Boundary Perturbation of the Laplace Eigenvalues and Applications to Electron Bubbles and Polygons

by

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B.A., Princeton University 1996

Submitted to the Department of Mathematics

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Abstract
We analyze the evolution of Laplace eigenvalues on a domain induced by the motion of the boundary. We apply our analysis to two problems:
1. We study the equilibrium and stability of electron bubbles. Electron bubbles are cavities formed around electrons injected into liquid helium. They can be treated as simple mathematical systems that minimize the energy with three terms: the energy of the electron proportional to a Laplace eigenvalue, the surface energy proportional to the surface area of the cavity, and the hydrostatic pressure proportional to its volume. This system possesses a surprising result: an instability of the 2S electron bubbles.
2. We compute the simple eigenvalues on a regular polygon with N sides. The polygon is treated as a perturbation of the unit circle and its eigenvalues are approximated by a Taylor series. The accuracy of our approach is measured by comparison with finite element estimates. For the lowest eigenvalue, the first Taylor term provides an estimate within $10^{-5}$ of the true value. The second term reduces the error to $10^{-7}$. We discuss how to utilize the available symmetry to obtain better finite element estimates. Finally, we briefly discuss the expansion of simple eigenvalues on regular polygons in powers of $1/N$.

Thesis Supervisor: Gilbert Strang
Title: Professor of Mathematics
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Chapter 1

Introduction

This work focuses on the perturbation of the Laplace eigenvalues of a domain $\Omega$. The perturbation is induced by a deformation of the boundary $S$. The eigenvalues $\lambda$ and the corresponding eigenfunctions $\psi$ are defined by the system

$$
\Delta \psi + \lambda \psi = 0, \text{ in the interior of } \Omega \quad (1.1a)
$$
$$
\int_{\Omega} d\Omega \psi^2 = 1, \text{ for normalization} \quad (1.1b)
$$
$$
\psi = 0, \text{ on the boundary } S \quad (1.1c)
$$

We show that the first order perturbation $\delta \lambda$ for a simple eigenvalue is given by

$$
\delta \lambda = - \int_{S} dS C \nabla^{i} \psi \nabla_{i} \psi, \quad (1.2)
$$

where $C$ is the infinitesimal deformation of the boundary. This result is derived in Chapter 4. An analogous expression is derived for multiple eigenvalues.

We present two applications of this theory.

1. The equilibrium and stability of electron bubbles is discussed in Chapter 5. In mathematical terms, the problem is to minimize the energy $E$ with respect to the location of the boundary $S$. The energy is given by

$$
E = \frac{h^2}{8\pi^2 m} \lambda + \sigma \int_{S} dS + P \int_{\Omega} d\Omega, \quad (1.3)
$$

where $h$ is Planck’s constant, $m$ is the electron mass, $\sigma$ is the surface tension and $P$ is the hydrostatic pressure. We will consider a more abstract expression for energy:

$$
E = \Psi \lambda + \Sigma \int_{S} dS + \Pi \int_{\Omega} d\Omega \quad (1.4)
$$

The positive constant $\Sigma$ corresponds to surface tension and $\Pi$ corresponds to pressure, which may be positive or negative. The resulting equilibrium equation ($B_{\alpha}^{\alpha}$ is curvature)

$$
\Psi \nabla^{i} \psi \nabla_{i} \psi + \Sigma B_{\alpha}^{\alpha} - \Pi = 0 \quad (1.5)
$$
is highly non-linear and in most cases can only be solved numerically. In certain situations, the solution is not unique. We analyze equation (1.5) for radially symmetric states in two and three dimensions. In both cases, this system yields a surprising result: the equilibrium spherical configuration for all but the lowest eigenvalue does not deliver a local minimum of the energy. Physically, this implies that the \(2S\) electron bubbles are unstable. We solve equation (1.5) by a gradient descent scheme for several of the lowest eigenvalues in two dimensions.

2. The Laplace eigenvalues of a regular \(N\)-sided polygon are discussed in Chapter 6. We treat the simple eigenvalues \(\lambda [N]_n\) on the polygon as perturbation of the simple eigenvalues \(\lambda_n\) on the unit circle. We present a Taylor series approximation for \(\lambda [N]_n\):

\[
\lambda [N]_n \approx 1 + \frac{d\lambda_n}{dt} + \frac{d^2\lambda_n}{dt^2},
\]

where \(t \in [0, 1]\) is a time-like parameter driving the perturbation. The derivatives are expressed in terms of \(\lambda_n\), \(N\), and Bessel functions \(J_m\). The second derivative contains an infinite series.

The Taylor series approach can be applied to more general shapes that are perturbations of domains whose eigenvalues are known. We can judge the accuracy of this method by comparing the results with the conventional finite element method with triangular elements and quadratic trial functions. For the lowest eigenvalue, the first Taylor term provides an estimate within \(10^{-5}\) of the true value. The second term reduces the error to \(10^{-7}\). For higher eigenvalues, the Taylor series actually beats finite elements and can be used to judge the accuracy of finite element estimates.

Finally, we briefly discuss the expansion of simple eigenvalues on regular polygons in powers of \(1/N\). This natural idea has not been developed in the existing literature.
Chapter 2

Analytical Background

The problems presented in this work rely heavily on tensor calculus and the invariant description of surfaces embedded in space. In addition, we make frequent use of the so-called $\frac{\delta}{\delta t}$-derivative which may also be called an invariant derivative with respect to a moving surface. We present its definition and summarize the key identities. This work assumes familiarity with the tensor notation.

There is a number of excellent textbooks on the subject of tensor calculus, but our favorite is McConnell's "Applications of Tensor Calculus" [31]. We also recommend [1], [20], [37], [28], [27], and [44].

2.1 Definition of the $\frac{\delta}{\delta t}$-derivative

Consider an evolving surface $S(t)$ and two nearby times $t$ and $t+h$. The $\frac{\delta}{\delta t}$-derivative applies to objects defined on $S(t)$. Let $A$ be a point on $S(t)$. The normal to $S(t)$ at point $A$ meets the surface $S(t+y)$ at point $A_h$. Then, $\frac{\delta D}{\delta t}$ is defined as in Figure 2-1:

$$\frac{\delta D(A)}{\delta t} = \lim_{h \to 0} \frac{D(A_h) - D(A)}{h} \quad (2.1)$$

This definition applies to vectors $D$ as well as scalars. The velocity $C$ of the surface along the normal $N$ is defined as the projection of the $\frac{\delta}{\delta t}$-derivative of the radius vector $z$ onto the normal $N$:

$$C = \frac{\delta z}{\delta t} \cdot N \quad (2.2)$$

Since $\delta z/\delta t$ is parallel to $N$ (Figure 2-1), we have $|C| = |\delta z/\delta t|$.

The surface velocity $C$ is a key quantity. It is analogous to the velocity of a material point and governs the evolution of the surface. However, its profound distinction from the partial derivative of $z$ is that it does not track material points but rather the surface as an invariant object. If a cylinder is rotating about its axis, $C = 0$ since the surface stays unchanged: $S(t+h)$ is the same as $S(t)$. While $\frac{\partial z}{\partial t} = 1$ is a straightforward PDE, its surface analog $C = 1$ is equivalent to the Eikonal equation.

The $\frac{\delta}{\delta t}$-derivative can also be defined analytically. Suppose that $\xi^\alpha$ are the surface coordi-
Figure 2-1: Geometric construction of the $\frac{\delta}{\delta t}$-derivative for $D$ (a scalar or vector) and its application to the radius vector $\mathbf{z}$ (which leads to $C$).

nates and that

$$z^i = z^i(\xi, t) \quad (2.3)$$

is a parametric equation for the surface. Our convention is to drop the superscript $\alpha$ from function arguments. Define the velocity object $v^i$ (which is not a tensor despite the upper index):

$$v^i(\xi, t) = \frac{\partial z^i(\xi, t)}{\partial t} \quad (2.4)$$

Its surface projection $v^\alpha$ is obtained by contraction with the shift tensor $z^\alpha_i$:

$$v^\alpha = z^\alpha_i v^i \quad (2.5)$$

The analytical definition of the $\frac{\delta}{\delta t}$-derivative for an invariant $D$ is:

$$\frac{\delta D}{\delta t} = \frac{\partial D(\xi, t)}{\partial t} - v^\alpha \nabla_\alpha D \quad (2.6)$$

The $\frac{\delta}{\delta t}$-derivative can also be defined for arbitrary tensors [11]. In the definition, there is a linear combination for each index and, as customary, we present the formula for a typical tensor $T^{ij}_{\alpha\beta}$:

$$\frac{\delta T^{ij}_{\alpha\beta}}{\delta t} = \frac{\partial T^{ij}}{\partial t} - v^\gamma \nabla_\gamma T^{ij}_{\alpha\beta} + v^m \Gamma^{ij}_{mk} T^{k\alpha\beta} - v^m \Gamma^{ij}_{mj} T^{k\alpha\beta} + \nabla_\gamma v^\alpha T^{ij\gamma}_{\beta\gamma} - \nabla_\beta v^\gamma T^{ij\alpha}_{\gamma\gamma} \quad (2.7)$$

$\Gamma^{ij}_{jk}$ is the Christoffel symbol. The definition (2.7) leads to a series of identities summarized in the next section.

2.2 Properties of the $\frac{\delta}{\delta t}$-derivative

The identities presented below assume the following notation for the standard space and surface objects:

1. The metrics. $z^i_\alpha$ is the shift tensor, $z_{ij}$ is the spatial metric tensor, $\xi_{\alpha\beta}$ is the surface metric tensor. Further, $z_{ijk}$ is the space permutation tensor and $\varepsilon_{\alpha\beta}$ is the surface permutation
tensor. In the case of curves embedded in surfaces, the surface permutation tensor has two
indices and the curve permutation tensor has one. Finally, \(z_i\) is the space covariant basis and
\(\xi_\alpha\) is the surface covariant basis.

2. \(N^i\) is the surface normal, \(B^0_\alpha\) is the curvature tensor. The trace of the curvature tensor
\(B^0_\alpha\) is known as the mean curvature.

Some objects defined on \(S(t)\) arise as surface restrictions of spatial fields (for example, the
flow around an airplane’s wing). If the field \(\phi(S,t)\) is the surface restriction of a spatial field
\(f(\mathbb{R}^3,t)\), the chain rule states

\[
\frac{\delta \phi}{\delta t} = \frac{\partial f(z_i,t)}{\partial t} + CN^i \nabla_i f
\]  

(2.8)

The \(\frac{\delta}{\delta t}\)-derivative obeys the Leibnitz or product rule:

\[
\frac{\delta (\phi \gamma)}{\delta t} = \frac{\delta \gamma}{\delta t} \phi + \frac{\delta \phi}{\delta t} \gamma
\]  

(2.9)

The general definition of the \(\frac{\delta}{\delta t}\)-derivative (2.7) leads to this much referenced table of identities:

\[
\frac{\delta z^i_\alpha}{\delta t} = \nabla_\alpha (CN^i) \tag{2.10a}
\]

\[
\frac{\delta \xi^0_\beta}{\delta t} = 0 \tag{2.10b}
\]

\[
\frac{\delta \xi_{\alpha\beta}}{\delta t} = -2CB_{\alpha\beta} \tag{2.10c}
\]

\[
\frac{\delta \xi_{\alpha\beta}}{\delta t} = 2CB^{\alpha\beta} \tag{2.10d}
\]

\[
\frac{\delta N^i}{\delta t} = -z^i_\alpha \nabla^\alpha C \tag{2.10e}
\]

\[
\frac{\delta B^i_\beta}{\delta t} = \nabla_\beta \nabla^\alpha C + CB^\alpha_\beta B^i_\beta \tag{2.10f}
\]

Identity (2.10b) shows that \(\frac{\delta}{\delta t}\) commutes with the operation of raising and lowering indices. The
chain rule (2.8) shows that \(\frac{\delta}{\delta t}\) "kills" all the spatial metrics:

\[
\frac{\delta z_i}{\delta t}, \frac{\delta z^i}{\delta t}, \frac{\delta z_{ij}}{\delta t}, \frac{\delta z^{ij}}{\delta t}, \frac{\delta z_{ijk}}{\delta t}, \frac{\delta z^{ijk}}{\delta t} = 0. \tag{2.11}
\]

\[\]  

2.3 Time differentiation of surface and volume integrals

Expressions for energy usually contain surface or volume integrals. We present rules for differ-
entiating such integrals. Consider an evolving domain \(\Omega(t)\) and its boundary \(S(t)\). Then

\[
\frac{d}{dt} \int_{\Omega(t)} d\Omega f = \int_{\Omega(t)} d\Omega \frac{\partial f}{\partial t} + \int_{S(t)} dSC f \tag{2.12}
\]
and
\[ \frac{d}{dt} \int_{S(t)} dS \phi = \int_{S(t)} dS \frac{\delta \phi}{\delta t} - \int_{S(t)} dS \left( \nabla_c B^c_\alpha \phi \right) \]
(2.13)

The vector or scalar field \( f \) is defined in the interior of \( \Omega(t) \) and may explicitly depend on \( t \). The vector or scalar field \( \phi \) is defined on \( S(t) \) and may also depend on \( t \). It may arise as a restriction of a spatial field or be defined exclusively on the surface, such as the normal \( N^i \). Formula (2.12) is the moving surface equivalent of the Fundamental Theorem of Calculus, while (2.13) has no analogue in one-dimensional calculus. In two dimensions, areas replace volumes and contours replace surfaces.

2.4 A reference for surface relationships

For the sake of future reference, we give a table of identities for the key surface tensors.

1. Surface metrics
\[ \xi_\alpha = \nabla_\alpha z^i z^i_\alpha \]
(2.14a)
\[ z^i_\alpha = \frac{\partial z^i}{\partial \xi^\alpha} = z^i \cdot \xi_\alpha \]
(2.14b)
\[ \xi_\alpha \cdot \xi_\beta = z_{ij} z^i_\alpha z^j_\beta \]
(2.14c)

2. Relationships involving the normal \( N^i \)
\[ N_i = \frac{1}{2} \epsilon^{\alpha\beta} z_{ijk} z^i_\alpha z^j_\beta \]
(2.15a)
\[ N_i z^i_\alpha = 0 \]
(2.15b)
\[ N^i N_i = 1 \]
(2.15c)

3. Projection formulas
\[ z^i_\alpha z^\beta_\alpha = \xi^\beta_\alpha \]
(2.16a)
\[ z^i_\alpha z^\alpha_\beta = z^i_j - N^i N_j \]
(2.16b)

4. Curvature tensor
\[ B_{\alpha\beta} = N_j \nabla_\alpha z^j_\beta \]
(2.17a)
\[ B_{\alpha\beta} = -z^j_\beta \nabla_\alpha N_j \]
(2.17b)
\[ \nabla_\alpha z^i_\beta = B_{\alpha\beta} N^i \]
(2.17c)

5. Curvature invariants for the circle, cylinder, and sphere
i. Circle of radius \( R \):
\[ B^\alpha_\alpha = -\frac{1}{R} \]
(2.18)
\[ B^\beta_\beta B^\beta_\alpha = \frac{1}{R^2} \]
(2.19)
ii. Sphere of radius \( R \):

\[
B_\alpha^\alpha = -\frac{2}{R} \tag{2.20}
\]

\[
B_\beta^\beta B_\alpha^\alpha = \frac{2}{R^2} \tag{2.21}
\]

iii. Cylinder of radius \( R \):

\[
B_\alpha^\alpha = -\frac{1}{R} \tag{2.22}
\]

\[
B_\beta^\beta B_\alpha^\alpha = \frac{1}{R^2} \tag{2.23}
\]

The tensor \( C_\mu^\alpha = B_\gamma^\alpha B_\mu^\gamma \) is known as the third groundform of \( S \). Identities (2.19), (2.21) and (2.23) give its trace.
Chapter 3

An Isolated Droplet: Discussion of Technique

3.1 Introduction

In this chapter we demonstrate the essential techniques on one of the simplest physical systems: an isolated droplet shown in Figure 3-1. "Isolated" means that the only physical phenomenon considered is surface tension. The equilibrium configuration is a sphere and it is stable with respect to small perturbations of the droplet's surface.

Our method for analyzing equilibrium and stability is based on minimizing the total potential energy [11], [23], [26], [39], [48] and ignores the dynamics of the system. The Navier-Stokes (or Euler) equations are not employed. As a matter of fact, the droplet need not be fluid. It may be an isotropic solid (in which case elastic energy must be added) or even a crystal. In the latter case, the surface energy density depends on the direction of the normal. For further discussions of the physical aspects of these problems, we refer the reader to the classic text by Landau "Statistical Mechanics" [23] as well as the following works: "Shape and Growth of Crystals" by Nozieres [34], "The surface tension in solids" by Shuttleworth [38]. Crystalline droplets are discussed in the book "Variational Theories of Liquid Crystals" by Virga [46]. An advanced reference on the variational methods in physics is [3].

The simple problem of an isolated droplet will illustrate many of the techniques used in later chapters. There we largely omit the analytic details by summing them up simply as "some algebra". Invariably, "some algebra" includes several steps:

1. (i) Computing the first energy variation \( \delta E \)
   (ii) Deriving the equilibrium conditions
   (iii) Formulating the quasi-static evolution equation by steepest descent

2. (i) Computing the second energy variation \( \delta^2 E \) in the vicinity of an equilibrium. This is analogous to finding \( \frac{d^2 f}{dx^2} \) at a point where \( \frac{df}{dx} = 0 \). The fact that the second energy variation is computed only in the vicinity of an equilibrium is critical from the technical point of view since the computation for an arbitrary configuration may be too complicated.

   (ii) Analyzing whether \( \delta^2 E \) can assume negative values for some allowable values of independent variations. For a spherical equilibrium configuration, we usually expand \( \delta^2 E \) in terms of the spherical harmonics \( Y_{lm} (\theta, \phi) \). This leads to an infinite-dimensional diagonal quadratic
Figure 3-1: An isolated spherical droplet of radius $R$ with surface tension $\sigma$.

form which yields the stability conditions.

There exists an alternative way to analyze stability. It is to solve the linearized quasi-static evolution equation obtained in 1(iii) and to determine whether small perturbation grow or decay.

3.2 "Some Algebra"

3.2.1 A one-parameter family of configurations

Consider a one-parameter family of attainable configurations of the system. A "configuration" is a collection of the values of physical parameters that may be independently varied. These depend on the problem and may include locations of material points, shape of an interface, electrostatic surface charge density, and dielectric polarization. The family of configurations is indexed by a time-like parameter $t$. The total energy of the system is then a function of $t$:

$$E \equiv E(t)$$

This expression can be differentiated with respect to $t$ in the sense of the ordinary calculus. By definition, the first variation $\delta E$ (for the chosen family of configurations) is given by:

$$\delta E = \frac{dE(t)}{dt} \bigg|_{t=0} \quad (3.1)$$
The second energy variation $\delta^2 E$ is computed only in the vicinity of equilibrium configurations. It is defined by:

$$\delta^2 E = \frac{d^2 E(t)}{dt^2} \bigg|_{t=0}$$

(3.2)

The equilibrium configuration is stable when $E$ attains a local minimum. In other words,

$$\delta^2 E > 0$$

(3.3)

for all allowable variations of the independent parameters. Of course, we are happy when we discover an instability for that constitutes a physical phenomenon! Instability occurs when

$$\delta^2 E < 0$$

for some variations.

(3.4)

### 3.2.2 The first variation

Suppose that $\Omega$ is the domain occupied by the droplet and $S$ is its boundary. The volume $V$ of the domain is

$$V = \int_{\Omega} d\Omega$$

(3.5)

and its surface area $A$ is

$$A = \int_{S} dS$$

(3.6)

The total energy of the system consists entirely of the surface tension energy $E_{ST}$. If the surface energy density (of the water/air interface) is $\sigma$, then

$$E_{ST} = \int_{S} dS \sigma$$

(3.7)

Conservation of volume is accounted for by a Lagrange multiplier $\lambda$:

$$E = E_{ST} - \lambda V = \int_{S} dS \sigma - \lambda \int_{\Omega} d\Omega$$

(3.8)

The surface energy density $\sigma$ is usually treated as a constant (as we do throughout this work), but not always. It may, for example, be a function of the surface charge density $\tau$, $\sigma = \sigma(\tau)$. For this reason we prefer to leave $\sigma$ inside the integral.

We compute the first variation by differentiating $E$:

$$\delta E = \frac{d}{dt} \int_{S} dS \sigma - \lambda \frac{d}{dt} \int_{\Omega} d\Omega$$

(3.9a)

by (2.12) and (2.13) = $- \int_{S} dS C \sigma B^\alpha_{\alpha} - \lambda \int_{S} dSC$

(3.9b)

Combining the two terms, we get

$$\delta E = - \int_{S} dSC \{ \sigma B^\alpha_{\alpha} + \lambda \}$$

(3.10)
Curly brackets \{\} are used for quantities that multiply independent variations. In our example, the independent variation is \( C \).

