MAU33E01: Engineering Mathematics V: Solving Partial Differential Equations with Separation Of Variables (Extra Question)

Liam Burke and Nikolaos Chatzarakis
School Of Mathematics, Trinity College Dublin

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NB: This worksheet is an additional unseen exercise for MAU33E01. It is not for module credit and is intended only as an additional resource for exam preparation.

Question 1 (The Wave Equation in Two Dimensions)

The Wave equation in two dimensions describes the evolution of a wave $u(t,x,y)$ in a two-dimensional medium. For a constant velocity c, this is

$$\frac{\partial^2 u}{\partial t^2} = c^2\Big(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\Big)\,.$$

Then, assume the boundary conditions on a fixed square

$$\begin{aligned} u(t,0,y) = 0 \quad &\text{and} \quad u(t,L,y) = 0 \\ u(t,x,0) = 0 \quad &\text{and} \quad u(t,x,L) = 0\,, \end{aligned}$$

(a) Derive the solution subject to these boundary conditions.
(b) If the initial conditions are

$$u(0,x,y) = 0 \qquad \text{and} \qquad \frac{\partial u}{\partial t}(0,x,y) = 1\,.$$

determine the solution?

Answer

(a)
Assume the solution takes the form $u(t,x,y) = w(t)f(x,y)$. Substituting this into the PDE, we have

$$\begin{aligned} \frac{\partial^2}{\partial t^2}(wf) &= c^2\Big(\frac{\partial^2}{\partial x^2}(wf) + \frac{\partial^2}{\partial y^2}(wf)\Big) \\ f(x,y)\frac{d^2 w}{dt^2} &= c^2 w(t)\Big(\frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2}\Big) \end{aligned}$$

Separating the the $t-$components on the left-hand side (essentially dividing by (wf)), we have

$$\frac{1}{w}\frac{d^2 w}{dt^2} = \frac{c^2}{f}\Big(\frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2}\Big) = \text{const.}$$

The two fractions are dependent on different variables, hecen being equal means they are both equal to a constant - let it be k. The two fractions are split into an ODE over t (left-hand side) and a PDE over x and y (right-hand side):

$$\begin{aligned}&\text{ODE: } \ddot{w} = kw\\&\text{PDE: } \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} = \frac{k}{c^2} f\end{aligned}$$

The new (reduced) PDE is known as the Helmholtz PDE and will be rediced in the same manner. Assume $f(x, y) = F(x)G(y)$ and substitute this into the Helmholtz equation. Then, following the same proccess, we arrive to

$$\begin{aligned}&G(y)F''(x) + F(x)G''(y) = \frac{k}{c^2} F(x)G(y)\\&\frac{F''(x)}{F(x)} + \frac{G''(y)}{G(y)} = \frac{k}{c^2} = \text{const.}\end{aligned}$$

Since the two fractions are dependent to a different variable and sum to a constant, must be equal to two constants - let them be κ_1 and κ_2, such that

$$\kappa_1 + \kappa_2 = \frac{k}{c^2}\,.$$

Then, there are two ODEs, one over x

$$F''(x) = \kappa_1 F(x)\,,$$

and one over y

$$G''(y) = \kappa_2 G(y)\,.$$

Note that the two of them are similar, so their solutions should be similar as well; we shall show the solution to the first and the second will follow accordingly.
Let $\kappa_1 = 0$, so $F''(x) = 0$ and thus

$$F(x) = \alpha_0 + \alpha_1 x\,,$$

where α_0, α_1 are real constants. Applying the boundary conditions,

$$\begin{aligned}&F(0) = F(L) = 0\\&\alpha_0 = \alpha_0 + \alpha_1 L = 0\end{aligned}$$

hence, $\alpha_0 = \alpha_1 = 0$. Thus, $F(x) = 0$ - a trivial solution.
Let $\kappa_1 = \lambda^2 > 0$ ($\lambda \in \mathbb{R}$), so $F''(x) = \lambda^2 F(x)$. Thus,

