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MIT (Fall 2014)

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1 Problem 140915 (First order phase transition)

Statement for problem 140915

In equilibrium statistical mechanics, one says that a system undergoes a ***first order phase transition*** when the system's thermodynamic equilibrium undergoes a discontinuity (finite jump) as some parameter crosses a critical value. The freezing of water into ice is an example of a first-order phase transition.

In mathematical terms: let V is the energy potential associated with the system. Then *thermodynamic equilibrium* corresponds to the state at which V is at a minimum (if such a minimum exists).[1] If the

[1] Note that local, but not absolute, minimums of V correspond to *meta-stable* equilibrium states. The system can stay in these states provided it is not perturbed too much.

potential depends on some parameter r, and at some value $r = r_c$ there is an exchange of minimums (some local minimum becomes the new absolute minimum, while the old absolute minimum becomes a local minimum), then a first order phase transition occurs at r_c.

Here *we will study a simple, 1-D model, for a first order phase transition.* Consider a small particle moving in a 1-D potential force field (in a heavily dissipative environment), while being "kicked" one way and the other by the action of thermal molecular motion. In dimensionless form the equation is

$$\dot{x} = F(x) + \frac{db}{dt}, \tag{1.1}$$

where

1. $\dot{x}$ is the dissipation and $F(x) = -\frac{dV}{dx} = r\,x + x^3 - x^5$ is the force produced by the potential.
2. $b = b(t)$ is Brownian motion, with a jump parameter size $\mu > 0$ (see hints) — $\frac{db}{dt}$ is white noise. *Assume that μ is small.*

Part a. Consider the potential V for the system (1.1), and *calculate* r_c. Here r_c is defined by the condition that V has three equally deep wells, i.e. the values of V at the three local minima are equal.[2] *Show that r_c corresponds to a first order phase transition.*

Part b. Note that the potential is left-right symmetric. What happens with the system state, at equilibrium, as r crosses r_c?

Part c/challenge. The pdf (probability distribution function) $\Phi = \Phi(x,\, t)$ for the position of the particle, is defined by

$$\text{Probability}\left\{|x(t) - s| < \frac{1}{2}ds\right\} = \Phi(s,\, t)\, ds. \tag{1.2}$$

c.1 Derive an equation for the time evolution of Φ.

c.2 Find the time independent, equilibrium pdf, Φ_0, by solving the equation derived in (c.1).

c.3 It can be shown that $\Phi \to \Phi_0$ as $t \to \infty$. What does Φ_0 tell you about the behavior of the system, as r crosses r_c?

Part d. Does the 1-D, deterministic, dynamical system

$$\dot{x} = F(x) = r\,x + x^3 - x^5 \tag{1.3}$$

have a bifurcation at $r = r_c$?

Hint for part (c.1)

The pdf Φ describes the probability of finding the particle somewhere in space, at any given time. A related function is the probability flux $\Psi(x,\, t)$, defined by

$$\Psi(x,\, t)\, dt = \text{Probability that the particle crosses } x \text{ left to right, during the time interval } [t,\, t + dt]. \tag{1.4}$$

Unlike Φ, Ψ need not be positive — $\Psi < 0$ means that the particle is moving right to left. In fact, $\int_{-\infty}^{\infty} \Psi dx = 0$.

[2] For this value of r, there is equal probability of finding the system in the state corresponding to any of the three minima.

From the definition of Ψ, it should be clear that

$$\int_a^b \Phi_t(x,\,t)\,dx = \underbrace{\frac{d}{dt}\int_a^b \Phi(x,\,t)\,dx = \Psi(a,\,t) - \Psi(b,\,t)}_{\text{conservation of probability}} = -\int_a^b \Psi_x(x,\,t)\,dx \tag{1.5}$$

for **any** $a < b$. Assuming that Φ_t and Ψ_x are continuous, this leads to the equation

$$\Phi_t + \Psi_x = 0. \tag{1.6}$$

Hence, **in order to do part (c.1), you need to write Ψ in terms of** Φ, and then use (1.6).

The flux Ψ is the sum of two parts. The flux produced by the deterministic term F in (1.1), plus the flux produced by the random Brownian motion fluctuations. The deterministic flux is easy to write, as it is the flux produced by motion at speed F — what is the flux of some density, when the things the density characterizes move at some known speed?

