Problem Set The Blume–Emery–Griffiths model

At low temperature, pure ⁴He changes from a normal fluid to a superfluid phase (the so-called λ transition). When ³He atoms are added, the transition is modified. In this Problem, we shall describe such a ³He-⁴He mixture. To do so, we will use a lattice model proposed by Blume, Emery, and Griffiths in 1971 [1]. Each of the N sites of the lattice is occupied by a ⁴He or ³He atom, and has z nearest neighbors. To each site is associated a fictitious spin S_i , taking the values 0 and ± 1 . A ³He atom at site *i* corresponds to $S_i = 0$ and a ⁴He atom to $S_i = \pm 1$. The spin degree of freedom describes the nature of the system: if $m = \langle S_i \rangle = 0$, the fluid is normal, while if $m \neq 0$, it is a superfluid.

1 Preliminaries

- (a) Show that the number of ³He and ⁴He atoms are given by $N_3 = \sum_{i=1}^{N} (1 S_i^2)$ and $N_4 = \sum_{i=1}^{N} S_i^2$, respectively, with $N = N_3 + N_4$.
- (b) Show that the average fraction x of ³He atoms on the lattice is given by $x = 1 \langle S_i^2 \rangle$.

2 Model Hamiltonian

We first introduce an Ising Hamiltonian with an external field H and a coupling constant -J between nearest neighbors which describes the tendency of the system to be superfluid at low temperature,

$$\mathcal{H}_1 = -J \sum_{\langle i,j \rangle} S_i S_j - H \sum_{i=1}^N S_i.$$

Here, $\langle i, j \rangle$ denotes a sum over nearest neighbor spins.

- (a) Briefly justify the use of the above Hamiltonian to describe the ${}^{3}\text{He-}{}^{4}\text{He}$ mixture. What is the sign of J?
- (b) We then want to describe the interactions between nearest neighbor atoms. Let us denote $-u_{33}$, $-u_{44}$, and $-u_{34} = -u_{43}$ the interaction energy between each type of pairs (³He-³He, ⁴He-⁴He, ³He-⁴He and ⁴He-³He, respectively). Show that

$$\mathcal{H}_{\text{int}} = -u_{44} \sum_{\langle i,j \rangle} S_i^2 S_j^2 - u_{33} \sum_{\langle i,j \rangle} \left(1 - S_i^2 \right) \left(1 - S_j^2 \right) - u_{34} \sum_{\langle i,j \rangle} \left[S_i^2 \left(1 - S_j^2 \right) + S_j^2 \left(1 - S_i^2 \right) \right].$$

(c) Finally, we take into account the chemical potentials μ_3 and μ_4 of the two species (³He and ⁴He, respectively). The full Hamiltonian then reads $\mathcal{H} = \mathcal{H}_1 + \mathcal{H}_{int} - \mu_3 N_3 - \mu_4 N_4$, where N_3 and N_4 are the number of ³He and ⁴He atoms, respectively. Show that the above Hamiltonian takes the form

$$\mathcal{H} = -J\sum_{\langle i,j\rangle} S_i S_j - K\sum_{\langle i,j\rangle} S_i^2 S_j^2 - H\sum_{i=1}^N S_i - \Delta \sum_{i=1}^N S_i^2 + C.$$
 (1)

Give the expressions of the constants K, Δ , and C as a function of the parameters of the problem. In what follows, we set C = 0. Why can we do so?



Figure 1: Phase diagram calculated from Eqs. (2) for H = 0 and K = 0. The tricritical point A separates the regions where first- and second-order phase transitions occur. Reproduced from Ref. [1].

3 Mean field approximation

Let us decompose the spin S_i into its average value $\langle S_i \rangle$ and the fluctuations δS_i around the latter: $S_i = \langle S_i \rangle + \delta S_i$. Let us further decompose S_i^2 into $\langle S_i^2 \rangle$ and δS_i^2 , the fluctuations of S_i^2 around $\langle S_i^2 \rangle$: $S_i^2 = \langle S_i^2 \rangle + \delta S_i^2$.

