Contents

1 Derivation of equations

We start with free energy for excluded volume.

$$F = \frac{C_{rest}}{C_\infty}\left(u\ln\left(\frac{u}{c_\infty - u - v}\right) + v\ln\left(\frac{v}{c_\infty - u - v}\right)\right) + c_\infty \ln\left(1 - \frac{u+v}{c_\infty}\right) \tag{1}$$

For the rest of this text I will use c instead of c_∞. Also I denote

$$R = c - u - v, A = \frac{C_{\text{rest}}}{c_\infty} \tag{2}$$

From free energy we get the chemical potentials

$$\mu_u = \frac{\partial F}{\partial u} = A\left(\left(\ln\frac{u}{R}\right) + \frac{R+u+v-c_\infty}{R}\right) = A\left(\ln\frac{u}{R}\right) = A\ln(u) - A\ln(R) \tag{3}$$

$$\mu_v = \frac{\partial F}{\partial v} == A\ln(v) - A\ln(R) \tag{4}$$

In the end we want to compute $\partial_x u \partial_x(\mu_u)$, because the full equation is

$$\dot{u} = \partial_x u \partial_x(\mu_u) + f_u(u,v). \tag{5}$$

The computations are contained in the next subchapter

1.1 Extended calculations

We want to compute

$$\mu_u = \frac{\partial F}{\partial u}, \tag{6}$$

where

$$F = u \ln \frac{u}{R} + v \ln \frac{v}{R} + c \ln \left(1 - \frac{u+v}{c}\right) \tag{7}$$

$$= u \ln u - u \ln R + v \ln v - v \ln R + c \ln R - c \ln c \tag{8}$$

We have

$$\begin{aligned}
&\frac{\partial}{\partial u}(u \ln u) = \ln u + 1, \\
&\frac{\partial}{\partial u}(-u \ln R) = -\ln R + \frac{u}{R}, \text{ (the mistakes were here)} \\
&\frac{\partial}{\partial u}(v \ln v) = 0, \\
&\frac{\partial}{\partial u}(-v \ln R) = \frac{v}{R}, \\
&\frac{\partial}{\partial u}(c \ln R) = -\frac{c}{R}, \\
&\frac{\partial}{\partial u}(-c \ln c) = 0.
\end{aligned}$$

So in the end we get

$$\mu_u = \ln u - \ln R = \ln u - \ln(c - u - v), \tag{9}$$

using

$$R = c - u - v. \tag{10}$$

Now we compute derivative We have

$$\partial_x \mu_u = \frac{u'}{u} - \frac{R'}{R} = \left(\frac{1}{u} + \frac{1}{R}\right) u' + \frac{1}{R} v' \tag{11}$$

So we would get

$$D_{uu} = (1 + \frac{u}{R}) = 1 + \frac{u}{c - u - v} \tag{12}$$

$$D_{uv} = \frac{u}{R} = \frac{u}{c - u - v} \tag{13}$$

So

$$\partial_x(u \partial_x \mu_u) = u'' + \frac{u'R - R'u}{R^2}(u' + v') + \frac{u}{R}(u'' + v'') \tag{14}$$

$$= u'' + \frac{u'}{R}(u' + v') + \frac{u}{R^2}(u' + v')^2 + \frac{u}{R}(u'' + v'') \tag{15}$$

$$= u'' - \frac{u(RR'' - (R')^2) + R'u'R}{R^2} \tag{16}$$

$$= u'' - \frac{u}{R} R'' + u \frac{(R')^2}{R^2} - \frac{R'u'}{R} \tag{17}$$

Or finally

$$\partial_x(u\partial_x\mu_u) = u'' + \frac{u'}{(c-u-v)}(u'+v') \tag{18}$$

$$+ \frac{u}{(c-u-v)^2}(u'+v')^2 + \frac{u}{(c-u-v)}(u''+v'') \tag{19}$$

And from this we get the linearization $u \to u + \delta u$, by also assuming $u', v', u'', v'' = 0$ and ignoring higher order terms.

