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Abstract

We study the scaling of bounds on heat transport in Rayleigh-Bénard convection of a layer of fluid between two infinite horizontal plates under various thermal boundary conditions. First we demonstrate how to establish an upper bound on the heat transport, measured by the Nusselt number $Nu$, as a function of the Rayleigh number $Ra$, using the Doering-Constantin approach of background profiles. Then we numerically compute the bounds using optimal piecewise linear background profiles. For each boundary condition we find that the $Nu$ is bounded above by a constant $C$ times the square root of $Ra$. In the fixed temperature case, we get $C = 0.045$; in the fixed flux case, we get $C = 0.078$; while for general thermal boundary conditions, we find numerically that the prefactor $C$ is similar to that in the fixed flux case, and depends, at best, weakly on the Biot number.
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Dedication

To my parents and Liyang.
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Chapter 1

Introduction

The motion of an enclosed fluid heated from below and cooled from above has been studied for a long time. Usually, a heated blob is less dense and experiences an upward buoyancy force; a cooler blob will tend to fall downward. At the lower heating rates, there is no motion due to the fluid's viscosity, which is a frictional force tending to resist fluid flow. When the heating is strong enough, the buoyancy force will overwhelm the fluid's viscosity, and the fluid begins to move. This resulting motion is referred to as 'convection'. We concentrate on Rayleigh-Bénard convection of flow between infinite horizontal parallel plates.

A quantity of fundamental interest in Rayleigh-Bénard convection is the Nusselt number $Nu$, which measures the total heat transport through the layer. The strength of the heating is usually given by the Rayleigh number $Ra$, a measure of the nondimensional temperature difference between the plates. A major goal of both theory and experiment is to establish the relation between $Nu$ and $Ra$. In high Rayleigh number flows, this relation is expected to take the scaling form $Nu \sim Ra^p$. Due to the complexity of the governing equations, it has not been possible to find the exact $Nu - Ra$ relation. However, many methods, both experimental and analytical ones, have been derived to obtain an upper bound of this relation.

In 1963, Howard made the first mathematical formulation of variational approach in the heat transport problem, without including incompressibility. A modification of Howard's variational problem including the incompressibility constraint was further developed by Busse in 1969. In 1992, a new method called the 'background method' was introduced by Doering and Constantin. This method, using an idea of Hopf (1941),
decomposes the velocity field into a 'background' component carrying the boundary conditions, and a 'fluctuation' component. They first used this method to derive an upper bound of the energy dissipation in plane Couette flows [4]. Their treatment of the convection problem was first published in 1996 [5], and has been improved and generalized in various papers since then.

The optimal upper bound for the Doering-Constantin method is difficult to obtain both analytically and numerically. There has been considerable effort at developing different ways to estimate or numerically compute the optimal upper bound using some appropriate set of test profiles. In 2002, Jesse Otero [9] applied this method and numerically computed the optimal piecewise linear solution to various different flows - Shear Flow, Porous Medium convection [10], Infinite Prandtl Number convection, etc. In this thesis, we adapt his method to the Rayleigh-Bénard convection problem, with the aim of obtaining a numerical estimate of the bound for large $Ra$. Unfortunately, direct calculation using Otero's method breaks down for large $Ra$ ($Ra > 10^5$). In 2004, Stephen C. Plasting [12] used the Doering-Constantin approach and Otero's method to study infinite Prandtl Number convection, but he first pushed the calculation up to $Ra = 10^{35}$ using multiple-precision arithmetic.

In this thesis, we first study how to use the Doering-Constantin method to formulate an upper bound of Rayleigh-Bénard convection for fixed temperature BCs [5], fixed flux BCs [11], as well as for general thermal BCs as recently derived by Ralf Wittenberg [13]. Then we numerically compute the upper bound under the piecewise linear profiles. By carefully rescaling the coefficient matrix, we can push the calculation up to about $Ra = 10^{35}$. It turns out that the exponents in the bound are always $\frac{1}{2}$ for all three boundary conditions.
Chapter 2

Equations and Boundary Conditions

A fluid heated from below will result in a tendency for the fluid to move as a result of the thermal expansion of the lower layers. When the heating is strong enough, this tendency will overwhelm the fluid’s viscosity, which tends to keep the fluid from flowing, and the fluid begins to move. The resulting motion is referred to as convection.

The models of Rayleigh-Bénard convection we will study here are based on the Boussinesq approximation, which presumes that the variations in density have appreciable effects only in the buoyancy forcing. The equations of motion are

\[
\frac{\partial \mathbf{u}^*}{\partial t^*} + \mathbf{u}^* \cdot \nabla \mathbf{u}^* + \frac{1}{\rho} \nabla P^* = \nu \nabla^2 \mathbf{u}^* + \alpha g (T^* - T_0) \hat{k},
\]

where \( \nu \) and \( \kappa \) are the diffusivity constants for momentum and temperature, \( \alpha \) is the thermal expansion coefficient, \( g \) is the acceleration due to gravity, \( \rho \) is the density at temperature \( T_0 \), and \( h \) is the height of the fluid layer. Variables with an asterisk are dimensional, and we take periodic boundary conditions in the horizontal directions. In the vertical direction \( \hat{k} \), we apply no-slip boundary condition for the velocity at \( z^* = 0, h \).

For the temperature, we consider fixed temperature, fixed flux or general thermal BCs
in this thesis:

fixed temperature BCs: $T^*|_{z^*=0} = T_{bot}$, $T^*|_{z^*=h} = T_{top}$,

fixed flux BCs: $\frac{\partial T^*}{\partial z^*}|_{z^*=0,h} = -\beta$,

general thermal BCs: $T^* - \eta^* \frac{\partial T^*}{\partial z^*}|_{z^*=0} = A_t$, $T^* + \eta^* \frac{\partial T^*}{\partial z^*}|_{z^*=h} = A_u$,

where $\beta$ is the heat flux at the boundaries and the general thermal boundary conditions are based on the Newton's Law of Cooling. Here we assume both top and bottom plates have the same Biot number.

The picture of this setup is shown in Figure 2.1.

![Figure 2.1: Rayleigh-Bénard convection. Periodic boundary conditions are imposed on the sidewalls. The boundary conditions for $u^*$ are $u^*|_{z^*=0,h} = 0$.](image)

Firstly, we want to non-dimensionalize the equations and boundary conditions. We take $h$ and $\frac{h^2}{\kappa}$ as the relevant space and time scales. The temperature scale $\Theta$ depends on different boundary conditions. For the fixed temperature case, we use $\Theta = T_{bot} - T_{top}$; for the fixed flux case, we use $\Theta = h\beta$; for the general thermal boundary conditions, we
use $\Theta = \frac{A_h - A_w}{1 + f \Delta T}$. (See [13] for details.) The equations in the non-dimensional velocity $u = (u, v, w)$ and temperature $T$ are

$$u_t + u \cdot \nabla u + \nabla P = \sigma \nabla^2 u + \sigma R T \kappa, \quad \nabla \cdot u = 0,$$

$$T_t + u \cdot \nabla T = \nabla^2 T,$$

where $R = \frac{\rho g h^3 \Theta}{\nu \kappa}$, and $\sigma = \frac{\nu}{\kappa}$ is the Prandtl number. The control parameter $R$ is not necessarily the same as the Rayleigh number $Ra = \frac{ag \Delta T^* h^3}{\gamma \kappa}$ (except in the fixed temperature case), but is related to it by

$$Ra = R \Delta T,$$

because of $\Delta T^* = \Theta \Delta T$. Note that $\Delta T^*$ is the dimensional averaged temperature difference between the two plates obtained by horizontal and time averaging,

$$\Delta T^* = \langle \overline{T}^* \rangle_{\Delta x = 0} - \langle \overline{T}^* \rangle_{\Delta x = h},$$

and $\Delta T$ is the corresponding nondimensional averaged temperature difference

$$\Delta T = \langle T \rangle_{z = 0} - \langle T \rangle_{z = 1}.$$

Note that for the conduction solution $T = 1 - z$, we have $\Delta T = 1$ and $Ra = R$.

The no-slip boundary condition for velocity is

$$u_{z = 0, 1} = 0.$$

The dimensionless boundary conditions for temperature will be one of the following

fixed temperature BCs: $T|_{z = 0} = 1, \quad T|_{z = 1} = 0,$

fixed flux BCs: $T_z|_{z = 0, 1} = -1,$

general thermal BCs: $\langle T - \eta T_z \rangle|_{z = 0} = 1 + \eta, \quad (T + \eta T_z)|_{z = 1} = -\eta,$

where $\eta$ is the Biot number. The Biot number is a dimensionless number used in unsteady-state heat transfer calculations. It relates the heat transfer resistance inside and at the surface of a body, and is named after the French physicist Jean-Baptiste Biot (1774-1862).
We can see that when $\eta = 0$, the general thermal BCs reduce to the fixed temperature case; when $\eta = \infty$, the general thermal BCs reduce to the fixed flux case.

While the fixed temperature [5] and fixed flux [11] formulations were originally derived quite differently, it turns out [13] that it is possible to set up the upper bound problem in a way that leads to a unified formulation and very similar numerical calculations for all the thermal boundary conditions.
Chapter 3

Statement of the Problem

Due to the similarities of the formulation for different BCs, we will establish and numerically compute the bounds for all BCs concurrently for comparison.

3.1 Notation and Definitions

We first introduce some notation: for functions \( f(x, y, z) \) and \( g(t) \), we define the horizontal and time averages by

\[
\bar{f}(z) = \frac{1}{A} \int f(x, y, z) dx dy, \quad (3.1)
\]

and

\[
\langle g \rangle = \lim_{t \to \infty} \sup_{t} \frac{1}{t} \int_{0}^{t} g(t') dt', \quad (3.2)
\]

where \( A \) is the non-dimensional area of the plates. In addition, \( \int f \) denotes a volume integral over the entire fluid layer. The \( L^{2} \) norms are defined by

\[
||u||^{2} = \int |u|^{2} = \int \sum_{i=1}^{3} u_{i}^{2},
\]

and we also have

\[
||\nabla u||^{2} = \int \sum_{i,j=1}^{3} \left( \frac{\partial u_{i}}{\partial x_{j}} \right)^{2} = \int \nabla u^{2},
\]

where \( u = (u, v, w) = (u_{1}, u_{2}, u_{3}) \) and \( x = (x, y, z) = (x_{1}, x_{2}, x_{3}) \).

In taking time averages, we frequently use the result that temperature \( T \) and the \( L^{2} \) norm \( ||T||, ||u|| \) are bounded (see [5]), so that the time averages of time derivatives of
those quantities vanish; for example, if $|T| \leq K$, then
\[ |\langle T_i \rangle| = \limsup_{t \to \infty} \frac{1}{t} \int_0^t \frac{dT}{dt} \, dt \]
\[ = \limsup_{t \to \infty} \frac{T(t) - T(0)}{t} \]
\[ \leq \limsup_{t \to \infty} \frac{2K}{t} = 0. \]

To define the Nusselt number $Nu$, we first write the heat equation (2.6) as
\[ T_t + \nabla \cdot J = 0, \]
where $J = uT + J_c$ is the heat current, and $J_c = -\nabla T$ is the conductive part of $J$. The Nusselt number is defined to be the ratio of the average total convective and conductive heat transport in the vertical direction to the purely conductive heat transport:
\[
Nu = \frac{\frac{1}{A} \langle \int J \cdot \hat{k} \rangle}{\frac{1}{A} \langle \int J_c \cdot \hat{k} \rangle} = \frac{\frac{1}{A} \langle \int wT \rangle + \frac{1}{A} \langle \int J_c \cdot \hat{k} \rangle}{\frac{1}{A} \langle \int J_c \cdot \hat{k} \rangle}. \tag{3.3}
\]
Since
\[
\frac{1}{A} \langle \int J_c \cdot \hat{k} \rangle = \frac{1}{A} \langle \int -T \rangle \]
\[ = \frac{1}{A} \left\langle \int \left( \int_0^1 -T_c \, dz \right) \, dx \, dy \right\rangle \]
\[ = \Delta T, \tag{3.4}
\]
we have
\[
Nu = 1 + \frac{\frac{1}{A} \langle \int wT \rangle}{\Delta T}. \tag{3.5}
\]
This expression may be further simplified by relating the quantities $\Delta T$ and $\langle \int wT \rangle$. We take the volume average of the heat equation (2.6) and then take the time average to get
\[
\frac{1}{A} \langle \int wT \rangle + \Delta T = \beta. \tag{3.6}
\]
Thus, we can get
\[
Nu = \frac{\beta}{\Delta T}. \tag{3.7}
\]
The above result is true for general thermal BCs. In the fixed temperature and fixed flux cases, this result may be simplified as
\[
\begin{align*}
\text{fixed temperature:} & \quad Nu = \beta \quad (\Delta T = 1), \\
\text{fixed flux:} & \quad Nu = \frac{1}{\Delta T} \quad (\beta = 1). \tag{3.8}
\end{align*}
\]
To obtain the next fundamental relation, we multiply the heat equation (2.6) by $T$ and take the volume and time average to find

$$\langle \| \nabla T \|^2 \rangle = A \langle T T_s \rangle_0. \quad (3.9)$$

Similarly, for the fixed temperature and fixed flux boundary conditions, we can rewrite the above general result as

$$\begin{cases} 
\text{fixed temperature:} & \langle \| \nabla T \|^2 \rangle = -A \langle T_s(0) \rangle = A \beta = A N u, \\
\text{fixed flux:} & \langle \| \nabla T \|^2 \rangle = A \Delta T = A N u^{-1}.
\end{cases} \quad (3.10)$$

Finally, we obtain the third basic equation by multiplying the momentum equation (2.5) by $u$ and taking the volume and time average to find

$$\frac{1}{R} \langle \| \nabla u \|^2 \rangle = \left\langle \int \frac{u}{T} \right\rangle = A \Delta T (N u - 1) = A (\beta - \Delta T). \quad (3.11)$$

For the fixed temperature and fixed flux boundary conditions, the above general result becomes

$$\begin{cases} 
\text{fixed temperature:} & \frac{1}{R} \langle \| \nabla u \|^2 \rangle = A (\beta - 1) = A (N u - 1), \\
\text{fixed flux:} & \frac{1}{R} \langle \| \nabla u \|^2 \rangle = A (1 - \Delta T) = A (1 - N u^{-1}).
\end{cases} \quad (3.12)$$

### 3.2 Doering-Constantin Background Method and Energy Identities

Using the idea of the Doering-Constantin method, we now decompose the temperature field into a background $\tau(z)$, which carries the thermal boundary conditions of the flow, and a disturbance $\theta(x, y, z, t)$:

$$T = \tau(z) + \theta(x, y, z, t). \quad (3.13)$$

We also decompose the velocity field into a zero background flow $U = 0$ and a disturbance $v(x, y, z, t)$:

$$u = U + v(x, y, z, t) = v(x, y, z, t). \quad (3.14)$$

Substituting (3.13) and (3.14) into the momentum equation (2.5) and heat equation (2.6), we get

$$v_t + v \cdot \nabla v = -\nabla P + \sigma \nabla^2 v + \sigma R T \dot{k}, \quad (3.15)$$
\[
\theta_t + \mathbf{v} \cdot \nabla \theta = \nabla^2 \theta + \tau'' - w\tau'.
\]

(3.16)

Using these two decompositions, we can also get

\[
\frac{1}{R} ||\nabla \mathbf{u}||^2 = \frac{1}{R} ||\nabla \mathbf{v}||^2,
\]

(3.17)

\[
||\nabla T||^2 = ||\nabla \theta + \tau' \mathbf{k}||^2 = ||\nabla \theta||^2 + \int \tau'^2 + 2 \int \theta \tau'.
\]

(3.18)

We multiply (3.15) by \(v\), integrate over the fluid, and integrate by parts (using incompressibility) to get:

\[
\frac{1}{2} \frac{1}{\sigma R} \frac{d}{dt} ||v||^2 = -\frac{1}{R} ||\nabla \mathbf{v}||^2 + \int \omega \tau
\]

\[
= -\frac{1}{R} ||\nabla \mathbf{v}||^2 + \int \omega \theta,
\]

(3.19)

where we used \(\int \omega \tau = 0\), because using incompressibility and horizontally periodic boundary conditions

\[
\partial_z \bar{w} = \frac{1}{A} \int w_z dxdy = \frac{1}{A} \int -(u_x + v_y)dxdy = 0
\]

\[
\Rightarrow \bar{w} = \bar{w}|_{z=0} = 0
\]

\[
\Rightarrow \int \omega \tau(z) = \int \tau(z) \left( \int w dxdy \right) dz = A \int \tau(z) \bar{w} dz = 0.
\]

Then, we multiply (3.16) by \(\theta\) and integrate by parts to get:

\[
\frac{1}{2} \frac{d}{dt} ||\theta||^2 = -||\nabla \theta||^2 - \int \theta \omega \tau' + A \theta T_z \bar{z}_{10} + \int \theta \tau''
\]

\[
= -||\nabla \theta||^2 - \int \theta \omega \tau' - \int \theta \tau' - A \theta T_z \bar{z}_{10},
\]

(3.20)

where the boundary term comes from the integration by parts on \(\int \theta \nabla^2 \theta\) and \(\int \theta \tau''\). For different boundary conditions, we can rewrite the above as

fixed temperature: \[
\frac{1}{2} \frac{d}{dt} ||\theta||^2 = -||\nabla \theta||^2 - \int \theta \omega \tau' - \int \theta \tau',
\]

(3.21)

fixed flux: \[
\frac{1}{2} \frac{d}{dt} ||\theta||^2 = -||\nabla \theta||^2 - \int \theta \omega \tau' - \int \theta \tau' + A \Delta \theta.
\]

(3.22)

However, later in the nonlinear stability analysis, we can see that, if we choose the background to be purely conduction solution \(\tau(z) = 1 - z\) (so \(\tau'' = 0\)), there is no
difference in the fixed temperature and fixed flux cases. Both boundary conditions give the following result for $\tau = 1 - z$:

$$\frac{1}{2} \frac{d}{dt} ||\theta||^2 = -||\nabla \theta||^2 + \int \theta_w. \quad (3.23)$$

We are now ready to do the stability analysis and discuss how we can establish an upper bound for the heat transport $Nu$ in terms of $Ra$. 
Chapter 4

Stability Analysis

In this chapter, we will do both linear and nonlinear stability analyses of the Rayleigh-Bénard convection flow. Firstly, we show that both lead to the same eigenvalue problem. Then we numerically compute the critical Rayleigh number $Ra_c$ for different boundary conditions.

4.1 Linear Stability Analysis

For the linear stability of the conduction solution $u_c = 0$, $\tau_c(z) = 1 - z$ and $P_c = P_0 - \frac{1}{2} \sigma R(1 - z)^2$, we consider a perturbation of the conduction solution

$$u = u_c + v = v,$$  

$$T = \tau_c(z) + \theta = 1 - z + \theta,$$  

$$P = P_c + q.$$  

Substituting these equations into (2.5), (2.6) and (2.7) gives evolution equations for the perturbation:

$$\nabla v + v \cdot \nabla v = -\nabla q + \sigma \nabla^2 v + \sigma R \theta \mathbf{k},$$

$$\nabla \cdot v = 0,$$

$$\theta + v \cdot \nabla \theta = \nabla^2 \theta + \omega,$$
where $v = (u, v, w)^T$. Linearize by dropping all the quadratic terms in the perturbations and assume an exponential time dependence $e^{-\lambda t}$ to get

\[
\nabla q - \sigma \nabla^2 v - \sigma R \theta \dot{k} = \lambda v, \\
\nabla \cdot v = 0, \\
-\nabla^2 \theta - w = \lambda \theta.
\]

Before looking into the solution of this problem, we will show that the nonlinear stability analysis leads to precisely the 'same' eigenvalue problem given in linear stability analysis.

### 4.2 Nonlinear Stability Analysis

For the nonlinear stability of the conduction solution $u = \bar{u}$ and $\tau(z) = 1 - z$, there is a detailed description in Chandrasekhar's book [3], but we put it here for completeness.