### 3.2.3 The equilibrium conditions and quasi-static evolution

We treat \( C \) as an independent variation. Therefore equation (3.10) yields the equilibrium condition for an isolated droplet:

\[
B_\alpha^2 = \text{Constant} \tag{3.11}
\]

The solution is a surface of constant curvature! A number of shapes have this property. The most obvious one is a sphere. A set of two disjoint spheres satisfies this condition as well, but this solution is not allowed. An infinite cylinder has constant mean curvature (2.22), as does any shape assumed by a thin film supported by a wire loop (in fact, its curvature is identically zero), but such surfaces are not closed.

In general, the equilibrium equation such as (3.11) is not easy to solve since its solution is the location of the interface itself. However, one can write an evolution system that should relax to stable equilibrium configurations. The idea is to deform the boundary by "gradient descent" to ensure that the energy is monotonically decreased. Since the total energy of an isolated droplet evolves according to

\[
\frac{dE_{ST}}{dt} = -\int_S dSC\sigma B_\alpha^2, \tag{3.12}
\]

a good suggestion for \( C \) is evolution by mean curvature:

\[
C = B_\alpha^2 \tag{3.13}
\]

for that would ensure that \( dE_{ST}/dt < 0 \). The problem with evolution (3.13) is that it does not conserve volume. This is a remediable problem.

According to equation (2.12), the rate of change of volume is given by

\[
\frac{dV}{dt} = \int_S dSC \tag{3.14}
\]

Therefore, to conserve volume, \( C \) must integrate to zero:

\[
\int_S dSC = 0 \tag{3.15}
\]

This condition is easy to satisfy. Suppose that \( X \) is any scalar field defined on the surface and \( \langle X \rangle \) is its average:

\[
\langle X \rangle = \frac{\int_S dS X}{\int_S dS} \tag{3.16}
\]

Then \( C \), defined by

\[
C = X - \langle X \rangle \tag{3.17}
\]

satisfies the volume conservation condition (3.15).
We now combine gradient descent with volume conservation:

\[ C = B_\alpha^a - \langle B_\alpha^a \rangle \]  \hspace{1cm} (3.18)

We must make sure that the adjustment did not affect the monotonic decrease in energy:

\[ \frac{dE_{ST}}{dt} = - \int_S dSB_\beta^a (B_\alpha^a - \langle B_\alpha^a \rangle) \]  \hspace{1cm} (3.19a)

\[ = - \left( \int_S dS (B_\alpha^a)^2 - \langle B_\alpha^a \rangle \int_S dSB_\beta^a \right) \]  \hspace{1cm} (3.19b)

\[ = - \left( \int_S dS (B_\alpha^a)^2 - \langle B_\alpha^a \rangle \langle B_\beta^a \rangle \int_S dS \right) \]  \hspace{1cm} (3.19c)

\[ = - \left( \langle (B_\alpha^a)^2 \rangle - \langle B_\alpha^a \rangle^2 \right) \int_S dS \]  \hspace{1cm} (3.19d)

The result is negative by convexity since the average of the square is greater than the square of the average.

There is a number of suitable choices for \( C \) that diminish total energy while conserving volume. Another good scheme is evolution by Laplacian:

\[ C = -\nabla_\gamma \nabla^\gamma B_\alpha^a \]  \hspace{1cm} (3.20)

The volume is conserved by the divergence theorem: there is no boundary term since there is no boundary! As for the evolution of energy, we have:

\[ \frac{dE_{ST}}{dt} = \int_S dSB_\beta^a \nabla_\gamma \nabla^\gamma B_\alpha^a \]  \hspace{1cm} (3.21a)

\[ = - \int_S dS \nabla_\gamma B_\beta^a \nabla_\gamma B_\alpha^a \]  \hspace{1cm} (3.21b)

This expression is negative since the integrand is \( |\nabla B_\alpha^a|^2 \). From the computational point of view, evolution by Laplacian has two disadvantages. It requires computation of fourth order derivatives and leads to stringent numerical stability requirements.

### 3.2.4 The second variation

The second energy variation reveals the stability properties of the equilibrium configuration. It is computed only in the vicinity of the equilibrium configuration. For a general configuration, we have:

\[ \delta^2 E = -\frac{d}{dt} \int_S dSC (B_\alpha^a \sigma + \lambda) \]  \hspace{1cm} (3.22a)

by (2.13) and (2.9) \[ = \left\{- \int_S dSC^2 B_\beta^a (\sigma B_\alpha^a + \lambda) + \int_S dS \frac{\delta^2 C}{\delta t} (\sigma B_\alpha^a + \lambda) \right\} \]  \hspace{1cm} (3.22b)

Since the equilibrium configuration satisfies equation (3.11), only the last integral survives. We
continue with that term:
\[
\delta^2 E = - \int_S dS \frac{\delta}{\delta t} \left( \sigma B^\alpha_\alpha + \lambda \right) \tag{3.23a}
\]
\[
= - \int_S dS \sigma \frac{\delta B^\alpha_\alpha}{\delta t} \tag{3.23b}
\]
by (2.10f) \[
= - \int_S dS \sigma \left( \nabla_\alpha \nabla^\alpha C + CB^\beta_\beta B^\alpha_\alpha \right) \tag{3.23c}
\]
For an equilibrium sphere of radius \( R \), we have by (2.21):
\[
\delta^2 E = - \int_S dS \sigma \left( \nabla_\alpha \nabla^\alpha C + C \frac{2}{R^2} \right) \tag{3.24}
\]
In rare cases it is possible to determine by a simple inspection whether \( \delta^2 E \) is positive for all admissible small variations of the independent parameters. For example, it is easy to see by convergence theorem that the first term in (3.24) is positive:
\[
- \int_S dS \sigma C \nabla_\alpha \nabla^\alpha C = \int_S dS \nabla_\alpha C \nabla^\alpha C = \int_S dS \sigma |\nabla C|^2 \tag{3.25}
\]
It is still unclear whether the overall expression is positive since the contribution of the second term is negative. We need a more robust way for analyzing \( \delta^2 E \).

### 3.2.5 Spherical harmonics expansion

Decompose \( C \) in terms of the spherical harmonics \( Y_{lm}(\theta, \phi) \):
\[
C = R \sum_{l\neq0,m} C_{lm} Y_{lm}(\theta, \phi) \tag{3.26}
\]
The factor of \( R \) is included in order to non-dimensionalize the expansion coefficients \( C_{lm} \). The term corresponding to \( l = 0 \) is omitted to conserve volume. Figure 3-2 shows perturbations of the sphere proportional to \( l = 0 \), \( l = 1 \), and \( l = 2 \) harmonics.

The spherical harmonics are eigenfunctions of the surface Laplacian on the unit sphere:
\[
\nabla_\alpha \nabla^\alpha Y_{lm} = -l(l+1)Y_{lm}, \quad S = \left\{ \mathbf{z} : |\mathbf{z}|^2 \equiv 1 \right\} \tag{3.27}
\]
On the sphere of radius \( R \), the surface Laplacian is scaled by \( R^{-2} \):
\[
\nabla_\alpha \nabla^\alpha Y_{lm} = -\frac{l(l+1)}{R^2} Y_{lm}, \quad S = \left\{ \mathbf{z} : |\mathbf{z}|^2 \equiv R^2 \right\} \tag{3.28}
\]
The spherical harmonics are chosen to form an orthonormal set on the unit sphere:
\[
\int_{|\mathbf{z}|^2 = 1} dS Y_{l_1 m_1}(\theta, \phi) Y_{l_2 m_2}(\theta, \phi) = \delta_{l_1 l_2} \delta_{m_1 m_2} \tag{3.29}
\]

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On the sphere of radius $R$, the normalization is scaled by $R^2$:

$$
\int_{|x|^2 = R^2} dS Y_{l_1 m_1} (\theta, \phi) Y_{l_2 m_2} (\theta, \phi) = R^2 \delta_{l_1 l_2} \delta_{m_1 m_2}
$$

(3.30)

The harmonic that corresponds to $l = m = 0$ is independent of $\theta$ and $\phi$.

$$
Y_{00} (\theta, \phi) = \frac{1}{\sqrt{4\pi}}
$$

(3.31)

This harmonic is responsible for radial perturbations of the sphere. In problems that conserve volume this harmonic is disallowed. Every other harmonic conserves volume (by orthogonality to $Y_{00}$).

There are three $l = 1$ harmonics:

$$
Y_{1,-1} (\theta, \phi) = \frac{1}{\sqrt{\frac{3}{4\pi}}} \cos \theta e^{-i\phi}
$$

(3.32a)

$$
Y_{1,0} (\theta, \phi) = \frac{1}{\sqrt{\frac{3}{4\pi}}} \cos \theta
$$

(3.32b)

$$
Y_{1,1} (\theta, \phi) = \frac{1}{\sqrt{\frac{3}{4\pi}}} \cos \theta e^{i\phi}
$$

(3.32c)

$Y_{10}$ is responsible for the vertical motion of the surface as a rigid body. As a set, $Y_{1,-1}$, $Y_{10}$, and $Y_{11}$ can move the surface as a rigid body in any direction.

The next set of five harmonics correspond to $l = 2$. These harmonics represent the simplest morphological perturbations of the sphere: transformation into an ellipsoid. Chapter 5 discusses this point in greater detail. There the reader will also find a simple recipe (proposed by Migdal) for testing the stability properties of physical systems with respect to ellipsoidal perturbations.

### 3.2.6 Completion of the second variation analysis

Substitute expansion (3.26) into the expression for the second energy variation (3.24)

$$
\delta^2 \Phi = \sigma \sum_{\ell \neq 0, m} |C_{\ell m}|^2 (\ell (\ell + 1) - 2) = \sigma \sum_{\ell \neq 0, m} |C_{\ell m}|^2 (\ell + 2) (\ell - 1)
$$

(3.33)

The result is an infinite-dimensional quadratic form in the $C_{\ell m}$. The factor of $(l - 1)$ is a common feature of problems in which the absolute location of the interface is immaterial. Therefore stability is neutral against motion as a rigid body.

Since (3.33) is diagonal in the $C_{\ell m}$, it is particularly easy to formulate the necessary conditions for stability:

$$
(l + 2) (l - 1) \geq 0
$$

(3.34)

This condition is satisfied for every $l \geq 2$ and we conclude that an the droplet is stable under the influence of surface tension.

The positive contribution of $(l + 2) (l - 1)$ grows with $l$. Therefore, destabilizing phenom-
\begin{align*}
Y_{0,0}(\theta, \phi) &= \frac{1}{\sqrt{4\pi}} \\
Y_{1,0}(\theta, \phi) &= \left(\frac{4}{3}\pi\right)^{-1/2} \cos \theta \\
Y_{2,0}(\theta, \phi) &= \left(\frac{16}{5}\pi\right)^{-1/2} (1+\cos 2\theta)
\end{align*}

Figure 3-2: The $l = 0$, $l = 1$, and $l = 2$ spherical harmonics.
ena, such as the electrical charge in the classical Rayleigh instability, have the best chance of destabilizing the $l = 2$ or $l = 3$ harmonic.

### 3.3 An alternative to the second variation

Second variation often leads to complicated computations. An alternative approach often lets us avoid this problem. It is based on solving the linearized evolution system in the vicinity of the equilibrium. Stability results if all infinitesimal perturbations decay with time.

We believe that this approach is equivalent to the second variation analysis although we do not have a proof. One potential difficulty is evident – evolution systems are not unique. We consider the second variation approach to be more sound. Nevertheless, the analysis presented in this section can be of great value in many situations in which the second energy variation is just too difficult to compute.

#### 3.3.1 Evolution by Laplacian

We first analyze evolution by Laplacian (3.20):

$$C = -\nabla_\gamma \nabla^\gamma B_\alpha$$  \hspace{1cm} (3.35)

Applying the $\frac{d}{dt}$-derivative to both sides yields:

$$\frac{\delta C}{\delta t} = \nabla_\gamma \nabla^\gamma \left( \nabla_\alpha \nabla^\alpha C + CB_\beta B_\alpha^\beta \right)$$  \hspace{1cm} (3.36)

The solution to this equation is a family of surfaces $S(t)$ such that (3.36) holds at every $t$. This equation is highly non-linear despite the fact that $C$ figures linearly in it. The source of the non-linearity is the motion of the interface.

We would like to rewrite equation (3.36) in a form that emphasizes the fact that all differentiations are carried out with respect to the metric of the surface $S_t$:

$$\frac{\delta C (S_t)}{\delta t} = \Delta_S \left( \Delta_{S_t} \nabla_{S_t} \nabla^\gamma \left( \nabla_\alpha \nabla^\alpha C + CB_\beta B_\alpha^\beta \right) \right)$$  \hspace{1cm} (3.37)

The linearization keeps the terms of order $C$ and replaces the metrics on $S_t$ with those on $S_0$. The linearized version of the evolution equation (3.36) is

$$\frac{\delta C}{\delta t} = \Delta_{S_0} \left( \Delta_{S_0} C + \left( B_\beta B_\alpha^\beta \right) \right)$$  \hspace{1cm} (3.38)

According to (2.21), $B_\beta^\gamma B_\alpha^\beta = 2R^{-2}$, so

$$\frac{\delta C}{\delta t} = \Delta_{S_0} \left( \Delta_{S_0} C + \frac{2C}{R^2} \right)$$  \hspace{1cm} (3.39)

This equation allows solutions of the form

$$C = c_{lm} e^{im\theta} Y_{lm} (\theta, \phi)$$  \hspace{1cm} (3.40)
where
\[ \eta_{lm} = -\frac{\nu}{R^2} (l - 1) l (l + 1) (l + 2) \] (3.41)

Therefore, all morphological perturbations of the interface decay for \( l \geq 2 \). The rigid body perturbation characterized by \( l = 0 \) neither grows nor decays indicating neutral stability. These conclusions agree entirely with the second variation analysis.

### 3.3.2 Evolution by mean curvature

Evolution by mean curvature can be analyzed in a similar fashion. \( C \) is given by
\[ C = B^\alpha_{\alpha} - \langle B^\alpha_{\alpha} \rangle = B^\alpha_{\alpha} - \frac{\int_S dSB^\alpha_{\alpha}}{\int_S dS} \] (3.42)

It is convenient to let \( C \) absorb \( \int_S dS \):
\[ C = B_{\alpha}^\alpha \int_S dS - \int_S dSB_{\alpha}^\alpha \] (3.43)

We once again apply the \( \frac{\delta}{\delta t} \)-derivative to both sides:
\[
\frac{\delta C}{\delta t} = \left( \left( \nabla^\alpha \nabla_\alpha C + CB_{\beta}^\beta B_{\alpha}^\beta \right) \int_S dS - B_{\alpha}^\alpha \int_S dSCB_{\beta}^\beta \right) - \int_S dS \left( \nabla^\alpha \nabla_\alpha C + CB_{\beta}^\beta B_{\alpha}^\beta \right) - \int_S dSCB_{\beta}^\beta B_{\alpha}^\alpha
\]

by divergence theorem
\[
= \left( \left( \Delta_S C + CB_{\beta}^\beta B_{\alpha}^\beta \right) \int_S dS - B_{\alpha}^\alpha \int_S dSCB_{\beta}^\beta \right) - \int_S dSCB_{\beta}^\beta B_{\alpha}^\alpha \int_S dSCB_{\beta}^\beta B_{\alpha}^\alpha
\] (3.44)

The linearized version of this equation is
\[
\frac{\delta C}{\delta t} = 4\pi R^2 \left( \Delta_S C + \frac{2}{R^2} C - \frac{2}{R^2} \int_S dSC \right)
\] (3.45)

The integral term vanishes by (3.15) since \( C \) must conserve volume leaving us with a perfectly linear equation:
\[
\frac{\delta C}{\delta t} = \Delta_S C + \frac{2}{R^2} C
\] (3.46)

This equation allows a solution of the form
\[ C = c_{lm} e^{\eta_{lm}t} Y_{lm} (\theta, \phi) \] (3.47)

where
\[ \eta_{lm} = - (l - 1) (l + 2) \] (3.48)

This expression indicates that \( \eta_{00} = 0 \) and \( \eta_{lm} < 0 \) for \( l > 1 \), which leads to precisely the same stability properties as the evolution by Laplacian.
3.3.3 A demonstration of evolution by mean curvature

Figure 3-3 illustrates evolution by mean curvature (3.18). The initial configuration is an ellipsoid with principal semi-axes 1, 1, and 2. The ellipsoid evolves into a perfect sphere. This may not take place if the initial configuration is too far away from the sphere. If the eccentricity of the ellipsoid is too high, it will tend to break up into smaller droplets. This behavior is related to the so-called Rayleigh instability which we discuss next.

3.4 An instability induced by surface tension

A spherical droplet is stable under the influence of surface tension. Surprisingly, surface tension can be a source of instability for some geometries. This is called the Rayleigh instability — not to be confused with the instability of an electrostatically charged droplet. Consider a slender cylinder is radius $R$ and height $L$. An orthogonal basis on the surface of the cylinder is given by

$$L_{mn}(z,\alpha) = e^{im\alpha}e^{i2\pi nz/L}, \quad -\infty < m, n < \infty.$$

Since the cylinder allows a Cartesian coordinate system, the Laplacian is given by

$$\nabla_\gamma \nabla_\gamma = \frac{1}{R^2} \frac{\partial^2}{\partial \alpha^2} + \frac{\partial^2}{\partial z^2}$$  \hspace{0.5cm} (3.49)

Therefore, the $L_{mn}$ are eigenfunctions of $\nabla_\gamma \nabla_\gamma$:

$$\nabla_\gamma \nabla_\gamma L_{mn} = -\left(\frac{m^2}{R^2} + \frac{4\pi^2 n^2}{L^2}\right) L_{mn}$$  \hspace{0.5cm} (3.50)

Expand the normal velocity $C$ in terms of the $L_{mn}$

$$C = R \sum_{m,n} C_{mn}Z_{mn}$$  \hspace{0.5cm} (3.51)

and substitute this expansion into the second energy variation (3.24):

$$\delta^2 E = -\int_S dS\sigma C \left(\nabla_\alpha \nabla_\alpha C + \frac{4\pi^2 R^2}{L^2} B_\beta B_\beta^\alpha\right)$$  \hspace{0.5cm} (3.52a)

$$= \sum_n 2\pi RL\sigma C_{mn}^2 \left(m^2 + \frac{4\pi^2 R^2}{L^2} - n^2 - 1\right)$$  \hspace{0.5cm} (3.52b)

The general stability criterion is

$$m^2 + \frac{4\pi^2 R^2}{L^2} - n^2 > 1$$  \hspace{0.5cm} (3.53)

Instability is only possible for $m = 0$ and if it does occur for some $n$, then it also occurs for $n = 1$. Therefore, the stability condition need only address perturbations proportional to $L_{1,0}$. We thus obtain the Rayleigh stability criterion

$$2\pi R > L$$  \hspace{0.5cm} (3.54)
Figure 3-3: Evolution by mean curvature. The initial configuration is an ellipsoid with semiaxes 1, 1, and 2. If the initial ellipsoid has significantly higher eccentricity, it might evolve into two spheres.
This criterion is violated by a cylinder whose height is greater than its circumference.

3.4.1 Demonstrations of the Rayleigh instability

Figure 3-4 displays evolution by mean curvature for a periodic cylindrical droplet of height $L = 12$ and radius $R = \frac{1}{2}$. A perturbation $10^{-3} e^{i4\pi z/L}$ along the normal was planted to accelerate the onset of the Rayleigh instability.

Figure 3-5 displays the same evolution for a periodic cylindrical droplet of height $L = 12$ and radius $R = 2$. This droplet does satisfy the Rayleigh criterion (3.54) and we expect it to return to the equilibrium cylindrical configuration. A perturbation of $10^{-1} e^{i3\pi z/2L}$ can be seen in the initial configuration. As expected, the droplet evolves into a perfect cylinder.

