Heat Diffusion on Higher Dimensions

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1 Introduction and Outline

Heat equation in one-dimensional space is unarguably the most well-analyzed topic throughout the course of the semester. Needless to say, heat equation has great physical significance thanks to its capacity in modelling the diffusion of energy/particles, a key area of interest in particle diffusion, Brownian motion, and thermodynamics, to name but a few. However, it should be clearly realized that most physical activities occur on higher dimensions, specifically on 2D and 3D. Hence, as an attempt to expand the range of phenomenon that we can tackle with the help of heat equations, it is worthy of us to analyze how heat diffusion happen in higher dimensions.

In this final report, our group aims to derive heat equations on 1D, 2D, and 3D spaces, on unbounded regions and bounded regions, respectively. As a review and general setup, we will begin by discussing the derivation and general solution of 1D heat equation. Boundary conditions and their Sturm-Liouville problem setup will also be considered. Following from this, we will analyze the derivation and general solution of 2D heat equation. Diffusion on 2D disks (section 3.4) will be integral to our discussion. Visualization of 2D diffusion will also be presented. For bounded scenarios, several boundary conditions will be discussed. Armed with our previous conclusions, we will venture on to provide a complete and contingent investigation into heat diffusion on 3-dimensional space, assumptions applied. Aside from derivation of general solution, we will consider the solution to homogeneous heat equations. Our tour of inspection shall terminate after this.

Different mathematical toolboxes will be employed in our exploration. Fourier transforms, separation of variables, application of Sturm-Liouville problem, and solving eigenvalue problem, to name but a few, are among the most extensively used. They will prove to be essential in our analysis in addition.

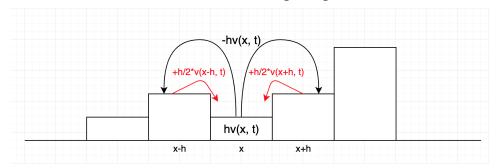
2 Heat Diffusion in 1D

2.1 1D heat diffusion on unbounded domains

2.1.1 Derivation

Since heat is the result of the movement of tiny particles in solids, liquids and gases, we are going to derive the heat equation by modeling diffusion as the random walk of particles.

Let v(x,t) be the concentration of particles at position x and time t. For a small $0 < h \ll 1$, hv(x,t) is approximately the number of particles on the interval $\left[x - \frac{h}{2}, x + \frac{h}{2}\right]$.



Assuming each particle moves one interval on the real axis to the left or to the right with equal probability $\frac{1}{2}$ and does not remain in the same position for time from t to $t + \tau$, where $0 < \tau \ll 1$ is a small time interval,

we have:

$$hv(x,t+\tau) = hv(x,t) + \frac{h}{2}v(x-h,t) + \frac{h}{2}v(x+h,t) - hv(x,t)$$

$$\Leftrightarrow \frac{v(x,t+\tau) - v(x,t)}{\tau} = \frac{h^2}{2\tau} \cdot \frac{v(x-h,t) - 2v(x,t) + v(x+h,t)}{h^2}$$
(1)

By expanding v(x-h,t) and v(x+h,t) in (1) using **Taylor series**, we get:

$$\frac{v(x,t+\tau) - v(x,t)}{\tau} = \frac{h^2}{2\tau} \cdot \frac{hv_x(x,t) + \frac{h^2}{2}v_{xx}(x,t) + (-h)v_x(x,t) + \frac{(-h)^2}{2}v_{xx}(x,t) + O(h^3)}{h^2}$$

$$\frac{v(x,t+\tau) - v(x,t)}{\tau} = \frac{h^2}{2\tau}(v_{xx} + O(h))$$
 (2)

Let $\frac{h^2}{2\tau} \to D$ as $h, \tau \to 0$, (2) converges to $v_t = Dv_{xx}$.

We usually choose an initial condition v(x,0) = f(x), where f(x) satisfies the following properties:

- f(x) can be differentiated infinitely many times.
- $\forall \alpha, \beta \in \mathbb{N}, \sup_{x \in R} |x^{\alpha} \frac{d^{\beta}}{dx^{\beta}} f(x)| < \infty$

Finally, we arrive at the 1D heat equation on an unbounded domain:

$$\begin{cases} v_t = Dv_{xx} & \text{for } x \in \mathbb{R}, t > 0 \\ v(x, 0) = f(x) & \text{for } x \in \mathbb{R} \end{cases}$$
 (3)

2.1.2 Solution

We apply Fourier transform with respect to x to our PDE (3):

$$\int_{-\infty}^{\infty} e^{ikx} v_t(x,t) dx = D \int_{-\infty}^{\infty} e^{ikx} v_{xx}(x,t) dx$$
$$\frac{\partial}{\partial t} \int_{-\infty}^{\infty} e^{ikx} v(x,t) dx = D \int_{-\infty}^{\infty} -ike^{ikx} v_x(x,t) dx$$
$$\frac{\partial}{\partial t} \hat{v}(k,t) = (-ik)^2 D \hat{v}(k,t)$$
$$\hat{v}(k,t) = \hat{v}(k,0) e^{-DK^2 t}$$

Given initial condition v(x,0) = f(x), we arrive at $\hat{v}(k,t) = \hat{f}(k)e^{-DK^2t}$. Apply the convolution with inverse Fourier transform, we get

$$v(x,t) = \mathcal{F}^{-1}(e^{-DK^2t}\hat{f}(k)) = (G*F)(x),$$

where $G(x,t) = \mathcal{F}^{-1}(e^{-DK^2t}) = \frac{1}{\sqrt{4\pi Dt}}e^{\frac{-x^2}{4Dt}}$ and $F(x) = \mathcal{F}^{-1}\hat{f}(k) = f(x)$ The solution v(x,t) of (3) is given by:

$$v(x,t) = \frac{1}{\sqrt{4\pi Dt}} \int_{-\infty}^{\infty} e^{\frac{-(x-y)^2}{4Dt}} f(y) dy$$

2.2 1D heat diffusion on bounded domains

When we are investigating the diffusion of heat on a bounded domain, e.g. a metal rod, our heat equation is only defined on an interval \mathcal{I} in \mathbb{R} :

$$\begin{cases} v_t = Dv_{xx} & \text{for } x \in \mathcal{I}, t > 0 \\ v(x,0) = f(x) & \text{for } x \in \mathcal{I} \end{cases}$$
Certain boundary conditions (BC) satisfied by $v(x,t)$

2.2.1 Sturm-Liouville Probelm

Recall that in class, we have constructed solutions to the heat equation as a Sturm-Liouville problem. The following is a brief summary of conclusions from the Sturm-Liouville problem for the sake of later use in our analysis.

