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

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

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

$$\begin{aligned} F =& u \ln \frac{u}{R} + v \ln \frac{v}{R} + c \ln \left(1 - \frac{u+v}{c}\right) && (7) \\ =& u \ln u - u \ln R + v \ln v - v \ln R + c \ln R - c \ln c && (8) \end{aligned}$$

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

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

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

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

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

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

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

or in the case of $D_1 = D_2$

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

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

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

The trace is equal to

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

We also have

$$B = \frac{a^3 D_1 - \frac{b^2 D_2}{a} - abD_1 + abD_2 + \frac{bD_2}{a}}{c - a - \frac{b}{a}} + a^2 D_1 - bD_2 + D_2 \tag{40}$$

and

$$q_c^2 = -\frac{-a^2cD_1 + a(2b(D_1 - D_2) + D_2) + (b - 1)cD_2}{2cD_1D_2} \tag{41}$$

2.3 Determinant neutral curve

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

$$b(q) = \frac{D_1D_2cq^4 + D_1a^2cq^2 - D_2aq^2 + D_2cq^2 - a^3 + a^2c}{2D_1aq^2 - 2D_2aq^2 + D_2cq^2 + a} \tag{42}$$

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

$$b = \frac{D^2cq^4 + Dq^2(a^2c - a + c) - a^3 + a^2c}{Dcq^2 + a} \tag{43}$$

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

$$b(q) = \frac{L}{c} + (a^2 - \frac{3a}{c} + 1) + \frac{a(1 - ac)(2a - c)}{cL}, \tag{44}$$

where $L = Dcq^2 + a$. The minimum occurs at $L^2 = a(1 - ac)(2a - c) = a^2c^2 + 2a^2 - ac - 2a^3c$ and is equal to

$$b(q_{crit}) = 1 + a^2 + \frac{2\sqrt{a(1 - ac)(2a - c)} - 3a}{c}. \tag{45}$$

For a minimum to exist we must have $L^2 > 0$, which means that $a \in (\frac{1}{c}, \frac{c}{2})$. Otherwise the only minimum is at $q = 0$ and is equal to $ca - a^2$. That means that c can't be too small if we want Turing patterns, i.e if $a > \frac{c}{2}$, then we only get minimum at $q = 0$ This means that $\det A_q$ is always positive for the $b's$ we're allowed to use. We also must have $\sqrt{a(1-ac)(2a-c)} - a \geq 0.$, which is the condition $L > 0.1$

2.3.1 Different diffusion coefficients

For different diffusion coefficient we can repeat the same trick, but the expressions are much more involved.

$$b(q) = B_0 L + B_1 + \frac{B_2}{L}, \tag{46}$$

where

$$L = 2aD_1q^2 - 2aD_2q^2 + cD_2q^2 + a \tag{47}$$

$$B_0 = \frac{cD_1D_2}{(2a(D_1 - D_2) + cD_2)^2} \tag{48}$$

$$B_1 = \frac{2a^3cD_1^2 - 2a^3cD_1D_2 + a^2c^2D_1D_2 - 2a^2D_1D_2 + 2a^2D_2^2 - 3acD_2^2 + c^2D_2^2}{(2aD_1 - 2aD_2 + cD_2)^2} \tag{49}$$

$$B_2 = -\frac{a(2a-c)(aD_1 - aD_2 + cD_2)\left(2a^2D_1 - 2a^2D_2 + acD_2 - D_2\right)}{(2aD_1 - 2aD_2 + cD_2)^2} \tag{50}$$

The coefficients were derived using Mathematica. As before we can find the minimum at

$$L^2 = \frac{B_2}{B_0} \tag{51}$$

2.3.2 Comparison of with the case of no interactions

For the no interaction case we have

$$b_{cN} = (1 + a\sqrt{\frac{D_1}{D_2}})^2, \tag{52}$$

which reduces to

$$b_{cN} = (1 + a)^2, \tag{53}$$

which is derived from

$$b(q) = \frac{a^2}{D_2q^2} + \frac{D_2 + D_1a^2}{D_2} + D_1q^2 \tag{54}$$

2.3.3 Monotonicity

Let's check how changing the parameters shifts the neutral curve. Let's start with the minimum, ie. b_{crit}. We can rewrite is as

$$b_{crit} = b_c^T = 1 + a^2 + 2\sqrt{a^2 + \frac{a}{c}(2\frac{a}{c} - 2a^2 - 1)} - 3\frac{a}{c} \tag{55}$$

