Exercise 3

A quantum-mechanical particle on the line with an infinite potential outside the interval $(0, l)$ ("particle in a box") is given by Schrödinger's equation $u_t = iu_{xx}$ on $(0, l)$ with Dirichlet conditions at the ends. Separate the variables and use (8) to find its representation as a series.

Solution

The PDE we have to solve is the one-dimensional Schrödinger equation.

$$u_t = iu_{xx}, \quad 0 < x < l$$

Its boundary conditions are

$$\begin{aligned} u(0, t) &= 0 \\ u(l, t) &= 0. \end{aligned}$$

Assume an arbitrary initial condition.

$$u(x, 0) = \phi(x)$$

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

$$u_t = iu_{xx} \quad \rightarrow \quad XT' = iX''T$$

and the boundary conditions.

$$\begin{aligned} u(0, t) = X(0)T(t) = 0 \quad &\rightarrow \quad X(0) = 0 \\ u(l, t) = X(l)T(t) = 0 \quad &\rightarrow \quad X(l) = 0 \end{aligned}$$

Separate variables now.

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

Note that i 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.

$$\frac{T'}{iT} = \frac{X''}{X} = k$$

Values of k 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: $k = \mu^2$

Assuming k 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.

$$X(0) = C_1 = 0$$
$$X(l) = C_1 \cosh \mu l + C_2 \sinh \mu l = 0$$

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

Determination of the Zero Eigenvalue: $k = 0$

Assuming k 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.

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

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

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

Assuming k 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.

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

The second equation simplifies to $C_6 \sin \lambda l = 0$. To avoid getting the trivial solution, we insist that $C_6 \neq 0$. Doing so yields an equation for the eigenvalues.

$$\sin \lambda l = 0$$

Solve for λl.

$$\lambda l = n\pi, \quad n = 1, 2, \ldots$$

So then

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

The eigenfunctions associated with these eigenvalues are

$$X(x) = C_6 \sin \lambda x \quad \rightarrow \quad X_n(x) = \sin \lambda_n x, \quad n = 1, 2, \ldots.$$

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

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

Multiply both sides by i.

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

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

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

Integrate both sides with respect to t.

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

Exponentiate both sides.

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

Use a new constant of integration.

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

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.

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

Therefore,

$$\boxed{u(x,t) = \sum_{n=1}^{\infty} A_n e^{-i\frac{n^2\pi^2}{l^2}t} \sin \frac{n\pi x}{l}}.$$

The final task is to use Fourier's method and the initial condition to determine A_n.

$$u(x,0) = \sum_{n=1}^{\infty} A_n \sin \frac{n\pi x}{l} = \phi(x)$$

Multiply both sides by $\sin \lambda_m x$, where m is a positive integer.

$$u(x,0) = \sum_{n=1}^{\infty} A_n \sin \frac{n\pi x}{l} \sin \frac{m\pi x}{l} = \phi(x) \sin \frac{m\pi x}{l}$$

Integrate both sides with respect to x over the domain the PDE is defined.

$$\int_0^l \sum_{n=1}^{\infty} A_n \sin \frac{n\pi x}{l} \sin \frac{m\pi x}{l}\, dx = \int_0^l \phi(x) \sin \frac{m\pi x}{l}\, dx$$

Bring the integral inside the sum on the left.

$$\sum_{n=1}^{\infty} A_n \int_0^l \sin \frac{n\pi x}{l} \sin \frac{m\pi x}{l}\, dx = \int_0^l \phi(x) \sin \frac{m\pi x}{l}\, dx$$

Since n and m are integers,

$$\int_0^l \sin \frac{n\pi x}{l} \sin \frac{m\pi x}{l}\, dx = \begin{cases} \frac{l}{2} & n = m \\ 0 & n \neq m \end{cases},$$

as can be verified with trigonometric identities. This implies that every term in the infinite series vanishes except for the $n = m$ term.

$$A_n \cdot \frac{l}{2} = \int_0^l \phi(x) \sin \frac{n\pi x}{l}\, dx$$

Therefore, the coefficient is

$$\boxed{A_n = \frac{2}{l} \int_0^l \phi(x) \sin \frac{n\pi x}{l}\, dx.}$$