$$\delta\dot{u} = \delta u'' + \frac{u}{c-u-v}(\delta u'' + \delta v'') + \text{ reaction kinetics part}$$

If we introduce the coefficient in free energy we'll get

$$\delta\dot{u} = D_1\left(\delta u'' + \frac{u}{c-u-v}(\delta u'' + \delta v'')\right) + \text{ reaction kinetics part}$$

Or

$$\delta\dot{u} = (D_{uu}\delta u'' + D_{uv}\delta v'')$$

for $\delta w = (\delta u, \delta v)$

$$\delta\dot{w} = \begin{pmatrix} D_1(1+\frac{u}{c-u-v}) & D_1\frac{u}{c-u-v} \\ D_2\frac{v}{c-u-v} & D_2(1+\frac{v}{c-u-v}) \end{pmatrix}\delta w'' + \text{ reaction kinetics part}$$

So the end result is the same

1.2 Linearization

The linearized equation looks like

$$\delta\dot{w} = \bar{D}\delta w'' + A(w)\delta w, \tag{20}$$

where

$$\bar{D} = \begin{pmatrix} D_1(1+\frac{u}{c-u-v}) & D_1\frac{u}{c-u-v} \\ D_2\frac{v}{c-u-v} & D_2(1+\frac{v}{c-u-v}) \end{pmatrix} \tag{21}$$

As usual taking $\delta w = v_q \exp iqx + \sigma t$ leads to the eigenvalue problem

$$\sigma v_q = (-q^2\bar{D} + A)v_q \tag{22}$$

2 Eigenvalue analysis

We want to find the eigenvalues $\sigma(q)$. Thus we look at the characteristic polynomial

$$\det(A - q^2\bar{D} - \sigma\mathbf{1}) = 0 \tag{23}$$

We can denote $A_q = A - q^2\bar{D}$. Then we get

$$\sigma^2 - \mathrm{tr}A_q\sigma + \det A_q = 0 \tag{24}$$

with the solutions

$$\sigma = \frac{1}{2}\left(\mathrm{tr}A_q \pm \sqrt{(\mathrm{tr}A_q)^2 - 4\det A_q}\right) \tag{25}$$

As before the condition for stability is

$$\mathrm{tr}A_q < 0, \det A_q > 0.$$

2.1 The determinant

We have the following expresssion for the determinant

$$\det A_q = \det A - q^2(d_{uu}a_{vv} + d_{vv}a_{uu} - d_{uv}a_{vu} - d_{vu}a_{uv}) + q^4 \det \bar{D}. \tag{26}$$

We'll write this as

$$\det A_q = \det A - Bq^2 + Cq^4, \tag{27}$$

We can see that

$$C = D_1 D_2 \frac{c}{c-u-v}, \tag{28}$$

or

$$\det A_q = \det A - q^2(D_2 a_{uu} + D_1 a_{vv} + B') + q^4(D_1 D_2 + C'), \tag{29}$$

where B', C' are the terms occuring solely due to the interactions. We find that the minimum occurs at $q^2_{crit} = \frac{B}{2C}$ and

$$\det A_{q_{crit}} = \det A - \frac{B^2}{4C} \tag{30}$$

Since $C > 0$, it follows that $B > 0$ as well.

2.2 The brusselator

In the case of Brusselator we have

$$A = \begin{pmatrix} b-1 & a^2 \\ -b & -a^2 \end{pmatrix} \tag{31}$$

$$\mathrm{tr}A = b - 1 - a^2 \tag{32}$$

$$\det A = a^2 \tag{33}$$

$$u = a, v = \frac{b}{a}(\text{fixed point}) \tag{34}$$

$$f_u = a - (b+1)u + u^2 v, f_v = bu - u^2 v \tag{35}$$

$$B = \frac{D_1(2ab - a^2 c) + D_2(a - c + bc - 2ab)}{R} \tag{36}$$

or in the case of $D_1 = D_2$

$$B = \frac{a - c + bc - a^2 c}{R}, \tag{37}$$

where $R = c - a - \frac{b}{a}$. Thus

$$\det A_q = a^2 - q^2 \frac{D_1(2ab - a^2 c) + D_2(a - c + bc - 2ab)}{c - a - \frac{b}{a}} + q^4 \frac{c}{c - a - \frac{b}{a}} \tag{38}$$