Theorem 1. Consider a Sturm-Liouville problem given by:

$$\begin{cases} v_{xx} + q(x)v = \lambda v, & \text{for } a < x < b \\ v(a)\cos\alpha + v_x(a)\sin\alpha = 0 \\ v(b)\cos\beta + v_x(b)\sin\beta = 0 \end{cases}$$
 (5)

- 1. (5) has infinitely many solutions. The eigenvalues λ_n are all real, and we have $\lambda_n \to -\infty$ as $n \to \infty$
- 2. For each eigenvalue λ_n , there is a single linearly independent eigenfunction $v_n \in L^2(a,b)$
- 3. We have $\langle v_n, v_m \rangle = 0$ for $n \neq m$. This means that v_n and v_m are orthogonal.
- 4. for each $f \in L^2(a,b)$, we have $f = \sum_{n=1}^{\infty} a_n v_n$, where:

$$a_n = \frac{\langle f, v_n \rangle}{\|v_n\|_{L^2}^2} = \frac{1}{\|v_n\|_{L^2}^2} \int_a^b f(x)v_n(x)dx$$

Theorem 2. Consider (5), if f(x) is continuously differentiable on [a,b] and satisfy the boundary conditions that are part of the (5), then:

$$\lim_{N \to \infty} \max_{a \le x \le b} |f(x) - \sum_{n=1}^{N} a_n v_n(x)| = 0$$

Theorem 3. Assume that $f_n(x,t):[a,b]\times[T_0,T_1]\to\mathbb{R}$ can be differentiated infinitely often. Let $K,L\in\mathbb{N}$. If:

$$\lim_{N \to \infty} \sum_{n=N}^{\infty} \max_{\substack{a \le x \le b \\ T_0 < t < T_1}} \mid \frac{\partial^{k+l} f_n}{\partial x^k \partial t^l}(x,t) \mid = 0$$

for each $0 \le k \le K$, $0 \le l \le L$, then there is a function u(x,t) such that:

$$\lim_{N \to \infty} \max_{\substack{a \le x \le b \\ T_0 \le t \le T_1}} \mid \frac{\partial^{k+l} u}{\partial x^k \partial t^l}(x,t) - \sum_{n=1}^N \frac{\partial^{k+l} f_n}{\partial x^k \partial t^l}(x,t) \mid = 0$$

Moreover, $u(x,t) = \sum_{n=1}^{\infty} f_n(x,t)$ and its derivatives are continuous in (x,t). In other words, one can differentiate u(x,t) in terms of x and t as often as one likes.

2.2.2 Example: Dirichlet boundary condition

Consider the following system of equations:

$$\begin{cases} u_t = u_{xx} & \text{for } 0 < x < \pi, t > 0 \\ u(o, t) = 0 = u(\pi, t) & t > 0 \\ u(x, 0) = f(x) & 0 < x < \pi \end{cases}$$
(6)

It could be translated to an SL problem by plugging $u(x,t) = e^{\lambda t}v(x)$ into the system of equation. The SL problem kicks in the form of:

$$\begin{cases} \lambda v = v_{xx} & 0 < x < \pi \\ v(0) = 0 = v(\pi) & 0 < x < \pi \end{cases}$$

$$(7)$$

Solving (7), we can derive that:

$$u(x,t) = \sum_{n=1}^{\infty} a_n e^{-n^2 t} \sin nx,$$

where $\forall n \in \mathbb{Z}^+, a_n = \frac{2}{\pi} \int_0^{\pi} f(x) \sin nx \, dx$

By referring to the theorems, we can also know that:

- 1. $\max_{0 \le x \le \pi} |u(x,t)| \to 0 \text{ as } t \to \infty$
- 2. u(x,t) can be differentiated infinitely often in (x,t) for t>0, although this is not necessarily true for t=0.

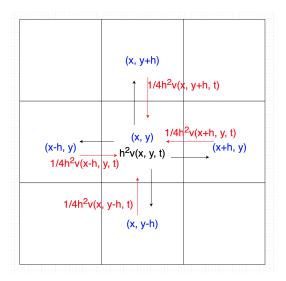
2.3 Wrap-up for 1D heat diffusion

Again, we would like to state the theorems because the SL problem will be one of our analytical focuses in solving 2D and 3D diffusion problems. We do not cover these theorems in depth since they are covered in class. At this stage, we believe that we can finish our tour of 1D heat diffusion, and we shall proceed with 2D heat diffusion models.

3 Heat Diffusion in 2D

3.1 Derivation

We are going to derive the heat equation from random walk of particles similar as above but on a plane. Consider a point (x, y) on a 2-D plane. For a small $0 < h \ll 1$, $[x - \frac{2}{h}, x + \frac{2}{h}] \times [y - \frac{2}{h}, y + \frac{2}{h}]$ would be the area around it. We can thus transform the plane into a grid composed of squares of length h and area h^2 . Let v(x, y, t) be the concentration of particles at position (x, y) at time t, then $h^2v(x, y, t)$ will be approximately the number of particles on that square area.



Assuming each particle moves one square to up, down, left, or right with equal probability $\frac{1}{4}$ and does not stay at the same position for time from t to $t + \tau$, we have:

$$\begin{split} &h^2v(x,y,t+\tau)\\ &=h^2v(x,y,t)-h^2v(x,y,t)+\frac{h^2v(x+h,y,t)}{4}+\frac{h^2v(x-h,y,t)}{4}+\frac{h^2v(x,y+h,t)}{4}+\frac{h^2v(x,y-h,t)}{4}\\ &=\frac{1}{4}h^2(v(x+h,y,t)+v(x-h,y,t)+v(x,y+h,t)+v(x,y-h,t)) \end{split}$$

