Final exam : Physics of complex systems

Correction

Coupled order parameters (Y. Imry 1975)

Notations and reasoning inspired by D. Arovas Lecture Notes.

- 1. The free energy must satisfy the $M \to -M$ and $\phi \to -\phi$ symmetries and is an expansion for small M and ϕ . Thus, the lowest non-trivial coupling is $M^2 \times \phi^2$ and the other terms are usual ϕ^4 theory terms.
- 2. For g = 0: at large T, the disorder phase will correspond to $M = \phi = 0$. When T is lowered, first $t < 0 < \tau$ so M gets ordered first, then, when $t < \tau < 0$, ϕ gets ordered and both order are non-zero (mixed phase). There are at least two transitions on this line.
- 3. When $M = \phi = 0$, the coupling is ineffective. When $M \neq 0$, g < 0 favours the ordering of ϕ , it increases the critical temperature of the mixed phase while g > 0 decreases this temperature. The last phase could be a $(M = 0, \phi \neq 0)$ phase. This could be possible for $T < T_2$ if the ordering of ϕ is much faster than that of M and g sufficiently positive to disfavour M while keeping ϕ finite.
- 4. One obtains

$$r = \frac{a}{\alpha} \sqrt{\frac{\delta}{d}}, \quad \varepsilon = \frac{a\alpha}{\sqrt{d\delta}}; \quad \lambda = \frac{g}{\sqrt{d\delta}}$$
 (1)

5. The rescaling is $\tilde{m} \to m = \tilde{m} \times r^{1/4}$ and $\tilde{\phi} \to \varphi = \tilde{\phi}/r^{1/4}$ so that $q = \sqrt{r}$.

6. We can write

$$f = \frac{1}{4} \begin{pmatrix} m^2 & \varphi^2 \end{pmatrix} \begin{pmatrix} 1 & \lambda \\ \lambda & 1 \end{pmatrix} \begin{pmatrix} m^2 \\ \varphi^2 \end{pmatrix} + \frac{1}{2} \begin{pmatrix} qt & \tau/q \end{pmatrix} \cdot \begin{pmatrix} m^2 \\ \varphi^2 \end{pmatrix}$$
(2)

The free energy must be bound from below in the positive quarter of the plane since the vector $\vec{v} = \begin{pmatrix} m^2 \\ \varphi^2 \end{pmatrix}$ has positive components. Diagonalizing the $A = \begin{pmatrix} 1 & \lambda \\ \lambda & 1 \end{pmatrix}$ matrix, we get the eigenvalues/eigenvectors $1 + \lambda/\vec{v}_+ = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$ and $1 - \lambda/\vec{v}_- = \begin{pmatrix} 1 \\ -1 \end{pmatrix}$. On the two axis $\varphi = 0$ and m = 0, the free energy diverges thanks to the positive coefficients of the quartic terms of the expansion. In the first quarter, divergence along the \vec{v}_+ direction is ensured by requiring that $1 + \lambda > 0$. We get the following condition : $\lambda > -1$. NB : we don't have to take into account the \vec{v}_- direction and the corresponding eigenvalue since it does not affect the stability in the first quarter of the plane.

7. Minimization of the free energy gives :

$$\frac{\partial f}{\partial m} = 0 = qtm + m^3 + \lambda m\varphi^2 \tag{3}$$

$$\frac{\partial f}{\partial \varphi} = 0 = q^{-1}\tau\varphi + \varphi^3 + \lambda m^2\varphi \tag{4}$$

8. We obtain, after some basic algebra :

$$\begin{array}{ll} \text{phase I} & (m = 0, \varphi = 0) & f_{\text{I}} = 0 \\ \text{phase II} & (m^2 = -qt, \varphi = 0) & f_{\text{II}} = -(qt)^2/4 \\ \text{phase III} & (m = 0, \varphi^2 = -\tau/q) & f_{\text{III}} = -(\tau/q)^2/4 \\ \text{phase IV} & \left(m^2 = \frac{\lambda \tau/q - qt}{1 - \lambda^2}, \varphi^2 = \frac{\lambda qt - \tau/q}{1 - \lambda^2}\right) & f_{\text{IV}} = \frac{1}{4(1 - \lambda^2)} \left(2\lambda t\tau - q^2t^2 - q^{-2}\tau^2\right) \\ \end{array}$$

