Study of the λ and phase separation transitions in ^{3}He-^{4}He mixtures

Based on [*Phys. Rev. A* **4** 3, 1071 (1971)]

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Outline of the talk

1. Introduction

2. Lattice gas model

3. Mean-field approximation

4. Landau theory for $K/J = 0$

Introduction to the Blume-Emery-Griffiths (BEG) model

Consider a nearest-neighbor spin-1 Ising model, consisting of spin variables

$$S_i \in \{0, +1, -1\},$$

with Hamiltonian

$$H = -J \sum_{<i,j>} S_i S_j - K \sum_{<i,j>} S_i^2 S_j^2 + \Delta \sum_i S_i^2 + H \sum_i S_i,$$

this model is called BEG model. Interesting theoretical features are:

- It describes a tricritical point.
- In certain regimes, it shows a triple point.
- It shows the competition of the coupling K and J in the description of the first-order transition.

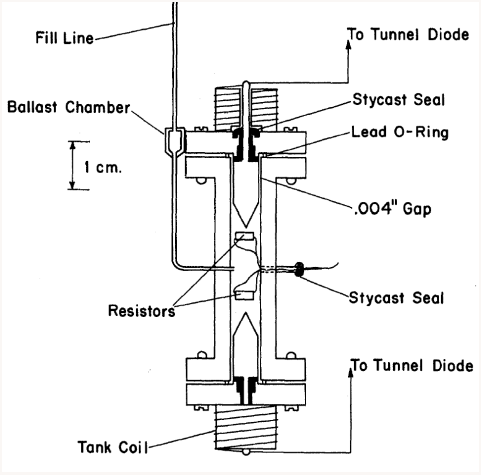
A simplification of the model is called Blume-Capel model, corresponding to $K = 0$.

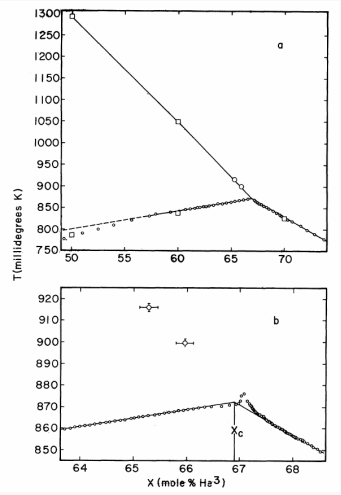
Results from literaure

The BEG was used to study many phenomena in statistical mechanics. Two notable examples are:

- First-order paramagnetic-ferromagnetic transition in UO_2 [Phys. Rev. **141**, 517-524 (1966)].
- Lambda transition and phase separation in ^{3}He-^{4}He mixtures [*Phys. Rev. A* **4**, 1071 (1971)].

Physics of ^{3}He-^{4}He mixtures





[E. H. Graf, D. M. Lee and J. D. Reppy, *Phys. Rev. Lett.* **19** 8, 417 (1967)]

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Lattice gas of the mixture

The spin-1 Ising model is used, in the context of the mixture, to represent a **lattice gas**, without vacancies, in which the Helium atoms are:

$$S_i = \begin{cases} 0 & {}^3\mathrm{He} \\ \pm 1 & {}^4\mathrm{He} \end{cases}$$

the apparently fictitious double value for the ^{4}He is assigned for being able to write an order parameter changing its sign. The lattice is a three-dimensional one, with an arbitrary shape. In fact, the number of nearest neighbors considered in the interaction will be absorbed in the coupling.

Definition of thermodynamic variables

In the lattice gas framework, we define the average magnetization

$$M = N^{-1} \sum_{i=1}^{N} \langle S_i \rangle \,,$$

the variables corresponding to the number of ^{3}He and ^{4}He atoms

$$N_3 = \sum_{i=1}^{N} \left(1 - S_i^2\right) ,$$

$$N_4 = \sum_{i=1}^{N} S_i^2 .$$

The concentration of ^{3}He is represented by the variable

$$x = \frac{1}{N} \langle N_3 \rangle \,.$$

Definition of thermodynamic variables

In a translationally symmetric system, it is possible to simplify the averages and take

$$M = \langle S_i \rangle ,$$

for the average magnetization, and

$$x = 1 - \left\langle S_i^2 \right\rangle ,$$

for the density of ^{3}He. These two variables correspond, respectively, to **superfluid** ordering, and **population imbalance**, and are the order parameters of the system. In the context of magnetism, M is named **magnetization**, and $1 - x$ is named **quadrupole moment**.