By expanding v(x+h,y,t), v(x-h,y,t), v(x,y+h,t), v(x,y-h,t) with **Taylor Series**, we have:

$$v(x \pm h, y, t) = v(x, y, t) \pm hv_x(x, y, t) + \frac{h^2}{2}v_{xx}(x, y, t) + O(h^3)$$

$$v(x, y \pm h, t) = v(x, y, t) \pm hv_y(x, y, t) + \frac{h^2}{2}v_{yy}(x, y, t) + O(h^3)$$

$$\frac{1}{4}h^2(v(x + h, y, t) + v(x - h, y, t) + v(x, y + h, t) + v(x, y - h, t)) = h^2(v(x, y, t) + \frac{h^2}{4}(v_{xx} + v_{yy}) + O(h^3))$$
Then,
$$h^2v(x, y, t + \tau) = h^2(v(x, y, t) + \frac{h^2}{4}(v_{xx} + v_{yy}) + O(h^3))$$

$$\frac{v(x, y, t + \tau) - v(x, y, t)}{\tau} = \frac{h^2}{4\tau}(v_{xx} + v_{yy} + O(h))$$

Let $h, \tau \to 0$ in such a way that $\frac{h^2}{4\tau} \to c^2 > 0$, the above converges to $v_t = c^2(v_{xx} + v_{yy})$. Suppose the size of the plate is $a \times b$, then the equation is valid for 0 < x < a, 0 < y < b.

Let's then consider the boundary condition. The simplest would be homogeneous Dirichlet conditions where the density on each side is 0.

left and right side:
$$v(0, y, t) = v(a, y, t) = 0$$
, $0 \le y \le b, t \ge 0$
upper and lower side: $v(x, 0, t) = v(x, b, t) = 0$, $0 \le x \le a, t \ge 0$ (8)

Finally, the way the plate is heated initially could be given by the initial condition:

$$v(x, y, 0) = f(x, y), \quad (x, y) \in [0, a] \times [0, b]$$

To sum it up, we derive the heat equation in 2D:

$$\begin{cases} v_t = c^2(v_{xx} + v_{yy}), & 0 < x < a, 0 < y < b, t > 0 \quad (a) \\ v(0, y, t) = v(a, y, t) = 0, & 0 \le y \le b, t \ge 0 \quad (b) \\ v(x, 0, t) = v(x, b, t) = 0, & 0 \le x \le a, t \ge 0 \quad (c) \\ v(x, y, 0) = f(x, y), & (x, y) \in [0, a] \times [0, b] \quad (d) \end{cases}$$

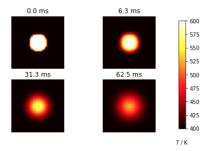
$$(9)$$

3.2 Visualization

Given the diffusion equation $v_t = c^2(v_{xx} + v_{yy})$ where c^2 is the diffusion coefficient. A simple numerical solution on the domain of the unit square $0 \le x < 1, 0 \le y < 1$ approximates v(x, y, t) by the discrete function $v_{i,j}^{(n)}$ where $x = i\Delta x, y = j\Delta y$ and $t = n\Delta t$. Applying finite difference approximations yields

$$\frac{v_{i,j}^{(n+1)} - v_{i,j}^{(n)}}{\Delta t} = c^2 \left[\frac{v_{i+1,j}^{(n)} - 2v_{i,j}^{(n)} + v_{i-1,j}^{(n)}}{(\Delta x)^2} + \frac{v_{i,j+1}^{(n)} - 2v_{i,j}^{(n)} + v_{i,j-1}^{(n)}}{(\Delta y)^2} \right]$$

Using the formula above, we can visualize how heat diffuse in 2D. Let's assume we have a 6×6 plane isolated from outer environment and the diffusion rate is $c^2 = 4$. The initial condition is that at the center of plane (3, 3), there is a circle of radius 1 having temperature 600 and the temperature of everywhere else is 400. With the help of JupyterLab [5], we get the following result:



3.3 Solution

3.3.1 Diffusion on 2D Rectangles

To solve (9), we first assume that v is separable so that v(x, y, t) = X(x)Y(y)T(t). Plugging into the heat equation (a) and boundary condition (b) (c), we get the following equations [2]:

$$X'' - BX = 0, X(0) = 0, X(a) = 0$$
(10)

$$Y'' - CY = 0, Y(0) = 0, Y(b) = 0$$
(11)

$$T' - c^2(B+C)T = 0 (12)$$

Now, let's look at them separately. The first equation (10), given by

$$X'' = BX$$

$$X(0) = 0 = X(a),$$

is a Sturm-Liouville problem! Therefore, we need to find all $B \in \mathbb{C}$ and non-trivial X(x) of the SL problem. By Theorem 1 from class, we know that $B \in \mathbb{R}$ and there is a single linearly independent solution X(x) for each B. There are three cases regarding the value of B [3]:

i. Let $B = -k^2$ for $k \in \mathbb{R}^+$. We then check whether $X(x) = \alpha \cos kx + \beta \sin kx$ satisfies X'' = BX:

LHS =
$$X''(x) = -\alpha k^2 \cos kx - \beta k^2 \sin kx$$

RHS = $BX = -k^2 (\alpha \cos kx + \beta \sin kx)$
 \Rightarrow LHS = RHS

We also check the boundary conditions:

$$X(0) = \alpha \cos 0 + \beta \sin 0 = \alpha \stackrel{!}{=} 0$$

$$\Rightarrow \alpha = 0$$

Hence, $X(x) = \beta \sin kx$ and we get:

$$X(a) = \beta \sin ka \stackrel{!}{=} 0$$

 $\Rightarrow b = 0 \text{ (trivial) or } \sin ka = 0$

Since we are looking for non-trivial X(x), we need to set $\sin ka = 0$, which implies that

$$ka = m\pi, \ m \in \mathbb{Z}^+$$

This is equivalent to $k = \frac{m\pi}{a}$. Therefore, $B_m = -k^2 = -\frac{m^2\pi^2}{a^2}$ with $X(x) = \sin m\pi x$ satisfies the SL problem for $m \in \mathbb{Z}^+$.

ii. Let $B = k^2$ for $k \in \mathbb{R}^+$. We then check whether $X(x) = \alpha e^{kx} + \beta e^{-kx}$ satisfies X'' = BX:

