THERMAL DISTRIBUTIONS AROUND AN INSULATED BARRIER AT THE INTERFACE OF GRADED COATING AND A HOMOGENEOUS SUBSTRATE

by

Nurdane GÜDÜK

July 2006

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APPROVAL PAGE

I certify that this thesis satisfies all the requirements as a thesis for the degree of Master of Science.

____
Assist.Prof.Dr. Ali ŞAHİN

This is to certify that I have read this thesis and in my opinion it is fully adequate, in scope and quality, as a thesis for the degree of Master of Science.

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July 2006

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M.S. Thesis-Mathematics Department
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Supervisor: Assist. Prof. Dr. Ali ŞAHİN

ABSTRACT

The main purpose of this study is to examine the effect of thermal flux or heat applied to an insulated barrier at the interface between the inhomogeneous composite coating and homogeneous metallic substrate. Using the superposition method the geometry was simplified and then applying Fourier integral transform method to steady state nonlinear heat conduction equation the problem was translated to the solution of an integral equation with Cauchy type of singularity. Eliminating the singularities with known numerical techniques the thermal distribution around the barrier was obtained in terms of orthogonal polynomials. The effect of inhomogeneity and thickness parameters was shown in figures. The obtained results could be used to evaluate the stress distribution around the barrier and also stresses are stimulated to find stress intensity factors on the barrier (at this point barrier turns to crack).

Keywords: Composite Materials, Heat Equation, Integral Transform, Cauchy type Singularity, Thermal Distribution.

DERECELENDİRİLMİŞ TABAKA VE HOMOJEN ORTAM ARASINDAKİ YÜZEYDE İZOLE EDİLMİŞ BİR BARİYERİN ETRAFINDAKİ ISI DAĞILIMI

Nurdane GÜDÜK

Yüksek Lisans Tezi-Matematik Bölümü
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Tez Danışmanı: Yrd.Doç.Dr. Ali ŞAHİN

ÖZET

Bu çalışmanın asıl amacı homojen olmayan malzemeden oluşmuş bir tabaka ile homojen olan metal bir malzeme arasındaki izole edilmiş bir bariyerin yüzeyine uygulanan termik akışın veya ısının etkisini incelemektir. Süperpozisyon metodu kullanılarak problem basitleştirilmiş, zamandan bağımsız lineer olmayan ısı denklemine Fourier integral transform metodu uygulanılarak problem Cauchy tipinde tekil integral denklemin çözümüne indirgenmiştir. Tekilliklerin bilinen nümerik tekniklerle yok edilmesi sonucu bariyer etrafındaki ısı dağılımı ortogonal polinomlar cinsinden elde edilmiştir. Homojen olmayan malzemenin ve kalınlığının parametrelerinin etkisi figürlerde gösterilmiştir. Elde edilen sonuçlar bariyer etrafındaki gerilimlerin şiddetlerinin hesabınde kullanılabilirler ve hatta bu gerilimler bariyerin üzerindeki gerilim yoğunluk faktörlerinin bulunmasında kullanılabilirler.

Anahtar Kelimeler: Komposit malzemeler, ısı denklemi, integral dönüşümleri, Cauchy tekillikleri, sıcaklık dağılımı.

DEDICATION

To my parents

ACKNOWLEDGEMENT

I express my thanks to Assist. Prof. Dr. Ali ŞAHİN for all his done. For his patience and understanding to complete for this study.

I express my thanks to my family for their motivation.

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CHAPTER 1

INTRODUCTION

The concept of various types of composites and bonded materials which are progressively changing properties to improve material performance has been used in many technological applications such as microelectronics, transportation and aerospace. Due to severe environment conditions, conventional materials do not seem to be adequate to meet the requirements of new technologies. The new developments in science and technology are heavily depend on new materials like composites, intermetallics and alloys to provide the necessary flexibility in the design and processing of these new materials. For most of the industrial applications, in which the uniformity in material properties is a general requirement, it is essential that every part of the material in use exhibits uniform properties. Last decades the considerable effort in development of composites has been put into determining how to uniformly mix the dispersoid within the matrix [1].

Composite materials can be prepared using several techniques including Chemical Vapor Deposition (CVD), Physical Vapor deposition (PVD), etc. Over the past several decades considerable progress has been made in using ceramic coatings to protect metallic components from high temperature environments. As a result of such coating progress some metallic parts in a surface of spacecraft can be protected as high as $1700^{\circ}C$, while the inside is cooled to about $700^{\circ}C$. The success of spacecraft construction relies on the successful ceramic coatings, commonly referred to as Thermal Barrier Coatings (TBCs), which can protect the craft from severe environments. Most TBCs are structurally as well as functionally complex and, therefore, should be considered and studied as a material system. TBC system can be used, for example, in aircraft engines typically that consist of a thick thermally insulating ceramic layer on the metallic substrate.

From a practical standpoint, the conventional approach for accommodating the material mismatch between the metallic substrate and ceramic coating is to make the ceramic layer compliant by incorporating structural defects, such as microcracks and porosity as well as vertically segmented columns. However, in terms of achieving long-term durability, several major problems are associated with the presence of these microstructural defects. Thus, increased temperature and prolonged time exposure become an important issue, resulting in, for example, increase in thermal conductivity and decrease in coating compliance.

In high temperature applications, which is one of the important technological areas, metals and metal alloys appear to be very susceptible to oxidation, creep and generally to loss of structural integrity. Low strength and low toughness have always been the disadvantages of ceramics. Thus, as an alternative to conventional thermal barrier ceramic coatings, in 1980's the concept of Functionally Graded Materials (FGMs) was proposed. For extensive information see [2-26].

FGMs are very attractive for high temperature applications and wear protective coatings. It is essentially two-phase particulate composites synthesized in such a way that the volume fractions of the constituents vary continuously in the thickness direction to give a predetermined composition profile. The composition profile which varies from 0% ceramic at the interface to 100% ceramic near the surface, in turn, is selected in such a way that the resulting nonhomogeneous material exhibits the desired thermomechanical properties. The concept of FGMs could provide great flexibility in material design by controlling both composition profile and microstructure. Current and potential applications of the concept of FGMs include not only thermal barrier coatings of high temperature components but also wear-resistant coatings on load transfer components, armors or shields with improved impact resistance, and thermoelectric cells. In addition to the fabricated FGMs, some materials naturally possess the same physical properties that vary continuously across the interfacial region or through the thickness as a natural consequence of material processing.

The main purpose of this study is to examine the interaction between the composite coating, which is nonhomogeneous material, and the metallic substrate, which is homogeneous one, under high temperature or heat flux. The constant heat flux has been applied to the surface of coating and the effect of heat on the insulated barrier at the interface between composite coating and metallic substrate has been investigated. In Chapter 2, it was summarized the heat equation and its solution in different techniques such as separation of variable and integral transform methods for finite and infinite media (geometries), respectively. In Chapter 3, some numerical integration techniques were studied. Main part of the work here is in Chapter 4, which is the part related to the modeling of temperature distribution around the barrier at the interface between composite coating and metallic substrate. In this chapter, superposition method was used to simplify the geometry of the problem and then by using Fourier integral transform method, the problem with the boundary conditions was translated to the integral equation with Cauchy type of singularity. Moreover, in Chapter 4 using a known standard technique, the integral equation was solved and the thermal distributions on the insulated barrier at the interface between coating and substrate were represented for different inhomogeneity and thickness parameters in Chapter 5. The results were compared with the homogeneous infinite and semi-infinite geometries and it was shown that results are perfectly matched and converged.

CHAPTER 2

SUMMARIES ON DIFUSSION EQUATION AND ITS SOLUTION

2.1 DERIVATION OF THE HEAT EQUATION

Suppose that we have a one dimensional rod of length L for which we make the following assumptions

1. The rod is made of a single homogeneous conducting material
2. The rod is laterally insulated (heat flows only in the x direction)
3. The rod is thin(The radius is very small compared to the length L).

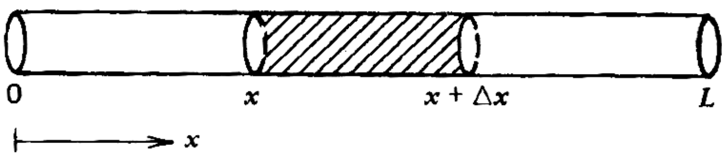


Figure 2.1: Thin Conducting Rod

If we apply the principle of conservation of heat segment $(x, x+\Delta x)$ we can claim that the net change of heat inside $(x, x+\Delta x)$ is equivalent to the addition of the net flux of heat across the boundaries and the total heat generated inside $(x, x+\Delta x)$. Now inasmuch as the total amount of heat inside $(x, x+\Delta x)$ at any time t is measured by [29] as

$$(x, x+\Delta x) = \int_{x}^{x+\Delta x} c\rho Au(s,t)\,ds\,, \tag{2.1}$$

where c and ρ are the thermal capacity and the density of the rod, respectively, as cross sectional area of the rod is given by A. We can write the conservation of energy

$$\frac{d}{dt}\int_{x}^{x+\Delta x} c\rho Au(s,t)\,ds = c\rho A\int_{x}^{x+\Delta x} \frac{d}{dt}u(s,t)\,ds$$

$$= kA\left[u_x\left(x+\Delta x,t\right)-u_x\left(x,t\right)\right]+A\int_x^{x+\Delta x} f\left(s,t\right)ds, \tag{2.2}$$

where k is the thermal conductivity of the rod and $f\left(x,t\right)$ is the external heat. From the mean value theorem, if $f\left(x\right)$ is a continuous function on $\left[a,b\right]$ then there exist at least one number $\xi,\ a<\xi<b,$ that satisfies

$$\int_a^b f\left(x\right)dx = f\left(\xi\right)\left(b-a\right). \tag{2.3}$$

Applying this result to Equation (2.2) we arrive at the following equation:

$$c\rho Au_t\left(\xi,t\right)\Delta x = kA\left[u_x\left(x+\Delta x,t\right)-u_x\left(x,t\right)\right]+Af\left(\xi,t\right)\Delta x, \qquad x<\xi<x+\Delta x \tag{2.4}$$

or

$$u_t\left(\xi,t\right)=\frac{k}{c\rho}\left\{\frac{u_x\left(x+\Delta x,t\right)-u_x\left(x,t\right)}{\Delta x}\right\}+\frac{1}{c\rho}f\left(\xi,t\right). \tag{2.5}$$

Finally, letting $\Delta x\to 0$ we have the desired result

$$u_t\left(x,t\right)=\alpha^2 u_{xx}\left(x,t\right)+F\left(x,t\right) \tag{2.6}$$

where $\alpha^2 = k/cp$ is called the diffusivity of the rod and the function $F\left(x,t\right)=\left(c\rho\right)^{-1}f\left(x,t\right)$ is named as the heat source density.

Suppose that the rod were not laterally insulated and that heat can flow in and out across the lateral boundary at a rate proportional to the difference between the temperature $u\left(x,t\right)$ and the surrounding medium that we keep at zero. In this case, the conservation of heat principle will give

$$u_t = \alpha^2 u_{xx} - \beta u + F\left(x,t\right) \tag{2.7}$$

where β is the rate constant $\left(\beta>0\right)$ for the lateral heat flow.

2.2 HEAT EQUATION IN CARTESIAN COORDINATES

Suppose that we have a thin homogeneous bar of uniform cross section placed along the x-axis from 0 to $L.$ Assume that the sides of the bar are sufficiently well insulated that no heat energy is lost through them and that the bar is sufficiently thin that temperature at any given time is constant on any given cross section perpendicular to the x-axis. Then the temperature u is a function of x and t only. To derive an equation for $u(x,t)$, begin with the experimentally observed fact that the amount of heat energy per unit time passing between two parallel plates of area A, distance d apart, and temperatures T_1 and T_2, is proportional to $A|T_1 - T_2|/d$, and flows from the warmer to the cooler plate. Let k be the constant of proportionality. Then the amount of heat energy per unit time flowing from the warmer to the cooler plate can be expressed as $k(A|T_1 - T_2|)/d$ where k is the coefficient of thermal conductivity and depends upon the material in the plates.

Now, by conservation of energy, the rate at which heat flows into any portion of the bar must equal the rate at which that part of the bar absorbs heat energy. We will obtain an equation for $u(x,t)$ by calculating the flux and absorption terms and setting them equal.

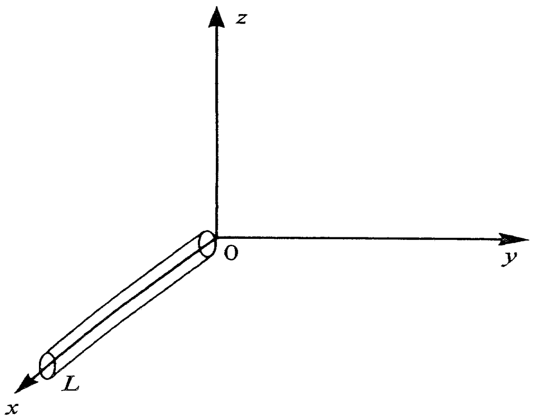


Figure 2.2: A thin homogeneous bar of uniform cross section placed along the x-axis.

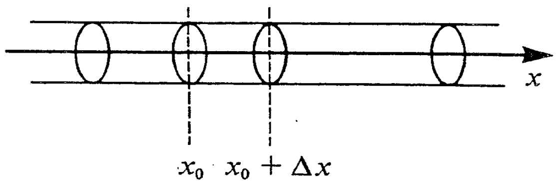


Figure 2.3: A portion of the bar between x_0 and $x_0 + \Delta x$.

For the flux term, look at a portion of the bar between x_0 and $x_0 + \Delta x$, as shown in Figure 2. We imagine that Δx is very small. The instantaneous rate of energy transfer from left to right across the section at x_0 at time t is [30]

$$R(x_0,t) = -\lim_{d\to 0} \frac{kA\left[u\left(x_0 + \frac{1}{2}d, t\right) - u\left(x_0 - \frac{1}{2}d, t\right)\right]}{d}. \tag{2.8}$$

The minus sign in front of the limit is due to the fact that energy flows left to right exactly when the temperature left of x_0 is greater than to the right of x_0. Similarly, the rate of energy transfer from left to right at $x_0 + \Delta x$ is

$$R\left(x_0 + \Delta x, t\right) = -\lim_{d \to 0} \frac{kA\left[u\left(x_0 + \Delta x + \frac{1}{2}d, t\right) - u\left(x_0 + \Delta x - \frac{1}{2}d, t\right)\right]}{d}. \tag{2.9}$$

We recognize these limits as

$$R\left(x_0, t\right) = -kA\frac{\partial u}{\partial x}\left(x_0, t\right) \qquad \text{and} \qquad R\left(x_0 + \Delta x, t\right) = -kA\frac{\partial u}{\partial x}\left(x_0 + \Delta x, t\right), \tag{2.10}$$

assuming that both k and the cross-sectional area A are constants. The net rate F at which heat energy flows into the portion between x_0 and $x_0 + \Delta x$ is then

$$F = R\left(x_0, t\right) - R\left(x_0 + \Delta x, t\right) = kA\left(\frac{\partial u}{\partial x}\left(x_0 + \Delta x, t\right) - \frac{\partial u}{\partial x}\left(x_0, t\right)\right). \tag{2.11}$$

The amount of heat entering this portion of the bar in time Δt is then $F\,\Delta t,$ or

$$kA\left(\frac{\partial u}{\partial x}\left(x_0 + \Delta x, t\right) - \frac{\partial u}{\partial x}\left(x_0, t\right)\right)\Delta t \tag{2.12}$$

which is the flux term. For the absorption term, the average change Δu in temperature over the time Δt is directly proportional to the flux $F\,\Delta t,$ and inversely proportional to the mass $\Delta m.$ Thus, for some constants

$$\Delta u = \frac{F\,\Delta t}{s\,\Delta m}. \tag{2.13}$$

Since $\Delta m = \rho A \Delta x,$ in which ρ is the density, then

$$\Delta u = \frac{F\,\Delta t}{s\rho A\,\Delta x}. \tag{2.14}$$

Now, the average change Δu is equal to the actual temperature change at some point $\overline{x}$ between x_0 and $x_0 + \Delta x.$ Then, from

$$\Delta u = u\left(\overline{x}, t + \Delta t\right) - u\left(\overline{x}, t\right) = \frac{F\,\Delta t}{s\rho A\,\Delta x} \tag{2.15}$$

the flux can be written as

$$F\,\Delta t = s\rho A\left[u\left(\overline{x}, t + \Delta t\right) - u\left(\overline{x}, t\right)\right]\Delta x. \tag{2.16}$$

By equating absorption and flux terms (Equ. 2.11 and 2.16 respectively)

$$kA\left(\frac{\partial u}{\partial x}\left(x_0 + \Delta x, t\right) - \frac{\partial u}{\partial x}\left(x_0, t\right)\right)\Delta t = s\rho A\left[u\left(\overline{x}, t + \Delta t\right) - u\left(\overline{x}, t\right)\right]\Delta x \tag{2.17}$$

and upon dividing by $A\Delta x\Delta t,$ we have

$$k\frac{\frac{\partial u}{\partial x}(x_0+\Delta x,t)-\frac{\partial u}{\partial x}(x_0,t)}{\Delta x}=s\rho\left(\frac{u(\overline{x},t+\Delta t)-u(\overline{x},t)}{\Delta t}\right). \tag{2.18}$$

Let $\Delta x\to 0$ and $\Delta t\to 0,$ noting that $\overline{x}\to x_0$ as $\Delta x\to 0.$ Then, Equation (2.2) can be written as

$$k\frac{\partial^2 u}{\partial x^2}=s\rho\frac{\partial u}{\partial t} \tag{2.19}$$

or in more general form as

$$\frac{\partial u}{\partial t}=a^2\frac{\partial^2 u}{\partial x^2} \tag{2.20}$$

where $a^2=k/s\rho$ is called the thermal diffusivity of the bar. To determine $u(x,t)$ for all $t\geq 0$ and $0\leq x\leq L,$ we need boundary conditions and initial data.

Associated with the heat conduction equation

$$\frac{\partial u}{\partial t}=a^2\frac{\partial^2 u}{\partial x^2},\qquad (t>0,\quad 0\leq x\leq L) \tag{2.21}$$

there are different initial and boundary conditions depends on the physical definition of a problem. As an example, if ends of the bar were kept at constant temperature T_1 and the temperature at the beginning $(t=0)$ on point x is given as $f(x),$ then the boundary and initial temperature conditions are, respectively, defined as

$$u(0,t)=u(L,t)=T_1,\qquad (t>0), \tag{2.22}$$

$$u(x,0)=f(x),\qquad (0\leq x\leq L). \tag{2.23}$$

If the bar is insulated from both ends then the boundary and initial conditions are defined as

$$\frac{\partial u}{\partial x}(0,t)=\frac{\partial u}{\partial x}(L,t)=0,\qquad (t>0), \tag{2.24}$$

$$u(x,0)=f(x),\qquad (0\leq x\leq L) \tag{2.25}$$

where the boundary conditions specify no heat flow across the ends of the bar. In two and three dimensional cartesian coordinate systems, the heat equation can be given, respectively, as follows:

$$\frac{\partial u}{\partial t}=a^2\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}\right), \tag{2.26}$$

$$\frac{\partial u}{\partial t} = a^2 \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right). \tag{2.27}$$

Corresponding boundary and initial conditions would have to accompany these partial differential equations to determine a unique solution.

2.3 SEPARATION OF VARIABLES

Separation of variables is one of the oldest techniques for solving initial-boundary-value problems and applies to problems where

1. The PDE is linear and homogeneous.
2. The boundary conditions are of the form

$$\alpha u_x(0,t) + \beta u(0,t) = 0, \tag{2.28}$$

$$\gamma u_x(1,t) + \delta u(1,t) = 0, \tag{2.29}$$

where α, β, γ and δ are constants. To show how method works let us apply it to a specific problem. Consider the initial boundary value problem (IBVP) (heat conduction equation)

$$\frac{\partial u}{\partial t} = \alpha^2 \frac{\partial^2 u}{\partial x^2}, \qquad (t > 0, \quad 0 \le x \le 1), \tag{2.30}$$

along with the following boundary and initial conditions, respectively,

$$u(0,t) = u(1,t) = 0, \qquad (t > 0), \tag{2.31}$$

$$u(x,0) = \Phi(x), \qquad (0 \le x \le 1). \tag{2.32}$$

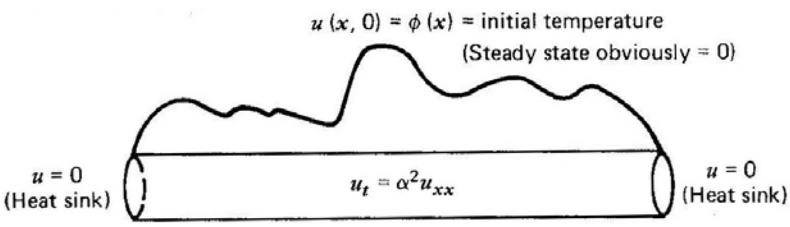


Figure 2.4: Diagram of the diffusion problem

Here we have a finite rod where temperature at the ends is fixed at zero. We are also given data for the problem in the form of an initial condition; our goal is to find the temperature $u(x,t)$ at later points in time. As an overview, separation of variables looks for simple type solutions to the PDE of the form

$$u(x,t) = X(x)T(t) \tag{2.33}$$

where $X(x)$ is some function of x and $T(t)$ is some function of t. The solutions are simple because any temperature $u(x,t)$ of this form will retain its basic shape for different values of time t [29].