- (a) We define the two correlation functions $C_{ij} = \langle S_i S_j \rangle \langle S_i \rangle \langle S_j \rangle$ and $\tilde{C}_{ij} = \langle S_i^2 S_j^2 \rangle \langle S_i^2 \rangle \langle S_j^2 \rangle$. Show that $C_{ij} = \langle \delta S_i \delta S_j \rangle$ and $\tilde{C}_{ij} = \langle \delta S_i^2 \delta S_j^2 \rangle$. What are the values of C_{ij} and \tilde{C}_{ij} within the mean field approximation (MFA)?
- (b) In the MFA, show that the Hamiltonian (1) reads

$$\mathcal{H} \simeq \frac{Nz}{2} \left[Jm^2 + K(1-x)^2 \right] - (H+zJm) \sum_{i=1}^N S_i - \left[\Delta + zK(1-x) \right] \sum_{i=1}^N S_i^2.$$

- (c) Deduce from the previous question an expression for the grand-canonical partition function Ξ and the grand potential Ω .
- (d) Show that the two self-consistent equations determining m and x are given by

$$m = \frac{2 \exp\left(\beta [\Delta + zK(1-x)]\right) \sinh\left(\beta [H+zJm]\right)}{1 + 2 \exp\left(\beta [\Delta + zK(1-x)]\right) \cosh\left(\beta [H+zJm]\right)}$$
(2a)

$$x = \frac{1}{1 + 2\exp\left(\beta[\Delta + zK(1-x)]\right)\cosh\left(\beta[H+zJm]\right)},\tag{2b}$$

where $\beta = 1/k_{\rm B}T$.

The numerical solution of Eqs. (2), at vanishing external field (H = 0) and for K = 0 (which typically corresponds to the experimental situation; why?), give the phase diagram of Fig. 1.

4 Description of the phase transition

In the following, we aim at better understanding the phase diagram displayed in Fig. 1. We therefore look at the properties of the system close to the phase transition, i.e., the order parameter m is close to zero. From now on, we consider the case where K = 0.



Figure 2: Experimental phase diagram. Reproduced from Ref. [2].

- (a) Let us introduce the potential $G(m) = \Omega(H) + Hm$. Justify the use of such a potential in order to study the phase transition at vanishing external field (H = 0).
- (b) We now aim at expanding G(m) in powers of the order parameter m as

$$G(m) = G(0) + \frac{1}{2}a\,m^2 + \frac{1}{4}b\,m^4 + \frac{1}{6}c\,m^6 + \mathcal{O}(m^8).$$

Limiting the expansion above to second order in m, show that $a = \delta k_{\rm B}T - zJ$, where we set $\delta = 1 + e^{-\beta\Delta}/2$. <u>Hint</u>: Expand Eq. (2a) for both $\beta H \ll 1$ and $m \ll 1$ in order to obtain H as a series expansion in m.

In what follows, we will admit that $b = \frac{k_{\rm B}T}{8}\delta^2(1-\frac{\delta}{3})$ and $c = \frac{k_{\rm B}T}{12}\delta^3(1-\frac{3\delta}{4}+\frac{3\delta^2}{20})$.

- (c) Let us assume that c > 0. Sketch $\Delta G(m) = G(m) G(0)$ as a function of m when b > 0. Then show that there exists a second-order phase transition at the critical temperature $T_{\rm c}(x) = T_{\rm c}(0)(1-x)$, with $k_{\rm B}T_{\rm c}(0) = zJ$.
- (d) Sketch $\Delta G(m)$ for b < 0. What happens in this case? Show that the equation for the first-order phase transition line is given by $a = 3b^2/16c$.
- (e) Show that there exists a tricritical point (T_t, x_t) . Calculate T_t and x_t .
- (f) Compare your theoretical predictions with the experimental results in Fig. 2.

References

- M. Blume, V.J. Emery, R.B. Griffiths, Ising model for the λ transition and phase separation in ³He-⁴He mixtures, Phys. Rev. A 4, 1071 (1971).
- [2] E.H. Graf, D.M. Lee, J.D. Reppy, Phase separation and the superfluid transition in liquid ³He-⁴He mixtures, Phys. Rev. Lett. 19, 417 (1967).