Ising model from physical couplings

In order to derive the BEG model, we assume the Hamiltonian as a sum of three terms

$$H = H_S + H_I - \mu_3 N_3 - \mu_4 N_4.$$

The term H_S is the term responsible for superfluidity, written as a ferromagnetic Ising Hamiltonian in zero field

$$H_S = -J \sum_{<i,j>} S_i S_j,$$

with the usual sum over nearest neighbors. The term H_I is modeling all the other possible interaction in nearest neighbors

$$\begin{aligned} H_I = &- K_{33} \sum_{\langle i,j \rangle} \left(1 - S_i^2\right)\left(1 - S_j^2\right) - K_{44} \sum_{\langle i,j \rangle} S_i^2 S_j^2 \\ &- K_{34} \sum_{\langle i,j \rangle} \left[S_i^2 \left(1 - S_j^2\right) + S_j^2 \left(1 - S_i^2\right)\right], \end{aligned}$$

where K_{ij} is the interaction between ${}^{i}\mathrm{He}$, ${}^{j}\mathrm{He}$. One expects all of the K_{ij} to be equal since the interatomic force is equal for the isotopes, but differences in mass and statistics lead to different effective interaction. Expanding the products and rearranging we can rewrite the Hamiltonian as

$$H = -J \sum_{\langle i,j \rangle} S_i S_j - K \sum_{\langle i,j \rangle} S_i^2 S_j^2 + \Delta \sum_i S_i^2 - N \left(z K_{33} + \mu_3 \right),$$

where generalized couplings has been defined as

$$K = K_{33} + K_{44} - 2K_{34},$$

and

$$\Delta = \mu_3 - \mu_4 + 2z \left(K_{33} - K_{44} \right),$$

where z is the valence, or coordination number of the lattice.

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Mean-field ansatz

We now derive mean-field equations of state. In the original paper they are derived by using a variational procedure.

Here we propose an alternative, based on a simpler writing of the probability distribution. As usual in the mean-field approximation, we assume to have independence of the probabilities related to a single site. Let $\bar{\rho}(\mathbf{S})$, be the joint probability distribution of the configuration $\mathbf{S}$, then

$$\bar{\rho}(\mathbf{S}) = \prod_i \rho_i(S_i),$$

moreover, by translational symmetry, $\rho_i = \rho_j =: \rho \; \forall \; i, j$. We can express the single-site probability as

$$\rho(S) = q_1 \; \delta_{S,1} + q_0 \; \delta_{S,0} + q_{-1} \; \delta_{S,-1},$$

requiring

$$\sum_i q_i = 1.$$

Mean-field ansatz

By computing the averages, we can relate the distribution to the magnetization M and the quadrupole moment $1 - x$ as follows

$$\begin{aligned} q_1 - q_{-1} &= M \\ q_1 + q_{-1} &= 1 - x, \end{aligned}$$

and solving for $\{q_i\}_i$, we have

$$\begin{aligned} q_0 &= x \\ q_1 &= \frac{(1-x) + M}{2} \\ q_{-1} &= \frac{(1-x) - M}{2}. \end{aligned}$$

Mean-field ansatz

The mean-field free energy per site, neglecting constant terms, can be obtained by direct substitution, where we redefine the couplings taking into account the valence number z: $zK \to K$ and $zJ \to J$,

$$f_{MF} = -\frac{J}{2}M^2 - \frac{K}{2}(1-x)^2 + \Delta(1-x) + \frac{1}{\beta}\left[x\ln x + \frac{(1-x)+M}{2}\ln\left(\frac{(1-x)+M}{2}\right) + \frac{(1-x)-M}{2}\ln\left(\frac{(1-x)-M}{2}\right)\right].$$

Minimizing the free energy with respect to M and x we obtain the equations of state

$$\frac{\partial f_{MF}}{\partial M} = -JM + \frac{1}{2\beta}\left[\ln\left(\frac{(1-x)+M}{2}\right) - \ln\left(\frac{(1-x)-M}{2}\right)\right] = 0.$$

$$\frac{\partial f_{MF}}{\partial x} = K(1-x) - \Delta + \frac{1}{2\beta}\left[-\ln\left(\frac{(1-x)+M}{2}\right) - \ln\left(\frac{(1-x)-M}{2}\right) + 2\ln x\right] = 0.$$

Mean-field ansatz

By exponentiating:

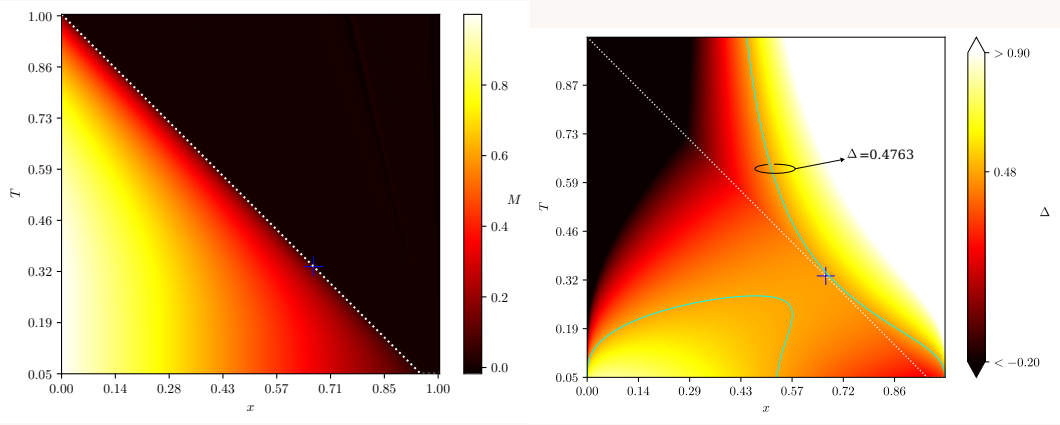
$$e^{2\beta(\Delta - K(1-x))} = \frac{4x^2}{(1-x)^2 - M^2},$$
$$(1-x)\sinh(\beta JM) - M\cosh(\beta JM) = 0.$$

By using simple algebra, the above equations are equivalent to the mean-field equations of Blume, Emery and Griffiths [Eq.(3.7), (3.8), *Phys. Rev. A* **4** 3, 1071 (1971)]. Once we show they are equivalent, we can use the same arguments for the Landau theory near the critical point. Those equations are

$$1 - x = \frac{2\cosh\beta JM}{\exp[\beta(\Delta - K(1-x))] + 2\cosh\beta JM},$$
$$M = \frac{2\sinh\beta IM}{\exp[\beta(\Delta - K(1-x))] + 2\cosh\beta JM}.$$

Phase diagrams

The numerical solution has been carried out using a nonlinear solver based on Newton-Rhapson metod for the joint system of equations. The results below correspond to $K/J = 0$.



We can observe that the coefficient M transit from a null value to a finite value in correspondence to a straight line. This can be easily checked by expanding Eq. (3.10):

$$1 - x = M \coth(\beta J M)$$

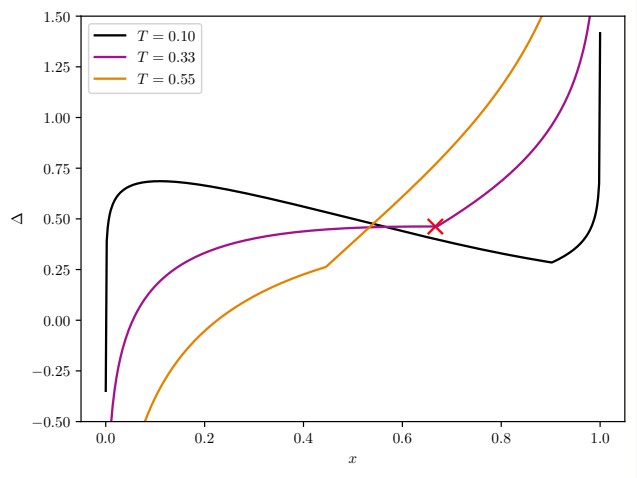
for small M, leading to the superfluid transition temperature

$$\frac{T_S}{J} = 1 - x.$$

We also observe the peculiar behaviour of the $\Delta = 0.4763$ line, which is suggesting unphysical behaviour.

Computation of first-order transition line

As usually happens with (approximate) equations of state, the description of the first-order transition is **unphysical**. In order to find the first-order transition lines, it is necessary to regularize the behaviour of the equation of state. This is routinely done by **Maxwell construction**, an example is the Van der Waals equation. In fact, we observe, looking at isothermal lines, that the isothermal compressibility becomes positive.