- 9. In order to find the phase diagram, we must look for the lowest free energy among the four possible phases and check that $m^2 > 0$ and $\varphi^2 > 0$ whenever they are non-zero. We always have $\tau > t$ since $T_1 > T_2$.
 - a) When $\tau > t > 0$, phases II and III are not possible because $m^2 > 0$ or $\varphi^2 > 0$ not possible.
 - b) We take $\lambda > 1$. Phase IV is possible provided $m^2 > 0$ and $\varphi^2 > 0$, which translates into

phase IV:
$$\lambda > 1 \implies \lambda \tau < q^2 t \text{ and } \lambda q^2 t < \tau$$
 (5)

In general, one has to be careful that λ , t and τ can be either positive or negative so dividing these inequalities will change the order depending on the respective signs. Here, we can write $\lambda < x = q^2 t/\tau$ and $\lambda < 1/x = \tau/q^2 t$. Necessarily, either x or 1/x is smaller than one so $\lambda < 1$, which contradicts the hypothesis.

c) Here, we have :

phase IV:
$$\lambda^2 < 1 \implies \lambda \tau > q^2 t \text{ and } \lambda q^2 t > \tau$$
 (6)

which yields $\lambda > x$ and $\lambda > 1/x$ so $\lambda > 1$, in contradiction with the hypothesis. In conclusion, phase IV cannot be stabilized and the only stable phase for t > 0 is phase I.

- 10. In the case where $\tau>0>t$:
 - a) As t < 0, $f_{\rm II} < 0 = f_{\rm I} = f_{\rm III}$ (since $\tau > 0$) so only phases II and IV can compete. Computing their energy difference gives

$$f_{\rm IV} - f_{\rm II} = -\frac{1}{1 - \lambda^2} \left(\tau/q - \lambda tq\right)^2 \tag{7}$$

Consequently, $\lambda > 1 \Rightarrow f_{\rm IV} > f_{\rm II}$ so II is realized in this case.

- b) we have $\tau = t + \Delta T_c$ so $\tau > 0 > t \Rightarrow -\Delta T_c < t < 0$.
- c) we then assume $\lambda^2 < 1$ so that $f_{IV} < f_{II}$. Still, one must also satisfy (6). Taking care that $\tau > 0$ while t < 0, they can be rewritten as an interval

$$\lambda_{-}(t) = \frac{q^{2}t}{t + \Delta T_{c}} < \lambda < \lambda_{+}(t) = \frac{t + \Delta T_{c}}{q^{2}t}$$

$$\tag{8}$$

- d) $\lambda_{+}(t) = \frac{1}{q^2} + \frac{\Delta T_c}{q^2 t}$ decreases from $1/q^2$ to $-\infty$ as $t \to 0$ while $\lambda_{-}(t) = q^2 \frac{q^2 \Delta T_c}{t + \Delta T_c}$ is an increasing function, starting at q^2 at $t \to -\infty$, diverging at $t = -\Delta T_c$ and reaching 0 when $t \to 0$. The crossing points are solutions of the equation $\frac{q^2 t}{t + \Delta T_c} = \frac{t + \Delta T_c}{q^2 t}$, which roots are $t_G = -\frac{\Delta T_c}{1 + q^2}$ and $t_K = -\frac{\Delta T_c}{1 q^2}$. In (8), G of abscissa t_G corresponds to $\lambda = -1$ while K corresponds to $\lambda = 1$ with $t_K < 0$ only for q < 1. Notice that $t_K < -\Delta T_c < t_G < 0$ so that only t_G matters for the current interval (though these results will be reused below).
- e) From the above graphical analysis, we understand that (8) is fulfilled when $-\Delta T_c \leq t \leq t_G$ in which $-1 < \lambda < \lambda_+(t)$. This is the region where IV is realized and has the minimum energy. For $\lambda > \lambda_+(t)$, only phase II is possible (see Fig. 1).
- 11. Last, in the case where $0>\tau>t$:
 - a) phases II and III have negative free energies so I has to be excluded.
 - b) In addition to (7), we obtain