#### 4.2.1 Fixed Temperature and Fixed Flux BCs

We add (3.19) and (3.23) to get

\[
\frac{1}{2} \frac{d}{dt} (||\theta||^2 + \frac{1}{\sigma R} ||v||^2) = -\int \left( \frac{1}{R} |\nabla v|^2 - 2w\theta + |\nabla \theta|^2 \right).
\]

Let

\[
E(t) = ||\theta||^2 + \frac{1}{\sigma R} ||v||^2,
\]

and

\[
Q[v, \theta] = \int \left( \frac{1}{R} |\nabla v|^2 - 2w\theta + |\nabla \theta|^2 \right).
\]

If $Q[v, \theta] \geq cE(t)$ for some $c > 0$, then we have $\frac{1}{2} \frac{dE}{dt} \leq -cE$, so $E(t)$ must decay exponentially in time. The optimal value of $c$ may be found by finding the minimum of $Q$ over all divergence-free vector fields $v$ and scalar fields $\theta$ satisfying the appropriate boundary conditions and a normalization condition (in this case, $||\theta||^2 + \frac{1}{\sigma R} ||v||^2 = 1$).

Thus, we introduce the quadratic form $L(\theta, v)$, incorporating the Lagrange multipliers $\lambda$ enforcing the normalization condition and $P(\alpha)$ enforcing incompressibility:

\[
L(\theta, v) = \int \frac{1}{R} |\nabla v|^2 + 2w\theta' + |\nabla \theta|^2 - \lambda \left( ||\theta||^2 + \frac{1}{\sigma R} ||v||^2 \right) - P \nabla \cdot v.
\]
CHAPTER 4. STABILITY ANALYSIS

Minimizing $L(\theta, v)$, and using some integration by parts, we can see that the Euler-Lagrange equations for both the fixed temperature and fixed flux cases are

\[ \nabla \tilde{P} - \sigma \nabla^2 v - \sigma R\theta \dot{k} = \lambda v, \]
\[ \nabla \cdot v = 0, \]
\[ -\nabla^2 \theta - w = \lambda \theta, \]

(4.12) (4.13) (4.14)

where $\tilde{P} = \frac{1}{2} \sigma RP$.

Therefore, the Euler-Lagrange equations are the same as the linear stability equations for both the fixed temperature and fixed flux cases.

4.2.2 General Thermal BCs

We add (3.19) and (3.20) (with $\tau = 1 - z$) to get

\[ \frac{1}{2} \frac{d}{dt} (||\theta||^2 + \frac{1}{\sigma R} ||v||^2) = - \int (\frac{1}{R} |\nabla v|^2 - 2w\theta + |\nabla \theta|^2) + A\bar{\theta}_z|_0^1. \]

As before, let

\[ E(t) = ||\theta||^2 + \frac{1}{\sigma R} ||v||^2, \]

and

\[ Q[v, \theta] = \int (\frac{1}{R} |\nabla v|^2 - 2w\theta + |\nabla \theta|^2) + A\bar{\theta}_z|_0^1. \]

Note that there is an extra boundary term compared to the fixed temperature and fixed flux cases. However, proceeding as before, it turns out that when we derive the Euler-Lagrange equations, the boundary term $A\bar{\theta}_z|_0^1$ disappears. The same thing happens for the upper bound formulation in the later chapter. We will give a detailed derivation of how that boundary term disappears in Chapter 7. Therefore, we get the same Euler-Lagrange equations as in the fixed temperature and fixed flux cases:

\[ \nabla \tilde{P} - \sigma \nabla^2 v - \sigma R\theta \dot{k} = \lambda v, \]
\[ \nabla \cdot v = 0, \]
\[ -\nabla^2 \theta - w = \lambda \theta, \]

(4.16) (4.17) (4.18)

where $\tilde{P} = \frac{1}{2} \sigma RP$.

We shall see in Chapter 7 that these Euler-Lagrange equations are the same as those which appear in our numerical upper bound calculation, except that there we will use an effective Rayleigh number $R_{\text{eff}}$ instead of $R$. This explains why all the figures of the numerical bounds calculation bifurcate at the (linear and nonlinear) stability boundary.
4.3 Solution to the Euler-Lagrange equations

From the previous two sections, we can see that both linear and nonlinear stability analyses lead to the same eigenvalue problem. It turns out that this is because one can rewrite the operator here to make it self-adjoint. Thus, the critical Rayleigh numbers for linear and nonlinear stability analyses are the same. This is not true, for instance, for the Shear Flow problem, because in that case one cannot make the operator self-adjoint (see [6] for details).

Therefore, there must exist a critical Rayleigh number $Ra_c (= R_c)$ for instability for the different thermal boundary conditions. If $Ra < Ra_c$, the conduction solution is energy stable; if $Ra > Ra_c$, the conduction solution is linearly unstable and any perturbation will grow exponentially in time. One can refer to [3] for details, but we summarize the derivation here for completeness.

The critical value of $R$ occurs when $\lambda = 0$. Setting $\lambda = 0$ and eliminating pressure, $u$ and $v$ give

$$
\nabla^4 w + R\nabla^2_H \theta = 0,
$$
$$
\nabla^2 \theta + w = 0,
$$

(4.19) \hspace{1cm} (4.20)

where $\nabla^2_H$ denotes the horizontal Laplacian $\partial_x^2 + \partial_y^2$. Using the periodicity of $w$ and $\theta$ we may decompose them as

$$
w(x, y, z) = \sum_k w_k(z)e^{i(k_1 x + k_2 y)},
$$
$$
\theta(x, y, z) = \sum_k \theta_k(z)e^{i(k_1 x + k_2 y)},
$$

(4.21) \hspace{1cm} (4.22)

where $k^2 = k_1^2 + k_2^2$, and we write $w_k$ for $w_{k_1, k_2}$ for convenience. Then the Euler-Lagrange equations become

$$
(D^2 - k^2)^2 w - k^2 R\theta = 0,
$$
$$
(D^2 - k^2)\theta + w = 0,
$$

(4.23) \hspace{1cm} (4.24)

where we drop the subscript $k$ for convenience, and define $D = d/dz$. We can also eliminate $\theta$ to get

$$
(D^2 - k^2)^3 w + k^2 Rw = 0.
$$
This is a $6^{th}$-order linear constant coefficient ODE, with characteristic equation

$$(p^2 - k^2)^3 + k^2 R = 0,$$

and the solutions to the characteristic equation are

$$p_{1,2} = \pm \sqrt{k^2 - (k^2 R)^{\frac{1}{3}}},$$

$$p_{3,4} = \pm \sqrt{k^2 + \frac{1}{2}(1 + i\sqrt{3})(k^2 R)^{\frac{1}{3}}},$$

$$p_{5,6} = \pm \sqrt{k^2 + \frac{1}{2}(1 - i\sqrt{3})(k^2 R)^{\frac{1}{3}}}.$$  

The solution of the Euler-Lagrange equations is then

$$w(z) = \sum_{i=1}^{6} A_i e^{p_i z},$$

$$\theta(z) = \frac{1}{k^2 R} \sum_{i=1}^{6} q_i A_i e^{p_i z},$$

where $q_i = (p_i^2 - k^2)^2$, and the $A_i$s are unknown constants.

Note that the value of $Ra_c$ does not depend on the Prandtl number $\sigma$ and is the same in 2D and 3D.

### 4.3.1 Numerical Results - Fixed Temperature BCs

For the fixed temperature BCs, imposing the six boundary conditions $w, Dw, \theta|_{z=0,1} = 0$ on (4.28) and (4.29) leads to the following system of equations

$$
\begin{pmatrix}
1 & 1 & 1 & 1 & 1 & 1 \\
p_1 & p_2 & p_3 & p_4 & p_5 & p_6 \\
q_1 & q_2 & q_3 & q_4 & q_5 & q_6 \\
e^{p_1} & e^{p_2} & e^{p_3} & e^{p_4} & e^{p_5} & e^{p_6} \\
p_1 e^{p_1} & p_2 e^{p_2} & p_3 e^{p_3} & p_4 e^{p_4} & p_5 e^{p_5} & p_6 e^{p_6} \\
q_1 e^{p_1} & q_2 e^{p_2} & q_3 e^{p_3} & q_4 e^{p_4} & q_5 e^{p_5} & q_6 e^{p_6}
\end{pmatrix}
\begin{pmatrix}
A_1 \\
A_2 \\
A_3 \\
A_4 \\
A_5 \\
A_6
\end{pmatrix} = \begin{pmatrix}
0 \\
0 \\
0 \\
0 \\
0 \\
0
\end{pmatrix}.
$$

In order to obtain non-trivial solutions, we require the coefficient matrix to have vanishing determinant. This gives $Ra$ implicitly as a function of $k$; a graph of this relation is shown below in Figure 4.1. For a given value of $k$ the corresponding value of $Ra$ is...
the critical Rayleigh number for that Fourier mode. In order to ensure that all modes are stable, we choose the minimum value of $Ra$ over all $k$. This minimum value is the critical Rayleigh number $Ra_c$. The result is:

$$Ra_c = 1707.76 \text{ for } k = 3.116.$$  

This result tells us the wave number $k_c = 3.116$ is the ‘most unstable’ mode. For $Ra < Ra_c$, the system is in the pure conductive state $u = 0$ and $T = 1 - z$, in which case the long time averaged heat transport is conductive ($Nu = 1$).
4.3.2 Numerical Results - Fixed Flux BCs

For the fixed flux BCs, imposing the six boundary conditions \( w, Dw, D\theta|_{z=0,1} = 0 \) on (4.28) and (4.29) leads to the following system of equations

\[
\begin{pmatrix}
1 & 1 & 1 & 1 & 1 & 1 \\
p_1 & p_2 & p_3 & p_4 & p_5 & p_6 \\
q_1p_1 & q_2p_2 & q_3p_3 & q_4p_4 & q_5p_5 & q_6p_6 \\
e^{p_1} & e^{p_2} & e^{p_3} & e^{p_4} & e^{p_5} & e^{p_6} \\
p_1e^{p_1} & p_2e^{p_2} & p_3e^{p_3} & p_4e^{p_4} & p_5e^{p_5} & p_6e^{p_6} \\
q_1p_1e^{p_1} & q_2p_2e^{p_2} & q_3p_3e^{p_3} & q_4p_4e^{p_4} & q_5p_5e^{p_5} & q_6p_6e^{p_6}
\end{pmatrix}
\begin{pmatrix}
A_1 \\
A_2 \\
A_3 \\
A_4 \\
A_5 \\
A_6
\end{pmatrix}
= \begin{pmatrix}
0 \\
0 \\
0 \\
0 \\
0 \\
0
\end{pmatrix}.
\]

Just as in the fixed temperature case, in order to obtain non-trivial solutions, we require the coefficient matrix to have vanishing determinant. This gives \( R \) implicitly as a function of \( k \); a graph of this relation is shown below in Figure 4.2. For a given value of \( k \) the corresponding value of \( R \) is the critical Rayleigh number for that Fourier mode.

In order to ensure that all modes are stable, we choose the minimum value of \( R \) over all \( k \). This minimum value is the critical Rayleigh number \( Ra_c \). The result is:

\[ Ra_c = 720 \text{ for } k_c = 0. \]

This result tells us the wave number \( k_c = 0 \) is the 'most unstable' mode. For \( Ra < Ra_c \), the system is in the pure conductive state \( u = \bar{0} \) and \( T = 1 - z \), in which case the long time averaged heat transport is conductive (\( Nu = 1 \)).

4.3.3 Numerical Results - General Thermal BCs

For the general BCs, we still need to impose the boundary conditions \( w, Dw|_{z=0,1} = 0 \). However, we need to change the temperature boundary conditions to be

\[
\begin{align*}
\theta - \eta \theta_z &= 0 \quad \text{at } z = 0, \\
\theta + \eta \theta_z &= 0 \quad \text{at } z = 1.
\end{align*}
\]

This leads to the following system of equations

\[
\begin{pmatrix}
1 \\
p_1 \\
e^{p_1} \\
p_1e^{p_1} \\
q_1(1 + \eta p_1)e^{p_1} \\
q_2(1 + \eta p_2)e^{p_2} \\
q_3(1 + \eta p_3)e^{p_3} \\
q_4(1 + \eta p_4)e^{p_4} \\
q_5(1 + \eta p_5)e^{p_5} \\
q_6(1 + \eta p_6)e^{p_6}
\end{pmatrix}
\begin{pmatrix}
A_1 \\
A_2 \\
A_3 \\
A_4 \\
A_5 \\
A_6
\end{pmatrix}
= \begin{pmatrix}
0 \\
0 \\
0 \\
0 \\
0 \\
0
\end{pmatrix}.
\]
As before, in order to obtain non-trivial solutions, we require the coefficient matrix to have vanishing determinant. This gives $R$ implicitly as a function of $k$ and $\eta$. For a fixed Biot number $\eta$, given any value of $k$ the corresponding $R$ is the critical Rayleigh number for that mode. In order to ensure that all modes are stable, we choose the minimum value over all $k$. This minimum value is the critical Rayleigh number $Ra_c$ for that Biot number $\eta$. Also, the values of $Ra_c(\eta)$ do not depend on the Prandtl number $\sigma$ and are the same in 2D and 3D.

We can see from the Figure 4.3 that the critical Rayleigh number $Ra_c$ is a decreasing function of Biot number $\eta$. When $\eta \to 0$, $Ra_c \to 1707.76$ which is the fixed temperature case; when $\eta \to \infty$, $Ra_c \to 720$ which is the fixed flux case. We can also see from the Figure 4.4 that the critical wavelength $k_c$ is also a decreasing function of Biot number $\eta$. When $\eta \to 0$, $k_c \to 3.116$ which is the fixed temperature case; when $\eta \to \infty$, $k_c \to 0$ which is the fixed flux case. All these results agree with the definition of the general thermal BCs (2.14). Note that the transition between the fixed temperature and fixed flux limits happens largely for a range $10^{-2} \lesssim \eta \lesssim 10^2$ near $\eta = 1$.

We can also plot $k_c$ as a function of $\eta$ in a log-log plot, like Figure 4.5. We can get the asymptotic scaling $k_c = 2.7146\eta^{-0.24999}$ for large $\eta$. The $-\frac{1}{4}$ scaling agrees with a previously obtained analytical result.
Figure 4.3: General thermal boundary conditions: Stability Analysis, $Ra_c(\eta)$.

Figure 4.4: General thermal boundary conditions: Stability Analysis, $k_c(\eta)$.

Figure 4.5: General thermal boundary conditions: Stability Analysis, log-log plot of $k_c(\eta)$. We have the asymptotic scaling $k_c = 2.7146\eta^{-0.2499}$ for large $\eta$. 
Chapter 5

Formulation of a Bound

Now we are ready to establish an upper bound for different boundary conditions. This formulation, derived in a way to allow a unified description, was obtained by Ralf Wittenberg [13].

5.1 Formulation of a Bound - Fixed Temperature BCs

For the fixed temperature boundary conditions, we have $\Delta T = 1$ and $Ra = R$. We can directly find an upper bound of $\text{Nu}$ in terms of $Ra$. First, we add (3.18) and twice (3.21) to get:

$$\frac{d}{dt}||\theta||^2 + \frac{1}{R}||\nabla \theta||^2 = -||\nabla \theta||^2 + \int \tau^2 - 2 \int \theta w' .$$

(5.1)

Then, we take a weighted average of two equations, $b$ (5.1) + $(1 - b)$ (3.17), to get:

$$b \frac{d}{dt}||\theta||^2 + b||\nabla T||^2 + \frac{1 - b}{R}||\nabla u||^2 = b \int \tau^2 - \int \left( \frac{b - 1}{R} ||\nabla v||^2 + 2b \tau \theta w + b ||\nabla \theta||^2 \right).$$

(5.2)

Taking the time average of the above equation (using (3.10) and (3.12)) gives

$$bANu + (1 - b)A(Nu - 1) = b \int \tau^2 - \left< \int \left( \frac{b - 1}{R} ||\nabla v||^2 + 2b \tau \theta w + b ||\nabla \theta||^2 \right) \right> .$$

(5.3)

Hence

$$Nu = 1 - b + b \int_0^1 \tau^2 dz - \frac{b}{A} Q[\theta, v],$$

(5.4)
where

\[ Q[\theta, v] = \frac{b - 1}{b R} \int \left( |\nabla \theta|^2 + 2 \tau' \theta w + |\nabla \theta|^2 \right). \]  

(5.5)

This gives an upper bound of \( Nu \) as a function of \( Ra \). Specifically, we have

\[ Nu \leq 1 - b + b \int_0^1 \tau^2 dz, \]  

(5.6)

provided \( Q[\theta, v] \geq 0 \). So if one can find \( \tau(z) \) and \( b > 0 \) so that \( Q[\theta, v] \geq 0 \) for all \( \theta \) and divergence-free fields \( v \), then we have an upper bound for \( Nu \).

### 5.2 Formulation of a Bound - Fixed Flux BCs

For the fixed flux boundary conditions, we have \( \beta = 1 \) and \( Nu = \frac{1}{2 \Delta T} \). We need to bound the temperature difference \( \Delta T \) from below in terms of \( R \), thereby bounding \( Nu = \frac{1}{2 \Delta T} \) from above in terms of \( R \). Finally, using the relationship \( Ra = R \Delta T \), we can bound \( Nu \) in terms of the Rayleigh number \( Ra \). Reference [11] gave a detailed description, and we briefly summarize the formulation here for completeness.

Firstly, we add (3.18) and twice (3.22) to get:

\[ d\|T\|^2 + \frac{d}{dt} \|\theta\|^2 = -\|\nabla \theta\|^2 + \int \tau^2 - 2 \int \theta \omega \tau' + 2 A \Delta \theta. \]  

(5.7)

Then, we take a weighted average of two equations, \( b \) (5.7) + \( (1 - b) \) (3.17), to get:

\[ b \frac{d}{dt} \|\theta\|^2 + b \|\nabla T\|^2 + \frac{1 - b}{R} \|\nabla u\|^2 = 2b A (\Delta T - \Delta \tau) + \int \tau^2 \]

\[ - \int \left( \frac{b - 1}{R} |\nabla v|^2 + 2b \tau' \theta w + b |\nabla \theta|^2 \right). \]  

(5.8)

Taking the time average of above equation gives

\[ b A \Delta T + (1 - b) A (1 - \Delta T) = 2b A (\Delta T - \Delta \tau) + \int \tau^2 \]

\[ - \left\langle \int \left( \frac{b - 1}{R} |\nabla v|^2 + 2b \tau' \theta w + b |\nabla \theta|^2 \right) \right\rangle. \]  

(5.9)

Hence

\[ \Delta T = 1 - b + 2b \Delta \tau - b \int_0^1 \tau^2 dz + \frac{b}{A} Q[\theta, v], \]  

(5.10)

where

\[ Q[\theta, v] = \left\langle \int \left( \frac{b - 1}{b R} |\nabla v|^2 + 2b \tau' \theta w + |\nabla \theta|^2 \right) \right\rangle. \]  

(5.11)
This gives a lower bound of $\Delta T$ as a function of $R$. Specifically, we have

$$\Delta T \geq 1 - b + 2b\Delta r - b \int_0^1 \tau^2 dz,$$

(5.12)

provided $Q[\theta, \nu] \geq 0$. So if one can find $\tau(z)$ and $b$ so that $Q[\theta, \nu] \geq 0$ for all $\theta$ and $\nu$, then we have a lower bound for $\Delta T$, and hence an upper bound for $Nu$.

### 5.3 Formulation of a Bound - General Thermal BCs

Recently the first analytical bound for general thermal BCs has been derived by Ralf Wittenberg [13], and we summarize the derivation below.

#### 5.3.1 Boundary Conditions and Some Identities

For the general thermal boundary conditions

$$T - \eta T_z = 1 + \eta \quad \text{at } z = 0,$$

(5.13)

$$T + \eta T_z = -\eta \quad \text{at } z = 1,$$

(5.14)

where $\eta$ is the Biot number.