$$F(x) = \alpha_1 e^{\lambda x} + \alpha_2 e^{-\lambda x}\,,$$

where α_1, α_2 are real constants. Applying the boundary conditions,

$$\begin{aligned}&F(0) = F(L) = 0\\&\alpha_1 + \alpha_2 = \alpha_1 e^{2\lambda L} + \alpha_2 = 0\end{aligned}$$

which are impossible unless $\lambda = 0$. This is the previous case ($\kappa_1 = 0$) which was disgarded as trivial.
Let $\kappa_1 = -\lambda^2 < 0$ ($\lambda \in \mathbb{R}$), so $F''(x) = -\lambda^2 F(x)$. Thus,

$$F(x) = \alpha_1 \cos(\lambda x) + \alpha_2 \sin(\lambda x)\,,$$

where α_1, α_2 are real constants. Applying the boundary conditions,

$$\begin{aligned}&F(0) = F(L) = 0\\&\alpha_1 = 0 \quad \text{and} \quad \alpha_1 \cos(\lambda L) + \alpha_2 \sin(\lambda L) = 0\end{aligned}$$

which can be true if

$$\lambda = \frac{n\pi}{L} \quad , \quad n \in \mathbb{N} \,.$$

Thus, the solution is

$$F_n(x) = \alpha_n \sin\left(\frac{n\pi}{L}x\right) .$$

In the same manner,

$$G_n(y) = \beta_n \sin\left(\frac{n\pi}{L}y\right) .$$

Since $\kappa_1 = \kappa_2 = -\Big(\frac{n\pi}{L}\Big)^2$, then

$$\begin{aligned} \frac{k}{c^2} &= \kappa_1 + \kappa_2 = -\Big(\frac{n\pi}{L}\Big)^2 - \Big(\frac{n\pi}{L}\Big)^2 \\ k &= -2\Big(\frac{n\pi}{cL}\Big)^2 \quad , \quad n \in \mathbb{N} \end{aligned}$$

and thus $k < 0$. Cosequently, the ODE over t becomes

$$\ddot{w} = -2\Big(\frac{n\pi}{cL}\Big)^2 w \,.$$

Its solution is

$$w_n(t) = \gamma_n \cos\left(\frac{\sqrt{2}n\pi}{cL}t\right) + \delta_n \sin\left(\frac{\sqrt{2}n\pi}{cL}t\right) .$$

where γ_n, δ_n are real constants.
The solution for the given boundary conditions is

$$u(t,x,y) = \sum_{n=0}^{\infty} u_n(t,x,y)$$

where

$$\begin{aligned} u_n(t,x,y) = w_n(t)F_n(x)G_n(y) &= A_n \cos\left(\frac{\sqrt{2}n\pi}{cL}t\right) \sin\left(\frac{n\pi}{L}x\right) \sin\left(\frac{n\pi}{L}y\right) + B_n \sin\left(\frac{\sqrt{2}n\pi}{cL}t\right) \sin\left(\frac{n\pi}{L}x\right) \sin\left(\frac{n\pi}{L}y\right) \\ &= \Big[\frac{A_n}{2} \cos\left(\frac{\sqrt{2}n\pi}{cL}t\right) + \frac{B_n}{2} \sin\left(\frac{\sqrt{2}n\pi}{cL}t\right)\Big] \sin\left(\frac{n\pi}{2L}(x+y)\right) \cos\left(\frac{n\pi}{2L}(x-y)\right) \end{aligned}$$

(b)
If the initial conditions are

$$u(0,x,y) = 0 \qquad \text{and} \qquad \frac{\partial u}{\partial t}(0,x,y) = 1 \,.$$

