Exercise 3

In the cube $(0, a)^3$, a substance is diffusing whose molecules multiply at a rate proportional to the concentration. It therefore satisfies the PDE $u_t = k\Delta u + \gamma u$, where γ is a constant. Assume that $u = 0$ on all six sides. What is the condition on γ so that the concentration does not grow without bound?

Solution

Here we will solve the following initial boundary value problem.

$$\begin{aligned} u_t = k\Delta u + \gamma u, \quad 0 < x, y, z < a,\ t > 0 \\ u(0, y, z, t) = 0 \qquad u(x, 0, z, t) = 0 \qquad u(x, y, 0, t) = 0 \\ u(a, y, z, t) = 0 \qquad u(x, a, z, t) = 0 \qquad u(x, y, a, t) = 0 \\ u(x, y, z, 0) = f(x, y, z) \end{aligned}$$

Because the PDE and its associated boundary conditions are linear and homogeneous, the method of separation of variables can be applied to solve for u. Assume a product solution of the form $u(x, y, z, t) = X(x)Y(y)Z(z)T(t)$ and substitute it into the PDE

$$u_t = k(u_{xx} + u_{yy} + u_{zz}) + \gamma u \quad \to \quad XYZT' = k(X''YZT + XY''ZT + XYZ''T) + \gamma XYZT$$

and the boundary conditions.

$$\begin{aligned} u(0, y, z, t) = 0 \quad &\to \quad X(0)Y(y)Z(z)T(t) = 0 \quad \to \quad X(0) = 0 \\ u(a, y, z, t) = 0 \quad &\to \quad X(a)Y(y)Z(z)T(t) = 0 \quad \to \quad X(a) = 0 \\ u(x, 0, z, t) = 0 \quad &\to \quad X(x)Y(0)Z(z)T(t) = 0 \quad \to \quad Y(0) = 0 \\ u(x, a, z, t) = 0 \quad &\to \quad X(x)Y(a)Z(z)T(t) = 0 \quad \to \quad Y(a) = 0 \\ u(x, y, 0, t) = 0 \quad &\to \quad X(x)Y(y)Z(0)T(t) = 0 \quad \to \quad Z(0) = 0 \\ u(x, y, a, t) = 0 \quad &\to \quad X(x)Y(y)Z(a)T(t) = 0 \quad \to \quad Z(a) = 0 \end{aligned}$$

Separate variables in the PDE: divide both sides by $kXYZT$ so that the left side is a function of t and the right side is a function of x, y, and z.

$$\frac{T'}{kT} = \frac{X''}{X} + \frac{Y''}{Y} + \frac{Z''}{Z} + \frac{\gamma}{k}$$

Bring γ/k to the left side.

$$\underbrace{\frac{T'}{kT} - \frac{\gamma}{k}}_{\text{function of } t} = \underbrace{\frac{X''}{X} + \frac{Y''}{Y} + \frac{Z''}{Z}}_{\text{function of } x \text{ and } y \text{ and } z}$$

The only way a function of t can be equal to a function of x, y, and z is if both are equal to a constant λ.

$$\frac{T'}{kT} - \frac{\gamma}{k} = \frac{X''}{X} + \frac{Y''}{Y} + \frac{Z''}{Z} = \lambda$$

Subtract both sides of the second equation by Z''/Z.

$$\underbrace{\frac{X''}{X} + \frac{Y''}{Y}}_{\text{function of } x \text{ and } y} = \underbrace{\lambda - \frac{Z''}{Z}}_{\text{function of } z}$$

The only way a function of x and y can be equal to a function of z is if both are equal to another constant μ.

$$\frac{X''}{X} + \frac{Y''}{Y} = \lambda - \frac{Z''}{Z} = \mu$$

Bring Y''/Y to the right side.

$$\underbrace{\frac{X''}{X}}_{\text{function of } x} = \underbrace{\mu - \frac{Y''}{Y}}_{\text{function of } y}$$

The only way a function of x can be equal to a function of y is if both are equal to another constant η.

$$\frac{X''}{X} = \mu - \frac{Y''}{Y} = \eta$$

As a result of applying the method of separation of variables, the PDE has been reduced to a system of four ODEs—one in x, one in y, one in z, and one in t.