Letting $T = \tau(z) + \theta$ as before, where $\tau(z)$ satisfies the thermal BCs at $z = 0, 1$, we have

$$\tau - \eta \tau_z = 1 + \eta \quad \text{at } z = 0,$$

(5.15)

$$\tau + \eta \tau_z = -\eta \quad \text{at } z = 1,$$

(5.16)

and

$$\theta - \eta \theta_z = 0 \quad \text{at } z = 0,$$

(5.17)

$$\theta + \eta \theta_z = 0 \quad \text{at } z = 1.$$

(5.18)

We take the difference of (5.13) and (5.14), then take the horizontal and time averages:

$$\Delta T + 2\eta \beta = 1 + 2\eta.$$

(5.19)

Similarly, we take the difference of (5.15) and (5.16):

$$\Delta \tau + 2\eta \gamma = 1 + 2\eta,$$

(5.20)
where
\[
\Delta \tau = \tau(0) - \tau(1),
\]
and
\[
\gamma = -\tau'(0) = -\tau'(1). \tag{5.21}
\]
Finally, we subtract (5.20) from (5.19) to get:
\[
\Delta \theta + 2\eta(\beta - \gamma) = 0, \tag{5.22}
\]
where \(\Delta \theta = (\bar{\theta}(0) - \bar{\theta}(1))\).

### 5.3.2 Formulation of a Bound

Firstly, we add (3.18) and twice (3.20) to get
\[
||\nabla T||^2 + \frac{d}{dt}||\theta||^2 = ||\nabla \theta||^2 + \int \tau'^2 + 2 \int \theta \tau' - 2 \int \theta w \tau' - 2 \int \theta z \tau' + 2 A \bar{\theta} T_z |_{z=0}^1 \tag{5.23}
\]
\[
= - ||\nabla \theta||^2 + \int \tau'^2 - 2 \int \theta w \tau' + 2 A \bar{\theta} T_z |_{z=0}. \tag{5.24}
\]
We multiply (5.24) by \(b\) and (3.17) by \((1 - b)\), then take the time average of the sum to get:
\[
b \langle ||\nabla T||^2 \rangle + \frac{1 - b}{R} \langle ||\nabla u||^2 \rangle = b \int \tau'^2 + 2bA(\bar{\theta} T_z |_{z=0}^1) - b Q[\theta, v], \tag{5.25}
\]
where \(Q[\theta, v] = (\int \frac{1}{\delta R} ||\nabla v||^2 + 2\tau' w + ||\nabla \theta||^2)\); note that the quadratic form \(Q[\theta, v]\) is the same as for fixed temperature and fixed flux BCs. Using (3.9) and (3.11) in (5.25), we get
\[
bA(\bar{T}T_z |_{z=0}^1) + (1 - b)A(\beta - \Delta T) = bA \int_0^1 \tau'^2 dz + 2bA(\bar{\theta} T_z |_{z=0}^1) - b Q[\theta, v]. \tag{5.26}
\]
Thus, using (5.17), (5.18) and (5.21) we obtain
\[
\begin{align*}
\bar{\theta} z_{i=1} &= \bar{\theta} z_{i=0} = -\eta(\bar{\theta}_z(1) + \bar{\theta}_z(0)), \tag{5.27} \\
\langle \bar{\theta} \tau' |_{z=0} \rangle &= \gamma \Delta \theta = \gamma(\Delta T - \Delta \tau), \tag{5.28}
\end{align*}
\]
Therefore,
\[
\begin{align*}
\langle \overline{\theta T_z} |_{z=0} \rangle &= \langle \bar{\theta} z |_{z=0} \rangle + \langle \bar{\theta} \tau' |_{z=0} \rangle \\
&= -\eta(\bar{\theta}_z(1) + \bar{\theta}_z(0)) + \gamma(\Delta T - \Delta \tau), \tag{5.29}
\end{align*}
\]
and
\[
\langle T_2^2 \rangle_0 = \langle \tau T_2^2 \rangle_0 + \langle \theta T_2^2 \rangle_0
\]
\[
= -\beta \tau_0 + \langle \theta T_2^2 \rangle_0
\]
\[
= \beta \Delta \tau + \gamma (\Delta T - \Delta \tau) - \eta \langle \theta_2^2(1) + \theta_2^2(0) \rangle.
\]
(5.30)

Substituting (5.29) and (5.30) into (5.26) gives:
\[
b (\beta \Delta \tau - \gamma (\Delta T - \Delta \tau) - \beta + \Delta T) + \beta - \Delta T
\]
\[
= b \int_0^1 \tau^2 dz - b \left( \eta \langle \theta_2^2(1) + \theta_2^2(0) \rangle + \frac{Q[\theta, v]}{A} \right).
\]
(5.31)

Now we eliminate \(\Delta T\) and \(\Delta \tau\) using (5.19) and (5.20):
\[
(1 + 2\eta) \beta = 1 + 2\eta + b \left( -(1 + 2\eta) + 2\eta \gamma^2 + \int_0^1 \tau^2 dz \right) - \frac{b}{A} \dot{Q},
\]
(5.32)

where using (5.27),
\[
\dot{Q} = \eta A \left( \theta_2^2(1) + \theta_2^2(0) \right) + Q[\theta, v]
\]
\[
= -A \langle \theta T_2^2 \rangle_0 + \left( \int \frac{1}{R_{\text{eff}}} |\nabla v|^2 + |\nabla \theta|^2 + 2\theta \omega \tau' \right)
\]
\[
= - \left( \int \nabla \cdot \hat{n} \cdot \nabla \theta \right) + \left( \int \frac{1}{R_{\text{eff}}} |\nabla v|^2 + |\nabla \theta|^2 + 2\theta \omega \tau' \right)
\]
\[
= \left( \eta \int \nabla \cdot \hat{n} \cdot \nabla \theta \right) + \left( \int \frac{1}{R_{\text{eff}}} |\nabla v|^2 + |\nabla \theta|^2 + 2\theta \omega \tau' \right).
\]
(5.33)

since by (5.17) and (5.18) we have \(\theta = -\eta \hat{n} \cdot \nabla \theta\) at \(z = 0, 1\); we have defined the "effective Rayleigh number"
\[
R_{\text{eff}} = \frac{bR}{b - 1} \geq R.
\]
(5.34)

This gives an upper bound of \(\beta\) as a function of \(R\). Specifically, we have
\[
\beta \leq 1 - b + \frac{b}{1 + 2\eta} \left( 2\eta \gamma^2 + \int_0^1 \tau^2 dz \right),
\]
(5.35)

provided \(\dot{Q}[\theta, v] \geq 0\). So if one can find \(\tau(z)\) and \(b\) so that \(\dot{Q}[\theta, v] \geq 0\) for all \(\theta\) and divergence-free fields \(v\), then we have an upper bound for \(\beta\). Using the relation (5.19) between \(\beta\) and \(\Delta T\), we can find a lower bound of \(\Delta T\) as a function of \(R_{\text{eff}}\). Finally, the upper bound of \(Nu\) as a function of \(R_{\text{eff}}\) is given by \(\frac{\partial R}{\partial T}\); and we can find the best optimal upper bound for \(Nu(R)\) by minimizing over \(b > 0\).
5.4 Piecewise Linear Profiles

Instead of working with the full optimization problem we introduce a family of profiles indexed by a single parameter $\delta \leq \frac{1}{2}$

$$\tau(z) = \tau_\delta(z) = \begin{cases} -\gamma z + 2\gamma \delta, & 0 \leq z \leq \delta \\ \gamma \delta, & \delta < z < 1 - \delta \\ -\gamma z + \gamma, & 1 - \delta \leq z \leq 1 \end{cases}$$

which is shown in Figure 5.1. The parameter $\delta$ corresponds physically to the thickness of the thermal boundary layer. Note that $\tau'(0) = \tau'(1) = -\gamma$ as required. We also compute $\Delta \tau = 2\gamma \delta$, and $\int_0^1 \tau'^2 dz = 2\delta \gamma^2 = \gamma \Delta \tau$.

![Figure 5.1: Piecewise Linear Profiles for $\tau_\delta(z)$](image)

- For the fixed temperature BCs, we should choose $\gamma = \frac{1}{2\delta}$ so that $\Delta \tau = 1$. Therefore, $\int_0^1 \tau'^2 dz = \frac{1}{2\delta}$, and the upper bound on $Nu$ from (5.4) becomes:

$$Nu \leq 1 - b + \frac{b}{2\delta} - \frac{b}{A} Q[\theta, v].$$

(5.37)

- For the fixed flux BCs, we should choose $\gamma = 1$. Therefore, $\Delta \tau = \int_0^1 \tau'^2 dz = 2\delta$, and the lower bound on $\Delta T$ from (5.10) becomes:

$$\Delta T \geq 1 - b + 2b\delta + \frac{b}{A} Q[\theta, v],$$

(5.38)
and $Nu = \frac{1}{\Delta T}$.

- For the general thermal BCs, we substitute $\Delta T = 2\gamma \delta$ into (5.20) to obtain the value of $\gamma$ (for given $\delta$ and $\eta$) for which the piecewise linear profile satisfies the BCs:

$$\gamma = \frac{1 + 2\eta}{2(\delta + \eta)} \quad \text{or} \quad \gamma - 1 = \frac{1 - 2\delta}{2(\delta + \eta)}.$$ 

Therefore, $2\eta \gamma^2 + \int_0^1 r^2 dz = 2\eta \gamma^2 + 2\delta \gamma^2 = 2\gamma^2 (\eta + \delta) = (1 + 2\eta) \delta$, and from (5.32) the upper bound on $\beta$ becomes:

$$\beta \leq 1 - b + b\gamma - \frac{b}{A(1 + 2\eta)} \dot{Q}.$$ 

Note that when $\eta = 0$, we have $\beta = Nu$ and $\gamma = \frac{1}{2}\delta$. Therefore, in this limit the above upper bound for the general thermal BCs reduces to the upper bound on $Nu$ for the fixed temperature BCs.

Using the relation (5.19) between $\beta$ and $\Delta T$, for $\eta > 0$ the upper bound on $\beta$ is equivalent to a lower bound on $\Delta T$:

$$\Delta T \geq 1 + 2b\eta (1 - \gamma) + \frac{2b\eta}{1 + 2\eta} \dot{Q},$$

and we then compute $Nu = \frac{\beta}{\Delta T}$.

When $\eta = \infty$, we have $\Delta T = \frac{1}{Nu}$ and $\gamma = 1$, so that, in this case, the lower bound on $\Delta T$ for the general thermal BCs reduces to the lower bound on $\Delta T$ for the fixed flux BCs.

However, in the later Chapters 6 and 7, we can see that the upper bound of $Nu - Ra$ relationship for general thermal BCs is quite close to the bound for the fixed flux case, no matter what the Biot number $\eta$ is. That's because for both fixed flux BCs and general thermal BCs, we cannot get an accurate $\Delta T$. Instead, we have to obtain a lower bound of $\Delta T$ in order to get an upper bound of $Nu$. On the contrary, we know $\Delta T$ is exactly 1 for the fixed temperature BCs.
Chapter 6

Analytical Upper Bound

From the previous chapter, we can see that both fixed temperature BCs and fixed flux BCs lead to the same quadratic form $Q[\theta, u]$:

$$Q[\theta, u] = \left\langle \int \frac{1}{R_{\text{eff}}} |\nabla u|^2 + 2\theta w r' + |\nabla \theta|^2 \right\rangle.$$  \hspace{1cm} (6.1)

For the general thermal BCs, we have

$$\tilde{Q}[\theta, u] = \left\langle \eta \int_{\partial \Omega} (\hat{n} \cdot \nabla \theta)^2 + \int \frac{1}{R_{\text{eff}}} |\nabla u|^2 + 2\theta w r' + |\nabla \theta|^2 \right\rangle \geq \left\langle \int \frac{1}{R_{\text{eff}}} |\nabla u|^2 + 2\theta w r' + |\nabla \theta|^2 \right\rangle = Q[\theta, u],$$

where $R_{\text{eff}} = \frac{bR}{k-1}$. Therefore, for all three boundary conditions, we can derive the analytical upper bound from the same quadratic form (6.1).

The following Cauchy-Schwarz analysis was first derived in [11] for fixed flux BCs; see also [9]. The basic idea is to consider the one-parameter family of piecewise linear background profiles for which the quadratic form $Q[\theta, u]$ is positive definite.

To impose the incompressibility constraint, we use the horizontal periodicity of the layer and recast the problem in Fourier variables:

$$w(\bar{x}, z) = \sum_k w_k(z) e^{ik\bar{x}}, \hspace{1cm} (6.2)$$

$$\theta(\bar{x}, z) = \sum_k \theta_k(z) e^{ik\bar{x}}, \hspace{1cm} (6.3)$$
where $\vec{x} = (x, y)$ and $\vec{k}$ is the horizontal wave vector. Using incompressibility we may express the quadratic form as

$$Q \geq \sum_k Q_k,$$

with

$$Q_k = \left( \int_0^1 \left( \frac{1}{R_{\text{eff}}} \left( \frac{1}{k^2} |D^2 w_k|^2 + 2|D w_k|^2 + k^2 |w_k|^2 \right) + |D\theta_k|^2 + k^2 |\theta_k|^2 + 2Re[\theta_k w_k^* r'] \right) dz \right).$$

(6.5)

where we define $w_k^* = \text{complex conjugate of } w_k$ and $k = |\vec{k}|$. Note that the quadratic form $Q[\theta, u]$ is positive definite if $Q_k \geq 0$ for all $k$.

Because $w_k(z)$ vanishes at $z = 0$ for all $k$, so does $\theta_k w_k$. Hence, for $z \leq \frac{1}{2}$, we have

$$|\theta_k w_k^*| = \left| \int_0^z D(\theta_k w_k^*)d\zeta \right| \leq \int_0^z |\theta_k D w_k^*|d\zeta + \int_0^z |D\theta_k w_k^*|d\zeta.$$ 

(6.6)

Furthermore, since $w_k$ and $D w_k$ both vanish at $z = 0$, we can estimate the last two terms using the Cauchy-Schwarz inequality

$$|w_k(z)| \leq \sqrt{z} \left( \int_0^{1/2} |D w_k(\zeta)|^2d\zeta \right)^{1/2} = \sqrt{z} \|D w_k\|_{[0, 1/2]},$$

(6.7)

$$|D w_k(z)| \leq \sqrt{z} \left( \int_0^{1/2} |D^2 w_k(\zeta)|^2d\zeta \right)^{1/2} = \sqrt{z} \|D^2 w_k\|_{[0, 1/2]}.$$ 

(6.8)

We substitute these two estimates into (6.6). Then we use the Cauchy-Schwarz inequality again, and the inequality $AB \leq \frac{1}{2}(A^2/\alpha + \alpha B^2)$ for any $\alpha > 0$ to get

$$|\theta_k w_k^*| \leq \|D^2 w_k\|_{[0, 1/2]} \int_0^z \sqrt{\zeta} \theta_k d\zeta + \|D w_k\|_{[0, 1/2]} \int_0^z \sqrt{\zeta} |D\theta_k|d\zeta$$

$$\leq \left( \|D^2 w_k\|_{[0, 1/2]} \|\theta_k\|_{[0, 1/2]} + \|D w_k\|_{[0, 1/2]} \|D\theta_k\|_{[0, 1/2]} \right) \frac{z}{\sqrt{2}},$$

(6.9)

$$\leq \left( \frac{\alpha_1}{k^2} \|D^2 w_k\|_{[0, 1/2]}^2 + \frac{k^2}{\alpha_1} \|\theta_k\|_{[0, 1/2]}^2 + \frac{1}{\alpha_2} \|D\theta_k\|_{[0, 1/2]}^2 \right) \frac{z}{2\sqrt{2}},$$

(6.10)

where $\alpha_1, \alpha_2 > 0$. A similar estimate holds for $z \geq \frac{1}{2}$:

$$|\theta_k w_k^*| \leq \left( \frac{\alpha_1}{k^2} \|D^2 w_k\|_{[1/2, 1]}^2 + \frac{k^2}{\alpha_1} \|\theta_k\|_{[1/2, 1]}^2 + \frac{1}{\alpha_2} \|D\theta_k\|_{[1/2, 1]}^2 \right) \frac{z}{2\sqrt{2}}.$$ 

(6.11)
CHAPTER 6. ANALYTICAL UPPER BOUND

Note that above analysis is independent of boundary conditions, and without using piecewise linear background profiles.

From now on, we will consider the piecewise linear background profiles introduced in Section 5.4. As before, we define \( \tau'(0) = \tau'(1) = -\gamma \). Then, on the whole domain \([0, 1]\), we obtain

\[
\left| \int_0^1 \theta_k w_k^* \tau' \right| \leq \gamma \left( \int_0^\delta |\theta_k w_k^*| + \int_{1-\delta}^1 |\theta_k w_k^*| \right)
\leq \frac{\gamma \delta^2}{4\sqrt{2}} \left( \frac{\alpha_1}{k^2} ||D^2 w_k||^2 + \alpha_2 ||D w_k||^2 + \frac{k^2}{\alpha_1} ||\theta_k||^2 + \frac{1}{\alpha_2} ||D \theta_k||^2 \right). \tag{6.13}
\]

Therefore, we have

\[
\int_0^1 2\Re[\theta_k w_k^* \tau''] dz = \int_0^1 (\theta_k w_k^* \tau' + \theta_k w_k^* \tau') \geq -\frac{\gamma \delta^2}{2\sqrt{2}} \left( \frac{\alpha_1}{k^2} ||D^2 w_k||^2 + \alpha_2 ||D w_k||^2 + \frac{k^2}{\alpha_1} ||\theta_k||^2 + \frac{1}{\alpha_2} ||D \theta_k||^2 \right). \tag{6.14}
\]

Finally, we substitute this into (6.5) to get

\[
Q_k \geq \left( \frac{k^2}{R_{\text{eff}}} ||w_k||^2 + \left( \frac{2}{R_{\text{eff}}} - \frac{\gamma \delta^2 \alpha_2}{2\sqrt{2}} \right) ||D w_k||^2 + \left( \frac{1}{R_{\text{eff}}} - \frac{\gamma \delta^2 \alpha_1}{2\sqrt{2}} \right) \frac{1}{k^2} ||D^2 w_k||^2 \right.
\]
\[\left. + \left(1 - \frac{\gamma \delta^2}{2\sqrt{2} \alpha_1}\right) k^2 ||\theta_k||^2 + \left(1 - \frac{\gamma \delta^2}{2\sqrt{2} \alpha_2}\right) ||D \theta_k||^2 \right). \tag{6.15}
\]

In order to ensure \( Q_k \geq 0 \), we can choose

\[
\alpha_1 = \alpha_2 = \frac{\gamma \delta^2}{2\sqrt{2}}, \tag{6.16}
\]

so that coefficients of \( ||\theta_k||^2 \) and \( ||D \theta_k||^2 \) are both zero. Therefore, the inequality (6.17) becomes

\[
Q_k \geq \left( \frac{k^2}{R_{\text{eff}}} ||w_k||^2 + \left( \frac{2}{R_{\text{eff}}} - \frac{\gamma^2 \delta^4}{8} \right) ||D w_k||^2 + \left( \frac{1}{R_{\text{eff}}} - \frac{\gamma^2 \delta^4}{8} \right) \frac{1}{k^2} ||D^2 w_k||^2 \right). \tag{6.17}
\]

Now we are ready to derive the analytical bounds for different boundary conditions. Given \( \gamma = \gamma(\delta) \) for different boundary conditions, we need to choose \( \delta \) so that \( Q_k \geq 0 \). In order to get the lowest upper bound on \( \beta \) and \( Nu \), or the highest lower bound on \( \Delta T \), we need to choose \( \delta \) so that \( Q_k \) is as small as possible.
6.1 Analytic Bound - Fixed Temperature BCs

For the fixed temperature BCs, we have $\gamma = \frac{1}{32}$. In order to guarantee each term in (6.19) be non-negative, we just need to make the coefficient of $||D^2w_k||^2$ be zero.

$$\frac{1}{R_{\text{eff}}} = \frac{\delta^2}{32} \implies \delta = 4\sqrt{2}R_{\text{eff}}^{-\frac{1}{2}}.$$  \hspace{1cm} (6.20)

So, we have

$$Nu \leq 1 - b + b \int_0^1 \tau^2 dz = 1 - b + \frac{b}{2\delta}$$
$$= 1 - b + \frac{b}{8\sqrt{2}}R_{\text{eff}}^{\frac{1}{2}}$$
$$= 1 - b + \frac{1}{8\sqrt{2}}b^{\frac{3}{4}}(b - 1)^{-\frac{1}{2}}Ra^{\frac{1}{2}}. \hspace{1cm} (6.21)$$

