Analysis and computation of a quadratic matrix polynomial with Schur-products and applications to the Barboy-Tenne model

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Abstract

Quadratic matrix polynomials of the form $Y^2 + \tau \circ Y = B + \tau \circ C$, where $Y, \tau, B$, and $C$ are real, symmetric 3x3 matrices and the dot $\circ$ denotes the Schur product, arise in the Barboy-Tenne equations of statistical mechanics [1]. In this paper we discuss the number of solutions for $Y$, and devise and implement algorithms solving equations of this form. We will focus our attention on solving the equations in two specific cases and discuss the existence of a solution in the general case.
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1 Introduction

The Barboy-Tenne equations of statistical mechanics [1], which describe the interaction of \( N \) species of sticky sphere particles, give rise to quadratic matrix polynomials of the form

\[ Y^2 + \tau \circ Y = B + \tau \circ C. \]

Here, \( Y, \tau, B, \) and \( C \) are real, symmetric 3x3 matrices and the dot \( \circ \) denotes the Schur product. In this paper we investigate the solutions, \( Y \), of quadratic matrix polynomials of this form and methods for solving these equations, and we will discuss why these solutions are of interest to us. We will look at these polynomials in the case where \( N = 1 \) and \( N = 2 \) and we will analyze the existence of a solution for all \( N \) as well as the number of solutions for \( N = 1 \) and \( N = 2 \).

2 The Barboy-Tenne Equations

Here we introduce the Barboy-Tenne equations of statistical mechanics [1] and show how they can be written in the form of a quadratic matrix polynomial, allowing us to solve for a set of the parameters of interest, \( \lambda \).

The Barboy-Tenne equations of statistical mechanics describe the interaction of \( N \) species of sticky sphere particles. The problem that this paper sets out to solve is concerned with a mixture of \( N \) types of particles and how they interact. Each type of particle has a specific diameter and density, and for any two given particles, we have a parameter that describes the distance between their centers. We want to analyze the behavior of these particles. How do they interact? Our particles have an attraction factor that determines how colliding particles will behave. When two or more particles collide, they may behave like hard spheres and repel each other, they may behave like sticky spheres and have some resistance to separation, or they may behave like something between hard and sticky spheres.

We will discuss some critical transitions of our mixture of particles as well. We will look at the spinodal — the point where our mixture is no longer smooth, but breaks down, and determine how this affects the interaction of our particles. We will also determine how the attraction factor between any two given particles affects our being able to solve the Barboy-Tenne Equations for our parameter of interest.

We define several parameters before stating the equations. Let \( \rho_\gamma \) be the density of particle \( \gamma \). Let \( d_{\alpha\alpha} \) be the diameter of particle \( \alpha \) and \( d_{\alpha\beta} = \frac{d_{\alpha\alpha} + d_{\beta\beta}}{2} \) be the distance of the closest centers of particles \( \alpha \) and \( \beta \), where \( \alpha, \beta = 1, 2, ..., N \).

For the convenience of a more simplified equation we define \( \xi_i = \frac{\pi}{6} \sum_\gamma \rho_\gamma d_{\gamma\gamma}^3 \). The measure of attraction between particle \( \alpha \) and particle \( \beta \) is given by the
dimensionless parameter $\tau_{\alpha\beta}$. When $\tau_{\alpha\beta}$ is 0, we have strong adhesion between particles $\alpha$ and $\beta$, and when $\tau_{\alpha\beta}$ is infinite, particles $\alpha$ and $\beta$ behave like hard spheres. Our interest lies in solving the equations for $\lambda_{\alpha\beta}$, a dimensionless function of $\rho_\gamma$, $d_{\gamma\gamma}$, and $\tau_{\alpha\beta}$. The Barboy-Tenne equations are given by:

$$\frac{\pi d_{\alpha\beta}}{12(1 - \xi_3)} \sum_\gamma \rho_\gamma d_{\gamma\gamma}^2 (\lambda_{\alpha\gamma} - 6) (\lambda_{\beta\gamma} - 6) - \tau_{\alpha\beta} \lambda_{\alpha\beta} = \frac{9d_{\alpha\beta}\xi_2}{(1 - \xi_3)} - \frac{6d_{\alpha\beta}^2}{d_{\alpha\alpha}d_{\beta\beta}}$$  \hspace{1cm} (2.1)$$

We will use Eq. (2.1) and find all possible values of $\lambda$ for the interaction of a species with itself (one-component) and for the interaction of two species (two-component), and we will discuss how these values are used to compute things of interest. These one and two component cases are discussed in sections 3 and 4.

### 2.1 Quadratic Matrix Polynomial of the Barboy-Tenne Equations

We will show how the Barboy-Tenne equations can be put into the form $Y^2 + \tau \circ Y = B + \tau \circ C$. Let $\tilde{\tau} = \tau \frac{12(1 - \xi_3)}{\pi d_{\alpha\beta}}$. We divide both sides of Eq. (2.1) by $\frac{\pi d_{\alpha\beta}}{12(1 - \xi_3)}$ and then add $6\tilde{\tau}_{\alpha\beta}$ to both sides which allows us to rewrite Eq. (2.1) as:

$$\sum_\gamma \rho_\gamma d_{\gamma\gamma}^2 (\lambda_{\alpha\gamma} - 6)(\lambda_{\beta\gamma} - 6) - \tilde{\tau}_{\alpha\beta} (\lambda_{\alpha\beta} - 6) = \left( \frac{9d_{\alpha\beta}\xi_2}{(1 - \xi_3)} - \frac{6d_{\alpha\beta}^2}{d_{\alpha\alpha}d_{\beta\beta}} \right) \left( \frac{12(1 - \xi_3)}{\pi d_{\alpha\beta}} \right) + 6\tilde{\tau}_{\alpha\beta}$$  \hspace{1cm} (2.2)$$

Let the matrices $L$, $D$, $\tilde{B}$, and $\tilde{C}$ be given as follows:

$$L = \begin{bmatrix} \lambda_{11} - 6 & \lambda_{12} - 6 & \cdots \\ \lambda_{12} - 6 & \lambda_{22} - 6 & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix}$$

$$D = \begin{bmatrix} \sqrt{\rho_1}d_{11} \\ \sqrt{\rho_2}d_{22} \\ \vdots \end{bmatrix}$$

$$\tilde{B} = \begin{bmatrix} \left( \frac{9d_{\alpha\beta}\xi_2}{(1 - \xi_3)} - \frac{6d_{\alpha\beta}^2}{d_{\alpha\alpha}d_{\beta\beta}} \right) \left( \frac{12(1 - \xi_3)}{\pi d_{\alpha\beta}} \right) & \cdots \\ \vdots & \ddots \end{bmatrix}$$
\[ \hat{C} = \begin{bmatrix} 6 & 6 & \cdots \\ 6 & 6 & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix} \]