2.4 Trace minimal curve

The neutral curve for trace is more complicated.

$$0 = -b^2 + b\left(ac + D_1q^2 + 1\right) + a^4 - a^3c + a^2\left(D_2q^2 + 1\right) - acD_1q^2 - acD_2q^2 - ac \tag{56}$$

or for $D_1 = D_2$

$$0 = -b^2 + b\left(ac + Dq^2 + 1\right) + a^4 - a^3c + a^2 - ac + Dq^2(a^2 - 2ac) \tag{57}$$

It seems like the minimum is still at $q = 0$, and the curve is closed and resembles ellipse. Actually. We know that $b = 1 + a^2$ works and it seems like $b = ca - a^2$ also works. Similar thing seems to happen when $a \approx \frac{c}{2}$. The curve suddenly flips around the maximum possible b and the minimum occurs at $q = 0$ and is equal to $ca - a^2$, which means that for these parameters the system is stable. But it's not exactly $\frac{c}{2}$ As this is a quadratic equation in b we can solve it explicitly, which will give us a square root term. We have two solutions for the square root to be equal to zero.

$$a_{crit} = \frac{1}{4}(c \pm \sqrt{c^2 - 8}) \tag{58}$$

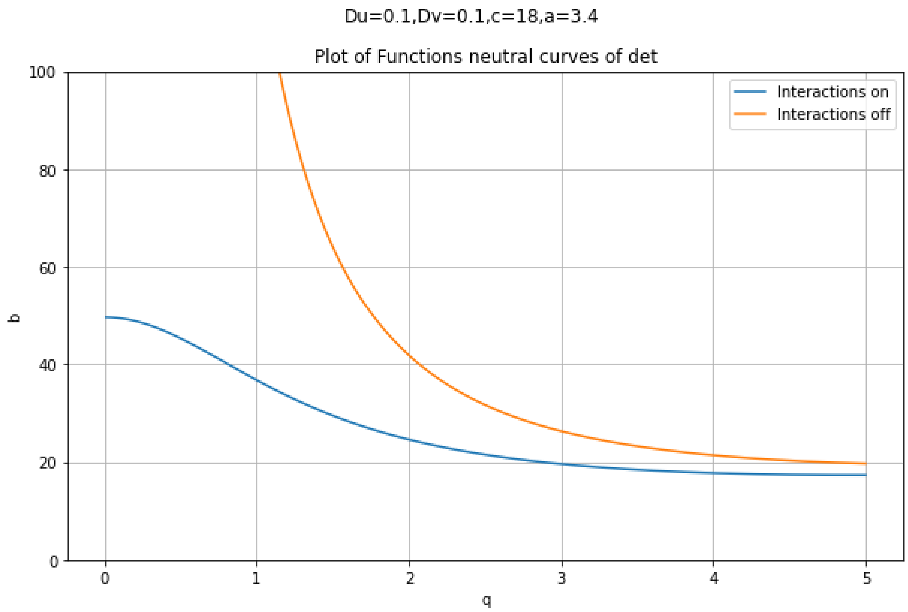
This is kind of weird since it implies c^2 can't be smaller than 8. So for $a < a_{\text{crit\_minus}}$ or $a > a_{\text{crit\_plus}}$ we have only $\text{tr}A_q < 0$ for any permissible b.