We want to get the lowest upper bound of $Nu$ in terms of $Ra$. In other words, we need to minimize $Nu$ over all $b > 1$. By minimizing $b^{\frac{3}{4}}(b - 1)^{-\frac{1}{2}}$ over all $b > 1$, we get $b = \frac{3}{2}$. Therefore we can get an upper bound on the Nusselt number as a function of $R_{\text{eff}}$

$$Nu \leq -\frac{1}{2} + \frac{3\sqrt{2}}{32}R_{\text{eff}}^{\frac{1}{2}}, \hspace{1cm} (6.23)$$

and an upper bound on $Nu(Ra)$:

$$Nu \leq -\frac{1}{2} + \frac{3\sqrt{6}}{32}Ra^{\frac{1}{2}} < -\frac{1}{2} + 0.230 Ra^{\frac{1}{2}}. \hspace{1cm} (6.24)$$

6.2 Analytic Bound - Fixed Flux BCs

For the fixed flux BCs, we have $\gamma = 1$. This upper bound formulation has been derived in [11], but we include it here for completeness. Making the coefficient of $||D^2w_k||^2$ be zero gives

$$\frac{1}{R_{\text{eff}}} = \frac{\delta^4}{8} \implies \delta = 8^{\frac{1}{4}}R_{\text{eff}}^{-\frac{1}{4}}. \hspace{1cm} (6.25)$$

We choose $b = 1 + c\delta$ with $c > 0$ (so $\Delta T > 0$). So we have

$$b = 1 + c\delta \implies R_{\text{eff}} = \frac{(1 + c\delta)R}{c\delta} \approx \frac{R}{c\delta}. \hspace{1cm} (6.26)$$

Combining the above two equations gives

$$\delta = (8c)^{\frac{1}{2}}R^{-\frac{1}{2}}. \hspace{1cm} (6.27)$$
Therefore, we have
\[ \Delta T \geq 1 - b + b(2\Delta - \int_0^1 \tau^2 dz) = 1 + b(2\delta - 1) \]
\[ = 1 + (1 + c\delta)(2\delta - 1) \]
\[ \approx (2 - c)\delta \quad \text{(get rid of } O(\delta^2)) \]
\[ = (8c)^{\frac{1}{3}}(2 - c)R^{-\frac{1}{3}}. \quad (6.28) \]

The coefficient above has a maximum value of \( 3/2^{1/3} \) when \( c = \frac{1}{2} \). (Later we get the numerical result \( c \approx 0.4861 \) for \( b \) and \( \delta \) in Figure 7.31.) This results in the bound
\[ \Delta T \geq \frac{3}{2^{1/3}}R^{-\frac{1}{3}}. \quad (6.29) \]

Using the relations \( Ra = R\Delta T \) and \( Nu = \frac{1}{3}Ra \), we can obtain the bound on \( Nu(Ra) \) and \( Nu(R) \):
\[ Nu \leq \left( \frac{2}{27} \right)^{\frac{1}{3}} Ra^{\frac{1}{3}} \approx 0.272 Ra^{\frac{1}{3}}, \quad (6.30) \]
\[ Nu \leq \frac{2^{\frac{4}{3}}}{3} R^{\frac{1}{3}}, \quad (6.31) \]

Moreover, if we substitute \( c = \frac{1}{2} \) into (6.27), we can obtain
\[ \delta = (4)^{\frac{1}{3}}R^{-\frac{1}{3}}. \quad (6.32) \]

Combining (6.31) and (6.32) with the relation \( Reff \approx \frac{R}{3} \), we can obtain
\[ Nu \leq \frac{2^{\frac{4}{3}}}{3} Reff^{\frac{1}{3}}. \quad (6.33) \]

### 6.3 Analytic Bound - General Thermal BCs

For the general thermal BCs, choosing \( \alpha_1 = \alpha_2 = \frac{2\delta^2}{2\sqrt{2}} \) leads to (6.19):
\[ Q_k \geq \left( \frac{k^2}{Reff} ||w_k||^2 + \left( \frac{2}{Reff} - \frac{\gamma^2\delta^4}{8} \right) ||Dw_k||^2 + \left( \frac{1}{Reff} - \frac{\gamma\delta^4}{8} \right) \frac{1}{k^2} ||D^2w_k||^2 \right), \]
where \( \gamma = \frac{4+2\eta}{2(6+\eta)} \) from (5.39). Making the coefficient of \( ||D^2w_k||^2 \) be zero gives
\[ \frac{1}{Reff} = \frac{\gamma^2\delta^4}{8} \implies \gamma\delta^2 = 2\sqrt{2Reff^{-\frac{1}{2}}} \quad (6.34) \]
6.3.1 For large $\eta$

For large $\eta$ (say $\eta > \frac{1}{2} \implies \delta < \eta$), we have

$$1 = \frac{1 + 2\eta}{1 + 2\eta} \leq \gamma \leq \frac{1 + 2\eta}{2\eta} = 1 + \frac{1}{2\eta},$$

$$\implies \gamma \approx 1,$$

$$\implies \delta \approx \delta^4 R_{\text{eff}}^{-\frac{1}{4}}.$$

which is the same as the fixed flux case. This tells us that when $\eta$ is large ($\eta > \frac{1}{2}$), the scalings for the general thermal BCs should be the same as for the fixed flux BCs.

6.3.2 For small $\eta$

For small $\eta$, the scaling depends on how large $R$ is. When $R$ is sufficiently small, we have

$$\delta \gg \eta \implies \gamma = \frac{1 + 2\eta}{2(\delta + \eta)} \sim \frac{1}{2\delta} \implies \delta \sim R_{\text{eff}}^{-\frac{1}{2}}; \quad (6.35)$$

in this case, the scalings look like the fixed temperature case.

When $R$ is large enough, we have $\delta \to 0$ and thus eventually we have $\delta \ll \eta$. Hence we get $\gamma \sim 1$, and the scalings will look asymptotically like the fixed flux case.

Therefore, for any small $\eta > 0$, the scalings for the general thermal BCs will be like the fixed temperature case first; but will change to be like the fixed flux case once $R$ is large enough.

6.3.3 Analytic Bound on $Nu$

We want to find the asymptotic upper bound, so $\delta \ll \eta$ must be true for sufficiently large $R$. By the relationship between $\beta$ and $\Delta T$ (5.19), and the upper bound on $\beta$, we
can derive a lower bound on $\Delta T$

$$
\Delta T = 1 + 2\eta - 2\eta \beta \\
\geq 1 - 2b\eta(\gamma - 1) \\
= 1 - 2\eta b^2 (\delta + \eta) \\
= 1 - b^2 \frac{1 - 2\delta}{1 + \frac{\delta}{\eta}} \\
= 1 - b(1 - 2\delta) \left(1 - \frac{\delta}{\eta} + O(\delta^2)\right) \\
= 1 - b + b\delta(2 + \frac{1}{\eta}) + O(\delta^2),
$$

(6.36)

where we used the Taylor expansion of $\frac{1}{1 + \frac{\delta}{\eta}}$, because $\frac{\delta}{\eta}$ is small for sufficiently large $R$. In order to have $\Delta T > 0$ (for $b > 1$) in the limit $R \to \infty$ (which implies $\delta \to 0$), we need to have that $b - 1$ approaches 0 as $\delta \to 0$. Therefore, we can let $b = 1 + c\delta$. Then the upper bound on $\Delta T$ becomes

$$
\Delta T \geq 1 - (1 + c\delta)(1 - 2\delta) \left(1 - \frac{\delta}{\eta} + O(\delta^2)\right) \\
= \left(1 + \frac{2\eta}{\eta} - c\right) \delta + O(\delta^2). 
$$

(6.37)

We will later compute $c = c(\eta)$ analytically and numerically.

Similarly, we can obtain an upper bound on $\beta$

$$
\beta \leq 1 + b(\gamma - 1) \\
= 1 + \frac{(1 + c\delta)(1 - 2\delta)}{2\eta(1 + \frac{\delta}{\eta})} \\
= 1 + \frac{1}{2\eta} (1 + c\delta)(1 - 2\delta) \left(1 - \frac{\delta}{\eta} + O(\delta^2)\right) \\
= 1 + \frac{1}{2\eta} \left(1 + \left(c - \frac{1 + 2\eta}{\eta}\right) \delta + O(\delta^2)\right) \\
= \frac{1 + 2\eta}{2\eta} + \frac{1}{2\eta} \left(c - \frac{1 + 2\eta}{\eta}\right) \delta + O(\delta^2).
$$

(6.38)
Finally, we can get an upper bound on $Nu$

$$Nu = \frac{b}{\Delta T} \leq \frac{1+c\delta}{2\eta} \left( \frac{c - 1+c\delta}{1+c\delta} \right) \delta + O(\delta^2)$$

$$= \frac{1+c\delta}{1+c\delta} \delta + O(1)$$

or equivalently

$$= \frac{1+2\eta}{2(1+(2-c)\eta)} + O(1). \quad (6.39)$$

For very large $R$, we have $\delta \ll \eta$. Hence,

$$R_{\text{eff}} = \frac{bR}{b-1} = \frac{(1+c\delta)R}{c\delta} \approx \frac{R}{c\delta}, \quad (6.40)$$

and

$$\gamma = \frac{1+2\eta}{2(\delta + \eta)} \approx \frac{1+2\eta}{2\eta}. \quad (6.41)$$

Combining with $\gamma \delta^2 = 2\sqrt{2} R_{\text{eff}}^{-\frac{1}{2}}$, we have

$$\left( \frac{1+2\eta}{2\eta} \right)^2 = 2\sqrt{2}(c\delta)^{\frac{1}{2}} R^{-\frac{1}{2}}, \quad (6.42)$$

or equivalently

$$\delta^{-1} = (8c)^{-\frac{1}{2}} \left( \frac{1+2\eta}{2\eta} \right)^{\frac{3}{2}} R^{\frac{1}{2}}. \quad (6.43)$$

Therefore, by substituting the above result into (6.39), we have

$$Nu \leq \frac{1+2\eta}{2\eta}^{\frac{3}{2}} \frac{1+2\eta}{4c^{\frac{1}{2}}(1+(2-c)\eta)} R^{\frac{1}{2}} \quad (6.44)$$

For each Biot number $\eta$, we want to find the lowest upper bound of $Nu$ in terms of $R$. By maximizing $c^{\frac{1}{2}}(1+(2-c)\eta)$ we get

$$c(\eta) = \frac{1+2\eta}{4\eta}. \quad (6.45)$$

We can see that for very small $\eta$, $c$ looks like $0.25\eta^{-1}$; for very large $\eta$, $c$ is approximately 0.5. This agrees with our numerical calculation, Figure 7.77, in Chapter 7.
Now we can substitute \( c = \frac{1 + 2\eta}{4\eta} \) into (6.37) and (6.44), to get the following results

\[
Nu \leq \frac{1}{3} \left( \frac{1 + 2\eta}{\eta} \right)^{\frac{1}{2}} R^{\frac{3}{2}}, \tag{6.46}
\]

\[
\Delta T \geq \frac{3}{2} \left( \frac{1 + 2\eta}{\eta} \right)^{\frac{3}{2}} R^{-\frac{1}{2}}. \tag{6.47}
\]

Using the relation \( Ra = R\Delta T \) and the lower bound (6.47), we have

\[
Ra = R\Delta T \geq \frac{3}{2} \left( \frac{1 + 2\eta}{\eta} \right)^{\frac{3}{2}} R^{\frac{3}{2}}, \tag{6.48}
\]

or equivalently,

\[
R^{\frac{3}{2}} \leq \left( \frac{2}{3} \right)^{\frac{1}{2}} \left( \frac{\eta}{1 + 2\eta} \right)^{\frac{3}{2}} Ra^{\frac{1}{2}}. \tag{6.49}
\]

Therefore, we can get an analytical upper bound of \( Nu \) in terms of \( Ra \):

\[
Nu \leq \frac{1}{3} \left( \frac{1 + 2\eta}{\eta} \right)^{\frac{3}{2}} R^{\frac{3}{2}} \tag{6.50}
\]

\[
\leq \left( \frac{2}{27} \right)^{\frac{1}{2}} Ra^{\frac{1}{2}} \approx 0.272 Ra^{\frac{1}{2}}. \tag{6.51}
\]

Interestingly, this analytical upper bound is independent of Biot number \( \eta \). And also, this bound is exactly the same as the analytical upper bound for the fixed flux case.

### 6.3.4 Other analytic scaling results

By combining the above estimates, we can obtain numerous other analytic bounds which we will compare with numerical results in Chapter 7.

**Critical \( \delta \) as a function of \( R \):**

We can combine (6.43) and (6.45) to get

\[
\delta_c = 2^{\frac{3}{2}} \left( \frac{2\eta}{1 + 2\eta} \right)^{\frac{1}{2}} R^{-\frac{1}{2}} \tag{6.52}
\]

\[
\approx 2\eta^{\frac{1}{2}} R^{-\frac{1}{2}} \quad \text{for small } \eta. \tag{6.53}
\]

We can also see that the prefactor(\( \eta \)) for \( \delta_c(R) \) scales as \( 2\eta^{\frac{1}{2}} \).
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Critical $\delta$ as a function of $R_{\text{eff}}$:

We can also combine (6.52) and (6.40) to get

$$\delta_c = 2^{\frac{3}{4}} \left( \frac{2\eta}{1 + 2\eta} \right)^{\frac{1}{4}} R_{\text{eff}}^{-\frac{1}{4}}$$

(6.54)

$$\approx 2^{\frac{3}{4}} \eta^{\frac{1}{4}} R_{\text{eff}}^{-\frac{1}{4}} \quad \text{for small } \eta.$$  

(6.55)

Therefore, the prefactor($\eta$) for $\delta_c(R_{\text{eff}})$ scales as $2^{\frac{3}{4}} \eta^{\frac{1}{4}}$.

Critical $\delta$ as a function of $Ra$:

Using the equation (6.52) and the relation between $R$ and $Ra$, (6.49), one can get $\delta_c(Ra)$:

$$\delta_c \geq 6^{\frac{1}{2}} Ra^{-\frac{1}{4}}.$$  

(6.56)

Therefore, the prefactor($\eta$) for $\delta_c(Ra)$ should be a constant $6^{\frac{1}{2}}$.

Critical $b$ as a function of $R$:

Now we substitute equations (6.52) and (6.45) into $b = 1 + c\delta$ to obtain the relation between $b_c$ and $R$:

$$b_c = 1 + 2^{-\frac{1}{4}} \left( \frac{1 + 2\eta}{2\eta} \right)^{\frac{1}{4}} R^{-\frac{1}{4}}$$

(6.57)

$$\approx 1 + \frac{1}{2} \eta^{\frac{1}{2}} R^{-\frac{1}{4}} \quad \text{for small } \eta.$$  

(6.58)

Therefore, the prefactor($\eta$) for $b_c - 1$ as the function of $R$ should scale as $\eta^{-\frac{1}{4}}$.

Critical $b$ as a function of $R_{\text{eff}}$:

We substitute equations (6.54) and (6.45) into $b = 1 + c\delta$ to obtain the relation between $b_c$ and $R_{\text{eff}}$:

$$b_c = 1 + 2^{-\frac{1}{4}} \left( \frac{1 + 2\eta}{2\eta} \right)^{\frac{1}{4}} R_{\text{eff}}^{-\frac{1}{4}}$$

(6.59)

$$\approx 1 + 2^{-\frac{3}{4}} \eta^{\frac{1}{4}} R_{\text{eff}}^{-\frac{1}{4}} \quad \text{for small } \eta.$$  

(6.60)

Therefore, the prefactor($\eta$) for $b_c - 1$ as the function of $R_{\text{eff}}$ should scale as $\eta^{-\frac{1}{4}}$. 

Critical $b$ as a function of $Ra$:

Similarly, we substitute equations (6.56) and (6.45) into $b = 1 + c\delta$ to obtain the relation between $b_c$ and $Ra$:

$$b_c \geq 1 + 6^{\frac{1}{2}} \frac{1 + 2\nu}{4\eta} Ra^{-\frac{1}{2}}$$

$$\approx 1 + \left(\frac{3}{8}\right)^{\frac{1}{2}} \eta^{-1} Ra^{-\frac{1}{2}}.$$  \hspace{1cm} (6.61)

(6.62)

Therefore, the prefactor($\eta$) for $b_c - 1$ as the function of $Ra$ should scale as $\eta^{-1}$. 


Chapter 7

Numerical Upper Bound Calculation

Using a numerical approach, we can compute the optimal piecewise linear solution to the Doering-Constantin background method. The numerical upper bound should be better than the analytical upper bound. It turns out that the exponent is still $\frac{1}{2}$, but we can get an improved prefactor.

7.1 Euler-Lagrange equations

We first show that all thermal boundary conditions lead to the same eigenvalue problem.

7.1.1 Fixed Temperature and Fixed Flux BCs

We already know that both fixed temperature BCs and fixed flux BCs lead to the same quadratic form $Q[\theta, u]$:

$$Q[\theta, u] = \int \frac{1}{R_{\text{eff}}} |\nabla u|^2 + 2\theta \omega \tau' + |\nabla \theta|^2,$$

where $R_{\text{eff}} = \frac{b\theta}{\kappa - 1}$.

The upper bound of $N_u$ for the fixed temperature case, or the lower bound of $\Delta T$ for the fixed flux case, may be obtained by minimizing this quadratic form over all background profiles $\tau$ satisfying the spectral condition $Q[\theta, u] \geq 0$, subject to the normalization condition and divergence-free condition. In other words, we just need to
make sure that the lowest eigenvalue of the Euler-Lagrange equations $\lambda_0$:

$$\lambda_0 = \inf_{u, \theta} Q[u, \theta]$$

(7.2)
is always $\geq 0$, subject to the boundary conditions, divergence-free condition $\nabla \cdot u = 0$, and normalization condition $||\theta||^2 + \frac{1}{\sigma R} ||u||^2 = 1$. Thus, we introduce $L(\theta, u)$:

$$L(\theta, u) = \int \frac{1}{R_{\text{eff}}} |\nabla u|^2 + 2\theta w r' + |\nabla \theta|^2 - \lambda \left( |\theta|^2 + \frac{1}{\sigma R} |u|^2 \right) - P \nabla \cdot u,$$

(7.3)

where $P = P(\vec{x})$ is the Lagrange multiplier enforcing the divergence-free condition and $\lambda$ is the Lagrange multiplier enforcing the normalization for the eigenfunctions. Then we have

$$L(\theta + \epsilon \phi, u + \epsilon \vec{\mu}) = \int \frac{1}{R_{\text{eff}}} |\nabla u + \epsilon \nabla \vec{\mu}|^2 - \lambda (\theta + \phi)^2 - \frac{\lambda}{\sigma R} |u + \epsilon \vec{\mu}|^2 - P (\nabla \cdot u + \epsilon \nabla \cdot \vec{\mu})$$

$$= \int \frac{1}{R_{\text{eff}}} |\nabla u|^2 + 2 \epsilon \nabla \theta \cdot \nabla \phi + \frac{1}{R_{\text{eff}}} (|\nabla u|^2 + 2 \epsilon \nabla \phi 
abla \vec{\mu})$$

$$+ 2(\theta w + \epsilon \phi w + \epsilon \theta \mu_z) r' - \lambda (\theta^2 + 2 \epsilon \phi) - \frac{\lambda}{\sigma R} (|u|^2 + 2 \epsilon u \cdot \vec{\mu})$$

$$- P (\nabla \cdot u + \epsilon \nabla \cdot \vec{\mu}) + O(\epsilon^2),$$

where the vector $\vec{\mu} = (\mu_x, \mu_y, \mu_z)^T$; thus (integrating by parts in the second equality)

$$\frac{L(\theta + \epsilon \phi, u + \epsilon \vec{\mu}) - L(\theta, u)}{\epsilon} = \int \frac{2}{R_{\text{eff}}} \nabla u \cdot \nabla \vec{\mu} + 2 \phi w r'$$

$$+ 2 \theta \mu_z r' - 2 \lambda \phi \phi - \frac{2 \lambda}{\sigma R} u \cdot \vec{\mu} - P \nabla \cdot \vec{\mu}$$

$$= \int (-2 \nabla^2 \theta + 2 w r' - 2 \lambda \phi) \phi$$

$$+ (\frac{2}{R_{\text{eff}}} \nabla^2 u - \frac{2 \lambda}{\sigma R} u + \nabla P) \cdot \vec{\mu} + 2 \theta r' \mu_z.$$

Therefore, the corresponding Euler-Lagrange equations are

$$P_x - \frac{2}{R_{\text{eff}}} \nabla^2 u = \lambda \frac{2}{\sigma R} u,$$

$$P_y - \frac{2}{R_{\text{eff}}} \nabla^2 v = \lambda \frac{2}{\sigma R} v,$$

$$P_z - \frac{2}{R_{\text{eff}}} \nabla^2 w + 2 \theta r' = \lambda \frac{2}{\sigma R} w,$$

(7.4)

$$w r' - \nabla^2 \theta = \lambda \theta,$$

$$u_x + v_y + w_z = 0.$$
It is important to note that $\lambda$, initially introduced as a Lagrange multiplier in (7.3) and appearing as an eigenvalue in (7.4), is in fact the value of the quadratic form $Q[u, \theta]$ at the extremizing $u$ and $\theta$. Given a solution $u = (u, v, w),$ $\theta,$ $P$ of (7.4), we can multiply the first equation by $\frac{1}{2}u$, the second by $\frac{1}{2}v$, the third one by $\frac{1}{2}w$ and the fourth by $\theta$, add and integrate, to obtain

$$\lambda \int \frac{1}{\sigma R} |u|^2 + \theta^2 = \int u \cdot \nabla P - \frac{1}{R_{\text{eff}}} u \cdot \nabla^2 u + \theta w \tau' - \theta \nabla^2 \theta.$$ 

Integrating by parts and using the normalization and divergence-free conditions, we get

$$\lambda \left( \frac{1}{\sigma R} ||u||^2 + ||\theta^2||^2 \right) = \int \frac{1}{R_{\text{eff}}} |\nabla u|^2 + \theta w \tau' + |\nabla \theta|^2 - P \nabla \cdot u$$

$$\implies \lambda = Q[u, \theta].$$

It follows that $\lambda$ is real. Note also that for each $\tau'$, the quadratic functional $Q[u, \theta]$ is bounded below.

