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, lets 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,

$$F = \int d^3r \; a\,\bar{t}\,m^2(r)/2 + b\,m^4(r)/4 + c\,|\nabla m(r)|^2 - h(r)m(r),$$

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

$$F/V = a\bar{t}m^2/2 + bm^4/4 - hm,$$

and the model-A dynamics read

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

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

Solution 1.1. Note: the problem originally had a factor of 2 missing in the free energy density. With the correct factor,

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

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

Solution 1.2.

$$\tau = \frac{1}{\Gamma a t}.$$

You should find that $\tau \to \infty$ as $T \to T_c$. 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?

Solution 1.3. First we need to find the equilibrium value of m,

$$\partial F/\partial m = a\bar{t}m + bm^3 = 0,$$

which gives $m_0^2 = -a\bar{t}/b$ Setting $m = m_0 + \delta$, we find

$$\partial F/\partial\delta = a\bar{t}\delta + 3bm_0^2\delta = -2a\bar{t}\delta,$$

which implies

$$\tau = \frac{1}{2\Gamma a|\bar{t}|}.$$

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

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

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 **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 dependance.

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

Solution 2.1.

$$\frac{\partial n}{\partial t} = Ma\bar{t}\nabla^2 n - 2M\lambda\nabla^2\left(\nabla^2 n\right).$$

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 $\omega(k)$?

Solution 2.2. Writing

$$n(r,t) = \int \frac{d\omega}{2\pi}\frac{d^3k}{(2\pi)^3} e^{-i\omega t + ik\cdot r} n(k,\omega)$$

we have

$$-i\omega n = (-Ma\bar{t}k^2 - 2M\lambda k^4)n,$$

which requires

$$\omega = -i\left(2M\lambda k^4 + Ma\bar{t}k^2\right).$$

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

Solution 2.3. For $\bar{t} > 0$ the system is stable (the imaginary part of all frequencies are negative). For $\bar{t} < 0$, the least stable wavevector is found from

$$\frac{\partial \omega}{\partial k^2} = 4M\lambda k^2 + Ma\bar{t} = 0,$$

which gives a wavelength

$$\lambda_0 = \frac{2\pi}{k_0} = 4\pi\sqrt{\frac{\lambda}{a(-\bar{t})}}$$

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

$$\begin{aligned} Z &= \int_{-\infty}^{\infty} d\epsilon \sum_{\{\sigma_i\}} e^{-\beta H} && (1)\\ &= \int_{-\infty}^{\infty} d\epsilon\, Z_\sigma e^{-N\beta\omega\epsilon^2} && (2)\\ &= \int_{-\infty}^{\infty} d\epsilon\, e^{-\beta N g(\epsilon)}, && (3) \end{aligned}$$

which defines the spin partition function Z_σ and the spin free energy $g(\epsilon)$.

If $g(\epsilon)$ has an aboslute 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

$$Z_\sigma = \mathrm{Tr}(\mathbf{PQ})^{N/2},$$

where

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

Solution 3.1. The argument is the same as the one given in class.

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

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

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

Solution 3.2. By definition,

$$g(\epsilon) = \omega\epsilon^2 - \frac{1}{N\beta}\log Z_\sigma.$$

Let $\lambda_\pm$ be the two eigenvalues of $\mathbf{PQ}$ with $\lambda_+ > \lambda_-$. We have $Z_\sigma = \lambda_+^{N/2} + \lambda_-^{N/2} \approx \lambda_+^{N/2}$, from which the desired equation directly follows.

3.3. Show that

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

Solution 3.3. Direct multiplication gives

$$\mathbf{PQ} = \begin{pmatrix} 2\cosh(2\beta) & 2\cosh(2\beta\epsilon) \\ 2\cosh(2\beta\epsilon) & 2\cosh(2\beta) \end{pmatrix},$$

with eigenvalues

$$\lambda_{\pm} = 2[\cosh(2\beta) \pm \cosh(2\beta\epsilon)].$$

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

Solution 3.4. Following the hint, for small ϵ, the free energy is

$$g(\epsilon) = a + b\epsilon^2 + c\epsilon^4 + \cdots.$$

The important term is

$$b = \omega - \frac{\beta}{1 + \cosh(2\beta)}.$$

The second order phase transition occurs when this term vanishes, which for $\omega = 0.2$ gives $\beta = 0.52$.

We also should verify that $c > 0$ at this point. A little algebra gives

$$c = \frac{\beta^3}{12} \frac{\cosh(2\beta) - 2}{\cosh^4(\beta)} \approx 0.003 > 0.$$

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.

Solution 3.5. At the first order phase transition $g(\epsilon^*) = g(0)$ where $\epsilon^* \neq 0$ is a local minimum of the free energy.
As an example, we can do this in mathematica by defining the free energy as

```
g[b_, eps_, w_] := -1/(2 b) Log[2 Cosh[2 b] + 2 Cosh[2 b eps]] + w  eps^2
```

where `b` is β, `eps` is ϵ and w is ω. One can make a routine which finds the difference $g(\epsilon^*) - g(0)$ as

```
mn[b_?NumericQ] := First@FindMinimum[g[b, x, 0.24] - g[b, 0, 0.24], {x, 2}]
```

The place where this difference vanishes is then found with

```
FindRoot[mn[b] == 0, {b, 1, 1.2}]
```

which gives $\beta = 1.09$.
An equally valid approach is to plot $g(\epsilon)$ at different values of β and find the graph for which the two minima look like they have the same value.

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.

Solution 3.6. This can always be done numerically, but the easiest way to estimate these values is to note that the tricritical point will be given by the point where the expansion coefficients c and b simultaneously vanish [exercise: convince yourself why this is true]. From $c = 0$ we have $\cosh(2\beta) = 2$, and from $b = 0$ we have $w = \beta/(1 + \cosh(2\beta)$. Together this means $\beta = 0.658$ and $w = \beta/3 = 0.219$.

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

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

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

Solution 4.1. Stable: $m = 2$; Unstable: $m = 0$; Metastable: $m = -1$.

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?

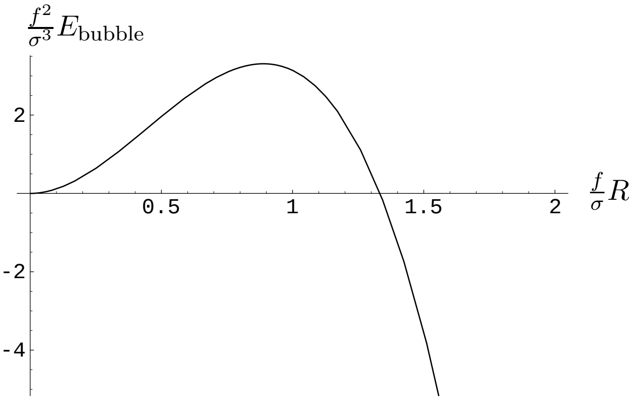
Solution 4.2. The Free energy per unit volume of the stable phase is $\mathcal{F}_2 = (-8/3)f$, while the energy per unit volume of the metastable phase is $\mathcal{F}_{-1} = (-5/12)f$. A bubble of radius R has volume $V = 4/3\pi R^3$, so the free energy savings is

$$\delta F = [\mathcal{F}_{-1} - \mathcal{F}_2]V = 3f\pi R^3.$$

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.l

Solution 4.3.

$$E_{\text{bubble}}(R) = 4\sigma\pi R^2 - 3f\pi R^3$$



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?

Solution 4.4. Setting $\partial E/\partial R = 0$, we find $R_c = (8/9)\sigma/f$, and $E_c = 256\pi\sigma^3/(243f^2)$.

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.