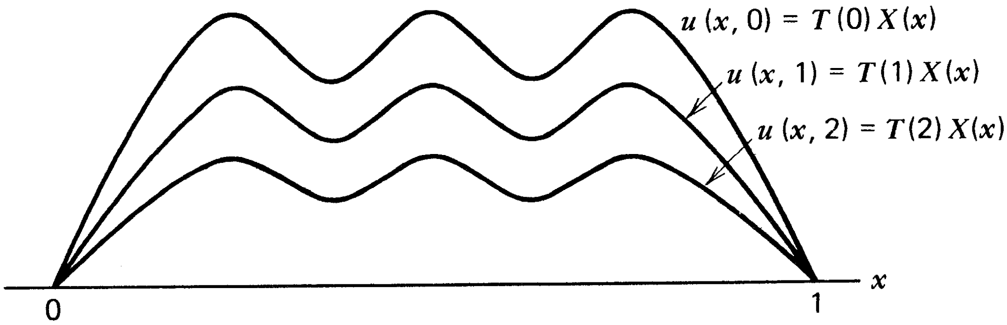


Figure 2.5: Graph of $X(x)T(t)$ for different values of t.

The general idea is that it is possible to find an infinite number of these solutions to the PDE. These simple functions $u_n(x,t) = X_n(x)T_n(t)$ are the building blocks of our problem, and the solution $u(x,t)$ is found by adding the simple fundamental solutions $X_n(x)T_n(t)$ in such a way that the resulting sum

$$\sum_{n=1}^{\infty} A_n X_n(x)T_n(t) \tag{2.34}$$

satisfies the initial conditions. Inasmuch as this sum still satisfies the PDE and the BCs, we now have the solution to our problem. Let us solve the given problem above as an example of the method.

Step 1: Finding elementary solutions to the PDE in Equation (2.30-2.32)

To begin we look for solutions of the form $u(x,t) = X(x)T(t)$ by substituting $X(x)T(t)$ into the PDE and solving for $X(x)T(t)$. Making this substituting gives

$$X(x)T'(t) = \alpha^2 X''(x)T(t). \tag{2.35}$$

Now here is the part that makes all this work: If we divide each side of this equation by $\alpha^2 X(x)T(t)$ we have

$$\frac{T'(t)}{\alpha^2 T(t)} = \frac{X''(x)}{X(x)} \tag{2.36}$$

and obtain what is called separated variables, that is, the left side of the equation depends only on t and the right side only on x. Inasmuch as x and t are independent of each other, each side must be a fixed constant; hence we can write

$$\frac{T'}{\alpha^2 T} = \frac{X''}{X} = k \tag{2.37}$$

or

$$\begin{aligned} T' - k\alpha^2 T &= 0, \\ X'' - kX &= 0. \end{aligned} \tag{2.38}$$

So now we can solve each of these two ordinary differential equations (ODEs) and then multiply them together to get a solution to the PDE. However, we make an important observation, namely, that we want the separation constant k to be negative. With this in mind it is general practice to rename $k = -\lambda^2$ where λ is nonzero. Calling our separation constant by its new name, we can write the two ODEs as

$$T' - \lambda^2\alpha^2 T = 0, \tag{2.39}$$

$$X'' - \lambda^2 X = 0. \tag{2.40}$$

We will now solve these equations. Both equations are standard type ODEs and have solutions

$$T(t) = Ae^{-\lambda^2\alpha^2 t} \quad , \qquad (A \text{ an arbitrary contant}) \tag{2.41}$$

$$X(x) = A\sin(\lambda x) + B\cos(\lambda x) \qquad (A, B \text{ arbitrary}) \tag{2.42}$$

and hence all functions

$$u(x,t) = e^{-\lambda^2\alpha^2 t}\left[A\sin(\lambda x) + B\cos(\lambda x)\right] \tag{2.43}$$

will satisfy the PDE $u_t = \alpha^2 u_{xx}$. At this point, we have an infinite number of functions that satisfy the PDE.

Step 2: Finding solutions to the PDE and the BCs

We are now to the point where we have many solutions to the PDE but not all of them satisfy the BCs or the IC. The next step is to choose a certain subset of our current crop of solutions that satisfy the boundary conditions in Equation (2.31-2.32). To do this, we substitute our solutions (2.43) into BCs given in Equation (2.31) and we will obtain the coefficient B as follows:

$$u(0,t) = Be^{-\lambda^2\alpha^2 t} = 0 \quad \Rightarrow \quad B = 0, \tag{2.44}$$

$$u(1,t) = Ae^{-\lambda^2\alpha^2 t}\sin\lambda = 0 \quad \Rightarrow \quad \sin\lambda = 0. \tag{2.45}$$

The last BC restricts the separation constant λ from being any nonzero number, it must be a root of the equation $\sin\lambda = 0$. In other words, in order that $u(1,t) = 0$, it is necessary to pick

$$\lambda = \pm\pi, \pm 2\pi, \pm 3\pi, \ldots \qquad \text{or} \qquad \lambda_n = \pm n\pi \qquad n = 1, 2, 3, \ldots \tag{2.46}$$

Note that last BC could also $A = 0$, but if we choose this, we would get the zero solution in Equation (2.43). We have now finished the second step and have found an infinite number of functions

$$u_n(x,t) = A_n e^{-(n\pi\alpha)^2}\sin(n\pi x), \qquad n = 1, 2, 3, \ldots \tag{2.47}$$

Each n value satisfies the PDE and BCs given in Equation (2.47). These are building blocks of the problem, and our desired solution will be a certain sum of these simple functions; the specific sum will depend on the initial condition

Step 3: Finding the Solution to the PDE, BCs and the IC

The last step is to add the fundamental solutions

$$u(x,t) = \sum_{n=1}^{\infty} A_n e^{-(n\pi\alpha)^2}\sin(n\pi x) \tag{2.48}$$

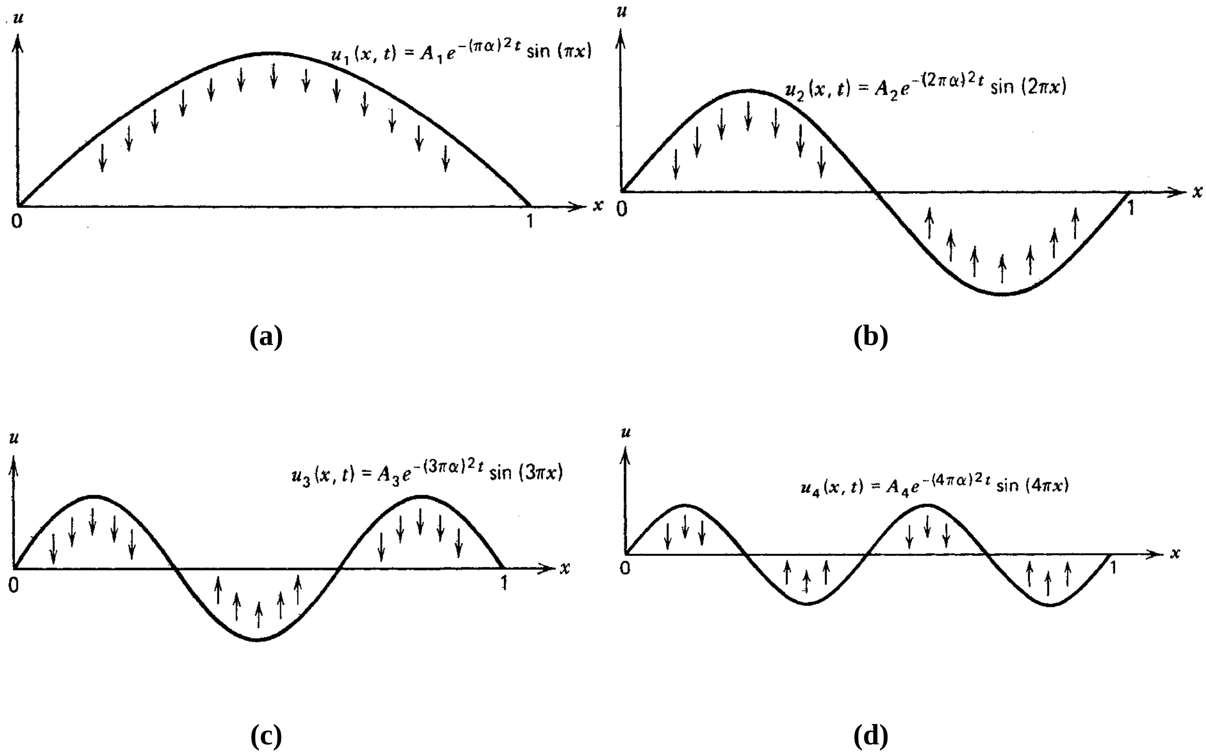
in such a way that the initial condition (2.33) is satisfied. Substituting the sum into the IC gives

$$\Phi(x) = \sum_{n=1}^{\infty} A_n \sin(n\pi x) \tag{2.49}$$

Is it possible to expand the initial temperature $\Phi(x)$ as the sum of the elementary functions as follows?

$$A_1\sin(\pi x) + A_2\sin(2\pi x) + A_3\sin(3\pi x) + \ldots \tag{2.50}$$

How to find the coefficients A_n .



(a) **(b)** **(c)** **(d)**

Figure 2.6: Fundamental solutions $u_n(x,t) = A_n e^{-(n\pi\alpha)^2 t} \sin(n\pi x)$ where **(a)** $u_1(x,t)$ **(b)** $u_2(x,t)$ **(c)** $u_3(x,t)$ **(d)** $u_4(x,t)$

One uses a property of the functions

$$\{\sin(n\pi x); \qquad n = 1,2,...\} \tag{2.51}$$

known as orthogonality. It turns out that these functions are orthogonal to each other in the sense of

$$\int_0^1 \sin(m\pi x)\sin(n\pi x)\,dx = \begin{cases} 0 & m \neq n \\ 1/2 & m = n \end{cases} \tag{2.52}$$

This property can be illustrated by at the graphs of these functions Figure 4. So, we are now in position to solve for the coefficients in the expression

$$\Phi(x) = A_1 \sin(\pi x) + A_2 \sin(2\pi x) + A_3 \sin(3\pi x) + ... \tag{2.53}$$

We multiply each side of this equation by $\sin(m\pi x)$ $(m, \text{an arbitrary integer })$ and integrate from zero to one; we get

$$\int_0^1 \Phi(x)\sin(m\pi x)dx = A_m \int_0^1 \sin^2(m\pi x)dx = \frac{1}{2}A_m. \tag{2.54}$$

Solving for A_m gives

$$A_m = 2\int_0^1 \Phi(x)\sin(m\pi x)\ dx. \tag{2.55}$$

The solution is

$$u(x,t) = \sum_{n=1}^{\infty} A_n e^{-(n\pi\alpha)^2 t} \sin(n\pi x) \tag{2.56}$$

where the coefficient A_n are given by Equation (2.55).

2.4 SUPERPOSITION METHOD

Let us mention the solution of nonhomogeneous heat equation by superposition method. Suppose we have the linear problem

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \sin(\pi x), \qquad (t > 0, \quad 0 \le x \le 1) \tag{2.57}$$

along with the following boundary and initial conditions [31], respectively,

$$u(0,t) = u(1,t) = 0, \qquad (t > 0), \tag{2.58}$$

$$u(x,0) = \sin(2\pi x), \qquad (0 \le x \le 1). \tag{2.59}$$

Here we have a nonhomogeneous heat equation, so separation of variables is not a viable method of attack. We could use the finite sine transform on the variable x or the Laplace transform on $t,$ but still another idea would be to consider two subproblems P_1 and P_2 of main problem P as follows:

$$(P_1) \qquad \frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \sin(\pi x), \qquad (t > 0, \quad 0 \le x \le 1) \tag{2.60}$$

along with

$$u(0,t) = u(1,t) = 0, \qquad (t > 0), \tag{2.61}$$

$$u(x,0) = 0, \qquad (0 \le x \le 1) \tag{2.62}$$

and

$$(P_2) \qquad \frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}, \qquad (t > 0, \quad 0 \le x \le 1) \tag{2.63}$$

along with

$$u(0,t) = u(1,t) = 0, \qquad (t > 0), \tag{2.64}$$

$$u(x,0) = \sin(2\pi x), \qquad (0 \le x \le 1). \tag{2.65}$$

These two problems can be solved individually with a little effort and it should be clear here that the sum of the solutions to P_1 and P_2 is the solution to the original problem P: that is

$$u(x,t) = \frac{1}{\pi^2}\left(1 - e^{-\pi^2 t}\right)\sin(\pi x) + e^{-(2\pi)^2 t}\sin(2\pi x). \tag{2.66}$$

2.5 INTEGRAL TRANSFORM METHOD

Integral transforms can use superposition; for instance, let us show how the finite sine transform uses this principle. Consider the nonhomogeneous heat equation [31]

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + f(x,t), \qquad (t > 0, \quad 0 \le x \le 1) \tag{2.67}$$

along with the following boundary and initial conditions, respectively,

$$u(0,t) = u(1,t) = 0, \qquad (t > 0), \tag{2.68}$$

$$u(x,0) = 0, \qquad (0 \le x \le 1) \tag{2.69}$$

and consider its solution by use of the finite sine transform. We start by expanding the Equation (2.67) into a sine series like

$$\sum_{n=1}^{\infty} A_n \sin(n\pi x) = \sum_{n=1}^{\infty} B_n \sin(n\pi x) + \sum_{n=1}^{\infty} F_n \sin(n\pi x) \tag{2.70}$$

where

$$A_n(t) = 2\int_0^1 u_t(x,t)\sin(n\pi x)\,dx, \tag{2.71}$$

$$B_n(t) = 2\int_0^1 u_{xx}(x,t)\sin(n\pi x)\,dx, \tag{2.72}$$

$$F_n(t) = 2\int_0^1 f(x,t)\sin(n\pi x)\,dx. \tag{2.73}$$

Note that coefficients A_n, B_n and F_n are actually functions of t since we started with functions of x and t. We have resolved the input $f(x,t)$ into simple components $F_n(t)$. We would add the $U_n(t)$ to get the solution $u(x,t)$. To find the simple responses $U_n(t)$ we must take our resolved PDE and perform a little calculus on the coefficient $A_n(t)$ and $B_n(t)$, so that the integrands contain u instead of u_t and u_{xx}. Integration of by parts given us

$$A_n(t) = 2\int_0^1 u_t(x,t)\sin(n\pi x)\,dx = \frac{d}{dt}\left[2\int_0^1 u(x,t)\sin(n\pi x)\,dx\right] = \frac{dU_n(t)}{dt}, \tag{2.74}$$

$$B_n(t) = 2\int_0^1 u_{xx}(x,t)\sin(n\pi x)\,dx = -(n\pi)^2 U_n(t) + 2n\pi\left[u(0,t)+(-1)^{n+1}u(1,t)\right] \tag{2.75}$$

where $U_n(t)$ is the sine transform of $u(x,t)$. Substituting our BCs in Equation (2.68) into (2.75), we have

$$B_n(t) = -(n\pi)^2 U_n(t) \tag{2.76}$$

and the resolved PDE becomes

$$\sum_{n=1}^{\infty}\left[U_n' + (n\pi)^2 U_n - F_n(t)\right]\sin(n\pi x) = 0. \tag{2.77}$$

Since this is identity in x, the coefficients must be zero; that is

$$U_n' + (n\pi)^2 U_n = F_n(t). \tag{2.78}$$

Hence, we have our input-output relationship between F_n and U_n. Before we can solve for $U_n(t)$, however we must go to initial condition given in Equation (2.69). If we expand $u(x,0)$ as a sine series and set it equal to zero we get

$$\sum_{n=1}^{\infty} U_n(0)\sin(n\pi x) = 0. \tag{2.79}$$

Hence, the initial condition is given as

$$U_n(0) = 0, \qquad n = 1, 2, \ldots. \tag{2.80}$$

We have now resolved our original initial boundary value problem into the simple input output problems. We can solve each of these problems by using an integrating factor in any case, we get

$$U_n(t) = e^{-(n\pi)^2 t}\int_0^t e^{(n\pi)^2 \tau} F_n(\tau)\,d\tau. \tag{2.81}$$

We have now found the responses $U_n(t)$ to the simple inputs $F_n(t)$. The final step is to sum of these simple responses

$$u(x,t) = \sum_{n=1}^{\infty} U_n(t)\sin(n\pi x) \tag{2.82}$$

to obtain the solution to the original problem [31].

2.6 THE FOURIER TRANSFORM

It is possible to find an analogous representation for some of functions. Without going through the details of the proofs, we can show that the Fourier series representation of a function $f(x)$ can be given as

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty}\left[a_n \cos(n\pi x/L) + b_n \sin(n\pi x/L)\right]$$

and also it can be turned into the Fourier integral representation (continuous frequency resolution) like

$$f(x) = \int_0^{\infty} a(\xi)\cos(\xi x)\,d\xi + \int_0^{\infty} b(\xi)\sin(\xi x)\,d\xi$$

where

$$a(\xi) = \frac{1}{\pi}\int_{-\infty}^{+\infty} f(x)\cos(\xi x)\,dx \qquad \text{and} \qquad b(\xi) = \frac{1}{\pi}\int_{-\infty}^{+\infty} f(x)\sin(\xi x)\,dx$$

for nonperiodic functions $f(x)$ defined on $(-\infty, +\infty)$. Here, we see that the Fourier integral representation has solved the function $f(x)$ into all frequencies $0<\xi<\infty$ (and not just multiples of one basic frequency, as with periodic functions). The frequency spectrum is defined as

$$C(\xi) = \sqrt{a^2(\xi) + b^2(\xi)}$$

which measures the composition of the function $f(x)$ in terms of its frequencies. Note that functions $f(x)$ that have sharp corners give rise to frequency spectra with large frequencies, since sharp corners require high-frequency components to represent them. On the other hand, the simple periodic function $f(x) = \sin(\xi x)$ obviously has a frequency spectrum that is zero everywhere except at $\xi = \xi_0$.

We are now in a position to define what a general form is as the exponential Fourier transform. By use of Euler's equation $e^{i\theta} = \cos\theta + i\sin\theta$, we can rewrite equation after a little effort as

$$f(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\left[\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} f(x)e^{-i\xi x}dx\right]e^{i\xi x}d\xi$$

which is known as Fourier integral representation. From this, we can write the two equations

$$\Im\left[f(x)\right] \equiv F(\xi) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} f(x)\, e^{-i\xi x}\, dx,$$

$$\Im^{-1}\left[F\right] \equiv f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} F(\xi) e^{i\xi x} d\xi$$

that are the Fourier and inverse Fourier transform, respectively [31].