The system (7.4) has a countable infinity of increasing eigenvalues. In order to ensure that $Q[u, \theta] \geq 0$ for all $u$ and $\theta$, we require that the lowest eigenvalue $\lambda_0 \geq 0$. It turns out that the set of allowed background fields $\tau(z)$ is convex, so that the optimal profile $\tau$ yielding the minimum bound for $Nu$ lies on the boundary of the convex set (See [5] or Chapter 4 in [9] for details of this argument). Thus it is sufficient to consider only profiles $\tau(z)$ for which $\lambda_0 = \inf_{u, \theta} Q[u, \theta] = 0$; that is, the lowest eigenvalue of (7.4) is 0.

Setting $\lambda = 0$ in (7.4), we have

$$P_x - \frac{2}{R_{\text{eff}}} \nabla^2 u = 0,$$

$$P_y - \frac{2}{R_{\text{eff}}} \nabla^2 v = 0,$$

$$P_z - \frac{2}{R_{\text{eff}}} \nabla^2 w + 2\theta \tau' = 0,$$

$$w \tau' - \nabla^2 \theta = 0,$$

$$u_x + v_y + w_z = 0.$$ 

Using the horizontal periodicity of $u$, we may decompose it as

$$u(x, y, z) = \sum_k u_k(z) e^{i(k_1 x + k_2 y)}.$$
where $k^2 = k_1^2 + k_2^2$; we perform the same decomposition for $v$, $w$, $\theta$ and $P$. Then the E-L equations in (7.5) become

\[
\begin{align*}
  ik_1 P - \frac{2}{R_{\text{eff}}} (D^2 - k_1^2 - k_2^2) u &= 0, \\
  ik_2 P - \frac{2}{R_{\text{eff}}} (D^2 - k_1^2 - k_2^2) v &= 0, \\
  DP - \frac{2}{R_{\text{eff}}} (D^2 - k_1^2 - k_2^2) w + 2\theta \tau' &= 0, \\
  w \tau' - (D^2 - k_1^2 - k_2^2) \theta &= 0, \\
  ik_1 u + ik_2 v + Dw &= 0.
\end{align*}
\]

where we drop the subscript $k$ for convenience, and define $D = d/dz$.

First we show, following [5], that when there is no background flow field, the 3D problem can be reduced to a 2D problem. Motivated by the rotational symmetry of the system about the vertical $z$-axis, we introduce a change of variables which essentially amounts to a coordinate rotation in the horizontal direction. The change of dependent variables from $u$ and $v$ to $u \cos \varphi + v \sin \varphi$ and $-u \sin \varphi + v \cos \varphi$, where $\tan \varphi = k_2/k_1$, yields

\[
\begin{align*}
  ikP - \frac{2}{R_{\text{eff}}} (D^2 - k^2) u &= 0, \\
  \frac{2}{R_{\text{eff}}} (D^2 - k^2) v &= 0, \\
  DP - \frac{2}{R_{\text{eff}}} (D^2 - k^2) w + 2\theta \tau' &= 0, \\
  w \tau' - (D^2 - k^2) \theta &= 0, \\
  iku + Dw &= 0.
\end{align*}
\]

The second equation in (7.7) is uncoupled from the others. The remaining equations are reduced to a 2D problem. Eliminating the pressure $P$ and introducing $\tilde{u} = iku$ yields

\[
\begin{align*}
  D(D^2 - k^2) \tilde{u} + k^2(D^2 - k^2) w - k^2 \tau' R_{\text{eff}} \theta &= 0, \\
  w \tau' - (D^2 - k^2) \theta &= 0, \\
  \tilde{u} + Dw &= 0.
\end{align*}
\]
CHAPTER 7. NUMERICAL UPPER BOUND CALCULATION

7.1.2 General Thermal BCs

First, we introduce $L(\theta, u)$, as before,

$$L(\theta, u) = \eta \int_{\partial \Omega} (\hat{n} \cdot \nabla \theta)^2 + \int \frac{1}{R_{\text{eff}}} |\nabla u|^2 + 2\theta w \tau' + |\nabla \theta|^2 - \lambda \left( |\theta|^2 + \frac{1}{\sigma R} |u|^2 \right) - P \nabla \cdot u.$$

So, we have

$$L(\theta + \epsilon \phi, u + \epsilon \mu)$$

$$= \eta \int_{\partial \Omega} (\hat{n} \cdot (\nabla \theta + \epsilon \nabla \phi))^2 + \int |\nabla \theta + \epsilon \nabla \phi|^2 + \frac{1}{R_{\text{eff}}} |\nabla u + \epsilon \nabla \mu|^2$$

$$+ 2(\theta + \epsilon \phi)(w + \epsilon \mu_z)\tau' - \lambda(\theta + \epsilon \phi)^2 - \frac{\lambda}{\sigma R} |u + \epsilon \mu|^2 - P (\nabla \cdot u + \epsilon \nabla \cdot \mu)$$

$$= \eta \int_{\partial \Omega} (\hat{n} \cdot \nabla \theta)^2 + 2\epsilon (\hat{n} \cdot \nabla \theta)(\hat{n} \cdot \nabla \phi) + \int |\nabla \theta|^2 + 2\epsilon |\nabla \theta \cdot \nabla \phi$$

$$+ \frac{1}{R_{\text{eff}}} (|\nabla u|^2 + 2\epsilon |\nabla u \cdot \nabla \mu|) + 2(\theta w + \epsilon \phi w + \epsilon \theta \mu_z)\tau' - \lambda(\theta^2 + 2\epsilon \theta \phi)$$

$$- \frac{\lambda}{\sigma R} (|u|^2 + 2\epsilon u \cdot \mu) - P(\nabla \cdot u + \epsilon \nabla \cdot \mu) + O(\epsilon^2).$$

Therefore, we have

$$\frac{L(\theta + \epsilon \phi, u + \epsilon \mu) - L(\theta, u)}{\epsilon}$$

$$= \int 2\nabla \cdot \nabla \phi + \frac{2}{R_{\text{eff}}} \nabla u : \nabla \mu + 2\phi w \tau' + 2\theta \mu_z \tau' - 2\lambda \theta \phi - \frac{2\lambda}{\sigma R} u \cdot \mu - P \nabla \cdot \mu$$

$$+ 2\eta \int_{\partial \Omega} (\hat{n} \cdot \nabla \theta)(\hat{n} \cdot \nabla \phi)$$

$$= \int (-2\nabla^2 \theta + 2\omega \tau' - 2\lambda \theta) \phi + \left(-\frac{2}{R_{\text{eff}}} \nabla^2 u - \frac{2\lambda}{\sigma R} u + \nabla P \right) : \mu + 2\theta \tau' \mu_z$$

$$+ 2 \int (\hat{n} \cdot \nabla \theta) \phi + 2\eta \int (\hat{n} \cdot \nabla \theta)(\hat{n} \cdot \nabla \phi)$$

$$= \int (-2\nabla^2 \theta + 2\omega \tau' - 2\lambda \theta) \phi + \left(-\frac{2}{R_{\text{eff}}} \nabla^2 u - \frac{2\lambda}{\sigma R} u + \nabla P \right) : \mu + 2\theta \tau' \mu_z$$

$$+ 2 \int (\hat{n} \cdot \nabla \theta)(\phi + \eta \hat{n} \cdot \nabla \phi)$$

$$= \int (-2\nabla^2 \theta + 2\omega \tau' - 2\lambda \theta) \phi + \left(-\frac{2}{R_{\text{eff}}} \nabla^2 u - \frac{2\lambda}{\sigma R} u + \nabla P \right) : \mu + 2\theta \tau' \mu_z,$$

where we used a lot of integration by parts. Note that the boundary term vanished due to the boundary conditions for $\phi$. This results in exactly the same Euler-Lagrange equations (7.4) - (7.8) as the fixed temperature and fixed flux cases.
7.2 Solutions for the Piecewise Linear Profiles

A solution of the above system (7.8) would yield the best upper bound for pure conductive background flow that this formulation of the Doering-Constantin method has to offer. A computation of this optimal bound, even from a numerical point of view, is difficult. However, the optimal upper bound may be estimated from above by performing the optimization over certain background profiles $\tau(z)$. Here, we will choose a one-parameter family of piecewise linear profiles; in this case, $\tau'(z)$ is piecewise constant, so that the equations (7.8) are piecewise constant coefficient ODEs, and can be solved analytically explicitly in each region in which $\tau'$ is constant.

Thus we introduce the family of profiles indexed by a single parameter $\delta$ introduced in Section 5.4 (See Figure 5.1)

$$\tau_\delta(z) = \begin{cases} 
-\gamma z + 2\gamma \delta, & 0 \leq z \leq \delta \\
\gamma \delta, & \delta < z < 1 - \delta \\
-\gamma z + \gamma, & 1 - \delta \leq z \leq 1
\end{cases}$$

(7.9)

where $\gamma = \frac{1}{2\delta}$ for the fixed temperature BCs; $\gamma = 1$ for the fixed flux BCs; and $\gamma = \frac{1+2\eta}{2(\delta+\eta)}$ for the general thermal BCs.

Denote the regions $[0, \delta]$ and $[\delta, \frac{1}{2}]$ as Regions I and II, respectively. Because the lowest eigenfunctions for the vertical velocity $w$ and temperature $\theta$ are even about $z = \frac{1}{2}$, we only need to solve the problem on half of the unit interval. (See the similar discussion in Appendix C of [9] for a discussion of evenness of the lowest eigenfunction in a similar problem.) Note that $\overline{u}$ is odd about $z = \frac{1}{2}$ due to the relation $\overline{u} = -Dw$.

Inserting the chosen profiles (7.9) into (7.8), we obtain a set of equations in Region I, where $\tau' = -\gamma$:

$$\begin{align*}
D(D^2 - k^2)\overline{u} + k^2(D^2 - k^2)w + k^2\gamma R_{\text{eff}}\theta &= 0, \\
\gamma w + (D^2 - k^2)\theta &= 0, \\
\overline{u} + Dw &= 0,
\end{align*}$$

Region I: (7.10)
which is a linear constant coefficient ODE system. The solution in exponential form is:

$$\begin{align*}
\ddot{u} &= -[A_1p_1e^{p_1z} - A_2p_2e^{p_2z} + A_3p_3e^{p_3z} - A_4p_4e^{-p_4z} + A_5p_5e^{p_5z} - A_6p_6e^{-p_6z}], \\
\dot{w} &= A_1e^{p_1z} + A_2e^{-p_1z} + A_3e^{p_3z} + A_4e^{-p_3z} + A_5e^{p_5z} + A_6e^{-p_5z}, \\
\theta &= -\frac{p^2}{2k^2\gamma_{\text{ref}}}(1 - i\sqrt{3})(A_1e^{p_1z} + A_2e^{-p_1z}) + (1 + i\sqrt{3})(A_3e^{p_3z} + A_4e^{-p_3z}) \\
&\quad - 2(A_5e^{p_5z} + A_6e^{-p_5z}),
\end{align*}$$

(7.11)

or, in the hyperbolic form:

$$\begin{align*}
\ddot{u} &= -[A_1p_1\sinh(p_1z) + A_2p_1\cosh(p_1z) + A_3p_2\sinh(p_2z) \\
&\quad + A_4p_2\cosh(p_2z) + A_5p_3\sinh(p_3z) + A_6p_3\cosh(p_3z)], \\
\dot{w} &= A_1\cosh(p_1z) + A_2\sinh(p_1z) + A_3\cosh(p_3z) + A_4\sinh(p_3z) \\
&\quad + A_5\cosh(p_3z) + A_6\sinh(p_3z), \\
\theta &= -\frac{p^2}{2k^2\gamma_{\text{ref}}}(1 - i\sqrt{3})(A_1\cosh(p_1z) + A_2\sinh(p_1z)) \\
&\quad + (1 + i\sqrt{3})(A_3\cosh(p_3z) + A_4\sinh(p_3z)) \\
&\quad - 2(A_5\cosh(p_3z) + A_6\sinh(p_3z)),
\end{align*}$$

(7.12)

where $\rho = (k^2\gamma_{\text{ref}})^{\frac{3}{2}}, p_{1,2} = \sqrt{k^2 + \frac{\rho}{2}(1 \pm i\sqrt{3})}$ and $p_3 = \sqrt{k^2 - \rho}$.

In the second region, where $\tau' = 0$, we have

$$\begin{align*}
\text{Region II:} & \\
\begin{cases}
D(D^2 - k^2)\ddot{u} + k^2(D^2 - k^2)\dot{w} = 0, \\
(D^2 - k^2)\theta = 0, \\
\ddot{u} + Dw = 0,
\end{cases}
\end{align*}$$

(7.13)

the general solution of which in exponential form is:

$$\begin{align*}
\ddot{u} &= -[B_1e^{\kappa z} + B_2(1 + k\kappa)e^{\kappa z} - B_3e^{-k\kappa z} + B_4(1 - k\kappa)e^{-k\kappa z}], \\
\dot{w} &= B_1e^{\kappa z} + B_2e^{k\kappa z} + B_3e^{-k\kappa z} + B_4e^{-\kappa z}, \\
\theta &= B_5e^{\kappa z} + B_6e^{-k\kappa z},
\end{align*}$$

(7.14)

or, in the hyperbolic form:

$$\begin{align*}
\ddot{u} &= -[B_1\sinh(k\zeta) + B_2k\cosh(k\zeta) + B_3(\cosh(k\zeta) + k\zeta \sinh(k\zeta)) \\
&\quad + B_4(\sinh(k\zeta) + k\zeta \cosh(k\zeta))], \\
\dot{w} &= B_1\cosh(k\zeta) + B_2\sinh(k\zeta) + B_3\cosh(k\zeta) + B_4\cosh(k\zeta), \\
\theta &= B_5\cosh(k\zeta) + B_6\sinh(k\zeta),
\end{align*}$$

(7.15)

where $\zeta = z - \frac{1}{2}$. 
7.3 Boundary Conditions

The boundary condition for $\theta$ at $z = 0$ depends on different thermal boundary conditions.

\[
\begin{aligned}
\text{fixed temperature BCs:} & \quad \theta(0) = 0 \\
\text{fixed flux BCs:} & \quad \theta'(0) = 0 \\
\text{general thermal BCs:} & \quad \theta(0) - \eta \theta'(0) = 0
\end{aligned}
\]

The other boundary conditions are as follows:

\[
\begin{aligned}
(\bar{u}, u, Dw)_{z=0} = 0; & \quad \text{boundary conditions at } z = 0 \\
(\bar{u}, D^2\bar{u}, Dw, D\theta)_{z=\frac{1}{2}} = 0; & \quad \text{symmetry conditions} \\
[D^j \bar{u}]_\delta = 0 & \text{for } j = 0, 1, 2; \\
[D^j w]_\delta = 0 & \text{for } j = 0, 1; \\
[D^j \theta]_\delta = 0 & \text{for } j = 0, 1;
\end{aligned}
\]

where we used the notation $[f]_z = f(z^+) - f(z^-)$ to indicate the jump in a function across the value $z$.

Due to the relation $\bar{u} = -Dw$, some of the above conditions are the same:

\[
\begin{aligned}
\bar{u}|_{z=0} &= Dw|_{z=0} = 0, \\
\bar{u}|_{z=\frac{1}{2}} &= Dw|_{z=\frac{1}{2}} = 0, \\
[D\bar{u}]_\delta &= [Dw]_\delta = 0.
\end{aligned}
\]

Therefore, there are 12 boundary conditions. Now will impose those 12 boundary conditions to construct the coefficient matrix. We will do that for solutions in both exponential form and hyperbolic form, because we will need both of them later.