Then,

$$u(0,x,y) = 2\sum_{n=0}^{\infty} A_n \sin\left(\frac{n\pi}{2L}(x+y)\right) \cos\left(\frac{n\pi}{2L}(x-y)\right) = 0$$

and eventually, $A_n = 0$. And

$$\frac{\partial u}{\partial t}(0,x,y) = \sqrt{2}\frac{L}{\pi c} \sum_{n=0}^{\infty} \frac{B_n}{n} \sin\left(\frac{n\pi}{2L}(x+y)\right) \cos\left(\frac{n\pi}{2L}(x-y)\right) = 1$$

which means that $\dfrac{\sqrt{2}LB_n}{n\pi c}$ are the "odd" coefficients of the Fourier expansion of 1.

$$\begin{aligned}\frac{\sqrt{2}LB_n}{n\pi c} &= \frac{2}{L}\int_0^L\int_0^L \sin\Big(\frac{n\pi}{L}x\Big)\sin\Big(\frac{n\pi}{L}y\Big)dxdy = \frac{2}{L}\Big[\int_0^L \sin\Big(\frac{n\pi}{L}x\Big)dx\Big]\Big[\int_0^L \sin\Big(\frac{n\pi}{L}y\Big)dy\Big]\\ &= \frac{2}{L}\Big[\frac{L}{n\pi}\cos\Big(\frac{n\pi}{L}\Big)\Big]_0^L\Big[\frac{L}{n\pi}\cos\Big(\frac{n\pi}{L}\Big)\Big]_0^L = \frac{8L}{n^2\pi^2}\sin^4\Big(\frac{\pi n}{2}\Big)\\ B_n &= \frac{4\sqrt{2}c}{n\pi}\sin^4\Big(\frac{\pi n}{2}\Big)\end{aligned}$$

Thus, the solution becomes

$$u(t,x,y) = \sum_{n=0}^{\infty}\frac{2\sqrt{2}c}{n\pi}\sin^4\Big(\frac{\pi n}{2}\Big)\sin\Big(\frac{\sqrt{2}n\pi}{cL}t\Big)\sin\Big(\frac{n\pi}{2L}(x+y)\Big)\cos\Big(\frac{n\pi}{2L}(x-y)\Big)$$

Question 2 (The Schrödinger Equation)

The Schrödinger equation is a partial differential equation that describes the wave function $\psi(t,x)$ of a quantum mechanical system. It can be thought of as the quantum mechanical analog of Newton's Second Law in Classical Mechanics. For a time independent potential $V(x,t) := V(x)$, it is given by

$$i\hbar\frac{\partial}{\partial t}\psi(t,x) = \Big(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\Big)\psi(t,x)$$

where $\hbar, m$ are constants.
(a) Derive the *stationary state* solution

$$\psi(t,x) = F(x)e^{-\frac{iE}{\hbar}t},$$

where E is a constant.
(b) Derive the solution for the *obstacle* potential

$$V(x) = \begin{cases} 0 & x<0 \\ V_0 & x\geq 0\end{cases},$$

where V_0 a real constant, and the continuity conditions

$$\psi(t,0)\big|_{x^-} = \psi(t,0)\big|_{x^+} \qquad \text{and} \qquad \frac{\partial\psi}{\partial x}\Big|_{x^-} = \frac{\partial\psi}{\partial x}\Big|_{x^+}.$$

Answer

(a)
Assume the solution takes the form $\psi(t,x) = F(x)G(t)$. Substitute this solution into the PDE to get

$$\begin{aligned}i\hbar\frac{\partial}{\partial t}(FG) &= -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}(FG) + V(x)FG\\ i\hbar FG' &= -\frac{\hbar^2}{2m}F''G + V(x)FG\end{aligned}$$

Now we exploit the usual trick of getting everything involving x to one side only and everything involving t to one side only. We see this can be done by dividing across by FG.

$$\begin{aligned}\frac{i\hbar FG'}{FG} &= \frac{-\frac{\hbar^2}{2m}F''G}{FG} + \frac{V(x)FG}{FG}\\ i\hbar\frac{G'}{G} &= -\frac{\hbar^2}{2m}\frac{F''}{F} + V(x) = \text{const} = E\end{aligned}$$