2.6.1 Useful Properties of the Fourier Transform

2.6.1.1 *Linear Transformation*

The Fourier transform is a linear transformation; that is, it can be written as

$$\Im\left[af + bg\right] = a\Im\left[f\right] + b\Im\left[g\right].$$

2.6.1.2 *Transformation of Derivatives*

If the Fourier transform transforms the $x-$variable and if the function being transformed is a partial derivative of a function $u(x,t)$ with respect to x, then the rules of transformation are

$$\Im\left[u_x\right] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} u_x(x,t) e^{-i\xi x}\, dx = i\xi\, \Im\left[u\right],$$

$$\Im\left[u_{xx}\right] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} u_{xx}(x,t) e^{-i\xi x} dx = -\xi^2\, \Im\left[u\right].$$

On the other hand, if we transform the partial derivative $u_t(x,t)$ then the transform is given by

$$\Im\left[u_t\right] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} u_t(x,t) e^{-i\xi x} dx = \frac{\partial}{\partial t} \Im\left[u\right],$$

$$\Im\left[u_{tt}\right] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} u_{tt}(x,t) e^{-i\xi x} dx = \frac{\partial^2}{\partial t^2} \Im\left[u\right].$$

2.6.1.3 *Convolution Property*

The general idea is that the transform of a product of two functions $f(x)g(x)$ is not the product of the individual transforms; that is

$$\Im\left[f(x)g(x)\right] \neq \Im[f]\Im[g].$$

We now derive the aforementioned time convolution theorem. Suppose that

$$h(x) = f(x) * g(x)$$

then, given that $\Im\{f(x)\} = F(\xi)$, $\Im\{g(x)\} = G(\xi)$ and $\Im\{h(x)\} = H(\xi)$, it can be written as

$$H(\xi) = \Im\{f(x) * g(x)\} = \Im\left\{\int_{-\infty}^{+\infty} f(\beta)g(x-\beta)d\beta\right\} = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\left[\int_{-\infty}^{+\infty} f(\beta)g(x-\beta)d\beta\right]e^{-i\xi x}dx,$$

$$H(\xi) = \int_{-\infty}^{+\infty} f(\beta)\left[\int_{-\infty}^{+\infty} g(x-\beta)e^{-i\xi x}dx\right]d\beta = G(\xi)\int_{-\infty}^{+\infty} f(\beta)e^{-i\xi\beta}d\beta = G(\xi)F(\xi).$$

It can be shown that the Fourier transform of a product, that is commutative, is given by the convolution of the individual transforms as

$$H(\xi) = G(\xi)F(\xi) = F(\xi)G(\xi).$$

Example 2.1: For given two functions $f(x) = x$ and $g(x) = e^{-x^2}$ the convolution is

$$(f * g)(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}(x-\xi)e^{-\xi^2}d\xi = \frac{x}{\sqrt{2}}$$

that is a new function and the following identity is used to arrive this value

$$\int_{-\infty}^{+\infty} e^{-\xi^2}d\xi = \sqrt{\pi}.$$

2.6.1.4 *Scaling Property*

If $\Im\{f(x)\} = F(s)$ then for a nonzero real constant $a > 0$ it can be written that

$$\Im\{f(ax)\} = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} f(\beta)e^{-i\xi\frac{\beta}{a}}\frac{d\beta}{a} = \frac{1}{a}\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} f(\beta)e^{-i\frac{\xi}{a}\beta}d\beta = \frac{1}{a}F\left(\frac{\xi}{a}\right).$$

From this, the time scaling property, it is evident that if the width of a function is decreased while its height is kept constant, then its Fourier transform becomes wider and shorter. If its width is increased, its transform becomes narrower and taller.

2.6.1.5 *Shifting Property*

If $\Im\{f(x)\} = F(s)$ and x_0 is a real constant, then

$$\Im\{f(x-x_0)\} = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} f(x-x_0)e^{-i\xi x}dx = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} f(\beta)e^{-i\xi(\beta+x_0)}d\beta = e^{i\xi x_0}F(\xi).$$

This time shifting property states that the Fourier transform of a shifted function is just the transform of the unshifted function multiplied by an exponential factor having a linear phase. Likewise, the frequency shifting property states that if $F(\xi)$ is shifted by a constant s_0, its inverse transform is multiplied by e^{ixs_0}

$$\Im\{f(x)e^{i2\pi x s_0}\} = F(s-s_0).$$

2.6.2. The Solution of Partial Differential Equations by Means of Fourier Transform

2.6.2.1 *Laplace's Equation*

In this subsection we will consider some problem involving Laplace's equations

$$\Delta_n u(r) = 0$$

where n is the dimension of the space, $u(r)$ is a function of the position vector $r = (x_1, x_2, ..., x_n)$ and Δ_n denotes the Laplacian operator

$$\Delta_n = \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + ... + \frac{\partial^2}{\partial x_n^2}.$$

2.6.2.2 *Laplace's Equation in a Half Plane*

Here we wish to determine a function $u(x, y)$ satisfying Laplace‘s equation

$$\Delta_2 u(x,y) = 0$$

in the half plane $y \geq 0$ subject to the boundary condition

$$u(x,0) = f(x), \qquad -\infty < x < \infty$$

and the limiting condition

$$u(x,y) \to 0, \qquad \rho \to \infty, \quad \rho = \sqrt{x^2 + y^2}.$$

If we introduce the Fourier transform

$$U(\xi, y) = \Im\left[u(x,y); x \to \xi\right]$$

then it follows that Laplace's equation is equivalent to the equation

$$\left(\frac{\partial^2}{\partial y^2} - \xi^2\right) U(\xi, y) = 0$$

and the boundary condition is also equivalent to the condition

$$U(\xi, 0) = F(\xi)$$

where $F(\xi) = \Im\left[f(x); \xi\right]$ and the limiting condition implies the condition

$$U(\xi, y) \to 0, \qquad y \to \infty.$$

The condition $u(x,y) \to 0$ as $|x| \to \infty$ follows from the Riemann-Lebesque lemma. We therefore obtain the expression

$$U(\xi, y) = F(\xi) e^{-|\xi| y}$$

for the Fourier transform of the function $u(x,y)$. Using the convolution theorem we see that

$$u(x,y) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(t) g(x-t)\, dt$$

where

$$g(x) = \Im^{-1}\left[e^{-|\xi| y}; \xi \to x\right] = \sqrt{\frac{2}{\pi}} \frac{y}{x^2 + y^2}.$$

Substituting this result into the last equation we obtain the expression

$$u(x,y) = \frac{y}{\pi} \int_{-\infty}^{\infty} \frac{f(t)\, dt}{(x-t)^2 + y^2}, \qquad (y > 0)$$

for the required function.

CHAPTER 3

METHODS OF NUMERICAL INTEGRATION

3.1 THE RIEMANN INTEGRAL

We shall be dealing entirely with functions that are integrable in the sense of Riemann. In the case of functions of one variable, this concept can be developed as follows. Suppose that $y = f(x)$ is a bounded function on the finite interval $[a,b]$. Partition the interval $[a,b]$ in to n subintervals by the points $a = x_0 < x_1 < ... < x_n = b.$ Let ξ_1 be any point in the ith subinterval: $x_{i-1} \le \xi_i \le x_i$, and form the sum

$$\sum_{i=1}^{n} f(\xi_i)(x_i - x_{i-1}). \tag{3.1}$$

Sums of this sort are called Riemann sums [32]. Let the maximum length of the subintervals be denoted by $\Delta : \Delta = \max(x_i - x_{i-1})$, and consider a sequence of sums of type (3.1) as $S_1, S_2, S_3, ..., S_m, ...$ whose corresponding maximum subintervals $\Delta_1, \Delta_2, \Delta_3, ..., \Delta_m, ...$ approach zero, $\lim_{m \to \infty} \Delta_m = 0.$ If, for any sequence of this type and corresponding to any choice of ξ_i , the sequence $\{S_m\}$ have a common limit S, then $f(x)$ is said to have the Riemann integral S over $[a,b]$ and shown as

$$S = \int_a^b f(x)dx. \tag{3.2}$$

A necessary and sufficient condition that a bounded function $f(x)$ have a Riemann integral is that $f(x)$ be continuous almost everywhere. In particular, if $f(x)$ continuous on $[a,b]$, it has a Riemann integral. Also, $f(x)$ is bounded on $[a,b]$ and continuous except for a finite number of points of discontinuity, it has a Riemann integral.

The following properties of the Riemann integral are fundamental. It is assumed that $f(x)$ and $g(x)$ are bounded and Riemann-integrable on $[a,b]$ then

$$\int_a^a f(x)dx = 0, \tag{3.3}$$

$$\int_a^b f(x)dx = \int_{a+h}^{b+h} f(x-h)dx, \tag{3.4}$$

$$\int_a^b f(x)dx = -\int_b^a f(x)dx, \tag{3.5}$$

$$\int_a^b f(x)dx + \int_b^c f(x)dx = \int_a^c f(x)dx, \tag{3.6}$$

$$\int_a^b cf(x)dx = c\int_a^b f(x)dx, \tag{3.7}$$

$$\int_a^b \left(f(x)+g(x)\right)dx = \int_a^b f(x)dx + \int_a^b g(x)dx. \tag{3.8}$$

If $f(x) \le g(x)$ almost everywhere on $[a,b]$, then

$$\int_a^b f(x)dx \le \int_a^b g(x)dx. \tag{3.9}$$

In particular, if $f(x) \ge 0$ on $[a,b]$, then $\int_a^b f(x)dx \ge 0$. If $f(x)$ and $g(x)$ are both increasing or both decreasing on $[a,b]$, then

$$(b-a)\int_a^b f(x)g(x)dx \ge \left(\int_a^b f(x)dx\right)\left(\int_a^b g(x)dx\right). \tag{3.10}$$

If $f(x)$ and $g(x)$ are opposite type, then the inequality is reversed. If $f(x)$ is bounded Riemann-integrable function on $[a,b]$, then so is $|f(x)|$, and

$$\left|\int_a^b f(x)dx\right| \le \int_a^b |f(x)|dx. \tag{3.11}$$

3.2 GENERALIZED MEAN-VALUE THEOREM

Let $f(x)$ and $g(x)$ be continuous and also $g(x) \geq 0$ on $a \leq x \leq b$. Then, there exists a value $\xi, (a < \xi < b)$, such that

$$\int_a^b f(x)g(x)dx = f(\xi)\int_a^b g(x)dx. \tag{3.12}$$

3.2.1 First Mean-Value Theorem

Let $f(x)$ be continuous on $a \leq x \leq b$. Then, there exists a value $\xi, (a < \xi < b)$, such that

$$\int_a^b f(x)dx = (b-a)f(\xi). \tag{3.13}$$

If $m \leq f(x) \leq M$ over $a \leq x \leq b$, then $m(b-a) \leq \int_a^b f(x)dx \leq M(b-a)$.

3.2.2 The Fundamental Theorem of Integral Calculus

If $F(x)$ is differentiable on $[a,b]$ and $F'(x)$ is Riemann-integrable there then

$$\int_a^b F'(x)dx = F(b) - F(a). \tag{3.14}$$

A formulation that is sufficient for our purposes is: If $f(x)$ is continuous on $a \leq x \leq b$ and $F(x)$ is any indefinite integral of $f(x)$ then

$$\int_a^b f(x)dx = F(b) - F(a). \tag{3.15}$$

3.2.3 Integration by Parts

$$\int_a^b f(x)g'(x)dx = f(b)g(b) - f(a)g(a) - \int_a^b f'(x)g(x)dx. \tag{3.16}$$

It is sufficient to assume that $f(x)$ and $g(x)$ are continuously differentiable on $a \le x \le b.$ A special Riemann sum arises when $[a,b]$ is subdivided into n equal parts and ξ_i is taken at the right-hand end point of its subinterval:

$$S_n = h\sum_{k=1}^{n} f(a+kh) \tag{3.18}$$

where $h=(b-a)/n.$ If ξ_i is taken at the left-hand end point of its subinterval, we obtain

$$S_n = h\sum_{k=0}^{n-1} f(a+kh). \tag{3.19}$$

3.3 IMPROPER INTEGRALS

Integrals whose range or integrand is unbounded are known as improper integrals. Such integrals are defined as the limits of certain integrals.

3.3.1 Integrals over $[0,\infty)$

Whenever the limit exists the following definition can be written

$$\int_0^{\infty} f(x)\,dx = \lim_{r\to\infty}\int_0^{r} f(x)\,dx. \tag{3.20}$$

Similar definitions are used for $\int_a^{\infty} f(x)\,dx$ and for $\int_{-\infty}^{a} f(x)\,dx.$

3.3.2 Integrals over $(-\infty,\infty)$

Here two definitions are employed. The first commonly employed definition says

$$\int_{-\infty}^{\infty} f(x)\,dx = \int_{-\infty}^{0} f(x)\,dx + \int_0^{\infty} f(x)\,dx. \tag{3.21}$$

The second one

$$\int_{-\infty}^{\infty} f(x)\,dx = \lim_{r\to\infty}\int_{-r}^{r} f(x)\,dx \tag{3.22}$$

which is known as the Cauchy principal value of the integral frequently designated by

$$P\int_{-\infty}^{\infty} f(x)\,dx. \tag{3.23}$$

Whenever both limits exist, the limiting values in the first and the second definitions will be identical, but the limit in the second one may exist in cases where that in the first definition does not.

3.3.3 Unbounded Integrals

Assume that $f(x)$ is defined on $(a,b]$ and is unbounded in the neighborhood of $x=a$ then the integral over the interval $(a,b]$ can be given as

$$\int_a^b f(x)\,dx = \lim_{r\to a^+}\int_r^b f(x)\,dx \tag{3.24}$$

whenever the latter limit exists. A similar definition applies to integrands that are unbounded in the neighborhood of the upper limit of integration. Suppose that $a<c<b$ and $f(x)$ is unbounded in the vicinity of $x=c$. The Cauchy Principal Value of the integral, is defined by the limit

$$P\int_a^b f(x)\,dx = \lim_{r\to 0^+}\left[\int_a^{c-r} f(x)\,dx + \int_{c+r}^{b} f(x)\,dx\right]. \tag{3.25}$$

A common principal value integral is the Hilbert transform which is defined as

$$g(x) = P\int_a^b \frac{f(t)}{t-x}dt, \qquad -\infty\le a<b\le\infty, \qquad a\le x\le b. \tag{3.26}$$

A sufficient condition for the existence of the Hilbert transform is that $f(t)$ satisfy a Lipshitz condition in $[a,b]$. This mean that there are constants $k>0$ and $0<\alpha<1$ such that for any two points t_1 and t_2 in $[a,b]$ we have

$$\left|f(t_1)-f(t_2)\right|\le k\left|t_1-t_2\right|^{\alpha}. \tag{3.27}$$

3.4 HIGHER RULES AS AN EXAMPLE OF RIEMANN SUMS

It follows from the definition (3.1) that an integration formula [33]

$$\int_a^b f(x)\,dx \approx \sum_{i=1}^{n} w_i f(\xi_i) \tag{3.28}$$

will be a Riemann sum if we can find points $a = x_0 < x_1 < \ldots < x_n = b$ such that

$$x_1 - x_0 = w_1, \ldots, x_n - x_{n-1} = w_n \text{ and } x_{i-1} \le \xi_i \le x_i. \tag{3.29}$$

Many higher rules qualify as Riemann sums. Thus, the trapezoidal rule, Simpson's rule and the Newton-Cotes rules of order $n = 4, 5, 6, 7$ are all Riemann sums. It has been proved that the Romberg rules are Riemann sums. The Gauss rules, G_n, of all orders are also Riemann sums.

3.4.1 Simpson's Rule

This rule is by far the most frequently used in obtaining approximate integrals. As one of the famous scientist Milton Abramowitz [33] used to say-somewhat in jest-that 95% of all practical work in numerical analysis boiled down to application of Simpson's rule and linear interpolation.

***Theorem 3.1*:** Let $f(x) \in C^4[a,b]$; then for $a < \xi < b$,

$$\int_a^b f(x)\,dx - \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right] = -\frac{(b-a)^5}{2880} f^{(4)}(\xi). \tag{3.30}$$

The Simpson approximation

$$\int_a^b f(x)\,dx \approx \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right] \tag{3.31}$$

is therefore exact for all polynomials of degree three or less. Simpson's rule is most frequently applied in its extended or compound form. The interval $[a,b]$ is divided into a number of equal subintervals or panels and Simpson's rule is applied to each. Let $a = x_0 < x_1 < \ldots < x_{2n-1} < x_{2n} = b$ be a sequence of equally spaced points in $[a,b]$: $x_{i+1} - x_i = h, \quad i = 0, \ldots, 2n-1.$ Set $f_i = f(x_i)$. Then the compound Simpson's rule is

$$\int_{x_0}^{x_{2n}} f(x)\,dx = \frac{h}{3}\left[f_0 + 4(f_1 + f_3 + \ldots + f_{2n-1}) + 2(f_2 + f_4 + \ldots + f_{2n-2}) + f_{2n}\right] + E_n. \tag{3.32}$$

The remainder E_n is given by

$$E_n = -\frac{nh^5}{90} f^{(4)}(\xi), \quad a < \xi < b. \tag{3.33}$$

If N designates the number of subdivisions of $[a,b]$, then $N = 2n$ and $h = (b-a)/N$, so that

$$E_n = -\frac{(b-a)^5}{180N^4} f^{(4)}(\xi), \qquad a < \xi < b. \tag{3.34}$$

For functions that have four continuous derivatives, Simpson's rule converges to the true value of the integral with rapidly N^{-4} at worst. In practice, therefore, one might expect that the use of ten subintervals would secure about four decimals, and the use of 100 subintervals would secure about eight decimals.

Example 3.1**:** Integrate the functions

$$f_1(x) = \frac{1}{1+x}, \qquad f_2(x) = \frac{x}{e^x - 1}, \qquad f_3(x) = x^{3/2} \qquad \text{and} \qquad f_4(x) = x^{1/2}$$

over $[0,1]$ by Simpson's rule.

n	$f_1(x)$	$f_2(x)$	$f_3(x)$	$f_4(x)$
1	.6944 4444	.7774 9413	.4023 6892	.6380 7119
2	.6932 5395	.7775 0400	.4004 3191	.6565 2627
4	.6931 5450	.7775 0446	.4000 7723	.6630 7925
8	6931 4759	.7775 0450	.4000 1368	.6653 9814
16	.6931 4708	.7775 0438	.4000 0235	.6662 1804
32	.6931 4683	.7775 0416	.4000 0033	.6665 0782
64	.6931 4670	.7775 0411	.3999 9984	.6666 1024
128	.6931 4664	.7775 0407	.3999 9973	.6666 4641
Exact value	.6931 4718	.7775 0463	.4000 0000	.6666 6667

The theoretical error bound may be easily computed for the first function. We select $n = 8$ we have

$$E_n \le -\frac{1}{18016^4} \max_{0 \le x \le 1} \left| f^{(4)}(x) \right|.$$

Now $f_1^{(4)}(x) = 24(1+x)^{-5}$, so that $\max_{0 \le x \le 1} \left| f_1^{(4)}(x) \right| = 24.$ Therefore

$$E_n \le 24/180.16^4 \approx .000002.$$

The observed error at $n = 8$ is 0.0000004. Note that after $n = 16$, the accuracy of the answer has deteriorated due to round off.

The second function is a Debye function. It has only an apparent singularity at $x=0,$ and we have $\lim_{x\to 0} f_2(x)=1.$ The value 1 was inserted at $x=0.$ Since $f_2(x)$ has derivatives of all orders in $[0,1],$ we can use the error estimate, but we have to compute the fourth derivative of $x/(e^x-1)$ and estimate its maximum value. This is a troublesome computation; we can avoid it by using the series expansion for $x/(e^x-1)$. We have

$$f_2(x)=\frac{x}{e^x-1}=\sum_{n=0}^{\infty}\frac{B_n}{n!}x^n$$

where B_n is the nth Bernoulli number. Hence

$$\left(\frac{x}{e^x-1}\right)^{(4)}=B_4+\frac{B_6}{2!}x^2+\frac{B_8}{4!}x^4+...$$

and

$$m=\max_{0\le x\le 1}\left|f_2^{(4)}(x)\right|\le B_4+\frac{B_6}{2!}+\frac{B_8}{4!}+...\le 0.5$$

selecting we have $|E|\le .05/180.4^4\approx 10^{-6}.$ This high accuracy is borne out by comparison with the exact value.