Then we can rewrite Eq.(2.2) using the above matrices and the substitution \( Y = -DLD \) to obtain:

\[ Y^2 + \tilde{\tau} \circ Y = B + \tilde{\tau} \circ C \quad (2.3) \]

### 3 One Component Case

In this section we consider the interaction of sticky spheres of a single species. From the Barboy-Tenne model where \( \alpha = \beta = 1 \) we obtain a quadratic equation in \( \lambda \) from which we calculate the spinodal — the point at which phase separation occurs in our model. Phase separation is when our mixture of particles separates into groups where we can see a heavy concentration of one particular type of particle in each group. In the case in which we have two types of particles (corresponding to indices \( \alpha \) and \( \beta \)), we can say phase separation has occurred when we see two groups — one made up of mostly particles of type \( \alpha \) with a few of type \( \beta \), and one made up mostly of particles of type \( \beta \) with a few of type \( \alpha \).

#### 3.1 The Spinodal and the Hessian

In order to understand what the spinodal is mathematically, we must first introduce the Hessian. We introduce a simplified factorization of \( Q[2] \), used to compute the Hessian which is given by \( Q^TQ \) [3].

\[
\rho = \begin{bmatrix} \rho_1 \\ \rho_2 \\ \vdots \end{bmatrix}, \quad X = \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}, \quad S = \begin{bmatrix} s_{11} & s_{12} & \cdots \\ s_{21} & s_{22} & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix}, \quad \gamma = \begin{bmatrix} 1 & \frac{d_1}{d_1} & \cdots \\ \frac{d_2}{d_1} & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix}, \quad U = \begin{bmatrix} 1 & 1 & \cdots \\ 1 & 1 & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix}
\]

\[
Q = \sqrt{\rho} X^{-1} (I + XS \circ \gamma)(I + XU) X \sqrt{\rho}^{-1}
\]
$S$ is a symmetric matrix where $s_{ij} = 3 - \lambda_{ij}$. We note that the factor of $(I + XS \circ \gamma)$ is singular when $\frac{x^{-1}}{\gamma} + S$ is singular.

The matrix $(I + XU)$ has $N - 1$ eigenvalues of 1 whose corresponding eigenvectors are:

\[
\begin{bmatrix}
1 \\
-1 \\
0 \\
0 \\
\vdots \\
0
\end{bmatrix}, \begin{bmatrix}
1 \\
0 \\
-1 \\
0 \\
\vdots \\
0
\end{bmatrix}, \ldots, \begin{bmatrix}
1 \\
0 \\
0 \\
\vdots \\
-1
\end{bmatrix}
\]

and an $N$th eigenvalue of $1 + x_1 + x_2 + x_3 + \ldots + x_N$ with corresponding eigenvector

\[
\begin{bmatrix}
x_1 \\
x_2 \\
x_3 \\
x_4 \\
\vdots \\
x_N
\end{bmatrix}
\]

Since all the values of $x_i$ are non-negative, the matrix $(I + XU)$ has $N$ non-zero eigenvalues, thus it is non-singular.

Our Hessian is a symmetric matrix composed of the second partial derivatives of the free energy as a function of composition and gives us insight on the stability of our mixtures. If the Hessian has only positive eigenvalues then it will be a positive definite matrix, meaning we have a stable mixture.

The issue of the spinodal occurs when our Hessian matrix is singular, or in other words, when $Q$ in singular. As we saw above, $Q$ will be singular when the factor $(I + XS \circ \gamma)$ is singular.

### 3.2 The One Component Equation

For interaction of a single species with itself we obtain the following quadratic equation:

\[
\frac{\pi d_{11}}{12(1 - \xi_3)}\rho_1 d_{11}^2 (\lambda_{11} - 6)^2 - \tau_{11} \lambda_{11} = 9 \frac{d_{11} \xi_2}{1 - \xi_3} - 6
\]
By multiplying both sides of the equation by a factor of 2 and using the substitution $\xi_3 = \frac{\pi}{6}d_{11}^3\rho_1$ we obtain:

$$\frac{\xi_3}{1 - \xi_3}\rho_1 d_{11}^2(\lambda_{11} - 6)^2 - 2\tau_{11}\lambda_{11} = 18\frac{\xi_3}{1 - \xi_3} - 12$$

Now we make the substitution $x = \frac{\xi_3}{1 - \xi_3}$ which yields:

$$(\lambda_{11} - 6)^2 - 2\frac{\tau}{x}\lambda_{11} = 18 - \frac{12}{x}$$

We can complete the square and use the quadratic formula to solve for $\lambda$ to obtain:

$$\lambda = \frac{\tau}{x} + 6 \pm \sqrt{\left(\frac{\tau}{x} + 6\right)^2 - \left(18 + \frac{12}{x}\right)} \quad (3.1)$$

For our one-component case, we have two roots and we know the right solution, the solution that should be used in other computations, to a certain limit. In order for a root to be of interest to us, we need to see continuity—a smooth change in the value of $\lambda_{\alpha\beta}$ that reflects a change in the value of $\tau_{\alpha\beta}$. If we apply this idea of continuity to the two roots found in the one component case, then the value of $\lambda$ that has meaning to us will approach zero as $x$ approaches infinity. Therefore, our root of interest will be the negative square root, shown in Eq.(3.2), as it satisfies this condition.

$$\lambda = \frac{\tau}{x} + 6 - \sqrt{\left(\frac{\tau}{x} + 6\right)^2 - \left(18 + \frac{12}{x}\right)} \quad (3.2)$$

### 3.2.1 Critical Transitions

Here we consider two critical transitions that affect the model of particle interaction. It is possible that we lose our root, meaning the value of $\lambda$ becomes complex. At this point, we still accurately represent the physics, but our model breaks down before phase separation occurs. A second possibility is that $\lambda$ is real and our model is still accurate, but our mixture breaks down and we experience phase separation. The point at which phase separation occurs is called the spinodal. We can calculate the curve (in the one-component case) or the surface (in the two-component case) of the spinodal by determining when the Hessian matrix—the matrix of the second partial derivatives of the Gibbs free energy as a function of composition—is singular.

