12.D.3. Linear Stability Analysis

For convenience, we shall call a perturbation in the form (12.60-1) or (12.62-3) a mode $\omega(\boldsymbol{k})$.

Stability of the uniform steady state (12.55) against a perturbation of mode $\omega(\boldsymbol{k})$ is determined entirely by the character of $\omega(\boldsymbol{k})$ [see Appendix C]. In particular, it is unstable against modes with $\operatorname{Re}\omega(\boldsymbol{k}) > 0$.

All discussions here are based on the text "Self-Organization in Non-equilibrium Systems" by G.Nicolis & I. Prigogine (1977).

12.D.1. Real Frequency $\omega(\boldsymbol{k})$

According to (12.67),

both $\omega_\pm(\boldsymbol{k})$ are real if $(C_1 + C_2)^2 - 4A^2 B > 0$ (12.68)

Assuming (12.68) is satisfied, then

$$\omega_+(\boldsymbol{k}) > 0 \quad \text{if} \quad C_1 - C_2 + \sqrt{(C_1 + C_2)^2 - 4A^2 B} > 0$$

$$\omega_-(\boldsymbol{k}) > 0 \quad \text{if} \quad C_1 - C_2 - \sqrt{(C_1 + C_2)^2 - 4A^2 B} > 0$$

Let

$$\sqrt{(C_1 + C_2)^2 - 4A^2 B} \geq 0 \tag{12.68a}$$

then $\omega_+(\boldsymbol{k}) > 0$ if

$$\sqrt{(C_1 + C_2)^2 - 4A^2 B} > C_2 - C_1 \qquad \forall\ C_1,\ C_2$$

$$\rightarrow \quad (C_1 + C_2)^2 - 4A^2 B > (C_2 - C_1)^2$$

$$C_1 C_2 - A^2 B > 0 \tag{12.69}$$

Thus, the uniform steady state is unstable if (12.69) is satisfied.

More importantly,

$$C_1 C_2 = A^2 B \quad \rightarrow \quad \omega_+(\boldsymbol{k}) = 0 \tag{12.69a}$$

so that the singular point (or uniform steady state) becomes a center [see Appendix C]. Unless $\omega_-(\boldsymbol{k})$ also vanishes, the system will possess another (necessarily non-uniform) steady state, i.e., it bifurcates.

Putting (12.66) into (12.69) gives

$$(B - 1 - D_X k^2)(A^2 + D_Y k^2) - A^2 B > 0$$

$$\rightarrow \quad B > \frac{1}{D_Y k^2}(1 + D_X k^2)(A^2 + D_Y k^2)$$

$$= (1 + D_X k^2)\left(\frac{A^2}{D_Y k^2} + 1\right)$$

$$= 1 + \frac{D_X}{D_Y} A^2 + \frac{A^2}{D_Y k^2} + D_X k^2 \tag{12.69a}$$

For a 1-D reaction chamber of length L,

$$k^2 = \left(\frac{n\pi}{L}\right)^2 \qquad n = 1, 2, 3, \ \ldots \tag{12.69b}$$

(12.69a) then simplifies to

$$B > 1 + \frac{D_X}{D_Y} A^2 + \frac{A^2}{D_Y n^2} \left(\frac{L}{\pi}\right)^2 + D_X n^2 \left(\frac{\pi}{L}\right)^2 \equiv B_n \tag{12.70}$$

According to (12.69a),

$$\omega_+(\boldsymbol{k}) = 0 \qquad \text{if} \qquad B = B_n \tag{12.70a}$$

The onset of instability is marked by the critical curve $B_n(n)$ with n taken as a real number [see Fig.12.4]. Combining (12.69b) & (12.70a), we see that bifurcation points are given by $B = B_n(n)$ with $n =$ integer.