***Example 3.2*:** Determine the value of the elliptic integral

$$I=\int_2^3\left[\left(2x^2+1\right)\left(x^2-2\right)\right]^{-1/2}dx.$$

Using Simpson's rule with an interval of 0.1 yields $I=.141117,$ an alternative computation of this integral can be made from tables of the elliptic integral of the first kind; it yields the same value of $I=.141117.$

3.4.2 Integration Rules of Gauss Type

Let $w(x)\ge 0$ be a fixed weight function defined on $[a,b]$ then the integral

$$\int_a^b w(x)f(x)g(x)dx=(f,g) \tag{3.35}$$

is known as the inner product of the functions $f(x)$ and $g(x)$ over the interval $[a,b]$ with respect to the weight $w(x)$. For a given weight $w(x)$, it is possible to define a sequence of polynomials $p_0(x), p_1(x), \dots$ which are orthogonal and which $p_n(x)$ is of exact degree n:

$$(p_m, p_n) = \int_a^b w(x)\, p_m(x)\, p_n(x)\, dx = 0, \qquad m \neq n. \tag{3.36}$$

By multiplying each $p_n(x)$ by an appropriate constant we can produce a set of polynomials p_n^*, which are orthonormal:

$$(p_m^*, p_n^*) = \int_a^b w(x)\, p_m^*(x)\, p_n^*(x)\, dx = \delta_{mn} = \begin{cases} 0 & if \quad m \neq n. \\ 1 & if \quad m = n. \end{cases} \tag{3.37}$$

The leading coefficient of p_n^* can be taken as positive:

$$p_n^* = k_n x^n + \dots, \qquad k_n > 0. \tag{3.38}$$

***Theorem 3.2*:** The zeros of orthogonal polynomials are real, simple and located in the interior of $[a,b]$.

***Theorem 3.3*:** The orthonormal polynomials p_n^* satisfy a three-term recurrence relationship

$$\begin{aligned} & p_n^* = (a_n x + b_n)\, p_{n-1}^*(x) - c_n p_{n-2}^*(x), \qquad n = 1,2,3,\dots, \\ & a_n, c_n \neq 0 \quad \text{and} \quad p_{-1}^*(x) = 0, \quad p_0^*(x) = \left(\int_a^b w(x)\, dx \right)^{1/2}. \end{aligned} \tag{3.39}$$

The following recurrence is particularly convenient for systematic computation.

$$\begin{aligned} & p_{-1}^*(x) = 0, \\ & p_0(x) = 1, \\ & \quad \vdots \\ & p_{n+1}(x) = x p_n^*(x) - (x p_n^*, p_n^*)\, p_n^*(x) - (p_n, p_n)^{1/2}\, p_{n-1}^*(x), \\ & p_n^*(x) = p_n(x) / (p_n, p_n)^{1/2}, \qquad n = 0,1,2,\dots \end{aligned} \tag{3.40}$$

If n distinct points $x_1, \dots, x_n$ of the interval $[a,b]$ are specified in advance, then we know that we can find coefficients $w_1, \dots, w_n$ such that the rule

$$\int_a^b w(x) f(x) dx \approx \sum_{k=1}^{n} w_k f(x_k) \tag{3.41}$$

will be exact for all polynomials of class $\wp_{n-1}$. If we treat both the x's and the w's as $2n$ unknowns, and determine them carefully perhaps we can arrange matters so that the rule will be exact for polynomials of class $\wp_{2n-1}$, that is, for linear combinations of the $2n$ powers $1, x, x^2, ..., x^{2n-1}$. This is possible, and the solution is intimately related to the orthogonal polynomials generated by the weight function $w(x)$.

Theorem 3.4: Let $w(x) \geq 0$ be a weight function defined on $[a,b]$ with corresponding orthonormal polynomials p_n^*. Let the zeros of $p_n^*(x)$ be $a < x_1 < x_2 < ... < x_n < b$. Then we can find positive constants $w_1, ..., w_n$ such that

$$\int_a^b w(x) p(x) dx = \sum_{k=1}^{n} w_k p(x_k) \tag{3.42}$$

whenever $p(x)$ is a polynomial of class $\wp_{2n-1}$ and where the weights w_k have the explicit representation like

$$w_k = -\frac{k_{n+1}}{k_n} \frac{1}{p_{n+1}^*(x_k) p_n^{*\prime}(x_k)}. \tag{3.43}$$

When abscissas and weights have been determined as this theorem, we say that the resulting integration rule is of Gauss type. We shall frequently refer to the n-point Gauss rule with the weight $w(x) \equiv 1$ by the symbol G_n. It should be observed that if $w(x)$ is a symmetric function like

$$w\left(\frac{1}{2}(a+b)+x\right) = w\left(\frac{1}{2}(a+b)-x\right), \tag{3.44}$$

then the abscissas x_k are located symmetrically in the interval $[a,b]$ and the weights corresponding to symmetric points are equal. Thus, in this case, half the work of the computation of these fundamental constants can be saved. The error incurred in Gaussian integration is governed by the following estimate.

Theorem 3.5: Let $w(x)$, $x_1, ..., x_n$, $w_1, ..., w_n$ be as in the previous theorem. Then, if $f(x) \in C^{2n}[a,b]$,

$$E_n(f)=\int_a^b w(x)f(x)dx-\sum_{k=1}^{n}w_k f(x_k)=\frac{f^{(2n)}(\xi)}{(2n)!k_n^2}, \qquad a<\xi<b. \tag{3.45}$$

***Corollary*:** In the case of the Jacobi weight function [33]

$$w(x)=(1-x)^{\alpha}(1+x)^{\beta}, \quad \alpha>-1 \quad \beta>-1 \tag{3.46}$$

over the interval $[-1,1]$, the error is given by, for $-1<\xi<1$,

$$E_n(f)=\frac{2^{2n+\alpha+\beta+1}\Gamma(n+\beta+1)\Gamma(n+\alpha+\beta+1)n!}{\Gamma(2n+\alpha+\beta+1)\Gamma(2n+\alpha+\beta+2)(2n)!}f^{(2n)}(\xi). \tag{3.47}$$

***Corollary*:** In the case of the weight $w(x)\equiv 1$ over $[-1,1]$, the error is given by

$$E_n(f)=\frac{2^{2n+1}(n!)^4}{(2n+1)\left[(2n)!\right]^3}f^{(2n)}(\xi), \quad -1<\xi<1. \tag{3.48}$$

In general, over the interval $[a,b]$ and for the weight $w(x)\equiv 1$ the error is given by

$$E_n(f)=\frac{(b-a)^{2n+1}(n!)^4}{(2n+1)\left[(2n)!\right]^3}f^{(2n)}(\xi), \quad a<\xi<b. \tag{3.49}$$

Thus, we see that Gauss rules are best in the sense that integrate exactly polynomials of as high degree as possible with a formula of the type $\sum_{k=1}^{n}w_k f(x_k)$. This optimality often carries over to near-optimality when this term has been defined in the language of normed spaces. The positive weights are also useful in keeping down roundoff error.

There are several disadvantages to Gauss rules. The weights and abscissas of the Gauss rules are generally irrational numbers. If computing is done by hand, it is an error-liable nuisance to deal with many digits, and so in years gone by, the Gauss rules were not popular. Digital computers, on the other hand, do not distinguish between simple numbers such as 0.5000000 and more complicated numbers such as 0.577350269. The Gauss rules which integrate exactly polynomials of maximal degree are excellent for large classes of functions arising in practice and are now very popular. But the old difficulty of rational versus irrational still comes into play in that the preparation of a program for Gauss integration requires the typing up and checking of many irrational numbers.

3.5 PROCEEDING TO THE LIMIT

The basic definition

$$\int_0^\infty f(x)\,dx = \lim_{r\to\infty}\int_0^r f(x)\,dx \tag{3.50}$$

suggests a primitive mode of procedure. Let $0 < r_0 < r_1 < \ldots$ be a sequence of numbers that converge to infinity. Write

$$\int_0^\infty f(x)\,dx = \int_0^{r_0} f(x)\,dx + \int_{r_0}^{r_1} f(x)\,dx + \ldots. \tag{3.51}$$

Each of the integrals on the right-hand side is proper, and the evaluations are terminated when $\left|\int_{r_n}^{r_{n+1}} f(x)\,dx\right| \le \varepsilon.$ This is only a practical termination criterion and is not correct theoretically. The interval is frequently doubled at each step; that is, $r^n = 2^n.$ The idea behind this selection is that if an arithmetic sequence is used $(\text{like } r_n = cn)$ the contribution of each additional step may be too insignificant to be worth a special computation. Furthermore, it may be less then $\varepsilon,$ thus stopping the process.

***Example 3.3*:** $I_n = \int_0^{r_n} \frac{e^{-x}}{1+x^4}\,dx, \qquad r_n = 2^n$

n	I_n	Number of functional evaluations
0	.5720 2582	35
1	.6274 5952	52
2	.6304 3990	100
3	.6304 7761	178
4	.6304 7766	322
Exact value	.6304 7783	

3.5.1 Speed-Up of Convergence

The method just described may be speeded up if one can obtained a reasonably good asymptotic expansion for the tail $\int_r^\infty f(x)\,dx.$

Example 3.4: Using the first term of the shifted Laguerre rule that $\int_r^\infty \frac{e^{-x}}{1+x^4}dx \approx \frac{ce^{-r}}{1+r^4}$.

We shall now use Richardson's extrapolation to infinity in the form

$$I_n' = \frac{I_n\phi(r_{n+1}) - I_{n+1}\phi(r_n)}{\phi(r_{n+1}) - \phi(r_n)}, \qquad \phi(r) = \frac{e^{-r}}{1+r^4}, \qquad r_n = 2^n. \tag{3.52}$$

This yields

n	I_n
0	.6299 6722
1	.6304 6682
2	.6304 7765
3	.6304 7766

Note that I_1' is much better than I_2 and I_2' is almost identical to I_4. Speed-up methods using the epsilon algorithm have been applied to integrals over an infinite range with limited success.

3.5.2 Nonlinear Transformation

Speed-up methods similar to those used for accelerating the convergence of slowly convergent series may be applied to infinite integrals. Let $f(x) \in C[a,\infty]$ and assume that

$$F(t) = \int_a^t f(x)\,dx \tag{3.53}$$

converges to S as $t \to \infty$. A function $F_1(t)$ is said to converge more rapidly to S than $F(t)$ if

$$\lim_{t\to\infty} \frac{S - F_1(t)}{S - F(t)} = 0. \tag{3.54}$$

Let us now define $R(t;k) = \frac{f(t+k)}{f(t)}$, $k > 0$ for $f(t) \neq 0$ and denote by $R(k)$, $\lim_{t\to\infty} R(t;k)$, if it exists. We are now in a position to define the G-transform of F and give some of its properties.

***Definition*:** The G-transform of F is given by

$$G[F;t,k]=\frac{F(t+k)-R(t,k)F(t)}{1-R(t,k)}, \qquad R(t,k)\neq 1 \tag{3.55}$$

for any k such that $R(t,k)\neq 1$ and $G[F;t,k]$ converges to S. If $R(k)\neq 0$ or $R(k)\neq 1$ the convergence is more rapid than that of $F(t+k)$. A limiting case of G-transform, which also converges more rapidly than $F(t+k)$, may be defined in which $R(t,k)$ is replaced by $R(k)$ in Equation (3.55).

***Example 3.5*:** $F(t)=\int_0^t \frac{\sin x}{x}dx \to \frac{\pi}{2}=1{,}5707963...$

$$R(t,k)=\frac{\sin(t+k)}{\sin t}\frac{t}{t+k}.$$

With $k=\pi$ and $R(t,\pi)=-t/(t+\pi)\to -1=R(\pi)$,

$$G[F;t,\pi]=\frac{t+\pi}{2t+\pi}\int_0^{t+\pi}\frac{\sin x}{x}dx+\frac{1}{2t+\pi}\int_0^{t}\frac{\sin x}{x}dx$$

for $t=9\pi$ and $G\approx 1{,}5707886$. Using the Euler transformation on the same range the value yields 1.5707911.

In case $R(k)=1$, we may be able to achieve better convergence with the Q-transform which, when defined, converges more rapidly than $F(t+1)$ and $G[F;t,1]$. Let $q=\lim_{r\to\infty} t[1-R(t,1)]$. If $q\neq 1$, we define the Q-transform of $F(t)$ by

$$Q[F;t]=(qG[F;t,1]-F(t))/(q-1). \tag{3.56}$$

***Example 3.6*:** $F(t)=\int_0^t \frac{1}{(1+x)^2}dx=1-\frac{1}{1+t}.$

In this case we can work everything out analytically. We have that $R(t,1)=((t+1)/(t+2))^2$,

$q=2,\ S=1,\ G[F;t,1]=1-\frac{1}{2t+3}$ and $Q[F;t,1]=1+\frac{1}{(1+t)(2t+3)}.$

Similar to the G-transform is the B-transform. Let $\rho(t;k)=k\dfrac{f(tk)}{f(t)},\ k>1,\ f(t)\neq 0$ and let $\rho(k)=\lim_{t\to\infty}\rho(t;k)$ exist. The B-transform is given by

$$B[F;t,k]=\frac{F(kt)-\rho(t,k)F(t)}{1-\rho(t,k)},\qquad \rho(t,k)\neq 1. \tag{3.57}$$

If $\rho(k)\neq 1,\ B[F;t,k]$ converges to S more rapidly than $F(t)$ while if $\rho(k)\neq 0$ or $\rho(k)\neq 1$ convergence is more rapid than that of $F(kt)$. As previously, a limiting case may be defined where $\rho(t,k)$ is replaced by $\rho(k)\neq 0$ or $\rho(k)\neq 1$ in Equation (3.57). This transformation also converges more rapidly than $F(kt)$.

***Example 3.7*:** $F(t)=\int_0^t \dfrac{dx}{1+x^2}\to\dfrac{\pi}{2}.$ For $k=1.1,\ \ t=18,\ B(F;t,k)=1.57099504$ with an error less than 0.0002.

3.5.3 Truncation of the Infinite Interval

We may also reduce the infinite interval to a finite interval by ignoring the “tail” of the integrand. Rigorous application of this method requires that the analyst be able to estimate this tail by some simple analytical device.

***Example 3.8*:** Determine numerically $\int_0^\infty e^{-x^2}dx\leq\int_k^\infty e^{-kx}dx=\dfrac{e^{-k^2}}{k}.$

For $k=4$, we have $e^{-k^2}/k\approx 10^{-8}$. For a seven-figure computation, it suffices to evaluate $\int_0^4 e^{-x^2}dx$ by some standard method.

***Example 3.9*:** Determine numerically $\int_0^\infty \dfrac{\sin x}{1+x^2}dx.$

We have $\left|\int_{2k\pi}^\infty \dfrac{\sin x}{1+x^2}dx\right|=\left|r_1+r_2+\ldots\right|$ where $r_j=\int_{(2k+j-1)\pi}^{(2k+j)\pi}\dfrac{\sin x}{1+x^2}dx.$ Since $r_{2n}<0,\ r_{2n+1}>0$ and $|r_1|>|r_2|>\ldots,$ we have

$$\left|r_1 + r_2 + ...\right| < r_1 = \int_{2k\pi}^{(2k+1)\pi} \frac{\sin x}{1+x^2}\,dx < \int_{2k\pi}^{(2k+1)\pi} \frac{dx}{x^2} < \frac{1}{4\pi k^2}.$$

For a truncation error 10^{-4}, this analysis suggests that $k \approx 28$.

3.5.4 Reducing the Intensity of the Singularity

Suppose it is possible to express the integrand $f(x)$ in the form $f(x) = g(x) + r(x)$ where $\int_0^\infty g(x)\,dx$ is available in closed form or from other sources and where the remainder $r(x) \to 0$ more rapidly than $f(x)$ as $x \to \infty$. The burden of evaluation is now thrown to $\int_0^\infty r(x)\,dx$ which presumably will be attended by less numerical difficulty. Repeated application of this principle can lead to convergent or asymptotic expansions.

***Example 3.10*:** Evaluate $\int_0^\infty \frac{x\sin x}{1+x^2}\,dx$ more rapidly.

$$\int_0^\infty \frac{x}{1+x^2}\sin x\,dx = \int_0^\infty \frac{\sin x}{x}\,dx - \int_0^\infty \frac{1}{1+x^2}\frac{\sin x}{x}\,dx = \frac{\pi}{2} - \int_0^\infty \frac{1}{1+x^2}\frac{\sin x}{x}\,dx.$$

3.6 ELIMINATING SINGULARITIES IN THE EVALUATION OF SINE AND COSINE INTEGRAL OVER THE INTERVAL $(0, \infty)$.

We find the iterative formula for the evaluation of integral whose integrand is given as a rational trigonometric function like $t^{-n} f(\sin at, \cos at)$ where n is a positive integer. Before starting the process of formulation we should know the identities of special functions $Si(t)$ and $Ci(t)$, sine and cosine integrals, respectively, as follows:

3.6.1 Sine and Cosine Integrals

The sine and cosine integrals are defined, respectively, as [31]

$$Si(x) = \int_0^x \frac{\sin t}{t} dt, \tag{3.58}$$

$$Ci(x) = \int_0^x \frac{\cos t}{t} dt. \tag{3.59}$$

The main purpose of this section is obtaining an iterative method to evaluate the following integrals

$$\int_A^\infty \frac{\sin \theta\omega}{\theta^n} d\theta \qquad \text{and} \qquad \int_A^\infty \frac{\cos \theta\omega}{\theta^n} d\theta. \tag{3.60}$$

First of all, we will start from the definition of integration by parts such as

$$(uv)' = u'v + uv' \tag{3.61}$$

and rewriting the Equation (3.61) again using an exact integral

$$\int_a^b v\,du + \int_a^b u\,dv = uv\Big|_a^b \quad \Rightarrow \quad \int_a^b u\,dv = uv\Big|_a^b - \int_a^b v\,du. \tag{3.62}$$

Using the integration by parts technique along with definitions given in Equation (3.58) as follows

$$Si(x) = \int_0^x \frac{\sin t}{t} dt = \left(\int_0^\infty \frac{\sin t}{t} dt - \int_x^\infty \frac{\sin t}{t} dt \right) = \frac{\pi}{2}\frac{|x|}{x} - \int_x^\infty \frac{\sin t}{t} dt \tag{3.63}$$

then one can obtain that

$$\int_x^\infty \frac{\sin t}{t} dt = \frac{\pi}{2}\frac{|x|}{x} - Si(x). \tag{3.64}$$

Similarly, with the definition of $Ci(x)$

$$Ci(x) = \int_0^x \frac{\cos t}{t} dt = \gamma_0 + \log|x| - \int_0^{|x|} \frac{1-\cos t}{t} dt, \tag{3.65}$$

$$\int_x^\infty \frac{\cos t}{t} dt = -Ci(x) = -\gamma_0 - \log|x| + \int_0^{|x|} \frac{1-\cos t}{t} dt \tag{3.66}$$

where γ_0 is called as Euler's constant and its value is $\gamma_0 = 0.57721566490.$ Now, let us solve the integral by using the integration by parts technique as follows:

$$S_2 = \frac{\omega}{|\omega|}\int_A^\infty \frac{\sin \alpha|\omega|}{\alpha^2} d\alpha = \frac{\omega}{|\omega|}\left(\frac{\sin \alpha|\omega|}{-\alpha}\Bigg|_A^\infty + |\omega|\int_A^\infty \frac{\cos \alpha|\omega|}{\alpha} d\alpha \right). \tag{3.67}$$

The last integral in Equation (3.67) is $-Ci(x)$ integral then the S_2 becomes

$$S_2 = \frac{\omega}{|\omega|}\int_A^\infty \frac{\sin\alpha|\omega|}{\alpha^2}d\alpha = \frac{\omega}{|\omega|}\frac{\sin A|\omega|}{A} - |\omega| Ci\left(A|\omega|\right) \tag{3.68}$$

where $\lim_{\alpha\to\infty}\frac{\sin\alpha|\omega|}{\alpha} = 0.$ Similarly for the integral

$$C_2 = \int_A^\infty \frac{\cos\alpha|\omega|}{\alpha^2}d\alpha = \left.\frac{\cos\alpha|\omega|}{-\alpha}\right|_A^\infty - |\omega|\int_A^\infty \frac{\sin\alpha|\omega|}{\alpha}d\alpha \tag{3.69}$$

and using the Equation (3.58) for $Si(x)$ the value C_2 becomes

$$C_2 = \int_A^\infty \frac{\cos\alpha|\omega|}{\alpha^2}d\alpha = \frac{\cos A|\omega|}{A} - |\omega|\left(\frac{\pi}{2}\frac{|A|\omega||}{A|\omega|} - Si\left(A|\omega|\right)\right) \tag{3.70}$$

where $\lim_{\alpha\to\infty}\frac{\cos\alpha|\omega|}{\alpha} = 0.$

In general, for integer $k \geq 2$, the recursive formula can be obtained by using integration by parts technique as follow:

$$S_k = \frac{\omega}{|\omega|}\int_A^\infty \frac{\sin\alpha|\omega|}{\alpha^k}d\alpha = \frac{\omega}{|\omega|}\left(\left.\frac{\sin\alpha|\omega|}{(1-k)\alpha^{k-1}}\right|_A^\infty - \frac{|\omega|}{1-k}\int_A^\infty \frac{\cos\alpha|\omega|}{\alpha^{k-1}}d\alpha\right),$$

$$S_k = \frac{\omega}{|\omega|}\left(\frac{\sin A|\omega|}{(k-1)A^{k-1}} + \frac{|\omega|}{k-1}\int_A^\infty \frac{\cos\alpha|\omega|}{\alpha^{k-1}}d\alpha\right),$$

$$S_k = \frac{\omega}{|\omega|}\left(\frac{\sin A|\omega|}{(k-1)A^{k-1}} + \frac{|\omega|}{k-1}C_{k-1}\right). \tag{3.71}$$

Similarly,

$$C_k = \int_A^\infty \frac{\cos\alpha|\omega|}{\alpha^k}d\alpha = \left.\frac{\cos\alpha|\omega|}{(1-k)\alpha^{k-1}}\right|_A^\infty + \frac{1}{1-k}\int_A^\infty \frac{\sin\alpha|\omega|}{\alpha^{k-1}}d\alpha,$$

$$C_k = \frac{\cos A|\omega|}{(k-1)A^{k-1}} - \frac{|\omega|}{k-1}\int_A^\infty \frac{\sin\alpha|\omega|}{\alpha^{k-1}}d\alpha,$$

$$C_k = \frac{\cos A|\omega|}{(k-1)A^{k-1}} - \frac{|\omega|}{k-1}S_{k-1}. \tag{3.72}$$

Once we obtain the value of S_1 and C_1 then the rest of the integrals for $k \geq 2$ can be evaluated by using the recursive formula. Some examples are given below.