Now we will Use Eq.(3.2) to determine what values of $\tau$ yield complex roots.
We begin by solving the inequality of the discriminant being less than 0 for $\tau$:

\[
\left( \frac{\tau}{x} + 6 \right)^2 - \left( 18 + \frac{12}{x} \right) < 0
\]

\[
\tau < \sqrt{(18x^2 + 12x) - 6x}
\] (3.3)

### 3.3 One Component Spinodal

Our interest now lies in the single component spinodal equation, which follows from $\det(Q) = 0$, and is given by:

\[
1 + x(3 - \lambda) = 0
\] (3.4)

We will investigate when our roots become complex — before or after we reach the spinodal. From the equation of the spinodal we obtain a new expression for lambda given by:

\[
\lambda = \frac{1}{x} + 3
\] (3.5)

By equating the expressions for lambda given in Eq.(3.2) and Eq.(3.5) we obtain:

\[
\frac{\tau}{x} + 6 - \sqrt{\left( \frac{\tau}{x} + 6 \right)^2 - \left( 18 + \frac{12}{x} \right)} = \frac{1}{x} + 3
\] (3.6)

By solving Eq.(3.6) for $\tau$ we find the curve of the spinodal in terms of $x$:

\[
\left( \frac{\tau}{x} + 6 \right) = \frac{18 + \frac{12}{x} + \left( \frac{1}{x} + 3 \right)^2}{2 \left( \frac{1}{x} + 3 \right)}
\]

\[
\frac{\tau}{x} = \frac{18 + \frac{12}{x} + \left( \frac{1}{x} + 3 \right)^2}{2 \left( \frac{1}{x} + 3 \right)} - 6
\]

Multiplying through by $\frac{x^2}{x}$ isolates $\tau$ on the left hand side and tells us at what point phase separation occurs. These values of $\tau$ are given in Eq.(3.7):

\[
\tau = \frac{18x^2 + 12x + (1 + 3x)^2}{2(1 + 3x)} - 6x
\] (3.7)
3.4 One Component Phase Diagram

Now we introduce the curve of the spinodal and the curve defining when the roots turn complex. The equations for these curves are respectively given by:

\[ \tau = \frac{18x^2 + 12x + (1 + 3x)^2}{2(1 + 3x)} - 6x \]  \hspace{1cm} (3.8)

\[ \tau = \sqrt{18x^2 + 12x} - 6x \]  \hspace{1cm} (3.9)

The following plot displays the curves defined by Eq.(3.8) and Eq.(3.9) in the \( \tau - x \) plane. It is crucial to note that the curve of the spinodal defined by the root of interest does not begin until the two curves reach a critical point at the \( x \) value 0.137. Thus, for values of \( x \) less than 0.137, or values of \( \tau \) less than approximately 0.585, our roots will turn complex before phase separation occurs.

Figure 1: Curves of the Spinodal and Roots Turning Complex

Figure 1 shows that for low values of \( x \) our model will break down before we reach phase separation, whereas for high values of \( x \), phase separation occurs before the model breaks down.
4 Two Component Case

4.1 The Two Component Equations

For interaction of two species we obtain the following coupled quadratic equations from Eq.(2.1):

\[
\frac{\pi d_{11}}{12(1 - \xi)} \left( \rho_1 d_{11}^2 (\lambda_{11} - 6)^2 + \rho_2 d_{22}^2 (\lambda_{12} - 6)^2 \right) - \tau_{11} \lambda_{11} = \frac{9 d_{11} \xi_2}{1 - \xi} - 6 \quad (4.1)
\]

\[
\frac{\pi d_{12}}{12(1 - \xi)} \left( \rho_1 d_{11}^2 (\lambda_{11} - 6)(\lambda_{12} - 6) + \rho_2 d_{22}^2 (\lambda_{12} - 6)(\lambda_{22} - 6) \right) - \tau_{12} \lambda_{12} = \frac{9 d_{12} \xi_2}{1 - \xi} - \frac{6 d_{12}^2}{d_{22}d_{11}} \quad (4.2)
\]

\[
\frac{\pi d_{22}}{12(1 - \xi)} \left( \rho_1 d_{11}^2 (\lambda_{12} - 6)^2 + \rho_2 d_{22}^2 (\lambda_{22} - 6)^2 \right) - \tau_{22} \lambda_{22} = \frac{9 d_{22} \xi_2}{1 - \xi} - 6 \quad (4.3)
\]

We can reformat Eq.(4.1), Eq.(4.2), and Eq.(4.3) as a a single sixth degree equation. Assuming we know all of the roots of a sixth degree equation, we will have a complete characterization of the roots of the two-component case. We will find these roots numerically.

4.1.1 Sixth Degree Polynomial

Our quadratic matrix polynomial can be written as \( Y^2 + \tilde{\tau} \circ Y = B + \tilde{\tau} \circ C \) where \( Y = \begin{bmatrix} y_{11} & y_{12} \\ y_{12} & y_{22} \end{bmatrix} \). We begin by letting \( R = B + \tilde{\tau} \circ C \) so that our matrix polynomial becomes \( Y^2 + \tilde{\tau} \circ Y = R \) and we obtain:

\[
y_{11}^2 + y_{12}^2 + \tilde{\tau}_{11} y_{11} = R_{11} \quad (4.4)
\]

\[
y_{22}^2 + y_{12}^2 + \tilde{\tau}_{22} y_{22} = R_{22} \quad (4.5)
\]

\[
y_{12}(y_{11} + y_{22}) + \tilde{\tau}_{12} y_{12} = R_{12} \quad (4.6)
\]

Now we let \( y_{11} = u + v \) and \( y_{22} = u - v \) and use this substitution to rewrite Eq.(4.4) and Eq.(4.5) to obtain:
\[
\begin{align*}
\dot{u}^2 + 2uv + v^2 + y_{12}^2 + \tilde{\tau}_{11}(u + v) &= R_{11} \quad (4.7) \\
\dot{u}^2 - 2uv + v^2 + y_{12}^2 + \tilde{\tau}_{22}(u - v) &= R_{22} \quad (4.8)
\end{align*}
\]

By summing Eq.(4.7) and Eq.(4.8) we obtain:

\[
2\dot{u}^2 + 2v^2 + 2y_{12}^2 + u(\tilde{\tau}_{11} + \tilde{\tau}_{22}) + v(\tilde{\tau}_{11} - \tilde{\tau}_{22}) = R_{11} + R_{22} \quad (4.9)
\]

