

01160611 — SELECT TOPICS IN LIVING SYSTEMS

LECTURES

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The document is provided as is and likely contains many errors.*

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1 PHASE TRANSITIONS IN EQUILIBRIUM

1.1 Motivation

Phase is a distinct state of matter which can be described by an "order parameter". We'll focus on isotropic polar phase transition. In this case the order parameter is the polarization $\vec{p} = \langle \hat{n} \rangle$ where \hat{n} is the unit vector of the particles' direction.

Phase transition: in certain areas of physics we see systems which aren't ordered at high temperatures but become ordered at low temperatures. Why? A competition between energy and entropy (Free energy being $F = U - TS$). The temperature at which order emerges is called the critical temperature, marked T_C and the change in the system is called a phase transition.

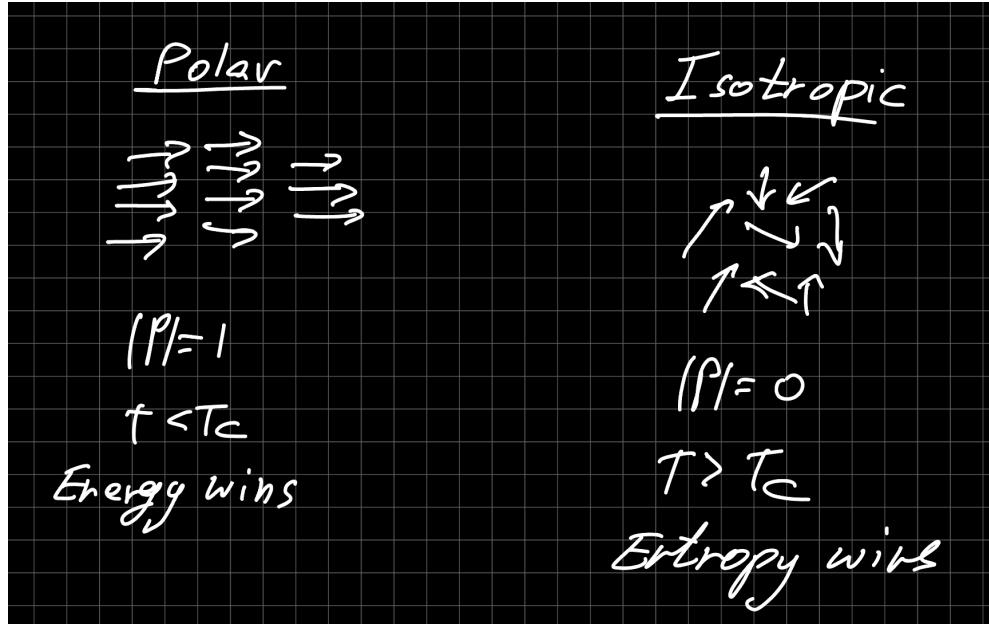


Figure 1: Polar and Isotropic ordering of matter.

1.2 Physical description

We'll assume free energy of the following form:

$$F(T, N, \psi) = F_0(T, N) + F_\psi(T, N, \psi) \quad (1)$$

where ψ is the order parameter. ψ is not a conserved quantity but rather a degree of freedom of the system (in contrast to the number of particles, for example). Therefore under equilibrium we find

$$F_{eq}(T, N, \psi) = F_0(T, N) + F_\psi(T, N, \psi_{eq}) \quad (2)$$

and the equilibrium value is determined by

$$\frac{\partial F_\psi}{\partial \psi} \Big|_{\psi=\psi_{eq}} = 0 \quad (3)$$

and the following is true:

$$\psi_{eq}(T > T_C) = 0 \quad (4)$$

$$\psi_{eq}(T < T_C) \neq 0 \quad (5)$$

We'll focus on phase transition of 2nd order, for which the order parameter changes continuously, thus $\psi_{eq}(T = T_C) = 0$. Otherwise the phase transition is of first order.

1.3 Landau Theory of Phase Transitions

The theory was developed by Lev Landau, for which he earned the Nobel Prize in Physics in 1962.