LHS =
$$X''(x) = \alpha k^2 e^{kx} + \beta (-k)^2 e^{-kx}$$

RHS = $BX = k^2 (\alpha e^{kx} + \beta e^{-kx})$
 \Rightarrow LHS = RHS

This is the general solution, since

$$e^{kx}(e^{-kx})' - (e^{kx})'e^{-kx} = -2ke^0 = -2k \neq 0$$
 for $k \neq 0$

We also check the boundary conditions:

$$X(0) = \alpha + \beta = 0$$

$$X(a) = \alpha e^{ka} + \beta e^{-ka} = 0$$

Since $\alpha + \beta = 0$, we have $\alpha = -\beta$. This implies that

$$X(a) = \alpha(e^{ka} - e^{-ka}) = 0$$

For $k \neq 0$, $e^{ka} - e^{-ka} \neq 0$, so α must be 0, i.e. $\alpha = \beta = 0$. Thus, X(x) is trivial in this case.

iii. Let B = 0. We then check whether $X(x) = \alpha + \beta x$ satisfies X'' = BX:

LHS =
$$X''(x) = (\alpha + \beta x)'' = 0$$

RHS = $BX = 0$
 \Rightarrow LHS = RHS

This is the general solution, since

$$1 \cdot \frac{\mathrm{d}x}{\mathrm{d}x} - \frac{\mathrm{d}1}{\mathrm{d}x}x = 1 - 0 = 1 \neq 0$$

We also check the boundary conditions:

$$X(0) = \alpha \stackrel{!}{=} 0$$

$$X(a) = \alpha + \beta a = \beta a \stackrel{!}{=} 0$$

Therefore, $\alpha = \beta = 0$, which means that X(x) is also trivial in this case.

Putting these together, we have all eigenvalues given by

$$B = -\mu_m^2, \ \mu_m = \frac{m\pi}{a}, \ m \in \mathbb{Z},$$

and the corresponding linearly independent eigenfunctions are

$$X_m(x) = \sin \mu_m x$$

On the other hand, the second equation (11), given by

$$Y'' = CX$$

$$Y(0) = 0 = Y(b),$$

is a Sturm-Liouville problem as well. By exactly the same argument, one can obtain all eigenvalues:

$$C = -\psi_n^2, \ \psi_n = \frac{n\pi}{b}, \ n \in \mathbb{Z},$$

and the corresponding linearly independent eigenfunctions are

$$Y_n(y) = \sin \psi_n y$$

Now, we have:

$$X_m(x) = \sin \mu_m x, \quad \mu_m = \frac{m\pi}{a}, \quad B = -\mu_m^2$$
$$Y_n(y) = \sin \psi_n y, \quad \psi_n = \frac{n\pi}{b}, \quad C = -\psi_n^2$$

Using these values in (12), we get

$$T_{mn}(t) = e^{-\lambda_{mn}^2 t} \text{ for } \lambda_{mn} = c\sqrt{\mu_m^2 + \psi_n^2} = c\pi\sqrt{\frac{m^2}{a^2} + \frac{n^2}{b^2}}$$
 (13)

Assembling these results, we find that for any pair $m, n \geq 1$ we have the normal mode

$$v_{mn}(x, y, t) = X_m(x)Y_n(y)T_{mn}(t) = \sin \mu_m x \sin \psi_n y e^{-\lambda_{mn}^2 t}$$

For any choice of constants A_{mn} , by the principle of superposition we then have the **general solution** to (9-a), (9-b), and (9-c) as:

$$v(x, y, t) = \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} A_{mn} \sin \mu_m x \sin \psi_n y e^{-\lambda_{mn}^2 t}$$

But what are the coefficients A_{mn} ? To figure out, we now need to determine the values of A_{mn} in order to satisfy the initial condition (9-d). Setting t = 0 and imposing the condition v(x, y, 0) = f(x, y) gives

$$f(x,y) = v(x,y,0) = \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} A_{mn} \sin \frac{m\pi}{a} x \cdot \sin \frac{n\pi}{b} y \cdot e^0 = \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} A_{mn} \sin \frac{m\pi}{a} x \cdot \sin \frac{n\pi}{b} y$$

Here, we denote $w_{mn}(x,y) = \sin \frac{m\pi}{a} x \cdot \sin \frac{n\pi}{b} y$, which are the eigenfunctions of the 2D Sturm-Liouville problem on a rectangle. Multiplying both sides by $w_{\hat{m}\hat{n}}(x,y)$ for dummy variables $\hat{m}, \hat{n} = 1, 2, 3, ...$ and integrating over the rectangle (denoted by D) gives

$$\iint_D f(x,y)w_{\hat{m}\hat{n}}(x,y)dA = \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} A_{mn} \iint_D w_{mn}(x,y)w_{\hat{m}\hat{n}}(x,y)dA,$$
(14)

where dA = dxdy. Then, notice that

$$\iint_{D} w_{mn}(x,y)w_{\hat{m}\hat{n}}(x,y)dA$$

$$= \int_{0}^{a} \sin\frac{m\pi}{a}x\sin\frac{\hat{m}\pi}{a}xdx \times \int_{0}^{b} \sin\frac{n\pi}{b}y\sin\frac{\hat{n}\pi}{b}ydy$$

$$= \begin{cases} \frac{ab}{4}, & \text{if } m = \hat{m} \text{ and } n = \hat{n} \\ 0, & \text{otherwise} \end{cases}$$

Thus, (14) becomes

$$\iint_D f(x,y)w_{\hat{m}\hat{n}}(x,y) dA = \frac{ab}{4} A_{\hat{m}\hat{n}}$$

Since \hat{m}, \hat{n} are dummy variables, we can replace \hat{m}, \hat{n} by m, n respectively to obtain

$$A_{mn} = \frac{4}{ab} \iint_D f(x, y) w_{\hat{m}\hat{n}}(x, y) dA$$
$$= \frac{4}{ab} \int_0^a \int_0^b f(x, y) \sin \frac{m\pi}{a} x \cdot \sin \frac{n\pi}{b} y dy dx$$

To sum up, the solution to (9), including diffusion equation, boundary condition, and initial condition would be the following:

$$\begin{cases} v(x,y,t) = \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} A_{mn} \sin \mu_m x \sin \psi_n y \, e^{-\lambda_{mn}^2 t} \\ A_{mn} = \frac{4}{ab} \int_0^a \int_0^b f(x,y) \sin \frac{m\pi}{a} x \sin \frac{n\pi}{b} y \, \mathrm{d}y \mathrm{d}x \end{cases}$$
(15)

where $\mu_m = \frac{m\pi}{a}$, $\psi_n = \frac{n\pi}{b}$, and $\lambda_{mn} = c\sqrt{\mu_m^2 + \psi_n^2}$

3.3.2 Diffusion on 2D Disks

Suppose we are given a circular, planar disk of radius R > 0 whose initial temperature is a univariate function f(r) that only depend on the distance of a point on the disk to the center of the disk. The diffusion itself occurs in the same way as described in section 3.1: $u_t = c^2(u_{xx} + u_{yy})$, where $c^2 := k > 0$ as the diffusivity and u(x, y, t) is our solution to heat diffusion.