To write the flux associated with Brownian motion, you need to know what Brownian motion is. There are many ways to define Brownian motion. A very simple one (albeit mathematically rather sloppy) is this:

In a time interval dt, the particle jumps a distance $\mu\sqrt{dt}$,
to the right or left — with probability $\frac{1}{2}$ in each direction. (1.7)

By considering the probability of the particle being in the intervals $[x - \mu\sqrt{dt},\, x]$ and $[x,\, x + \mu\sqrt{dt}]$, at some time t, and the above definition, you can compute the flux across x in a time interval dt. Expanding, and neglecting all quantities with orders higher than dt, should then give you Ψ written in terms of Φ. ♣

Hint for part (c.2)

To find Φ_0 you will have to solve a second order ode. It is easy to integrate this ode once, reducing the problem to that of solving a first order linear ode. Because the problem is a second order ode, the solutions involve two free constants. These free constants are picked uniquely by that Φ has to be integrable, non-negative, and satisfy $\int_{-\infty}^{\infty} \Phi_0(x)\,dx = 1$.

2 Problem 140916 (Model problem on singular limits)

Statement for problem 140916

Consider the *linear* differential equation

$$\epsilon\frac{d^2x}{dt^2} + \frac{dx}{dt} + x + \sin(t) = 0, \quad \text{where} \quad 0 < \epsilon \ll 1, \tag{2.1}$$

subject to the initial conditions $x(0) = 1$ and $\dot{x}(0) = 0$.

a. Solve the problem analytically, for any $0 < \epsilon < 1/4$.

b. Show that, for $0 < \epsilon \ll 1$, there are two widely separated time scales in the solution, and estimate them in terms of ϵ. *Hint: expand all the constants in the solution in powers of ϵ.*

c. What do you conclude about the validity of replacing (2.1) by its singular limit $\dot{x} + x + \sin(t) = 0$? *Hint: inspect the behavior of the leading order in of the solution that you just obtained, for* $t \gg \epsilon$.

d. Give a mechanical example where this equation arises. Then find the dimensionless combination of parameters corresponding to ϵ, and state the physical meaning of the limit $0 < \epsilon \ll 1$.

e. Graph $x(t)$ and $\dot{x}(t)$ for $\epsilon 0.15$. Compare with the solution to the singular limit.

3 Problem 140924 (Excitable systems)

Statement for problem 140924

(Excitable systems). Consider the situation when a neuron is stimulated. For a small enough stimulus, not much happens: the neuron increases its membrane potential slightly, and then relaxes back to its *rest state*. Beyond a *critical threshold*, the neuron "fires", and produces a large voltage spike before returning to rest. Interestingly, the spike's size is almost independent of the stimulus' size — anything above the threshold produces essentially the same response. Similar phenomena occur for other types of cells and some chemical reactions.[3] These systems are called **excitable.** An excitable system is characterized by the properties:

1. It has a unique, globally attracting *rest state*.

2. A stimulus above some *threshold* sends the system orbit on an $O(1)$ excursion through phase space, before it returns to the rest state.

A very simple excitable system (one of the simplest possible) is

$$\frac{d\theta}{dt} = 1 + \xi \sin\theta, \tag{3.1}$$

where ξ is slightly larger than 1 ($0 < \xi - 1 \ll 1$).

a. Show that this system satisfies the properties above. Identify the rest state and the threshold.

b. Let $V(t) = \cos\theta(t)$. Plot V for various initial conditions — V is the neuron's membrane potential analog, and the initial conditions correspond to different perturbations from the rest state.[4]

c. Is there another range of values for ξ which make (3.1) an excitable system?

[3] Winfree, A., T. (1980) *The Geometry of Biological Time* (Springer, New York).
Rinzel, J., and Ermentrout, G. B. (1989) Analysis of neural excitability and oscillations. In C. Koch and I. Sergev, eds. *Methods in Neuronal Modeling: From Synapses to Networks.* (MIT Press, Cambridge, MA).
Murray, J. (1989) *Mathematical Biology* (Springer, New York).

