Diffusion over unbounded, semi-infinite and bounded domains

For this homework we will study the effect of boundary conditions on diffusion, starting with unbounded diffusion over the infinite domain $-\infty < x < \infty$, then diffusion with one-sided boundary over the semi-infinite domain $0 \leq x < \infty$, and finally the familiar two-sided boundary conditions over the domain $0 \leq x < L$. Except for the latter, we’ll use Laplace and Fourier transforms to find solutions rather than the usual separation of variables.

This homework will also serve as an exercise in finding Green’s functions. Green’s functions reduce the problem of finding the solution to the diffusion equation for general space- and time-varying source activation, time-varying boundary conditions, and/or space-varying initial conditions, to finding a set of simpler solutions for just a single-location and single-instance source activation $f(x, t) = \delta(x - x_0)\delta(t - t_0)$ and zero initial and boundary conditions. The set of such solutions $u(x, t)$ for each activation location $x_0$ and each activation instance $t_0$ defines the Green’s function $G(x, t; x_0, t_0)$. Because diffusion is linear, the general solution is then a linear combination of these, which can be expressed as integrals of the Green’s function over all the activations in space $x_0$ and time $t_0$ as given by the non-zero source terms and/or initial/boundary conditions.

a (10 pts)

Show that the Green’s function $G(x, t; x_0, t_0)$ for general diffusion can be written as $G(x, t - t_0; x_0, 0)$, where $G(x, t; x_0, 0)$ is obtained as the solution $u(x, t)$ to the homogeneous diffusion problem with initial conditions $u(x, 0) = \delta(x - x_0)$. We will consider this simplified homogeneous diffusion setting for finding Green’s functions, with single-location initial conditions rather than single-location single-instance source activation, for the rest of this homework.

b (25 pts)

Consider homogeneous diffusion over the infinite domain $-\infty < x < \infty$ with single-location activation in the initial conditions:

$$\frac{\partial u}{\partial t} = D \frac{\partial^2 u}{\partial x^2}; \quad u(x, 0) = \delta(x - x_0)$$

Using Fourier transforms in space, and Laplace transforms in time, show that the solution $u(x, t)$ for $t > 0$ is Gaussian in $x$ centered around mean $x_0$ with standard deviation $\sqrt{2Dt}$:

$$u(x, t) = N(x_0, \sqrt{2Dt}) = \frac{1}{\sqrt{4\pi Dt}} \exp \left(-\frac{(x - x_0)^2}{4Dt}\right)$$

(2)

c (15 pts)

Now consider the same diffusion problem (1) in Part a but now over the semi-infinite domain $0 \leq x < \infty$ with zero-flux boundary condition at $x = 0$:

$$\frac{\partial u}{\partial t} = D \frac{\partial^2 u}{\partial x^2}; \quad \begin{cases} u(x, 0) = \delta(x - x_0) \\ \frac{\partial u}{\partial x}(0, t) = 0 \end{cases}$$

(3)

Show that the solution $u(x, t)$ for $t > 0$ can be written as the sum of the solution over the infinite domain (2) as the Gaussian $N(x_0, \sqrt{2Dt})$ centered at $x_0$, and its mirrored version $N(-x_0, \sqrt{2Dt})$ centered at $-x_0$:

$$u(x, t) = N(x_0, \sqrt{2Dt}) + N(-x_0, \sqrt{2Dt})$$

(4)

Hint: Show that $u(x, t)$ in (4) satisfies the PDE with the initial conditions over the semi-infinite domain, and that the boundary conditions are trivially satisfied.
d (50 pts)

Finally, consider the diffusion problem now over the two-sided domain $0 \leq x < L$ with zero-flux boundary condition at $x = 0$ and zero-flux boundary condition at $x = L$:

$$\frac{\partial u}{\partial t} = D \frac{\partial^2 u}{\partial x^2}; \quad \begin{cases} u(x, 0) = \delta(x - x_0) \\ \frac{\partial u}{\partial x}(0, t) = 0 \\ \frac{\partial u}{\partial x}(L, t) = 0 \end{cases} \quad (5)$$

Using similar arguments as in Part c, show that the solution $u(x, t)$ for $t > 0$ can be written as an infinite recursion of mirroring operations (4) around $x = 0$ and $x = L$:

$$u(x, t) = \sum_{k=-\infty}^{+\infty} \left( \mathcal{N}(2kL + x_0, \sqrt{2Dt}) + \mathcal{N}(2kL - x_0, \sqrt{2Dt}) \right) \quad (6)$$

Compare this solution (6) with the infinite series of eigenmodes $u(x, t) = \sum_l c_l \Phi_l(x) \exp(-D\lambda_l t)$ you obtain by separation of variables. What happens when you truncate either of the two infinite series? Which one is more accurate for $t \to 0$, and which is more accurate for $t \to \infty$? For $x_0 = L/3$, and for $0 \leq x \leq L$ and $0 \leq t \leq L^2/D$ plot: i) the truncated recursively mirrored series solution (6) with six Gaussians ($k = -1, 0, +1$); ii) the truncated eigenmode series solution with the first six eigenmodes ($l = 1, \ldots 6$); and iii) the numerical solution using Matlab’s `pdepe` or an equivalent PDE solver. For the surface plots you may use Matlab’s `surf`. Without loss of generality, assume $L = 1$ cm, and $D = 1$ cm$^2$/s.