We now have two separate ODE's, but from the question we see that we do not need to solve the ODE for $F(x)$. We thus solve the ODE for $G(t)$ only. This ODE is

$$i\hbar G' = EG$$

Multiply across by i and remember that $i^2 = -1$ to rewrite the ODE as

$$G' + \frac{i}{\hbar}EG = 0$$

This is a first order ODE with constant coefficients. We thus take our solutions to be exponential solutions of the form $G(t) = e^{\lambda t}$. Substitute this back into the ODE to get

$$\lambda e^{\lambda t} + \frac{i}{\hbar}Ee^{\lambda t} = 0$$
$$\implies e^{\lambda t}(\lambda + \frac{i}{\hbar}E) = 0$$

We thus get $\lambda = -\frac{iE}{\hbar}$. We have one linearly independent solution and thus the appropriate linear combination is

$$G(t) = Ae^{-\frac{iE}{\hbar}t}$$

where A is a constant which can absorbed into $F(x)$. This yields the solution.

$$\psi(t,x) = F(x)e^{-\frac{iE}{\hbar}t},$$

(b)

Given the potential

$$V(x) = \begin{cases} 0 & x < 0 \\ V_0 & x \geq 0 \end{cases},$$

the physical problem is the scattering of a particle (described by the wave function) over a step potential. Hence, the ODE over x is split; on the negative half-space, it is

$$-\frac{\hbar^2}{2m}\frac{F''(x)}{F(x)} = E$$
$$F''(x) + \frac{2m}{\hbar^2}EF(x) = 0\,,$$

and on the positive half-space, it is

$$-\frac{\hbar^2}{2m}\frac{F''(x)}{F(x)} + V_0 = E$$
$$F''(x) + \frac{2m}{\hbar^2}\big(E - V_0\big)F(x) = 0\,.$$

And the continuity conditions are such that the two solutions and their first-order derivatives should be equal in $x = 0$,

$$F(0)\big|_{x^-} = F(0)\big|_{x^+} \qquad \text{and} \qquad F'(0)\big|_{x^-} = F'(0)\big|_{x^+}\,.$$

On the negative half-space,

$$F''(x) + \frac{2m}{\hbar^2}EF(x) = 0$$

and the solution is

$$F(x)\big|_{x^-} = A_1\cos\Big(\frac{\sqrt{2mE}}{\hbar}x\Big) + A_2\sin\Big(\frac{\sqrt{2mE}}{\hbar}x\Big)\,.$$

Note that the solution is unique, since m and E are positive.
On the positive half-space,

$$F''(x) + \frac{2m}{\hbar^2}\big(E - V_0\big)F(x) = 0$$

- If $E = V_0$, then $F''(x) = 0$ and
$$F(x)\big|_{x^+} = B_0 + B_1 x\,,$$
where B_0, B_1 are real constants. Applying the continuity conditions, we have
$$\begin{aligned} &F(x)\big|_{x^-} = F(x)\big|_{x^+} \\ &A_1 = B_0 \end{aligned}$$
and
$$\begin{aligned} &F'(0)\big|_{x^-} = F'(0)\big|_{x^+} \\ &A_2 \frac{\hbar}{\sqrt{2mE}} = B_1 \end{aligned}$$
Thus, the solution is
$$\psi(t,x) = \begin{cases} \Big[A_1 \cos\Big(\frac{\sqrt{2mE}}{\hbar}x\Big) + A_2 \sin\Big(\frac{\sqrt{2mE}}{\hbar}x\Big)\Big] e^{-\frac{iE}{\hbar}t} & x < 0 \\ \Big(A_1 + \frac{\hbar A_2}{\sqrt{2mE}} x\Big) e^{-\frac{iE}{\hbar}t} & x \geq 0 \end{cases}$$