7.4 Constructing the Coefficient Matrix

We will construct the coefficient matrices in both exponential form and hyperbolic form.
7.4.1 Exponential Matrix

We impose those 12 boundary conditions on the solution of exponential form:

1. \( u(0) = 0 : p_1 A_1 - p_1 A_2 + p_2 A_3 - p_2 A_4 + p_3 A_5 - p_3 A_6 = 0. \)
2. \( w(0) = 0 : A_1 + A_2 + A_3 + A_4 + A_5 + A_6 = 0. \)
3. *fixed temperature* \[ \theta(0) = 0 : \]
   \[
   (1 - i\sqrt{3}) A_1 + (1 - i\sqrt{3}) A_2 + (1 + i\sqrt{3}) A_3 + (1 + i\sqrt{3}) A_4 - 2A_5 - 2A_6 = 0.
   \]
4. *fixed flux* \[ \theta'(0) = 0 : \]
   \[
   (1 - i\sqrt{3}) p_1 A_1 - (1 - i\sqrt{3}) p_2 A_2 + (1 + i\sqrt{3}) p_2 A_3 - (1 + i\sqrt{3}) p_2 A_4 - 2p_3 A_5 + 2p_3 A_6 = 0.
   \]
5. *general thermal BCs* \[ \theta(0) = 0 : \]
   \[
   (1 - i\sqrt{3})(1 - \eta p_1) A_1 + (1 - i\sqrt{3})(1 + \eta p_1) A_2 + (1 + i\sqrt{3})(1 - \eta p_2) A_3 + (1 + i\sqrt{3})(1 + \eta p_2) A_4 - 2(1 - \eta p_3) A_5 - 2(1 + \eta p_3) A_6 = 0.
   \]
6. \( u(\frac{1}{2}) = 0 : \)
   \[
   k e^B_1 + (1 + \frac{k}{2})e^B_2 - ke^{-\frac{k}{2}} B_3 + (1 - \frac{k}{2})e^{-\frac{k}{2}} B_4 = 0.
   \]
7. \( u''(\frac{1}{2}) = 0 : \)
   \[
   ke^B_1 + (3 + \frac{k}{2})e^B_2 - ke^{-\frac{k}{2}} B_3 + (3 - \frac{k}{2})e^{-\frac{k}{2}} B_4 = 0.
   \]
8. \( \theta'(\frac{1}{2}) = 0 : \)
   \[
   e^B_5 - e^{-\frac{k}{2}} B_6 = 0.
   \]
9. \[ [u]_\delta = 0 : \]
   \[
   [A_1 p_1 e^{p_1 \delta} - A_2 p_1 e^{-p_1 \delta} + A_3 p_2 e^{p_2 \delta} - A_4 p_2 e^{-p_2 \delta} + A_5 p_3 e^{p_3 \delta} - A_6 p_3 e^{-p_3 \delta}] - [B_1 k e^{k \delta} + B_2 (1 + k \delta) e^{k \delta} - B_3 k e^{-k \delta} + B_4 (1 - k \delta) e^{-k \delta} = 0.\]
10. \[ [D]_\delta = 0 : \]
   \[
   [A_1 p_1^2 e^{p_1 \delta} + A_2 p_1^2 e^{-p_1 \delta} + A_3 p_2^2 e^{p_2 \delta} + A_4 p_2^2 e^{-p_2 \delta} + A_5 p_3^2 e^{p_3 \delta} + A_6 p_3^2 e^{-p_3 \delta}] - [B_1 k^2 e^{k \delta} + B_2 k^2 (2 + k \delta) e^{k \delta} - B_3 k^2 e^{-k \delta} + B_4 k^2 (2 - k \delta) e^{-k \delta} = 0.\]
11. \[ [D^2 u]_\delta = 0 : \]
   \[
   [A_1 p_1^3 e^{p_1 \delta} + A_2 p_1^3 e^{-p_1 \delta} + A_3 p_2^3 e^{p_2 \delta} + A_4 p_2^3 e^{-p_2 \delta} + A_5 p_3^3 e^{p_3 \delta} + A_6 p_3^3 e^{-p_3 \delta}] - [B_1 k^3 e^{k \delta} + B_2 k^3 (3 + k \delta) e^{k \delta} - B_3 k^3 e^{-k \delta} + B_4 k^3 (3 - k \delta) e^{-k \delta} = 0.\]
12. \[ [w]_\delta = 0 : \]
   \[
   [A_1 e^{p_1 \delta} + A_2 e^{-p_1 \delta} + A_3 e^{p_2 \delta} + A_4 e^{-p_2 \delta} + A_5 e^{p_3 \delta} + A_6 e^{-p_3 \delta}] - [B_1 k e^{k \delta} + B_2 k e^{k \delta} + B_3 e^{-k \delta} + B_4 e^{-k \delta} = 0.\]
13. \[ [\theta]_\delta = 0 : \]
   \[
   \frac{\rho^2}{2k^2 \eta p_3} [(1 + i\sqrt{3}) (A_1 e^{p_1 \delta} + A_2 e^{-p_1 \delta}) + (1 + i\sqrt{3}) (A_3 e^{p_3 \delta} + A_4 e^{-p_3 \delta}) - 2(A_5 e^{p_3 \delta} + A_6 e^{-p_3 \delta})] + [B_5 k e^{k \delta} + B_6 e^{-k \delta} = 0.\]
14. \[ [D\theta]_\delta = 0 : \]
   \[
   \frac{\rho^2}{2k^2 \eta p_3} [(1 - i\sqrt{3}) p_1 (A_1 e^{p_1 \delta} - A_2 e^{-p_1 \delta}) + (1 + i\sqrt{3}) p_2 (A_3 e^{p_3 \delta} - A_4 e^{-p_3 \delta}) - 2p_3 (A_5 e^{p_3 \delta} - A_6 e^{-p_3 \delta})] + [B_5 k e^{k \delta} - B_6 k e^{-k \delta} = 0.\]
We can see that we have 12 unknowns $A_1, \ldots, A_6, B_1, \ldots, B_6$, and one should get a 12 by 12 matrix of coefficients. A nontrivial solution will exist only if the coefficient matrix has a vanishing determinant. This provides an implicit functional relation between $\delta$, $k$ and $R$. To obtain a profile $\tau_\delta(z)$ for which $Q[u, \theta] \geq 0$ for all $u$, $\theta$, our choice of $\delta$ must satisfy the spectral constraint for all $k$. This uniformity in $k$ is achieved by minimizing $\delta(k, R)$ as a function of $k$ for each $R$. In this way, one obtains the desired relation between $\delta$ and $R$. We will talk about the details of the algorithm later.

7.4.2 Hyperbolic Matrix

For convenience, we let $\zeta = \delta - \frac{1}{2}$. Then, we impose those 12 boundary conditions:

1. $\bar{u}(0) = 0 : p_1 A_2 + p_2 A_4 + p_3 A_6 = 0$.
2. $u(0) = 0 : A_1 + A_3 + A_5 = 0$.

3. fixed temperature $[\theta(0) = 0]$ :
   
   $(1 - i\sqrt{3}) A_1 + (1 + i\sqrt{3}) A_3 - 2 A_5 = 0$.

fixed flux $[\theta'(0) = 0]$ :
   
   $(1 - i\sqrt{3}) p_1 A_2 + (1 + i\sqrt{3}) p_2 A_4 - 2 p_3 A_6 = 0$.

general thermal BCs $[\theta(0) - \eta \theta'(0) = 0] :
   
   (1 - i\sqrt{3}) A_1 - \eta (1 - i\sqrt{3}) p_1 A_2 + (1 + i\sqrt{3}) A_3 - \eta (1 + i\sqrt{3}) p_2 A_4 - 2 A_5 + 2 \eta p_3 A_6 = 0$.

4. $\bar{u}'(\frac{1}{2}) = 0 : k B_2 + B_3 = 0$.
5. $\bar{u}''(\frac{1}{2}) = 0 : k B_2 + 3 B_3 = 0$.

Note: From the above two equations, we can see that $B_2$ and $B_3$ are identically zero.

6. $\theta'(\frac{1}{2}) = 0 : B_6 = 0$.

7. $[\bar{u}]_\delta = 0$ :
   
   $[A_1 p_1 \sinh(p_1) + A_2 p_1 \cosh(p_1) + A_3 p_2 \sinh(p_2) + A_4 p_2 \cosh(p_2) + A_5 p_3 \sinh(p_3) + A_6 p_3 \cosh(p_3)] - [B_1 k \sinh(k) + B_4 (\sinh(k) + k \cosh(k))] = 0$.

8. $[D \bar{u}]_\delta = 0$ :
   
   $[A_1 p_1^2 \cosh(p_1) + A_2 p_1^2 \sinh(p_1) + A_3 p_2^2 \cosh(p_2) + A_4 p_2^2 \sinh(p_2) + A_5 p_3^2 \cosh(p_3) + A_6 p_3^2 \sinh(p_3)] - [B_1 k^2 \sinh(k) + B_4 (2 k \cosh(k) + k^2 \cosh(k))] = 0$.

9. $[D^2 \bar{u}]_\delta = 0$ :
   
   $[A_1 p_1^3 \sinh(p_1) + A_2 p_1^3 \cosh(p_1) + A_3 p_2^3 \sinh(p_2) + A_4 p_2^3 \cosh(p_2) + A_5 p_3^3 \sinh(p_3) + A_6 p_3^3 \cosh(p_3)] - [B_1 k^3 \sinh(k) + B_4 (3 k^2 \sinh(k) + k^3 \cosh(k))] = 0$.

10. $[u]_\delta = 0$ :
   
   $[A_1 \cosh(p_1) + A_2 \sinh(p_1) + A_3 \cosh(p_2) + A_4 \sinh(p_2) + A_5 \cosh(p_3) + A_6 \sinh(p_3)] -$
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From the conditions 4, 5 and 6, we can see that $B_2$, $B_3$ and $B_6$ are identically zero. Therefore, there are essentially 9 unknowns, and one should get a 9 by 9 matrix. This reduction is due to the utility of the symmetry of hyperbolic functions $\sinh(k\zeta)$ and $\cosh(k\zeta)$. The algorithm is the same as using the exponential matrix.

Now, we will investigate how to get an numerical upper bound for both fixed temperature BCs and fixed flux BCs.

In order to get an asymptotic relation of $Nu \sim Ra^p$, we need to compute a bound for asymptotically large Rayleigh numbers. However, in our experience the determinant of the matrix gives numerical overflow (using double precision arithmetic in Matlab) for large $Reff$. Without performing any of the rescalings that we will talk about later, we can only do the calculation up to $Reff = 10^{6.0}$ for the fixed temperature case, and $Reff = 10^{13.4}$ for the fixed flux case, in Matlab. Note that these two limits to the numerics are the same for the Hyperbolic Matrix and Exponential Matrix form of equations.

One way of solving this problem is to use multiple-precision arithmetic, as implemented by Plasting (2004). He was able to attain $Ra = 10^{35}$ using this method in the infinite Prandtl number convection problem (which is numerically more subtle than our problem of finite Prandtl number convection).

However, for our Rayleigh Bénard convection flow, we have been able to make considerable progress for larger $Reff$ just by carefully rescaling the coefficient matrix. Using this method, we can push the calculation up to a very large Rayleigh number in Matlab without using multiple-precision arithmetic.


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7.5 Numerical Results - Fixed Temperature BCs

The following algorithm is used to get the optimized upper bounds for the case of fixed temperature BCs ($\eta = 0; \theta(0) = 0$).

7.5.1 Rescaled matrix

Our goal is to find the approximate scaling of $Nu \sim Ra^p$. However, when $Ra$ becomes very large ($Ra_{\text{eff}} > 10^8$), the entries of the matrix become very large, such that the determinant blows up in double precision as used by Matlab. In this case, we have to rescale the matrix in order to push the calculation further for large $Ra$.

After the initial calculation for $Ra_{\text{eff}} \leq 10^8$, we found that $k_c \sim Ra_{\text{eff}}^{0.5}$ and $\delta_c \sim Ra_{\text{eff}}^{-0.5}$. Thus we estimate

$$k_c \sim Ra_{\text{eff}}^{0.5} \text{ and } \delta_c \sim Ra_{\text{eff}}^{-0.5} \implies \gamma = \frac{1}{2\delta} \sim Ra_{\text{eff}}^{0.5}$$

$$\implies \rho = (k^2\gamma^2 Ra_{\text{eff}})^{\frac{1}{2}} \sim Ra_{\text{eff}}$$

$$\implies p_i \sim (k^2 - \rho)^{\frac{1}{2}} \sim Ra_{\text{eff}}^{0.5}$$

$$\implies p_i \delta_c \sim O(1)$$

$$\implies \sinh(p_i \delta_c) \text{ and } \cosh(p_i \delta_c) \sim O(1),$$

and

$$k_c \sim Ra_{\text{eff}}^{0.5} \text{ and } \delta_c \sim Ra_{\text{eff}}^{-0.5} \implies k_c \delta_c \sim O(1)$$

$$\implies k_c \zeta = k_c (\delta_c - \frac{1}{2}) = k_c \delta_c - \frac{1}{2} k_c \sim -Ra_{\text{eff}}^{0.5}.$$ 

Rescale the Hyperbolic Matrix

If we investigate the hyperbolic matrix, we can see that the possible large entries are $\sinh(p_i \delta)$, $\cosh(p_i \delta)$, $\sinh(k \zeta)$ and $\cosh(k \zeta)$. If we always optimize over the correct interval, the entries involving $\sinh(p_i \delta)$ and $\cosh(p_i \delta)$ will never blow up. Thus, we just need to rescale $\sinh(k \zeta)$ and $\cosh(k \zeta)$. However, we should not compute $\sinh(k \zeta)$ and $\cosh(k \zeta)$ and then rescale them, because those numbers will become NaN in Matlab and therefore cannot be rescaled.
The correct method is to rescale those entries "in advance" by "redefining" the functions \( \sinh(k\zeta) \) and \( \cosh(k\zeta) \) we use. We can do that due to the special structure of the matrix shown in Figure 7.1. Only the entries inside the rectangular area contain \( \sinh(k\zeta) \) or \( \cosh(k\zeta) \). Because \( k\zeta \) will be a very large negative number \((-R^{0.5})\) as shown above, one way to avoid numerical overflow is to define variables '\( \sinh k\zeta \)' and '\( \cosh k\zeta \)' as following:

\[
\sinh k\zeta = \frac{1}{2}(e^{2k\zeta} - 1), \\
\cosh k\zeta = \frac{1}{2}(e^{2k\zeta} + 1).
\]

We use those two new variables '\( \sinh k\zeta \)' and '\( \cosh k\zeta \)' in place of the hyperbolic functions \( \sinh(k\zeta) \) and \( \cosh(k\zeta) \). This is *mathematically equivalent to* multiplying the last three columns by \( e^{k\zeta} \). The difference is that we never actually compute \( \sinh(k\zeta) \) and \( \cosh(k\zeta) \), which will blow up for large \( Ra \).

Also note that, we should rescale the rows having \( p^n_i \) or \( k^n \) \((n = 1, 2, 3)\) as the common factors; and also rescale the number \( \frac{\rho^2}{k^2\gamma R_{\text{eff}}} \sim R_{\text{eff}}^{0.5} \) for the last two boundary conditions.
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Rescale the Exponential Matrix

For the exponential matrix, the possible large entries are $e^{\pm p_\delta}$ and $e^{\pm k\delta}$. If we always optimize over the correct interval, both $p_\delta$ and $k\delta$ are $O(1)$ and those entries will never blow up. We do not need to rescale any columns (or equivalently, redefine functions) for the Exponential Matrix.

Therefore, we just need to rescale the rows having $p_\delta$ or $k^n$ ($n = 1, 2, 3$) as the common factors; and also rescale the number $\frac{p_\delta^2}{k^{2n}R_{\text{eff}}}$ $\sim R_{\text{eff}}^{-0.5}$ for the last two boundary conditions.

After this rescaling, we can do the calculation up to $R_{\text{eff}} = 10^{36}$ using either the Hyperbolic Matrix or Exponential Matrix! For $R_{\text{eff}} > 10^{36}$, the determinant of our coefficient matrix no longer appears to be a smooth function of $\delta$ due to numerical error. Therefore, the calculation breaks down. Note that both matrices yield the same bounds. The Exponential Matrix yields a more accurate eigenfunction around $\delta_c$; and the Hyperbolic Matrix is good to recover the eigenfunction around $z = \frac{1}{2}$. We care more about the accuracy at $\delta_c$, because all bounds depend on $\delta_c$. Therefore, we will use the Exponential Matrix for the calculation, although both forms of the coefficient matrix yield the same bound.

The coefficient matrix is a function of $k$, $R_{\text{eff}}$ and $\delta$, and we denote it by $M_0(\delta, k, R_{\text{eff}}) = M_0(\delta)$.  

7.5.2 Critical $\delta$ and $k$ values

We fix $k$ and $R_{\text{eff}} = \frac{bR}{\delta^{2.5}}$, graph the determinant of $M_0(\delta, k, R_{\text{eff}})$ versus $\delta$ and find the minimum $\delta$ such that the determinant equals zero; label this $\delta_0$. Thus, we can find a function $\delta_0(k)$ for the given $R_{\text{eff}}$.

We plot the real and imaginary parts of the determinant as a function of $\delta$, for $k = 14$ and $R_{\text{eff}} = 10^5$. From Figure 7.2, we can see that the real part of the determinant is essentially zero to our numerical precision. Therefore, we just need to find the zero of imaginary part.

Note that there might be many zeros for the $\text{det}(M_0(\delta))$. We need to compute the minimum one. In order to do that, we first scan over all $\delta$ when $Ra < 10^5$, for which the minimum zero $\delta_0$ is relatively big, so it is not hard to find it. After the scan, we can get the approximate scalings of the critical $\delta \sim R_{\text{eff}}$ and the critical $k \sim R_{\text{eff}}$. This gives
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Figure 7.2: Fixed temperature boundary conditions: real and imaginary parts of det(Mo(δ)), for k = 14 and Reff = 10^5. The real part of det(Mo(δ)) is always zero.

us the approximate interval within which to search. Therefore, we can always optimize over the correct interval to get the smallest zero we want. We cannot simply scan over δ values for large Rayleigh numbers, because we would have to use extremely small step sizes in δ and that would make the scan extremely slow.

The next step is to minimize δ0 over all k to get δc(Reff) and kc. For a given Reff, the picture of δ0(k) always looks like a parabola concave up. Figure 7.3 shows δ0 as a function of k for Reff = 10^5.

We use the command 'fminbnd' in Matlab to minimize δ0 = δ0(k, Reff) over all k, and label this δc = δc(Reff). Then δc corresponds to the largest δ for which the condition Q[δ, v] ≥ 0 holds, and hence we get the optimal numerical upper bound

\[ Nu \leq 1 - b + \frac{b}{2\delta_c(Reff)} = 1 - b + \frac{b}{2\delta_c(\frac{\text{Ra}}{b-1})}, \]  

(7.24)

for the piecewise linear background profiles.

7.5.3 Upper bound for Nu(Ra)

Having found δc(Reff), we now minimize Nu over all b > 1 to get bc and an upper bound for Nu(Ra).

In order to guarantee that (6.1) is positive definite, we need to choose b > 1. Therefore, we minimize Nu from (7.24) over all b > 1 to get the lowest upper bound of Nu.
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Figure 7.3: Fixed temperature boundary conditions: \( \delta_0(k) \), for \( R_{\text{eff}} = 10^5 \).

Figure 7.4: Fixed temperature boundary conditions: \( Nu < 0.045 \ Ra^{0.5} \), where the numerical exponent is 0.5+2e-13. The vertical line segment indicates that we can recover the eigenfunctions successfully up to that Rayleigh number (we will discuss this in section 7.5.5). We will put a corresponding small line segment in all the figures below.

Figure 7.5: Fixed temperature boundary conditions: \( Nu(Ra) \) when \( Ra \) is close to 1707.76.
as a function of $R (= Ra)$ for piecewise linear profiles, as shown in Figure 7.4. We can see that $Nu$ scales as
\[ Nu \leq 0.045 \, Ra^{0.5}. \] (7.25)

The 0.5 exponent agrees with our analytical result (6.24)
\[ Nu \leq -\frac{1}{2} + 0.230 \, Ra^{0.5}, \]
but the prefactor is much smaller.

We can also plot the function $Nu(Ra)$ when $Ra$ is very close to 1707.76. From Figure 7.5, we can see that $Nu(Ra)$ bifurcates at the right place with $b \rightarrow \infty$ (so $Reff \rightarrow Ra$). This verifies our stability analysis result from Section 4.3.1.

### 7.5.4 Other interesting scaling results

We also obtain some other interesting scalings:
- $Nu \leq 0.026 \, Reff^{\frac{1}{2}}$ in Figure 7.6;
  - The $\frac{1}{2}$ exponent agrees with our analytical result (6.23) obtained using Cauchy-Schwarz estimates: $Nu \leq -\frac{1}{2} + \frac{3\sqrt{2}}{32} \, Reff^{\frac{1}{2}}$.
- $\delta_c = 16.6525 \, Ra^{-\frac{1}{2}}$ in Figure 7.7;
- $\delta_c = 28.8430 \, Reff^{-\frac{1}{2}}$ in Figure 7.8;
  - The $-\frac{1}{2}$ exponent agrees with our analytical result (6.20): $\delta = 4\sqrt{2} \, Reff^{-\frac{1}{2}}$.
- $k_c = 0.0722 \, Ra^{\frac{1}{2}}$ in Figure 7.9;
- $k_c = 0.0417 \, Reff^{\frac{1}{2}}$ in Figure 7.10.

In summary, all our numerical scalings agree with our analytical results, but have a much smaller prefactor.
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Figure 7.6: Fixed temperature boundary conditions: $Nu < 0.026 \ R_{eff}^{0.5}$, where the numerical exponent is $0.5-1e-09$.

Figure 7.7: Fixed temperature boundary conditions: $\delta_c = 16.6525 \ Ra^{-0.5}$, where the numerical exponent is $-0.5-8e-10$.

Figure 7.8: Fixed temperature boundary conditions: $\delta_c = 28.8430 \ R_{eff}^{-0.5}$, where the numerical exponent is $-0.5-2e-15$. 
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Figure 7.9: Fixed temperature boundary conditions: \( k_c = 0.0722 \, Ra^{0.5} \), where the numerical exponent is 0.5 + 5e-10.