By dividing Eq.(4.9) by 2 and completing the square for \(u\) and \(v\) we obtain:

\[
\left[u + \frac{1}{4}(\tilde{\tau}_{11} + \tilde{\tau}_{22})\right]^2 + \left[v + \frac{1}{4}(\tilde{\tau}_{11} - \tilde{\tau}_{22})\right]^2 + y_{12}^2 = \frac{1}{2}(R_{11} + R_{22}) + \frac{1}{16}\left((\tilde{\tau}_{11} + \tilde{\tau}_{22})^2 + (\tilde{\tau}_{11} - \tilde{\tau}_{22})^2\right) \quad (4.10)
\]

Now we let \(\hat{u} = [u + \frac{1}{4}(\tilde{\tau}_{11} + \tilde{\tau}_{22})]\) and \(\hat{v} = [v + \frac{1}{4}(\tilde{\tau}_{11} - \tilde{\tau}_{22})]\) and substitute to obtain:

\[
\hat{u}^2 + \hat{v}^2 + y_{12}^2 = \frac{1}{2}(R_{11} + R_{22}) + \frac{\tilde{\tau}_{11}^2 + \tilde{\tau}_{22}^2}{8} \quad (4.10)
\]

By subtrating Eq.(4.5) from Eq.(4.4) we obtain:

\[
4uv + u(\tilde{\tau}_{11} - \tilde{\tau}_{22}) + v(\tilde{\tau}_{11} + \tilde{\tau}_{22}) = R_{11} - R_{22}
\]

Now we divide both sides of the equation by 4 and complete the product to obtain:

\[
uv + \frac{1}{4}u(\tilde{\tau}_{11} - \tilde{\tau}_{22}) + \frac{1}{4}v(\tilde{\tau}_{11} + \tilde{\tau}_{22}) = \frac{R_{11} - R_{22}}{4}
\]

\[
(u + \frac{1}{4}u(\tilde{\tau}_{11} + \tilde{\tau}_{22}))(v + \frac{1}{4}u(\tilde{\tau}_{11} - \tilde{\tau}_{22})) = \frac{R_{11} - R_{22}}{4} + \frac{\tilde{\tau}_{11}^2 - \tilde{\tau}_{22}^2}{16}
\]

\[
\hat{u} \cdot \hat{v} = \frac{R_{11} - R_{22}}{4} + \frac{\tilde{\tau}_{11}^2 - \tilde{\tau}_{22}^2}{16} \quad (4.11)
\]

Now we can rewrite Eq.(4.6) using the substitution \(u = y_{11} + y_{22}\) to obtain:

\[
(u + \frac{1}{2}\tilde{\tau}_{12})y_{12} = \frac{1}{2}R_{12} \quad (4.12)
\]
Since \( \hat{u} = u + \frac{1}{4}(\bar{\tau}_{11} + \bar{\tau}_{22}) \) we have \( u = \hat{u} - \frac{1}{4}(\bar{\tau}_{11} + \bar{\tau}_{22}) \) and if we substitute this into Eq.(4.12) we obtain:

\[
[\hat{u} - \frac{1}{4}(\bar{\tau}_{11} - 2\bar{\tau}_{12} + \bar{\tau}_{22})]y_{12} = \frac{1}{2}R_{12}
\]  

(4.13)

By solving Eq.(4.11) for \( \hat{v} \) and solving for \( y_{12} \) in terms of \( \hat{u} \) in Eq.(4.13) then substituting these into Eq.(4.10) we obtain a rational polynomial expression in \( \hat{u} \):

\[
\hat{u}^2 + \left( \frac{R_{11} - R_{22}}{4} + \frac{\bar{\tau}_{11}^2 - \bar{\tau}_{22}^2}{16} \right) - \frac{(\frac{1}{2}R_{12})^2}{\hat{u}^2} = \frac{R_{11} + R_{22}}{2} + \frac{\bar{\tau}_{11}^2 + \bar{\tau}_{12}^2}{8}
\]

(4.14)

To rewrite Eq.(4.14) as a sixth degree polynomial expression we multiply by \( \hat{u}^2[\hat{u} - \frac{1}{4}(\bar{\tau}_{11} - 2\bar{\tau}_{12} + \bar{\tau}_{22})]^2 \) and obtain:

\[
\hat{u}^4[\hat{u} - \frac{1}{4}(\bar{\tau}_{11} - 2\bar{\tau}_{12} + \bar{\tau}_{22})]^2 + [\hat{u} - \frac{1}{4}(\bar{\tau}_{11} - 2\bar{\tau}_{12} + \bar{\tau}_{22})]^2 \left[ \frac{R_{11} - R_{22}}{4} + \frac{\bar{\tau}_{11}^2 - \bar{\tau}_{22}^2}{16} \right]
\]

\[
+ \hat{u}^2 \left( \frac{1}{2}R_{11} \right)^2 = \hat{u}^2[\hat{u} - \frac{1}{4}(\bar{\tau}_{11} - 2\bar{\tau}_{12} + \bar{\tau}_{22})]^2 \left[ \frac{R_{11} + R_{22}}{6} + \frac{\bar{\tau}_{11}^2 + \bar{\tau}_{12}^2}{8} \right]
\]

(4.15)

Now we wish to find the roots of this polynomial in order to determine the values of \( \lambda \) and find the correct root - the root that has meaning in the relevant physics problem.

### 4.1.2 Solving the Sixth Degree Polynomial

To solve Eq.(4.15), we use an eigenvalue routine. Suppose we look at the companion matrix, \( M \), for Eq.(4.15). Let

\[
M = \begin{bmatrix}
0 & 1 & 0 & \cdots \\
0 & 0 & 1 & \cdots \\
\vdots & \vdots & \vdots & \ddots \\
-a_0 & -a_1 & \ldots & -a_{N-1}
\end{bmatrix}
\]

Then \( \det(M - \lambda I) = \lambda^N + a_{n-1}\lambda^{N-1} + \ldots + a_0 \). Therefore, if we expand Eq.(4.15) and let \( a_k \) be the coefficient of \( \hat{u}^k \), the eigenvalues of \( M \) will be the
roots of the polynomial.

