

Problem set 5

March 5, 2013

to submit by Thursday the 21st of March

0.1 Second and first order phase transitions

Let us consider the following phenomenological free energy density of a given system described in terms of a real homogeneous order parameter m (Landau's mean-field theory):

$$\frac{f(m)}{V} = f_0 + a(T - T_c)m^2 + \frac{b}{2}m^4, \quad (1)$$

where $a > 0$ and $b > 0$ are two constant positive parameters.

1. If the state that minimises the free energy is the physically realised state, describe the second order phase transition across $T = T_c$ and find how the minimum m_0 changes with the temperature.
2. Now let's imagine that a system is instead described by the following free energy

$$\frac{f(m)}{V} = f_0 + a(T - T_c)m^2 + \frac{b}{2}m^4 + \frac{c}{3}m^6, \quad (2)$$

where the coefficient $c > 0$ for stability, but the coefficient of the fourth order term, b , can now change sign (as before $a > 0$). Show that, for $T > T_c$, two (symmetric) secondary minima develop in the free energy density at finite values of the order parameter m and that, for a critical temperature $T = T_{first} > T_c$, a first order transition can be identified where the minimum for $m = 0$ and the one for $m \neq 0$ have the same energy. Describe the system phase diagram as a function of the system parameters.

1 Two-component condensates

Let us consider the case of a gas formed by a mixture of two types of bosons of equal densities. We indicate with ψ_\uparrow and ψ_\downarrow the BEC order parameter for each boson — we can think of them as, e.g., the same boson in two different spin state. Now the system is characterised by an intra-species interaction strength $U_{\uparrow\uparrow} = U_{\downarrow\downarrow} = U_0$ (which we are assuming to be the same for the two species and repulsive) and an inter-species interaction strength, which we indicate as

$U_{\uparrow\downarrow} = U_0 - 2U_1$, and that can be either attractive or repulsive. The free energy of the system can be thus written as:

$$\begin{aligned}
E[\psi_{\uparrow}, \psi_{\uparrow}^*, \psi_{\downarrow}, \psi_{\downarrow}^*] &= \int d\mathbf{r} \left[\sum_{\sigma=\uparrow,\downarrow} \psi_{\sigma}^* \left(-\frac{\hbar^2 \nabla^2}{2m_{\sigma}} - \mu \right) \psi_{\sigma} \right. \\
&\quad \left. + \frac{U_0}{2} (|\psi_{\uparrow}|^4 + |\psi_{\downarrow}|^4) + (U_0 - 2U_1) |\psi_{\uparrow}|^2 |\psi_{\downarrow}|^2 \right] \\
&= \int d\mathbf{r} \left[\sum_{\sigma=\uparrow,\downarrow} \psi_{\sigma}^* \left(-\frac{\hbar^2 \nabla^2}{2m_{\sigma}} - \mu \right) \psi_{\sigma} \right. \\
&\quad \left. + \frac{U_0 - U_1}{2} (|\psi_{\uparrow}|^2 + |\psi_{\downarrow}|^2)^2 + \frac{U_1}{2} (|\psi_{\uparrow}|^2 - |\psi_{\downarrow}|^2)^2 \right]. \quad (3)
\end{aligned}$$

3. Evaluate the two coupled Gross-Pitaevskii equations associated to (3).
4. Consider now the case of uniform field solutions. Show that the the free energy (3) has a minimum for $|\psi_{\uparrow}| = |\psi_{\downarrow}|$ if $U_1 > 0$, while the minimum occurs for either $(|\psi_{\uparrow}| \neq 0, |\psi_{\downarrow}| = 0)$ or $(|\psi_{\uparrow}| = 0, |\psi_{\downarrow}| \neq 0)$ when $U_1 < 0$ — Note that, for stability, one has to require that $U_0 > 0$ and $U_0 - U_1 > 0$. Discuss what happens when either $U_0 < 0$ or $U_0 - U_1 < 0$. Find the values of the minima in terms of the chemical potential. Plot the system phase diagram in the (U_0, U_1) space.
5. Evaluate the Bogoliubov spectra of excitation separately for both cases $U_1 > 0$ and $U_1 < 0$ and discuss your results — now assume that $U_0 > 0$ and $U_0 - U_1 > 0$.

2 Vortex line solutions

We have derived in class that a solution of the time-independent Gross-Pitaevskii equation (GPE) is the one describing a vortex line of charge j :

$$\Psi_v(\mathbf{r}) = e^{ij\varphi} |\Psi_v(r)|, \quad (4)$$

where (r, φ, z) are the cylindrical coordinates, i.e. φ is the azimuthal angle.

6. Show that, by parametrising the amplitude of the vortex solution $|\Psi_v(r)|$ in terms of a dimensionless function of $\tilde{r} = r/\xi$, where $\xi = \hbar/\sqrt{2mU_0\bar{n}}$ is the healing length and $\bar{n} \simeq \mu/U_0$ is the uniform density solution,

$$|\Psi_v(r)| = \sqrt{\bar{n}} f(\tilde{r}), \quad (5)$$

the GPE can be equivalently rewritten as

$$\frac{1}{\tilde{r}} \frac{d}{d\tilde{r}} \left(\tilde{r} \frac{df(\tilde{r})}{d\tilde{r}} \right) + \left(1 - \frac{j^2}{\tilde{r}^2} \right) f(\tilde{r}) - f^3(\tilde{r}) = 0. \quad (6)$$

7. Show that (in a cylindrical container of height L and radius R , thus with volume $V = L\pi R^2$) the free energy of the vortex solution minus the free

energy of the homogeneous solution ($E'_0 = V(\frac{U_0\bar{n}^2}{2} - \mu\bar{n}) = -\frac{L\pi R^2}{2}U_0\bar{n}^2$) can be written as

$$E'_v - E'_0 = \frac{\pi Ln\hbar^2}{m} \int_0^{R/\xi} d\tilde{r}\tilde{r} \left[\left(\frac{df}{d\tilde{r}} \right)^2 + \frac{j^2}{\tilde{r}^2} f^2 + \frac{1}{2} (f^2 - 1)^2 \right]. \quad (7)$$

Note that we use the notation $E' = E - \mu N$.

8. For the case of a vortex of charge $|j| = 1$, consider the following variational solution

$$f(\tilde{r}) = \frac{\tilde{r}}{\sqrt{\alpha + \tilde{r}^2}}, \quad (8)$$

and use it as a trial form for the real solution $f(\tilde{r})$ of (6), i.e., substitute (8) into (7) and minimise the energy expression with respect to the parameter in the trial function α . Show that the optimal value is $\alpha = 2$.

9. **(Optional:)** Show that for the optimal solution, one gets

$$E'_v - E'_0 = \frac{\pi Ln\hbar^2}{m} \ln \left(\frac{1.497R}{\xi} \right), \quad (9)$$

which is very close to the exact (numerical) result $E'_v - E'_0 = \frac{\pi Ln\hbar^2}{m} \ln(1.464R/\xi)$.