Example 3.11**:** Find the recursive formula for S_3 and C_3.

Now, let us solve the following integrals by using the integration by part

$$S_3 = \frac{\omega}{|\omega|}\int_A^\infty \frac{\sin\theta|\omega|}{\theta^3}d\theta = \frac{\omega}{|\omega|}\int_{A|\omega|}^\infty \frac{\sin\alpha}{\left(\alpha/|\omega|\right)^3}\frac{d\alpha}{|\omega|} = \omega\int_{A|\omega|}^\infty \frac{\sin\alpha}{\alpha^3}d\alpha,$$

$$S_3 = \omega\left(\left.\frac{\sin\alpha}{-\alpha^2}\right|_{A|\omega|}^\infty + \int_{A|\omega|}^\infty \frac{\cos\alpha}{\alpha^2}d\alpha\right) = \omega\left(\frac{\sin A|\omega|}{A|\omega|} - C_2\right),$$

$$C_2 = \int_{A|\omega|}^\infty \frac{\cos\alpha}{\alpha^2}d\alpha = \left.\frac{\cos\alpha}{-\alpha}\right|_{A|\omega|}^\infty - \int_{A|\omega|}^\infty \frac{\sin\alpha}{\alpha}d\alpha = \frac{\cos A|\omega|}{A|\omega|} - S_1.$$

Back substitution along with the value of the integral S_1 given in Equation (3.64) results the value of integral S_3. Similarly

$$C_3 = \int_A^\infty \frac{\cos\theta|\omega|}{\theta^3}d\theta = \int_{A|\omega|}^\infty \frac{\cos\alpha}{\left(\alpha/|\omega|\right)^3}\frac{d\alpha}{|\omega|} = |\omega|^2\int_{A|\omega|}^\infty \frac{\cos\alpha}{\alpha^3}d\alpha,$$

$$C_3 = |\omega|^2\left(\left.\frac{\cos\alpha}{-\alpha^2}\right|_{A|\omega|}^\infty - \int_{A|\omega|}^\infty \frac{\sin\alpha}{\alpha^2}d\alpha\right) = |\omega|^2\left(\frac{\cos A|\omega|}{\left(A|\omega|\right)^2} - S_2\right),$$

$$S_2 = \int_{A|\omega|}^\infty \frac{\sin\alpha}{\alpha^2}d\alpha = \left.\frac{\sin\alpha}{-\alpha}\right|_{A|\omega|}^\infty + \int_{A|\omega|}^\infty \frac{\cos\alpha}{\alpha}d\alpha = \frac{\sin A|\omega|}{A|\omega|} + C_1.$$

Applying back substitution along with the value of the integral C_1 given in Equation (3.66) the value of C_3 can be obtained.

CHAPTER 4

THERMAL DISTRIBUTIONS AROUND AN INSULATED BARRIER AT THE INTERFACE OF A GRADED COATING AND A HOMOGENEOUS SUBSTRATE

4.1 DEFINITION OF THE PROBLEM

Starting with the diffusion equation in xyz -coordinate [31]

$$\frac{\partial T}{\partial t}=\frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(k\frac{\partial T}{\partial y}\right)+\frac{\partial}{\partial z}\left(k\frac{\partial T}{\partial z}\right) \quad , \tag{4.1}$$

which can be reduced to the following form for steady-state conduction in 2-D problem

$$\frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(k\frac{\partial T}{\partial y}\right)=0 \quad , \tag{4.2}$$

where k is conductivity which can be expressed exponential function [29] such as

$$k(y)=k_0e^{\beta y}, \qquad k_0,\beta: \text{ constants.} \tag{4.3}$$

Suppose that heat is supplied over the area $-a<x<a$ in the plane $z=0$ at rate depending on y only. The diffusion equation can be written in a simple form for the temperature $T(x,y)$ as

$$\frac{\partial^2 T}{\partial x^2}+\beta\frac{\partial T}{\partial y}+\frac{\partial^2 T}{\partial y^2}=0. \tag{4.4}$$

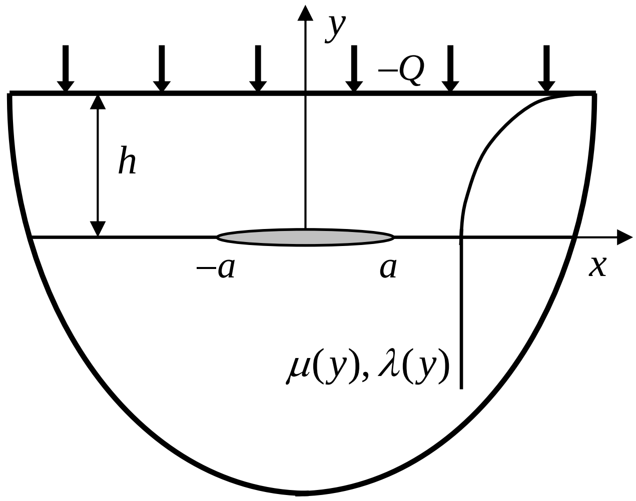


Figure 4.1: Geometry of the heat conduction problem

We will solve the problem given in Figure 4.1 using superposition method such that the temperature function $T(r,z)$ will be addition of two problems. The first problem is the one – dimensional problem

$$\beta\frac{\partial T_1}{\partial y}+\frac{\partial^2 T_1}{\partial y^2}=0 \tag{4.5}$$

on y-axis along with the boundary conditions,

$$k(y)\frac{\partial}{\partial y}T_1(x,y)\rightarrow \textit{finite} \text{ as } \rho\rightarrow-\infty \text{ where } \rho=\sqrt{x^2+y^2}, \tag{4.6}$$

$$T_1(x,0^+)=T_1(x,0^-), \qquad -\infty<x<\infty, \quad y=0, \tag{4.7}$$

$$k(y)\frac{\partial}{\partial y}T_1(x,y)\Big|_{y=h}=Q_0\ , \quad -\infty<x<\infty, \quad y=h \tag{4.8}$$

and the second problem is two-dimensional heat conduction problem

$$\frac{\partial^2 T_2}{\partial x^2}+\beta\frac{\partial T_2}{\partial y}+\frac{\partial^2 T_2}{\partial y^2}=0 \tag{4.9}$$

on (x,y) plane along with the boundary conditions,

$$k(y)\frac{\partial}{\partial y}T_2(x,y)\rightarrow \textit{finite} \text{ as } \rho\rightarrow-\infty \text{ where } \rho=\sqrt{x^2+y^2}, \tag{4.10}$$

$$k(y)\frac{\partial}{\partial y}T_2(x,y)\Big|_{y=h}=0\,, \qquad y=h, \quad -\infty<x<\infty, \tag{4.11}$$

$$\frac{\partial}{\partial y}T_2\left(x,0^+\right)=\frac{\partial}{\partial y}T_2\left(x,0^-\right), \qquad y=0, \quad a<|x|<\infty, \tag{4.12}$$

$$T\left(x,0^+\right)=T\left(x,0^-\right), \qquad y=0, \quad a<|x|<\infty, \tag{4.13}$$

$$k\left(y\right)\frac{\partial}{\partial y}T\left(x,y\right)=-Q_0, \qquad y=0, \quad -a<x<a. \tag{4.14}$$

4.2 ONE-DIMENSIONAL HEAT CONDUCTION PROBLEM $T_1\left(y\right)$

One-dimensional heat conduction problem given in Figure 4.2 can be obtained by solving (4.5) such that

$$T_1\left(y\right)=\begin{cases} A+Be^{-\beta y}, & 0<y<h, \\ C+Dy, & y<0. \end{cases} \tag{4.15}$$

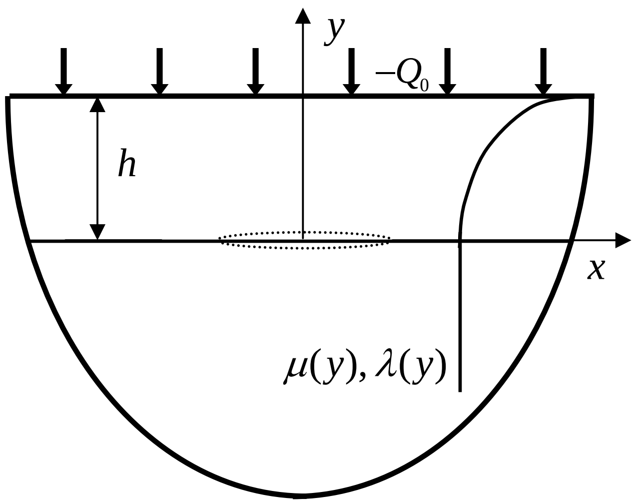


Figure 4.2: Geometry of the one dimensional heat conduction problem

Using regularity condition (4.6) the coefficient D should be zero and from boundary conditions (4.7) and (4.8)

$$A+B=C \quad \text{as} \quad y=0, \tag{4.16}$$

$$k_0e^{\beta y}\left(-\beta Be^{-\beta h}\right)=Q_0 \quad \Rightarrow \quad B=-\frac{Q_0}{\beta k_0} \text{ and } C=A-\frac{Q_0}{\beta k_0}. \tag{4.17}$$

Then, the solution of (4.5) will be determined by arbitrarily choosing $A=0$ as

$$T_1(y)=\begin{cases}-\dfrac{Q_0}{\beta k_0}e^{-\beta y}, & 0<y<h,\\ -\dfrac{Q_0}{\beta k_0}, & y<0.\end{cases} \tag{4.18}$$

4.3 TWO-DIMENSIONAL HEAT CONDUCTION PROBLEM $T_2(x,y)$

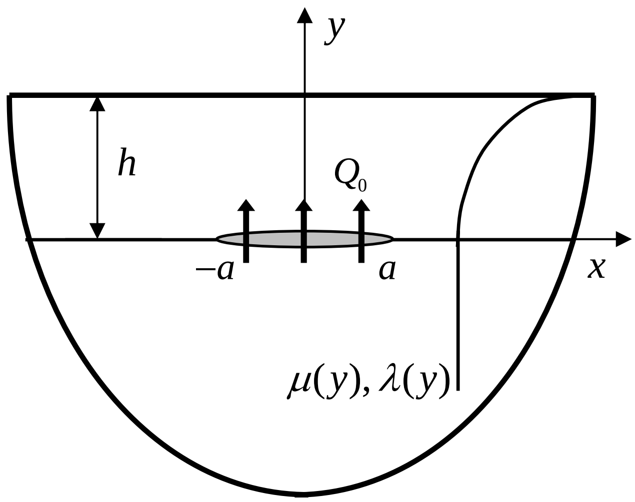


Figure 4.3: Geometry of the two dimensional heat conduction problem

We will solve Equation (4.9) by using Fourier integral transform method for plane-strain problem. Defining temperature distribution [27] $T_2(x,y)$,

$$T_2(x,y)=\frac{1}{2\pi}\int_{-\infty}^{+\infty}\tau(\xi,y)e^{i\xi x}d\xi, \tag{4.19}$$

and substituting it into (4.9) it will be obtained as

$$\frac{\partial}{\partial^2 y}\int_{-\infty}^{+\infty}\tau(\xi,y)e^{i\xi x}d\xi+\beta\frac{\partial}{\partial y}\int_{-\infty}^{+\infty}\tau(\xi,y)e^{i\xi x}d\xi+\frac{\partial^2}{\partial^2 x}\int_{-\infty}^{+\infty}\tau(\xi,y)e^{i\xi x}d\xi=0. \tag{4.20}$$

Using the properties of Fourier transform [31],

$$\Im\left\{\frac{\partial^n}{\partial x^n}f(x,y)\right\}=(i\xi)^n F(\xi,y) \tag{4.21}$$

Equation (4.20) can be expressed in terms of an ordinary differential equation as

$$\left(D^2+\beta D-\xi^2\right)\tau(\xi,y)=0 \tag{4.22}$$

where D is the differential operator, $D = d/dy$. The solution of the differential equation can be obtained by using the characteristic equation of the Equation (4.22) and it can be given as

$$\tau(\xi, y) = \begin{cases} A_1(\xi)e^{r_1 y} + A_2 e^{r_2 y}, & 0 < y < h, \\ B_1(\xi)e^{|\xi| y} + B_2(\xi)e^{-|\xi| y}, & y < 0 \end{cases} \tag{4.23}$$

where

$$r_1 = -\frac{\beta}{2} + \frac{1}{2}\sqrt{4\xi^2 + \beta^2} \quad \text{and} \quad r_2 = -\frac{\beta}{2} - \frac{1}{2}\sqrt{4\xi^2 + \beta^2} \tag{4.24}$$

are the roots of the characteristic equation in (4.22). Let us examine the sign of the roots as follows

$$r_1 = m_2 - m_1 = \frac{1}{2}\sqrt{4\xi^2 + \beta^2} - \frac{\beta}{2}, \tag{4.25}$$

$$r_2 = -(m_2 + m_1) = -\frac{1}{2}\sqrt{4\xi^2 + \beta^2} - \frac{\beta}{2} \tag{4.26}$$

where m_1 and m_2 are defined as

$$m_1 = \frac{\beta}{2} \quad \text{and} \quad m_2 = \frac{1}{2}\sqrt{4\xi^2 + \beta^2}. \tag{4.27}$$

Finally, we observed that

$$r_1 = -\frac{\beta}{2} + \frac{|\beta|}{2}\sqrt{1 + \left(\frac{2\xi}{\beta}\right)^2} > 0, \tag{4.28}$$

$$r_2 = -\frac{\beta}{2} - \frac{|\beta|}{2}\sqrt{1 + \left(\frac{2\xi}{\beta}\right)^2} < 0 \tag{4.29}$$

then

$$m_2 - m_1 > 0 \quad \text{and} \quad m_2 + m_1 > 0. \tag{4.30}$$

The solution of $\tau(\xi, y)$ that is transformed temperature now can be written in the following form

$$\tau(\xi, y) = \begin{cases} A_1(\xi)e^{(m_2 - m_1)y} + A_2(\xi)e^{(m_2 + m_1)y}, & 0 < y < h, \\ B_1(\xi)e^{|\xi| y} + B_2(\xi)e^{-|\xi| y}, & y < 0. \end{cases} \tag{4.31}$$

Since the transformed temperature function is bounded function at infinity then coefficient $B_2(\xi)$ becomes zero $\left(e^{-|\xi| y} \to \infty \ \text{ as } \ y \to -\infty\right)$. Also, using the boundary conditions (4.11) the coefficient $A_2(\xi)$ can be expressed in terms of coefficients $A_1(\xi)$ as

$$A_2 = \frac{m_2 - m_1}{m_2 + m_1} e^{2m_2} A_1 \tag{4.32}$$

and from the boundary condition (4.12) one can easily obtained $B_1(\xi)$ in terms of $A_1(\xi)$ like

$$B_1 = \left(1 - e^{2m_2 h}\right) \frac{m_2 - m_1}{|\xi|} A_1. \tag{4.33}$$

Finally, the transformed temperature function $\tau(\xi, y)$ can be written in terms of only one unknown constant $A_1(\xi)$ as follows:

$$\tau(\xi, y) = \begin{cases} e^{(m_2 - m_1)y} + \dfrac{m_2 - m_1}{m_2 + m_1} e^{2m_2} e^{-(m_2 + m_1)y} A_1(\xi), & 0 < y < h, \\ \left(1 - e^{2m_2}\right) \dfrac{m_2 - m_1}{|\xi|} e^{|\xi| y} A_1(\xi), & y < 0. \end{cases} \tag{4.34}$$

Now, we will define a new function, which is so-called the density function [37], to find unknown constant $A_1(\xi)$ at the interface of nonhomogeneous graded coating and homogeneous substrate like

$$\phi(x) = \frac{d}{dx}\left\{T_2\left(x, 0^+\right) - T_2\left(x, 0^-\right)\right\} \tag{4.35}$$

which satisfies

$$\int_{-a}^{a} \phi(\eta)\, d\eta = 0 \qquad \text{and} \qquad \phi(\eta) = 0 \qquad \text{at} \qquad a < |x| < \infty. \tag{4.36}$$

Let $\Phi(\xi)$ be defined as the Fourier transform of the density function $\phi(x)$ given in Equation (4.35). The transformed density function $\Phi(\xi)$, is identically zero at the outside of the barrier. We will obtained the last unknown constant $A_1(\xi)$ in terms of the new function $\Phi(\xi)$ such as,

$$\frac{1}{2\pi} \int_{-\infty}^{+\infty} \Phi_1(\xi) e^{i\xi x} d\xi = \frac{1}{2\pi} \int_{-\infty}^{+\infty} i\xi \left(\tau\left(\xi, 0^+\right) - \tau\left(\xi, 0^-\right)\right) e^{i\xi x} d\xi,$$

$$\Phi(\xi) = i\xi \left(\tau\left(\xi, 0^+\right) - \tau\left(\xi, 0^-\right)\right) \tag{4.37}$$

where

$$\tau\left(\xi,0^{+}\right)=\left(1+\frac{m_2-m_1}{m_2+m_1}e^{2m_2h}\right)A_1\left(\xi\right),\qquad \tau\left(\xi,0^{-}\right)=\left(1-e^{2m_2h}\right)\frac{m_2-m_1}{\left|\xi\right|}A_1\left(\xi\right). \tag{4.38}$$

By substituting the function values $\tau\left(\xi,0^{+}\right)$ and $\tau\left(\xi,0^{-}\right)$ into Equation (4.37) it may be obtained as

$$\Phi\left(\xi\right)=i\frac{\xi}{\left|\xi\right|}\frac{\left|\xi\right|\left(m_2+m_1\right)-m_2^2+m_1^2+\left(\left|\xi\right|\left(m_2-m_1\right)+m_2^2-m_1^2\right)e^{2m_2h}}{m_2+m_1}A_1\left(\xi\right).$$

From Equation (4.27), the last expression for $\Phi\left(\xi\right)$ can be reduced to the following form

$$\Phi\left(\xi\right)=i\frac{\xi}{\left|\xi\right|}\frac{\left|\xi\right|\left(m_2+m_1\right)-\left|\xi\right|^2+\left(\left|\xi\right|\left(m_2-m_1\right)+\left|\xi\right|^2\right)e^{2m_2h}}{m_2+m_1}A_1\left(\xi\right). \tag{4.39}$$

Then, using inverse Fourier transform the last unknown constant function, $A_1\left(\xi\right)$, can be obtained along with the condition (4.36) as

$$A_1\left(\xi\right)=\frac{1}{i\xi}\left(\frac{m_2+m_1}{\left(m_2+m_1\right)-\left|\xi\right|+\left(\left(m_2-m_1\right)+\left|\xi\right|\right)e^{2m_2h}}\right)\int_{-a}^{a}\phi\left(s\right)e^{-i\xi s}ds. \tag{4.40}$$

