Exercise 3

Solve the Schrödinger equation $u_t = iku_{xx}$ for real k in the interval $0 < x < l$ with the boundary conditions $u_x(0,t) = 0$, $u(l,t) = 0$.

Solution

Since the Schrödinger equation and its boundary conditions are linear and homogeneous, the method of separation of variables can be applied to solve it. Assume a product solution of the form, $u(x,t) = X(x)T(t)$, and plug it into the PDE

$$u_t = iku_{xx} \quad \rightarrow \quad XT' = ikX''T$$

and the boundary conditions.

$$\begin{aligned} u_x(0,t) = X'(0)T(t) = 0 \qquad &\rightarrow \qquad X'(0) = 0 \\ u(l,t) = X(l)T(t) = 0 \qquad &\rightarrow \qquad X(l) = 0 \end{aligned}$$

Separate variables now.

$$\frac{T'}{ikT} = \frac{X''}{X}$$

Note that ik is a constant and can go on either side. The final answer will be the same regardless. We have a function of t on the left side and a function of x on the right side. The only way both functions can be equal is if they are equal to a constant.

$$\frac{T'}{ikT} = \frac{X''}{X} = p$$

Values of p for which $X'(0) = 0$ and $X(l) = 0$ are satisfied are called the eigenvalues, and the nontrivial functions $X(x)$ associated with them are called the eigenfunctions.

Determination of Positive Eigenvalues: $p = \mu^2$

Assuming p is positive, the differential equation for X becomes

$$\frac{X''}{X} = \mu^2.$$

Multiply both sides by X.

$$X'' = \mu^2 X$$

The general solution can be written in terms of hyperbolic sine and hyperbolic cosine.

$$X(x) = C_1 \cosh \mu x + C_2 \sinh \mu x$$

Now use the boundary conditions to determine C_1 and C_2.

$$\begin{aligned} X'(0) &= C_2\mu = 0 \\ X(l) &= C_1 \cosh \mu l + C_2 \sinh \mu l = 0 \end{aligned}$$

We see that $C_1 = 0$ and $C_2 = 0$. Hence, only the trivial solution $X(x) = 0$ results from considering positive values for p, and there are no positive eigenvalues.

Determination of the Zero Eigenvalue: $p = 0$

Assuming p is zero, the differential equation for X becomes

$$\frac{X''}{X} = 0.$$

Multiply both sides by X.

$$X'' = 0$$

The general solution is a linear function.

$$X(x) = C_3 x + C_4$$

Now use the boundary conditions to determine C_3 and C_4.

$$X'(0) = C_3 = 0$$
$$X(l) = C_3 l + C_4 = 0$$

We see that $C_3 = 0$ and $C_4 = 0$. Hence, only the trivial solution $X(x) = 0$ results from considering $p = 0$, and zero is not an eigenvalue.

Determination of Negative Eigenvalues: $p = -\lambda^2$

Assuming p is negative, the differential equation for X becomes

$$\frac{X''}{X} = -\lambda^2.$$

Multiply both sides by X.

$$X'' = -\lambda^2 X$$

The general solution can be written in terms of sine and cosine.

$$X(x) = C_5 \cos \lambda x + C_6 \sin \lambda x$$

Now use the boundary conditions to determine C_5 and C_6.

$$X'(0) = C_6 \lambda = 0$$
$$X(l) = C_5 \cos \lambda l + C_6 \sin \lambda l = 0$$

The second equation simplifies to $C_5 \cos \lambda l = 0$. To avoid getting the trivial solution, we insist that $C_5 \neq 0$. Doing so yields an equation for the eigenvalues.

$$\cos \lambda l = 0$$

Solve for λl.

$$\lambda l = \frac{1}{2}(2n+1)\pi, \quad n = 0, 1, \ldots$$

So then

$$\lambda = \lambda_n = \frac{\pi}{2l}(2n+1), \quad n = 0, 1, \ldots.$$

The eigenfunctions associated with these eigenvalues are

$$X(x) = C_5 \cos \lambda x \quad \rightarrow \quad X_n(x) = \cos \lambda_n x, \quad n = 0, 1, \ldots.$$

Now solve the differential equation for $T(t)$.

$$\frac{T'}{ikT} = -\lambda^2$$

Multiply both sides by ik.

$$\frac{T'}{T} = -ik\lambda^2$$

The left side is just the derivative of $\ln T$.

$$\frac{d}{dt}(\ln T) = -ik\lambda^2$$

Integrate both sides with respect to t.

$$\ln T = -ik\lambda^2 t + C_7$$

Exponentiate both sides.

$$T(t) = e^{-ik\lambda^2 t + C_7} = e^{-ik\lambda^2 t} e^{C_7}$$

Use a new constant of integration.

$$T(t) = C_8 e^{-ik\lambda^2 t} \quad \rightarrow \quad T_n(t) = e^{-ik\lambda_n^2 t}$$

According to the principle of linear superposition, the solution to the PDE for $u(x,t)$ is a linear combination of all products $T_n(t)X_n(x)$ over all the eigenvalues.

$$\begin{aligned} u(x,t) &= \sum_{n=0}^{\infty} A_n T_n(t) X_n(x) \\ &= \sum_{n=0}^{\infty} A_n e^{-ik\lambda_n^2 t} \cos \lambda_n x \\ &= \sum_{n=0}^{\infty} A_n e^{-ik\left[\frac{\pi}{2l}(2n+1)\right]^2 t} \cos\left[\frac{\pi}{2l}(2n+1)x\right] \end{aligned}$$

Therefore,

$$u(x,t) = \sum_{n=0}^{\infty} A_n \exp\left[-ik\frac{\pi^2}{4l^2}(2n+1)^2 t\right] \cos\left[\frac{\pi}{2l}(2n+1)x\right].$$

If an initial condition were provided, A_n could be determined.