Close to the critical temperature T_C the physics of phase transitions is universal. For a phase transition of 2nd order, we will write F_ψ in a phenomenological form as a Taylor series expansion:

$$F_\psi = \frac{a}{2}\psi^2 + \frac{b}{4}\psi^4 \quad (6)$$

The terms being of even powers because we don't care about directions. The quadratic term's coefficient is of the form

$$a = a_0 \cdot \frac{T - T_C}{T_C} \quad (7)$$

Where $a_0 > 0$. This quantifies the competition between energy (which wins at $T < T_C$) and entropy (which wins at $T > T_C$). The parameter $b > 0$ ensures stability: ψ_{eq} receives finite values and does not approach infinity.

Because of a's sign, we find $\psi_{eq} \neq 0$ for $T < T_C$. Explicitly:

$$0 = \frac{\partial F}{\partial \psi} \Big|_{\psi=\psi_{eq}} = a\psi_{eq} + b\psi_{eq}^3 = b\psi_{eq} \left(\psi_{eq}^2 + \frac{a}{b} \right) \quad (8)$$

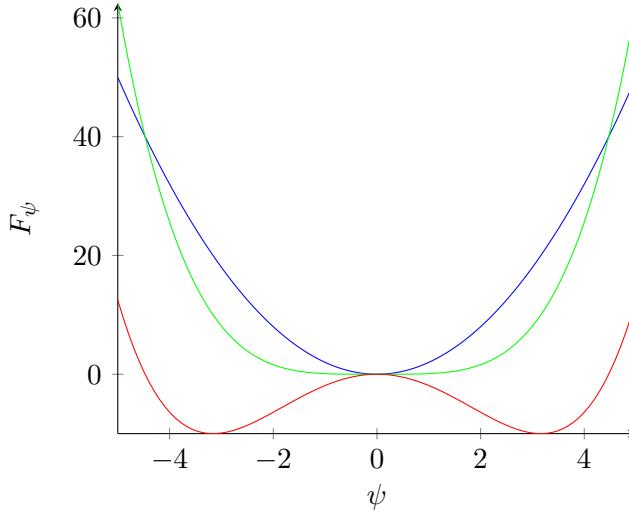


Figure 2: The graphs for the functions $2x^2$ (blue), $0.1x^4$ (green) and $0.1x^4 - 2x^2$ (red).

therefore

$$\psi_{eq} = 0, \pm \sqrt{\frac{a_o}{b} \cdot \frac{T - T_C}{T_C}} \quad (9)$$

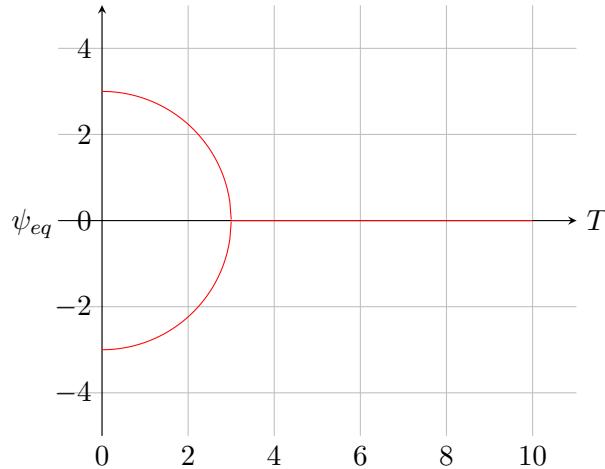


Figure 3: The possible solutions from equation 9.

There is no distinction between the positive and negative sign. Either can be chosen arbitrarily (spontaneous symmetry break). There will be a preference given an external field which will add an element of the form $-h\psi$ to the free energy.