$$\left.\begin{aligned} \frac{T'}{kT} - \frac{\gamma}{k} &= \lambda \\ \frac{X''}{X} &= \eta \\ \mu - \frac{Y''}{Y} &= \eta \\ \lambda - \frac{Z''}{Z} &= \mu \end{aligned}\right\}$$

Values of λ, η, and μ for which there exist nontrivial solutions to the ODEs are called the eigenvalues. The solutions themselves are called the eigenfunctions. Start by solving the ODE for X.

$$X'' = \eta X$$

Suppose first that η is positive: $\eta = \alpha^2$.

$$X'' = \alpha^2 X$$

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

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

Apply the boundary conditions to determine C_1 and C_2.

$$\begin{aligned} X(0) &= C_1 = 0 \\ X(a) &= C_1 \cosh \alpha a + C_2 \sinh \alpha a = 0 \end{aligned}$$

The second equation reduces to $C_2 \sinh \alpha a = 0$. No nonzero value of α satisfies this equation, so C_2 must be zero. This results in the trivial solution $X(x) = 0$, which means there are no positive eigenvalues for η. Suppose secondly that η is zero: $\eta = 0$. The ODE for X becomes

$$X'' = 0.$$

Integrate both sides with respect to x twice.

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

Apply the boundary conditions to determine C_3 and C_4.

$$\begin{aligned} X(0) &= C_4 = 0 \\ X(a) &= C_3 a + C_4 = 0 \end{aligned}$$

The second equation reduces to $C_3 a = 0$, so $C_3 = 0$. The trivial solution $X(x) = 0$ results, which means zero is not an eigenvalue for η. Suppose thirdly that η is negative: $\eta = -\beta^2$. The ODE for X becomes

$$X'' = -\beta^2 X.$$

The general solution is written in terms of sine and cosine.

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

Apply the boundary conditions to determine C_5 and C_6.

$$\begin{aligned} X(0) &= C_5 = 0 \\ X(a) &= C_5 \cos \beta a + C_6 \sin \beta a = 0 \end{aligned}$$

The second equation reduces to $C_6 \sin \beta a = 0$. To avoid the trivial solution, we insist that $C_6 \neq 0$. Then

$$\begin{aligned} \sin \beta a &= 0 \\ \beta a &= n\pi, \quad n = 1, 2, \ldots \\ \beta_n &= \frac{n\pi}{a}. \end{aligned}$$

There are negative eigenvalues $\eta = -n^2\pi^2/a^2$, and the eigenfunctions associated with them are

$$\begin{aligned} X(x) &= C_5 \cos \beta x + C_6 \sin \beta x \\ &= C_6 \sin \beta x \quad \rightarrow \quad X_n(x) = \sin \frac{n\pi x}{a}. \end{aligned}$$

Only positive values of n are used because negative integers give redundant values for η. With $\eta = -n^2\pi^2/a^2$, solve the ODE for Y now.

$$\mu - \frac{Y''}{Y} = -\frac{n^2\pi^2}{a^2}$$

$$Y'' = -\left(-\mu - \frac{n^2\pi^2}{a^2}\right) Y$$

Suppose first that μ is positive: $\mu = \xi^2$.

$$Y'' = \left(\xi^2 + \frac{n^2\pi^2}{a^2}\right) Y$$

The general solution is written in terms of hyperbolic sine and hyperbolic cosine, which results in the trivial solution $Y(y) = 0$ as before. There are no positive eigenvalues for μ. Suppose secondly that μ is zero: $\mu = 0$. The ODE for Y becomes

$$Y'' = \frac{n^2\pi^2}{a^2} Y.$$

Again, the general solution is in terms of hyperbolic functions, which results in the trivial solution $Y(y) = 0$. Zero is not an eigenvalue for μ. Suppose thirdly that μ is negative: $\mu = -\zeta^2$. The ODE for Y becomes

$$Y'' = -\left(\zeta^2 - \frac{n^2\pi^2}{a^2}\right) Y.$$

The general solution is written in terms of sine and cosine.

$$Y(y) = C_7 \cos\sqrt{\zeta^2 - \frac{n^2\pi^2}{a^2}}y + C_8 \sin\sqrt{\zeta^2 - \frac{n^2\pi^2}{a^2}}y$$

Apply the boundary conditions to determine C_7 and C_8.