$$f_{\rm II} - f_{\rm III} = \frac{1}{4} \left(\left(\tau/q \right)^2 - \left(qt\right)^2 \right)^2 \tag{9}$$

$$f_{\rm IV} - f_{\rm III} = -\frac{1}{4(1-\lambda^2)} \left(qt - \lambda\tau/q\right)^2 \tag{10}$$

Clearly, for $\lambda > 1$, phase IV cannot be stabilized. It remains the competition between II and III. The boundary between phase II and III is given by the equation $(\tau/q)^2 - (qt)^2 = 0$ which is the same as the roots for the crossing points. Since we had $t_K < -\Delta T_c < t_G < 0$ and are working in the interval $t < -\Delta T_c$, the boundary corresponds to a vertical line of abscissa t_K , provided it exists, i.e. provided q < 1. Otherwise, only phase II is realized.

c) we consider $\lambda^2 < 1$ so that $f_{\text{IV}} < f_{\text{II}}, f_{\text{III}}$. Still, one must also satisfy (6). Taking care that now $\tau < 0$ while t < 0, we obtain the conditions

$$\lambda < \lambda_{-}(t) = \frac{q^{2}t}{t + \Delta T_{c}} \text{ and } \lambda < \lambda_{+}(t) = \frac{t + \Delta T_{c}}{q^{2}t} \Leftrightarrow \lambda < \min(\lambda_{-}(t), \lambda_{+}(t))$$
(11)

From the previous graphical analysis, we must distinguish two cases : when q > 1, then $\lambda_{-}(t) < \lambda_{+}(t)$ in this range so the boundary is simply the continuation of the $\lambda_{-}(t)$ curve. When q < 1, we have $\lambda_{-}(t) < \lambda_{+}(t)$ for $t_{K} < t < t_{G}$ while $\lambda_{+}(t) < \lambda_{-}(t)$ for $t < t_{K}$ so that $\lambda_{+}(t)$ becomes the boundary in this range (see Fig. 1).

12. From the previous analysis, we can put the phases number on Fig. 1 corresponding to q > 1 and q < 1. Otherwise, using the $\lambda = 0$ intuitive results and the discussions of questions 2 and 3, we can name the phases.



FIGURE 1 – Typical phase diagrams for q > 1 (left) and q < 1 (right). The full lines are second order and the dashed line is first order.

Cahn-Hilliard equation

Statics

- 1. The g corresponds to an elastic energy cost in deforming the order parameter. For $T > T_c$, $f_L(\phi)$ has a single minimum at $\phi_m = 0$ with curvature $f''_L(0) = 2\tilde{a} > 0$. For $T < T_c$, $\phi_m = 0$ becomes a local maximum with curvature $f''_L(0) = 2\tilde{a} < 0$, while two minima appear at $\phi_m = \pm \sqrt{-\frac{\tilde{a}}{2d}}$ with curvature $f''_L(\phi_m) = -4\tilde{a} > 0$.
- 2. It satisfies $\frac{\delta F}{\delta \phi} = 0 \Rightarrow -2g\Delta \phi_0 + f_L'(\phi_0) = 0.$
- 3. Using $f'_L(\phi_0 + \delta\phi) \simeq f'_L(\phi_0) + f''_L(\phi_0)\delta\phi$, we have $-2g\Delta\phi_0 2g\Delta\delta\phi + f'_L(\phi_0) + f''_L(\phi_0)\delta\phi = 0 \Rightarrow [-2g\Delta + f''_L(\phi_0)]\delta\phi = 0$
- 4. Above T_c : the equation can be written $[-\Delta + \frac{1}{\xi^2}]\delta\phi = 0$ with $\xi = \sqrt{\frac{2g}{f_L''(0)}} = \sqrt{\frac{g}{\tilde{a}}}$. Perturbation typically decreases with distance over a length scale ξ which is the correlation length (growing solutions are possible with some confining).

