Exercise 12

The purpose of this exercise is to calculate $Q(x,t)$ approximately for large $t$. Recall that $Q(x,t)$ is the temperature of an infinite rod that is initially at temperature 1 for $x > 0$, and 0 for $x < 0$.

(a) Express $Q(x,t)$ in terms of $\text{erf}$.

(b) Find the Taylor series of $\text{erf}(x)$ around $x = 0$. (**Hint**: Expand $e^z$, substitute $z = -y^2$, and integrate term by term.)

(c) Use the first two nonzero terms in this Taylor expansion to find an approximate formula for $Q(x,t)$.

(d) Why is this formula a good approximation for $x$ fixed and $t$ large?

Solution

Part (a)

The initial value problem for $Q(x,t)$ is

$$Q_t = kQ_{xx}, \quad Q(x,0) = H(x) = \begin{cases} 1 & x > 0 \\ 0 & x < 0 \end{cases}. \quad (1)$$

To solve (1) we will use the similarity method. Since the Heaviside function $H(x)$ is dimensionless, $Q$ is dimensionless as well. Hence, the variables $x$ (meters), $t$ (seconds), and $k$ (meters$^2$/second) have to appear in the solution as a dimensionless combination. The combination variable $\eta$ is thus

$$\frac{x^2}{kt}$$

or any convenient multiple or power thereof. Choose

$$\eta = \frac{x}{\sqrt{4kt}}$$

to make the process of obtaining the final answer smoother. Hence,

$$Q = Q(\eta),$$

Write expressions for $Q_t$ and $Q_{xx}$ in terms of this new variable using the chain rule.

$$\frac{\partial Q}{\partial t} = \frac{dQ}{d\eta} \frac{\partial \eta}{\partial t} = \frac{dQ}{d\eta} \left( -\frac{x}{4\sqrt{kt^3}} \right)$$

$$\frac{\partial Q}{\partial x} = \frac{dQ}{d\eta} \frac{\partial \eta}{\partial x} = \frac{dQ}{d\eta} \left( \frac{1}{\sqrt{kt}} \right)$$

$$\frac{\partial^2 Q}{\partial x^2} = \frac{\partial}{\partial x} \left( \frac{\partial Q}{\partial x} \right) = \frac{\partial \eta}{\partial x} \frac{\partial Q}{\partial \eta} \left( \frac{\partial Q}{\partial x} \right) = \frac{d^2Q}{d\eta^2} \left( \frac{1}{4kt} \right)$$

Substituting these expressions into the diffusion equation gives

$$\frac{dQ}{d\eta} \left( -\frac{x}{4\sqrt{kt^3}} \right) = k \frac{d^2Q}{d\eta^2} \left( \frac{1}{4kt} \right).$$
Cancel common terms and bring all terms to one side.

\[ Q'' + \frac{x}{\sqrt{kt}}Q' = 0 \]

Use the combination variable \( \eta \).

\[ Q'' + 2\eta Q' = 0 \]

Make the substitution \( r = Q' = \frac{dQ}{d\eta} \).

\[ \frac{dr}{d\eta} + 2\eta r = 0 \]

This is a first-order differential equation that we can solve by separation of variables.

\[ \frac{dr}{r} = -2\eta d\eta \]

Integrate both sides.

\[ \ln |r| = -\eta^2 + C \]

Exponentiate both sides.

\[ |r| = e^{-\eta^2+C} \]

\[ r = \pm e^C e^{-\eta^2} \]

\[ r = C_1 e^{-\eta^2} \]

Now that we have \( r \), we can get \( Q \) by integrating the result.

\[ Q(\eta) = \int_0^\eta r \, ds + C_2 = \int_0^\eta C_1 e^{-s^2} \, ds + C_2 \]

The lower limit, 0, is arbitrary; choosing a different value leads to a different value for \( C_2 \). To evaluate the constants of integration, we look to the initial condition, \( Q(x, 0) = H(x) \). For \( x > 0 \), as \( t \to 0, \eta \to +\infty \). Conversely, for \( x < 0 \), as \( t \to 0, \eta \to -\infty \). Thus,

For \( x > 0 \):

\[ 1 = C_1 \int_0^\infty e^{-s^2} \, ds + C_2 \]

For \( x < 0 \):

\[ 0 = C_1 \int_0^{-\infty} e^{-s^2} \, ds + C_2 \]

The system of equations to solve is

\[ 1 = C_1 \cdot \frac{\sqrt{\pi}}{2} + C_2 \]

\[ 0 = -C_1 \cdot \frac{\sqrt{\pi}}{2} + C_2. \]

Solving it yields

\[ C_1 = \frac{1}{\sqrt{\pi}} \quad \text{and} \quad C_2 = \frac{1}{2}. \]

The solution is thus

\[ Q(\eta) = \frac{1}{\sqrt{\pi}} \int_0^\eta e^{-s^2} \, ds + \frac{1}{2} \operatorname{erf}(\eta) + \frac{1}{2} = \frac{1}{2} \operatorname{erf}(\eta) + 1. \]

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Figure 1: Plot of the dimensionless temperature $Q(x,t)$ with $k = 1 \text{ m}^2/\text{s}$ for six different times: $t = 0 \text{ s}$ (red), $t = 1 \text{ s}$ (orange), $t = 2 \text{ s}$ (yellow), $t = 5 \text{ s}$ (green), $t = 10 \text{ s}$ (blue), and $t = 20 \text{ s}$ (purple).