Figure 7.10: Fixed temperature boundary conditions: \( k_c = 0.0417 \, Ra^{0.5} \), where the numerical exponent is 0.5 - 4e-10.

Figure 7.11: Fixed temperature boundary conditions: \( b_c(Ra) = 1.5 + 16.841 \, Ra^{-0.50039} \). When \( Ra > 10^{15} \), \( b_c \) is very close to 1.5 and some values of \( b_c - 1.5 \) become negative due to numerical errors, so that the log-log graph is not a straight line any more.

Figure 7.12: Fixed temperature boundary conditions: \( b_c(R_{\text{eff}}) = 1.5 + 29.173 \, R_{\text{eff}}^{-0.50038} \).
7.5.5 Eigenfunctions

As a check on the correctness of the calculations, we can plot the eigenfunctions to verify whether the boundary conditions are satisfied, and whether the eigenfunctions are smooth at $\delta_c$.

For given $R_{\text{eff}}$, we compute the critical values $k_c$ and $\delta_c$ first, then compute the eigenfunctions corresponding to the zero eigenvalue of the matrix. Because we rescaled the matrix, the eigenfunctions ($A_1$ to $B_6$) need to be rescaled back. Hence we can recover the solutions $\tilde{u}(z)$, $w(z)$ and $\theta(z)$.

![Graphs showing eigenfunctions for $R_{\text{eff}} = 10^{20}$](image)

Figure 7.13: Fixed temperature boundary conditions: Eigenfunctions for $R_{\text{eff}} = 10^{20}$. The vertical line segments indicate the location of $z = \delta_c$. Because the boundary layer is very thin for large $R_{\text{eff}}$, here we only plot the range $[0, \delta]$ in order to see the boundary layer clearly.

For example, for the fixed $R_{\text{eff}} = 10^{20}$, we get $k_c = 416579356.1616$ and $\delta_c = 2.8843 \times 10^{-9}$. We substitute these into the $12 \times 12$ matrix $M_0(\delta_c, k_c, R_{\text{eff}})$ of the exponential
form to compute its eigenfunction corresponding to the zero eigenvalue. (Note that the exponential matrix is better than the hyperbolic matrix in order to get the correct $\delta_c$; hyperbolic matrix is better to guarantee the symmetry at $z = \frac{1}{2}$. In order to get the correct bounds, we care more about the accuracy of $\delta$ than the symmetry at $z = \frac{1}{2}$. That is why we should choose the exponential matrix.) Finally we can recover the solutions (7.11) and (7.14) to get Figure 7.13. The vertical line is $z = \delta_c$.

We can see that the boundary layer is very thin for large $R_{\text{eff}}$, but the eigenfunctions are still smooth at $\delta$ and all boundary conditions at $z = 0$ are satisfied. This means the eigenfunctions could be successfully recovered. It turns out that we can recover the eigenfunctions for $R_{\text{eff}}$ values as large as $R_{\text{eff}} = 10^{28}$. For $R_{\text{eff}} > 10^{28}$, the eigenfunctions are not smooth any more due to numerical error. The jump at $\delta$ indicates that the eigenfunctions cannot be correctly recovered. Note that in all our graphs of computed scalings, we have put a small vertical line segment at $R_{\text{eff}} = 10^{28}$; for $R_{\text{eff}} \leq 10^{28}$ and its corresponding $Ra$, we are confident that the scaling must be correct.

As another example, we want to plot the eigenfunctions for $R_{\text{eff}} = 10^6$ in order to see both the boundary layer and the symmetry at $z = \frac{1}{2}$. We can see from Figure 7.14 that the eigenfunctions are smooth at $\delta$ and all boundary conditions at $z = 0$ and $\frac{1}{2}$ are satisfied.

Finally, we can plot the eigenfunctions using the exponential matrix when $R_{\text{eff}} = 1708$, which is slightly above the critical Rayleigh number for the conduction state 1707.76. For this Rayleigh number, we get $k_c$ very close to the critical wave mode 3.1163, and $\delta_c = 0.49997$ very close to 0.5. This means that the conduction solution is just becoming unstable, and this is exactly as we predicted from the stability analysis. We can see from Figure 7.15 that all the boundary conditions at $z = 0$ are satisfied. Also we can see that both $w$ and $\theta$ are even at $z = \frac{1}{2}$; and $\bar{u}$ is odd at $z = \frac{1}{2}$. 
Figure 7.14: Fixed temperature boundary conditions: Eigenfunctions for $R_{\text{eff}} = 10^6$. The vertical line segments indicate the location of $z = \delta_c$. 

\[ R_{\text{eff}} = 1 \times 10^6, \ k_c = 41.6579, \ \delta_c = 0.028843 \]
Figure 7.15: Fixed temperature boundary conditions: Eigenfunctions for $R_{\text{eff}} = 1708$, near the critical Rayleigh number $Ra_c = 1707.76$. The $\delta_c$ is very close to 0.5.
7.6 Numerical Results - Fixed Flux BCs

For the fixed flux case, the numerical approach is exactly the same as the fixed temperature case, except that $\gamma = 1$ and the boundary condition for $\theta$ at $z = 0$ should be $D\theta|_{z=0} = 0$. The algorithm is very similar to the fixed temperature case.

7.6.1 Rescaled matrix

As for the fixed temperature case, we still need to rescale the matrix when $Ra$ is very large ($R_{\text{eff}} > 10^{13.4}$). After the initial calculation for small $R_{\text{eff}} \leq 10^{13.4}$, we found that $k_c \sim R_{\text{eff}}^{0.25}$ and $\delta_c \sim R_{\text{eff}}^{-0.25}$; we also know $\gamma = 1$. Thus we get:

$$k_c \sim R_{\text{eff}}^{0.25} \quad \text{and} \quad \delta_c \sim R_{\text{eff}}^{-0.25} \quad \Rightarrow \quad \rho = (k^2 \gamma^2 R_{\text{eff}})^{\frac{1}{2}} \sim R_{\text{eff}}^{0.5}$$

$$\Rightarrow \quad p_i \sim (k^2 - \rho)^{\frac{1}{2}} \sim R_{\text{eff}}^{0.25}$$

$$\Rightarrow \quad p_i \delta_c \sim O(1)$$

$$\Rightarrow \quad \sinh(p_i \delta_c) \quad \text{and} \quad \cosh(p_i \delta_c) \sim O(1),$$

and

$$k_c \sim R_{\text{eff}}^{0.25} \quad \text{and} \quad \delta_c \sim R_{\text{eff}}^{-0.25}, \quad \Rightarrow \quad k_c \delta_c \sim O(1),$$

$$\Rightarrow \quad k_c \zeta = k_c (\delta_c - \frac{1}{2}) = k_c \delta_c - \frac{1}{2} k_c \sim -R_{\text{eff}}^{0.25}.$$ 

Rescale the Hyperbolic Matrix

As for the fixed temperature case, we still need to rescale the same entries in advance (inside the rectangular area in Figure 7.1). The only difference is that now $k_c \zeta \sim -R_{\text{eff}}^{0.25}$. As before, we define two new variables ‘$\sinh k\zeta$’ and ‘$\cosh k\zeta$’ as following:

$$\sinh k\zeta = \frac{1}{2} (e^{2k\zeta} - 1), \quad (7.26)$$

$$\cosh k\zeta = \frac{1}{2} (e^{2k\zeta} + 1). \quad (7.27)$$

We use those two variables ‘$\sinh k\zeta$’ and ‘$\cosh k\zeta$’ in place of the hyperbolic functions $\sinh(k\zeta)$ and $\cosh(k\zeta)$. Therefore those entries will never lead to numerical overflow for large $Ra$, and our calculation can be pushed further.
We also note that we should rescale the rows having $p_i^a$ or $k^n \ (n = 1, 2, 3)$ as the common factors; and rescale the number $\frac{\alpha^2}{k^2 R_{\text{eff}}} \sim R_{\text{eff}}^{-0.5}$ for the last two boundary conditions.

Rescale the Exponential Matrix

As for the fixed temperature case, we do not need to rescale any columns for Exponential Matrix. We just need to rescale the rows having $p_i^a$ or $k^n \ (n = 1, 2, 3)$ as the common factors; and also rescale the number $\frac{\alpha^2}{k^2 R_{\text{eff}}} \sim R_{\text{eff}}^{-0.5}$ for the last two boundary conditions.

After this rescaling to improve the conditioning of our coefficient matrices, we can do the calculation up to $R_{\text{eff}} = 10^{61}$ (much higher than for the fixed temperature case) using either the Hyperbolic Matrix or the Exponential Matrix! We denote the coefficient matrix by $M_{\infty}(\delta) = M_{\infty}(\delta, k, R_{\text{eff}})$. For $R_{\text{eff}} > 10^{61}$, $\det(M_{\infty}(\delta))$ is no longer a smooth function of $\delta$ due to numerical error, and the calculation breaks down.

7.6.2 Critical $\delta$ and $k$ values

For fixed $k$ and $R_{\text{eff}} = \frac{5R}{b - 1}$, we graph the determinant versus $\delta$ and find the minimum $\delta$ such that $\det(M_{\infty}(\delta))$ equals zero; we label this $\delta_0$.

As in the fixed temperature case, we plot the real and imaginary parts of the determinant as a function of $\delta$, for $k = 20$ and $R_{\text{eff}} = 10^8$. From Figure 7.16, we can see that the real part of the determinant is essentially zero, which is the same property that holds for the fixed temperature case. Therefore we just need to find the zero of the imaginary part.

The next step is to minimize $\delta_0$ over all $k$ to get $\delta_c(R_{\text{eff}})$ and $k_c$. Figure 7.17 shows $\delta_0$ as a function of $k$ for $R_{\text{eff}} = 10^{20}$. We minimize $\delta_0$ over all $k$, and label this $\delta_c = \delta_c(R_{\text{eff}})$. Then $\delta_c$ corresponds to the largest $\delta$ for which the condition $Q[\theta, v] \geq 0$ holds, and hence we get an lower bound on $\Delta T$ of

$$
\Delta T \geq 1 - b + 2b \delta_c(R_{\text{eff}}) = 1 - b + 2b \delta_c \left( \frac{bR}{b - 1} \right) .
$$

(7.28)
Figure 7.16: Fixed flux boundary conditions: real and imaginary parts of $\text{det}(\delta)$, for $k = 20$ and $R_{\text{eff}} = 10^8$.

Figure 7.17: Fixed flux boundary conditions: $\delta_0(k)$, for $R_{\text{eff}} = 10^{20}$.
7.6.3 Lower bound for $\Delta T$ and upper bound for $Nu(Ra)$

Maximizing $\Delta T$ over all $b > 1$, one gets the largest lower bound of $\Delta T$ as a function of $R$ for piecewise linear profiles, as in Figure 7.19.

Using the relations $Nu = \frac{1}{\Delta T}$ and $Ra = R\Delta T$ one can finally get the upper-bound relation between $Nu$ and $Ra$. From Figure 7.18, we can see that $Nu$ scales as

$$Nu \leq 0.078 Ra^{0.5}. \tag{7.29}$$

The exponent 0.5 agrees with our analytical result (6.30)

$$Nu \leq 0.273 Ra^{0.5},$$

but with a much smaller prefactor.

![Figure 7.18: Fixed flux boundary conditions: $Nu \leq 0.078 Ra^{0.5}$, where the numerical exponent is 0.5+4e-6.](image1)

![Figure 7.19: Fixed flux boundary conditions: $Nu \leq 0.183 R^{\frac{1}{3}}$, where the numerical exponent is 0.5+2e-6.](image2)

This scaling is also bigger than the numerical upper bound for the fixed temperature case (see Figure 7.4)

$$Nu \leq 0.045 Ra^{0.5}.$$  

We can also plot the function $Nu(R)$ when $R$ is very close to 720, the value at which the conduction state becomes unstable. From the Figure 7.20, we can see that $Nu(R)$ bifurcates at the right place. This verifies our stability analysis result from Section 4.3.2.
7.6.4 Other interesting scaling results

We also obtained some other interesting scaling results:

- $\eta R^{-\frac{1}{3}}$ in Figure 7.19;
  
  This $\frac{1}{3}$ exponent agrees with our analytical result (6.31): $\eta R^{-\frac{1}{3}}$.
- $\eta R^{-\frac{1}{4}}$ in Figure 7.21;
  
  This $\frac{1}{4}$ exponent agrees with our analytical result (6.33): $\eta R^{-\frac{1}{4}}$.
- $b_c - 1 = 4.083 Ra^{-\frac{1}{3}}$ in Figure 7.22;
- $b_c - 1 = 1.750 R^{-\frac{1}{3}}$ in Figure 7.23;
- $b_c - 1 = 1.522 R^{-\frac{1}{4}}$ in Figure 7.24;
- $\delta_c = 8.441 Ra^{-\frac{1}{3}}$ in Figure 7.25;
- $\delta_c = 3.610 R^{-\frac{1}{3}}$ in Figure 7.26;
  
  This $\frac{1}{3}$ exponent agrees with our analytical result (6.32): $\delta = (4)^{\frac{1}{3}} R^{-\frac{1}{3}}$.
- $\delta_c = 3.193 R^{-\frac{1}{3}}$ in Figure 7.27;
  
  This $\frac{1}{3}$ exponent agrees with our analytical result (6.25): $\delta = 8^{\frac{1}{3}} R^{-\frac{1}{3}}$.
- $k_c = 0.073 Ra^{\frac{1}{3}}$ in Figure 7.28;
- $k_c = 0.171 R^{\frac{1}{3}}$ in Figure 7.29;
• \( k_c = 0.196 R_{\text{eff}}^{\frac{1}{4}} \) in Figure 7.30.
• \( b_c = 0.9977 + 0.4861 \delta_c \) in Figure 7.31.

All our numerical scalings agree with our analytical results, but have improved prefactors, as expected.
Figure 7.25: Fixed flux boundary conditions: $\delta = 8.441 \, Ra^{-0.4996}$.

Figure 7.26: Fixed flux boundary conditions: $\delta = 3.610 \, R^{-0.3331}$.

Figure 7.27: Fixed flux boundary conditions: $\delta = 3.139 \, R_{\text{eff}}^{-0.25000000008}$.  

Figure 7.28: Fixed flux boundary conditions: $k = 0.073 \, Ra^{0.4996}$. 
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Figure 7.29: Fixed flux boundary conditions: $k_c = 0.171 R^{0.3331}$.

Figure 7.30: Fixed flux boundary conditions: $k_c = 0.196 R_{\text{eff}}^{0.25000003}$.

Figure 7.31: Fixed flux boundary conditions: $b_c - 1 = 0.4861 \delta_c$. 
7.6.5 Eigenfunctions

As in the fixed temperature case, for given $R_{\text{eff}}$, we first compute the critical values $k_c$ and $\delta_c$, then compute the eigenfunction corresponding to the zero eigenvalue of the matrix. Because we rescaled the matrix, the eigenfunctions ($A_1$ to $B_6$) need to be rescaled back. Hence we can recover the solutions $\bar{u}(z)$, $w(z)$ and $\theta(z)$.

For example, for fixed $R_{\text{eff}} = 10^{20}$, we get $k_c = 19625.9222$ and $\delta_c = 3.1392 \times 10^{-5}$. We substitute these into the $12 \times 12$ matrix $M_{\infty}(\delta_c, k_c, R_{\text{eff}})$ of the exponential form to compute its eigenfunction corresponding to the zero eigenvalue. Finally we can recover the solutions (7.11) and (7.14) to get Figure 7.32. The vertical line indicates the location of $\delta_c$. We can see that the boundary layer is very thin for large $R_{\text{eff}}$, but the eigenfunctions are still smooth and all boundary conditions at $z = 0$ are satisfied. This means the eigenfunctions could be successfully recovered. It turns out that we can recover the eigenfunctions for $R_{\text{eff}}$ as large as $R_{\text{eff}} = 10^{28}$. This number is the same as for the fixed temperature case. For $R_{\text{eff}}$ larger than $10^{28}$, the eigenfunctions are no longer smooth. Note that we have put a small vertical line segment in all the pictures, indicating the location of $R_{\text{eff}} = 10^{28}$. For $R_{\text{eff}} < 10^{28}$ and its corresponding $Ra$, we are confident that the scaling must be correct.

As another example, we plot the eigenfunctions for $R_{\text{eff}} = 10^6$ in order to see both the boundary layer and the symmetry at $z = \frac{1}{2}$. We can see from Figure 7.33 that the eigenfunctions are smooth at $\delta$ and all boundary conditions at $z = 0$ and $\frac{1}{2}$ are satisfied.

Finally, we can plot the eigenfunctions when $R_{\text{eff}} = 720.1$, which is slightly greater than the critical Rayleigh number 720. For this Rayleigh number, we get $k_c = 0.0002089$ very close to the critical wave mode 0, and $\delta_c = 0.49998$ very close to 0.5. This means that the conduction solution is just becoming unstable, and this is exactly what we predicted from the stability analysis. We can see from Figure 7.34 that all the boundary conditions at $z = 0$ are satisfied. Also we can see that both $w$ and $\theta$ are even at $z = \frac{1}{2}$, and $\bar{u}$ is odd at $z = \frac{1}{2}$. 

Figure 7.32: Fixed flux boundary conditions: Eigenfunctions for $R_{\text{eff}} = 10^{30}$. The vertical line segments indicate the location of $z = \delta_c$. Because the boundary layer is very thin, we just plot the region $[0, \delta]$ in order to see the boundary layer clearly.
Figure 7.33: Fixed flux boundary conditions: Eigenfunctions for $R_{\text{eff}} = 10^6$. The vertical line segments indicate the location of $z = \delta_c$. 
Figure 7.34: Fixed flux boundary conditions: Eigenfunctions for $R_{\text{eff}} = 720.1$. 

\[ R_{\text{eff}} = 720.1, \ k_{\xi} = 0.0002089, \ \delta_{\xi} = 0.49998 \]
7.7 Numerical Results - General Thermal BCs

The following steps are for fixed Biot number $\eta$.

7.7.1 Rescaled matrix

As in the fixed temperature and fixed flux cases, we still need to rescale the coefficient matrix, denoted by $M_\eta(\delta) = M_\eta (\delta, k, R_{\text{eff}})$, using exactly the same approach.

For small $\eta$, for which the transition between fixed temperature and fixed flux scaling happens for large $R$ (as we will see later), ideally we should rescale differently for two different regions. However, I rescale the whole region by the fixed flux scaling for convenience, and this works for all $\eta \geq 10^{-8}$.

7.7.2 Critical $\delta$ and $k$ values

For the fixed $k$ and $R_{\text{eff}} = E$, we graph the determinant versus $\delta$ and find the minimum $\delta$ such that the determinant equals zero, and label this $\delta_0 = \delta_0(k, R_{\text{eff}})$.

Unlike in the fixed temperature and fixed flux cases, the real part of $\det(M_\eta(\delta))$ for the general boundary conditions is not always zero. Therefore, instead of using ‘fzero’ to find the zero of $\text{imag}(\det(M_\eta(\delta)))$, we use ‘fminbnd’ to find the minimum of the norm($\det(M_\eta(\delta))$), and this minimum is the zero of $\det(M_\eta(\delta))$ as long as we can always optimize over the correct interval. For example, when $k = 13$, $R_{\text{eff}} = 10^5$, and $\eta = 10^{-4}$, the graph of norm($\det(M_\eta(\delta))$) is illustrated in Figure 7.35.

Next, as before we minimize $\delta_0$ over all $k$, and label this $\delta_c$. Then $\delta_c$ corresponds to the largest $\delta$ for which condition $Q[\theta, v] \geq 0$ holds, and hence

$$\beta \leq 1 + b(\gamma - 1) = 1 + \frac{b}{\eta + \delta(R_{\text{eff}})}\left(1 - \frac{2\delta(R_{\text{eff}})}{\eta + \delta(R_{\text{eff}})}\right).$$

For example, when $R_{\text{eff}} = 10^5$ and $\eta = 10^{-4}$, the graph of $\delta_0(k)$ is shown in Figure 7.36.

