3.5.3 Diffusion within a sphere

As an application of spherical coordinates, let us consider the diffusion of a scalar density field $n(\vec{r},t)$ within a spherical volume of radius R. Assuming an initial condition that is spherically symmetric, i.e. a density $n(r,t=0)$ that depends only on the radial coordinate r and is independent of the angles θ and ϕ, the diffusion equation simplifies to

$$\frac{\partial n}{\partial t} = D\nabla^2 n = D\frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial n}{\partial r})\,. \tag{3.5.16}$$

Where D is the diffusion coefficient, and we have used the radial part of Eq. (3.6.35).

Looking for separable solutions of the form $n(r,t) = R(r)T(t)$ leads to the pair of equations

$$\frac{1}{R}\frac{1}{r^2}\frac{d}{dr}(r^2\frac{dR}{\partial r}) = -k^2\,, \quad \text{and} \quad \frac{\dot{T}}{T} = -Dk^2\,, \tag{3.5.17}$$

where for ease of later notation we have set the constant of proportionality to $-k^2$. The solution to $T(t)$ is an exponential decay. While not immediately apparent, a solution to the radial function is $\sin(kr)/r$ as can be checked by substitution. Thus the family of separable solutions, parametrized by k, have the simple form

$$n(r,t) \propto \frac{\sin(kr)}{r}e^{-Dk^2t}\,. \tag{3.5.18}$$

Possible boundary conditions for the diffusion equation are:

- Closed boundary conditions which forbid exit of material. The absence of flux leads to a Neumann boundary condition with $\vec{\nabla}n = \frac{\partial n}{\partial r}\hat{r} = 0$.
- Absorbing boundary conditions are an extreme of open boundary conditions in which the material disappears at the boundary (absorbed or escaping to far away), leading to the Dirichlet condition $n = 0$ at the boundary.

Here we shall consider absorbing boundary conditions with $n(R,t) = 0$. This condition quantizes possible values of k in Eq. (3.5.18) to

$$k_n = \frac{n\pi}{R}\,, \qquad \text{with} \quad n = 1, 2, 3, \cdots\,. \tag{3.5.19}$$

The division by r renders the functions $\sin(k_n R)/r$ non-orthogonal if simply integrated over r. However, the appropriate orthogonality condition pertains to spherically symmetric functions in three dimensions, and

$$\int_0^R (4\pi r^2\ dr)\frac{\sin(k_n r)}{r}\frac{\sin(k_m r)}{r} = 2\pi R\ \delta_{mn}\,. \tag{3.5.20}$$

Indeed, any radially symmetric function vanishing at R can be represented as a superposition of such functions, including the initial condition $n(r,t=0) = n_0(r)$, as

$$n_0(r) = \sum_{n=1}^{\infty} A_n \frac{\sin(k_n r)}{r}\,. \tag{3.5.21}$$

Integrating both sides of the equation after multiplication by $\sin(k_m r)/r$, and using Eq.(3.5.20), leads to

$$\int_0^R (4\pi r^2\, dr) n_0(r) \frac{\sin(k_m r)}{r} = 2\pi R A_m \,. \tag{3.5.22}$$

As an appropriate analog of the Dirac delta function, consider an initial "mass" M of diffusing material concentrated near to origin $r = 0$. Using the result $\lim_{r\to 0} \sin(k_m r)/r = k_m$, we then find

$$2\pi R A_m = k_m \int_0^R (4\pi r^2\, dr) n_0(r) = M \,, \quad \Rightarrow \quad A_m = \frac{M k_m}{2\pi R} = \frac{M}{2R^2} m \,. \tag{3.5.23}$$

The time evolution of this density is now given by

$$n(r,t) = \frac{M}{2R^2} \sum_{n=1}^{\infty} \frac{n}{r} \sin\left(\frac{\pi n r}{R}\right) \exp\left(-\frac{n^2 \pi^2 D t}{R^2}\right) \,. \tag{3.5.24}$$

The terms in the sum corresponding to larger values of n decay more rapidly, such that at very long times only the $n = 1$ survives and

$$n(r, t \gg R^2/D) = \frac{M}{2R^2} \frac{1}{r} \sin\left(\frac{\pi r}{R}\right) \exp\left(-\frac{\pi^2 D t}{R^2}\right) \,. \tag{3.5.25}$$