3 Results

If $2a > c$, then det is always positive. Can I manipulate

3.1 Neutral curve

Here are some comparisons between neutral curves of det, with and without interactions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Plot of Functions neutral curves of det
Interactions on
Interactions off
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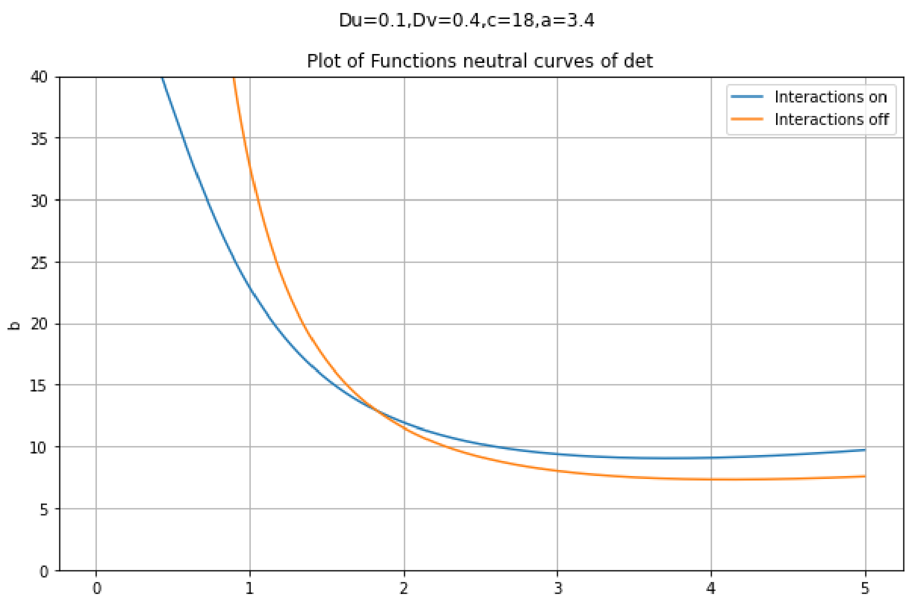
3
4
5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Plot of Functions neutral curves of det
Interactions on
Interactions off
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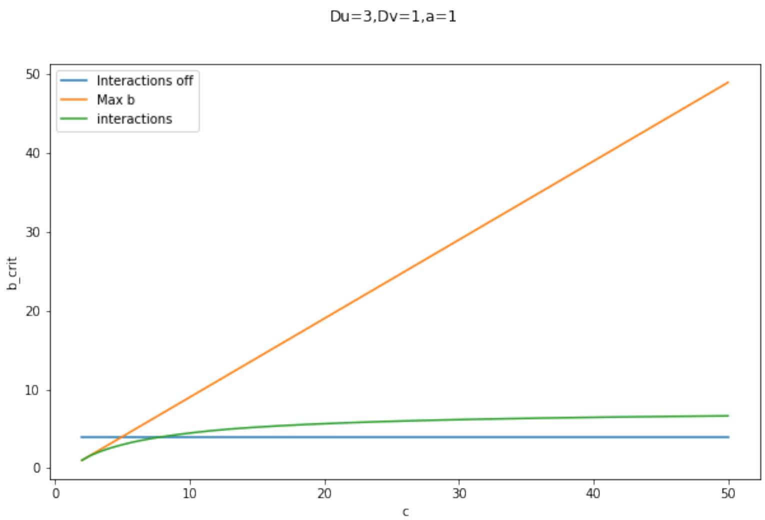
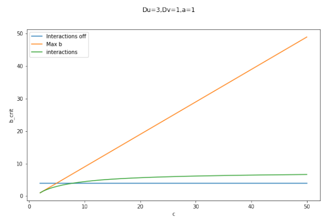
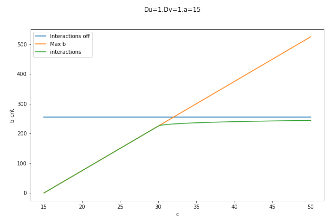
Comparison of critical parameter with and without interactions

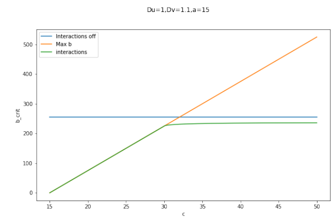




(a) Caption 1a



(b) Caption 1b



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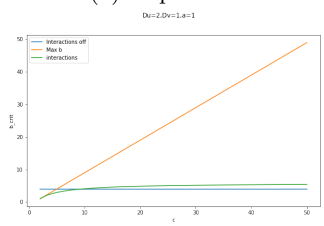

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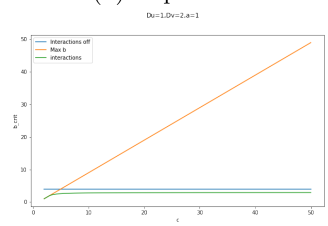

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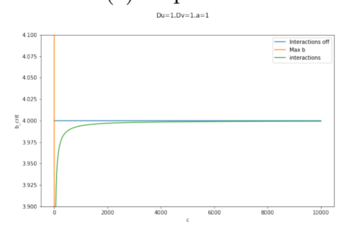

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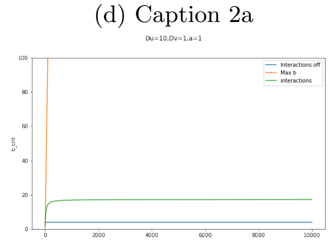