In terms of the original variables it is

$$Q(x,t) = \frac{1}{2} \left[ \text{erf} \left( \frac{x}{\sqrt{4kt}} \right) + 1 \right]. \quad (2)$$

**Part (b)**

Following the hint, we will write the Taylor series of $e^z$ about $z = 0$ (also known as the Maclaurin series), substitute $z = -y^2$, and then integrate the series term by term.

$$e^z = \sum_{n=0}^{\infty} \frac{z^n}{n!}$$

Now make the substitution.

$$e^{-y^2} = \sum_{n=0}^{\infty} \frac{(-y^2)^n}{n!} = \sum_{n=0}^{\infty} \frac{(-1)^n y^{2n}}{n!}$$

With this series in hand, we can now write the Taylor series expansion of $\text{erf} \ x$ about $x = 0$. Start
with the definition of \( \text{erf} x \).

\[
\text{erf} \ x = \frac{2}{\sqrt{\pi}} \int_0^x e^{-y^2} \, dy
\]

\[
= \frac{2}{\sqrt{\pi}} \int_0^x \sum_{n=0}^{\infty} \frac{(-1)^n y^{2n}}{n!} \, dy
\]

\[
= \frac{2}{\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{(-1)^n y^{2n}}{n!} \int_0^x \, dy
\]

\[
= \frac{2}{\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{(-1)^n y^{2n+1}}{2n+1} \bigg|_0^x
\]

Therefore, the Taylor series expansion of \( \text{erf} x \) centered at \( x = 0 \) is

\[
\text{erf} \ x = \frac{2}{\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{(-1)^n x^{2n+1}}{2n+1}.
\]

**Part (c)**

The series can be written term by term as follows.

\[
\text{erf} \ x = \frac{2}{\sqrt{\pi}} x - \frac{2}{3\sqrt{\pi}} x^3 + \frac{1}{5\sqrt{\pi}} x^5 - \frac{1}{21\sqrt{\pi}} x^7 + \cdots
\]

If we use only the first two nonzero terms we get an approximation for \( \text{erf} x \).

\[
\text{erf} \ x \approx \frac{2}{\sqrt{\pi}} x - \frac{2}{3\sqrt{\pi}} x^3
\]

The error function appears with an argument of \( x/\sqrt{4kt} \) in the solution for \( Q(x,t) \) in (2), so replace \( x \) with this expression in the Taylor series.

\[
\text{erf} \ \frac{x}{\sqrt{4kt}} \approx \frac{2}{\sqrt{\pi}} \left( \frac{x}{\sqrt{4kt}} \right) - \frac{2}{3\sqrt{\pi}} \left( \frac{x}{\sqrt{4kt}} \right)^3 = \frac{x}{\sqrt{\pi kt}} - \frac{1}{12} \frac{x^3}{\sqrt{\pi k^3 t^3}}
\]

That is,

\[
\text{erf} \ \frac{x}{\sqrt{4kt}} \approx \frac{x}{\sqrt{\pi kt}} \left( 1 - \frac{x^2}{12kt} \right).
\]

Plugging this two-term form for the error function into (2), we get an approximation for \( Q(x,t) \).

\[
Q(x,t) \approx \frac{1}{2} \left[ \frac{x}{\sqrt{\pi kt}} \left( 1 - \frac{x^2}{12kt} \right) + 1 \right]
\]

**Part (d)**

When \( x \) is fixed and \( t \) is large, the combination variable \( \eta = x/\sqrt{4kt} \ll 1 \). Therefore, higher-order terms in the Taylor series are negligible compared to the first two. This is why the approximation is a good one.
Figure 2: Plot of the two-term approximation to $Q(x,t)$ with $k = 1 \text{ m}^2/\text{s}$ for six different times: 
$t = 0 \text{ s (red)}, t = 1 \text{ s (orange)}, t = 2 \text{ s (yellow)}, t = 5 \text{ s (green)}, t = 10 \text{ s (blue)}, \text{ and } t = 20 \text{ s (purple)}$.

If we do a side-by-side comparison with the graph of the exact solution for $Q(x,t)$, we see that as time increases, the interval over which the approximation closely matches the exact solution increases.

Figure 3: Superposition of the plots of the exact solution for $Q(x,t)$ (solid lines) and the approximate solution for $Q(x,t)$ (dashed lines) with $k = 1 \text{ m}^2/\text{s}$ for six different times: 
$t = 0 \text{ s (red)}, t = 1 \text{ s (orange)}, t = 2 \text{ s (yellow)}, t = 5 \text{ s (green)}, t = 10 \text{ s (blue)}, \text{ and } t = 20 \text{ s (purple)}$. 

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