The Rayleigh instability can also be observed in a toroidal droplet with $R = 5$ and $r = \frac{1}{2}$, Figure 3-6. The torus is particularly easy to code. It is periodic in both of its coordinates, enabling the FFT [40], [45] can perform the necessary differentiations. Interestingly, a torus cannot be an equilibrium configuration. In fact, numerical simulations indicate that there are no equilibrium configurations that have the toroidal topology.
Figure 3-4: The Rayleigh instability for a cylinder. A small perturbation was planted to accelerate the onset of the instability. The height $L = 12$ and radius $R = \frac{1}{2}$ violate the Rayleigh stability criterion (3.54).
Figure 3-5: The Rayleigh instability for a cylinder. A small perturbation was planted to accelerate the onset of the instability. The height $L = 12$ and radius $R = 2$ satisfy the Rayleigh stability criterion (3.54).
Figure 3-6: Rayleigh instability for a toroidal droplet with $R = 5$ and $r = \frac{1}{2}$. The small box in the center is used to indicate the orientation of the scene. The two locations where the instability is most visible are marked by circles on the last image.
Chapter 4

Evolution of Laplace Eigenvalues Due to Deformation of the Boundary

4.1 What you will find in this chapter

The hardest part about writing this chapter was deciding what to leave out. In the end, we decided to cover the following topics:

1. Classical linear algebra perturbation theory of self-adjoint operators. Simple and degenerate cases are considered. Expressions for eigenvectors as well as eigenvalues are derived.

2. Boundary perturbation of simple Laplace eigenvalues. General expressions for the first and the second eigenvalue perturbations are derived. Eigenfunction perturbations can theoretically be obtained from the perturbed system of equations for any shape. However, analytical expressions can be obtained only for a handful of geometries (but arbitrary perturbations). We find those expressions for the circle and the sphere.

3. Boundary perturbation of degenerate eigenvalues. We present a general expression and as an example, consider an ellipsoidal perturbation of the sphere.

4. Migdal’s approach to eigenvalue perturbation. Ellipsoidal perturbations of the sphere can be effectively analyzed by an approach proposed by Migdal. The approach is based on introducing a new coordinate system in which the ellipsoid has the same equation as the sphere in the original system. The evolution of the boundary re-emerges as a perturbation of the Laplace operator and classical perturbation theory can be applied. Migdal’s approach can be employed in other energy minimization problems. It can reveal instabilities with respect to boundary perturbations, but only if the shape is unstable with respect to ellipsoidal perturbations. (This is not the case for the 2S electron bubbles.)

4.2 Introduction

The natural frequencies of a body are determined by its shape $\Omega$, its material properties, and the boundary conditions. In this chapter, we study one of these factors: the shape. The vibrations of a body are modeled by the wave equation, $\frac{\partial^2 u}{\partial t^2} = \nabla^2 \psi u$. Separation of variables leads to the eigenvalue equation

$$\nabla^2 \psi = -\lambda \psi$$
The primary focus of this chapter is the dependence of the solution to this equation on the shape of the boundary \( S \). In Chapter 5, we apply the techniques developed here to the quantum mechanical problem of equilibrium shape and morphological stability of electron bubbles. The energy of the trapped electron is the eigenvalue of the Schrödinger operator, which is proportional to the Laplacian. In Chapter 6, we present a way to estimate (to a great degree of accuracy) the eigenvalues of a regular polygon.

Different shapes generally have different eigenvalues, although this is not always the case. There exist isospectral domains of different shapes [5], [6], [7], [9]. Those shapes provide counterexamples to the long standing question: "Can you hear the shape of a drum?" [19].

The question of change in eigenvalues due to change in domain is relevant to the numerical solutions of PDE's, particularly the Finite Element method. In Finite Elements, the true domain is typically approximated by a polygon. If isoparametric elements are used, the original shape can be matched to a higher order but a discrepancy still exists. Therefore, an error is introduced into the problem before the discrete approximation is constructed. The paper by Strang and Berger [42] addresses this issue for the Poisson equation and we now do the same for the eigenvalue problem.

4.3 Overview of the classical eigenvalue perturbation theory

4.3.1 Introduction

In this section we focus on the classical Linear Algebra eigenvalue problem [41], [21]

\[
A \psi = \lambda \psi
\]  

(4.1)

We use a Greek letter to denote the eigenvector because later we shall apply the same approach to the eigenvalues of the Schrödinger operator. We assume that \( A \) and its perturbations are symmetric. Consider a family of matrices \( A(t) \) parametrized by a time-like parameter \( t \) such that

\[
A(0) = A
\]  

(4.2)

A typical family \( A(t) \) can be given by

\[
A(t) = A + tA_1 + t^2A_2 + ...
\]  

(4.3)

where all \( A_i \) are symmetric. Linear perturbation theory only uses \( A_1 \).

Suppose the typical eigenvalue of \( A(t) \) is \( \lambda(t) \) and the corresponding eigenvector is \( \psi(t) \):

\[
A(t) \psi(t) = \lambda(t) \psi(t)
\]  

(4.4)

We always normalize the eigenvector to unity:

\[
|\psi(t)|^2 = \langle \psi(t), \psi(t) \rangle = 1
\]  

(4.5)

Our primary goal is to compute \( d\lambda/dt, d\psi/dt \) and \( d^2\psi/dt^2 \). It can be shown that \( \lambda(t) \) and \( \psi(t) \) are differentiable with respect to \( t \). (This is not true if \( A \) is not symmetric.) At time
$t = 0$, the eigenvalues and eigenvectors of $A(t)$ coincide with those of $A$:

$$\lambda(0) = \lambda$$  \hspace{1cm} (4.6a)  

$$\psi(0) = \psi$$  \hspace{1cm} (4.6b)  

The first order perturbation equation is obtained by differentiating equation (4.4) with respect to $t$:

$$\frac{dA}{dt}\psi + A\frac{d\psi}{dt} = \frac{d\lambda}{dt}\psi + \lambda\frac{d\psi}{dt}$$  \hspace{1cm} (4.7)  

The second order perturbation equation is obtained by one more differentiation

$$\frac{d^2A}{dt^2}\psi + 2\frac{dA}{dt}\frac{d\psi}{dt} + A\frac{d^2\psi}{dt^2} = \frac{d^2\lambda}{dt^2}\psi + 2\frac{d\lambda}{dt}\frac{d\psi}{dt} + \lambda\frac{d^2\psi}{dt^2}$$  \hspace{1cm} (4.8)  

The derivatives $\frac{dA}{dt}$, $\frac{d\lambda}{dt}$, $\frac{d\psi}{dt}$ at $t = 0$ are the first order perturbations of $A$, $\lambda$, and $\psi$. The second derivatives $\frac{d^2A}{dt^2}$, $\frac{d^2\lambda}{dt^2}$, $\frac{d^2\psi}{dt^2}$ at $t = 0$ are the second order perturbations.

### 4.3.2 First order perturbation of simple eigenvalues and eigenvectors

Suppose that $\lambda$ is a simple eigenvalue (multiplicity 1) and that $\psi$ is the corresponding eigenvector. Construct the inner product of $\psi$ with the first perturbation equation (4.7):

$$\left< \psi, \frac{dA}{dt}\psi \right> + \left< \psi, A\frac{d\psi}{dt} \right> = \left< \psi, \frac{d\lambda}{dt}\psi \right> + \left< \psi, \lambda\frac{d\psi}{dt} \right>$$  \hspace{1cm} (4.9)  

Since $A$ is self-adjoint, it can be moved from $\frac{d\psi}{dt}$ to $\psi$ in the second term:

$$\left< \psi, \frac{dA}{dt}\psi \right> + \left< A\psi, \frac{d\psi}{dt} \right> = \left< \psi, \frac{d\lambda}{dt}\psi \right> + \left< \psi, \lambda\frac{d\psi}{dt} \right>$$  \hspace{1cm} (4.10)  

Substituting $A\psi = \lambda\psi$, we get

$$\frac{d\lambda}{dt} = \frac{\left< \psi, \frac{dA}{dt}\psi \right>}{\left< \psi, \psi \right>}$$  \hspace{1cm} (4.11)  

Since $\psi$ is normalized to unity (4.5), the final expression for the first perturbation of a simple eigenvalue is:

$$\frac{d\lambda}{dt} = \left< \psi, \frac{dA}{dt}\psi \right>$$  \hspace{1cm} (4.12)  

We now turn to the perturbation of the associated eigenvector $\psi$. Suppose that the full spectrum of $A$ is $\{\lambda_m, \psi_m\}$. Since $A$ is symmetric, the $\psi_m$ form a complete basis and can be chosen orthonormal. Our eigenvector $\psi$ is one of its members (if the sign is chosen correctly). Suppose that $\psi = \psi_M$ and $\lambda = \lambda_M$. The first derivative of $\frac{d\psi}{dt}$ can be decomposed with respect to the unperturbed basis $\{\psi_m\}$:

$$\frac{d\psi}{dt} = \sum_m c_m \psi_m$$  \hspace{1cm} (4.13)  

To determine the coefficient $c_m$, substitute this expansion into the first order perturbation
equation (4.7): 
\[ \frac{dA}{dt} \psi_M + A \sum_m c_m \psi_m = \frac{d\lambda}{dt} \psi_M + \lambda_M \sum_m c_m \psi_m \] (4.14) 

Since \( A\psi_m = \lambda_m \psi_m \), this becomes: 
\[ \frac{dA}{dt} \psi_M + \sum_m c_m \lambda_m \psi_m = \frac{d\lambda}{dt} \psi_M + \lambda_M \sum_m c_m \psi_m \] (4.15) 

Let \( N = \dim(A) \). The first \( N - 1 \) equations are obtained by constructing the inner products with \( \psi_n \) for \( n \neq M \): 
\[ \left< \psi_n, \frac{dA}{dt} \psi_M \right> + \sum_m \lambda_m c_m \left< \psi_n, \psi_m \right> = \frac{d\lambda}{dt} \left< \psi_n, \psi_M \right> + \lambda_M \sum_m c_m \left< \psi_n, \psi_m \right> \] (4.16) 

Since \( \psi_M \) is orthogonal to \( \psi_n \), \( \left< \psi_M, \psi_n \right> = \delta_{Mn} \), this is 
\[ \left< \psi_n, \frac{dA}{dt} \psi_M \right> + \lambda_n c_n = \lambda_M c_n \] (4.17) 

These \( N - 1 \) equations determine all but one of the components \( c_n \):
\[ c_n = \frac{\left< \frac{dA}{dt} \psi_M, \psi_n \right>}{\lambda_M - \lambda_n}, \quad n \neq M \] (4.18) 

The remaining component \( c_M \) vanishes since \( \frac{d\psi}{dt} \) is orthogonal to \( \psi \). This can be shown by differentiating the normalization condition (4.5) with respect to \( t \):
\[ 2 \left< \psi, \frac{d\psi}{dt} \right> = 0 \] (4.19) 

Thus \( c_M = 0 \).

4.3.3 Degenerate perturbation theory

Multiple eigenvalues arise in problems that possess symmetries, such as the eigenvalues on a sphere. The sphere is symmetric with respect to rotation and non-radial eigenfunctions lead to multiple eigenvalues. If the perturbation destroys the symmetry, the degeneracy is lifted and the spectrum splits.

Suppose that \( \lambda \) is a repeated eigenvalue of multiplicity \( M \) and that \( \psi_1, ..., \psi_M \) (or \( \psi_{m \leq M} \)) are corresponding eigenvectors. The unperturbed equation (4.4) only determines the \( M \)-dimensional subspace spanned by \( \psi_{m \leq M} \). If the perturbation lifts the degeneracy, there is a natural way to determine the unperturbed eigenvectors \( \psi_1, ..., \psi_M \) that we "should have chosen" as the limits of the perturbed eigenvectors:
\[ \psi_m = \lim_{t \to 0} \psi_m(t), \quad m \leq M \] (4.20) 

If the degeneracy is lifted only partially, this limit may only be computed for some of the
eigenvectors. For example, if a sphere is stretched along an axis into an ellipsoid, one of the 2l+1 eigenfunctions that correspond to \( \lambda_l = -l (l + 1) \) separates completely, while the remaining 2l form l degenerate pairs. If the degeneracy is lifted completely, then the first perturbation allows us to determine all of the unperturbed eigenvectors according to (4.20). We are about to show how to compute them algebraically rather than by taking a limit. But first we would like to make a special note of a characteristic shift: Every order perturbation of the eigenvectors is determined by the next order perturbation equation. Therefore, to determine the first order eigenfunction perturbations we have to analyze the second order perturbation equation which we do at the end of this section.

We start our analysis by collecting the terms containing \( \frac{d\psi}{dt} \) in the first perturbation equation (4.7):

\[
(A - \lambda I) \frac{d\psi}{dt} = \frac{d\lambda}{dt} \psi - \frac{dA}{dt} \psi
\]  

(4.21)

Since \( \lambda \) is an eigenvalue of \( A \) of multiplicity \( M \), \( (A - \lambda I) \) is singular. (Its rank \( N - M \).) The above linear system has a solution only if the right hand side is orthogonal to the nullspace of \( (A - \lambda I) \). Since the nullspace of \( (A - \lambda I) \) is spanned by \( \psi_{m \leq M} \), we have \( M \) equations that the unperturbed eigenvector \( \psi \) must satisfy:

\[
\left\langle \psi_{m}, \frac{d\lambda}{dt} \psi - \frac{dA}{dt} \psi \right\rangle = 0, \ m \leq M
\]  

(4.22)

These \( M \) equations are sufficient to determine \( \psi \), since we know the \( M \)-dimensional subspace to which it belongs. It is easy to decompose \( \psi \) in terms of the \( \psi_{m \leq M} \). Suppose that the components are \( d_m \):

\[
\psi = \sum_{m=1}^{M} d_m \psi_m
\]  

(4.23)

Substitute this expansion into the \( M \) equations (4.22):

\[
\sum_{m_1=1}^{M} \left\langle \psi_{m}, \frac{dA}{dt} \psi_{m_1} \right\rangle d_{m_1} = \frac{d\lambda}{dt} d_m
\]  

(4.24)

We get an \( M \times M \) eigenvalue problem with respect to the coefficients \( d_m \). It determines the unperturbed eigenvector \( \psi \) along with the first perturbation of the eigenvalue \( \frac{d\lambda}{dt} \). If all of its eigenvalues are distinct, this eigensystem yields \( M \) unperturbed eigenvectors and \( M \) first order eigenvalues corrections. If any of the \( M \) eigenvalue corrections are repeated then the original degeneracy has not been lifted entirely.

The first order eigenvector perturbations \( \frac{d\psi}{dt} \) can be determined in a similar fashion from the second order perturbation equation. Once again, we seek the decomposition of \( \frac{d\psi}{dt} \) with respect to the unperturbed eigenvectors (which are now known!):

\[
\frac{d\psi}{dt} = \sum_{m=1}^{N} e_m \psi_m
\]  

(4.25)
We need a total of $N$ equations to determine $\frac{d^2 \psi}{dt^2}$. As before, $N - M$ equations are readily available from the first order perturbation system (4.7). The remaining $M$ equation come from the second order perturbation equation (4.8). First, collect the terms containing $\frac{d^2 \psi}{dt^2}$

$$
(A - \lambda I) \frac{d^2 \psi}{dt^2} = \frac{d^2 \lambda}{dt^2} \psi + 2 \frac{d\lambda}{dt} \frac{d\psi}{dt} - \frac{d^2 A}{dt^2} \psi - 2 \frac{dA}{dt} \frac{d\psi}{dt}
$$

(4.26)

Similarly to linear system of equation (4.22), this system is singular. It is solvable only if the right hand side is orthogonal to the nullspace of $A$. This orthogonality property can be converted to $M$ equations in a way that parallels the analysis of $\frac{d\psi}{dt}$. The result is once again an $M \times M$ eigensystem that determines $\frac{d\psi}{dt}$ as well as the second order eigenvalue corrections $\frac{d^2 \lambda}{dt^2}$.

### 4.4 Perturbation of the Laplace operator

We now turn to the central part of this chapter, [24], [32], [36]. To the extent possible we proceed by analogy with the classical perturbation approach outlined above.

Suppose the unperturbed domain is $\Omega$, Figure 4-1. The system of equations that determines $\psi(z)$ consists of a bulk equation, a boundary condition and a normalization condition. The bulk equation is the standard Laplace eigenvalue equation:

$$
\nabla_i \nabla^i \psi + \lambda \psi = 0
$$

(4.27)

The sign in equation (4.27) is chosen according to the quantum mechanics convention and the operator is positive definite. The Dirichlet boundary condition is:

$$
\psi|_{z \in S} = 0
$$

(4.28)

Finally, $\psi$ is normalized to unity:

$$
\int_{\Omega} d\Omega \psi^2 = 1.
$$

(4.29)

The perturbation is induced by the moving boundary. The motion of the boundary is given as a family of curves $\Omega(t)$. Ideally, we would like to determine the following quantities:

1. First order perturbations of the eigenvalues $\lambda$
2. First order perturbations of the eigenfunctions $\psi$
3. Second order perturbations of the eigenvalues $\lambda$ ("Second Variation"). This computation will be performed in Chapter 5.

Depending on the symmetry of the initial domain and the complexity of the perturbation, we may be able to obtain closed form expressions for these quantities.
4.4.1 The perturbed system of equations

The system (4.27)-(4.29) is perturbed by differentiating the bulk in the $\frac{\partial}{\partial t}$ sense, the boundary condition in the $\frac{\partial}{\partial t}$ sense, and normalization condition in the $\frac{\partial}{\partial t}$ sense:

$$\nabla_i \nabla_i \frac{\partial \psi}{\partial t} + \frac{d\lambda}{dt} \psi + \lambda \frac{\partial \psi}{\partial t} = 0, \text{ in the interior of } \Omega \quad (4.30a)$$

$$\frac{\partial \psi}{\partial t} + C N^i \nabla_i \psi = 0, \text{ at the boundary } S \quad (4.30b)$$

$$\int_{\Omega} d\Omega \psi \frac{\partial \psi}{\partial t} = 0 \quad (4.30c)$$

$C$ is the velocity of the boundary $S$ (2.2), $\frac{d\lambda}{dt}$ is the perturbation of the eigenvalue, $\frac{\partial \psi}{\partial t}$ is the perturbation of the corresponding eigenfunction and $N^i$ is the normal to the boundary $S$ (2.15a).
4.4.2 Eigenvalue perturbation

First assume that the eigenvalue $\lambda$ is simple. We proceed by analogy with classical perturbation theory. Multiply the perturbed bulk equation (4.30a) by $\psi$ and integrate over $\Omega$:

\begin{equation}
0 = \int_{\Omega} d\Omega \left( \psi \nabla_i \psi_i \frac{\partial \psi_i}{\partial t} + \frac{d\lambda}{dt} \psi^2 + \lambda \frac{\partial \psi}{\partial t} \psi \right) \tag{4.31a}
\end{equation}

Integration by parts and (4.28), (4.29), (4.30c)

\begin{equation}
= -\int_{\Omega} d\Omega \nabla_i \psi \nabla_i \frac{\partial \psi_i}{\partial t} + \frac{d\lambda}{dt} \tag{4.31b}
\end{equation}

Divergence theorem and (4.30c)

\begin{equation}
= -\int_{S} dS i \nabla_i \psi \nabla_i \psi + \frac{d\lambda}{dt} \tag{4.31c}
\end{equation}

by (4.30b)

\begin{equation}
= \int_{S} dSC \left( N^i \nabla_i \psi \right)^2 + \frac{d\lambda}{dt} \tag{4.31d}
\end{equation}

Therefore

\begin{equation}
\frac{d\lambda}{dt} = -\int_{S} dSC \left( N^i \nabla_i \psi \right)^2 \tag{4.32}
\end{equation}

Equation (4.32) can be written slightly differently. Since $\psi$ vanishes at the boundary, the surface gradient $\psi$ is identically zero:

\begin{equation}
\nabla_\alpha \psi = 0 \tag{4.33}
\end{equation}

The surface gradient $\nabla_\alpha \psi$ is obtained from the spatial gradient $\nabla_i \psi$ by projection $\nabla_\alpha \psi = z_\alpha^i \nabla_i \psi$. Therefore

\begin{equation}
z_\alpha^i \nabla_i \psi = 0 \tag{4.34}
\end{equation}

We have:

\begin{equation}
0 = z_j^i z_\alpha^j \nabla_i \psi \tag{4.35a}
\end{equation}

by (2.16a)

\begin{equation}
= \left( \delta_j^i - N^i N_j \right) \nabla_i \psi \tag{4.35b}
\end{equation}

\begin{equation}
= \nabla_j \psi - N_j N^i \nabla_i \psi \tag{4.35c}
\end{equation}

Consequently, $\nabla_i \psi$ is colinear with the normal $N^i$:

\begin{equation}
\nabla_j \psi = N_j \left( N^i \nabla_i \psi \right) \tag{4.36}
\end{equation}

The gradient $\nabla_i \psi$ has essentially one degree of freedom - its magnitude. By "squaring" (4.36) we get:

\begin{equation}
\nabla_j \psi \nabla_j \psi = \left( N^i \nabla_i \psi \right)^2 \tag{4.37}
\end{equation}

This identity allows us to restate our central result:

\begin{equation}
\frac{d\lambda}{dt} = -\int_{S} dSC \nabla^i \psi \nabla_i \psi \tag{4.37}
\end{equation}

This is a central identity for us and will be referenced frequently throughout this work. It is analogous to the classical result (4.12). Equation (4.37) applies to arbitrary domains.