After all the derivative of transformed temperature is

$$\frac{d}{dy}\tau\left(\xi,y\right)=\begin{cases}\left(\left(m_2-m_1\right)e^{\left(m_2-m_1\right)y}-\left(m_2-m_1\right)e^{2m_2h}e^{-\left(m_2+m_1\right)y}\right)A_1\left(\xi\right), & 0<y<h,\\ \left(1-e^{2m_2h}\right)\left(m_2-m_1\right)e^{\left|\xi\right|y}A_1\left(\xi\right), & y<0\end{cases} \tag{4.41}$$

and from the boundary condition (4.14) as $y\to0^{-}$ one can reduced the problem into integral equation as follows:

$$\lim_{y\to0^{-}}e^{\beta y}\frac{1}{2\pi}\int_{-\infty}^{\infty}\left(1-e^{2m_2h}\right)\left(m_2-m_1\right)e^{\left|\xi\right|y}A_1\left(\xi\right)e^{i\xi x}d\xi=-\frac{Q_0}{k_0},$$

$$\lim_{y\to0^{-}}\frac{1}{2\pi}\int_{-\infty}^{\infty}e^{\left(\left|\xi\right|+\beta\right)y}\left[\frac{1}{i\xi}\frac{\left(1-e^{2m_2h}\right)\left(m_2^2-m_1^2\right)}{\left(m_2+m_1\right)-\left|\xi\right|+\left(\left(m_2-m_1\right)+\left|\xi\right|\right)e^{2m_2h}}\Phi\left(\xi\right)\right]e^{i\xi x}d\xi=-\frac{Q_0}{k_0},$$

$$\lim_{y\to0^{-}}\frac{1}{2\pi}\int_{-\infty}^{\infty}e^{\left(\left|\xi\right|+\beta\right)y}\left[\frac{1}{i\xi}\frac{\left(1-e^{2m_2h}\right)\xi^2\Phi\left(\xi\right)}{\left(m_2+m_1\right)-\left|\xi\right|+\left(\left(m_2-m_1\right)+\left|\xi\right|\right)e^{2m_2h}}\right]e^{i\xi x}d\xi=-\frac{Q_0}{k_0},$$

$$\lim_{y\to0^{-}}\frac{1}{2\pi}\int_{-\infty}^{\infty}e^{\left(\left|\xi\right|+\beta\right)y}\left[\frac{-i\xi\left(1-e^{2m_2h}\right)\int_{-a}^{a}\phi\left(s\right)e^{-i\xi s}ds}{\left(m_2+m_1\right)-\left|\xi\right|+\left(\left(m_2-m_1\right)+\left|\xi\right|\right)e^{2m_2h}}\right]e^{i\xi x}d\xi=-\frac{Q_0}{k_0},$$

$$-\frac{Q_0}{k_0}=\frac{1}{2\pi}\int_{-a}^{a}\phi(s)\,ds\lim_{y\to 0^-}\int_{-\infty}^{\infty}\frac{-i\xi\left(1-e^{2m_2h}\right)e^{(|\xi|+\beta)y}}{(m_2+m_1)-|\xi|+((m_2-m_1)+|\xi|)e^{2m_2h}}e^{-i\xi(s-x)}d\xi. \qquad (4.42)$$

Defining some values in Equation (4.42) in terms of basic variables and saying that $R=\frac{\beta}{2|\xi|}$, one may express as

$$m_2-m_1=\frac{1}{2}\sqrt{\beta^2+4\xi^2}-\frac{\beta}{2}=\frac{2|\xi|}{2}\sqrt{\left(\frac{\beta}{2|\xi|}\right)^2+1}-\frac{\beta}{2}\frac{|\xi|}{|\xi|}=|\xi|\sqrt{1+R^2}-|\xi|R, \qquad (4.43)$$

$$m_2+m_1=\frac{1}{2}\sqrt{\beta^2+4\xi^2}+\frac{\beta}{2}=\frac{2|\xi|}{2}\sqrt{\left(\frac{\beta}{2|\xi|}\right)^2+1}+\frac{\beta}{2}\frac{|\xi|}{|\xi|}=|\xi|\sqrt{1+R^2}+|\xi|R, \qquad (4.44)$$

$$e^{2m_2h}=e^{h\sqrt{\beta^2+4\xi^2}}=e^{2h|\xi|\sqrt{1+\left(\frac{\beta}{2\xi}\right)^2}}=e^{2h|\xi|\sqrt{1+R^2}}. \qquad (4.45)$$

Substituting Equations (4.43-4.45) into (4.42) it can be obtained as

$$-\frac{Q_0}{k_0}=\frac{1}{2\pi}\int_{-a}^{a}\phi(s)\,ds\lim_{y\to 0^-}\int_{-\infty}^{\infty}\frac{\xi\left(1-e^{2h|\xi|\sqrt{1+R^2}}\right)e^{(|\xi|+\beta)y}e^{-i\xi(s-x)}}{i|\xi|\left[\sqrt{1+R^2}+R-1+\left(\sqrt{1+R^2}-R+1\right)e^{2h|\xi|\sqrt{1+R^2}}\right]}d\xi. \qquad (4.46)$$

To solve the infinity integral in Equation (4.46) it will be used some identities related to the complex function properties of the integrand such as

$$\frac{1}{i}e^{-i\xi(s-x)}=-ie^{-i\xi(s-x)}=-i\left(\cos\xi(s-x)-i\sin\xi(s-x)\right),$$

$$=-\sin\xi(s-x)-i\cos\xi(s-x).$$

Since $\int_{-\infty}^{\infty}f(\xi)\,d\xi=\int_{-\infty}^{0}f(\xi)\,d\xi+\int_{0}^{\infty}f(\xi)\,d\xi$ and defining that

$$\xi\Big|_{-\infty}^{0}=-\xi\Big|_{\infty}^{0}\Rightarrow d\xi=-d\xi$$

It can be written that

$$\int_{-\infty}^{\infty}f(\xi)\,d\xi=\int_{-\infty}^{0}f(\xi)\,d\xi+\int_{0}^{\infty}f(\xi)\,d\xi,$$

$$=\int_{-\infty}^{0}f(-\xi)\,d(-\xi)+\int_{0}^{\infty}f(\xi)\,d\xi=\int_{0}^{\infty}f(-\xi)\,d\xi+\int_{0}^{\infty}f(\xi)\,d\xi.$$

After all of these simplifications the part that contains infinity integral in Equation (4.46) can be defined as

$$F(\xi)=\frac{\left(1-e^{2h\xi\sqrt{1+R^2}}\right)}{\left[\sqrt{1+R^2}+R-1+\left(\sqrt{1+R^2}-R+1\right)e^{2h\xi\sqrt{1+R^2}}\right]}$$

and the same equation can be written in the following form

$$\lim_{y\to 0^-}\int_0^\infty -F(\xi)e^{(\xi+\beta)y}\frac{e^{i\xi(s-x)}}{i}d\xi+\int_0^\infty F(\xi)e^{(\xi+\beta)y}\frac{e^{-i\xi(s-x)}}{i}d\xi,$$

$$=\lim_{y\to 0^-}\int_0^\infty iF(\xi)e^{(\xi+\beta)y}\left(i\cos\xi(s-x)-\sin\xi(s-x)\right)d\xi$$

$$+\lim_{y\to 0^-}\int_0^\infty F(\xi)e^{(\xi+\beta)y}\left(-\sin\xi(s-x)-i\cos\xi(s-x)\right)d\xi$$

$$=-2\int_0^\infty F(\xi)e^{(\xi+\beta)y}\sin\xi(s-x)d\xi.$$

As a result of these simplification Equation (4.46) can be reduced to the form of

$$-\frac{2Q_0}{k_0}=\frac{1}{\pi}\int_{-a}^{a}\phi(s)ds\lim_{y\to 0^-}\int_0^\infty -2F(\xi)e^{(\xi+\beta)y}\sin\xi(s-x)d\xi. \tag{4.47}$$

Now the next step is the asymptotically expand the integrand to separate the singular part if any. For this purposes we will examine the integrand $2F(\xi)$ as $\xi\to\infty$ (or $R\to 0$)

$$\frac{-2\left(1-e^{2h\xi\sqrt{1+R^2}}\right)}{\left[\sqrt{1+R^2}+R-1+\left(\sqrt{1+R^2}-R+1\right)e^{2h\xi\sqrt{1+R^2}}\right]}\frac{e^{-2h\xi\sqrt{1+R^2}}}{e^{-2h\xi\sqrt{1+R^2}}}$$

$$=\frac{-2\left(e^{2h\xi\sqrt{1+R^2}}-1\right)}{\left(\sqrt{1+R^2}+R-1\right)e^{-2h\xi\sqrt{1+R^2}}+\sqrt{1+R^2}-R+1},$$

$$=1-e^{-2h\xi}+\frac{1}{2}\left(e^{-2h\xi}-1\right)^2R+\left(e^{-2h\xi}h\xi-\frac{1}{4}\left(1-e^{-4h\xi}\right)-\frac{1}{4}\left(e^{-2h\xi}-1\right)^3\right)R^2$$

$$+\left[-\frac{1}{2}\left(e^{-2h\xi}-1\right)e^{-2h\xi}h\xi-\frac{1}{8}\left(e^{-4h\xi}-1\right)\left(e^{-2h\xi}-1\right).\right.$$

$$\left.-\frac{1}{2}\left(e^{-2h\xi}h\xi+e^{-4h\xi}-\frac{1}{4}e^{-6h\xi}-\frac{3}{4}e^{-2h\xi}\right)\left(e^{-2h\xi}-1\right)\right]R^3+0\left(R^4\right).$$

Simplifying the last expression as $\xi\to\infty$,

$$F(R)=1+\frac{1}{2}R-\frac{1}{8}R^3+\frac{1}{16}R^5-\frac{5}{128}R^7+\frac{7}{256}R^9-\frac{21}{1024}R^{11}+\frac{33}{2048}R^{13}-0\left(R^{13}\right), \tag{4.48}$$

$$F(\xi)=1+\frac{1}{2}\frac{\beta}{2\xi}-\frac{1}{8}\left(\frac{\beta}{2\xi}\right)^3+\frac{1}{16}\left(\frac{\beta}{2\xi}\right)^5-\frac{5}{128}\left(\frac{\beta}{2\xi}\right)^7+\frac{7}{256}\left(\frac{\beta}{2\xi}\right)^9-\frac{21}{1024}\left(\frac{\beta}{2\xi}\right)^{11}\ldots \quad (4.49)$$

As we realized the second part of the integrand which contains the exponential function tends to zero as $R\to 0$ $(\xi\to\infty)$. To eliminate the singularity, so called Cauchy type, let us write the integral equation (4.47) again like

$$\frac{1}{\pi}\int_{-a}^{a}\phi(s)ds\lim_{y\to 0^-}\int_0^\infty\left(-2F(\xi)-1+1\right)e^{(\xi+\beta)y}\sin\xi(s-x)d\xi=-\frac{2Q_0}{k_0}. \quad (4.50)$$

Separating the integrand as

$$\frac{1}{\pi}\int_{-a}^{a}\phi(s)ds\lim_{y\to 0^-}\int_0^\infty e^{(\xi+\beta)y}\sin\xi(s-x)d\xi$$

$$+\int_{-a}^{a}\phi(s)ds\lim_{y\to 0^-}\frac{1}{\pi}\int_0^\infty\left(-2F(\xi)-1\right)e^{(\xi+\beta)y}\sin\xi(s-x)d\xi=-\frac{2Q_0}{k_0}, \quad (4.51)$$

we will examine the first infinity integral to show the singularity part as follows:

$$\lim_{y\to 0^-}\int_0^\infty e^{\xi y}e^{\beta y}\sin\xi(s-x)d\xi$$

$$=\lim_{y\to 0^-}e^{\beta y}\left(\frac{xe^{\xi y}\cos\xi(s-x)-x-ye^{\xi y}\sin\xi(s-x)+s-se^{\xi y}\cos\xi(s-x)}{y^2+s^2-2sx+x^2}\right),$$

$$=\lim_{y\to 0^-}e^{\beta y}\left(\frac{(s-x)\left(1-e^{\xi y}\cos\xi(s-x)\right)-ye^{\xi y}\sin\xi(s-x)}{y^2+(s-x)^2}\right),$$

$$=\lim_{y\to 0^-}e^{\beta y}\left(\frac{(s-x)\left(1-e^{\xi y}\cos\xi(s-x)\right)}{y^2+(s-x)^2}-\frac{ye^{\xi y}\sin\xi(s-x)}{y^2+(s-x)^2}\right),$$

$$=\lim_{y\to 0^-}e^{\beta y}\frac{(s-x)\left(1-e^{\xi y}\cos\xi(s-x)\right)}{y^2+(s-x)^2}-\lim_{y\to 0^-}e^{\beta y}\frac{ye^{\xi y}\sin\xi(s-x)}{y^2+(s-x)^2}$$

$$=\frac{s-x}{(s-x)^2}-0=\frac{1}{s-x}$$

where the value $\frac{1}{s-x}$ is called as the dominant term of the integral equation. Then, the Equation (4.50) becomes

$$\frac{1}{\pi}\int_{-a}^{a}\frac{\phi(s)}{s-x}ds+\int_{-a}^{a}\phi(s)ds\lim_{y\to 0^-}\frac{1}{\pi}\int_0^\infty\left(-2F(\xi)-1\right)e^{(\xi+\beta)y}\sin\xi(s-x)d\xi=-\frac{2Q_0}{k_0} \quad (4.52)$$

and as $y \to 0^-$ the Equation (4.52) turn into

$$\frac{1}{\pi}\int_{-a}^{a}\frac{\phi(s)}{s-x}ds+\frac{1}{\pi}\int_{-a}^{a}\phi(s)\,ds\int_{0}^{\infty}k(\xi)\,\sin\xi(s-x)\,d\xi=-\frac{2Q_0}{k_0} \tag{4.53}$$

where

$$k(\xi)=\frac{-2\left(e^{-2h\xi\sqrt{1+R^2}}-1\right)}{\left(\sqrt{1+R^2}+R-1\right)e^{-2h\xi\sqrt{1+R^2}}+\sqrt{1+R^2}-R+1}-1. \tag{4.54}$$

Now, we will try to solve the infinity integral in Equation (4.53) by separating it into two parts over the interval $[0,A]$ and $[A,\infty]$

$$\frac{1}{\pi}\int_{-a}^{a}\frac{\phi(s)}{s-x}ds$$

$$+\frac{1}{\pi}\int_{-a}^{a}\phi(s)\,ds\left(\int_{0}^{A}k_c(\xi)\sin\xi(s-x)\,d\xi+\int_{A}^{\infty}k_a(\xi)\sin\xi(s-x)\,d\xi\right)=-\frac{2Q_0}{k_0} \tag{4.55}$$

where $k_c(\xi)=k(\xi)$ is a close form of the integrand and $k_a(\xi)$ is an asymptotic expansion of integrand as $\xi\to\infty$ given by

$$k_a(\xi)=\frac{1}{2}\frac{\beta}{2\xi}-\frac{1}{8}\left(\frac{\beta}{2\xi}\right)^3+\frac{1}{16}\left(\frac{\beta}{2\xi}\right)^5-\frac{5}{128}\left(\frac{\beta}{2\xi}\right)^7+\frac{7}{256}\left(\frac{\beta}{2\xi}\right)^9-\frac{21}{1024}\left(\frac{\beta}{2\xi}\right)^{11}-0\left(R^{13}\right)$$

or

$$k_a(\xi)=\frac{\beta}{2^2}\frac{1}{\xi}-\frac{\beta^3}{2^6}\frac{1}{\xi^3}+\frac{\beta^5}{2^9}\frac{1}{\xi^5}-\frac{5\beta^7}{2^{14}}\frac{1}{\xi^7}+\frac{7\beta^9}{2^{17}}\frac{1}{\xi^9}-\frac{21\beta^{11}}{2^{21}}\frac{1}{\xi^{11}}-0\left(R^{13}\right). \tag{4.56}$$

4.4 NUMERICAL PROCEDURE

Numerical procedure starts with non-dimensionalization process by defining that

$$s=at \quad\Rightarrow\quad ds=a\,dt, \qquad x=ar \quad\Rightarrow\quad dx=a\,dr, \qquad a\xi=\lambda \quad\Rightarrow\quad a\,d\xi=d\lambda, \tag{4.57}$$

$$h=al, \qquad\qquad a\beta=\kappa. \tag{4.58}$$

According to all new variables, the Equation (4.55) that is dimensionless anymore becomes

$$\frac{1}{\pi}\int_{-1}^{1}\frac{\phi(at)}{t-r}dt$$

$$+\frac{1}{\pi}\int_{-1}^{1}\phi(at)\,dt\left(\int_{0}^{A}k_c(\lambda)\sin\lambda(t-r)\,d\lambda+\int_{A}^{\infty}k_a(\lambda)\sin\lambda(t-r)\,d\lambda\right)=-\frac{2Q_0}{k_0} \tag{4.59}$$

where

$$k_c(\xi)=\frac{-2\lambda\left(e^{-l\sqrt{\kappa^2+4\lambda^2}}-1\right)}{\left(\frac{1}{2\lambda}\sqrt{\kappa^2+4\lambda^2}+\frac{\kappa}{2\lambda}-1\right)e^{-l\sqrt{\kappa^2+4\lambda^2}}+\frac{1}{2\lambda}\sqrt{\kappa^2+4\lambda^2}-\frac{\kappa}{2\lambda}+1}-1, \tag{4.60}$$

$$k_a(\lambda)=\frac{1}{2^2}\frac{\kappa}{\lambda}-\frac{1}{2^6}\frac{\kappa^3}{\lambda^3}+\frac{1}{2^9}\frac{\kappa^5}{\lambda^5}-\frac{5}{2^{14}}\frac{\kappa^7}{\lambda^7}+\frac{7}{2^{17}}\frac{\kappa^9}{\lambda^9}-\frac{21}{2^{21}}\frac{\kappa^{11}}{\lambda^{11}}-0\left(R^{13}\right). \tag{4.61}$$

Since we have some singularities in the interval $[-1,1]$ then we have to eliminate them. Let us examine the close form solution of the following integrals

$$\int_0^\infty \frac{\sin\lambda(t-r)}{\lambda}d\lambda=\frac{|t-r|}{t-r}\int_0^\infty \frac{\sin\lambda|t-r|}{\lambda}d\lambda$$

then using the transform $\lambda|t-r|=\theta$

$$\int_0^\infty \frac{\sin\lambda(t-r)}{\lambda}d\lambda=\frac{|t-r|}{t-r}\int_0^\infty \frac{\sin\theta}{\theta}d\theta=\frac{|t-r|}{t-r}\frac{\pi}{2}=\frac{\pi}{2}\operatorname{sgn}(t-r). \tag{4.62}$$

Now substituting these values into the integral equation in (4.59) like

$$\frac{1}{\pi}\int_{-1}^{1}\frac{\phi(t)}{t-r}dt+\frac{1}{\pi}\int_{-1}^{1}\phi(t)dt\left(H(t,r)-\frac{\pi}{2}\frac{\kappa}{4}\frac{|t-r|}{t-r}\right)+\frac{1}{\pi}\int_{-1}^{1}\frac{\pi}{2}\frac{\kappa}{4}\frac{|t-r|}{t-r}\phi(t)dt=-\frac{2Q_0}{k_0} \tag{4.63}$$

where

$$H(t,r)=\int_0^A k_c(\lambda)\sin\lambda(t-r)d\lambda+\int_A^\infty k_a(\lambda)\sin\lambda(t-r)d\lambda. \tag{4.64}$$

Let us simplify the looks of the integral equation by defining new functions like

$$\frac{1}{\pi}\int_{-1}^{1}\frac{\phi(t)}{t-r}dt+\int_{-1}^{1}\phi(t)X(t,r)dt+\int_{-1}^{1}\phi(t)Y(t,r)dt=-\frac{2Q_0}{k_0} \tag{4.65}$$

where

$$X(t,r)=\frac{1}{\pi}\left(H(t,r)-\frac{\pi\kappa}{8}\frac{|t-r|}{t-r}\right), \tag{4.66}$$

$$Y(t,r)=\frac{\kappa}{8}\frac{|t-r|}{t-r}. \tag{4.67}$$

To solve the integral equation we redefine the density functions $\phi(t)$ as series of orthogonal functions [31-33] such as

$$\phi(t)=\sum_{n=0}^{N}A_n\frac{\mathrm{T}_n(t)}{\sqrt{1-t^2}} \tag{4.68}$$

along with the conditions

$$\int_{-1}^{1}\phi(t)\,dt=0, \qquad \phi(x)=-\phi(-x) \tag{4.69}$$

where $\mathrm{T}_n(t)$ is called as the Chebyshev polynomial of the first kind which are orthogonal with respect to the weight function $\frac{1}{\sqrt{1-t^2}}$. Now, by using the single valuedness condition given in Equation (4.36) and noting that $T_0(t)=1$,

$$\int_{-1}^{1}\phi(t)\,dt=\sum_{n=0}^{N}A_n\int_{-1}^{1}\frac{\mathrm{T}_n(t)\mathrm{T}_0(t)}{\sqrt{1-t^2}}\,dt=0 \tag{4.70}$$

then $A_0=0$ due to the orthogonality properties of the Chebyshev polynomials. By using the oddness of $\phi(t)$ given in Equation (4.69), Equation (4.68) can be written in terms of odd indices of the Chebyshev polynomials like

$$\phi(t)=\sum_{n=1}^{N}A_n\frac{\mathrm{T}_{2n-1}(t)}{\sqrt{1-t^2}}. \tag{4.71}$$

