

P653 HW4

Due Sept. 22, 2005

Problem 1. Mean Field Dynamics

Here we wish to explore a crude, yet generic, model for the time dynamics of the order parameter near a critical point. For concreteness, let's think about the magnetization m . We know that if m takes on its equilibrium value, then it shouldn't change with time. Furthermore, we expect that m will tend to approach its equilibrium value.

The simplest model with this structure is

$$\frac{\partial m(r)}{\partial t} = -\Gamma \frac{\delta F}{\delta m(r)},$$

where Γ is some positive constant. This is known as "model A" dynamics.

We will use a quartic free energy,

$$F = \int d^3r \left[a t m^2(r)/2 + b m^4(r)/4 + c |\nabla m(r)|^2 - h(r)m(r) \right],$$

where $a, b, c > 0$ and all temperature dependence is given by $t = (T - T_c)/T_c$. Furthermore we will ignore the spatial dependence of m , assuming that it is uniform for all time. IE. the free energy per unit volume is simply

$$F/V = a t m^2 + b m^4/4 - h m,$$

and the model-A dynamics read

$$\frac{\partial m}{\partial t} = -\frac{\Gamma}{V} \frac{\partial F}{\partial m}.$$

1.1. Consider $t > 0$, and $h = 0$. Suppose m is small. To linear order in m , write the model A equation of motion for m .

1.2. What is the time-scale τ for m to fall by $1/e$?

You should find that $\tau \rightarrow \infty$ as $T \rightarrow T_c$. This is known as "critical slowing down." Dynamics get slow near a second order phase transition. For future reference, one defines the dynamical exponent y by $\tau \propto |t|^{-y}$.

1.3. For $t < 0$, what is the timescale for m to approach its equilibrium value?

Problem 2. Conservation Laws

Model A is the simplest dynamics one can write down for the relaxation of the order parameter. It does not, however, capture the behavior of a system with a conserved quantity.

Consider, for example, a binary alloy consisting of equal numbers two different atoms: A, B. In the high temperature phase, these are homogeneously mixed, while at low temperature the system prefers to be pure A or B.

The order parameter is

$$n = \frac{n_A - n_B}{n_A + n_B}$$

where n_A and n_B are the densities of each of the components. A free energy with the appropriate symmetry is

$$F = \int d^3r a \frac{T - T_c}{T_c} n^2/2 + b n^4/4 + \lambda (\nabla n)^2,$$

where all relevant temperature dependence is explicitly shown.

If the number of atoms is conserved, we must have a conservation law,

$$\frac{\partial n}{\partial t} + \nabla \cdot \mathbf{j} = 0,$$

where \mathbf{j} is the current associated with n .

The current must vanish when we are at a stationary point of the free energy. The simplest model we can take is then,

$$\mathbf{j}(r) = -M \nabla \frac{\delta F}{\delta m(r)},$$

where $M > 0$ is a constant. This is known as Model B dynamics.

Substituting this expression for \mathbf{j} into the continuity equation gives the Cahn-Hilliard equation,

$$\frac{\partial n}{\partial t} = M \nabla^2 \frac{\delta F}{\delta m(r)}.$$

Suppose we quench this binary alloy into the low temperature phase ($T < T_c$). Initially $n = 0$. Now, however, the system wants to phase separate. This process of phase separation is known as spinodal decomposition.

We can assume that the system follows Model B dynamics. In the initial stages of spinodal decomposition, where n is small, we can linearize the dynamics. Here we *must* keep the spatial dependence.

2.1. Linearize the Cahn-Hilliard equation to derive a linear partial differential equation for the short time behavior of $n(r, t)$.

2.2. Fourier transform this linearized equation with respect to space and time. You should be able to derive a relationship between the frequency ω and the wave vector k . What is $\omega(k)$?