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4.4.3 Eigenfunction perturbation

The PDE system (4.30a)-(4.30c) can be used to determine $\frac{\partial \psi}{\partial t}$ for simple eigenvalues. A closed-form solution may be obtained for the sphere and the circle.

4.5 Eigenfunction perturbations on the sphere

4.5.1 The unperturbed spectrum on the sphere

The unperturbed spectrum of the sphere of radius $R$ (Figure 4-2) is

$$\psi_{l,m,n}(r, \theta, \psi) = Kr^{-\frac{1}{2}}J_{l+\frac{1}{2}} \left( \frac{\rho_{l,n}}{R} \right) Y_{lm}(\theta, \alpha), \quad l \geq 0, \; |m| \leq l, \; n > 0 \quad (4.38)$$

The radial component $J_{l+\frac{1}{2}}(r)$ is a Bessel function of the first kind $[4], [25]$, $Y_{lm}(\theta, \alpha)$ is a spherical harmonic and $K$ is the appropriate normalization constant which depends on $l$ and $n$. Finally, $\rho_{l,n}$ is the $n$-th root of $J_{l+\frac{1}{2}}(r)$ and the eigenvalue

$$\lambda_{l,n} = \frac{\rho_{l,n}^2}{R^2} \quad (4.39)$$

has multiplicity $2l + 1$.

We first focus on the radial eigenfunctions $\psi_n(r)$ which lead to simple eigenvalues. These
eigenfunctions correspond to \( l = 0 \) in equation (4.38). The \( n \)-th root of \( J_{\frac{1}{2}} (r) \), \( \rho_n \) is

\[
\rho_n = \rho_{0,n} = n\pi
\]  

and the corresponding eigenvalue is

\[
\lambda_n = \lambda_{0,n} = \frac{n^2 \pi^2}{R^2}
\]

The normalized eigenfunction \( \psi_n (r) \) is given by

\[
\psi_n (r) = \frac{\rho_n^{1/2}}{2R} r^{-\frac{1}{2}} J_{\frac{1}{2}} \left( \frac{\rho_n r}{R} \right)
\]

4.5.2 Perturbation of the radial eigenfunctions

We attempt to represent the solution as an infinite series in spherical harmonics:

\[
\frac{\partial \psi}{\partial t} = \sum_{l,m} s_{lm} (r) Y_{lm} (\theta, \psi)
\]

Expand the perturbation of the boundary \( C \) as a series in spherical harmonics

\[
C = R \sum_{l,m} C_{lm} Y_{lm} (\theta, \psi)
\]

Since \( \psi_n (r) \) is radial, the application of the perturbation formula (4.37) is straightforward:

\[
\frac{d \lambda_n}{dt} = -2 \frac{n^2 \pi^2}{R^2} D_{00}, \text{ where } D_{00} = \frac{C_{00}}{\sqrt{4\pi}}
\]

To determine \( \frac{\partial \psi}{\partial t} \), substitute the expansion (4.43) into the perturbed bulk equation (4.30a):

\[
\sum_{l,m} \left( \frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{d}{dr} s_{lm} (r) \right) - l (l + 1) \frac{1}{2} s_{lm} (r) + \lambda s_{lm} (r) \right) Y_{lm} (\theta, \alpha) = 0
\]

The spherical harmonics form a linearly independent set; therefore the above equation decouples into individual equations for \( s_{lm} (r) \). The equation for \( s_{00} \) is unlike the rest in two ways: it contains an inhomogeneous term and the constant of integration is determined from the orthogonality condition (4.30c) and not from the boundary condition (4.30b). Therefore we analyze this equation separately.

4.5.3 The \( l = 0 \) equation

The \( l = 0 \) equation is obtained by collecting the terms proportional to \( Y_{00} (\theta, \alpha) \):

\[
\frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{d}{dr} s_{00} (r) \right) + \rho_n^2 R^2 s_{00} (r) - D_{00} \rho_n^{5/2} R^{-3} r^{-\frac{3}{2}} J_{\frac{1}{2}} \left( \frac{\rho_n r}{R} \right) = 0
\]
The homogeneous part of this equation is the standard Bessel equation. The inhomogeneous part of the solution can be guessed (see Appendix below):

\[ s_{00}(r) = A_n D_0 \rho n^{-1/2} J_{\frac{3}{2}} \left( \frac{\rho_n r}{R} \right) - \frac{1}{4} D_0 \rho n^{-1/2} R^{-1} r^{-1/2} \left( J_{\frac{3}{2}} \left( \frac{\rho_n r}{R} \right) + 2 \rho_n \frac{r}{R} J_{-\frac{3}{2}} \left( \frac{\rho_n r}{R} \right) \right) \]  

(4.48)

\( A_n \) is an undetermined constant. It is not determined by the boundary condition (as one might think) since the particular solution satisfies the boundary condition and the homogeneous part vanishes identically. Regardless of the value of \( A_n \), the boundary condition is satisfied. Instead, \( A_n \) is determined from the "orthogonality condition" (4.30c). Somewhat anticlimactically, \( A_n = 0 \) and \( s_{00}(r) \) is therefore given by

\[ s_{00}(r) = -\frac{1}{4} D_0 \rho n^{-1/2} R^{-1} r^{-1/2} \left( J_{\frac{3}{2}} \left( \frac{\rho_n r}{R} \right) + 2 \rho_n \frac{r}{R} J_{-\frac{3}{2}} \left( \frac{\rho_n r}{R} \right) \right) \]  

(4.49)

### 4.5.4 The \( l \neq 0 \) equation

The \( l \neq 0 \) equation is

\[ \frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{d}{dr} s_{lm} \right) - l (l + 1) \frac{1}{r^2} s_{lm} + \rho_n^2 R^{-2} s_{lm} = 0 \]  

(4.50)

It is the standard Bessel equation whose solution is:

\[ s_{lm}(r) = A_{lm} r^{-\frac{1}{2}} J_{l+\frac{1}{2}} \left( \frac{\rho_n r}{R} \right) \]  

(4.51)

This time, the constant \( A_{lm} \) is determined by the boundary condition (4.30b). Orthogonality is automatically satisfied since all spherical harmonics \( Y_{l,m} \) with \( l \neq 0 \) are orthogonal to the unperturbed radial eigenfunctions. We have:

\[ s_{lm}(r) = -\frac{1}{2} C_{lm} \rho n^{3/2} R^{-1} \frac{J_{-\frac{1}{2}} \left( \frac{\rho_n r}{R} \right)}{J_{l+\frac{1}{2}} \left( \frac{\rho_n r}{R} \right)} r^{-1/2} J_{l+\frac{1}{2}} \left( \frac{\rho_n r}{R} \right) \]  

(4.52)

This completes the first order perturbation analysis on the sphere and we now turn to the case of the circle.

### 4.6 Eigenfunction perturbations on the circle

We proceed in complete analogy with the sphere. We do not detail any of the steps and only provide a summary of the results. The unperturbed spectrum is given by:

\[ \psi_{m,n}(r, \theta) = K J_m \left( \frac{\rho_{m,n} r}{R} \right) e^{im\theta} \]  

(4.53)

where \( \rho_{m,n} \) is the \( n \)-th root of the Bessel function \( J_m(r) \) and the corresponding eigenvalue is:

\[ \lambda_{m,n} = \frac{\rho_{m,n}^2}{R^2} \]  

(4.54)
The radial eigenfunctions are given by \( m = 0 \). The normalization constant for the radial case \( K_n = K_{0,n} \) is given by \( K_n^{-2} = \pi R^2 J_1^2 (\rho_n) \). Therefore the radial eigenfunctions \( \psi_n (r) \) are given by

\[
\psi_n (r) = \psi_{0,n} (r, \theta) = \frac{1}{\sqrt{\pi R J_1^2 (\rho_n)}} J_0 \left( \rho_n \frac{r}{R} \right) \tag{4.55}
\]

The perturbation of the radial eigenvalues is obtained by an application of equation (4.37):

\[
\frac{d\lambda_n}{dt} = -2\lambda_n C_0 \tag{4.56}
\]

The eigenfunction perturbation \( \frac{\partial \psi_n}{\partial t} \) is

\[
\frac{\partial \psi_n}{\partial t} = \sum_{m=-\infty}^{\infty} s_{m,n} (r) e^{im\theta} \tag{4.57}
\]

where

\[
s_{0,n} (r) = -C_0 \frac{1}{\sqrt{\pi R J_1 (\rho_n)}} \left( J_0 \left( \rho_n \frac{r}{R} \right) + \rho_n \frac{r}{R} J_1 \left( \rho_n \frac{r}{R} \right) \right) \tag{4.58}
\]

\[
s_{m,n} (r) = C_m \frac{\rho_n}{\sqrt{\pi R J_m (\rho_n)}} J_m \left( \rho_n \frac{r}{R} \right) \tag{4.59}
\]

In Chapter 5 we consider a specific perturbation of the circle – a transformation to a regular polygon – where we will apply the expressions (4.56)-(4.59) that we have just obtained.

### 4.7 Energy splitting on the sphere

#### 4.7.1 Introduction and general theory

The eigenvalues \( \lambda_{l,n} \) on the sphere have multiplicity \( 2l+1 \). In this section, we shall drop the index \( l \) and label the eigenvalues \( \lambda_{l,n} \) simply as \( \lambda_n \). In general, the perturbation lifts the degeneracy, but if the perturbation itself has symmetry then the degeneracy may be partially preserved. For example, if the perturbation has azimuthal symmetry then of the \( 2l + 1 \) eigenvalues, one will separate completely and the rest will form \( l \) degenerate pairs.

Our analysis parallels the classical case. By analogy, the first order eigenfunction perturbation is determined from the second order perturbation equation. We do not go that far and content ourselves with the first order eigenvalue perturbation.

Consider the subspace (of dimension \( 2l + 1 \)) of eigenfunctions associated with eigenvalue \( \lambda_{l,m,n} \). Let \( \{ \psi_m, |m| \leq l \} \) be an orthonormal basis for this subspace. The standard choice of the basis is this (4.38). Suppose that a solution to the perturbed system (4.30a)-(4.30c) is decomposed with respect to \( \{ \psi_m, |m| \leq l \}; \)

\[
\psi = d^m \psi_m, \text{ summation over } m \text{ implied}
\]

Substitute \( \psi \) into the perturbed system (4.30a)-(4.30c). Multiply the bulk equation successively
by each $\psi^*_{m_1}$,

$$0 = \left\{ \int_\Omega d\Omega \psi^*_{m_1} \nabla_i \nabla^i \partial \psi + \frac{d\lambda}{dt} \int_\Omega d\Omega \partial \psi^*_{m_1} \psi^*_{m_1} \psi^*_{m_1} \right\} (4.60a)$$

Integration by parts twice,

divergence theorem twice

$$= \left\{ \int_S dS \nabla_i \psi^*_{m_1} \nabla^i \partial \psi - \int_\Omega d\Omega N^i \nabla_i \psi^*_{m_1} \partial \psi + \frac{d\lambda}{dt} \int_\Omega d\Omega \partial \psi^*_{m_1} \psi^*_{m_1} \right\} (4.60b)$$

Since $\nabla_i \nabla_i \psi_{m_1} = -\lambda \psi_{m_1}$

$$= \left\{ - \int_S dS \nabla_i \psi^*_{m_1} \nabla^i \partial \psi + \frac{d\lambda}{dt} \int_\Omega d\Omega \partial \psi^*_{m_1} \psi^*_{m_1} \right\} (4.60c)$$

Unperturbed

t boundary condition

$$= \left\{ - \int_S dS \nabla_i \psi^*_{m_1} \nabla^i \partial \psi + \frac{d\lambda}{dt} d_{m_1} \right\} (4.60d)$$

Orthonormality of the basis

$$= \int_S dS \nabla_i \psi^*_{m_1} \nabla^i \partial \psi + \frac{d\lambda}{dt} d_{m_1} \right\} (4.60e)$$

Perturbed

t boundary condition

$$= \int_S dS \nabla_i \psi^*_{m_1} \nabla^i \partial \psi + \frac{d\lambda}{dt} d_{m_1} \right\} (4.60f)$$

$$= \int_S dS C \nabla_i \psi^*_{m_1} \nabla^i \partial \psi + \frac{d\lambda}{dt} d_{m_1} \right\} (4.60g)$$

The unknown component $d^m$ and the corresponding eigenvalue corrections $\frac{d\lambda}{dt}$ are therefore determined from the eigenvalue problem:

$$\left( \int_S dS C \nabla_i \psi^*_{m_1} \nabla^i \partial \psi \right) d^m = -\frac{d\lambda}{dt} d_{m_1} \right\} (4.61)$$

This system applies to an arbitrary domain $\Omega$ and perturbation $C$. If the initial configuration $\Omega$ is the sphere then

$$N^i \nabla_i \psi_{m_1} \right|_{r=R} = \frac{\partial \psi_{m_1}}{\partial r} \right|_{r=R} \right\} (4.62a)$$

$$= K \frac{\rho_{l,n}}{R^{3/2}} \left( l_1 + \frac{1}{2} \right) (l_{1+n}) Y_{l} (\theta, \alpha) \right\} (4.62b)$$

Therefore, for the sphere the coefficients $d^m$ satisfy the following eigenvalue system:

$$B^m_{m_1} d^m + \frac{d\lambda}{dt} d_{m_1} = 0 \right\} (4.63)$$

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where

$$B_{m}^{m_1} = K^2 \lambda_{n,r}^{2} r_{l+\frac{1}{2}}^{2} \left( \rho_{n} \right) \left[ \begin{array}{c} \cdots \cr \int_{r=1}^{\infty} \frac{dS_{R}^{2}}{r_{RM}} Y_{lm} Y_{lm}^{*} \cr \cdots \cr \cdots \end{array} \right] \right] \right]$$

(4.64)

Matrix (4.64) can be expressed in closed form:

$$B_{m}^{m_1} = K^2 \lambda_{n,r}^{2} r_{l+\frac{1}{2}}^{2} \left( \rho_{n} \right) \left[ \begin{array}{c} \text{Typical term } B_{m}^{m_1} : \cr \sum_{L=0,M}^{\infty} C_{LM} \sqrt{\frac{2L+1}{4\pi}} (2l+1) \left( \begin{array}{ccc} L & l & l \\ 0 & 0 & 0 \\ M & m & -m_1 \end{array} \right) \end{array} \right]$$

(4.65)

where \( \left( \begin{array}{ccc} l_1 & l_2 & l_3 \\ m_1 & m_2 & m_3 \end{array} \right) \) is the Wigner 3j-symbol [47], [8].

This completes our analysis of the first order eigenvalue perturbation.

### 4.7.2 Example: ellipsoidal perturbation of the sphere

This problem was first studied by Migdal [32] who was interested in the energy spectrum of an electron trapped in an ellipsoidal cavity. Below we outline his approach and show that it leads to the same results as our methodology.

**Family of ellipsoids**

Consider the perturbation into the ellipsoid with semiaxes \( R (1 + \Delta X) \), \( R (1 + \Delta Y) \), and \( R (1 + \Delta Z) \). The ellipsoid is given parametrically as:

$$\begin{bmatrix} z^1 \\ z^2 \\ z^3 \end{bmatrix} = \begin{bmatrix} R (1 + \Delta X) \sin \theta \cos \phi \\ R (1 + \Delta Y) \sin \theta \sin \phi \\ R (1 + \Delta Z) \cos \theta \end{bmatrix}$$

(4.66)

Define the evolution of the ellipsoid by letting the semi-axes change linearly from the radius of the sphere to their eventual values. One such family is

$$\begin{bmatrix} z^1 \\ z^2 \\ z^3 \end{bmatrix} (\theta, \psi, t) = \begin{bmatrix} R (1 + \Delta X t) \sin \theta \cos \phi \\ R (1 + \Delta Y t) \sin \theta \sin \phi \\ R (1 + \Delta Z t) \cos \theta \end{bmatrix}$$

(4.67)

For future reference, the evolution of volume \( V(t) \) is

$$V(t) = \frac{4}{3} \pi R^3 (1 + \Delta X t) (1 + \Delta Y t) (1 + \Delta Z t)$$

(4.68)

The derivative of \( V(t) \) with respect to \( t \) at \( t = 0 \) is

$$\left. \frac{dV(t)}{dt} \right|_{t=0} = \frac{4\pi}{3} (\Delta X + \Delta Y + \Delta Z) \cdot$$

(4.69)
Consequently, the volume is instantaneously conserved at \( t = 0 \) if and only if \( \Delta x + \Delta y + \Delta z = 0 \).

We must now determine \( C \) so that we can construct the matrix \( B^{m_1}_m \). We follow the recipe outlined in Chapter 2. First determine the object \( v^i \) defined by equation (2.4)

\[
v^i (\theta, \psi, t) = \frac{\partial z^i (\theta, \psi, t)}{\partial t} = \begin{bmatrix} R \Delta x \sin \theta \cos \phi \\ R \Delta x \sin \theta \sin \phi \\ R \Delta z \cos \theta \end{bmatrix}
\]  
(4.70)

The object \( v^i \) does not depend on time.

The normal \( N^i \) at \( t = 0 \) (eqs. (2.15a)-(2.15c)) is given by

\[
N^i = \begin{bmatrix} \sin \theta \cos \psi \\ \sin \theta \sin \psi \\ \cos \theta \end{bmatrix}
\]
(4.71)

Thus, the velocity \( C \) (eq. 2.2) at \( t = 0 \) is

\[
C = v^i N_i = R \begin{bmatrix} \Delta x \sin \theta \cos \phi \\ \Delta y \sin \theta \sin \phi \\ \Delta z \cos \theta \end{bmatrix} \begin{bmatrix} \sin \theta \cos \phi \\ \sin \theta \sin \phi \\ \cos \theta \end{bmatrix} = R (\Delta x \sin^2 \theta \cos^2 \phi + \Delta y \sin^2 \theta \sin^2 \phi + \Delta z \cos^2 \theta)
\]
(4.72a)

\[
\begin{bmatrix} C_{2,-2} \\ C_{2,-1} \\ C_{2,0} \\ C_{2,1} \\ C_{2,2} \end{bmatrix} = \frac{1}{3 \sqrt{5}} R^2 \begin{bmatrix} \sqrt{6} (\Delta x - \Delta y) \\ 0 \\ 2 (-\Delta x + 2 \Delta z - \Delta y) \\ 0 \\ \sqrt{6} (\Delta x - \Delta y) \end{bmatrix}
\]
(4.72b)

Decomposition of \( C \) in terms of the spherical harmonics

It will prove insightful to represent \( C \) as a Fourier series. (This is not needed for the computation of the first order perturbation for simple eigenvalues.) The only non-zero \( C_{l,m} \) are:

\[
D_{00} = \frac{C_{00}}{\sqrt{4\pi}} = \frac{1}{3} (\Delta x + \Delta y + \Delta z)
\]
(4.72c)

\[
\begin{bmatrix} C_{2,-2} \\ C_{2,-1} \\ C_{2,0} \\ C_{2,1} \\ C_{2,2} \end{bmatrix} = \frac{1}{3 \sqrt{5}} R^2 \begin{bmatrix} \sqrt{6} (\Delta x - \Delta y) \\ 0 \\ 2 (-\Delta x + 2 \Delta z - \Delta y) \\ 0 \\ \sqrt{6} (\Delta x - \Delta y) \end{bmatrix}
\]
(4.72d)

The \( l = 0 \) component \( C_{0,0} \) is responsible for the radial expansion of the sphere. It vanishes when the volume is instantaneously conserved. The \( l = 1 \) components \( C_{1,m} \) move the sphere as a rigid body. These vanish also since our ellipsoid is transforming without moving as a whole. The \( l = 2 \) coefficients are non-zero and all of the remaining \( C_{l,m} \) are zero! This is why perturbations proportional to \( Y_{2,m} \) are called ellipsoidal.

Perturbation of the radial eigenvalues

We first compute the eigenvalue perturbations \( \frac{d \lambda_n}{dt} \) for radial eigenfunctions \( \psi_n \). These eigen-
values are not degenerate and we can therefore use equation (4.37):

\[
\frac{d\lambda_n}{dt} = \left\{ -\left(\frac{1}{2} (n\pi)^{3/2} R^{5/2} J_{\frac{n}{2}} (n\pi) \right)^2 \times \int_{-\pi}^{\pi} \int_0^\pi R \left( \Delta_X \sin^2 \theta \cos^2 \phi + \Delta_Y \sin^2 \theta \sin^2 \phi + \Delta_Z \cos^2 \theta \right) R^2 \sin \theta d\theta d\phi \right\} (4.73)
\]

Thus,

\[
\frac{d\lambda_n}{dt} = -\frac{2}{3} (\Delta_X + \Delta_Y + \Delta_Z) \lambda_n \tag{4.74}
\]

If the volume is instantaneously conserved (4.69), then the radial eigenvalues are also instantaneously unchanged.