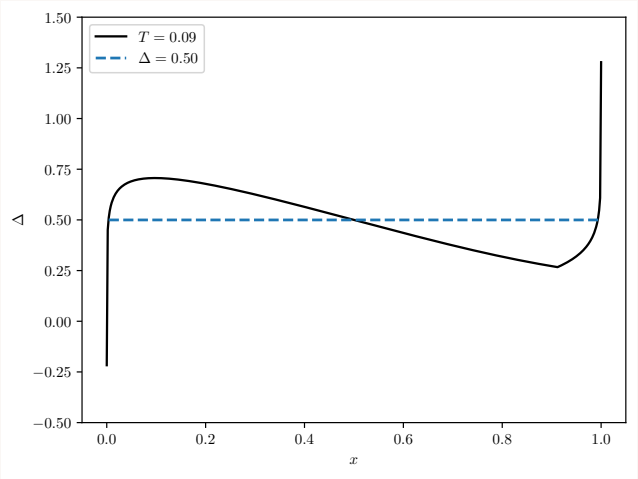


Computation of first-order transition line

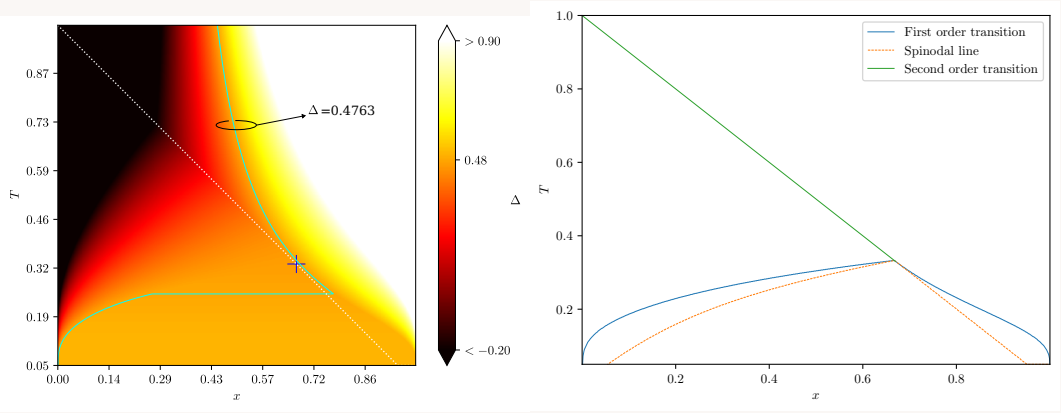
Imposing negativity of the isothermal compressibility, we have that physically meaningful points on the phase diagram satisfy

$$\left(\frac{\partial \Delta}{\partial x}\right)_T > 0$$

We proceed applying the standard Maxwell construction and get the phase diagrams, in which we have also a spinodal line.

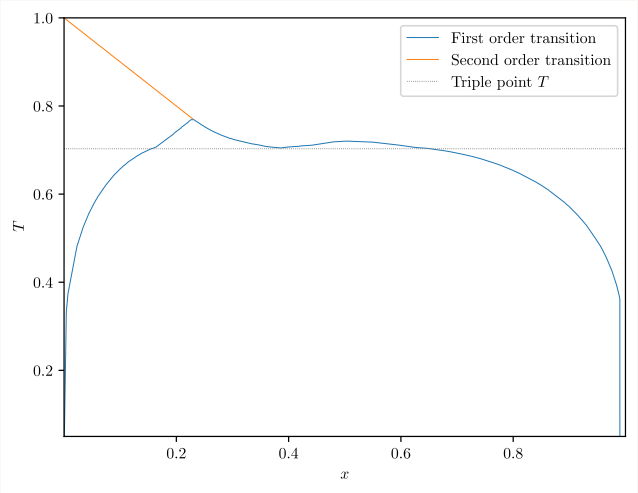


Computation of first-order transition line



Case of $K/J = 2.88$

Setting $K/J = 2.88$, an interesting feature of the phase diagram is appearing, namely a **triple point**, in which **three phases**, described by three different values of x, coexist. By using the lever rule, one can obtain the relative amount of the phases.