Expanding Eq.(4.15) we obtain:

\[
\hat{u}^6 - \frac{1}{2}(\bar{\tau}_{11} - 2\bar{\tau}_{12} + \bar{\tau}_{22})\hat{u}^5 + \left[\frac{1}{16}(\bar{\tau}_{11} - 2\bar{\tau}_{12} + \bar{\tau}_{22})^2 - \left(R_{11} + R_{22} + \frac{(\bar{\tau}_{11}^2 + \bar{\tau}_{12}^2)^2}{8}\right)\right]\hat{u}^4
\]

\[
+ \frac{1}{2}\left(\frac{R_{11} + R_{22}}{6} + \frac{(\bar{\tau}_{11}^2 + \bar{\tau}_{12}^2)^2}{8}\right)(\bar{\tau}_{11} - 2\bar{\tau}_{12} + \bar{\tau}_{22})\hat{u}^3 + \left[\frac{R_{11} - R_{22}}{4} + \frac{(\bar{\tau}_{11}^2 - \bar{\tau}_{22}^2)^2}{16}\right]\hat{u}^2
\]

\[
+ \left(\frac{1}{2}R_{11}\right)^2 - \frac{1}{16}\left(\frac{R_{11} + R_{22}}{6} + \frac{(\bar{\tau}_{11}^2 + \bar{\tau}_{12}^2)^2}{8}\right)(\bar{\tau}_{11} - 2\bar{\tau}_{12} + \bar{\tau}_{22})^2\hat{u}^2
\]

\[
- \frac{1}{2}\left[\frac{R_{11} - R_{22}}{4} + \frac{(\bar{\tau}_{11}^2 - \bar{\tau}_{22}^2)^2}{16}\right](\bar{\tau}_{11} - 2\bar{\tau}_{12} + \bar{\tau}_{22})\hat{u} + \frac{1}{16}(\bar{\tau}_{11} - 2\bar{\tau}_{12} + \bar{\tau}_{22})^2\left[\frac{R_{11} - R_{22}}{4} + \frac{(\bar{\tau}_{11}^2 - \bar{\tau}_{22}^2)^2}{16}\right] = 0
\]

(4.16)

Now we can define the \(a_k\)’s as:

\[
a_6 = 1
\]

\[
a_5 = -\frac{1}{2}(\bar{\tau}_{11} - 2\bar{\tau}_{12} + \bar{\tau}_{22})
\]

\[
a_4 = \left[\frac{1}{16}(\bar{\tau}_{11} - 2\bar{\tau}_{12} + \bar{\tau}_{22})^2 - \left(R_{11} + R_{22} + \frac{(\bar{\tau}_{11}^2 + \bar{\tau}_{12}^2)^2}{8}\right)\right]
\]

\[
a_3 = \frac{1}{2}\left(\frac{R_{11} + R_{22}}{6} + \frac{(\bar{\tau}_{11}^2 + \bar{\tau}_{12}^2)^2}{8}\right)(\bar{\tau}_{11} - 2\bar{\tau}_{12} + \bar{\tau}_{22})
\]

\[
a_2 = \left[\frac{R_{11} - R_{22}}{4} + \frac{(\bar{\tau}_{11}^2 - \bar{\tau}_{22}^2)^2}{16}\right] + \left(\frac{1}{2}R_{11}\right)^2 - \frac{1}{16}\left(\frac{R_{11} + R_{22}}{6} + \frac{(\bar{\tau}_{11}^2 + \bar{\tau}_{12}^2)^2}{8}\right)(\bar{\tau}_{11} - 2\bar{\tau}_{12} + \bar{\tau}_{22})^2
\]

\[
a_1 = -\frac{1}{2}\left[\frac{R_{11} - R_{22}}{4} + \frac{(\bar{\tau}_{11}^2 - \bar{\tau}_{22}^2)^2}{16}\right](\bar{\tau}_{11} - 2\bar{\tau}_{12} + \bar{\tau}_{22})
\]

\[
a_0 = \frac{1}{16}(\bar{\tau}_{11} - 2\bar{\tau}_{12} + \bar{\tau}_{22})^2\left[\frac{R_{11} - R_{22}}{4} + \frac{(\bar{\tau}_{11}^2 - \bar{\tau}_{22}^2)^2}{16}\right]
\]

Given these definitions of the \(a_k\)’s, we can substitute them into the 6x6 matrix \(M\) and find its eigenvalues, the roots of the sixth degree polynomial. This yields six values of \(\hat{u}\) which allows us to use Eq.(4.12) to find six values for \(y_{12}\). We then use the values of \(y_{12}\) to to solve for \(\hat{v}\) in Eq.(4.10), allowing us to then find six values for \(v\).

With six values each for \(u\) and \(v\) in hand, we use the substitutions that gave
rise to Eq.(4.7) and Eq.(4.6), namely \( y_{11} = u + v \) and \( y_{22} = u - v \), to find six values for \( y_{11} \) and \( y_{22} \). Once we know the values of \( Y = \begin{bmatrix} y_{11} & y_{12} \\ y_{12} & y_{22} \end{bmatrix} \) we can use the fact that \( Y = -DLD \) to find six values for \( \lambda \).

Reformulating our problem as finding the solutions of a sixth degree polynomial establishes that in the two component case there are six solutions for \( \lambda \), and reminds us of how powerful the Fundamental Theorem of Algebra really is. The MATLAB code used to generate these values of \( \lambda \) can be found in appendix B.

### 4.2 Two Component Spinodal

We define \( \eta_i = x_i(1 - \xi_3) \) and \( s_{ij} = 3 - \lambda_{ij} \) for \( i, j \in \{1, 2\} \) where the \( \lambda \)'s are all functions of \( \eta_1, \eta_2 \). The spinodal for the two component case is \( 1 + x_1 s_{11} + x_2 s_{22} + x_1 x_2 (s_{11}s_{22} - s_{12}^2) = 0 \). We analyze the spinodal first as a function of \( \tau_{11} \) by fixing the values of \( \tau_{12} \) and \( \tau_{22} \) and determining the values of \( \tau_{11} \) that make \( \det(I + X S \circ \gamma) \) equal to zero. Second, we analyze the spinodal as a function of \( \tau_{12} \) by fixing the values of \( \tau_{11} \) and \( \tau_{22} \) and determining the values of \( \tau_{12} \) that make \( \det(I + X S \circ \gamma) \) equal to zero.

### 4.3 Two Component Phase Diagram

Before beginning, we must understand the meaning of a value of \( \tau_{ij} \) being infinite. If \( \tau_{ij} \) is infinite its corresponding value of \( \lambda_{ij} \) will be zero, and when a particle of type \( i \) interacts with a particle of type \( j \), they will behave like hard spheres.