$$\begin{aligned} Y(0) &= C_7 = 0 \\ Y(a) &= C_7 \cos\sqrt{\zeta^2 - \frac{n^2\pi^2}{a^2}}a + C_8 \sin\sqrt{\zeta^2 - \frac{n^2\pi^2}{a^2}}a = 0 \end{aligned}$$

The second equation reduces to $C_8 \sin\sqrt{\zeta^2 - \frac{n^2\pi^2}{a^2}}a = 0$. To avoid getting the trivial solution, we insist that $C_8 \neq 0$. Then

$$\begin{aligned} \sin\sqrt{\zeta^2 - \frac{n^2\pi^2}{a^2}}a &= 0 \\ \sqrt{\zeta^2 - \frac{n^2\pi^2}{a^2}}a &= m\pi, \quad m = 1, 2, \ldots \\ \sqrt{\zeta^2 - \frac{n^2\pi^2}{a^2}} &= \frac{m\pi}{a} \\ \zeta^2 - \frac{n^2\pi^2}{a^2} &= \frac{m^2\pi^2}{a^2} \\ \zeta^2 &= \frac{\pi^2}{a^2}(m^2 + n^2) \\ \zeta_{mn} &= \frac{\pi}{a}\sqrt{m^2 + n^2}. \end{aligned}$$

There are negative eigenvalues $\mu = -\frac{\pi^2}{a^2}(m^2 + n^2)$, and the eigenfunctions associated with them are

$$\begin{aligned} Y(y) &= C_7 \cos\sqrt{\zeta^2 - \frac{n^2\pi^2}{a^2}}y + C_8 \sin\sqrt{\zeta^2 - \frac{n^2\pi^2}{a^2}}y \\ &= C_8 \sin\sqrt{\zeta^2 - \frac{n^2\pi^2}{a^2}}y \quad \rightarrow \quad Y_m(y) = \sin\frac{m\pi y}{a}. \end{aligned}$$

Only positive values of m are used because negative integers give redundant values for μ. With $\mu = -\frac{\pi^2}{a^2}(m^2 + n^2)$, solve the ODE for Z now.

$$\lambda - \frac{Z''}{Z} = -\frac{\pi^2}{a^2}(m^2 + n^2)$$

$$Z'' = -\left[-\lambda - \frac{\pi^2}{a^2}(m^2 + n^2)\right] Z$$

Suppose first that λ is positive: $\lambda = \rho^2$.

$$Z'' = \left[\rho^2 + \frac{\pi^2}{a^2}(m^2+n^2)\right] Z$$

The general solution is written in terms of hyperbolic sine and hyperbolic cosine, which results in the trivial solution $Z(z) = 0$ as before. There are no positive eigenvalues for λ. Suppose secondly that λ is zero: $\lambda = 0$. The ODE for Z becomes

$$Z'' = \frac{\pi^2}{a^2}(m^2+n^2)Z.$$

Again, the general solution is in terms of hyperbolic functions, which results in the trivial solution $Z(z) = 0$. Zero is not an eigenvalue for λ. Suppose thirdly that λ is negative: $\lambda = -\omega^2$. The ODE for Z becomes

$$Z'' = -\left[\omega^2 - \frac{\pi^2}{a^2}(m^2+n^2)\right] Z$$

The general solution is written in terms of sine and cosine.

$$Z(z) = C_9 \cos\sqrt{\omega^2 - \frac{\pi^2}{a^2}(m^2+n^2)}z + C_{10}\sin\sqrt{\omega^2 - \frac{\pi^2}{a^2}(m^2+n^2)}z$$

Apply the boundary conditions to determine C_9 and C_{10}.

$$\begin{aligned} Z(0) &= C_9 = 0 \\ Z(a) &= C_9 \cos\sqrt{\omega^2 - \frac{\pi^2}{a^2}(m^2+n^2)}a + C_{10}\sin\sqrt{\omega^2 - \frac{\pi^2}{a^2}(m^2+n^2)}a = 0 \end{aligned}$$