The trace is equal to

$$\mathrm{tr} A_q = b - 1 - a^2 - q^2 \left(\frac{D_1(c - \frac{b}{a}) + D_2(c - a)}{c - a - \frac{b}{a}}\right) \tag{39}$$

2.3 Neutral curves

To find the neutral curve we set $\det A_q = 0$. From this we solve for b. We get

$$b(q) = \frac{D_1 D_2 c q^4 + D_1 a^2 c q^2 - D_2 a q^2 + D_2 c q^2 - a^3 + a^2 c}{2 D_1 a q^2 - 2 D_2 a q^2 + D_2 c q^2 + a} \tag{40}$$

In the case of $D_1 = D_2$ it simplifies to

$$b = \frac{D^2 c q^4 + D q^2 (a^2 c - a + c) - a^3 + a^2 c}{D c q^2 + a} \tag{41}$$

It's important to remember that $R > 0$ i.e $c - a - \frac{b}{a} > 0$, which gives us a bound on b.
One can also write it as

$$b(q) = \frac{L}{c} + (a^2 - \frac{3a}{c} + 1) + \frac{a(1 - ac)(2a - c)}{cL}, \tag{42}$$

where $L = Dcq^2 + a$. The minimum occurs at $L^2 = a(1 - ac)(2a - c)$ and is equal to

$$b(q_{crit}) = 1 + a^2 + \frac{2\sqrt{a(1 - ac)(2a - c)} - 3a}{c}. \tag{43}$$

For it to exist we must have $L^2 > 0$, which means that $a \in (\frac{1}{c}, \frac{c}{2})$.

The neutral curve for trace is more complicated.

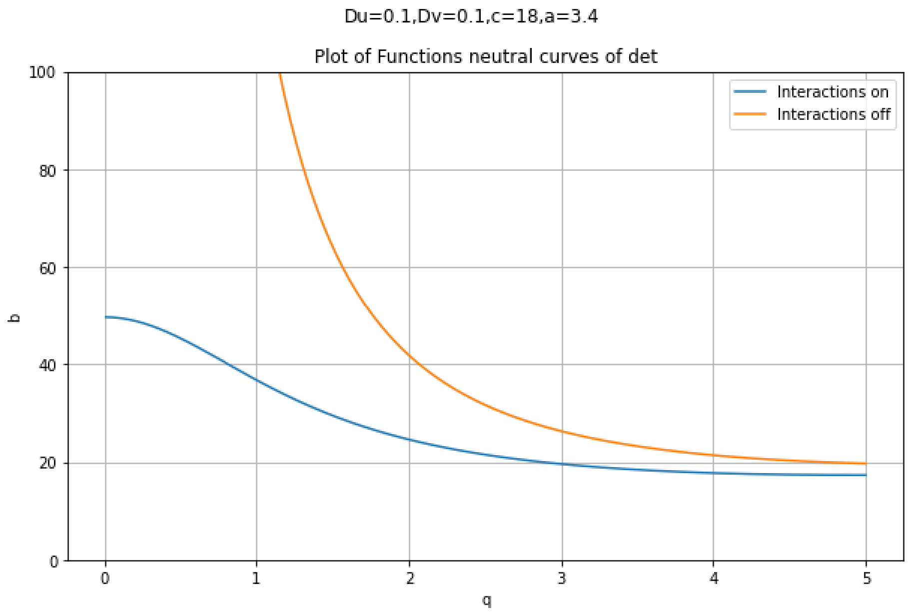
$$0 = -b^2 + b\left(ac + D_1 q^2 + 1\right) + a^4 - a^3 c + a^2\left(D_2 q^2 + 1\right) - acD_1 q^2 - acD_2 q^2 - ac \tag{44}$$