For convenience we define \( \phi_i = \frac{\pi}{6} \rho_i d_i^3 \). For our first case, we let \( \tau_{12} = 5 \) and let \( \tau_{22} \) be infinite and we obtain the following surface representing the spinodal in the two-component case as a function of \( \tau_{11} \).
Figure 2: Surface of the Spinodal as a function of $\tau_{11}$

In Figure 2 we see a clear trend that as $\phi_1$ and $\phi_2$ increase, the value of $\tau_{11}$ at which we reach the spinodal increases.

For the second case, we let $\tau_{11} = .56$ and let $\tau_{22}$ again be infinite and we obtain the following surface representing the spinodal in the two component case as a function of $\tau_{12}$. 
Figure 3: Surface of the Spinodal as a function of $\tau_{12}$

5 Analysis of Solutions

5.1 Existence of a Solution

We have shown that in the one component case we have two solutions, and in the two component case we have six solutions. This leaves the case for general $N$ open. We will establish that there is at least one real root in the general case, given that $\tau_{ij}$ is not too small, in other words, that our spheres are not “too sticky”.

Before showing that there is at least one real root, we wish to establish certain bounds on the matrices $B$, $C$, and $Z = Y - C$, which we will regard as vectors in $R^{N^2}$. Let $T_{\text{max}} = \max\{\tau_{ij}\}$ and let $T_{\text{min}} = \min\{\tau_{ij}\}$, as we will later bound certain norms in terms of the largest and smallest components of $\tau$.

We would like to establish a bound for $||Z^2||$. Let $Z_i$ denote the $i^{th}$ row of $Z$, and $Z_j$ denote the $j^{th}$ column of $Z$. Let’s begin by looking at $||Z^2||^2$:

$$||Z^2||^2 = \sum_{ij} |Z_{ij}|^2 = \sum_{ij} |Z_i \cdot Z_j|^2$$
By the Cauchy-Schwarz inequality we have

\[ \sum_{ij} |Z_i \cdot Z_j|^2 \leq \sum_{ij} ||Z_i||^2 ||Z_j||^2 \]

so we obtain:

\[ ||Z^2||^2 \leq \sum_{ij} ||Z_i||^2 ||Z_j||^2 \]
\[ = \sum_i ||Z_i||^2 \sum_j ||Z_j||^2 \]
\[ = \sum_i ||Z_i||^2 \sum_j \sum_k |Z_{kj}|^2 \]
\[ = \sum_i ||Z_i||^2 ||Z_i||^2 \]
\[ = ||Z||^4 \]

By taking the square root of both sides we obtain the desired bound:

\[ ||Z^2|| \leq ||Z||^2 \]

Note that the symbol \( \cdot \) is regarded as an \( \mathbb{R}^{N^2} \) dot product and not the Schur product in establishing our bounds. We find the following bounds by using the Cauchy-Schwarz inequality to obtain:

\[ ||Z \cdot B|| \leq ||Z|| ||B|| \]
\[ 0 \leq ||Z||^2 \cdot T \leq Z \cdot \tau \circ Z \text{ where } T = \min \tau_{ij} \]
\[ ||Z \cdot C^2|| \leq ||Z|| ||C^2|| \]
\[ ||Z \cdot Z^2|| \leq ||Z|| ||Z^2|| \leq ||Z||^3 \]
\[ ||C \cdot Z|| = ||Z \cdot C|| \leq ||Z|| ||C|| \]

We will use the bounds just established to help us prove the following theorem on the existence of a solution.

**Theorem:** For any \( N \), and any symmetric matrices \( B \) and \( C \), if \( T_{\text{min}} > \)
$2(\sqrt{||C^2 - B|| + ||C||})$ then Eq.(2.3) has at least one real root [4].

**Proof:** Note that if $B = C^2$ we have the trivial case resulting in the equation $Y^2 + \tau \circ Y = C^2 + \tau \circ C$ and our solution is $Y = C$. Now we concern ourselves with the case $B \neq C^2$. Consider $Y^2 + \tau \circ Y = B + \tau \circ C$ and make the substitution $Z = Y - C$ to obtain:

\[(Z + C)^2 + \tau \circ (Z + C) = B + \tau \circ C\]

\[Z^2 + ZC + CZ + C^2 + \tau \circ Z - B = 0\] (5.1)

We would like to turn our root finding problem into a problem of finding fixed points of a mapping. To do so, we will introduce $\varepsilon > 0$. We can rewrite Eq. (5.1) as

\[Z - \varepsilon(Z^2 + ZC + CZ + C^2 + \tau \circ Z - B) = Z\] (5.2)

for any $\varepsilon > 0$. If we define our mapping as

\[Z' = Z - \varepsilon(Z^2 + ZC + CZ + C^2 + \tau \circ Z - B)\]

then finding fixed points of this mapping will be finding roots to Eq (5.2), and thus roots of Eq.(5.1). Now that our root finding problem is a problem of finding the fixed points of a mapping, we need to establish that this mapping takes the domain and maps it back into itself. If we can show this, then Brouwer’s Fixed Point Theorem ensures that there is a fixed point of our mapping [5].

We want to show that for some $\delta$, if $||Z|| < \delta$, then $||Z'|| < \delta$. By the triangle inequality we have:

\[||Z'|| \leq ||Z - \varepsilon \tau \circ Z|| + \varepsilon||Z^2 + ZC + CZ + C^2 - B||\]

Assume $||Z|| \leq \delta$, and we will show that if $\varepsilon < \frac{1}{T_{\min} + T_{\max}}$ then $||Z'|| \leq \delta$ if $T_{\min}$ is sufficiently large.

\[||Z - \varepsilon \tau \circ Z||^2 = \sum_{ij} \left(1 - \frac{\tau_{ij}}{T_{\min} + T_{\max}}\right)^2 Z_{ij}^2 \leq \left(\frac{T_{\max}}{T_{\min} + T_{\max}}\right)^2 ||Z||^2\]

So:

\[||Z - \varepsilon \tau \circ Z|| \leq \frac{T_{\max}}{T_{\min} + T_{\max}} ||Z|| < \frac{T_{\max}}{T_{\min} + T_{\max}} \delta\]
and
\[ \varepsilon\|Z^2 + ZC + CZ + C^2 - B\| \leq \frac{1}{T_{\min} + T_{\max}} (\delta^2 + 2\delta\|C\| + \|C^2 - B\|) \]

Now, we want
\[ \frac{T_{\max}}{T_{\min} + T_{\max}} \delta + \frac{1}{T_{\min} + T_{\max}} (\delta^2 + 2\delta\|C\| + \|C^2 - B\|) \leq \delta \]

which will be true for \( T_{\min} > \frac{\delta^2 + 2\delta\|C\| + \|C^2 - B\|}{\delta} \).

\[ \square \]

Our proof provides a relationship between \( T_{\min} \) and \( \delta \) which we summarize in the following corollary.