For simplicity, we transform (x,y) to polar coordinates (r,θ) by $\begin{cases} x = r\cos\theta \\ y = r\sin\theta \end{cases}$. The solution u becomes a

function of radius r, angle θ and time t, i.e. $u(r, \theta, t)$. We perform the differentiation with respect to r and θ using for our 'new' solution u(x, t).

$$\frac{\partial u}{\partial r} = \frac{\partial u}{\partial x} \cdot \frac{\partial x}{\partial r} + \frac{\partial u}{\partial y} \cdot \frac{\partial y}{\partial r} = \cos \theta \cdot \frac{\partial u}{\partial x} + \sin \theta \cdot \frac{\partial u}{\partial y}$$

$$\begin{split} \frac{\partial^2 u}{\partial r^2} &= \frac{\partial}{\partial r} (\frac{\partial u}{\partial r}) = \frac{\partial}{\partial r} (\cos \theta \cdot \frac{\partial u}{\partial x} + \sin \theta \cdot \frac{\partial u}{\partial y}) \\ &= \cos \theta (\frac{\partial^2 u}{\partial x^2} \cdot \frac{\partial x}{\partial r} + \frac{\partial^2 u}{\partial x \partial y} \cdot \frac{\partial y}{\partial r}) + \sin \theta (\frac{\partial^2 u}{\partial x \partial y} \cdot \frac{\partial x}{\partial r} + \frac{\partial^2 u}{\partial y^2} \cdot \frac{\partial y}{\partial r}) \\ &= \cos^2 \theta \frac{\partial^2 u}{\partial x^2} + 2 \sin \theta \cos \theta \frac{\partial^2 u}{\partial x \partial y} + \sin^2 \theta \frac{\partial^2 u}{\partial y^2} \end{split}$$

$$\frac{\partial u}{\partial \theta} = \frac{\partial u}{\partial x} \cdot \frac{\partial x}{\partial \theta} + \frac{\partial u}{\partial y} \cdot \frac{\partial y}{\partial \theta} = -r \sin \theta \frac{\partial u}{\partial x} + r \cos \theta \frac{\partial u}{\partial y}$$

$$\begin{split} \frac{\partial^2 u}{\partial \theta^2} &= \frac{\partial}{\partial \theta} (\frac{\partial u}{\partial \theta}) = \frac{\partial}{\partial \theta} (-r \sin \theta \frac{\partial u}{\partial x} + r \cos \theta \frac{\partial u}{\partial y}) \\ &= [-r \cos \theta \frac{\partial u}{\partial x} - r \sin \theta (-r \sin \theta \frac{\partial^2 u}{\partial x^2} + r \cos \theta \frac{\partial^2 u}{\partial x \partial y})] + [-r \sin \theta \frac{\partial u}{\partial y} + r \cos \theta (-r \sin \theta \frac{\partial^2 u}{\partial x \partial y} + r \cos \theta \frac{\partial^2 u}{\partial y^2})] \\ &= -r (\cos \theta \frac{\partial u}{\partial x} + \sin \theta \frac{\partial u}{\partial y}) + r^2 (\sin^2 \theta \frac{\partial^2 u}{\partial x^2} - 2 \sin \theta \cos \theta \frac{\partial^2 u}{\partial x \partial y} + \cos^2 \theta \frac{\partial^2 u}{\partial y^2}) \end{split}$$

By observation, the first part of $\frac{\partial^2 u}{\partial \theta^2}$ contains $\frac{\partial u}{\partial r}$ and the second part of $\frac{\partial^2 u}{\partial \theta^2}$ can cancel with $\frac{\partial^2 u}{\partial r^2}$:

$$\begin{split} \frac{\partial^2 u}{\partial r^2} + \frac{1}{r^2} \cdot \frac{\partial^2 u}{\partial \theta^2} &= \cos^2 \theta \frac{\partial^2 u}{\partial x^2} + 2 \sin \theta \cos \theta \frac{\partial^2 u}{\partial x \partial y} + \sin^2 \theta \frac{\partial^2 u}{\partial y^2} \\ &- \frac{1}{r} \cdot \frac{\partial u}{\partial r} + \sin^2 \theta \frac{\partial^2 u}{\partial x^2} - 2 \sin \theta \cos \theta \frac{\partial^2 u}{\partial x \partial y} + \cos^2 \theta \frac{\partial^2 u}{\partial y^2} \\ &= -\frac{1}{r} \cdot \frac{\partial u}{\partial r} + (\sin^2 \theta + \cos^2 \theta) \frac{\partial^2 u}{\partial x^2} + (\sin^2 \theta + \cos^2 \theta) \frac{\partial^2 u}{\partial y^2} \\ &= -\frac{1}{r} \cdot \frac{\partial u}{\partial r} + (\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}) \end{split}$$

This gives $u_{xx} + u_{yy} = u_{rr} + \frac{1}{r}u_r + \frac{1}{r^2}u_{\theta\theta}$. It follows that $u_t = k(u_{xx} + u_{yy}) = k(u_{rr} + \frac{1}{r}u_r + \frac{1}{r^2}u_{\theta\theta})$. The heat equation on a disk written by polar coordinates is:

$$\begin{cases} u_t = k(u_{rr} + \frac{1}{r}u_r + \frac{1}{r^2}u_{\theta\theta}) & k > 0, t > 0, 0 \le r < R \\ u(r,0) = f(r) & 0 \le r < R \end{cases}$$
Some Boundary Condition for $r = R$ (16)

We assume that the initial condition f(r) that we choose entails high temperature at (or around) the center of the disk [4]. Then the heat would emanate from the center along the line the radius is on, pointing away from the center. Hence, there is no angular diffusion that we need to consider, and we can simplify our solution form to u(r,t). The $u_{\theta\theta}$ term inside of our PDE vanishes. Here we proceed with the Dirichlet Boundary Condition u(R,t)=0. This boundary condition corresponds to the scenario of cooling a disk, since heat energy escapes from the disk at its boundary.