7.7.3 Bounds for $\beta$, $\Delta T$ and $Nu$

Minimizing $\beta$ over all $b \geq 1$, one can get the lowest upper bound of $\beta$ as a function of $R$. Note that we can not minimize $Nu$ over all $b \geq 1$. The reason is that $\Delta T$ might be negative at some values of $b$, although it is always positive at $b_c$. Therefore, $Nu = \frac{\beta}{\Delta T}$ might not be smooth, and will make the optimization much harder.
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Figure 7.35: General thermal boundary conditions: norm of \( \text{det}(M_k(b)) \), for \( k = 13 \), \( R_{\text{eff}} = 10^5 \), and \( \eta = 10^{-4} \).

Figure 7.36: General thermal boundary conditions: \( \delta_0(k) \), for \( R_{\text{eff}} = 10^5 \), and \( \eta = 10^{-4} \).

For example, if we plot \( \beta(b) \), \( \Delta T(b) \) and \( \text{Nu}(b) \) for \( R = 10^{15} \) and \( \eta = 10^{-4} \), we can see from the Figure 7.37 that \( \Delta T \) turns from positive to negative at about \( b = 1.035 \) and \( \text{Nu} \) is not smooth at that turning point. That is why we choose to optimize \( \beta(b) \) instead of \( \text{Nu}(b) \).

We next compute \( \Delta T \) by \( \Delta T = 1 + 2\eta(1 - \beta) \); then one can get an upper bound of \( \text{Nu} = \frac{\partial}{\partial \Delta T} \) as a function of \( R \) for the fixed Biot number \( \eta \). Figure 7.38 shows the bound for \( \eta = 10^{-4} \); we see that \( \text{Nu} \) scales as \( R^{1/3} \) for large \( R \). For comparison, Figure 7.39 shows \( \text{Nu}(R) \) for a smaller \( \eta = 10^{-8} \); note that the transition between fixed temperature scaling (\( \text{Nu} \sim R^{1/4} \)) and fixed flux scaling (\( \text{Nu} \sim R^{1/3} \)) occurs for higher \( R \).

Using the relation \( Ra = R\Delta T \), one can finally get the upper-bound relation between \( \text{Nu} \) and \( Ra \). Figure 7.40 shows the bound for \( \eta = 10^{-4} \), and Figure 7.41 shows the bound for a smaller \( \eta = 10^{-8} \). Our final bounds for these values of \( \eta \) are

\[
\text{Nu} \leq 0.0782 \, Ra^{1/2} \quad \text{for } \eta = 10^{-4}, \quad \text{Nu} \leq 0.0781 \, Ra^{1/2} \quad \text{for } \eta = 10^{-8}.
\] (7.30)

Note that we find a numerical exponent of \( \frac{1}{2} \), as in the fixed temperature and fixed flux cases and agreeing with our analytical bound (6.51), and also that the prefactors for different \( \eta \) values are very similar. We discuss this in Section 7.7.9 below.
Figure 7.37: General thermal boundary conditions: \( \beta(b), \Delta T(b) \) and \( Nu(b) \) for \( R = 10^{15} \) and \( \eta = 10^{-4} \).

### 7.7.4 Other interesting scaling results

We have done all calculations for several values of \( \eta \). For comparison, in Figures 7.38 to 7.61, the left one is for \( \eta = 10^{-4} \) and the right one is for \( \eta = 10^{-8} \). These figures include \( Nu(Ra), Nu(R), Nu(Reff), k_c(Ra), k_c(R), k_c(Reff), \delta_c(Ra), \delta_c(R), \delta_c(Reff), b_c(Ra), b_c(R) \) and \( b_c(Reff) \); the scaling results we obtained are indicated in the figure captions.
Figure 7.38: General thermal boundary conditions: $Nu < 3.1278 R^0.3333$ for $\eta = 10^{-4}$. The scaling before the transition has exponent 0.5.

Figure 7.39: General thermal boundary conditions: $Nu < 67.325 R^0.3333$ for $\eta = 10^{-8}$. The scaling before the transition has exponent 0.5.

Figure 7.40: General thermal boundary conditions: $Nu < 0.0782 Ra^{0.5000}$ for $\eta = 10^{-4}$.

Figure 7.41: General thermal boundary conditions: $Nu < 0.0781 Ra^{0.5000}$ for $\eta = 10^{-8}$.
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Figure 7.42: General thermal boundary conditions: $Nu < 14.69 \, R_{\text{eff}}^{0.2500}$ for $\eta = 10^{-4}$. The scaling before the transition has exponent 0.5.

Figure 7.43: General thermal boundary conditions: $Nu < 1488.49 \, R_{\text{eff}}^{0.2501}$ for $\eta = 10^{-8}$. The scaling before the transition has exponent 0.5.

Figure 7.44: General thermal boundary conditions: $k_c = 0.0738 \, Ra^{0.5001}$ for $\eta = 10^{-8}$.

Figure 7.45: General thermal boundary conditions: $k_c = 0.0731 \, Ra^{0.4999}$ for $\eta = 10^{-4}$. 
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Figure 7.46: General thermal boundary conditions: \( k_c = 2.9543 \ R^{0.3334} \) for \( \eta = 10^{-4} \). The scaling before the transition has exponent 0.5.

Figure 7.47: General thermal boundary conditions: \( k_c = 62.8978 \ R^{0.3332} \) for \( \eta = 10^{-8} \). The scaling before the transition has exponent 0.5.

Figure 7.48: General thermal boundary conditions: \( k_c = 13.8776 \ R^{0.2500} \) for \( \eta = 10^{-4} \).

Figure 7.49: General thermal boundary conditions: \( k_c = 1389.37 \ R^{0.2500} \) for \( \eta = 10^{-8} \).
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Figure 7.50: General thermal boundary conditions: $\delta_c = 8.3421 \, Ra^{-0.5001}$ for $\eta = 10^{-4}$.

Figure 7.51: General thermal boundary conditions: $\delta_c = 8.4377 \, Ra^{-0.4999}$ for $\eta = 10^{-8}$.

Figure 7.52: General thermal boundary conditions: $\delta_c = 0.2085 \, R^{-0.3334}$ for $\eta = 10^{-4}$. The scaling before the transition has exponent $-0.5$.

Figure 7.53: General thermal boundary conditions: $\delta_c = 0.0098 \, R^{-0.3332}$ for $\eta = 10^{-8}$. The scaling before the transition has exponent $-0.5$. 
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**Figure 7.54:** General thermal boundary conditions: $\delta_c = 0.0444 R_{\text{eff}}^{-0.2500}$ for $\eta = 10^{-4}$. The scaling before the transition has exponent $-0.5$.

**Figure 7.55:** General thermal boundary conditions: $\delta_c = 0.00044 R_{\text{eff}}^{-0.2500}$ for $\eta = 10^{-8}$. The scaling before the transition has exponent $-0.5$.

**Figure 7.56:** General thermal boundary conditions: $b_c = 1 + 2 \times 10^4 Ra^{-0.5003}$ for $\eta = 10^{-4}$.

**Figure 7.57:** General thermal boundary conditions: $b_c = 1 + 2 \times 10^8 Ra^{-0.4995}$ for $\eta = 10^{-8}$. 
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Figure 7.58: General thermal boundary conditions: $b_c = 1 + 486.9 \, R^{-0.3335}$ for $\eta = 10^{-4}$.

Figure 7.59: General thermal boundary conditions: $b_c = 1 + 2.4 \times 10^5 \, R^{-0.3330}$ for $\eta = 10^{-8}$.

Figure 7.60: General thermal boundary conditions: $b_c = 1 + 103.6 \, R_{\text{eff}}^{-0.2501}$ for $\eta = 10^{-4}$.

Figure 7.61: General thermal boundary conditions: $b_c = 1 + 1.1 \times 10^4 \, R_{\text{eff}}^{-0.2498}$ for $\eta = 10^{-8}$.
7.7.5 Verification of the bifurcation point $R_c$.

In Sections 4.2.2 and 4.3.3, we did the stability analysis for the general thermal BCs. Now we can actually verify that all the figures bifurcate at the right place.

For example, we found $R_c \approx 1511.28$ and $k_c \approx 2.941$ for $\eta = 0.1$ in the stability analysis; see Figures 4.3 and 4.4. If we plot $Nu(R)$, $k(R)$ and $\delta(R)$ for $R$ close to $R_c$, we can see from the Figures 7.62, 7.63 and 7.64 that they do bifurcate at the right place, which gives us confidence in our other results.

![Figure 7.62: General thermal boundary conditions: Bifurcation of $Nu(R)$ for $\eta = 0.1$.](image1)

![Figure 7.63: General thermal boundary conditions: Bifurcation of $k_c(R)$ for $\eta = 0.1$.](image2)

![Figure 7.64: General thermal boundary conditions: Bifurcation of $\delta_c(R)$ for $\eta = 0.1$.](image3)
7.7.6 Eigenfunctions

As a further check on the accuracy of our computation, for given \( R_{\text{eff}} \), we compute the critical values \( k_c \) and \( \delta_c \) first, then compute the eigenfunction corresponding to the zero eigenvalue of the matrix. Because we rescaled the matrix, the eigenfunctions (\( A_1 \) to \( B_6 \)) need to be rescaled back. Hence, we can recover the solutions \( \bar{u}(z) \), \( w(z) \) and \( \theta(z) \).

For example, for given \( \eta = 1 \) and fixed \( R_{\text{eff}} = 10^{20} \), we get \( k_c = 24036.1864 \) and \( \delta_c = 2.5632 \times 10^{-5} \). We substitute these into the \( 12 \times 12 \) matrix \( M_{\eta} \) of the exponential form to compute its eigenfunction corresponding to the zero eigenvalue. Finally we can recover the solutions (7.11) and (7.14) to get Figure 7.65. The vertical line is \( z = \delta_c \). We can see that the boundary layer is very thin for large \( R_{\text{eff}} \), but the eigenfunctions are still smooth and all boundary conditions at \( z = 0 \) are satisfied. This means the eigenfunctions could be successfully recovered. It turns out that we can recover the eigenfunctions up to \( R_{\text{eff}} = 10^{24} \) for different Biot number \( \eta \). For larger \( R_{\text{eff}} \), the eigenfunctions are not smooth anymore. We can see from Figure 7.65 that the boundary conditions for \( \bar{u} \) and \( w \) at \( z = 0 \) are satisfied. Also we can see that both \( w \) and \( \theta \) are even at \( z = \frac{1}{2} \); and \( \bar{u} \) is odd at \( z = \frac{1}{2} \).

As another example, for given \( \eta = 1 \) we plot the eigenfunctions for \( R_{\text{eff}} = 10^7 \) in order to see both the boundary layer and the symmetry at \( z = \frac{1}{2} \). We can see from Figure 7.66 that the eigenfunctions are smooth at \( \delta \) and all boundary conditions at \( z = 0 \) and \( \frac{1}{2} \) are satisfied.
Figure 7.65: General thermal boundary conditions: Eigenfunctions for $R_{eff} = 10^{20}$ and $\eta = 1$. The vertical line segments indicate the location of $z = \delta_c$. Because the boundary layer is very thin, we just plot $[0, \delta]$ in order to see the boundary layer clearly.

7.7.7 Biot number - dependence of prefactors

We can also plot the prefactors as a function of $\eta$ for $\delta_c(R)$, $\delta_c(R_{eff})$, $\delta_c(Ra)$, $b_c(R)$, $b_c(R_{eff})$, $b_c(Ra)$, $k_c(R)$, $k_c(R_{eff})$, and $k_c(Ra)$, as shown from Figures 7.67 to 7.72. It is particularly interesting that all of our numerically obtained scaling results agree with the analytical results of Sections 6.3.3 and 6.3.4.
Figure 7.66: General thermal boundary conditions: Eigenfunctions for $R_{\text{eff}} = 10^7$ and $\eta = 1$. The vertical line segments indicate the location of $z = \delta_c$.

7.7.8 Scalings of $b_c$ with $\eta$

In Section 6.3.3, we showed that the balance parameter $b$ must satisfy $b = 1 + c(\eta)\delta$. For each Biot number $\eta$, we can numerically compute $b_c - 1$ as a function of $\delta_c$. For example, we compute $b_c - 1$ versus $\delta_c$ for $\eta = 10^{-4}$ to get $c \approx 2504.4$ as shown in Figure 7.76.

We numerically compute the dependence of $c$ on the Biot number $\eta$ to get Figure 7.77. We can see that our numerical result is very close to the numerical result (6.45), $c(\eta) = \frac{1 + 2\delta_c}{4\eta}$, we got previously. Both the analytical result and the numerical result indicate the following:

- For large $\eta$, we have $c \to 0.5$. This agrees with our analytical result $c = 0.5$ ([11]) in the fixed flux case; and is also very close to the numerical result $c = \frac{b - 1}{\delta} \approx 0.4861$ in
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Figure 7.67: General thermal boundary conditions: Prefactor(\(\eta\)) for \(\delta_c(R)\). The \(\frac{1}{3}\) scaling agrees with the analytical result (6.53).

Figure 7.68: General thermal boundary conditions: Prefactor(\(\eta\)) for \(\delta_c(R_{\text{eff}})\). The \(\frac{1}{2}\) scaling agrees with the analytical result (6.55).

Figure 7.69: General thermal boundary conditions: Prefactor(\(\eta\)) for \(\delta_c(Ra)\). The weak dependence on \(\eta\) agrees with the analytical result (6.56).

Figure 7.70: General thermal boundary conditions: Prefactor(\(\eta\)) for \(b_{c}(R)\). The \(-\frac{5}{3}\) scaling agrees with the analytical result (6.58).
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Figure 7.71: General thermal boundary conditions: Prefactor($\eta$) for $b_c(R_{\text{eff}})$. The $-\frac{1}{3}$ scaling agrees with the analytical result (6.60).

Figure 7.72: General thermal boundary conditions: Prefactor($\eta$) for $b_c(Ra)$. The $-1$ scaling agrees with the analytical result (6.62).

Figure 7.73: General thermal boundary conditions: Prefactor($\eta$) for $k_c(R)$.

Figure 7.74: General thermal boundary conditions: Prefactor($\eta$) for $k_c(R_{\text{eff}})$.

Figure 7.75: General thermal boundary conditions: Prefactor($\eta$) for $k_c(Ra)$.
the fixed flux case.

For small $\eta$, we have $b = 1 + \frac{1}{4} \delta$. The fact that $c(\eta)$ blows up for small $\eta$ is consistent with our analytical result $b = 1.5 + c\delta$ in the fixed temperature case.

Figure 7.76: General thermal boundary conditions: $b_\infty - 1 = 2505.4$ for $\eta = 0$.

Figure 7.77: General thermal boundary conditions: $c(\eta)$ in $b_\infty = 1 + c(\eta)\delta$. The solid line is the analytical result $c(\eta) = \frac{1+2\eta}{4\eta}$; the stars indicate our numerical result.
7.7.9 Dependence of scaling transition and bounds on Biot number $\eta$

We can see that, for small $R$, the scalings (mainly in the exponent) involving $R$ and $R_{\text{eff}}$ behave as in the fixed temperature case; for very large $R$, all quantities scale as in the fixed flux case. The transitions are obvious from our figures. (Note: There is no difference for the scalings exponents for $Nu(Ra)$ between fixed temperature BCs and fixed flux BCs; thus there is no crossover in this case. It is interesting that the prefactor for the $Ra$ scaling does not appear to change significantly at the transition.)

Moreover, as $\eta$ decreases, the general thermal BCs (2.14) are increasingly close to the fixed temperature BCs (2.12), and the figures scale as in the fixed temperature case for a large range of $R$. The transition values of $R$ and $R_{\text{eff}}$ are both decreasing functions of $\eta$, and diverge proportional to $\eta^{-2}$ as $\eta$ decreases to 0, as seen in Figures 7.78 and 7.79. However, for all $\eta > 0$ no matter how small, all quantities scale as in the fixed flux case for sufficiently large $R$ or $R_{\text{eff}}$. All those results agree with the analytical results in [13], and in Chapter 6.

For the general boundary conditions, we have computed the upper bounds of $Nu(Ra)$ for different $\eta$. All of our bounds have yielded the same exponent $p = \frac{1}{2}$, up to small numerical errors; the largest deviation from $p = \frac{1}{2}$ is of order $10^{-5}$. In other words, we get $Nu \leq C(\eta)Ra^{\frac{1}{2}}$. From Figure 7.80, one can see that the prefactors $C(\eta)$ depend only very weakly on $\eta$. All prefactors are between 0.0781 and 0.0786. This means that the scalings we got using the Doering-Constantin method are almost independent of the Biot number $\eta$. Once again, it is gratifying that this $\eta$-independence (for $\eta > 0$) agrees with our analytical prediction (6.51).
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Figure 7.78: General thermal boundary conditions: \( R_{\text{transition}}(\eta) = 3162.27766 \eta^{-2} \).

Figure 7.79: General thermal boundary conditions: \( R_{\text{eff, transition}}(\eta) = 472.3121 \eta^{-2.0061} \).

Figure 7.80: General thermal boundary conditions: \( C(\eta) \) as a function of \( \eta \) for \( Nu \leq C(\eta) Ra^{1/4} \).
Chapter 8

Conclusions

In this thesis, we have studied the scaling of bounds on heat transport in Rayleigh-Bénard convection of a layer of fluid between two infinite horizontal plates under various thermal boundary conditions.

First, for completeness we have rederived the stability analyses for the conduction solution $u_c = 0$ and $\tau_c(z) = 1 - z$, and verified that both linear and nonlinear stability analyses lead to precisely the same eigenvalue problem. We have computed the critical Rayleigh number $Ra_c$ and its corresponding wavelength $k_c$ for different boundary conditions. For the fixed temperature case, we get $Ra_c \approx 1707.76$ and $k_c \approx 3.116$; for the fixed flux case, we get $Ra_c = 720$ and $k_c = 0$; for the general thermal boundary conditions, we can compute $Ra_c$ and $k_c$ for any given Biot number $\eta$, as shown in Figures 4.3, 4.4 and 4.5.

Then, based on the recent results of [13] (see also [11]), we demonstrated how to establish an upper bound on the heat transport, measured by the Nusselt number $Nu$, as a function of the Rayleigh number $Ra$, using the Doering-Constantin approach of background profiles. Using the Cauchy-Schwarz inequality and choosing the one-parameter piecewise linear background profiles, we derived the analytical upper bounds for different boundary conditions:

- fixed temperature BCs: $Nu \leq -0.5 + 0.230 Ra^{0.5}$,
- fixed flux BCs: $Nu \leq 0.272 Ra^{0.5}$,
- general thermal BCs: $Nu \leq 0.272 Ra^{0.5}$.

In particular, we found that the analytical upper bound for the general thermal BCs is
independent of the Biot number $\eta$, and is also exactly the same as the bound for the fixed flux case.

Finally, in the main original contribution of this thesis, we have numerically computed the bounds using optimal piecewise linear background profiles by imposing the boundary conditions on the Euler-Lagrange equations. The choice of piecewise linear background profiles does not sacrifice much in the quality of the bounds, and the numerical upper bounds for each thermal boundary condition are

\[
\begin{align*}
\text{fixed temperature BCs:} & \quad Nu \leq 0.0450 \, Ra^{0.5}, \\
\text{fixed flux BCs:} & \quad Nu \leq 0.0781 \, Ra^{0.5}, \\
\text{general thermal BCs:} & \quad Nu \leq C(\eta) \, Ra^{0.5}, \text{ with } C(\eta) \in [0.0781, 0.0786].
\end{align*}
\]

where the numerical upper bound for the general thermal BCs depends weakly on $\eta$, and is very close to the bound for the fixed flux case.

In real convection experiments, a more realistic boundary condition would be to have plates of finite conductivity above and below the fluid layer. A study of this problem is necessary to better understand the effect that different boundary conditions might have on the heat transport of Rayleigh-Bénard convection. It turns out [13] that the analytical upper bound formulation is quite similar to that presented in this thesis, and numerical investigation of this is continuing.

This study of fixed flux and general thermal BCs was initially motivated by the hope of lowering the exponent of the $Nu - Ra$ scaling, and of finding a prefactor $c(\eta)$ that would interpolate between the fixed temperature and fixed flux limits $\eta = 0$ and $\eta = \infty$, respectively; however, our results so far did not confirm these expectations. It remains for future investigations to determine whether a better optimal study, for instance by choosing more complicated background profiles (see [12]), would modify these conclusions.
Bibliography