**Non-radial eigenvalues**

We form the matrix \(B\) from equation (4.64). For eigenvalue \(\lambda_{l,n}\) of multiplicity \(2l + 1\), \(B\) is a \((2l + 1) \times (2l + 1)\) matrix. In this example, we study the splitting of \(\lambda_{2,1}\):

\[
R^2 \int_{-\pi}^{\pi} \int_0^1 dx d\phi R \left( \Delta_X \left(1 - x^2\right) \cos^2 \phi + \Delta_Y \left(1 - x^2\right) \sin^2 \phi + \Delta_Z x^2 \right) \times
\[
\begin{bmatrix}
B_{-2}^{-1} \\
B_{-1}^{-1} \\
B_0^{-1} \\
B_1 \\
B_2 
\end{bmatrix}
= 
\begin{bmatrix}
\left(\frac{1}{4} \sqrt{\frac{15}{2\pi}} \right)^2 (1 - x^2) \\
\left(\frac{1}{4} \sqrt{\frac{15}{2\pi}} \right)^2 x^2 (1 - x^2) \\
\left(\frac{5}{4\pi} \left(\frac{3}{2} x^2 - \frac{1}{2}\right)\right)^2 \\
\left(\frac{3}{4\pi} \left(\frac{3}{2} x^2 - \frac{1}{2}\right)\right)^2 \\
\left(\frac{1}{4} \sqrt{\frac{15}{2\pi}} \right)^2 (1 - x^2)^2
\end{bmatrix} (4.75)
\]

which yields:

\[
\begin{bmatrix}
B_{-2}^{-1} \\
B_{-1}^{-1} \\
B_0^{-1} \\
B_1 \\
B_2 
\end{bmatrix}
= \frac{R^3}{7} \begin{bmatrix}
3\Delta_Y + 3\Delta_X + \Delta_Z \\
2\Delta_Y + 2\Delta_X + 3\Delta_Z \\
\frac{5}{3}\Delta_Y + \frac{5}{3}\Delta_X + \frac{11}{3}\Delta_Z \\
2\Delta_Y + 2\Delta_X + 3\Delta_Z \\
3\Delta_Y + 3\Delta_X + \Delta_Z
\end{bmatrix} (4.76)
\]

Consequently, the final expression for \(B_{m1}\) is:

\[
B_{m1} = \frac{1}{7} R^3 \begin{bmatrix}
A = 3\Delta_Y + 3\Delta_X + \Delta_Z & 0 & 0 & 0 & 0 \\
0 & B = 2\Delta_Y + 2\Delta_X + 3\Delta_Z & 0 & 0 & 0 \\
0 & 0 & C = \frac{5}{3}\Delta_Y + \frac{5}{3}\Delta_X + \frac{11}{3}\Delta_Z & 0 & 0 \\
0 & 0 & 0 & B & A
\end{bmatrix}
\]

(4.77)

The eigenvalue corrections appear on the main diagonal. The degeneracy is not lifted completely since the eigenvalue corrections \(A\) and \(B\) are repeated.
4.8 Migdal’s approach to eigenvalue perturbation

Migdal was interested in the calculation of the spectrum of a quantum particle trapped in an ellipsoidal cavity [32], [24]. Migdal’s idea was to adjust the coordinate system in such a way that the ellipsoid becomes a sphere. Then the perturbation of the interface re-emerges as a perturbation of the operator and standard theory is applied.

Suppose that \( \beta \) is a small parameter and that \( RX(\beta) \), \( RY(\beta) \), and \( RZ(\beta) \) are the semiaxes of the ellipsoid:

\[
\begin{align*}
X(\beta) &= 1 + \beta \Delta_X \tag{4.78a} \\
Y(\beta) &= 1 + \beta \Delta_Y \tag{4.78b} \\
Z(\beta) &= 1 + \beta \Delta_Z \tag{4.78c}
\end{align*}
\]

where \( \Delta_X \), \( \Delta_Y \), and \( \Delta_Z \) are on the order of unity and characterize the relative magnitudes of the perturbations of the semiaxes.

For a given value of \( \beta \), introduce new variables

\[
\begin{align*}
z'^1 &= z^1 / X(\beta) \tag{4.79a} \\
z'^2 &= z^2 / Y(\beta) \tag{4.79b} \\
z'^3 &= z^3 / Z(\beta) \tag{4.79c}
\end{align*}
\]

In this new coordinate system, the ellipsoid has the same equation as the sphere in the original coordinate system. A simple change of variables yields the Laplacian in the new coordinate system. For example,

\[
\frac{\partial^2 \psi}{\partial x^2} = \frac{\partial}{\partial x} \left( \frac{\partial \psi}{\partial x} \right) \tag{4.80a}
\]

\[
= \frac{\partial}{\partial x'} \left( \frac{\partial \psi}{\partial x'} \frac{\partial x'}{\partial x} \right) \frac{\partial x'}{\partial x} = \frac{\partial^2 \psi}{\partial x'^2} \left( \frac{1}{X(\beta)} \right)^2 \tag{4.80b}
\]

\[
= \frac{\partial^2 \psi}{\partial x'^2} \left( 1 - 2\beta \Delta_X + O(\beta^2) \right) \tag{4.80c}
\]

Suppose that \( H' \) is the linear correction to the Laplacian in the new coordinate system. It is defined by the following identity

\[
\Delta' = \Delta + \beta H' + O(\beta^2). \tag{4.81}
\]

The \( H' \) is given by

\[
H' = -2\Delta_X \frac{\partial^2 \psi}{\partial x'^2} + 2\Delta_Y \frac{\partial^2 \psi}{\partial y'^2} + 2\Delta_Z \frac{\partial^2 \psi}{\partial z'^2} \tag{4.82a}
\]

\[
= -2 \left( \Delta_X \frac{\partial^2 \psi}{\partial x'^2} + \Delta_Y \frac{\partial^2 \psi}{\partial y'^2} + \Delta_Z \frac{\partial^2 \psi}{\partial z'^2} \right) \tag{4.82b}
\]

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Perturbation of radial eigenvalues

The eigenvalue correction can now by computed by applying equation (4.11). To perform the necessary integration, express $\frac{\partial^2 \psi_n}{\partial z^2}$ in polar coordinates:

\[
\frac{\partial^2 \psi_n}{\partial z^2} = \frac{\partial}{\partial z'} \left( \frac{d\psi_n}{dr} \left( \frac{\partial r}{\partial z'} \right) \right)
\]
\[
= \frac{d^2 \psi_n}{dr^2} \left( \frac{\partial r}{\partial z'} \right)^2 + \frac{d\psi_n}{dr} \frac{\partial^2 r}{\partial z'^2}
\]
\[
= \frac{d^2 \psi_n}{dr^2} \cos^2 \theta + \frac{d\psi_n}{dr} \frac{1}{r} \sin^2 \theta
\]

Then

\[
\left\langle \psi, 2\Delta_z \frac{\partial^2}{\partial z^2} \psi \right\rangle = -2\pi \int_0^\pi \left( \int_0^R \psi \left( \frac{d^2 \psi}{dr^2} \cos^2 \theta + \frac{d\psi}{dr} \frac{1}{r} \sin^2 \theta \right) r^2 \sin \theta dr \right) d\theta
\]
\[
= \frac{1}{3} n^2 \pi^2 = \frac{2}{3} \Delta_z \lambda_n
\]

Combining the $\frac{\partial^2 \psi}{\partial \beta^2}$, $\frac{\partial^2 \psi}{\partial \beta^2}$, and $\frac{\partial^2 \psi}{\partial z^2}$ terms we get

\[
\frac{d\lambda_n}{d\beta} = -\frac{2}{3} (\Delta_X + \Delta_Y + \Delta_z) \lambda_n.
\]

This is entirely consistent with our previous result (4.74).

4.9 Appendix: Solution of the inhomogeneous "l = 0" equation

As we stated in the text, the solution of the "l = 0" equation

\[
\frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{d}{dr} s_{00} (r) \right) + \frac{\rho_n}{R^2} s_{00} (r) - \frac{\sigma/2}{R^3} r^{-1/2} J_1 \left( \rho_n \frac{r}{R} \right) C_{00} = 0
\]

can be easily guessed. Roughly speaking, $s_{00} (r)$ represents the perturbation of the radial eigenfunctions corresponding to the radial perturbation of the boundary. However, such correction can be found directly. Let

\[
R (t) = R (1 + Y_{00} C_{00} t)
\]

and so

\[
\psi_n (r, t) = \frac{\rho_n^{1/2}}{2R (1 + D_{00} t)} r^{-1/2} J_1 \left( \rho_n \frac{r}{R} \right) \left( \rho_n \frac{r}{R} \right)
\]

Therefore,

\[
\frac{\partial \psi_n (r, t)}{\partial t} \bigg|_{t=0} = -\frac{1}{4} D_{00} \rho_n^{1/2} r^{-1/2} R^{-1} \left( J_{-1/2} \left( \rho_n \frac{r}{R} \right) + 2J_{-1/2} \left( \rho_n \frac{r}{R} \right) \rho_n \frac{r}{R} \right)
\]

We can reasonably expect that this function satisfies the "l = 0" equation and, in fact, it does!
Chapter 5

Electron Bubbles: Shapes That Minimize $\Psi \lambda + \sum \int_S dS + \Pi \int_\Omega d\Omega$

5.1 Introduction

Electron bubbles are an area of active research, past [33], [16] and present [10], [17], [18], [29], [30], [22], [14]. They form when electrons penetrate liquid helium. The electrons repel the helium atoms and form a cavity virtually free of helium. We study their equilibrium and stability properties. In particular, we would like to determine the equilibrium stable shapes assumed by bubbles occupied by electrons in excited states [30], [22].

In mathematical terms, the problem of equilibrium is to minimizing the energy

$$E = \frac{h^2}{8\pi^2 m} - \lambda + \sigma \int_S dS + P \int_\Omega d\Omega,$$

where $\sigma$ is the surface tension density, $P$ is the hydrostatic pressure and $\lambda$ is the eigenvalue of the Laplace operator. $h$ is Planck's constant and $m$ is the mass of the electron.

Electrons can be in excited states and this adds a great deal of richness to this problem. Excited states correspond to the different eigenvalues of the Laplace operator and it is valuable to discover the equilibrium shapes for each eigenvalue. The states are classified according the value of spherical harmonic number $l$ and the number of the root $n$. The electrons in radially symmetric states $l = 0$ are known as the $S$ electrons. The ground state, $n = 1$, electrons are known as the $1S$, and the next radially symmetric energy state $n = 2$ is known as the $2S$, etc. The $l = 1$ electrons are known as the $P$ electrons and the $l = 2$ electrons are the $D$ electrons. Our study shall focus on the $1S$, $2S$, $1P$, and the $1D$ electrons. We shall talk about the surprising result that the equilibrium spherical configuration for the $2S$ electron bubbles is morphologically unstable [14]. In fact, all of the $S$ electrons are morphologically unstable for $n \geq 2$ but only the $2S$ are physically significant. We shall indicate the non-spherical stable configurations for these electron bubbles.
5.2 Equilibrium Equations

5.2.1 Equilibrium equation for general geometries

We analyze the energy expression

\[ E = \Psi \lambda + \Sigma \int_S dS + \Pi \int_\Omega d\Omega \quad (5.2) \]

Our goal is to minimize this energy with respect to the location of the interface \( S \). Equation (4.37) from Chapter 4 states that the derivative of the eigenvalue \( \lambda \) is given by

\[ \frac{d\lambda}{dt} = - \int_S dSC \nabla^i \psi \nabla_i \psi, \quad (5.3) \]

where \( \psi \) is the corresponding eigenfunction. By application of (2.12) and (2.13) from Chapter 2, we have

\[ \frac{d}{dt} \int_S dS = - \int_S dSC B_\alpha \]
\[ \frac{d}{dt} \int_\Omega d\Omega = \int_\Omega d\Omega C \]

Combining the three ingredients we obtain a complete expression for the first energy variation

\[ \delta E = \int_S dSC \left( -\Psi \nabla^i \psi \nabla_i \psi - \Sigma B_\alpha + \Pi \right), \quad (5.4) \]

We treat \( C \) as an independent variation and thus derive the equilibrium equation

\[ \Psi \nabla^i \psi \nabla_i \psi + \Sigma B_\alpha - \Pi = 0. \quad (5.5) \]

This equation defines the unknown location of the interface. This equation is highly nonlinear and, in general, can only be solved numerically. There is one family of equilibrium configurations that is easy to analyze. It is circles in two dimensions and spheres in three dimensions. For both geometries, the equilibrium equation becomes an algebraic equation that determines the equilibrium radius \( \Gamma \). We will consider both cases throughout this chapter.

5.2.2 Equilibrium equation for the sphere

For the sphere of radius \( \Gamma \), the radial eigenfunctions are given by

\[ \psi_n (r) = \frac{\rho_n^{1/2}}{2 \Gamma} r^{-\frac{1}{2}} J_{\frac{1}{2}} \left( \rho_n \frac{r}{\Gamma} \right), \] \text{ with } \rho_n = n\pi, \text{ and } \lambda_n = \frac{\rho_n^2}{\Gamma^2} \quad (5.6) \]

where \( J_m (r) \) is the Bessel function of order \( m \), \( \rho_n \) is its \( n \)-th root.

Due to the radial symmetry of \( \psi_n \), its gradient contains only a radial component. Since the
radial derivative of \( \psi_n \) is given by

\[
\frac{d\psi_n}{dr} = -\frac{1}{2} \frac{\rho_n^{3/2}}{r} r^{-1/2} J_5 \left( \frac{\rho_n}{\Gamma} \right),
\]

the equilibrium equation becomes

\[
\frac{\Psi n^2 \pi}{4 \Sigma} \frac{1}{\Gamma^5} \frac{1}{\Gamma} = 1 - \frac{\Pi}{2 \Sigma} = 0
\]

(5.8)

For \( \Pi = 0 \), this equation allows a single positive solution. Correspondingly, for the ground state electron \( (n = 1) \), the equilibrium radius \( \Gamma_0 \) is given by:

\[
\Gamma_0 = 4 \sqrt{\frac{\pi \Psi}{4 \Sigma}}
\]

(5.9)

We use the characteristic length scale \( \Gamma_0 \) to non-dimensionalize the equilibrium equation (5.5). Introduce two dimensionless parameters \( y \) and \( a \):

\[
y = \frac{\Gamma_0}{\Gamma}; \quad a = \frac{\Pi \Gamma_0}{2 \Sigma}
\]

(5.10)

The parameter \( y \) is dimensionless length and \( a \) is the ratio of pressure to surface tension. In particular, \( a > 0 \) if and only if \( \Pi > 0 \). In terms of \( y \), \( a \), and \( n \), the equilibrium equation reads:

\[
n^2 y^5 - y - a = 0
\]

(5.11)

The graph of \( n^2 y^5 - y - a \) can be seen in Figure 5-1 for several values of \( a \).

5.2.3 Equilibrium configuration for the circle

The radial eigenfunctions \( \psi_n \) are given by

\[
\psi_n (r) = \frac{1}{\sqrt{\pi \Gamma^3 J_1 (\rho_n)}} J_0 \left( \frac{\rho_n}{\Gamma} \right), \text{ with } \lambda_n = \frac{\rho_n^2}{\Gamma^2}
\]

(5.12)

where \( J_m (r) \) is the Bessel function of order \( m \) and \( \rho_n \) is the \( n \)-th root of \( J_0 \). First six zeros of \( J_0 \) and the corresponding radial eigenvalues for the circle are given in Table 5.1.

<table>
<thead>
<tr>
<th>Bessel root</th>
<th>Eigenvalue</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \rho_1 = 2.40482555769577 )</td>
<td>( \lambda_1 = 5.783188596294677 )</td>
</tr>
<tr>
<td>( \rho_2 = 5.5200711028631 )</td>
<td>( \lambda_2 = 30.4712623436621 )</td>
</tr>
<tr>
<td>( \rho_3 = 8.65372791291101 )</td>
<td>( \lambda_3 = 74.8870679096951 )</td>
</tr>
<tr>
<td>( \rho_4 = 11.7915344390143 )</td>
<td>( \lambda_4 = 139.040284426460 )</td>
</tr>
<tr>
<td>( \rho_5 = 14.9309177084878 )</td>
<td>( \lambda_5 = 222.932303617635 )</td>
</tr>
<tr>
<td>( \rho_6 = 18.0710639679109 )</td>
<td>( \lambda_6 = 326.563426434833 )</td>
</tr>
</tbody>
</table>

Table 5.1: Six lowest roots of \( J_0 \) and corresponding eigenvalues.
Figure 5-1: The graph of $y^5 - y - a$. The positive root indicates an equilibrium spherical electron bubbles. At some negative pressures, there are two equilibrium bubbles. Only the smaller one (larger root) is radially stable. However, it is quite common for a physical system to be radially stable but morphologically unstable [12], [13].

Due to the radial symmetry of $\psi_n$, its gradient contains only a radial component. Since the radial derivative of $\psi_n$ is

$$\frac{d\psi_n}{dr} = -\frac{1}{\sqrt{\pi \Gamma^2}} \frac{\rho_n}{J_1(\rho_n)} J_1(\rho_n \frac{r}{\Gamma})$$

(5.13)

the equilibrium equation for a circle of radius $\Gamma$ is given by.

$$\Psi \frac{\rho_n^2}{\pi \Sigma \Gamma^4} - \frac{1}{\Gamma} - \frac{\Pi}{\Sigma} = 0$$

(5.14)

For $\Pi = 0$, this equation allows a single solution. For the ground state configuration $n = 1$, we have:

$$\Gamma_0 = \sqrt[3]{\frac{\Psi \rho_1^2}{\pi \Sigma}}$$

(5.15)

The dimensionless parameters $y$ and $a$ are defined a little differently from 5.10):

$$y = \frac{\Gamma_0}{\Gamma}; \quad a = \frac{\Pi \Gamma_0}{\Sigma}$$

(5.16)

The dimensionless equilibrium equation is

$$\frac{\lambda_n}{\lambda_1} y^4 - y - a = 0$$

(5.17)
5.3 The second energy variation and the stability criteria

5.3.1 Expression for general geometries

The second energy variation is obtained by differentiating the equilibrium equation (5.5) with respect to t:

$$
\delta^2 E = -\frac{d}{dt} \int_S dS \left( \psi \nabla^i \psi \nabla_i \psi + \Sigma B_\alpha^a \right)
$$

(5.18a)

by (2.13) = \left\{ \begin{array}{l}
\int_S dS \frac{\delta}{\delta t} \left( C \left( \psi \nabla^i \psi \nabla_i \psi + \Sigma B_\alpha^a \right) \right) \\
- \int_S dS \frac{\delta^2 C}{\delta t^2} \left( \psi \nabla^i \psi \nabla_i \psi + \Sigma B_\alpha^a \right)
\end{array} \right\}

(5.18b)

by (2.9) = \left\{ \begin{array}{l}
\int_S dS \frac{\delta}{\delta t} \left( \psi \nabla^i \psi \nabla_i \psi + \Sigma B_\alpha^a \right) \\
+ \int_S dS \frac{\delta^2 C}{\delta t^2} \left( \psi \nabla^i \psi \nabla_i \psi + \Sigma B_\alpha^a \right) \\
- \int_S dS \frac{\delta^2 C}{\delta t^2} \left( \psi \nabla^i \psi \nabla_i \psi + \Sigma B_\alpha^a \right)
\end{array} \right\}

(5.18c)

The most significant simplification comes from the fact that the second energy variation is of interest only for equilibrium configurations. Therefore, the equilibrium equation (5.5) kills the first and the last terms:

$$
\delta^2 E = \int_S dS \frac{\delta}{\delta t} \left( \psi \nabla^i \psi \nabla_i \psi + \Sigma B_\alpha^a \right)
$$

(5.19)

by (2.9) and (2.10f) = \int_S dS \left( 2\psi \nabla^i \left( \frac{\delta \psi}{\delta t} + C N^i \nabla_i \psi \right) \nabla_i \psi + \Sigma \left( \nabla^a \nabla_a C + C B^a_\beta B_\beta^a \right) \right)

The final expression for the second energy variation that applies to equilibrium configuration of arbitrary shapes is obtained by a single application of the Chain Rule (2.8) to the \( \frac{\delta \psi}{\delta t} \) term:

$$
\delta^2 E = \int_S dS \left( 2\psi \nabla^i \left( \frac{\partial \psi}{\partial t} + C N^i \nabla_i \psi \right) \nabla_i \psi + \Sigma \left( \nabla^a \nabla_a C + C B^a_\beta B_\beta^a \right) \right)
$$

(5.20)

For spherically symmetric equilibrium configurations only radial components of the gradients survive (requires care: \( \nabla^i \partial \psi / \partial t \) has non-radial components):

$$
\delta^2 E = \int_S dS \left( 2\psi \left( \frac{\partial \psi}{\partial r \partial t} + C \frac{d \psi}{d r} \right) \frac{d \psi}{d r} + \Sigma \left( \nabla^a \nabla_a C + C B^a_\beta B_\beta^a \right) \right)
$$

(5.21)

5.3.2 Closed-form expression for the sphere

We represent the surface perturbation \( C \) as a series:

$$
C = \Gamma \sum_{l,m} C_{lm} Y_{lm}(\theta, \alpha)
$$

(5.22)

and, once again, introduce a scaled constant term

$$
D_{00} = \frac{C_{00}}{\sqrt{4\pi}}
$$

(5.23)
For ease of reference, we copy the key terms appearing equation (5.21) from the previous chapter.

