Statistical Mechanics Problems III
(Assessed as extra credit at a value of 3% of total course mark. Due 26 September, 2008. **Hand in to Simon Tyler!**)

Questions on Mean Field theory.

(a) Lattice gas models are often used to examine properties of interacting systems of particles. The idea is to divide a volume V into atomic-size cubes each of volume v_o and the cubes are stacked on top of each other so as to form a sort of simple cubic lattice. Due to short-ranged repulsion between atoms there can be no more than one gas atom in each of these sites. There is also an attractive interaction between atoms which is also treated as short ranged and only important between atoms in neighbouring cells. The model classical Hamiltonian has the form

$$H = -\varepsilon \sum_{(i,j)} n_i \, n_j$$

where the sum is only over nearest neighbours. The occupation numbers n_i are 1 if a cell is occupied and 0 if it is empty. Show that the mean field classical Hamiltonian is

$$H_{mf} = \sum_{i=1}^{N} (3 \varepsilon n^2 - 6 \varepsilon n n_i) .$$

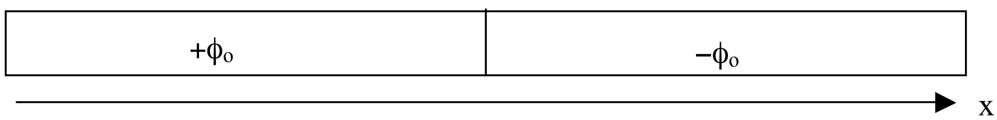
(b) For certain systems that undergo an order-disorder transition, the free energy density $f[\phi(\mathbf{r})]$ may be written as

$$f[\varphi(\mathbf{r})] = -\frac{\alpha}{2} (T_C - T) \varphi^2 + \frac{b}{4} \varphi^4 + \frac{\lambda}{2} (\nabla\varphi)^2$$

where $\phi(\mathbf{r})$ is the order parameter and T is close to, but less than, T_C.

i) What is the value ϕ_o of the order parameter that minimizes the free energy if the sample is uniformly ordered?

ii) Suppose that the sample is ordered in one region with $+\phi_o$, and in another region with $-\phi_o$.



If the sample is infinite, then the profile of how the order parameter varies form + to – ϕ can be calculated as a function of position. The equation governing the profile can be found by using the calculus of variations on the free energy equation to derive a differential equation that minimizes the total free energy:

$$\frac{\delta f[\varphi]}{\delta\varphi} = 0 \Rightarrow \lambda \frac{\partial^2}{\partial x^2} \varphi = -\alpha (T_C - T) \varphi + b \varphi^3 .$$

Show by substitution that a solution to this equation is $\varphi(x) = \phi_O \tanh(x/L)$,
and determine ϕ_O and L in terms of α, T and b. This solution describes a boundary wall between phases and is mathematically known as a topological soliton.

NOT FOR ASSESSMENT! Example exam questions on applications of Mean Field theory.

(a) Consider a system in the Landau-Ginzburg theory. The free energy density f is

$$f = -\frac{\alpha}{2}(T_C - T)\varphi^2 + \frac{b}{4}\varphi^4$$

where φ is the order parameter.

i) Sketch the general form of f as a function of φ for two cases: (i) $T > T_C$ and (ii) $T < T_C$. Explain in words why this free energy describes a continuous phase transition from one phase to another at T_C. Find the allowed values of φ for cases (i) and (ii) in terms of α and b.

ii) The superfluid order parameter is complex and can be written as $\varphi = A\exp(iS)$ where A and S are real numbers. What is the physical interpretation of $|\varphi|^2 = A^2$?

(b) Consider a region within the superfluid. If φ is evaluated along a circle in this region, then we expect that φ is the same at the start and finish of the circle. This means that φ could change only in phase, not magnitude so that $\varphi(S) = \varphi(S+2\pi n)$ where n is an integer.

i) Argue that as long as the circle contains no discontinuities in φ, it then follows that the velocity must be uniform and independent of position. (Hint: recall that the momentum operator is proportional to ∇S and viscosity requires a gradient in velocity). Argue that if the circle contains a line of normal fluid at the centre, then it is possible to have quantized circulation of the superfluid (a vortex).

ii) Suppose that a term $\frac{\lambda}{2}|\nabla\varphi|^2$ is included in the free energy, and A is allowed to vary with position along the x axis. If $T < T_C$, there are two solutions that minimise the free energy f but which have A independent of x. Another solution exists in which A does change with position x. Sketch the form of this third solution for A(x) as a function of x. Explain the physical significance of this solution, noting the value of A as $x \to \pm\infty$.