

Lecture 10: Diffusion equation. We will now derive the fundamental solution for the diffusion equation in three space dimensions:

$$(10.1) \quad u_t = k\Delta u = k(u_{xx} + u_{yy} + u_{zz}), \quad u(\mathbf{x}, 0) = f(\mathbf{x}).$$

We claim that

$$(10.2) \quad u(\mathbf{x}, t) = \frac{1}{(4\pi kt)^{3/2}} \iiint \exp\left(-\frac{|\mathbf{x} - \mathbf{y}|^2}{4kt}\right) f(\mathbf{y}) d\mathbf{y} = \iiint S_3(\mathbf{x} - \mathbf{y}, t) f(\mathbf{y}) d\mathbf{y},$$

solves (10.1). To prove this let

$$S(x, t) = \frac{1}{(4\pi kt)^{1/2}} e^{-x^2/4kt}$$

be the one dimensional source function. Note that we can write the 3 dimensional source function

$$\begin{aligned} S_3(x, y, z, t) &= S(x, t)S(y, t)S(z, t) \\ &= \frac{1}{(4\pi kt)^{1/2}} e^{-x^2/4kt} \frac{1}{(4\pi kt)^{1/2}} e^{-y^2/4kt} \frac{1}{(4\pi kt)^{1/2}} e^{-z^2/4kt} = \frac{1}{(4\pi kt)^{3/2}} e^{-(x^2+y^2+z^2)/4kt} \end{aligned}$$

If we take derivative we get

$$\partial_t(S(x, t)S(y, t)S(z, t)) = S_t(x, t)S(y, t)S(z, t) + S(x, t)S_t(y, t)S(z, t) + S(x, t)S(y, t)S_t(z, t)$$

and

$$(\partial_x^2 + \partial_y^2 + \partial_z^2)(S(x, t)S(y, t)S(z, t)) = S_{xx}(x, t)S(y, t)S(z, t) + S(x, t)S_{yy}(y, t)S(z, t) + S(x, t)S(y, t)S_{zz}(z, t)$$

Since S is the one dimensional source function $S_t(x, t) = S_{xx}(x, t)$, $S_t(y, t) = S_{yy}(y, t)$, $S_t(z, t) = S_{zz}(z, t)$ so we have shown that

$$\partial_t S_3 = k\Delta S_3.$$

It follows that u given by (10.2) is a solution of the diffusion equation in (10.1), but we must show that it satisfies the initial conditions in (10.1) as well. For this we must take a limit as in section 3.5. We need to show that

$$(10.3) \quad u(\mathbf{x}, t) = \frac{1}{(4\pi kt)^{3/2}} \iiint \exp\left(-\frac{|\mathbf{z}|^2}{4kt}\right) f(\mathbf{x} + \mathbf{z}) d\mathbf{z} \rightarrow f(\mathbf{x}), \quad t \rightarrow 0,$$

where we have made the change of variables $\mathbf{z} = \mathbf{y} - \mathbf{x}$. If we make the further change of variables $\mathbf{y} = \mathbf{z}/\sqrt{4kt}$ we get

$$u(\mathbf{x}, t) = \frac{1}{(\pi)^{3/2}} \iiint \exp(-|\mathbf{y}|^2) f(\mathbf{x} + \mathbf{y}\sqrt{4kt}) d\mathbf{y}$$

If we subtract off $f(\mathbf{x})$ we get

$$u(\mathbf{x}, t) - f(\mathbf{x}) = \frac{1}{\pi^{3/2}} \iiint \exp(-|\mathbf{y}|^2) [f(\mathbf{x} + \mathbf{y}\sqrt{4kt}) - f(\mathbf{x})] d\mathbf{y}$$

since $\pi^{-3/2} \iiint e^{-|\mathbf{y}|^2} f(\mathbf{x}) d\mathbf{y} = f(\mathbf{x})\pi^{-3/2} \iiint e^{-|\mathbf{y}|^2} d\mathbf{y} = f(\mathbf{x})$. Suppose now that f satisfies

$$(10.4) \quad |f(\mathbf{x}) - f(\mathbf{y})| \leq K|\mathbf{x} - \mathbf{y}|$$

Then we can estimate

$$|u(\mathbf{x}, t) - f(\mathbf{x})| \leq \frac{1}{(\pi)^{3/2}} \iiint \exp(-|\mathbf{y}|^2) K|\mathbf{y}\sqrt{4kt}| d\mathbf{y} = K \frac{\sqrt{4kt}}{\pi^{3/2}} \iiint \exp(-|\mathbf{y}|^2) |\mathbf{y}| d\mathbf{y} = C\sqrt{t}.$$

(Here the integral is easily seen to be finite, e.g. by introducing spherical coordinates.)