1. The radial eigenfunction, indexed by $n$:

$$
\psi_n (r) = \frac{\rho_n^{1/2}}{2R} r^{-3/2} J_{\frac{3}{2}} \left( \frac{\rho_n}{R} \right) \tag{5.24}
$$

and its radial derivatives at the boundary:

$$
\frac{d\psi_n}{dr} \bigg|_{r=R} = \frac{1}{2} \rho_n^{3/2} R^{-5/2} J_{-\frac{5}{2}} \left( \rho_n \right) \tag{5.25a}
$$

$$
\frac{d^2\psi_n}{dr^2} \bigg|_{r=R} = -\rho_n^{3/2} R^{-7/2} J_{-\frac{7}{2}} \left( \rho_n \right) \tag{5.25b}
$$

2. The perturbation of the radial eigenfunctions:

$$
\begin{aligned}
\left\{ \frac{\partial \psi_n}{\partial r} = \sum_{l,m} s_{lm} (r) Y_{lm} (\theta, \alpha) \right.
\left. \frac{\partial \psi_n}{\partial \theta} = \sum_{l,m} \frac{ds_{lm}(r)}{dr} Y_{lm} (\theta, \alpha) \right\} \text{ index } n \text{ dropped on the RHS}, \tag{5.26}
\end{aligned}
$$

where

$$
\begin{aligned}
s_{00} (r) &= -\frac{1}{4} D_{00} \rho_n^{3/2} R^{-1} r^{-1/2} \left( J_{\frac{3}{2}} \left( \frac{\rho_n}{R} \right) + 2 \rho_n \frac{r}{R} J_{-\frac{1}{2}} \left( \frac{\rho_n}{R} \right) \right) \tag{5.27a} \\
s_{lm} (r) &= -\frac{1}{2} C_{lm} \rho_n^{3/2} R^{-1} \frac{J_{\frac{5}{2}} \left( \frac{\rho_n}{R} \right)}{J_{l+\frac{1}{2}} \left( \frac{\rho_n}{R} \right)} r^{-1/2} J_{l+\frac{1}{2}} \left( \frac{\rho_n}{R} \right) \tag{5.27b}
\end{aligned}
$$

and their radial derivatives at the boundary are:

$$
\begin{aligned}
\frac{ds_{00}}{dr} \bigg|_{r=R} &= -\frac{1}{4} D_{00} \rho_n^{3/2} R^{-5/2} J_{-\frac{5}{2}} \left( \rho_n \right) \tag{5.27c} \\
\frac{ds_{lm}}{dr} \bigg|_{r=R} &= \frac{1}{2} C_{lm} \rho_n^{3/2} R^{-5/2} J_{-\frac{7}{2}} \left( \rho_n \right) \left( l + 1 \right) - \rho_n \frac{J_{l+\frac{1}{2}} \left( \rho_n \right)}{J_{l+\frac{1}{2}} \left( \rho_n \right)} \tag{5.27d}
\end{aligned}
$$

Finally, recall that $B_{\beta}^3 B_{\alpha}^\beta = 2/\Gamma^2$ and that $\nabla_\alpha \nabla^\alpha Y_{lm} = -l (l + 1) \Gamma^{-2} Y_{lm}$.

We now have all the ingredients in place to substitute in (5.21) and obtain the final expression:

$$
\delta^2 E = \left\{ \right. + \sum \left\{ \Psi \Gamma^{-2} \pi \left( \frac{|C_{00}|^2 \left( \frac{3}{2} \Psi \pi^2 \Gamma^{-2} - 2 \Sigma \Gamma^2 \right)}{J_{l+\frac{1}{2}} \left( \Psi \pi^2 \pi \right)} - (l - 1) \right) \right. + \Sigma \Gamma^2 \left( l + 2 \right) (l - 1) \left. \right. \right. \right.
\right.
$$

by (5.9) and (5.10) = \Sigma \Gamma^2 \left\{ \right. + \sum \left\{ 4n^2 y^4 \left( \frac{|C_{00}|^2 \left( 5y^4 - 1 \right)}{J_{l+\frac{1}{2}} \left( \Psi \pi^2 \pi \right)} - (l - 1) \right) \right. + \left( l + 2 \right) (l - 1) \right. \right. \}
Therefore, the criterion for morphological stability is given by

\[ P^l_n (y) = 4n^2 y^4 \left( \frac{n \pi J_{l-\frac{1}{2}}(n \pi)}{J_{l+\frac{1}{2}}(n \pi)} -(l - 1) \right) + (l + 2)(l - 1) > 0 \]  

(5.28)

At zero pressure \( \Pi = 0 \), the dimensionless equilibrium equation (5.11) yields: \( y_0 = \pi^{-1/2} \). Table 5.2 shows the values of

\[ P^l_n (y_0) = 4 \left( \frac{n \pi J_{l-\frac{1}{2}}(n \pi)}{J_{l+\frac{1}{2}}(n \pi)} - (l - 1) \right) + (l + 2)(l - 1) \]  

(5.29)

for the 6 lowest radial eigenvalues and 10 lowest spherical harmonics. All electron bubbles are neutrally stable with respect to the \( Y_{1,m} \) harmonic. This should be expected since motion as a rigid body does not change the energy of the system.

<table>
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<th>( \lambda_2 )</th>
<th>( \lambda_3 )</th>
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Table 5.2: The value of \( P^l_n(y_0) \) for the 6 lowest eigenvalues and 10 lowest spherical harmonics.

5.3.3 Instability of the \( S \) electron bubbles

We observe that the 1\( S \) electron bubble is stable against all infinitesimal perturbations. All of the remaining \( S \) electrons are unstable against \( Y_{3,m} \) and all but the 2\( S \) bubbles are unstable against against other harmonics as well. This is a very surprising fact, which at the present time does not have a simple intuitive explanation. We believe that it is possible to verify this prediction experimentally, [14].

In all cases there exist non-spherical stable configurations. Non-surprisingly, the equilibrium shapes look like perturbations proportional to \( Y_{3,m} \). However, we are not making the claim that they should. Our analysis is linear and only states the very fact of instability.
5.3.4 Closed-form expression for the circle

Express the normal velocity $C$ is expressed as a Fourier series:

$$C = \Gamma \sum_{m}^{\infty} C_m e^{im\theta}$$  \hspace{1cm} (5.30)

We remind the reader of the values for some of the ingredients in the above expression.

1. The eigenfunction $\psi_n$ and its normal derivatives at the boundary:

$$\psi_n (r) = \frac{1}{\sqrt{\pi R^2} J_1 (\rho_n)} J_0 \left( \rho_n \frac{r}{R} \right)$$  \hspace{1cm} (5.31)

2. The time derivative of $\psi_n$ and its first normal derivative at the boundary:

$$\frac{\partial \psi}{\partial t} = \sum_{m=-\infty}^{\infty} s_m (r) e^{im\theta}$$  \hspace{1cm} (5.32)

where

$$s_0 (r) = \frac{C_0}{\sqrt{\pi R^2} J_1 (\rho_n)} \left( J_1 \left( \rho_n \frac{r}{R} \right) \rho_n \frac{r}{R} - J_0 \left( \rho_n \frac{r}{R} \right) \right)$$  \hspace{1cm} (5.33a)

$$s_m (r) = C_m \frac{\rho_n}{\sqrt{\pi R^2} J_m (\rho_n)} J_m \left( \rho_n \frac{r}{R} \right)$$  \hspace{1cm} (5.33b)

and

$$\frac{d}{dr} s_0 (r) \bigg|_{r=R} = C_0 \frac{\rho_n}{\sqrt{\pi R^2}}$$  \hspace{1cm} (5.33c)

$$\frac{d}{dr} s_m (r) \bigg|_{r=R} = C_m \frac{\rho_n^2}{\sqrt{\pi R^2} J_m (\rho_n)} J'_m (\rho_n)$$  \hspace{1cm} (5.33d)

Putting everything together and also recalling the value of the equilibrium radius (5.9), we get:

$$\frac{\delta^2 E}{\Sigma R} = \left( 4 \frac{\rho_n^2}{\rho_1^2} y^3 - 1 \right) |C_0|^2 + \sum_{m=-\infty}^{\infty} \left( 2 \frac{\rho_n^2}{\rho_1^2} y^3 \left( \frac{\rho_n J'_m (\rho_n)}{J_m (\rho_n)} + 1 \right) + (m+1) (m-1) \right) |C_m|^2$$  \hspace{1cm} (5.34)

The bubble is morphologically stable if

$$P_m^n = 2 \frac{\rho_n^2}{\rho_1^2} y^3 \left( \frac{\rho_n J'_m (\rho_n)}{J_m (\rho_n)} + 1 \right) + (m+1) (m-1) > 0$$  \hspace{1cm} (5.35)

At $\Sigma = 0$, the equilibrium circle is characterized by $y_0 = \sqrt[3]{\rho_1^2 / \rho_2^2}$. Table 5.3 contains the values of

$$P_m^n (y_0) = (m+1)^2 - 2 \rho_n \frac{J_{m+1} (\rho_n)}{J_m (\rho_n)} > 0$$  \hspace{1cm} (5.36)

for the 6 lowest radial eigenvalues and 10 lowest spherical harmonics. The two dimensional
The situation is very similar to the three-dimensional one. The 1S electron bubble is stable against all perturbation. The 2S and the higher energy radially symmetric states are unstable with respect to the $m = 3$ harmonic. The $l \geq 3$ states are also unstable with respect to the fifth harmonic.

<table>
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Table 5.3: The value of $P_\pi^m(y_0)$ for the 6 lowest eigenvalues and 10 lowest spherical harmonics.

### 5.4 Stable equilibrium shapes

#### 5.4.1 Relevant physical parameters and non-dimensionalization

Our simulations target the actual electron bubbles whose energy is given by (5.1). The relevant physical parameters in SI units are

\[
h = 6.6262 \times 10^{-34} \text{J} \cdot \text{s} \tag{5.37a}
\]

\[
m = 9.1095 \times 10^{-31} \text{kg} \tag{5.37b}
\]

\[
\sigma = 3.41 \times 10^{-4} \text{J/m}^3 \tag{5.37c}
\]

The equilibrium radius $R_0$ for the 1S electron bubbles at zero pressure is

\[
R_0 = \sqrt[4]{\frac{\hbar^2}{32\pi m \sigma}} = 1.936 \times 10^{-9} \text{m} \tag{5.38}
\]

This radius is treated as the characteristic length scale all of the dimensions in the figures below are given in the units of $R_0$. Introduce the dimensionless parameter $a$

\[
a = \frac{PR_0}{2\sigma} \tag{5.39}
\]

In terms of $R_0$, $a$, the new dimensionless eigenvalue $\lambda'$, area $S'$, and volume $V'$, the dimensionless energy $E' = E/\sigma R_0^2$ is given by:

\[
E' = \frac{4}{\pi} \lambda'_{ \text{mn} } + S' + 2aV' \tag{5.40}
\]
Therefore the actual physical problem can be expressed in canonical form by letting

\[
\begin{align*}
\Phi &= \frac{4}{\pi} \\
\Sigma &= 1 \\
\Pi &= 2a
\end{align*}
\]  

(5.41a, 5.41b, 5.41c)

Varying the pressure \( P \) will only affect the value of \( \Pi \).

### 5.4.2 Analytical formulation

The equilibrium equation (5.5) cannot be solved in closed form for non-spherical configurations. We propose two numerical schemes that can reveal non-spherical stable shapes. Both schemes fall under the gradient descent category. The first one is analogous to the evolution given by equation (3.13) in Chapter 3:

\[
C = \Psi \nabla \psi \nabla \psi + \Sigma B^\alpha - \Pi, 
\]

(5.42)

There is no need to subtract out the mean in this case since there are no volume constraints. This approach is faster than the alternative one, but requires computing curvatures and normals which is a challenging task in three dimensions. Thus, in three dimensions we employ another technique that follows the philosophy of the Finite Element method. We replace the differentiable shape with a polyhedron and solve the new approximate problem exactly. Suppose that \( \Omega_N \) is the polyhedron that approximates the electron bubble and \( S_N \) is its boundary. The energy of the system is given by

\[
E = \Psi \times \text{Finite Element Estimate} (\lambda) + \Sigma \times \text{Area} (S_N) + \Pi \times \text{Volume} (\Omega_N)
\]

We must note that it is somewhat inaccurate to say that the bubble is replaced by a polyhedron since the finite element method also implies that a mesh is constructed in the interior of the polyhedron.

### 5.4.3 Numerical simulations

1S electron bubbles

We concentrate on the three dimensional simulation. We use tetrahedral elements with linear trial functions. The interface is advanced by a forward Euler scheme. All of the simulations use time step \( \Delta t = \frac{1}{10} \) and are performed on a mesh created by Per-Olof Persson [35]. The mesh contains 1843 nodes and 9084 tetrahedrons.

We first consider the 1S electron bubble. At zero pressure the stable equilibrium radius is \( R_0 \) or, in dimensionless terms, 1. The initial configuration for the simulation shown in Figure 5-2) is a sphere of radius 1.414. The bounding box in the figure indicates the size of the theoretical equilibrium configuration (\( L = 2 \)). We make several observations concerning the numerical simulation.

1. The numerical solution converges (or "settles"). We conclude that the equilibrium configuration is stable with respect to arbitrary perturbations of the boundary.
Figure 5-2: The quasi-static evolution for the 1S electron bubble at zero pressure. The initial sphere has radius 1.414. The bounding box fits a sphere of radius 1.
2. The accuracy of our method is quite high. The radius of the equilibrium sphere (computed as $\sqrt[3]{\frac{3V}{4\pi}}$) is about 1.003.

3. The computed energy for the polyhedron does not decrease monotonically for near equilibrium configurations towards the end of the simulation. This is not cause for concern. This happens for two reasons. First, the configuration often overshoots the equilibrium. Second, when computing the eigenvalue gradient by moving the nodes and recomputing the eigenvalue estimate is not actually recomputed since that would take too long. Instead, the perturbation to the constructed FE matrices is computed and classical perturbation theory is employed at that point. This introduces a small error into the eigenvalue gradient computation.

2S electron bubbles

Our central result is that the 2S electron bubbles are unstable for $P > -1.23$. The 2S electron bubble corresponds to the second radial eigenvalue which is 10-th overall. Figures 5-3 and 5-4 present the evolution for a 2S electron bubble at $P = -0.75$ bars ($\Pi = -0.4258944$). The initial configuration is a sphere of radius $\sqrt{2}$ which corresponds to the equilibrium (unstable!) spherical configuration for the 2S bubble at zero pressure. The eventual equilibrium configuration has tetrahedral symmetry. The particular evolution that takes place is determined by "random" factors such as the specifics of the mesh and round off. Therefore, different evolutions will be observed if we significantly perturb the initial configuration in different ways. In Figure 5-3 the initial sphere was perturbed along $\Re Y_{3,1} (\theta, \phi)$ while in Figure 5-4 it was perturbed along $\Re Y_{3,3} (\theta, \phi)$. In the latter case, the evolution immediately developed into a "pear" shape and stayed on that plateau for a great number of iterations. We show 12 frames to highlight this fact. This evolution suggested to us that "pear" might be a stable equilibrium configuration. However, we persisted with this evolution and realized that the "pear" is not an equilibrium shape.

An interesting effect occurs for a range of pressures: eigenvalue crossing. Figure 5-5 shows an evolution of the 2S electron bubble at zero pressure. The bubble develops into the same eventual shape as the 1D electron bubble. It is unclear whether this crossing occurs in nature (although Professor Maris of Brown believes that it does!). All we can state with confidence is that at those pressures, equilibrium stable configurations do not exist for the 10-th eigenvalue. It is difficult to pinpoint the exact pressure at which this phenomenon begins to take place. We have determined that it happens somewhere between $-0.75$ and $-0.50$ bars.

1P electron bubbles

A sphere cannot be an equilibrium configuration for the 1P electron bubbles since the eigenstate does not have spherical symmetry. The existence of an equilibrium shape is difficult to ascertain analytically. However, we are able to provide a numerical answer: an equilibrium configuration does exist. Figure 5-6 shows an evolution of the 1P electron bubble at 0.75 bars. It proves that an equilibrium stable configuration exists. At most pressures it is shaped like a peanut although at pressures below approximately $-1.50$ bars the waist disappears and the shape becomes convex. In all cases the eventual equilibrium shape and the evolution possess axial symmetry.
Figure 5-3: Evolution of a 2S electron bubble at \(-0.75\) bars. The bounding box fits a sphere of radius \(\sqrt{2}\). The eventual configuration has tetrahedral symmetry.
Figure 5-4: Evolution of a 2S electron bubble at \(-0.75\) bars. The bounding box fits a sphere of radius \(\sqrt{2}\). An interesting feature of this evolution is how much time the bubble spends in a "pear" shape.
Figure 5-5: Evolution of the 2S electron bubble at zero pressure. In this instance, eigenvalues cross and must conclude that the equilibrium stable shape does not exist for \( \lambda_2 \).
Figure 5-6: Evolution of a $1P$ electron bubble at $-0.75$ bars. The initial configuration is a sphere of radius 1.
1D electron bubbles

The 1D electron bubbles correspond to eigenfunctions that typically do not have axial symmetry. We therefore expected to uncover a variety of equilibrium configurations. But that did not happen! While we did observe a variety of evolutions, the eventual configurations were identical (except for orientation). Figures 5-7 and 5-8 are two examples of different evolutions.
Figure 5-7: Evolution of the 1D electron bubble at -0.75 bars.
Figure 5-8: Another evolution of the 1D electron bubble at -0.75 bars.
Chapter 6

Laplace Eigenvalues on Regular Polygons

We discuss the application of our central technique to computing simple eigenvalues on regular polygons with $N$ sides, (Figure 6-1). The effectiveness of our approach can be measured by comparison with the finite element estimates. For higher eigenvalues, our method actually beats finite elements and can be used to judge the accuracy of finite element estimates.

At the end of this chapter we discuss the expansion of simple eigenvalues on regular polynomials in powers of $1/N$. Surprisingly, this natural idea has not been developed in the existing literature. The material presented in this chapter can be found in a more condensed form in [15].

6.1 The Taylor Series Approach

6.1.1 Example: expanding circle

A simple example will illustrate what we want to accomplish. If $\lambda_n$ is an eigenvalue on the unit circle, then the corresponding eigenvalue $\lambda_n^{[\Delta R]}$ on a circle of radius $1 + \Delta R$ is

$$\lambda_n^{[\Delta R]} = \frac{\lambda_n}{(1 + \Delta R)^2}$$

(6.1)

In order to estimate this value, imagine a family of uniformly expanding circles $\Omega(t)$ whose radii evolve as $1 + t\Delta R$. Thus $\Omega(0)$ is the unit circle and $\Omega(1)$ is the circle of radius $1 + \Delta R$. Suppose that the radial eigenvalues of $\Omega(t)$ are $\lambda_n(t)$, and we want $\lambda_n(1)$. We represent $\lambda_n(t)$ as a Taylor series:

$$\lambda_n(t) = \frac{\lambda_n}{(1 + t\Delta R)^2} = \lambda_n \left(1 - 2t\Delta R + 3t^2\Delta R^2 + O(t^3\Delta R^3)\right)$$

(6.2)

We arrive at an approximation for $\lambda_n^{[\Delta R]}$ by evaluating this series at $t = 1$ and keeping the first two terms:

$$\lambda_n^{[\Delta R]} = \lambda_n \left(1 - 2\Delta R + 3\Delta R^2 + O(\Delta R^3)\right)$$

(6.3)
The first two Taylor coefficients are $-2\lambda_n$ and $6\lambda_n$. An exact computation will also be possible for regular polygons, although the expression for the second term will contain an infinite series. Another difference is that the polygon perturbation is only piecewise smooth. In our experience, the discontinuities do not affect the Taylor series expansion in the first two terms. It remains to determine whether the Taylor series approximation holds in higher terms. Also note that we have evaluated the Taylor approximation far from the origin ($\Delta t = 1$). Nevertheless, the approximation is valid since $\Delta R$ is small.