[4] Of course, **equation (3.1) is much too simple to take it seriously as a model for a neuron.**

4 Problem 05.01.02 - Strogatz (Asymptotic behavior as $t \to \infty$)

Statement for problem 05.01.02

Consider the system $\dot{x} = ax$, $\dot{y} = -y$, where $a < -1$. Show that all trajectories become parallel to the y-direction as $t \to \infty$, and parallel to the x-direction as $t \to -\infty$.
Hint: Examine the slope $\dfrac{dy}{dx} = \dot{y}/\dot{x}$.
Strictly speaking, not all trajectories satisfy these two statements. What are the exceptions?

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5 Problem 140922 (Attracting and Liapunov stable)

Statement for problem 140922

Recall the *definitions for the various types of stability* that concern critical points:
Let $\mathbf{x}^*$ be a fixed point of the system $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x})$. Then:

1. $\mathbf{x}^*$ is **attracting** if there is a $\delta > 0$ such that $\lim_{t\to\infty} = \mathbf{x}^*$ whenever $\|\mathbf{x}(0) - \mathbf{x}^*\| < \delta$. That is: any trajectory that starts within δ of $\mathbf{x}^*$ *eventually* converges to $\mathbf{x}^*$. Note that trajectories that start nearby $\mathbf{x}^*$ *need not stay close in the short run*, but *must* approach $\mathbf{x}^*$ *in the long run.*
2. $\mathbf{x}^*$ is **Liapunov stable** if for each $\epsilon > 0$, there is a $\delta > 0$ such that $\|\mathbf{x}(t) - \mathbf{x}^*\| < \epsilon$ for $t > 0$, whenever $\|\mathbf{x}(0) - \mathbf{x}^*\| < \delta$. Thus, trajectories that start within δ of $\mathbf{x}^*$ stay within ϵ of $\mathbf{x}^*$ for all $t > 0$.
In contrast with attracting, Liapunov stability requires nearby trajectories to remain close *for all* $t > 0$.
3. $\mathbf{x}^*$ **is asymptotically stable** if it is *both* attracting and Liapunov stable.
4. $\mathbf{x}^*$ is **repeller** if there are $\epsilon > 0$ and $\delta > 0$ such that if $0 < \|\mathbf{x}(0) - \mathbf{x}^*\| < \delta$, after some critical time $\|\mathbf{x}(t) - \mathbf{x}^*\| > \epsilon$ applies (i.e., for $t > t_c$). Repellers are a special kind of *unstable* critical points.

For each of the following systems, decide whether the origin is attracting but not Liapunov stable, Liapunov stable, asymptotically stable, repeller, or unstable but not a repeller.

a) $\dot{x} = 2\,y$ and $\dot{y} = -3\,x$.

b) $\dot{x} = y\,\cos(x^2 + y^2)$ and $\dot{y} = -x\,\cos(x^2 + y^2)$.

c) $\dot{x} = -x$ and $\dot{y} = -|y|\,y$.

d) $\dot{x} = 2\,x\,y$ and $\dot{y} = y^2 - x^2$. *Hint: what happens along $x = 0$?*

e) $\dot{x} = x - 2\,y\,x^2 - 4\,y^3$ and $\dot{y} = y + x^3 + 2\,x\,y^2$.

f) $\dot{x} = y$ and $\dot{y} = x$.

g) Finally, consider the critical point $(x,\, y) = (1,\, 0)$, for the system

$$\dot{x} = (1 - r^2)\,x - (1 - \tfrac{x}{r})\,y \quad \text{and} \quad \dot{y} = (1 - r^2)\,y + (1 - \tfrac{x}{r})\,x, \tag{5.1}$$

defined in the “punctured” plane $r = \sqrt{x^2 + y^2} > 0$. *Hint: write the equations in polar coordinates.*

Additional hints. In some cases you can get the answer by finding a function $\mathcal{J} = \mathcal{J}(x, y)$ with a local minimum at the origin such that $\frac{d\mathcal{J}}{dt} > 0$ along trajectories — or maybe one such $\frac{d\mathcal{J}}{dt} < 0$, or maybe one such $\frac{d\mathcal{J}}{dt} = 0$. In other cases look for special trajectories that either leave, or approach, the origin.