The second equation reduces to $C_{10}\sin\sqrt{\omega^2 - \frac{\pi^2}{a^2}(m^2+n^2)}a = 0$. To avoid the trivial solution, we insist that $C_{10} \neq 0$. Then

$$\begin{aligned} \sin\sqrt{\omega^2 - \frac{\pi^2}{a^2}(m^2+n^2)}a &= 0 \\ \sqrt{\omega^2 - \frac{\pi^2}{a^2}(m^2+n^2)}a &= p\pi, \quad p = 1, 2, \ldots \\ \sqrt{\omega^2 - \frac{\pi^2}{a^2}(m^2+n^2)} &= \frac{p\pi}{a} \\ \omega^2 - \frac{\pi^2}{a^2}(m^2+n^2) &= \frac{p^2\pi^2}{a^2} \\ \omega^2 &= \frac{\pi^2}{a^2}(m^2+n^2+p^2) \\ \omega_{mnp} &= \frac{\pi}{a}\sqrt{m^2+n^2+p^2}. \end{aligned}$$

There are negative eigenvalues $\lambda = -\frac{\pi^2}{a^2}(m^2+n^2+p^2)$, and the eigenfunctions associated with them are

$$\begin{aligned} Z(z) &= C_9 \cos\sqrt{\omega^2 - \frac{\pi^2}{a^2}(m^2+n^2)}z + C_{10}\sin\sqrt{\omega^2 - \frac{\pi^2}{a^2}(m^2+n^2)}z \\ &= C_{10}\sin\sqrt{\omega^2 - \frac{\pi^2}{a^2}(m^2+n^2)}z \quad \rightarrow \quad Z_p(z) = \sin\frac{p\pi z}{a}. \end{aligned}$$

Only positive values of p are used because negative integers give redundant values for λ. With $\lambda = -\frac{\pi^2}{a^2}(m^2+n^2+p^2)$, solve the ODE for T now.

$$\frac{T'}{kT} - \frac{\gamma}{k} = -\frac{\pi^2}{a^2}(m^2+n^2+p^2)$$

$$T' = k\left[\frac{\gamma}{k} - \frac{\pi^2}{a^2}(m^2+n^2+p^2)\right]T$$

The general solution is written in terms of the exponential function.

$$T(t) = C_{11}\exp\left\{k\left[\frac{\gamma}{k} - \frac{\pi^2}{a^2}(m^2+n^2+p^2)\right]t\right\}$$

For the solution to remain bounded as $t \to \infty$, it's necessary that the coefficient of t in the exponent is not positive.

$$\frac{\gamma}{k} - \frac{\pi^2}{a^2}(m^2+n^2+p^2) \leq 0$$

$$\frac{\gamma}{k} \leq \frac{\pi^2}{a^2}(m^2+n^2+p^2)$$

$$\gamma \leq \frac{k\pi^2}{a^2}(m^2+n^2+p^2)$$

This inequality must hold for all values of m, n, and p. The smallest values of m, n, and p are $m=1$, $n=1$, and $p=1$.

$$\gamma \leq \frac{k\pi^2}{a^2}(1+1+1)$$

Therefore,

$$\boxed{0 < \gamma \leq \frac{3k\pi^2}{a^2}.}$$

This answer is in disagreement with the answer at the back of the book, $-\infty < \gamma \leq 3k\pi^2/a^2$. Recall that the PDE is

$$u_t = k\Delta u + \gamma u.$$

If γ is negative, then the number of molecules decays rather than multiplies at a rate in proportion to the concentration. In addition, allowing γ to be zero does not take into account the fact that molecules multiply, resulting in an inaccurate model of the phenomenon.

According to the principle of superposition, the general solution to the PDE for u is a linear combination of $X(x)Y(y)Z(z)T(t)$ over all the eigenvalues.

$$u(x,y,z,t) = \sum_{p=1}^{\infty}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty} B_{mnp}\exp\left\{\left[\gamma - \frac{k\pi^2}{a^2}(m^2+n^2+p^2)\right]t\right\}\sin\frac{n\pi x}{a}\sin\frac{m\pi y}{a}\sin\frac{p\pi z}{a}$$

The coefficients B_{mnp} are determined by using the initial condition.

$$u(x,y,z,0) = \sum_{p=1}^{\infty}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty} B_{mnp}\sin\frac{n\pi x}{a}\sin\frac{m\pi y}{a}\sin\frac{p\pi z}{a} = f(x,y,z)$$

$$\rightarrow \quad B_{mnp} = \frac{8}{a^3}\int_0^a\int_0^a\int_0^a f(x,y,z)\sin\frac{n\pi x}{a}\sin\frac{m\pi y}{a}\sin\frac{p\pi z}{a}\,dx\,dy\,dz$$