One way to tackle this problem is to use the **separation of variables**. Suppose our solution u(r,t) can be written as the product of two univariate functions v(r) and w(t), i.e. u(r,t) = y(r)g(t). Substituting this into the PDE, we obtain:

$$LHS = u_t = y(r)g'(t) \quad RHS = k(u_{rr} + \frac{1}{r}u_r) = kg(t)(y''(r) + \frac{1}{r}y'(r))$$

$$LHS = RHS \Rightarrow y(r)g'(t) = kg(t)(y''(r) + \frac{1}{r}y'(r)) \Leftrightarrow \frac{g'(t)}{kq(t)} = \frac{y''(r) + \frac{1}{r}y'(r)}{y(r)} := -\lambda$$

Solving $\frac{g'(t)}{kg(t)} = -\lambda$, we have $g(t) = e^{-\lambda kt}$. Hence, the bulk is to solve $\frac{y''(r) + \frac{1}{r}y'(r)}{y(r)} = -\lambda$.

Hence, the bulk is to solve
$$\frac{y''(r) + \frac{1}{r}y'(r)}{y(r)} = -\lambda$$

$$\Leftrightarrow ry''(r) + y'(r) = -\lambda ry(r)$$

$$\Leftrightarrow -(ry')' = \lambda ry \qquad \text{(Sturm-Liouville Problem)}$$

$$\Leftrightarrow \int_0^R -(ry')'y \, dr = \lambda \int_0^R ry^2 \, dr \quad \text{(multiply by } y \text{ then integrate)}$$

$$\Leftrightarrow -ry'y \Big|_0^R + \int_0^R r(y')^2 \, dr = \lambda \int_0^R ry^2 \, dr$$

$$\Leftrightarrow (-Ry'(R) \cdot 0) - (-0 \cdot y'(0)y(0)) + \int_0^R r(y')^2 \, dr = \lambda \int_0^R ry^2 \, dr$$

Since $\int_0^R r(y')^2 dr \ge 0$ and $\int_0^R ry^2 dr \ge 0$, $\lambda \ge 0$.

When $\lambda = 0$, we have $g(t) = e^0 = 1$ and $-(ry')' = 0 \cdot ry = 0$. Further solving for y(r):

$$-ry' = b \Rightarrow y' = -\frac{b}{r} \Rightarrow y(r) = a + b \ln r \quad (a, b \in \mathbb{R})$$

Since r=0 is possible, we have b=0. Since u(R,t)=y(R)g(t)=0 for all t>0 (Dirichlet Boundary Condition), we have y(R) = 0 = a. Hence a = b = 0. The solution is trivial when $\lambda = 0$.

Therefore, we consider the case where $\lambda > 0$.

We have $\frac{y''(r) + \frac{1}{r}y'(r)}{y(r)} = -\lambda \Leftrightarrow r^2 \frac{d^2y}{dr^2} + r \frac{dy}{dr} + \lambda r^2 y(r) = 0.$ Let $x = \sqrt{\lambda}r$. Then $r = \frac{x}{\sqrt{\lambda}}, \frac{dx}{dr} = \sqrt{\lambda}, \frac{dy}{dr} = \sqrt{\lambda} \frac{dy}{dx}, \frac{d^2y}{dr^2} = \frac{d}{dr}(\frac{dy}{dr}) = \lambda \frac{d^2y}{dx^2}$. The above becomes:

$$x^{2}\frac{d^{2}y}{dx^{2}}(x) + x\frac{dy}{dx}(x) + x^{2}y(x) = 0$$
(17)

We proceed with **Frobenius Method** and suppose $y = x^{\alpha}(a_0 + a_1x + a_2x^2 + \ldots + a_kx^k + \ldots) = \sum_{k=0}^{\infty} a_kx^{k+\alpha}$ where $\alpha \in \mathbb{N}$, $a_i \in \mathbb{R}$ ($\forall i \in \mathbb{N}$) and $a_0 \neq 0$. Then, the **Bessel equation** (17) reads:

$$x^{2} \sum_{k=0}^{\infty} (k+\alpha)(k+\alpha-1)a_{k}x^{k+\alpha-2} + x \sum_{k=0}^{\infty} (k+\alpha)a_{k}x^{k+\alpha-1} + x^{2} \sum_{k=0}^{\infty} a_{k}x^{k+\alpha} = 0$$

$$\Leftrightarrow \sum_{k=0}^{\infty} (k+\alpha)^{2} a_{k}x^{k+\alpha} + \sum_{k=0}^{\infty} a_{k}x^{k+\alpha+2} = 0$$

$$\Leftrightarrow \alpha^{2} a_{0}x^{\alpha} + (\alpha+1)^{2} a_{1}x^{\alpha+1} + \sum_{k=2}^{\infty} ((k+\alpha)^{2} a_{k} + a_{k-2})x^{k+\alpha} = 0$$

Since the above holds for all values of x that satisfies $0 \le \frac{x}{\sqrt{\lambda}} < R$, we let the coefficients of x equal to zero: $\alpha^2 a_0 = (\alpha + 1)^2 a_1 = (k + \alpha)^2 a_k + a_{k-2} = 0 \text{ for } k = 2, 3, \dots$

This yields $\alpha=0, a_1=a_3=a_5=\ldots=0, a_k=\frac{-a_{k-2}}{k^2}$. Let k=2m for $m=1,2,\ldots$, we have: $a_{2m}=\frac{(-1)^m a_0}{2^{2m}(m!)^2}$. Then, we have our solution $y=a_0\sum_{m=0}^{\infty}\frac{(-1)^m}{m!\Gamma(m+1)}(\frac{x}{2})^{2m}$, since $\Gamma(m+1)=m!$ for $m\in\mathbb{N}$.

The first kind of Bessel function has the form $J_{\nu}(x)=\sum_{n=0}^{\infty}\frac{(-1)^n}{n!\Gamma(n+\nu+1)}(\frac{x}{2})^{2n+\nu}$ [1], where ν is its order.

The solution y we have corresponds to the Bessel function with $\nu = 0$. Hence, we have:

$$y(r) = a_0 J_0(\sqrt{\lambda}r) = a_0 \sum_{m=0}^{\infty} \frac{(-1)^m}{m!\Gamma(m+1)} (\frac{\sqrt{\lambda}r}{2})^{2m}$$
(18)

Now we apply the boundary condition to (18), we have $y(R) = a_0 J_0(\sqrt{\lambda}R) = 0$. Hence, $\sqrt{\lambda}R = z_n, n = 0$ $1, 2, 3, \ldots$, where z_n are the zeros of the Bessel function of first kind with order 0.