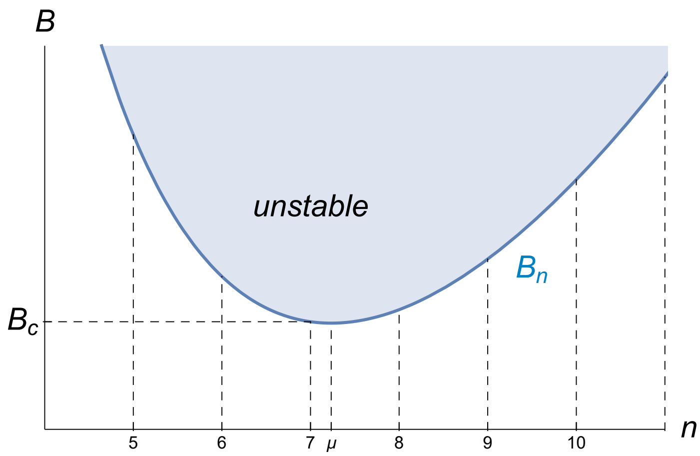

Fig.12.4. Linear stability diagram for bifurcation to a spatially oscillatory steady state.
The blue line is B_n and the shaded area is the unstable region ($B > B_n$).
First bifurcation occurs at $B_c = B_n(7)$, which is close to but not at the minimum $B_n(\mu)$.

Code

```
Clear["Global`*"]

Bn[n_] := 1 + Dx/Dy A^2 + (A^2 L^2)/(Dy π^2 n^2) + Dx (π/L)^2 n^2

par = {A → 2, L → 1, Dx → 2 × 10^-3, Dy → 7.5 × 10^-3, B → 4.17};

μ = Abs[n] /. (NSolve[Bn'[n] == 0 /. par, n, Reals] // Flatten)

7.2334

(* Fig.12.4 *)
Plot[Bn[n] /. par // Evaluate, {n, 2, 12},
    PlotRange → {{4, 11}, {3.8, 5}},
    AxesLabel → {"n", "B"},
    Filling → Top, Ticks → {{5, 6, 7, 8, 9, 10, {μ, "μ"}}, {{Bn[7] /. par, "Bc"}}},
    Epilog → {Dashed, Line[{{0, Bn[7]}, {7, Bn[7]}} /. par],
  Table[Line[{{n, 0}, {n, Bn[n] /. par}}], {n, 5, 12}],
  Line[{{n, 0}, {n, Bn[n] /. par}}] /. n → μ,
  Text["unstable", {7, 4.5}], Text["Bn", {9.5, 4.3}]}
]
```

12.D.2.1. Complex Frequency $\omega(\boldsymbol{k})$

From (12.68), we see that $\omega_\pm$ is a complex conjugate pair if

$$(C_1 + C_2)^2 - 4 A^2 B < 0 \tag{12.71}$$

Using (12.66), this becomes

$$\left[B + A^2 - 1 + (D_Y - D_X) k^2 \right]^2 - 4 A^2 B < 0 \tag{12.71a}$$

Setting

$$\delta = 1 - (D_Y - D_X) k^2 \tag{12.71b}$$

(12.71a) becomes

$$\left(B + A^2 - \delta \right)^2 - 4 A^2 B < 0$$

$$\to \quad B^2 + 2 \left(A^2 - \delta\right) B + \left(A^2 - \delta\right)^2 - 4 A^2 B < 0$$

$$B^2 - 2 \left(A^2 + \delta\right) B + \left(A^2 - \delta\right)^2 < 0 \tag{12.71c}$$

The root of

$$B^2 - 2 \left(A^2 + \delta\right) B + \left(A^2 - \delta\right)^2 = 0$$

are

$$B_\pm = A^2 + \delta \pm \sqrt{\left(A^2 + \delta\right)^2 - \left(A^2 - \delta\right)^2}$$

$$= A^2 + \delta \pm 2 A \sqrt{\delta}$$

$$= \left(A \pm \sqrt{\delta}\right)^2 \tag{12.71d}$$

Since B , A & δ must be real, we have

$$\delta \geq 0 \tag{12.71e}$$

Writing (12.71c) as

$$(B - B_+) (B - B_-) < 0$$

gives

$$B_+ > B > B_-$$

$$\to \quad \left(A + \sqrt{\delta}\right)^2 > B > \left(A - \sqrt{\delta}\right)^2 \qquad \text{[(12.71d) used.]} \tag{12.71f}$$