When $t \rightarrow 0$ the right hand side tends to 0 so (10.3) follows. As far as the assumption (10.4). We have to make some assumption on f , say that its continuously differentiable. If in addition f has compact support or if the derivatives of f are uniformly bounded then (10.4) holds. However, its also possibly to get by with weaker assumptions.

Ex Find the solution to the diffusion equation with initial data $f(x, y, z) = xy^2z$:

$$\begin{aligned} u(x_0, y_0, z_0, t) &= \frac{1}{(4\pi kt)^{3/2}} \iiint \exp\left(-\frac{(x-x_0)^2 + (y-y_0)^2 + (z-z_0)^2}{4kt}\right) xy^2z \, dx dy dz \\ &= \frac{1}{(4\pi kt)^{3/2}} \iiint \exp\left(-\frac{x^2 + y^2 + z^2}{4kt}\right) (x+x_0)(y+y_0)^2(z+z_0) \, dx dy dz \\ &= \frac{1}{(4\pi kt)^{3/2}} \int e^{-x^2/4kt} (x+x_0) \, dx \int e^{-y^2/4kt} (y+y_0)^2 \, dy \int e^{-z^2/4kt} (z+z_0) \, dz \\ &= \frac{1}{(4\pi kt)^{3/2}} \int e^{-x^2/4kt} x_0 \, dx \int e^{-y^2/4kt} (y^2 + y_0^2) \, dy \int e^{-z^2/4kt} z_0 \, dz \end{aligned}$$

since the integral of odd powers cancel $\int e^{-x^2/4kt} x^{2k+1} \, dx = 0$. Moreover integrate by parts gives

$$\int e^{-y^2/4kt} y^2 \, dy = \int \frac{y}{2kt} e^{-y^2/4kt} 2kty \, dy = - \int e^{-y^2/4kt} 2kt \, dy = -2kt \int e^{-y^2/4kt} \, dy$$

Hence

$$u(x_0, y_0, z_0, t) = x_0(y_0^2 - 2kt)z_0 \frac{1}{(4\pi kt)^{3/2}} \int e^{-x^2/4kt} \, dx \int e^{-y^2/4kt} \, dy \int e^{-z^2/4kt} \, dz = x_0(y_0^2 - 2kt)z_0$$

Schrödinger equation. We claim that the fundamental solution for the Schrödinger equation in three space dimensions:

$$(10.5) \quad u_t = i\Delta u = i(u_{xx} + u_{yy} + u_{zz}), \quad u(\mathbf{x}, 0) = f(\mathbf{x}),$$

is given by

$$(10.7) \quad u(\mathbf{x}, t) = \frac{1}{(4\pi it)^{3/2}} \iiint \exp\left(-\frac{|\mathbf{x} - \mathbf{y}|^2}{4it}\right) f(\mathbf{y}) \, d\mathbf{y}.$$

Formally this is obtained by replacing k in (10.1)-(10.2) by the imaginary number i . However we must make a choice of square root $i^{1/2}$ in (10.6). For either possible choice $(i+1)/\sqrt{2}$ or $-(i+1)/\sqrt{2}$, (10.6) will satisfy the Schrödinger equation (10.4), but we must choose the square root in the right half plane $(i+1)/\sqrt{2}$ in order for the initial condition to be satisfied in (10.5). We will now see why the initial conditions are satisfied if we make this choice. We know that for k real and positive:

$$(10.7) \quad \frac{1}{(4\pi kt)^{3/2}} \iiint \exp\left(-\frac{|\mathbf{y}|^2}{4kt}\right) \, d\mathbf{y} = 1$$

The integral however converges absolutely for $\text{Re } k > 0$. Since both sides of (10.6) are analytic functions for $\text{Re } k > 0$ if we choose the square root with positive real part, they must be equal. Passing to the limit $k = i + \varepsilon$, $\varepsilon \rightarrow 0$, $\varepsilon > 0$, we get (10.7) with the square root defined with positive real part.