Therefore, the eigenvalues $\lambda_n = \frac{z_n^2}{R^2}, n = 1, 2, 3, \dots$ with the corresponding eigenfunctions $y_n(r) = J_0(\frac{z_n r}{R})$ and $g_n(t) = e^{-\lambda_n kt}$. Now that we have found infinitely many solutions to the PDE and its boundary condition, we can use the superposition principle of solutions to construct the general solution:

$$u(r,t) = \sum_{n=1}^{\infty} c_n e^{-\frac{z_n^2}{R^2}kt} J_0(\frac{z_n r}{R}), \text{ where } c_n \in \mathbb{R} \text{ are determined by } f(r)$$

The calculation of c_n can be done by the **orthogonality of Bessel functions with respect to the weight** function r [4]. That is $\int_0^R J_0(\frac{z_n r}{R}) J_0(\frac{z_m r}{R}) r \, dr = 0$ for $n \neq m$. The proof is as following:

Let $n, m \in \mathbb{Z}^+$ s.t. $n \neq m$. Denote the corresponding eigenvalues as λ_m, λ_n and the component Bessel functions as v_m, v_n , respectively. Since both pairs satisfy $-(ry')' = \lambda ry$, we obtain:

$$-(ry'_m)' = \lambda_m ry_m \dots (m), -(ry'_n)' = \lambda_n ry_n \dots (n)$$

By $y_n * (m) - y_m * (n)$, we get: $-y_n(ry'_m)' + y_m(ry'_n)' = (\lambda_m - \lambda_n)ry_my_n$. Integrate on both sides:

$$\int_0^R [-y_n(ry'_m)' + y_m(ry'_n)'] dr = (\lambda_m - \lambda_n) \int_0^R ry_m y_n dr$$

We focus on the LHS of above, and integrate it by parts using y(r) = 0:

$$\int_0^R \left[-y_n (ry'_m)' + y_m (ry'_n)' \right] dr = \left(-ry_n y'_m + ry_m y'_n \right) \Big|_0^R - \int_0^R \left(-ry'_n y'_m + ry'_m y'_n \right) dr = (0 - 0) + \int_0^R 0 \, dr = 0$$

Hence, $RHS = 0 = (\lambda_m - \lambda_n) \int_0^R r y_m y_n dr$. We have assumed $\lambda_m \neq \lambda_n$, so we obtain:

$$\int_0^R r y_m y_n \, dr = 0 \quad n \neq m \tag{19}$$

The final step is to satisfy the initial condition f(r). By Theorem 1 when addressing the Sturm-Liouville problem, we can calculate coefficients $c_n(n = 1, 2, 3, ...)$ with the following:

$$f(r) = \sum_{n=1}^{\infty} c_n J_0(\frac{z_n r}{r})$$

$$\Leftrightarrow f(r) J_0(\frac{z_m r}{r}) r = J_0(\frac{z_m r}{r}) r \sum_{n=1}^{\infty} c_n J_0(\frac{z_n r}{r}) \quad \forall m \in \mathbb{Z}^+$$

$$\Leftrightarrow \int_0^R f(r) J_0(\frac{z_m r}{r}) r \, dr = \sum_{n=1}^{\infty} c_n \int_0^R J_0(\frac{z_n r}{r}) J_0(\frac{z_m r}{r}) r \, dr$$

$$\Leftrightarrow \int_0^R f(r) J_0(\frac{z_m r}{r}) r \, dr = 0 + \dots + 0 + c_m \int_0^R J_0(\frac{z_m r}{r}) J_0(\frac{z_m r}{r}) r \, dr + 0 + \dots + 0 \quad \text{by (19)}$$

This gives us (by changing m to n):

$$c_n = \frac{\int_0^R f(r)J_0(\frac{z_n r}{R})r \, dr}{\int_0^R (J_0(\frac{z_n r}{R}))^2 r \, dr} \quad \forall n \in \mathbb{Z}^+$$

Conclusion: The solution to the following system $\begin{cases} u_t = k(u_{rr} + \frac{1}{r}u_r) & k > 0, t > 0, 0 \le r < R \\ u(r,0) = f(r) & 0 \le r < R \\ u(R,t) = 0 & t > 0 \end{cases}$ can be

written as:

$$u(r,t) = \sum_{n=1}^{\infty} \frac{\int_0^R f(r) J_0(\frac{z_n r}{R}) r \, dr}{\int_0^R (J_0(\frac{z_n r}{R}))^2 r \, dr} e^{-\frac{z_n^2}{R^2} kt} J_0(\frac{z_n r}{R}),$$

where $J_0(x) = \sum_{m=0}^{\infty} \frac{(-1)^m}{m!\Gamma(m+1)} (\frac{x}{2})^{2m}$ is the first kind Bessel function with order $\nu = 0$ and z_n $(n \in \mathbb{Z}^+)$ are its zeros.

4 Heat Diffusion on 3D

4.1 Derivation

Let Ω be an isotropic region composed of the same material in \mathbb{R}^3 where heat diffusion occurs. Denote its boundary as $\partial\Omega$. Denote its density and specific heat of as ρ and c. Let u(x,y,z,t) be the temperature at time t>0 at point $(x,y,z)\in\Omega\setminus\partial\Omega$. Let B be an arbitrary sphere in Ω .

The Conservation of Energy implies that:

Change of energy in system = Energy flux - Energy generated

We shall set up the three components of the above law for the arbitrary sphere B by considering the following:

1. Heat of B is given by

$$H_B = \iiint_B c\rho u \, dV$$

- 2. Denote the rate at which point (x, y, z) is generating heat at time t is denoted by the real-valued function f = f(x, y, z, t). If f > 0 at (x, y, z) then this point is a heat source; similarly, f < 0 implies a heat sink (absorber). The rate at which heat is generated in B is: $\iiint_B f \, dV$.
- 3. Denote $\Phi(x, y, z, t)$ as the heat flux at (x, y, z) at time t and its direction follows the heat flow. We assume that heat is emanating from B. Then the heat flow across the surface of B is given by:

$$\int_{\partial B} \Phi \cdot \vec{n} \, dA,$$

where \vec{n} is the normal vector over the surface.

