

Modified free energy and Tonks gas

Equation derivation

We have an 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

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

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 $u, v \ll 1$ 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

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

where D is the diffusion coefficient.

Eigenvalues

Thus we're looking for σ s.t.

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

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

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

And

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

Brusselator

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

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 $D = D(\mathbb{I} + P)$, ie. we'll denote by D the whole operator, along with diffusion coefficient.

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

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

where d_{ij} is just the coefficient of $D(\mathbb{I} + P)$.

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

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

And the B is equal to:

$$B = D \frac{a^4 - a^3c - a^2 + abc - b^2}{aR} = D \frac{a^4 - a^3c - a^2 + abc - b^2}{ca - a^2 - b}$$

We also must have

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

This is equivalent to

$$B > \sqrt{4C \det A}$$

$$D \frac{a^4 - a^3c - a^2 + abc - b^2}{aR} > 2a \sqrt{\frac{Dc}{R}}$$

or

$$D(a^4 - a^3c - a^2 + abc - b^2) > 2a^2 \sqrt{R} \sqrt{Dc}$$