1.3.1 Where a comes from

We'll assume a simple model of polarisation with energy

$$U = - \sum_{i,j \text{ neighbors}} u n_\alpha^i n_\alpha^j , \quad u > 0 \quad (10)$$

The energy is lower when i,j point in the same direction. Using mean field approximation the internal energy is

$$U = \frac{u}{2} \sum_{i,j} \langle n_\alpha^i \rangle \cdot \langle n_\alpha^j \rangle = -\frac{u}{2} N Z p_\alpha^2 \quad (11)$$

where $p_\alpha = \langle n_\alpha \rangle$, N is the number of particles, and Z the number of close neighbors. As for the entropy, we can find from a taylor expansion

$$S = S(p=0) - \alpha N p^2 \quad (12)$$

and summing it up we find

$$F = U - TS = N \left(\alpha T - \frac{u}{2} Z \right) p^2 = a_0 \cdot \frac{T - T_C}{T_C} p^2 \quad (13)$$

where

$$T_C = \frac{uZ}{2\alpha} \quad a_0 = \alpha N T_C \quad (14)$$

If instead of the vector n_α there is spin (\pm) then we find a similar result in the mean field framework. This model is called the Ising model, one of the most basic and useful models in statistical mechanics.

1.3.2 A dynamical description of the phase transition

We described the phase transition from the free energy but we can also describe it from dynamics. For a non-conserved order parameter we can write the dynamics as follows:

$$\dot{\psi} = -\Gamma_\psi \frac{\partial F}{\partial \psi} , \quad \Gamma_\psi > 0 \quad (15)$$

the idea being that the dynamics guarantee that the free energy only gets smaller (the total entropy grows). We can see this using the chain rule:

$$\dot{F} = \frac{\partial F}{\partial \psi} \dot{\psi} = -\Gamma_\psi \left(\frac{\partial F}{\partial \psi} \right)^2 < 0 \quad (16)$$

this dynamics is called Model A (and often appears with a "noise" parameter). We'll insert F and find:

$$\dot{p} = -\Gamma_p(ap + bp^3) \quad (17)$$

the fixed points are $\frac{\partial F}{\partial p} = 0$, the extrema of the free energy. The stability of the solution is determined in phase space.

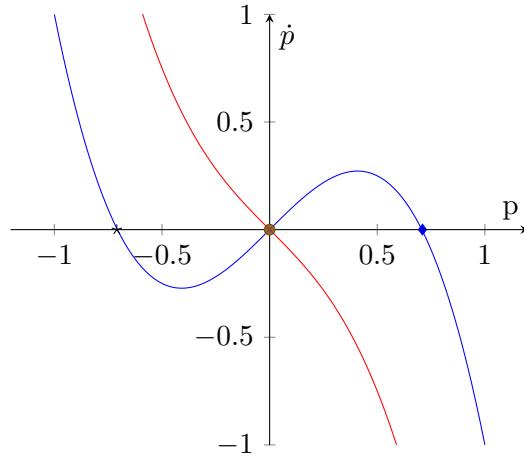


Figure 4: The graphs of $f(x) = x - 2x^3$ (blue) and $g(x) = -x - 2x^3$ (red). The positive and negative points marked on the x axis are stable points of equilibrium for $f(x)$. The point marked at $(0,0)$ is a stable point for $g(x)$ but an unstable one for $f(x)$.

in the language of dynamical systems, a phase transition is called a bifurcation. This approach is useful for out of equilibrium systems, for which we can't write down a free energy. Later on in the course, we'll come across dynamical equations of a similar form.

In general dynamical systems, when a function F whose derivative is strictly non-positive with a finite minimum exists (like free energy), then it's called a Lyapunov function.

1.4 Spatial Dependence: The Ginsburg-Landau Theory

We saw that the direction of \vec{p} is arbitrary, in practice different areas of the system will initially develop order in different directions. For simplicity, we'll assume $\vec{p} = p\hat{y}$ where p can be either positive or negative. We'll look at the case where \vec{p} points down at $x \rightarrow -\infty$ and up at $x \rightarrow \infty$.