By Gauss's Divergence Theorem,

$$\int_{\partial B} \Phi \cdot \vec{n} \, dA = \iiint_{B} \nabla \cdot \Phi dV$$

Hence, we obtain the equation of heat balance:

$$\frac{d}{dt} \iiint_{B} c\rho u \, dV = -\iiint_{B} \nabla \cdot \Phi \, dV + \iiint_{B} f \, dV$$

$$\Leftrightarrow \iiint_{B} (c\rho u_{t} + \nabla \cdot \Phi - f) \, dV = 0$$

This balance equation must hold for all $(x, y, z) \in \Omega$ and t > 0, since we can let $V_B \to 0$.

By **Fick's Law** in 3D, $\Phi = -D \cdot \nabla u$, where u is the concentration of the diffusing entity, and D > 0 is the diffusion coefficient. Then $\nabla \cdot \Phi = -D \cdot \nabla (\nabla u) = -D(u_{xx} + u_{yy} + u_{zz})$

Therefore, we obtain the heat equation for each point $(x, y, z) \in \Omega$ at time t > 0 as following:

$$c\rho u_t - D(u_{xx} + u_{yy} + u_{zz}) - f = 0$$

Let $\Delta u = u_{xx} + u_{yy} + u_{zz}$. We have:

$$c\rho u_t - D\Delta u = f$$

$$\Leftrightarrow u_t - k\Delta u = \frac{1}{c\rho} f, \text{ where } k = \frac{D}{c\rho} \text{ is the diffusivity of the medium.}$$
(20)

Note that in even higher dimensions (e.g. \mathbb{R}^n), the equation (20) still holds, yet u would be $u: \mathbb{R}^n \times [0, \infty) \to \mathbb{R}$ and the same for f.

As in the 1D scenario, the initial condition for heat equation in 3D is:

$$u(x, y, z, 0) = u_0(x, y, z)$$
 for $(x, y, z) \in \Omega \setminus \partial \Omega$.

4.2 Solution on Unbounded Domains, Homogeneous

For simplicity, let's consider the case where there is no heat source within the system, i.e. $f(x, y, z, t) = 0 \ \forall x, y, z \in \mathbb{R}, t \in \mathbb{R}^+$. Then, the problem becomes

$$\begin{cases} u_t = a^2 \Delta u = a^2 (u_{xx} + u_{yy} + u_{zz}) \\ u(x, y, z, 0) = \phi(x, y, z) \end{cases}$$
 (21)

Note that we write $k = a^2$ (a > 0) here since $k = \frac{D}{c\rho} > 0$.

We apply the Fourier transform with respect to x, y, z to our PDE and the initial condition (21), and denote them by:

$$\hat{u}(\lambda_1, \lambda_2, \lambda_3, t) = \mathcal{F}[u(x, y, z, t)]$$
$$\hat{\phi}(\lambda_1, \lambda_2, \lambda_3) = \mathcal{F}[\phi(x, y, z)]$$

In this way, we get

$$\begin{cases} \frac{\mathrm{d}\hat{u}}{\mathrm{d}t} = -a^2(\lambda_1^2 + \lambda_2^2 + \lambda_3^2)\hat{u} \\ \hat{u}(\lambda_1, \lambda_2, \lambda_3, 0) = \hat{\phi}(\lambda_1, \lambda_2, \lambda_3) \end{cases}$$
(22)

This becomes an ODE, where t is the only independent variable, and $\lambda_1, \lambda_2, \lambda_3$ are 3 parameters generated by the Fourier transform. Solve (22) using separation of variables, and we get

$$\hat{u}(\lambda_1, \lambda_2, \lambda_3, t) = \phi((\lambda_1, \hat{\lambda}_2, \lambda_3))e^{-a^2(\lambda_1^2 + \lambda_2^2 + \lambda_3^2)t}$$

Analogous to how we solve one-dimensional heat equation, we now need to apply the inverse Fourier transform with the convolution theorem. That is,

$$u(x, y, z, t) = (G * \phi)(x, y, z, t),$$

where

$$G(x, y, z, t) = \mathcal{F}^{-1}[e^{-a^2(\lambda_1^2 + \lambda_2^2 + \lambda_3^2)t}]$$

$$= \frac{1}{(2\pi)^3} \iiint_{\mathbb{R}^3} e^{-a^2(\lambda_1^2 + \lambda_2^2 + \lambda_3^2)t} e^{i(\lambda_1 x + \lambda_2 y + \lambda_3 z)} d\lambda_1 d\lambda_2 d\lambda_3$$

$$= \frac{1}{(2a\sqrt{\pi t})^3} \exp(-\frac{x^2 + y^2 + z^2}{4a^2t})$$

Therefore, the solution u(x, y, z, t) to the PDE with the initial condition is given by

$$u(x, y, z, t) = \frac{1}{(2a\sqrt{\pi t})^3} \iiint_{\mathbb{R}^3} \phi(\xi, \eta, \zeta) e^{-\frac{(x-\xi)^2 + (y-\eta)^2 + (z-\zeta)^2}{4a^2t}} d\xi d\eta d\zeta$$
$$= \frac{1}{(\sqrt{4k\pi t})^3} \iiint_{\mathbb{R}^3} \phi(\xi, \eta, \zeta) e^{-\frac{(x-\xi)^2 + (y-\eta)^2 + (z-\zeta)^2}{4kt}} d\xi d\eta d\zeta$$

5 Summary and Conclusions

In our final project, we presented our findings regarding heat diffusion in 1D, 2D, and 3D spaces in order. The endeavor is fruitful, and it, without any doubt, strengthened and consolidated our understanding on probably the most thoroughly covered topic in the course.

In our analysis concerning 2D heat diffusion, we have shown the derivation process of the general solution using random walk model and Taylor expansion, with several assumptions such as the separability of the expression v being made. We visualized the diffusion of heat on a 6×6 plane via JupyterLab. Using distinct approaches, we also explored the diffusion of heat on a circular, planar disk of radius R, and a rectangle, with given initial conditions, and succeeded in providing an account of the equation as precisely as possible. Mathematical methods such as Frobenius Method and Bessel equation were employed in our discussion.

Following from this, we set up our general derivation of 3D heat diffusion by applying the conservation of energy, divergence theorem, and Fick's law, to name a few. We considered the homogeneous case and were able to offer an discussion of this scenario at the very end of our presentation, finishing our inspection into the topic.

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