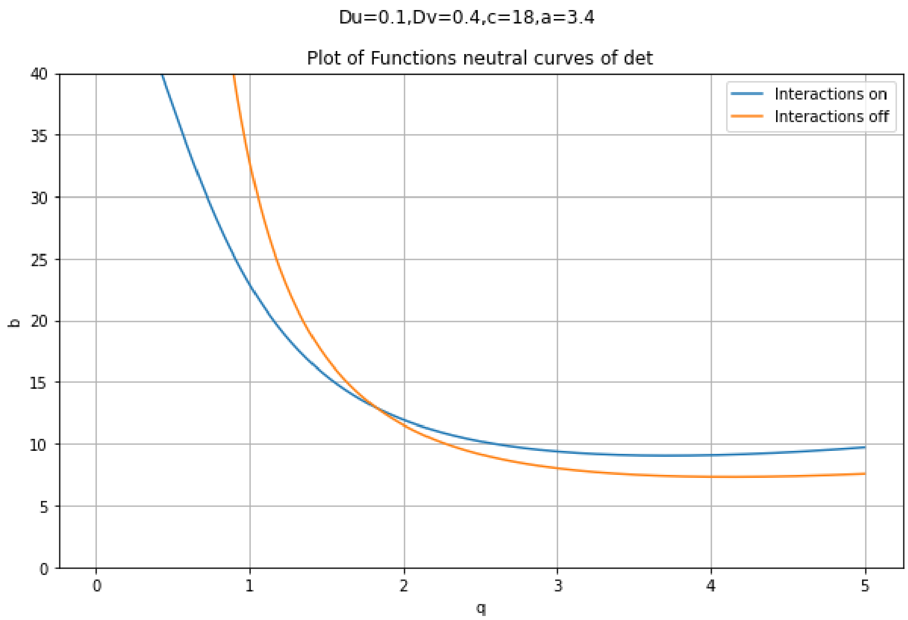
It seems like the minimum is still at $q = 0$, and the curve is closed and resembles ellipse.

3 Results

3.1 Neutral curve

Here are some comparisons between neutral curves of det, with and without interactions


Du=0.1,Dv=0.1,c=18,a=3.4
Plot of Functions neutral curves of det
Interactions on
Interactions off
b
q


Du=0.1,Dv=0.4,c=18,a=3.4
Plot of Functions neutral curves of det
Interactions on
Interactions off
b
q

ng

4 Collected equations

$$A = \begin{pmatrix} b-1 & a^2 \\ -b & -a^2 \end{pmatrix} \tag{45}$$

$$\mathrm{tr} A = b - 1 - a^2 \tag{46}$$

$$\det A = a^2 \tag{47}$$

$$u = a, v = \frac{b}{a}(\text{fixed point}) \tag{48}$$

$$f_u = a - (b+1)u + u^2 v, f_v = bu - u^2 v \tag{49}$$

$$\bar{D} = \begin{pmatrix} D_1(1+\frac{u}{c-u-v}) & D_1\frac{u}{c-u-v} \\ D_2\frac{v}{c-u-v} & D_2(1+\frac{v}{c-u-v}) \end{pmatrix} \tag{50}$$

$$\det A_q = \det A - q^2\left(d_{uu}a_{vv} + d_{vv}a_{uu} - a_{vu}d_{uv} - d_{vu}a_{uv}\right) + q^4 \det \bar{D}, \tag{51}$$

$$\det A_q = a^2 - q^2 \frac{D_1(2ab - a^2c) + D_2(a - c + bc - 2ab)}{c - a - \frac{b}{a}} + q^4 \frac{c}{c - a - \frac{b}{a}} \tag{52}$$

$$\mathrm{tr} A_q = \mathrm{tr} A - q^2 (D_1(1+\frac{u}{R}) + D_2(1+\frac{v}{R}) = b - 1 - a^2 - q^2 (\frac{D_1(c - \frac{b}{a}) + D_2(c-a)}{c - a - \frac{b}{a}}) \tag{53}$$

$$C = D_1 D_2 \frac{c}{R} \tag{54}$$