Modified free energy and Tonks gas

Equation derivation

We have and expression for free energy

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

I denoted

$$\frac{c_{rest}}{c_\infty}=A, R=c_\infty-u-v$$

Extended calculations

We have

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

if $u, v << 1$ then $R \approx c_\infty$. We would get $\mu_u=\ln u-\ln c_\infty$, which gives correct expression for diffusion term. But I'm not sure if we can approximate that early in the calculations.
We have

$$\partial_x(u\partial_x\mu_u)=u''-\frac{u(RR''-(R')^2)+R'u'R}{R^2}=u''-g(u,v,u',v',u'',v'')$$

But if u', v' also small, then we recover diluted solution case.

$$\partial_x(u\partial_x\mu_u)\approx u''-\frac{R'u'}{R}\approx u''$$

Linearization

We want to linearize. We assume that base state is stationary and stable, ie. u'=v'=0.
So we discard any terms that contain u', v', u'', v''
There is one term that does not contain u',v' etc.
It is $-\frac{u}{R}(-\delta u''-\delta v'')$
Thus we can get modified equation

$$\delta\dot{u}=\delta u''+\frac{u}{R}(\delta u''+\delta v'')+A\cdot(\delta u,\delta v)^T$$

The same for v but with u,v reversed.
Or with $w=(u,v)$

$$\delta\dot{w} = \delta w'' + P\delta w'' + A(w)\delta w$$

$$P = \frac{1}{R}\begin{pmatrix} u & u \\ v & v \end{pmatrix}.$$

If we assume $\delta w = \vec{v}_q \exp(iqx + \sigma t)$, then we get

$$\vec{v}_q \sigma = -q^2 D(\mathbb{1} + P)\vec{v}_q + A\vec{v}_q,$$

where D is the diffusion coefficient.

Eigenvalues

Thus we're looking for σ s.t.

$$\det(A - q^2 D(\mathbb{1} + P) - \sigma\mathbb{1}) = 0$$

for a given q. Denote $A - q^2 D(\mathbb{1} + P)$ by A_q. Then we get

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

And

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

To find neutral curve $b(q)$ we put $\Re\sigma = \frac{1}{2}\mathrm{tr} A_q = 0$.

$$0 = b - 1 - a^2 - q^2 D(2 + \frac{u+v}{R}) = b - 1 - a^2 - q^2 D(1 + \frac{c}{c - a - \frac{b}{a}})$$

Brusselator

$$\det A = a^2, \mathrm{tr} A = b - 1 - a^2$$

Stability analysis

The situation is the same as for typical brusselator except A_q looks different.
So we assume that without diffusion the situation is stable ie. Also for convenience let $D = D(\mathbb{1} + P)$, ie. we'll denote by D the whole operator, along with diffusion coefficient.

1. $\mathrm{tr} A < 0$ and $\det A > 0$. Thus $\mathrm{tr} A_q < \mathrm{tr} A < 0$.
2. Unstable, stationary case (Turing pattern) must have $\det A_q < 0$.

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

where d_{ij} is just the coefficient of $D(\mathbb{1}+P)$. ## I had an error here, gotta redo some calculations

Also we denote the coefficients of the polynomial by

$$B = (d_{uu}a_{vv} + d_{vv}a_{uu} - a_{vu}d_{uv} - d_{vu}a_{uv})$$
$$C = (d_{uu}d_{vv} - d_{vu}d_{vu}).$$

As before the maximum is at $q=0$ or $q_{crit}^2 = \frac{B}{2C}$.

In the second case we get

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

This should be negative for instability.

Since $\det A > 0$, this means that $C > 0$ and from this we infer that $B > 0$.

But $C > 0$ is satisfied by because

$$C = D^2(1+\frac{u}{R})(1+\frac{v}{R}) - \frac{uv}{R^2} = D\left(1+\frac{(u+v)}{R}\right) = D^2\frac{c_\infty}{R}$$

And the B is equal to:

$$B = D\frac{-a^2c - c + bc + u}{R} = D\frac{-a^2c + bc - c + a}{R} = D\frac{-a^3c + a^2 + abc - ac}{ca - a^2 - b}$$

The signs in B are correct (this is the new and correct B).

B must be positive and

We also must have

$$\det A_{q_{crit}} = \det A - \frac{B^2}{4C} < 0,$$

This is equivalent to

> Old inequality_incorrect
>
> ## Old inequality
>
> $$B > \sqrt{4C\det A}$$
>
> $$D\frac{a^4 - a^3c - a^2 + abc - b^2}{aR} > 2a\sqrt{\frac{Dc}{R}}$$
>
> or
>
> $$D(a^4 - a^3c - a^2 + abc - b^2) > 2a^2\sqrt{R}\sqrt{Dc}$$

New inequality

$$D\frac{-a^3c + a^2 + abc - ac}{ca - a^2 - b} > 2aD\sqrt{\frac{c}{R}}$$

Neutral curve

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