- If $E > V_0$, then $F''(x) + \dfrac{2m\lambda^2}{\hbar^2} F(x) = 0$, whose solution is
$$F(x)\big|_{x^+} = B_1 e^{\frac{\sqrt{2m(E-V_0)}}{\hbar}x} + B_2 e^{-\frac{\sqrt{2m(E-V_0)}}{\hbar}x}$$
where B_1, B_2 are real constants. Applying the continuity conditions, we have
$$\begin{aligned} &F(x)\big|_{x^-} = F(x)\big|_{x^+} \\ &A_1 = B_1 + B_2 \end{aligned}$$
and
$$\begin{aligned} &F'(0)\big|_{x^-} = F'(0)\big|_{x^+} \\ &A_2 \frac{\hbar}{\sqrt{2mE}} = \frac{\sqrt{2m(E-V_0)}}{\hbar}\big(B_1 - B_2\big) \\ &A_2 = \frac{2m}{\hbar^2}\sqrt{\frac{E}{E-V_0}}\big(B_1 - B_2\big) \end{aligned}$$
from where
$$B_1 = \frac{A_1}{2} + \sqrt{\frac{E-V_0}{E}}\frac{\hbar^2 A_2}{4m} \quad \text{and} \quad B_2 = \frac{A_1}{2} - \sqrt{\frac{E-V_0}{E}}\frac{\hbar^2 A_2}{4m}$$
Thus, the solution is
$$\psi(t,x) = \begin{cases} e^{-\frac{iE}{\hbar}t}\Big[A_1 \cos\Big(\frac{\sqrt{2mE}}{\hbar}x\Big) + A_2 \sin\Big(\frac{\sqrt{2mE}}{\hbar}x\Big)\Big] & x < 0 \\ e^{-\frac{iE}{\hbar}t}\Big[A_1 \cosh\Big(\frac{\sqrt{2m(E-V_0)}}{\hbar}x\Big) + \sqrt{\frac{E-V_0}{E}}\frac{\hbar^2 A_2}{2m} \sinh\Big(\frac{\sqrt{2m(E-V_0)}}{\hbar}x\Big)\Big] & x \geq 0 \end{cases}$$

- If $E < V_0$ (this is the physically interesting case), then $F''(x) - \dfrac{2m\lambda^2}{\hbar^2} F(x) = 0$, whose solution is
$$F(x)\big|_{x^+} = B_1 \cos\Big(\frac{\sqrt{2m(V_0-E)}}{\hbar}x\Big) + B_2 \sin\Big(\frac{\sqrt{2m(V_0-E)}}{\hbar}x\Big)$$

where B_1, B_2 are real constants. Applying the continuity conditions, we have

$$\begin{aligned} F(x)\big|_{x^-} &= F(x)\big|_{x^+} \\ A_1 &= B_1 \end{aligned}$$

and

$$\begin{aligned} F'(0)\big|_{x^-} &= F'(0)\big|_{x^+} \\ A_2 \frac{\hbar}{\sqrt{2mE}} &= \frac{\sqrt{2m(V_0 - E)}}{\hbar} B_2 \\ B_2 &= \frac{2m}{\hbar^2}\sqrt{\frac{E - V_0}{E}} A_2 \end{aligned}$$

Thus, the solutions is

$$\psi(t,x) = \begin{cases} e^{-\frac{iE}{\hbar}t}\Big[A_1 \cos\Big(\frac{\sqrt{2mE}}{\hbar}x\Big) + A_2 \sin\Big(\frac{\sqrt{2mE}}{\hbar}x\Big)\Big] & x < 0 \\ e^{-\frac{iE}{\hbar}t}\Big[A_1 \cos\Big(\frac{\sqrt{2m(E - V_0)}}{\hbar}x\Big) + \sqrt{\frac{E - V_0}{E}}\frac{\hbar^2 A_2}{2m} \sin\Big(\frac{\sqrt{2m(E - V_0)}}{\hbar}x\Big)\Big] & x \geq 0 \end{cases}$$

Note that this is a *general solution*, given that the real coefficients A_1, A_2 are not specified; to specify these further, one should employ boundary conditions. In the case of a wave function, the usual boundary conditions are at $-\infty$ and ∞, so they lie out of the scope of this presentation.