Let us write the integral equation (4.65) again by substituting functions $\phi(t)$ into integral equation such as

$$\sum_{n=1}^{N}A_n\frac{1}{\pi}\int_{-1}^{1}\frac{\mathrm{T}_{2n-1}(t)}{(t-r)\sqrt{1-t^2}}\,dt$$
$$+\sum_{n=1}^{N}A_n\int_{-1}^{1}\frac{\mathrm{T}_{2n-1}(t)}{\sqrt{1-t^2}}X(t,r)\,dt+\sum_{n=1}^{N}A_n\int_{-1}^{1}\frac{\mathrm{T}_{2n-1}(t)}{\sqrt{1-t^2}}Y(t,r)\,dt=-\frac{2Q_0}{k_0}. \tag{4.72}$$

Now we will examine each integral in the system above starting from the first integral. By using the following identity for Chebyshev polynomials

$$\frac{1}{\pi}\int_{-1}^{1}\frac{\mathrm{T}_k(t)}{(t-r)\sqrt{1-t^2}}\,dt=\begin{cases}0, & k=0\ ,-1<r<1,\\ \mathrm{U}_{k-1}(r), & k>0\ ,-1<r<1\end{cases} \tag{4.73}$$

then the first integral in Equation (4.72) becomes

$$\frac{1}{\pi}\int_{-1}^{1}\frac{\mathrm{T}_{2n-1}(t)}{(t-r)\sqrt{1-t^2}}\,dt=\mathrm{U}_{2n-2}(r) \tag{4.74}$$

where $\mathrm{U}_{2n-2}(r)$ the Chebyshev polynomial of the second kind and defined as

$$\mathrm{U}_k(r)=\frac{\sin\left[(k+1)\arccos(r)\right]}{\sin\left[\arccos(r)\right]} \tag{4.75}$$

for $k = 2n-2$ the second kind of Chebyshev polynomials can be expressed in terms of trigonometric function of sines and cosines as

$$\mathrm{U}_{2n-2}(r) = \frac{\sin\left[(2n-1)\arccos(r)\right]}{\sin\left[\arccos(r)\right]}. \tag{4.76}$$

For the other integrals in Equation (4.72) we will define a map such that

$$t = \cos\theta \quad \Rightarrow \quad dt = -\sin\theta \, d\theta, \quad t\,\Big|_{r}^{1} = \theta\,\Big|_{\arccos(r)}^{0} \quad \text{and} \quad t\,\Big|_{-1}^{r} = \theta\,\Big|_{\pi}^{\arccos(r)} \tag{4.77}$$

also, from the definition of Chebyshev polynomials of the first kind, it can be written that

$$\mathrm{T}_k(t) = \cos\left[k\arccos(t)\right] = \cos\left[k\arccos(\cos\theta)\right] = \cos(k\theta). \tag{4.78}$$

The second integral in Equation (4.72) can be expressed as in the form of

$$\int_{-1}^{1} \frac{\mathrm{T}_{2n-1}(t)}{\sqrt{1-t^2}} X(t,r)\,dt = \int_{\pi}^{0} \frac{\cos\left[(2n-1)\theta\right]}{\sin\theta} X(t,r)(-\sin\theta)\,d\theta,$$

$$= \int_{0}^{\pi} \cos\left[(2n-1)\theta\right] X(t,r)\,d\theta. \tag{4.79}$$

Because of the disadvantage of Gauss quadrature, the third integral in Equation (4.72) that contains sign function has to be rewritten to eliminate the singularity in the following form

$$\int_{-1}^{1} \frac{|t-r|}{t-r}\phi(t)\,dt = \int_{r}^{1}\phi(t)\,dt - \int_{-1}^{r}\phi(t)\,dt. \tag{4.80}$$

Then, the third integral can be expressed as

$$\int_{-1}^{r} \frac{\mathrm{T}_{2n-1}(t)}{\sqrt{1-t^2}} Y(t,r)\,dt = \int_{\pi}^{\arccos(r)} \frac{\cos\left[(2n-1)\theta\right]}{\sin\theta}(-\sin\theta)\frac{\kappa}{8}\,d\theta,$$

$$= \frac{\kappa}{8}\int_{\arccos(r)}^{\pi} \cos\left[(2n-1)\theta\right] d\theta \tag{4.81}$$

and

$$\int_{r}^{1} \frac{\mathrm{T}_k(t)}{\sqrt{1-t^2}} Y(t,r)\,dt = \int_{\arccos(r)}^{0} \frac{\cos\left[(2n-1)\theta\right]}{\sin\theta}(-\sin\theta)\frac{\kappa}{8}\,d\theta,$$

$$= \frac{\kappa}{8}\int_{0}^{\arccos(r)} \cos\left[(2n-1)\theta\right] d\theta. \tag{4.82}$$

Then the integral can be evaluated as

$$Y_E(r)=\int_{-1}^{1}\frac{T_{2n-1}(t)}{\sqrt{1-t^2}}Y(t,r)\,dt=-\frac{\kappa}{8}\int_{\arccos(r)}^{\pi}\cos\left[(2n-1)\theta\right]d\theta+\frac{\kappa}{8}\int_{0}^{\arccos(r)}\cos\left[(2n-1)\theta\right]d\theta,$$

$$=\frac{\kappa}{8}\left(-\int_{\arccos(r)}^{\pi}\cos\left[(2n-1)\theta\right]d\theta+\int_{0}^{\arccos(r)}\cos\left[(2n-1)\theta\right]d\theta\right),$$

$$=\frac{\kappa}{8}\left(-\frac{\sin\left[(2n-1)\theta\right]}{2n-1}\Bigg|_{\arccos(r)}^{\pi}+\frac{\sin\left[(2n-1)\theta\right]}{2n-1}\Bigg|_{0}^{\arccos(r)}\right),$$

$$Y_E(r)=\frac{\kappa}{4}\left(\frac{\sin\left[(2n-1)\arccos(r)\right]}{2n-1}\right)\quad,\quad n=1,2,3,,... \tag{4.83}$$

then the integral equation in (4.72) becomes

$$\sum_{n=1}^{N}A_n U_{2n-2}(r)+\sum_{n=1}^{N}A_n\int_0^{\pi}\cos\left[(2n-1)\theta\right]X(\cos\theta,r)\,d\theta+\sum_{n=1}^{N}A_nY_E(r)=-\frac{2Q_0}{k_0},$$

$$\sum_{n=1}^{N}A_n\left(U_{2n-2}(r)+\int_0^{\pi}\cos\left[(2n-1)\theta\right]X(\cos\theta,r)\,d\theta+Y_E(r)\right)=-\frac{2Q_0}{k_0} \tag{4.84}$$

where

$$X(\cos\theta,r)=\frac{1}{\pi}\left(H(\cos\theta,r)-\frac{\pi\kappa}{8}\frac{|\cos\theta-r|}{\cos\theta-r}\right). \tag{4.85}$$

and $H(\cos\theta,r)$ is defined in Equation (4.64). Defining

$$a_{in}(r_i)=U_{2n-2}(r)+\int_0^{\pi}\cos\left[(2n-1)\theta\right]X(\cos\theta,r)\,d\theta+Y_E(r) \tag{4.86}$$

as a new function then the integral equation can be turned into the system of algebraic equations for each discrete value of r_i in the interval $[-1,1]$, such as

$$\sum_{n=1}^{N}A_n a_{in}(r_i)=-\frac{2Q_0}{k_0}. \tag{4.87}$$

For example, when we choose the number of collocation points, r_i as 5 the following system can be obtained to be solved

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} & a_{15}\\ a_{21} & a_{22} & a_{23} & a_{24} & a_{25}\\ a_{31} & a_{32} & a_{33} & a_{34} & a_{35}\\ a_{41} & a_{42} & a_{43} & a_{44} & a_{45}\\ a_{51} & a_{52} & a_{53} & a_{54} & a_{55}\end{pmatrix}\begin{pmatrix}A_1\\A_2\\A_3\\A_4\\A_5\end{pmatrix}=\begin{pmatrix}2Q_0/k_0\\2Q_0/k_0\\2Q_0/k_0\\2Q_0/k_0\\2Q_0/k_0\end{pmatrix}. \tag{4.88}$$

From the solution of the system given by Equation (4.87), A_n are obtained at each collocation point. The temperature distribution around the insulated barrier may easily be calculated by using Equations (4.35) and (4.71) as follows:

$$\phi(x/a)=\frac{d}{dx}\left(T\left(x,0^+\right)-T\left(x,0^-\right)\right)=\sum_{n=1}^{N}A_n\frac{\mathrm{T}_{2n-1}\left(x/a\right)}{\sqrt{1-\left(x/a\right)^2}},$$

$$\int_{-a}^{x}\frac{d}{d\eta}\left(T\left(\eta,0^+\right)-T\left(\eta,0^-\right)\right)d\eta=\sum_{n=1}^{N}\int_{-a}^{x}A_n\frac{\mathrm{T}_{2n-1}\left(\eta/a\right)}{\sqrt{1-\left(\eta/a\right)^2}}d\eta,$$

$$T\left(\eta,0^+\right)-T\left(\eta,0^-\right)\Big|_{-a}^{x}=\sum_{n=1}^{N}\int_{-a}^{x}A_n\frac{\mathrm{T}_{2n-1}\left(\eta/a\right)}{\sqrt{1-\left(\eta/a\right)^2}}d\eta,$$

$$T\left(x,0^+\right)-T\left(x,0^-\right)=\sum_{n=1}^{N}\int_{-1}^{x/a}A_n\frac{\mathrm{T}_{2n-1}\left(\eta\right)}{\sqrt{1-\eta^2}}d\eta. \qquad (4.89)$$

The close form solution for the integral in Equation (4.89) can be shown to be

$$\int_{-1}^{x/a}\frac{\mathrm{T}_k\left(s\right)}{\sqrt{1-s^2}}ds=-\frac{1}{k}\mathrm{U}_{k-1}\left(x/a\right)\sqrt{1-\left(x/a\right)^2}, \qquad k>1. \qquad (4.90)$$

Or by defining a new variable

$$\eta=\cos\eta, \qquad \pi\le\theta\le\arccos\left(x/a\right), \qquad (4.91)$$

the value of the integral in Equation (4.89) can be obtained as

$$\int_{-1}^{x/a}\frac{\mathrm{T}_k\left(s\right)}{\sqrt{1-s^2}}ds=\int_{\pi}^{\arccos(x/a)}\cos\left[\left(2n-1\right)\theta\right]d\theta=\frac{\sin\left[\left(2n-1\right)\arccos\left(x/a\right)\right]}{2n-1}. \qquad (4.92)$$

Then the difference in temperature distribution on the plane of the insulated barrier may be obtained as

$$T\left(x,0^+\right)-T\left(x,0^-\right)=\sum_{n=1}^{N}A_n\frac{\sin\left(\left(2n-1\right)\arccos\left(x/a\right)\right)}{2n-1}. \qquad (4.93)$$

By using the relation in Equation (4.76), the temperature distribution on the plane of insulated barrier can be shown in terms of coefficients A_n and $\mathrm{U}_{2n-2}\left(x/a\right)$ as

$$T^*\left(x\right)=T\left(x,0^+\right)-T\left(x,0^-\right)=\sqrt{1-\left(x/a\right)^2}\sum_{n=1}^{N}A_n\frac{\mathrm{U}_{2n-2}\left(x/a\right)}{2n-1}. \qquad (4.94)$$

In the next section, temperature distribution difference on the barrier surface will be represented for different material nonhomogeneity parameter β.

CHAPTER 5

CONCLUSION OF THE STUDY

5.1 CONCLUSION AND DISCUSSION

At the end of the analytical part in Chapter 4, the temperature distribution on the barrier as a series of Chebyshev polynomials of the second kind with suitable coefficients A_n is obtained. The values of A_n are obtained from the Equation (4.87) as a solution of the system depends on the part of integral equation in (4.84) which contains the effect of nonhomogeneity parameter β. In the following figures the effect of the nonhomogeneity parameter β and the thickness of the nonhomogeneous coating h/a on the thermal distribution on the barrier are shown for different values.

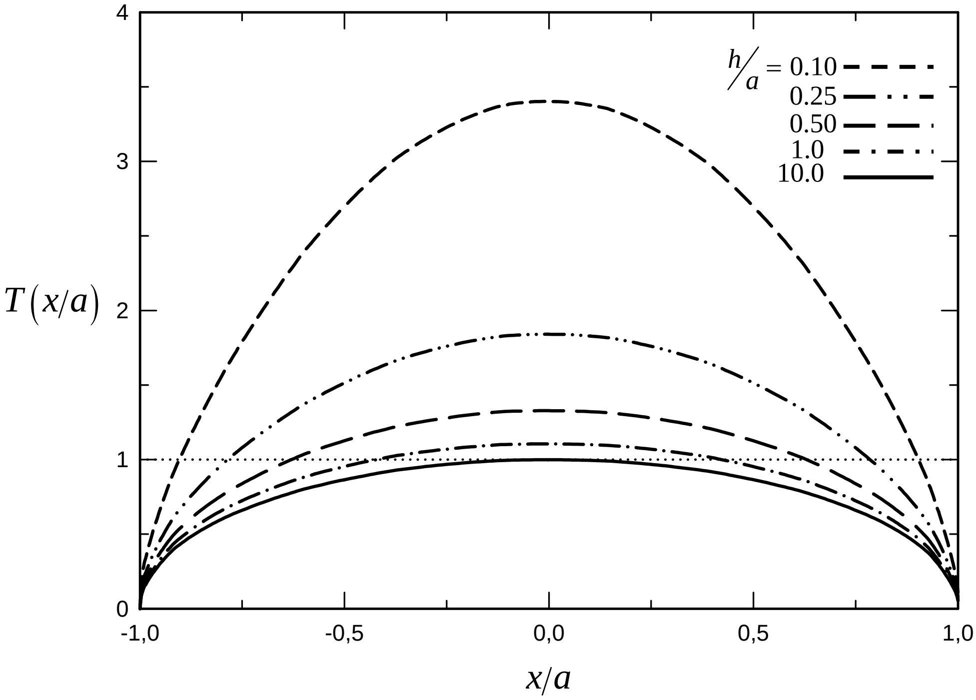


Figure 5.1: Temperature distribution on the barrier for various thicknesses of coating as nonhomogeneity parameter $\beta = 0$.

From the close form solution of a homogeneous infinite medium containing an insulated barrier the temperature distribution is given [27] as

$$T(x) = T(x,0^+) - T(x,0^-) = 2\pi \frac{Q_0}{k_0}\sqrt{a^2 - x^2}. \tag{5.1}$$

The results of this study were compared with Equation (5.1) for homogeneous medium ($\beta = 0$) with a large thickness parameter h/a. Assuming that $h/a = 10.0$ is large enough for comparing the homogeneous case in Equation (5.1) it was shown that there is a perfect agreement (Fig. 5.1). In this study, the results for homogeneous medium ($\beta = 0$) with different coating thicknesses h/a are perfectly match the results given in [27]. As it is expected the decreasing coating thickness increases the temperature distribution on the barrier. Due to the convergence of the numerical scheme used in this study the lowest coating thickness accepted as $h/a = 0.10$ which gives the highest temperature distribution on the barrier. The effect of the coating thickness on the temperature distribution increases as the thickness is getting smaller and smaller (Fig. 5.1).

Results for nonhomogeneous case of hardening coating material ($\beta > 0$) are represented in Figures 5.2–5.5. Observing the all four figures together one can easily see that the temperature distribution on the barrier is increasing with decreasing coating thickness h/a values. As it is seen in Figure 5.3, $\beta = 1.0$, temperature distribution on the barrier of infinite medium (semi-infinite coating on semi-infinite substrate) is decreasing in terms of the results given in Equation (5.1). As a result, in designing or manufacturing machine parts that work under constant thermal flux one can use the hardening coating material to be in need of low temperature distribution on the barrier. Once we obtained the thermal stress distribution around a barrier one can easily find the thermal stresses around it by using equilibrium equations and stress-strain relations [36, 28].

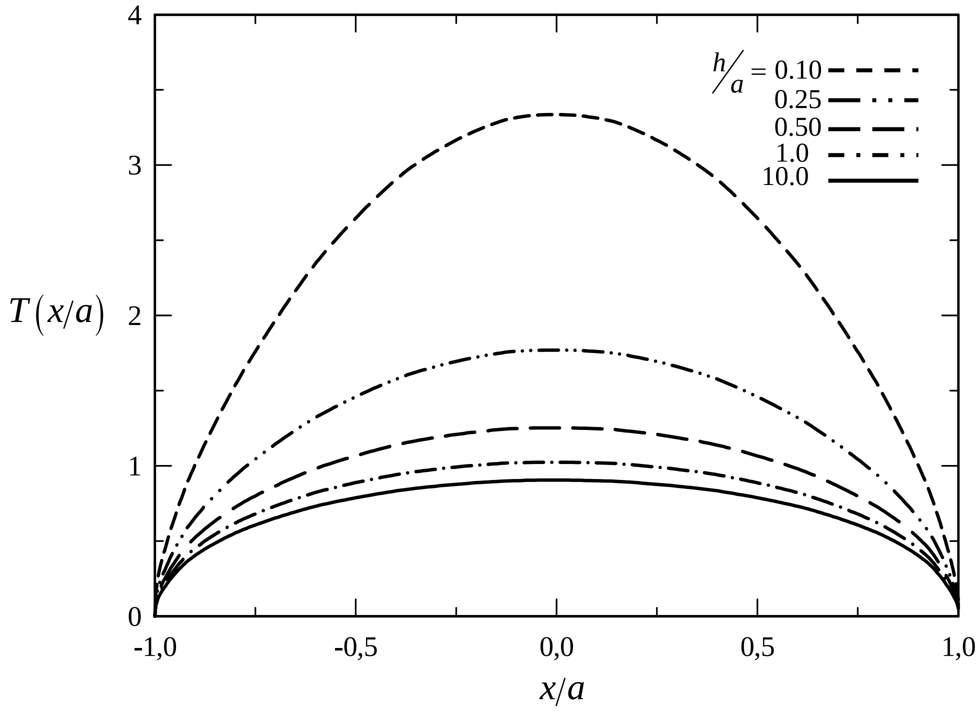


Figure 5.2: Temperature distribution on the barrier for various thicknesses of coating as nonhomogeneity parameter $\beta = 0.5$.

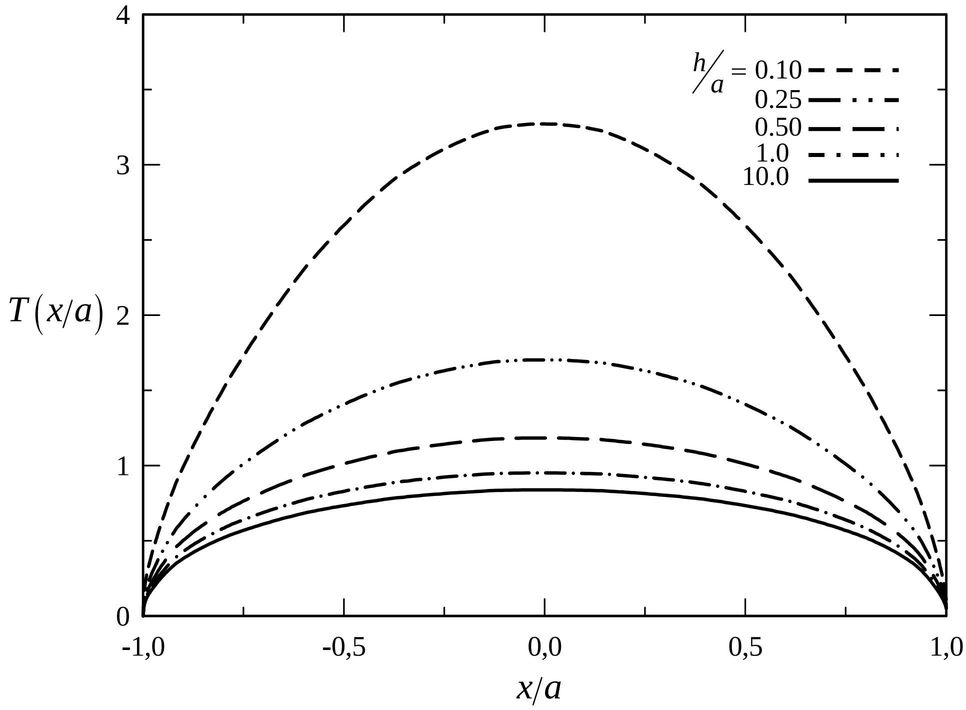


Figure 5.3: Temperature distribution on the barrier for various thicknesses of coating as nonhomogeneity parameter $\beta = 1.0$.