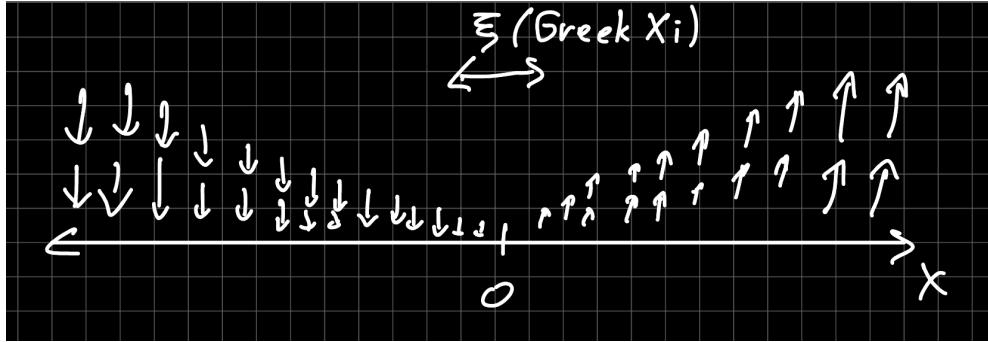


Figure 5: A smooth phase transition with Domain Wall ξ .

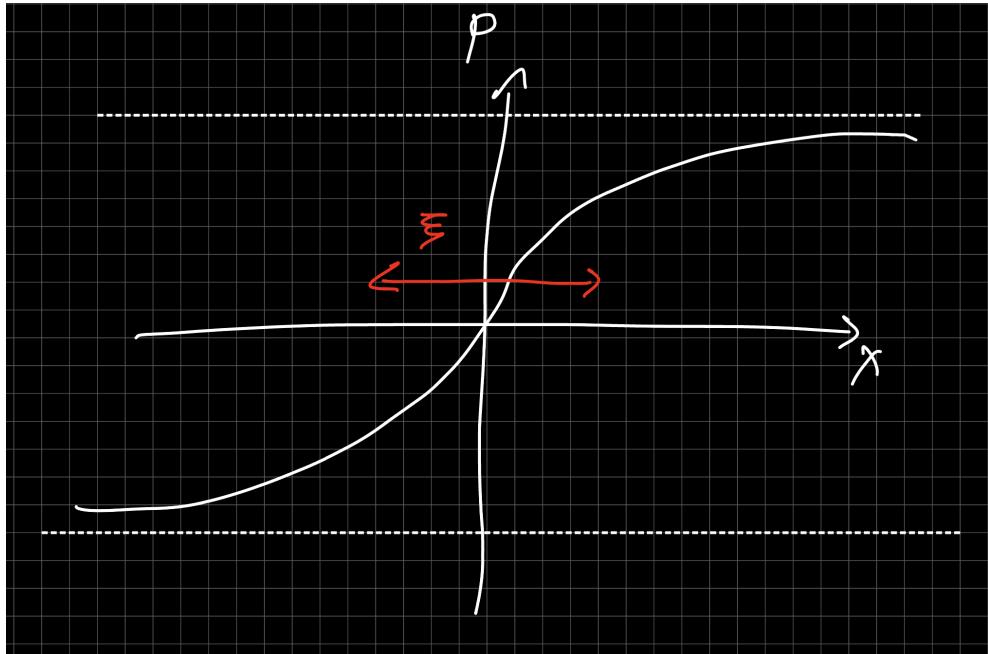


Figure 6: A smooth phase transition with Domain Wall ξ .

We'll find a finite range around 0 of width ξ in which $|p| \neq p_{eq}$. This region is called the Domain Wall.

To quantify the cost to change p in space we'll write the density of free energy per length unit:

$$F[p] = \int dx f = \int dx \left(\frac{a}{2} p^2 + \frac{b}{4} p^4 + \frac{k}{2} p'^2 \right) \quad (18)$$

where $k > 0$. The last element quantifies the cost to change p . In higher dimensions we'll have $(\vec{\nabla} p)^2$. Why is it like this? The cost comes from the gradient, and given there is no preferred direction, a positive and negative change should cost the same.

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