### 6.1.2 From a circle to a polygon – the second order perturbation of (simple) eigenvalues

Suppose that $\lambda^{[N]}_n$ is the $n$-th simple eigenvalue on the regular polygon $\Omega_N$ with $N$ sides (Figure 6-1). Consider an evolution of curves that depart from the circle at time $t = 0$ and arrive at the polygon at $t = 1$. In the course of this evolution, the $n$-th simple eigenvalue $\lambda_n(t)$ will change from $\lambda_n$ at $t = 0$ to $\lambda^{[N]}_n$ at $t = 1$. We approximate $\lambda^{[N]}_n$ by the truncated Taylor expansion:

$$\frac{d\lambda_n}{dt} \bigg|_{t=0} + \frac{1}{2} \frac{d^2\lambda_n}{dt^2} \bigg|_{t=0} \quad (6.4)$$

The linear term was computed in Chapter 4, (4.37):

$$\frac{d\lambda_n}{dt} \bigg|_{t=0} = - \int_S dSC \nabla_i \psi_n \nabla^i \psi_n \quad (6.5)$$
C is the velocity of the interface at $t = 0$ and $\psi_n$ is the unperturbed eigenfunction. The second derivative is obtained by differentiating (6.5) with respect to $t$.

\[
\frac{d^2 \lambda}{dt^2} = - \frac{d}{dt} \int_S dS C \nabla_i \psi_n \nabla^i \psi_n
\]

(6.6a)

by (2.13) = \[
\left\{ - \int_S dS \frac{\delta C}{dt} (C \nabla_i \psi_n \nabla^i \psi_n) \right\}
+ \int_S dS C^2 B^i_n \nabla^i \psi_n \nabla_i \psi_n
\]

(6.6b)

by (2.9) = \[
\left\{ - \int_S dS \frac{\delta C}{dt} (\nabla^i \psi_n \nabla_i \psi_n) \right\}
- 2 \int_S dS C \nabla_i \frac{\delta \psi_n}{\delta t} \nabla^i \psi_n
+ \int_S dS C^2 B^i_n \nabla^i \psi_n \nabla_i \psi_n
\]

(6.6c)

Finally, by chain rule (2.8), we have

\[
\frac{d^2 \lambda}{dt^2} = \left\{ - \int_S dS \frac{\delta C}{dt} (\nabla^i \psi_n \nabla_i \psi_n) \right\}
- 2 \int_S dS C \left( \nabla_i \frac{\delta \psi_n}{\delta t} + C N \nabla_j \nabla^i \psi_n \right) \nabla_i \psi_n
+ \int_S dS C^2 B^i_n \nabla^i \psi_n \nabla_i \psi_n
\]

(6.7)

In order to evaluate expressions (6.5) and (6.7), we must select a specific evolution of the boundary.

### 6.1.3 One-parameter family of curves

It is useful to consider a circle of radius $R$ rather than unity. Then dimensional analysis will assist with the algebra - the powers of $R$ must match among all terms. We divide the circle into $N$ equal parts and parameterize each arc by $\alpha \in \left[ \frac{-\pi}{N}, \frac{\pi}{N} \right]$ as in Figure 6-2. Introduce a useful ratio of cosines:

\[
\Omega^N_\alpha = \frac{\cos \frac{\pi}{N}}{\cos \alpha} < 1
\]

(6.8)

The derivative of $\Omega^N_\alpha$ with respect to $\alpha$ is

\[
\frac{d\Omega^N_\alpha}{d\alpha} = \Omega^N_\alpha \tan \alpha
\]

(6.9)

The circle evolves into a polygon in the following way: each point moves radially inward with constant velocity (depending on the point). All points arrive at their destination at $t = 1$.

The distance traveled by the point at angle $\alpha$ is $R \left( 1 - \Omega^N_\alpha \right)$ as seen in Figure 6-2. Then a reasonable parameterization for this evolution is:

\[
\begin{bmatrix}
  z^x (\alpha, t) \\
  z^y (\alpha, t)
\end{bmatrix}
= R \left( 1 - (1 - \Omega^N_\alpha) t \right) \begin{bmatrix}
  \cos \alpha \\
  \sin \alpha
\end{bmatrix}
\]

(6.10)

### 6.1.4 The essential ingredients

The goal of this section is to express the elements in (6.5) and (6.7) in terms of the fundamental geometric and kinematic quantities $\alpha$, $R$, $t$, and $\lambda_n$.

1) $C$ and $\frac{\delta C}{\delta t}$. The most fundamental ingredient is the velocity of the interface $C$ defined in
Figure 6-2: A single slice of a regular polygon with $N$ sides. The slice is centered around the $x$-axis.

(2.2). One might expect that $C$ is proportional to the distance traveled, $1 - \Omega_{\alpha}^N$. This is indeed the case for $v^i$, the radial velocity at each point, (2.4). However, since the normal $N_i$ depends on $t$, so does $C(t)$.

$\frac{\delta C}{\delta t}$ is obtained by a formal application of the $\frac{\delta C}{\delta s}$-derivative defined by (2.6). We must keep track of the time dependence of the fundamental geometric objects such as the normal $N^i$.

ii) The terms containing the gradient of the unperturbed eigenfunction $\psi_n$ will be computed by utilizing the closed form expressions for $\psi_n$, (4.53). It is important to note that only the normal components of the gradients $\frac{\partial}{\partial \alpha}$ will survive in (6.7) due to the symmetry of the original configuration. (This statement requires care since $\nabla_\alpha \frac{\partial \psi}{\partial t}$ has non-radial components.)

iii) The most challenging term in equation (6.7) is the gradient of the eigenfunction perturbation $\nabla_\alpha \frac{\partial \psi}{\partial t}$. It is computed by solving the perturbed eigensystem and is summarized in equations (4.57)-(4.59).

We pick the parameter $\alpha$ to be our surface coordinate while the standard Cartesian system will be utilized in the embedding plane space. The spatial indices are denoted by lower case Latin letters (although $n$ stands for the number of the eigenvalue). We can raise and lower spatial indices without multiplication by a metric.

**Basic surface tensors**

1. The shift tensor $z^i_\alpha$ needed to compute the surface metric tensor $z_{\alpha \beta}$ and the normal $N^i$:

$$
\begin{bmatrix}
  z^x_\alpha \\
  z^y_\alpha \\
\end{bmatrix}
= R \frac{\partial}{\partial \alpha}
\begin{bmatrix}
  (1 - (1 - \Omega_{\alpha}^N) t) \cos \alpha \\
  (1 - (1 - \Omega_{\alpha}^N) t) \sin \alpha \\
\end{bmatrix}
= R \begin{bmatrix}
  \Omega_{\alpha}^N (t - 1) \sin \alpha \\
  \Omega_{\alpha}^N \cos \alpha + (1 - t) \cos \alpha \\
\end{bmatrix}
$$

(6.11)
2. The covariant metric tensor $z_{\alpha \beta}$ is a $1 \times 1$ matrix:

$$z_{\alpha \beta} = z^i_{\alpha} z_{j\beta} = (1 \times 1) = R^2 \left[ (z^x_{\alpha})^2 + (z^y_{\alpha})^2 \right] =$$

$$= R^2 \left[ ((t - 1) \sin \alpha)^2 + \left( t \frac{\Omega^N_{\alpha}}{\cos \alpha} + (1 - t) \cos \alpha \right)^2 \right]$$

(6.12a)

(6.12b)

3. The normal $N^i$:

$$N^i = \frac{1}{2} \varepsilon^i_{\alpha} \varepsilon^j_{\alpha} z_{j \alpha} = \frac{1}{\sqrt{(z^x_{\alpha})^2 + (z^y_{\alpha})^2}} \left[ \frac{t \Omega^N_{\alpha}}{\cos \alpha} + (1 - t) \cos \alpha \right]$$

(6.13)

Evaluating $C$

4. $C = v^i N_i$ where the velocity "object" $v^i$ is

$$\begin{bmatrix} v^x \\ v^y \end{bmatrix} = R \frac{\partial}{\partial t} \left[ \frac{1 - (1 - \Omega^N_{\alpha}) t}{(1 - (1 - \Omega^N_{\alpha}) t) \sin \alpha} \right] = R \left( \Omega^N_{\alpha} - 1 \right) \begin{bmatrix} \cos \alpha \\ \sin \alpha \end{bmatrix}$$

(6.14)

It is seen to be independent of $t$. The word "object" emphasizes the fact that it is not a tensor. Nevertheless, we adhere to the tensorial notation for it.

5. The velocity of the surface $C$:

$$C = v^j N_j = R \frac{1}{\sqrt{(z^x_{\alpha})^2 + (z^y_{\alpha})^2}} \left[ \frac{t \Omega^N_{\alpha}}{\cos \alpha} + (1 - t) \cos \alpha \right] \cdot \left[ \frac{\Omega^N_{\alpha} - 1}{(1 - t) \sin \alpha} \right]$$

(6.15a)

$$= R \frac{t (\Omega^N_{\alpha} - 1)^2}{\sqrt{(z^x_{\alpha})^2 + (z^y_{\alpha})^2}} + R \frac{\Omega^N_{\alpha} - 1}{\sqrt{(z^x_{\alpha})^2 + (z^y_{\alpha})^2}}$$

(6.15b)

In particular, at time $t = 0$, $C$ equals the negative distance along a radial direction from the initial circle to the eventual polygon:

$$C|_{t=0} = R (\Omega^N_{\alpha} - 1)$$

(6.16)

Evaluating $\frac{\delta C}{\delta t}$ at time $t = 0$

According to the definition of the $\frac{\delta}{\delta t}$-derivative,

$$\frac{\delta C}{\delta t} = \frac{\partial C(\alpha, t)}{\partial t} - v^\alpha \nabla_\alpha C$$

(6.17)
6. The partial derivative of $C$ with respect to $t$ equals

$$\frac{\partial C(\alpha, t)}{\partial t} = R \frac{\partial}{\partial t} \left( \frac{t (\Omega_\alpha^N - 1)^2}{(z_\alpha^x)^2 + (z_\alpha^y)^2} + \frac{\Omega_\alpha^N - 1}{(z_\alpha^x)^2 + (z_\alpha^y)^2} \right)$$

$$= R \frac{(\Omega_\alpha^N - 1)^2}{(z_\alpha^x)^2 + (z_\alpha^y)^2} \frac{1/2}{2} \left( \frac{t (\Omega_\alpha^N - 1)^2 + (\Omega_\alpha^N - 1)}{(z_\alpha^x)^2 + (z_\alpha^y)^2} \right) \left( \frac{\partial x}{\partial t} \frac{\partial y}{\partial t} \right).$$

In particular, at time $t = 0$, $\frac{\partial C(\alpha, t)}{\partial t}$ vanishes:

$$\frac{\partial C(\alpha, t)}{\partial t} \bigg|_{t=0} = 0$$

(6.19)

7. The covariant surface derivative of $C$ at time $t = 0$:

$$\nabla_\alpha C \big|_{t=0} = R \Omega_\alpha^N \tan \alpha$$

(6.20)

8. The projection of the velocity object onto the surface:

$$v_\alpha = v^i z_{i\alpha} = R (\Omega_\alpha^N - 1) \left[ \begin{array}{c} \cos \alpha \\ \sin \alpha \end{array} \right] \cdot \left[ \begin{array}{c} (t - 1) \sin \alpha \\ t \Omega_\alpha^N \cos \alpha + (1 - t) \cos \alpha \end{array} \right] =$$

$$= R t (\Omega_\alpha^N - 1) \Omega_\alpha^N \tan \alpha$$

(6.21a)

In particular, at time $t = 0$, $v_\alpha$ vanishes:

$$v_\alpha \big|_{t=0} = 0$$

(6.21b)

9. Putting the ingredients 6-8 together, we find that $\frac{\delta C}{\delta t}$ vanishes at time $t = 0$:

$$\frac{\delta C}{\delta t} \bigg|_{t=0} = \frac{\partial C(\alpha, t)}{\partial t} - v_\alpha \nabla_\alpha C \bigg|_{t=0} = 0$$

(6.22)

**Fourier decomposition of $C$**

10. Below we make use of the Fourier series decomposition of $C$ at time $t = 0$:

$$C_{t=0}(\alpha) = R \sum_{m=-\infty}^{\infty} C^{[N]}_m e^{i m \alpha}$$

(6.23)

The coefficients $C^{[N]}_m$ are given by:

$$C^{[N]}_m = \begin{cases} 0, & m \neq k N \\ \frac{N}{2\pi} \int_{-\pi}^{\pi/N} \left( \frac{\cos \frac{\pi}{N} \cos \alpha - 1}{\cos \alpha} \right) e^{-i k \alpha} d\alpha, & m = k N \end{cases}$$

(6.24)
The constant term is.

\[ C_0^{[N]} = \frac{N}{2\pi} \int_{-\pi/N}^{\pi/N} \left( \cos \frac{\pi}{N} - 1 \right) d\alpha = \frac{N}{2\pi} \cos \frac{\pi}{N} \ln \frac{1 + \sin \frac{\pi}{N}}{1 - \sin \frac{\pi}{N}} - 1 \]  

(6.25)

Note that in the ongoing enumeration, this is the only equation that does not apply to a general evolution of the circle.

**The unperturbed eigenfunction and its gradients**

11. For the ease of reference, we copy the expression for the eigenfunction \( \psi_n \) (4.53) and present its normal derivatives at \( r = R \):

\[ \psi_n (r) = \frac{1}{\sqrt{\pi R^2 J_1 (\rho_n)}} J_0 \left( \frac{\rho_n r}{R} \right) \]  

(6.26a)

\[ \left. \frac{d\psi_n}{dr} \right|_{r=R} = \frac{\rho_n}{\sqrt{\pi R^4}} \]  

(6.26b)

\[ \left. \frac{d^2\psi_n}{dr^2} \right|_{r=R} = \frac{\rho_n}{\sqrt{\pi R^6}} \]  

(6.26c)

12. The combinations of gradients in equation (6.7) are:

a) \( N^j \nabla_j \nabla_i \psi \nabla_i \psi = \frac{\rho_n^2}{\pi R^8} \) by (6.26b) and (6.26c)

b) \( B_\alpha \nabla_i \psi \nabla_i \psi = -\frac{2\rho_n^3}{R^8} \) by (2.18) and (6.26b)

(6.27)

**The eigenfunction perturbation \( \frac{\partial \psi_n}{\partial t} \)**

13. For the ease of reference we copy equations (4.57) - (4.59) from Chapter 4.

\[ \frac{\partial \psi_n}{\partial t} = \sum_{l,m} s_m (r) e^{im\theta} \]  

(6.28)

The radial parts are given by

\[ s_0 (r) = -C_0 \frac{1}{\sqrt{\pi R^2 J_1 (\rho_n)}} J_0 \left( \frac{\rho_n r}{R} \right) + C_0 \frac{\rho_n}{\sqrt{\pi R^4 J_1 (\rho_n)}} r J_1 \left( \frac{\rho_n r}{R} \right) \]  

(6.29a)

\[ s_m (r) = C_m \frac{\rho_n}{\sqrt{\pi R^2 J_m (\rho_n)}} J_m \left( \frac{\rho_n r}{R} \right) \]  

(6.29b)

where \( C_m \) are the Fourier coefficients. The radial derivatives of \( s_m (r) \) at \( r = R \) are given by:

\[ \left. \frac{d}{dr} s_m (r) \right|_{r=R} = C_0 \frac{\rho_n}{\sqrt{\pi R^3}} \]  

(6.29c)

\[ \left. \frac{d}{dr} s_m (r) \right|_{r=R} = C_m \frac{\rho_n}{\sqrt{\pi R^3}} \left( m - \rho_n \frac{J_{m+1} (\rho_n)}{J_m (\rho_n)} \right) \]  

(6.29d)

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6.1.5 Evaluating $\frac{d\lambda_n}{dt}$

$\frac{d\lambda_n}{dt}$ is given by equation (4.56). The radially symmetric eigenfunction $\psi_n$ is constant on $S$ and can therefore be taken outside the integral. The velocity of the interface $C$ is then the only expression left inside the integral. Therefore, only the constant Fourier term $C_0$ survives:

$$\left. \frac{d\lambda_n}{dt} \right|_{t=0} = -2C_0\lambda_n$$  \hspace{1cm} (6.30)

For regular polygons the numerical answer is obtained by substituting equation (6.25) in (6.30):

$$\left. \frac{d\lambda_n}{dt} \right|_{t=0} = -2\lambda_n \left( \frac{N}{2\pi} \cos \frac{\pi}{N} \ln \frac{1 + \sin \frac{\pi}{N}}{1 - \sin \frac{\pi}{N}} - 1 \right)$$  \hspace{1cm} (6.31)

The first order perturbation has a particularly simple dependence on $n$: it is directly proportional to the unperturbed eigenvalue $\lambda_n$.

The negative sign is consistent with the fact that the eigenvalues diminish as the domain expands. In fact, the rate of change in the eigenvalues is directly proportional to rate of change in area since according to equation (2.12), $d\Omega(t)/dt = \int dSC$. Therefore

$$\frac{d\lambda_n}{dt} = -\lambda_n \frac{d\Omega}{\pi \frac{dt}{dt}}$$  \hspace{1cm} (6.32)

6.1.6 Evaluating $\frac{d^2\lambda_n}{dt^2}$

We now turn to the computation of the second order perturbation of the radial eigenvalues. Recall from equation (6.7):

$$\frac{d^2\lambda_n}{dt^2} = \left\{ -\int_S dS \frac{\delta^2}{\delta t^2} \left( \nabla_i \psi_n \nabla_i \psi_n \right) \right. -2 \int_S dSC \left( \nabla_i \frac{\partial \psi_n}{\partial t} + CN_j \nabla_j \nabla_i \psi_n \right) \nabla_i \psi_n \\
\left. + \int_S dSC^2 B_{\alpha \beta} \nabla^\alpha \nabla^\beta \psi_n \nabla_i \psi_n \right\}$$  \hspace{1cm} (6.33)

Combining all the terms derived above, we get

$$\frac{d^2\lambda_n}{dt^2} = \left\{ -2 \int_S dSC \left( \nabla_i \frac{\partial \psi_n}{\partial t} + CN_j \nabla_j \nabla_i \psi_n \right) \nabla_i \psi_n \right. + \int_S dSC^2 B_{\alpha \beta} \nabla^\alpha \nabla^\beta \psi_n \nabla_i \psi_n \\
\left. - \frac{2\pi^2}{R^2} \left( \frac{2\pi R}{(2\pi R)} \right) \sum_{m \neq 0} |C_m|^2 \left( m - \rho_n \frac{J_{m+1}(\rho_n)}{J_m(\rho_n)} \right) \right\}$$

$$+ \frac{\pi^2}{R^2} \int_S dSC^2 - \frac{\pi^2}{R^2} \int_S dSC^2$$  \hspace{1cm} (6.34a)

by (6.22) = \hspace{1cm} (6.34b)

by (6.27) and 
(6.28)-(6.29d) = \hspace{1cm} (6.34c)

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We finally obtain a rather compact expression for \( d^2 \lambda_n / dt^2 \):

\[
\frac{d^2 \lambda_n}{dt^2} = 4 \frac{\lambda_n}{R^2} \left( |C_0|^2 + \sum_{m \neq 0}^\infty |C_m|^2 \left( m - \rho_n \frac{J_{m+1}(\rho_n)}{J_m(\rho_n)} \right) \right)
\]

(6.35)

6.1.7 Summary

We approximate the simple eigenvalues \( \lambda_n^{[N]} \) of the regular polygons with \( N \) sides by a truncated Taylor series:

\[
\lambda_n^{[N]} \approx \lambda_n + \left. \frac{d\lambda_n}{dt} \right|_{t=0} + \frac{1}{2} \left. \frac{d^2 \lambda_n}{dt^2} \right|_{t=0},
\]

(6.36)

where \( \lambda_n \) is the \( n \)-th radial eigenvalue on the circle. The derivative terms can be expressed in closed form in terms of \( N, n, R \), and \( \lambda_n = \rho_n^2 / R^2 \):

\[
\left. \frac{d\lambda_n}{dt} \right|_{t=0} = -2\lambda_n \left( \frac{N}{2\pi} \cos \frac{\pi}{N} \ln \left( 1 + \sin \frac{\pi}{N} \right) - 1 \right)
\]

(6.37a)

\[
\left. \frac{d^2 \lambda_n}{dt^2} \right|_{t=0} = 4 \frac{\rho_n^2}{R^2} \left( |C_0|^2 + \sum_{m \neq 0} |C_m|^2 \left( m - \rho_n \frac{J_{m+1}(\rho_n)}{J_m(\rho_n)} \right) \right)
\]

(6.37b)

where

\[
C_m^{[N]} = \begin{cases} 
0, & m \neq kN \\
\frac{N}{2\pi} \int_{-\pi/N}^{\pi/N} \left( \frac{\cos \frac{\pi}{N}}{\cos \alpha} - 1 \right) e^{-i\kappa\alpha} d\alpha, & m = kN
\end{cases}
\]

(6.38)

The infinite series in (6.35) must be evaluated numerically (we use Matlab). For the purpose of computing polygonal eigenvalues it is sufficient to add up only a few of the lowest terms.