2.3. The mode with the largest imaginary frequency will grow fastest. What is its wavelength?

Problem 3. Tricritical Point – (Plischke and Bergersen 3.15) Consider an Ising chain with N spins $\sigma_i = \pm 1$ and periodic boundary conditions. The chain is coupled to an elastic field ϵ . Nonzero values of ϵ cause a dimerization of the chain, i.e. alternating bonds are strengthened and weakened. The Hamiltonian for the system, in reduced units, can be written as

$$H = - \sum_{i=1}^N [1 - \epsilon(-1)^i] \sigma_i \sigma_{i+1} + N\omega\epsilon^2.$$

The parameter ω represents the energy cost of dimerization.

The partition function for the system is

$$Z = \int_{-\infty}^{\infty} d\epsilon \sum_{\{\sigma_i\}} e^{-\beta H} \quad (1)$$

$$\int_{-\infty}^{\infty} d\epsilon Z_{\sigma} e^{-N\beta\omega\epsilon^2} \quad (2)$$

$$\int_{-\infty}^{\infty} d\epsilon e^{-\beta N g(\epsilon)}, \quad (3)$$

which defines the spin partition function Z_{σ} and the spin free energy $g(\epsilon)$.

If $g(\epsilon)$ has an absolute minimum at ϵ_0 , then at equilibrium $\epsilon = \epsilon_0$, and the free energy per spin is $g(\epsilon_0)$.

We will perform the sum over spins via the transfer matrix approach.

3.1. Prove that

$$Z_{\sigma} = \text{Tr}(\mathbf{P}\mathbf{Q})^{N/2},$$

where

$$\mathbf{P} = \begin{pmatrix} e^{\beta(1+\epsilon)} & e^{-\beta(1+\epsilon)} \\ e^{-\beta(1+\epsilon)} & e^{\beta(1+\epsilon)} \end{pmatrix}$$

$$\mathbf{Q} = \begin{pmatrix} e^{\beta(1-\epsilon)} & e^{-\beta(1-\epsilon)} \\ e^{-\beta(1-\epsilon)} & e^{\beta(1-\epsilon)} \end{pmatrix}$$

3.2. Show that in the limit $N \rightarrow \infty$,

$$g(\epsilon) = -(k_B T/2) \ln \lambda(\epsilon) + \omega\epsilon^2,$$

where $\lambda(\epsilon)$ is the largest eigenvalue of the matrix product $\mathbf{P}\mathbf{Q}$.

3.3. Show that

$$\lambda(\epsilon) = 2[\cosh(2\beta) + \cosh(2\beta\epsilon)].$$

3.4. Show that if $\omega = 0.20$, as a function of temperature, the system will undergo a second order phase transition to a dimerized state $\epsilon \neq 0$. Estimate the value of β at the transition.

Hint: expand free energy to quartic order

3.5. Show that if $\omega = 0.24$ the system will undergo a first order transition to a dimerized state. Estimate β at the transition.

Hint: You will probably need to do this graphically/numerically.

3.6. The point where a first order phase transition line turns into a second order phase transition line is known as the tricritical point. Estimate ω and β at the tricritical point.

As an aside, for $\omega > 0.25$ there is no phase transition.

Problem 4. Critical Droplets

Consider a three dimensional magnetic system in a finite magnetic field. The temperature and field are set so that the free energy is

$$F = \left[f \int d^3r m^4/4 - m^3/3 - m^2 \right].$$

4.1. What are the stable, metastable, and unstable values of m ? Take m to be uniform.

4.2. Suppose the system is initially uniform in the metastable phase. Suppose fluctuation generate a spherical bubble of the stable phase with radius R . What is the energy savings?

4.3. The edge of the bubble is a domain wall. This costs energy, proportional to its surface area $E_{\text{wall}} = \sigma A$. Including this domain wall energy, calculate the total free energy of forming a bubble $E_{\text{bubble}}(R)$. Plot this function as R is varied.

As you should see, a small bubble will tend to collapse, while a big bubble will grow.

4.4. What is the free energy, E_c , of the critical droplet, the smallest bubble which will grow?

Given that the probability of any given state is proportional to $e^{-\beta F}$, one expects that the timescale for nucleating a bubble is proportional to $e^{\beta E_c}$.

An estimate of the surface tension within Landau-Ginzburg can be found in section 4.4 of Plischke and Bergersen.