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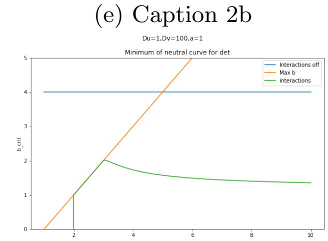

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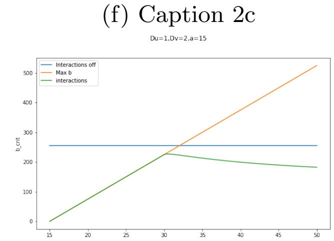
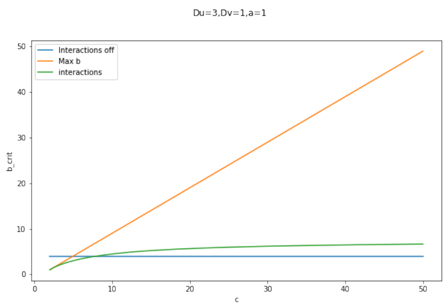
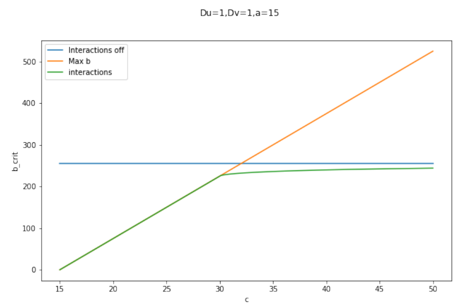


(i) Caption 3c

Figure 1: 3x3 grid of subfigures



(a) Caption 1a



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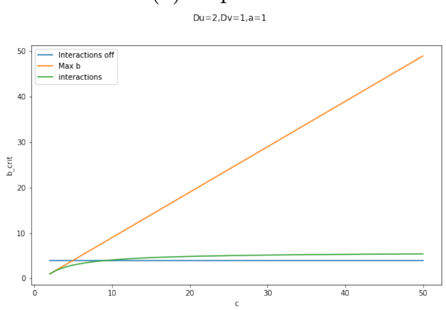

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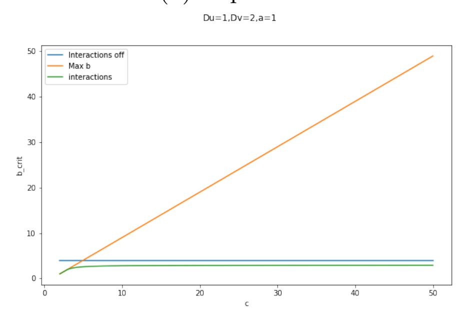

(d) Caption 2b

Figure 2

4 Collected equations

$$A = \begin{pmatrix} b-1 & a^2 \\ -b & -a^2 \end{pmatrix} \tag{59}$$

$$\mathrm{tr} A = b - 1 - a^2 \tag{60}$$

$$\det A = a^2 \tag{61}$$

$$u = a, v = \frac{b}{a} (\text{fixed point}) \tag{62}$$

$$f_u = a - (b+1)u + u^2 v, f_v = bu - u^2 v \tag{63}$$

$$\bar{D} = \begin{pmatrix} D_1(1 + \frac{u}{c-u-v}) & D_1 \frac{u}{c-u-v} \\ D_2 \frac{v}{c-u-v} & D_2(1 + \frac{v}{c-u-v}) \end{pmatrix} \tag{64}$$

$$\det A_q = \det A - q^2 \left(d_{uu} a_{vv} + d_{vv} a_{uu} - a_{vu} d_{uv} - d_{vu} a_{uv} \right) + q^4 \det \bar{D}, \tag{65}$$

$$\det A_q = a^2 - q^2 \frac{D_1(2ab - a^2 c) + D_2(a - c + bc - 2ab)}{c - a - \frac{b}{a}} + q^4 \frac{c}{c - a - \frac{b}{a}} \tag{66}$$

$$\mathrm{tr}A_q = \mathrm{tr}A - q^2(D_1(1+\frac{u}{R})+D_2(1+\frac{v}{R}) = b-1-a^2-q^2(\frac{D_1(c-\frac{b}{a})+D_2(c-a)}{c-a-\frac{b}{a}}) \tag{67}$$

$$C = D_1 D_2 \frac{c}{R} \tag{68}$$