6.2 Finite elements estimates

There are three fundamental difficulties in achieving high accuracy with finite elements [43], [2].

1. Accurate estimates require fine meshes. If the mesh has \( P \) nodes, the continuous eigenvalue problem is converted into a \( P \times P \) problem which can be sparsely represented by \( O(P) \) bytes. The conventional eigenvalue solvers perform an inversion with a shift which requires \( O(P^2) \) bytes. A mesh with \( 10^6 \) nodes will challenge our RAM reserves of 1 gigabyte.

The fine mesh requirement is particularly stringent for polygons with many sides, since a greater density of nodes is necessary near the boundary. Figure 6-3 shows a typical mesh (produced by Per-Olof Persson [35]) for a regular polygon with 128 sides.

2. The finite element errors grow as \( O(\lambda^3) \). This becomes a problem rather quickly as the fifth radial eigenvalue on the circle is about \( \lambda_5 = 223 \).

3. It is difficult to employ Richardson extrapolation – a standard tool in series acceleration – for two reasons:

i) The error in estimates for larger eigenvalues, \( \lambda > 100 \), exceeds the \( O(1) \) spacing between the consecutive eigenvalues. For the unit square, the eigenvalues are \( \pi^2 (n^2 + m^2) = \pi^2 r^2 \).
Figure 6-3: A typical mesh for a 128-sided regular polygon.

They have roughly the same distribution as points with integer coordinates in two dimensions. No eigenvalues with \( m \neq n \) are simple; they are at least double from the pairs \((m, n)\) and \((n, m)\).

- i) Eigenvalue crossing occurs for subsequent mesh refinements, as it does for

\[
A(t) = \begin{bmatrix} 2 + t & 0 \\ 0 & 4 - t \end{bmatrix}
\]  \tag{6.39}

The eigenvalues \( \lambda_1(t) \) and \( \lambda_2(t) \) change differentiably with \( t \) if defined according to

\[
\begin{align*}
\lambda_1(t) &= 2 + t \\
\lambda_2(t) &= 4 - t
\end{align*}
\]  \tag{6.40}

Then \( \lambda_1(t) \) and \( \lambda_2(t) \) are seen to "cross" at \( t = 1 \). If the index is chosen according to the relative magnitude

\[
\begin{align*}
\lambda_1(t) &= \min(2 + t, 4 - t) \\
\lambda_2(t) &= \max(2 + t, 4 - t)
\end{align*}
\]  \tag{6.41}

then the dependence on \( t \) is no longer differentiable and the evolution is more difficult to track.

### 6.2.1 Richardson extrapolation

Suppose that the limit of a sequence \( a^{(k)} \) is \( A_0 \) and the convergence is quadratic: \( a^{(k)} = A_0 + A_1 k^{-2} + O(k^{-3}) \). Then \( a^{(2k)} = A_0 + \frac{1}{4} A_1 k^{-2} + O(k^{-3}) \). Richardson extrapolation forms a new series \( b^{(k)} = \frac{1}{3} (4a^{(2k)} - a^{(k)}) \). The effect is the cancellation of the quadratic terms, \( b^{(k)} = R_{20} a^{(k)} = A_0 + O(k^{-3}) \). We can expect that \( b^{(k)} \) will converge more rapidly than \( a^{(k)} \). The new \( b^{(k)} \) series can be accelerated further by: \( c^{(k)} = R_{32} b^{(k)} = \frac{1}{4} (8b^{(2k)} - b^{(k)}) \). The two
steps, \( \mathcal{R}_2 \) and \( \mathcal{R}_3 \), may be combined into a single extrapolation \( \mathcal{R}_{2,3} \):

\[
\begin{align*}
\epsilon^{(k)} &= \frac{1}{7} \left( 8b^{(2k)} - b^{(k)} \right) \\
&= \frac{1}{7} \left( 8 \times \frac{1}{3} \left( 4a^{(4k)} - a^{(2k)} \right) - \frac{1}{3} \left( 4a^{(2k)} - a^{(k)} \right) \right) \\
&= \frac{1}{21} \left( 32a^{(4k)} - 12a^{(2k)} + a^{(k)} \right)
\end{align*}
\]  

These \( \mathcal{R}_{2,3} \) coefficients \( \frac{32}{21}, -\frac{12}{21}, \) and \( \frac{1}{21} \) are the convolution of \( \frac{4}{3}, -\frac{1}{3} \) from \( \mathcal{R}_2 \) and \( \frac{8}{7}, -\frac{1}{7} \) from \( \mathcal{R}_3 \).

Richardson extrapolation can be used with finite elements. With each refinement the characteristic mesh size \( h \) is cut in half. The corresponding eigenvalue estimate \( \lambda_h \) is a function of \( h \). For linear elements the order of convergence is \( h^2 \) and \( \mathcal{R}_2 \) produces a sequence that should converge at least as fast as \( h^3 \). In reality it converges as \( h^4 \). We can therefore use \( \mathcal{R}_4 \) to accelerate the convergence further. For quadratic elements on the same mesh (irregular but reasonable), the leading order in error is \( h^4 \) and the productive accelerations are \( \mathcal{R}_4, \mathcal{R}_6 \) and \( \mathcal{R}_8 \).

### 6.2.2 Considering a single slice

The symmetries offered by regular polygons overcome the obstacles to Richardson extrapolation described above. The trick (suggested by Per-Olof Persson) works for all simple eigenvalues and radially symmetric eigenfunctions. We replace the original polygon by a single slice with Neumann conditions (zero normal derivatives) along the sides. The original radial eigenfunctions are symmetric with respect to rotation by \( 2\pi/N \) and reflection about the sides of any slice. Therefore, they satisfy zero Neumann conditions and our new problem ought to pick them out. Figure 6-4 shows a slice of a 16-sided polygon and a typical eigenfunction with Neumann conditions on the sides.

The new PDE also picks up spurious solutions on the slice that cannot be extended to an eigenfunction on the polygon. An example of such a solution can be seen on Figure 6-5. If two such triangles are arranged side by side, the combined solution will not be continuous.

For eigenvalues \( \lambda < 10^4 \), there are only a few spurious solutions and we can simply exclude them. An alternative is to replace Neumann conditions with periodic conditions, but this requires a highly regular mesh: the node pattern along each side must be the same. Also, periodic conditions lead to more complicated code. We decided to employ Neumann conditions in the numerical experiments described below.

The main effect of using a slice with Neumann conditions is that the eigenvalues are primarily the ones that correspond to radial eigenfunctions allowing Richardson extrapolation.

What order terms should we cancel when we do not know the true eigenvalues? Our plan is to ascertain the order of convergence from the consecutive differences \( \lambda^{(k)} - \lambda^{(k+1)} \). If the \( \lambda^{(k)} \) converge to \( \lambda \) then the differences normally converge to zero at the same rate. We encounter two interesting effects which can be seen in Figure 6-6: the order of convergence depends on the eigenvalue and the curve for one of the eigenvalues is clearly "out of line". The latter is an example in which eigenvalues cross. The 26-th (radial) and the 27-th (non-radial) eigenvalue estimates are given in Table 6.1. The right choices (indicated in bold) can be made by inspecting
Figure 6-4: Eigenfunction on a slice of a regular polygon with 16 sides. The brightness indicates the value of the eigenfunction (min = black, max = white).

Figure 6-5: A spurious solution on a single slice of a regular polygon with 16 sides.
the shape of the eigenfunctions or by straightening out the difference curves as in Figure 6-7.

For the larger eigenvalues, the order is $O(h^4)$ and we therefore use $R_4$. For the first few eigenvalues, the order is less clear (Figure 6-7 shows a change in slope) and Richardson extrapolation needs more care. Fortunately, it is less critical for these eigenvalues since the direct unextrapolated values may be sufficiently accurate. Our eigenvalue estimates are given at the end of the next section.

6.3 Results and comparison

The finite element estimates in this section came from these parameters:

1. The regular polygon had $N = 128$ sides.

2. The finite elements were quadratic (6 parameters per triangle). For a given amount of RAM, this is better than using linear test and trial functions on a more refined mesh.

3. Richardson extrapolation used meshes that represent 6, 7, and 8 successive refinements of the slice. These meshes contained 2145, 8385, and 33153 nodes and 4096, 16384, and 65536 elements.

4. We employed the Richardson extrapolation $R_4$ that cancels the $h^4$ terms.

We do not know the true eigenvalues. Therefore we study the difference between the finite element and Taylor series estimates. That difference is plotted against the eigenvalue itself.

<table>
<thead>
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<th>$h^{-1}$</th>
<th>32</th>
<th>64</th>
<th>128</th>
<th>256</th>
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<td>26th estimate</td>
<td>6058.272</td>
<td>6049.884</td>
<td>6049.286</td>
<td>6048.509</td>
</tr>
<tr>
<td>27th estimate</td>
<td><strong>6263.288</strong></td>
<td>6064.930</td>
<td>6049.528</td>
<td>6049.247</td>
</tr>
</tbody>
</table>

Table 6.1: Consecutive eigenvalue estimates that demonstrate eigenvalue crossing.
on a log-log graph in Figure 6-10 and it is immaterial which of the estimates is used for the x-axis. The three curves correspond to the Taylor series estimates with one term ($\lambda_n$), two terms ($\lambda_n + \lambda'_n$) and three terms ($\lambda_n + \lambda'_n + \frac{1}{2} \lambda''_n$).

The data is consistent with the following conjecture. For $\lambda < 1000$, the finite element estimate is closer to the true polygon eigenvalue. Therefore, the difference between the estimates essentially represents the error in the Taylor series. Each term in that expansion reduces the error by a factor of 100. The error grows linearly with the eigenvalue. This is precisely what the "expanding circle" example would suggest.

For $\lambda > 1000$ the 3-term Taylor series wins over finite elements. The plotted difference is essentially the FE error, which grows as $\lambda^3$. Until roughly $\lambda = 10000$, the finite element estimate is better than the Taylor series with two terms. This is no longer true for $\lambda > 10000$ and soon the two lowest curves meet, for they both represent the finite element error.

Table (6.2) shows our estimates for the first ten simple eigenvalues on the regular 128-sided polygon.

| $\lambda_1$ | 5.78552 | $\lambda_6$ | 326.69528 |
| $\lambda_2$ | 30.48357 | $\lambda_7$ | 450.11529 |
| $\lambda_3$ | 74.91726 | $\lambda_8$ | 593.28245 |
| $\lambda_4$ | 139.09646 | $\lambda_9$ | 756.19675 |
| $\lambda_5$ | 223.02237 | $\lambda_{10}$ | 938.85822 |

Table 6.2: Best estimates for the 10 lowest radial eigenvalues for the regular polygon with 128 sides
6.4 Expansion in powers of $1/N$

This idea is so natural that we were surprised not to find any mention of it in the literature. Still, it seems very likely that this series has been established by earlier authors!

Suppose that $\lambda_n^{(N)}$ is the $n$-th simple eigenvalue for an $N$-sided regular polygon. We express $\lambda_n^{(N)}$ as a series in powers of $1/N$:

$$
\lambda_n^{(N)} = \lambda_n \left( 1 + a_{1n} \frac{1}{N} + a_{2n} \left( \frac{1}{N} \right)^2 + \ldots \right),
$$

where $\lambda_n$ is the corresponding eigenvalue on the circle.

The $a_{nm}$ can be determined from the Taylor series by expanding each term in powers of $1/N$. The first non-zero term is $O\left(1/N^2\right)$ and can be determined from the first Taylor term

$$
\frac{d\lambda_n(n)}{dt} = -2\lambda_n \left( \frac{N}{2\pi} \cos \frac{\pi}{N} \ln \left( 1 + \sin \frac{\pi}{N} \right) - 1 \right)
$$

$$
= \lambda_n \left( \frac{2}{3} \frac{\pi^2}{N^2} + \frac{2}{315} \frac{1}{N^6} + O\left( \frac{1}{N^8} \right) \right)
$$

Therefore $a_{1n} = 0$ and $a_{2n}$ is independent of $n$:

$$
a_{2n} = \frac{2}{3} \pi^2
$$

Figure 6-9 shows the difference between the first 10 simple eigenvalues on regular $N$-sided polygons and the circle. The slope of $-2$ tells us that convergence is quadratic.

To determine the next term in (6.43), we computed the difference $\Delta$ between $\lambda_n \left( 1 + \frac{2}{3} \frac{\pi^2}{N^2} \right)$ and
The difference $\lambda_n^{[N]} - \lambda_n$ decreases like $1/N^2$ for the first ten simple eigenvalues.

The slope was $-3$, indicating that the next term is $O(N^{-3})$. Numerically, the average for the quantity

$$\frac{\Delta}{N^3} = \frac{\lambda_n \left(1 + \frac{2}{3} \frac{\pi^2}{128^2}\right) - \lambda_n^{[128]}}{128^3}$$

over the first ten eigenvalues equals 5.1570. We can therefore conjecture that

$$\alpha_{3n} = \frac{\pi^3}{6}$$

We have therefore been able to obtain the first four terms in the desired series

$$\lambda_n^{(N)} = \lambda_n \left(1 + \frac{2}{3} \frac{\pi^2}{N^2} + \frac{1}{6} \frac{\pi^3}{N^3} + \ldots\right)$$

Finding a general expression for each term in this series remains an open problem. We anticipate that the general term of the series depends on $n$ – but this dependence does not seem to occur in the low terms.

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Conclusions and Acknowledgements

Conclusions

We have considered two problems: equilibrium and stability of electron bubbles and eigenvalues of regular polygons. These problems are united by a common theme: the change in eigenvalues is induced by the deformation of the boundary $S$. The latter is specified by the velocity of the boundary $C(t)$ along the normal $N(t)$. The first derivative of a simple eigenvalue $\lambda$ is given by

$$\frac{d\lambda}{dt} = \int_S dSC \nabla^i \psi \nabla_i \psi,$$

(C.49)

where $\psi$ is the corresponding eigenfunctions. Equation (C.49) applied to arbitrary domains and perturbations $C$. The second derivative can also be given by an expression applicable to arbitrary domains and perturbations:

$$\frac{d^2\lambda}{dt^2} = \left\{ \begin{array}{l}
-2 \int_S dSC \left( \nabla^i \frac{\partial \psi}{\partial t} + C N^i \nabla_j \nabla^i \psi \right) \nabla_i \psi \\
+ \int_S dSC^2 B_{\alpha}^i \nabla^i \psi \nabla_i \psi
\end{array} \right\}$$

(C.50)

The definition of the $\frac{\partial}{\partial t}$-derivative employed in that expression is defined by (2.6) in Chapter 2. The curvature tensor $B_{\alpha}^i$ is also discussed in Chapter 2.

The formulas (C.49) and (C.50) are derived in Chapter 5.

The eigenvalues of regular polygons are discussed in Chapter 6. The deformation of the unit circle into an $N$-sided regular polygon can be described by a motion such that at $t = 0$:

$$C_{t=0} = \frac{\cos \frac{\pi}{N}}{\cos \alpha} - 1$$

where $-\pi/N \leq \alpha \leq \pi/N$. For this particular motion, the derivatives of simple eigenvalues $\lambda_n$ at $t = 0$ are

$$\left. \frac{d\lambda_n}{dt} \right|_{t=0} = -2 \lambda_n \left( \frac{N}{2\pi} \cos \frac{\pi}{N} \ln \frac{1 + \sin \frac{\pi}{N}}{1 - \sin \frac{\pi}{N}} - 1 \right)$$

(C.51a)

$$\left. \frac{d^2\lambda_n}{dt^2} \right|_{t=0} = 4 \frac{\rho_n^2}{R^2} \left( |C_0|^2 + \sum_{m \neq 0} |C_m|^2 \left( m - \rho_n \frac{J_{m+1}(\rho_n)}{J_m(\rho_n)} \right) \right)$$

(C.51b)
where \( C_m^{[N]} \) is the \( m \)-th Fourier coefficient of \( C \)

\[
C_m^{[N]} = \begin{cases} 
\frac{N}{2\pi} \int_{-\pi/N}^{\pi/N} \left( \frac{\cos \frac{\pi}{N} - 1}{\cos \alpha} \right) e^{-ik\alpha} d\alpha, & m = kN \\
0, & m \neq kN 
\end{cases}
\]

and \( J_m \) is the Bessel function.

Given the exact values for eigenvalue derivatives, an estimate for simple eigenvalues \( \lambda_n^{[N]} \) on polygons can be obtained as a Taylor series

\[
\lambda_n^{[N]} \approx \lambda_n + \frac{d\lambda_n}{dt} \bigg|_{t=0} + \frac{1}{2} \frac{d^2\lambda_n}{dt^2} \bigg|_{t=0}.
\]

Closed form expressions do not exist for eigenvalues of regular polygons. Therefore, in order to test the efficiency of the Taylor series estimates, we must have an alternative way of computing eigenvalues and we do so by Finite Elements. There are a number of factors that inhibit the use of Finite Elements: a need for very fine meshes to capture the complicated geometry, \( O(\lambda^3) \) error and eigenvalue crossing. We overcome these obstacles by considering a single slice of a regular polygon and computing eigenvalues with zero Neumann boundary conditions along the equal sides. For \( \lambda < 1000 \), the FE estimate is closer to the true polygon eigenvalue than the Taylor series estimates. Therefore, the difference between the estimates essentially represents the error in the Taylor series. Each term in the series reduces the error by a factor of 100. For \( \lambda > 1000 \) the 3-term Taylor series wins over finite elements. The plotted difference is essentially the FE error, which grows as \( \lambda^3 \). Until roughly \( \lambda = 10000 \), the finite element estimate is better than the Taylor series with two terms. This is no longer true for \( \lambda > 10000 \) and soon the two lowest curves meet, for they both represent the FE error.

The equilibrium and stability of electron bubbles is discussed in Chapter 5. In mathematical terms, the problem is to minimize the energy \( E \) with respect to the location of the boundary \( S \). The energy is given by

\[
E = \frac{\hbar^2}{8\pi^2 m} \lambda + \sigma \int_S dS + P \int_\Omega d\Omega,
\]

where \( \hbar \) is Planck's constant, \( m \) is the electron mass, \( \sigma \) is the surface tension and \( P \) is the hydrostatic pressure. We consider a more abstract expression for energy:

\[
E = \Psi \lambda + \Sigma \int_S dS + \Pi \int_\Omega d\Omega
\]

The positive constant \( \Sigma \) corresponds to surface tension and \( \Pi \) corresponds to pressure, which may be positive or negative. The resulting equilibrium equation

\[
\Psi \nabla^2 \psi + \Sigma B^\alpha_{\alpha} - \Pi = 0
\]

is highly non-linear and in most cases can only be solved numerically. In certain situations, the solution is not unique. We analyze equation (C.56) for radially symmetric states in two and three dimensions. In both cases, this system yields a surprising result: the equilibrium spherical configuration for all but the lowest eigenvalue does not deliver a local minimum of the energy.
Figure 6-10: The difference between the FEM and the Taylor Series estimates for $\lambda < 20000$.

Physically, this implies that the $2S$ electron bubbles are unstable. We solve equation (C.56) by a gradient descent scheme for several of the lowest eigenvalues in two dimensions and discover stable non-spherical equilibrium shapes for each of the eigenvalues, such as $\lambda_2$ seen in Figure 6-11.
Figure 6-11: An equilibrium shape for the 2S-electron bubble at \(-0.75\) bars.

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There are very many people who contributed to my career at MIT of which this work is a culmination. I would like to begin by thanking two very special people: my academic advisor Gilbert Strang and my father Michael Grinfeld. Professor Strang took me under his wing three years ago and has guided me steadfastly ever since. He lit a fire in me with his vision and sustained it with a steady supply of exciting problems. Into a world in which I look for instabilities, he brought stability. I am eagerly looking forward to our working together on problems in the coming years.

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