Below T_c : for the local maximum we get $[-\Delta - \frac{1}{\xi^2}]\delta\phi = 0$ with $\xi = \sqrt{\frac{2g}{-f_L'(0)}} = \sqrt{-\frac{g}{\tilde{a}}}$. The solutions are oscillatory meaning that perturbations are stable, they propagate with distance, corresponding to the fact that the system is not stable. For the two oter minima, we get again $[-\Delta + \frac{1}{\xi^2}]\delta\phi = 0$ with $\xi = \sqrt{\frac{2g}{f_L'(\phi_m)}} = \sqrt{-\frac{g}{2\tilde{a}}}$.

Dynamics

5. We compute

$$\frac{\partial \overline{\phi}}{\partial t} = \frac{1}{V} \int_{V} \frac{\partial \phi}{\partial t}(\vec{r}, t) \, d\vec{r} = -\frac{1}{V} \iiint_{V} \vec{\nabla} \cdot \vec{J} \, d\vec{r} = \oiint_{S(V)} \vec{J} \cdot d\vec{S} = 0 \tag{12}$$

where S(V) is the surface of the system. Since the system is closed, the surface integral is zero. Close to equilibrium, the fluxes \vec{J} are opposed to the cause so, physically, $\Gamma > 0$.

6. In the lecture, we have seen the time-dependent Ginzburg-Landau equation :

$$\frac{\partial \phi}{\partial t} = -\Gamma \frac{\delta F}{\delta \phi} \tag{13}$$

for non-conserved order parameter. If one starts from a uniform state, it gives an evolution with a relaxation to the equilibrium uniform state. In Cahn-Hilliard, if we set $\phi = \text{const.}$, then $\vec{J} = \vec{0}$ and there is no evolution, even if ϕ is not the equilibrium order parameter.

7. We get $\vec{\nabla} \cdot \vec{J} = -\Gamma \vec{\nabla}^2 \frac{\delta F}{\delta \phi}$

$$\frac{\partial\phi}{\partial t} = \Gamma\Delta\left(-2g\Delta\phi + f'_L(\phi)\right) \tag{14}$$

8. Injecting $\phi(\vec{r},t) = \phi_m + \delta \phi(\vec{r},t)$ with $f'_L(\phi_m) = 0$, $\frac{\partial \phi_m}{\partial t} = 0$ and $\Delta \phi_m = 0$, we get

$$\frac{\partial \delta \phi}{\partial t} = \Gamma \Delta \left(-2g\Delta \delta \phi + f_L''(\phi_m) \delta \phi \right) = \left[-2g\Gamma \Delta^2 + \Gamma f_L''(\phi_m) \Delta \right] \delta \phi .$$
⁽¹⁵⁾

- 9. Consider the situation where ϕ_m is a minimum :
 - a) For a minimum, we can use $f''_L(\phi_m) = 2g/\xi^2$ so that the equation reads :

$$\left[\frac{\partial}{\partial t} + 2g\Gamma\Delta^2 - \frac{2g\Gamma}{\xi^2}\Delta\right]\delta\phi = 0.$$
(16)

b) By Fourier transformation, we get

$$-i\omega + 2g\Gamma(i\vec{k})^4 - \frac{2g\Gamma}{\xi^2}(i\vec{k})^2 = 0 \Rightarrow \omega(k) = -i\frac{2g\Gamma}{\xi^2}k^2\left(1 + \xi^2k^2\right)$$
(17)

The dispersion relation is of the form $\omega(k) = -i/\tau_{\vec{k}}$ with $\tau_{\vec{k}} = \frac{\xi^2}{2g\Gamma} \frac{1}{k^2(1+\xi^2k^2)}$. It means that the timeevolution of the modes will be of the form $e^{-t/\tau_{\vec{k}}}$: they will all be damped with time, in agreement with the fact that we expect the system to relax to the minimum (equilibrium). Still, the $\vec{k} = \vec{0}$ mode has an infinite relaxation rate so it is good to get the Green's function to have a better understanding.