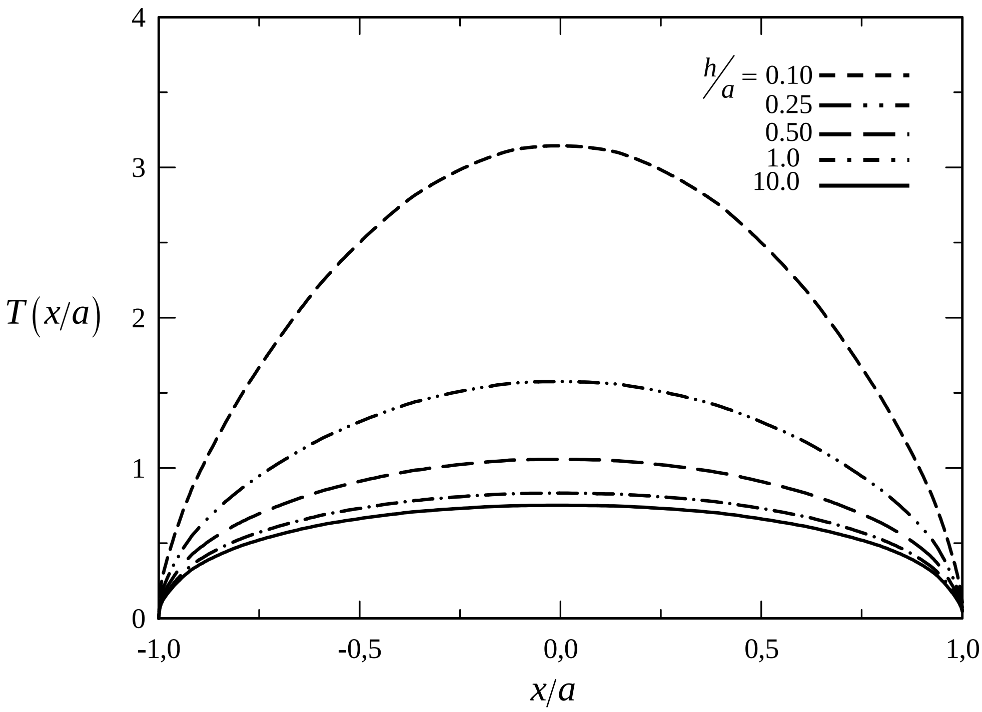


Figure 5.4: Temperature distribution on the barrier for various thicknesses of coating as nonhomogeneity parameter $\beta = 2.0$.

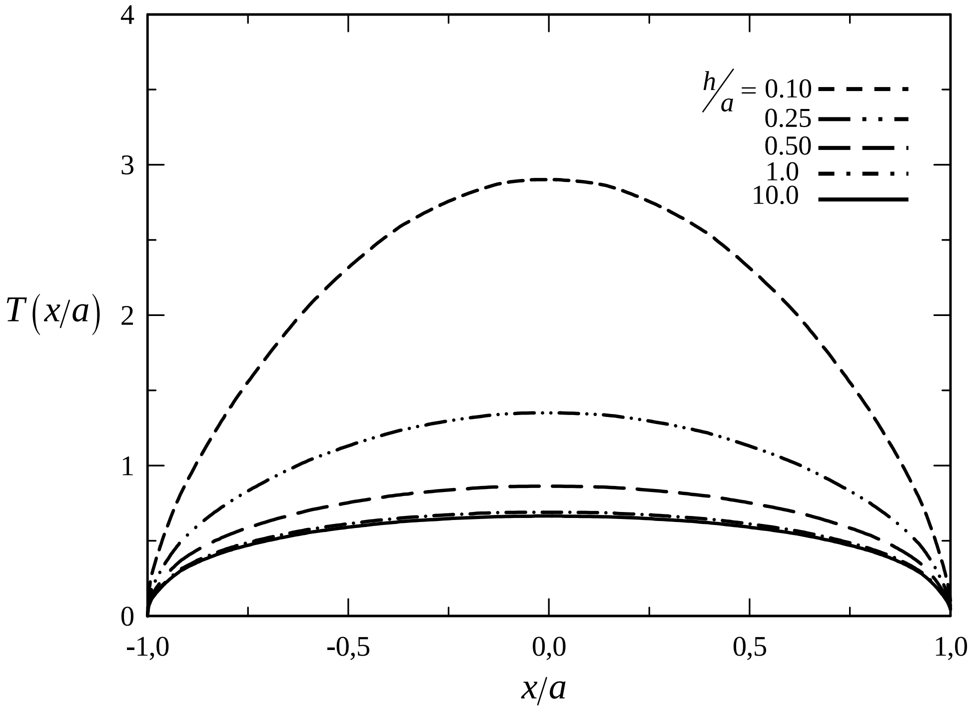


Figure 5.5: Temperature distribution on the barrier for various thicknesses of coating as nonhomogeneity parameter $\beta = 4.0$.

Similarly, observing the Figures 5.6–5.9 in which the nonhomogeneous coating is softening through the substrate ($\beta < 0$) it can be seen that the temperature distribution on the barrier is increasing when the thickness of the coating is decreasing as it is expected. When it is compared to homogeneous case given in Equation (5.1) the temperature distribution on the barrier of infinite medium (solid line) is increasing rapidly. In designing process it is not easy to find an application for this case due to high thermal stresses on the barrier caused by high temperature distribution.

In Figure 5.10, it is shown the effect of the nonhomogeneity parameter on the temperature distribution where the solid line represents the infinite medium and the values are matched with Equation (5.1) at $\beta = 0$. Observing the Figure 5.10, one can easily observe that the decreasing nonhomogeneity parameter β in coating increases the temperature distribution on the barrier. Also, the effect of the thickness of coating can be seen obviously on the same figure.

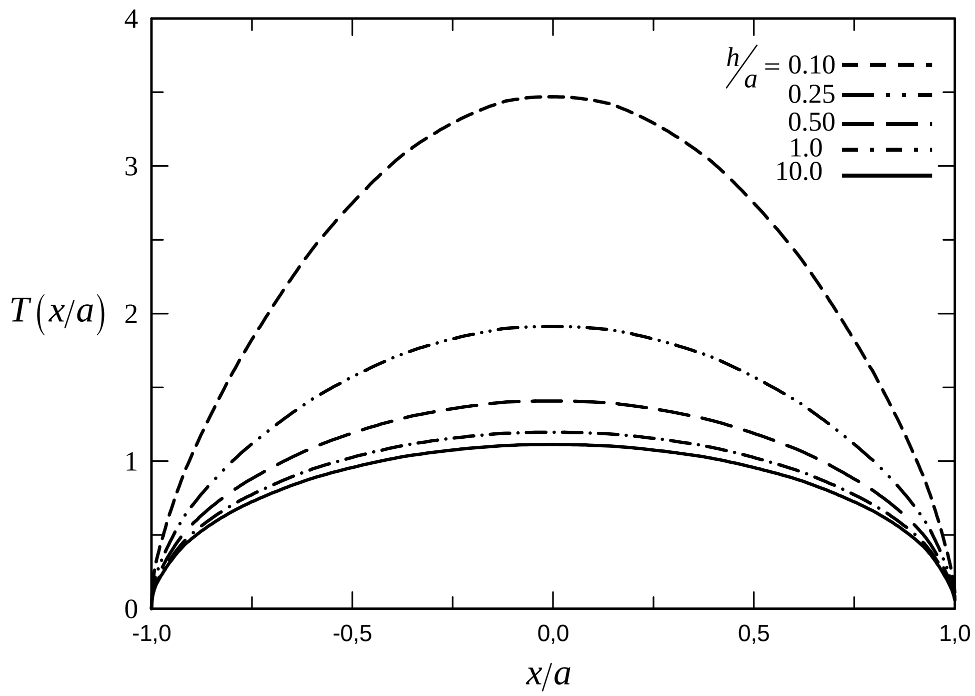


Figure 5.6: Temperature distribution on the barrier for various thicknesses of coating as nonhomogeneity parameter $\beta = -0.5$.

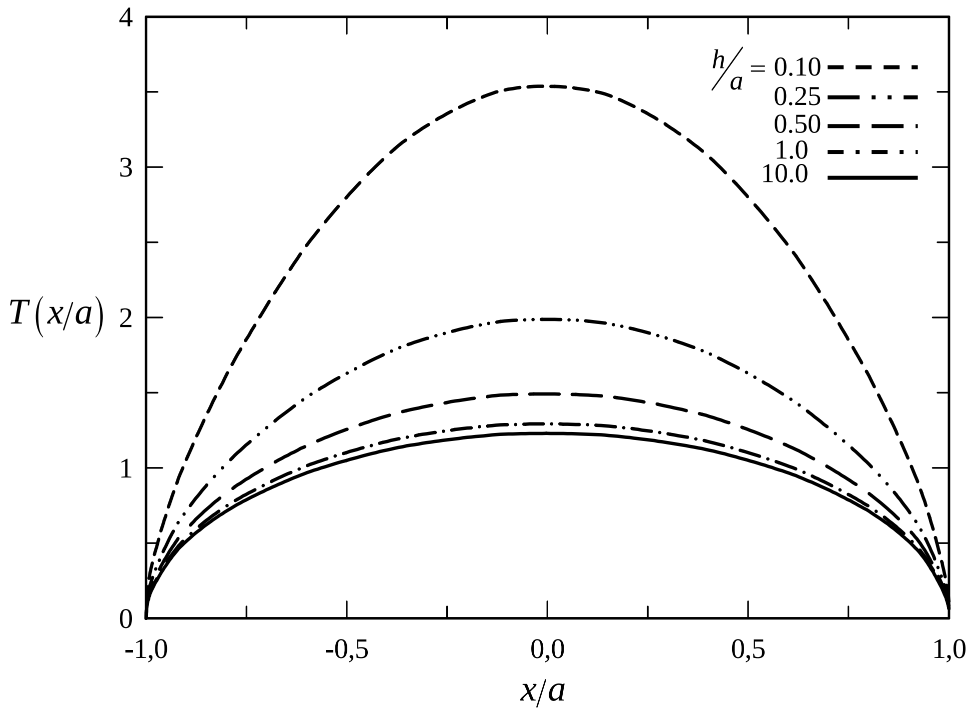


Figure 5.7: Temperature distribution on the barrier for various thicknesses of coating as nonhomogeneity parameter $\beta = -1.0$.

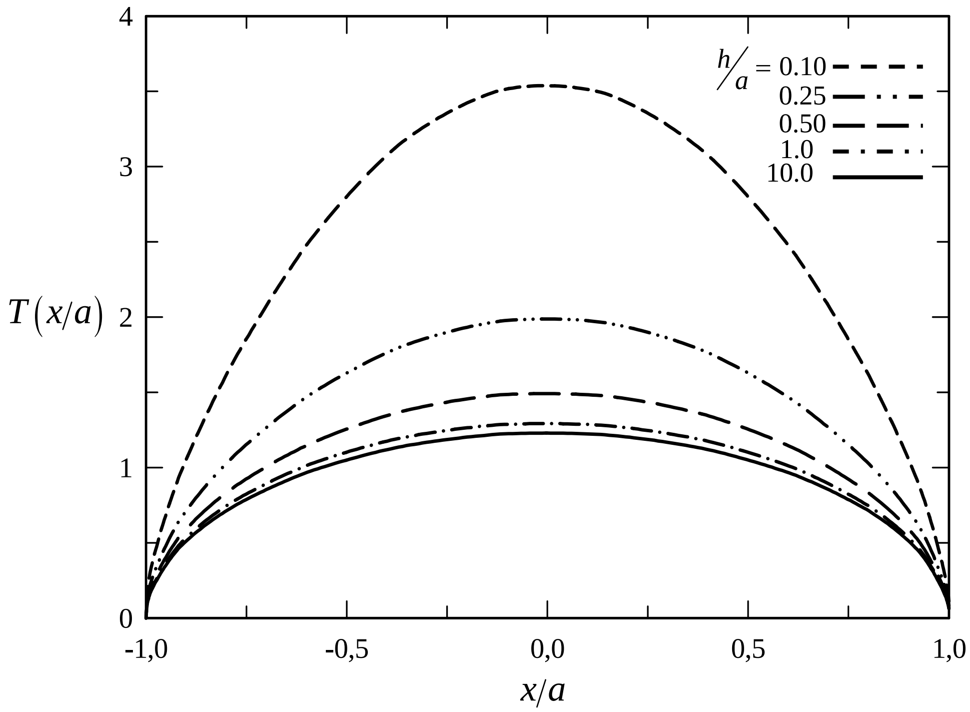


Figure 5.8: Temperature distribution on the barrier for various thicknesses of coating as nonhomogeneity parameter $\beta = -2.0$.

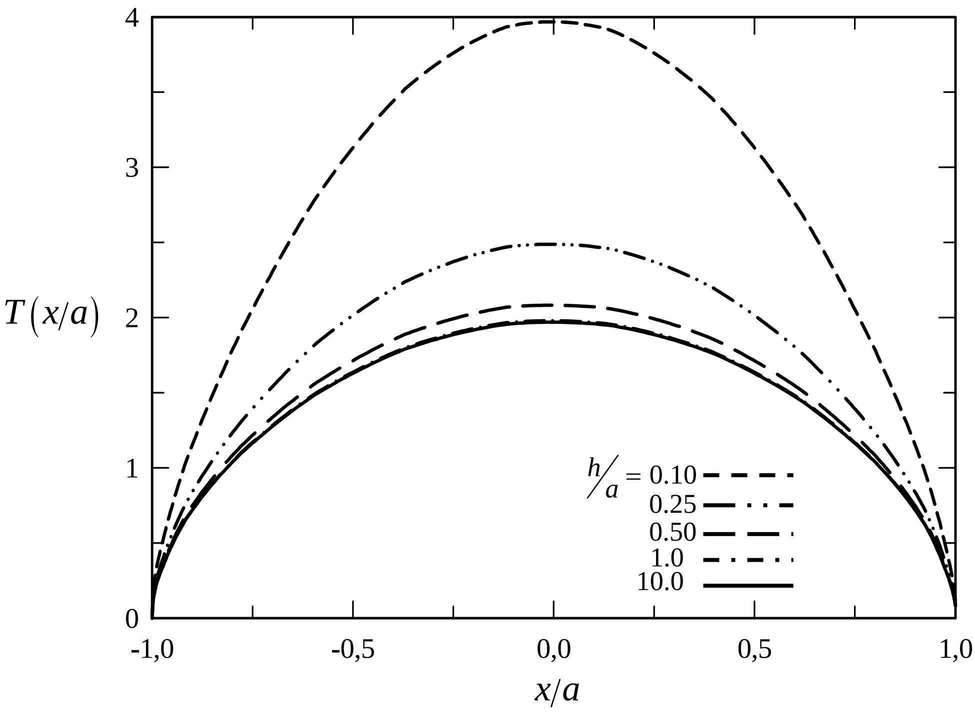


Figure 5.9: Temperature distribution on the barrier for various thicknesses of coating as nonhomogeneity parameter $\beta = -4.0$.

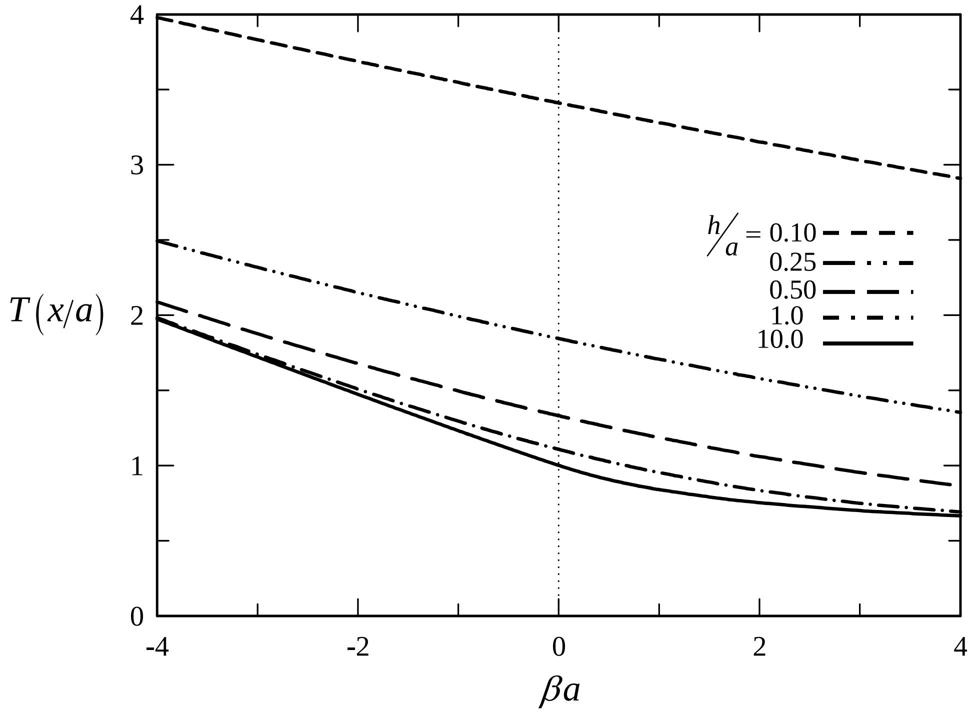


Figure 5.10: Temperature distribution on the barrier versus nonhomogeneity parameter β for various thicknesses of coating.

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APPENDIX A

CHEBYSHEV POLYNOMIAL OF THE FIRST KIND

$$\mathrm{T}_n(x) = \cos\left(n\cos^{-1}x\right) = x^n - \binom{n}{2}x^{n-2}\left(1-x^2\right) + \binom{n}{4}x^{n-4}\left(1-x^2\right)^2 - \ldots$$

SPECIAL CHEBYSHEV POLYNOMIALS OF THE FIRTS KIND

$$\mathrm{T}_0(x) = 1,$$
$$\mathrm{T}_1(x) = x,$$
$$\mathrm{T}_2(x) = 2x^2 - 1,$$
$$\mathrm{T}_3(x) = 4x^3 - 3x.$$

SPECIAL VALUES

$$\mathrm{T}_n(-x) = (-1)^n\,\mathrm{T}_n(x),$$
$$\mathrm{T}_n(1) = 1,$$
$$\mathrm{T}_n(-1) = (-1)^n,$$
$$\mathrm{T}_{2n}(0) = (-1)^n,$$
$$\mathrm{T}_{2n+1}(0) = 0.$$

ORTHOGONALITY

$$\int_{-1}^{1}\frac{\mathrm{T}_m(x)\,\mathrm{T}_n(x)}{\sqrt{1-x^2}}\,dx = 0, \qquad m \neq n,$$
$$\int_{-1}^{1}\frac{\left\{\mathrm{T}_n(x)\right\}^2}{\sqrt{1-x^2}}\,dx = \begin{cases}\pi & if \quad n = 0\\ \dfrac{\pi}{2} & if \quad n = 1, 2, \ldots\end{cases}$$

CHEBYSHEV POLYNOMIALS OF THE SECOND KIND

$$\mathrm{U}_n(x) = \frac{\sin\left\{(n+1)\cos^{-1}x\right\}}{\sin\left(\cos^{-1}x\right)} = \binom{n+1}{1}x^n - \binom{n+1}{3}x^{n-2}\left(1-x^2\right) + \binom{n+1}{5}x^{n-4}\left(1-x^2\right)^2 - \ldots$$

SPECIAL CHEBYSHEV POLYNOMIALS OF THE SECOND KIND

$\mathrm{U}_0(x) = 1,$ $\quad$ $\mathrm{U}_2(x) = 4x^2 - 1,$

$\mathrm{U}_1(x) = 2x,$ $\quad$ $\mathrm{U}_3(x) = 8x^3 - 4x.$

SPECIAL VALUES

$\mathrm{U}_n(-x) = (-1)^n \mathrm{U}_n(x),$ $\quad$ $\mathrm{U}_n(-1) = (-1)^n (n+1),$

$\mathrm{U}_{2n+1}(0) = 0,$

$\mathrm{U}_n(1) = n+1,$ $\quad$ $\mathrm{U}_{2n}(0) = (-1)^n .$

ORTHOGONALITY

$$\int_{-1}^{1} \sqrt{1-x^2}\, \mathrm{U}_m(x)\, \mathrm{U}_n dx = 0, \qquad m \neq n,$$

$$\int_{-1}^{1} \sqrt{1-x^2} \left\{ \mathrm{U}_n(x) \right\}^2 dx = \frac{\pi}{2}.$$

RELATIONS BETWEEN $\mathrm{T}_n(x)$ AND $\mathrm{U}_n(x)$

$$\mathrm{U}_n(x) = \frac{1}{\pi} \int_{-1}^{1} \frac{\mathrm{T}_{n+1}(v)\, dv}{(v-x)\sqrt{1-v^2}} .$$