Putting (12.7e) into (12.71b) gives

$$1 \geq (D_Y - D_X) k^2$$

$$\to \quad D_Y - D_X \leq \left(\frac{L}{n \pi}\right)^2 \tag{12.72}$$

To summarize, $\omega_\pm$ is a complex conjugate pair if either (12.72) is satisfied. In which case [see (12.67)],

$$\text{Re}\, \omega_\pm = \frac{1}{2} (C_1 - C_2)$$

$$= \frac{1}{2} \left(B - 1 - D_X k^2 - A^2 - D_Y k^2\right) \qquad \text{[(12.66) used.]}$$

Hence, the uniform steady state is unstable if

$$B > 1 + A^2 + (D_X + D_Y) k^2$$

$$= 1 + A^2 + (D_X + D_Y)\left(\frac{\pi}{L}\right)^2 n^2 \qquad \text{[(12.69b) used.]} \qquad (12.73)$$

$$\equiv B_n(n) \qquad (12.74)$$

Note that on the critical curve B_n,

$\text{Re}\,\omega_\pm = 0$ $\qquad$ $\omega_\pm$ = purely imaginary

and the singular point (or uniform steady state) becomes a limit cycle [see Appendix C].. Thus, the system bifurcates to a time-periodic state for $B = B_n(n)$ with n = integers. Furthermore, the state with $n = 0$ is spatially uniform, i.e., it is a chemical clock. For $n \neq 0$, we have travelling waves.

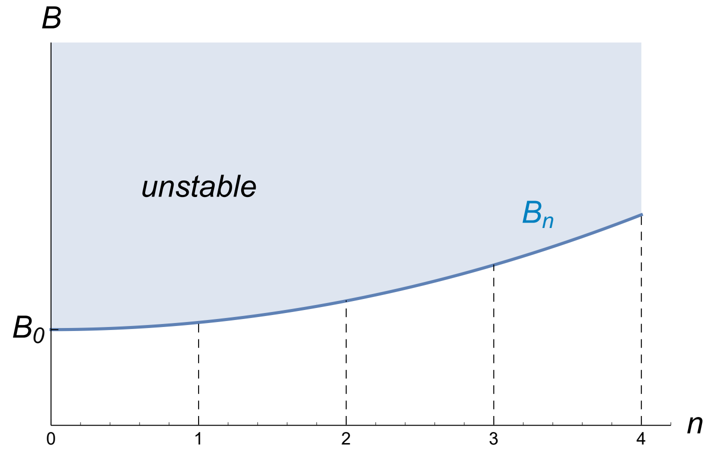

Fig.12.6. Linear stability diagram for the bifurcation to a time-periodic state.
The blue line is the critical curve B_n and the shaded area is the unstable region.
Bifurcation occurs at $B = B_n(n)$ with n = integers.
The first bifurcation at $B_0 = B_n(0)$ is spatially uniform.

Calculations of the bifurcation states involve solving the original nonlinear equations (12.53-4) with the indicated boundary conditions. Since these are stiff equations, the built-in routines in *Mathematica* are not adequate for the task. Our discussions of the problem must therefore end here.

Code

```
In[1]:= Clear["Global`*"]

In[2]:= Bn[n_] := 1 + A^2 + (Dx + Dy) (π/L)^2 n^2

In[3]:= par = {A → 2, L → 1, Dx → 0.5, Dy → 1.5};

In[4]:= par = {A → 2, L → 1, Dx → 1.6 × 10^-3, Dy → 6.0 × 10^-3, B → 4.17};
```

In[17]:=
```
(* Fig.12.4 *)
Plot[Bn[n] /. par // Evaluate, {n, 0, 4},
    PlotRange → {{0, 4.2}, {4, 8}},
    AxesLabel → {"n", "B"}, Ticks → {All, {{Bn[0] /. par, "B0"}}},
    Filling → Top,
    Epilog → {Dashed, Table[Line[{{n, 0}, {n, Bn[n] /. par}}], {n, 1, 5}],
  Text["unstable", {1, 6.5}], Text["Bn", {3.3, 6.2}]}
]
```