6 Problem 06.01.07 - Strogatz (Nullclines versus stable manifolds)

Statement for problem 06.01.07

(Nullclines versus stable manifolds). There is a confusing aspect of Example 6.1.1 in the book,[5] dealing with the system

$$\frac{dx}{dt} = x + e^{-y}, \qquad \text{and} \qquad \frac{dy}{dt} = -y. \tag{6.1}$$

The nullcline $\dot{x} = 0$ in Figure 6.1.3 has a similar shape and location as the stable manifold of the saddle, shown in Figure 6.1.4. But they are not the same curve! To clarify the relation between the two curves, plot both of them on the same phase portrait. *You have two options here.* Either:

1. Use a computer to do the plot, generating the stable manifold by numerically solving the equation; or
2. Find an explicit formula for the stable manifold, and then do a sketch of the phase portrait.

   Hint. Write the equation for $\boldsymbol{\frac{dy}{dx}}$*, and then solve it.*

   A sketch without an analytical justification is not an acceptable answer!

7 Problem 06.01.09 - Strogatz (Computer generated phase portrait)

Statement for problem 06.01.09

Plot a computer generated phase plane portrait for the "Dipole fixed point" system

$$\frac{dx}{dt} = 2\,x\,y \qquad \text{and} \qquad \frac{dy}{dt} = y^2 - x^2. \tag{7.1}$$

8 Problem 06.01.10 - Strogatz (Computer generated phase portrait)

Statement for problem 06.01.10

First, plot a computer generated phase plane portrait for the "two-eyed monster"

$$\frac{dx}{dt} = y + y^2 \qquad \text{and} \qquad \frac{dy}{dt} = -\frac{1}{2}\,x + \frac{1}{5}\,y - x\,y + \frac{6}{5}\,y^2. \tag{8.1}$$

[5] First edition: pp. 147-148. Second edition: pp. 148-149.

In particular, make a plot that covers the region $-5 \le x \le 3$ and $-3 \le y \le 2$.
Next find the critical points and classify them. Does what you observe in the plot match what the theory predicts? Explain any discrepancies.
Hint: Explore carefully what happens close to the critical points.

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9 Problem 06.01.13 - Strogatz (Draw a phase portrait)

Statement for problem 06.01.13

Draw a phase portrait that has exactly three closed orbits and one fixed point.

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10 Index for a critical point with zero determinant.

Statement: Index for a critical point with zero determinant.

Consider a phase plane system

$$\dot{x} = f(x, y) \quad \text{and} \quad \dot{y} = g(x, y), \tag{10.1}$$

where f and g are smooth functions of all of its arguments. Assume that:

1. The origin $\mathcal{O}$ is an isolated critical point. That is $f(0, 0) = g(0, 0) = 0$, and there are no solutions to $f(x, y) = g(x, y) = 0$ with $0 < x^2 + y^2 < \epsilon$ — for some ϵ.
2. Let A be the 2×2 matrix corresponding to the linearization near $\mathcal{O}$, with $\tau = \text{tr}(A)$ and $\Delta = \det(A)$. Suppose that $\boldsymbol{\Delta = 0}$ and $\boldsymbol{\tau > 0}$ — so that one eigenvalue of A vanishes, and the other equals τ.

This is a structurally unstable situation, in particular: the index for $\mathcal{O}$ is not determined at all by the linearized equations. **Construct examples of the above situation where:**

A. $\mathcal{I} = \text{index}(\mathcal{O}) = 1.$

B. $\mathcal{I} = \text{index}(\mathcal{O}) = -1.$

C. $\mathcal{I} = \text{index}(\mathcal{O}) = 0.$

Sketch the phase plane diagrams for the systems that you construct.

Hints. Consider the linear system $\dot{Y} = AY$, and then add a nonlinear correction which:

For part **A**. Makes $\mathcal{O}$ into a (nonlinear) node.

For part **B**. Makes $\mathcal{O}$ into a (nonlinear) saddle.

For part **C**. Makes $\mathcal{O}$ into a (nonlinear) saddle on one side, and a (nonlinear) node on the other.

THE END.

18.385J / 2.036J Nonlinear Dynamics and Chaos
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