**Corollary:** For any \( N \), and any symmetric matrices \( B \) and \( C \), if \( T_{\min} > \frac{\delta^2 + 2\delta\|C\| + \|C^2 - B\|}{\delta} \) then Eq.(2.3) has at least one real root in the sphere \( \|Z\| < \delta \).

The minimum value of \( g(\delta) = \frac{\delta^2 + 2\delta\|C\| + \|C^2 - B\|}{\delta} \) occurs when \( \delta = \sqrt{\|C^2 - B\|} \) which yields \( g(\sqrt{\|C^2 - B\|}) = 2(\sqrt{\|C^2 - B\|} + \|C\|) \). Therefore, for \( T_{\min} > 2(\sqrt{\|C^2 - B\|} + \|C\|) \), Eq.(5.1) will have at least one real root, and hence, Eq.(2.3) has a real solution \( Y \).

**Corollary:** For any \( N \), and any symmetric matrices \( B \) and \( C \), if \( T_{\min} > \frac{2(\sqrt{\|C^2 - B\|} + \|C\|)}{\delta} \) then Eq.(2.3) has at least one real root in the sphere \( \|Z\| < \delta \), where \( \delta = \sqrt{\|C^2 - B\|} \).

### 5.2 The Number of Solutions

Here we explore the possible number of solutions to Eq.(2.1) for both the general case in matrix form, and the two component case in polynomial form.

#### 5.2.1 Solutions of the General Case

From our analysis of the one-component and two-component cases above, it seems that we can expect at least \( 2^N \) solutions to a quadratic matrix polynomial as in Eq.(2.3) when \( \tau = 0 \). Consider diagonalizing the matrix \( Y^2 \). Then we obtain:
\[ Y^2 = M = QDQ^T \]
and for $Y$ we obtain:

$$Y = QZQ^T$$

Now,

$$Z^2 = D = \begin{bmatrix} d_{11} & d_{22} & \cdots & d_{NN} \\ \vdots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots \\ d_{NN} & \cdots & \cdots & d_{NN} \end{bmatrix}$$

Thus we obtain:

$$Z = \begin{bmatrix} \pm \sqrt{d_{11}} \pm \sqrt{d_{22}} \ldots \pm \sqrt{d_{NN}} \end{bmatrix}$$

So we can expect that Eq.(2.3) will have at least $2^N$ distinct solutions for distinct values of $d$. For the case $N = 2$, we have seen that there are in fact six solutions to our polynomial, so we use $2^N$ as a loose guideline for finding the number of roots in the general case.

### 5.2.2 Solutions of the Two Component Case

By restating our problem as a sixth degree polynomial we have established that there are six solutions in the two component case. Here we look at a second approach to determining these solutions. We turn our attention to Eq.(4.10), Eq.(4.11) and Eq.(4.13), and take a geometric approach to determine the number of solutions. Eq.(4.10) is the graph of a sphere, while both Eq.(4.11) and Eq.(4.13) are hyperbolas. We are interested in the intersections of these three equations as they correspond to the roots of our sixth degree polynomial in Eq.(4.16). From these values of $\hat{u}$ we can back substitute to find the corresponding values of $\lambda$ which solve the two component system of equations as stated in Eq.(4.1), Eq.(4.2), and Eq.(4.3).

By solving Eq.(4.11) for $\hat{v}$ and substituting it into Eq.(4.10) we can find an equation for $y_{12}$ as a function of $\hat{u}$. Let $K = \frac{R_{11} - R_{22}}{4} + \frac{\tau_{11} - \tau_{22}}{16}$ and $C^2 = \frac{R_{11} + R_{22}}{2} + \frac{\tau_{11} + \tau_{22}}{8}$ and from Eq.(4.11) we obtain:

$$\hat{u}^2 + \frac{K^2}{\hat{u}^2} + y_{12}^2 = C^2$$

$$y_{12} = \pm \sqrt{C^2 - \hat{u}^2 - \frac{K^2}{\hat{u}^2}}$$

(5.3) \hspace{1cm} (5.4)
The following graphs illustrate the intersections of these three equations for various values of $R_{ij}$ and $\tau_{ij}$ where $i, j \in \{1, 2\}$.

Fig. 4 shows four intersections of these curves when $R = \begin{bmatrix} 7.1420 & 9.7820 \\ 9.7820 & 27.7820 \end{bmatrix}$, $\rho_1 = 0.0003$, $\rho_2 = 0.0045$, $d = \begin{bmatrix} 7 \\ 7 \end{bmatrix}$, and $\tau = \begin{bmatrix} .56 \\ 1 \\ 4 \end{bmatrix}$.

Figure 4: Intersections of Eq.(4.10), Eq.(4.11), and Eq.(4.13)

The values of $\hat{u}$ where the graphs intersect can be used to back substitute and find the corresponding values of $\lambda$. In the particular case of Figure 4, we can see that there will be four roots to the two component equations.
6 Conclusions

For the interaction of sticky spheres of a single species we found that there are two solutions. We found these solutions by solving the quadratic equation that arises from Eq.(2.3). From these two candidates we used the idea of continuity — that our root varies continuously, and in fact smoothly, with the $\tau$’s — to pick out the root of interest, or the root that is physically realistic. By using the single component equation we can develop a graph of the spinodal, which gives us insight into whether we first reach phase separation or a break down in our model for certain values of $x$ and $\tau$.

For the two component equation we found that our matrix polynomial could be re-expressed as a sixth degree polynomial. We were able to quickly find all six solutions of the polynomial by finding the eigenvalues of its companion matrix. From these six solutions we used the idea of continuity to sort through our roots and determine which five are extraneous and which one is our root of interest. Again, we use the two-component equations to look at the surface defined by the spinodal to tell us for which values of $\phi_i$ and $\tau_{\alpha\beta}$ we expect phase separation to occur.

