ways.

D–22. Start with

$$\frac{1}{1-x} = 1 + x + x^2 + \cdots$$

Now let $x = 1/x$ to write

$$\frac{1}{1-\dfrac{1}{x}} = \frac{x}{x-1} = 1 + \frac{1}{x} + \frac{1}{x^2} + \cdots$$

Now add these two expressions to get

$$1 = \cdots + \frac{1}{x^2} + \frac{1}{x} + 2 + x + x^2 + \cdots$$

Does this make sense? What went wrong?

D–23. The energy of a quantum-mechanical harmonic oscillator is given by $\varepsilon_n = (n + \frac{1}{2})h\nu$, $n = 0, 1, 2, \ldots$, where h is the Planck constant and ν is the fundamental frequency of the oscillator. The average vibrational energy of a harmonic oscillator in an ideal gas is given by

$$\varepsilon_{\text{vib}} = (1 - e^{-h\nu/k_\text{B}T}) \sum_{n=0}^{\infty} \varepsilon_n e^{-nh\nu/k_\text{B}T}$$

where k_B is the Boltzmann constant and T is the kelvin temperature. Show that

$$\varepsilon_{\text{vib}} = \frac{h\nu}{2} + \frac{h\nu e^{-h\nu/k_\text{B}T}}{1 - e^{-h\nu/k_\text{B}T}}$$