c) If we neglect the Δ^2 term, we get a *diffusion equation*, writing $D = \frac{2g\Gamma}{\xi^2}$ (diffusion coefficient), the dispersion relation reads $\omega(k) = -iDk^2$ and the Green's function equation (by considering adding a

source term in the right hand side, not in
$$f_L$$
):

$$\left[\frac{\partial}{\partial t} - D\Delta\right]\chi(\vec{r}, t) = \delta(\vec{r}\,)\delta(t) \;. \tag{18}$$

In Fourier space, we obtain

$$\hat{\chi}(\vec{k},\omega) = \frac{1}{Dk^2 - i\omega} \tag{19}$$

Inverse Fourier transform starts by computing

$$\int \frac{d\omega}{2\pi} \frac{e^{-i\omega t}}{Dk^2 - i\omega} = \Theta(t)e^{-Dk^2t}$$
(20)

with the residue theorem (similar to the lectures). As in the lecture, the integral over \vec{k} is computed using Fourier transform of gaussian integrals.

$$\chi(\vec{r},t) = \Theta(t) \frac{1}{(4\pi Dt)^{d/2}} e^{-\vec{r}^{\,2}/(4Dt)} \,. \tag{21}$$

d) We can use, for t > 0, the fact that $\Delta \chi = \frac{1}{D} \frac{\partial \chi}{\partial t}$ to estimate the Δ^2 term. First, we have

$$\frac{\partial\chi}{\partial t} = \left[\frac{\vec{r}^2}{4Dt^2} - \frac{d}{2t}\right]\chi \Rightarrow \Delta^2\chi = \frac{1}{D^2}\frac{\partial^2\chi}{\partial t^2} = \frac{1}{D^2}\left[\left(\frac{\vec{r}^2}{4Dt^2} - \frac{d}{2t}\right)^2 - \left(\frac{\vec{r}^2}{2Dt^3} - \frac{d}{2t^2}\right)\right]\chi \tag{22}$$

In the long times regime, the contributions from the Δ^2 are then negligible w.r.t. the diffusive kernel. Physically, as the diffusion process smooths the profile, it is logical that high wave-length become negligible first.

- 10. Consider the situation where ϕ_m is a local maximum :
 - a) For the maximum, we can use $f''_L(\phi_m) = -2g/\xi^2$ so that the equation now reads :

$$\left[\frac{\partial}{\partial t} + 2g\Gamma\Delta^2 + \frac{2g\Gamma}{\xi^2}\Delta\right]\delta\phi = 0.$$
⁽²³⁾

It only changes the sign of the Δ term, but this has profound physical implications.

b) By Fourier transformation, we get

$$-i\omega + 2g\Gamma(i\vec{k})^4 + \frac{2g\Gamma}{\xi^2}(i\vec{k})^2 = 0 \implies \omega(k) = iDk^2\left(1 - \xi^2k^2\right)$$
(24)

Now, the imaginary part of $\omega(k)$ is positive for small k and negative at large k. The curve has an intermediate maximum corresponding to

$$k_{\max} = \frac{1}{\sqrt{2\xi}} \,. \tag{25}$$

c) Modes with positive imaginary part of the dispersion relation will grow with time as $e^{t/\tau_{\vec{k}}}$ with $\tau_{\vec{k}} = 1/\Im\omega(k)$. Modes with negative imaginary parts will be damped as before and correspond to short wave-lengths. The most unstable one is the one corresponding to k_{\max} , corresponding to the wave-length $\lambda_{\max} = 2\sqrt{2}\pi\xi$. At short times, the system is unstable towards the formation of domains of size governed by ξ (as for the case of conserved order parameter). When domains are formed, they are locally close to the equilibrium solution so there is little evolution in the bulk of the domain. The evolution is governed by the motion of the interfaces. In the conserved case, this motion is (slightly) different from the non-conserved case because the domains have to fulfil the global constraint (fixed area for black and white domains).