Now that we know there is always a solution to $Y^2 + \tau \circ Y = B + \tau \circ C$ given certain conditions, we can look toward solving Eq.(2.3) for the case $N = 3$, making a generalization to the number of solutions, and rewriting the problem to solve for these solutions.
References


APPENDIX

A Use of the Quadratic Formula

When attempting to find the solvents of a quadratic matrix polynomial, our first question might be whether the quadratic formula can be applied to equations of the form $Y^2 + \tau \circ Y = B + \tau \circ C$ when $Y$, $\tau$, $B$, and $C$ are real matrices. For the quadratic matrix polynomial in question, we will find a solution by completing the square for $Y^2 + BY + C = 0$.

\[ Y^2 + BY = -C \]

\[ Y^2 + BY + \frac{1}{4}B^2 = \frac{1}{4}B^2 - C \]

\[ (Y + \frac{1}{2}B)^2 = \frac{1}{4}B^2 - C \]

\[ Y = \sqrt{\frac{1}{4}B^2 - C} - \frac{1}{2}B \]

Our question now is if this can indeed be a solution to the quadratic matrix polynomial equation. We investigate this question by substituting the result of completing the square into the quadratic matrix polynomial.

\[ Y^2 + BY = -C \]

\[ \left( \sqrt{\frac{1}{4}B^2 - C} - \frac{1}{2}B \right)^2 + B \left( \sqrt{\frac{1}{4}B^2 - C} - \frac{1}{2}B \right) + C = 0 \]

\[ \frac{1}{4}B^2 - C - \frac{1}{2}B \left( \sqrt{\frac{1}{4}B^2 - C} \right) - \left( \sqrt{\frac{1}{4}B^2 - C} \right) \frac{1}{2}B + \frac{1}{4}B^2 + B \left( \sqrt{\frac{1}{4}B^2 - C} \right) - \frac{1}{2}B^2 + C = 0 \]

In order for this to work, $\frac{1}{4}B^2 - C$ must have a square root, and $B$ and $C$ must commute.

B MATLAB Code

B.1 CarriePoly.m
% To run this file define:
% a 2x2 matrix tau,
% a 1x2 matrix rho, and
% a 2x2 matrix d.

%Define rho using phi.
rho(1) = (6*phi(1))/(pi*(d(1,1)^3));
rho(2) = (6*phi(2))/(pi*(d(2,2)^3));

% Create the values used to find the spinodal and the hessian
eta1 = (pi/6)*(d(1,1)^3)*rho(1);
eta2 = (pi/6)*(d(2,2)^3)*rho(2);
x1 = eta1/(1-eta1-eta2);
x2 = eta2/(1-eta1-eta2);
X = [x1 0; 0 x2];
gamma = [1 d(1,1)/d(2,2); d(2,2)/d(1,1) 1];
U = ones(2);

% Create the matrices B and C.
C = [6 6; 6 6];

xi2 = (pi/6)*((rho(1)*(d(1,1)^2)+ rho(2)*(d(2,2)^2)));
xi3 = (pi/6)*((rho(1)*(d(1,1)^3)+ rho(2)*(d(2,2)^3)));

bval11 = (((9*d(1,1)*xi2)/(1-xi3)) - ((6*d(1,1)^2)/(d(1,1)*d(1,1))))* (12*(1-xi3)/(pi*d(1,1)));
bval12 = (((9*d(1,2)*xi2)/(1-xi3)) - ((6*d(1,2)^2)/(d(1,1)*d(2,2))))* (12*(1-xi3)/(pi*d(1,2)));
bval22 = (((9*d(2,2)*xi2)/(1-xi3)) - ((6*d(2,2)^2)/(d(2,2)*d(2,2))))* (12*(1-xi3)/(pi*d(2,2)));
B = [bval11 bval12; bval12 bval22];

% Account for tau absorbing the term (12*(1-xi3))/(pi*d_alphabet)
tau(1,1) = tau(1,1)*((12*(1-xi3))/(pi*d(1,1)));
tau(1,2) = tau(1,2)*((12*(1-xi3))/(pi*d(1,2)));
tau(2,1) = tau(2,1)*((12*(1-xi3))/(pi*d(2,1)));
tau(2,2) = tau(2,2)*((12*(1-xi3))/(pi*d(2,2)));

% Create the matrix D.
for ijk = 1:2
   D(ijk,ijk) = sqrt(rho(ijk))*d(ijk,ijk);
end

% Create the matrix R
R = D*B*D + D*tau.*C*D;

% Define some variables.
T = tau(1,1) - 2*tau(1,2) + tau(2,2);
S = ((R(1,1) - R(2,2))/4 + (tau(1,1)^2 - tau(2,2)^2)/16)^2;
P = (R(1,1) + R(2,2))/2 + (tau(1,1)^2 + tau(2,2)^2)/8;
a = zeros(6,0)';
% Define the coefficients of the 6th degree polynomial
a(1) = (1/16)*(T^2)*S;
a(2) = (-1/2)*T*S;
a(3) = S + (1/4)*R(1,2)^2 - (1/16)*(T^2)*P;
a(4) = (1/2)*T*P;
a(5) = (1/16)*(T^2) - P;
a(6) = (-1/2)*T;
a(7) = 1;

% Put the coefficients in a matrix
M = [0 1 0 0 0 0; 0 0 1 0 0 0; 0 0 0 1 0 0; 0 0 0 0 1 0; -a(1) -a(2) -a(3) -a(4) -a(5) -a(6)];

% Use the eigenvalues of the matrix to get uhat, vhat, u and v.

uhat = eig(M);
u = uhat - (1/4)*(tau(1,1) + tau(2,2));
vhat = ((R(1,1) - R(2,2))/(4*uhat)) + ((tau(1,1)^2 - tau(2,2)^2)/(16*uhat));
u = vhat - (1/4)*(tau(1,1) - tau(2,2));

% Find the matrix Y and use it to find the lambdas.
y11 = u + v;
y12 = (R(1,2))/(2*u + tau(1,2));
y22 = u - v;

for ijk = 1:length(uhat)
    Y = [y11(ijk) y12(ijk); y12(ijk) y22(ijk)];
    L = inv(D)*-1*Y*inv(D);
    lambda = L + [6 6; 6 6];

% Find the spinodal using each root.
SMatrix = [3 - lambda(1,1) 3-lambda(1,2); 3-lambda(1,2) 3-lambda(2,2)];
spinodal = det(eye(2) + (X*SMatrix).*gamma)
end

% Find the Q and the Hessian
for ijk = 1:2
    sqrtrho(ijk,ijk) = sqrt(rho(ijk));
end

for ijk = 1:2
    for k = 1:2
        Q = sqrtrho*inv(X)*(eye(2) + X*SMatrix.*gamma)*(eye(2) + X*U)*X*inv(sqrtrho);
    end
end
Hessian = Q'*Q;