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Power series expansion of the potential

$$G(M) = \Phi - MH$$

$$H = -\frac{\partial G}{\partial M}$$

Near the transition point, one can use the equation of state to get the expansion for the coefficients:

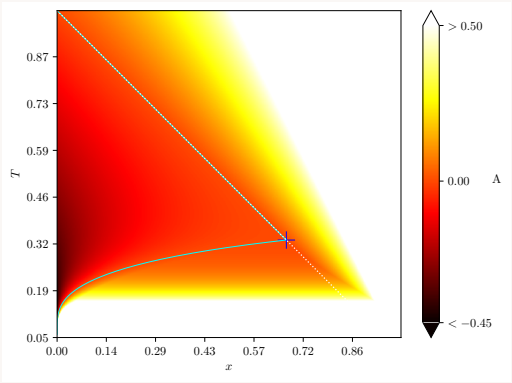
$$\begin{aligned} A &= \frac{\delta}{2\beta} - \tfrac{1}{2}\delta, \\ B &= \frac{1}{8\beta}\left(\delta^2 - \tfrac{1}{3}\delta^3\right), \\ C &= \frac{1}{6\beta}\left(\tfrac{1}{2}\delta^3 - \tfrac{3}{8}\delta^4 + \tfrac{3}{40}\delta^5\right), \end{aligned}$$

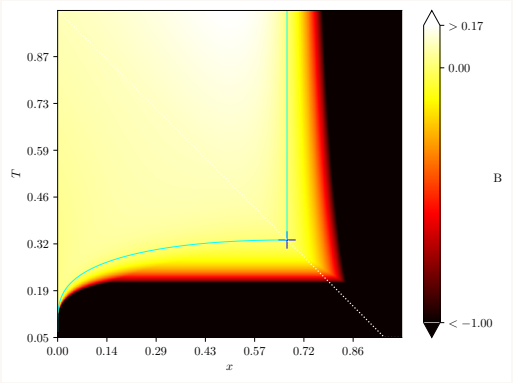
with

$$\delta = 1 + \frac{1}{2}e^{\beta\Delta}.$$

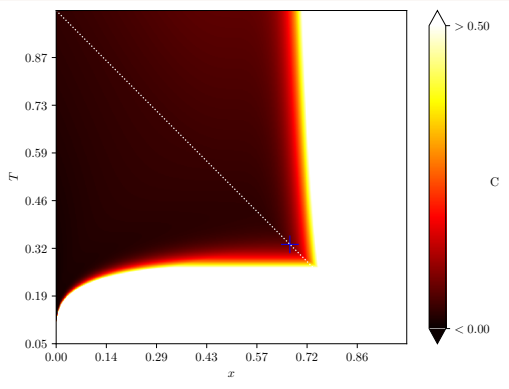
Where we can use the solution of the Δ found before, and draw transition lines.

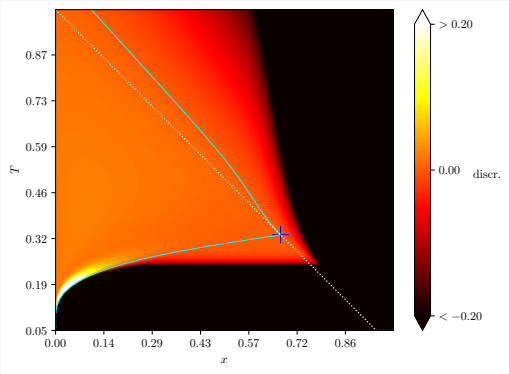
Transition lines



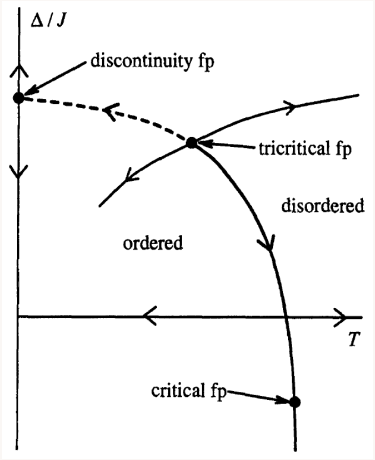


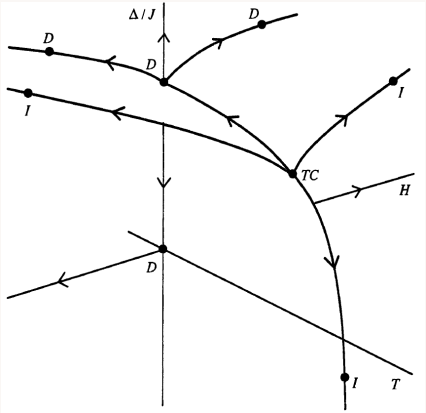
Transition lines





RG considerations for the Blume-Capel model





[J. Cardy, *Scaling and Renormalization in Statistical Physics*, Cambridge University Press (2015)]

Conclusions

- The BEG model has been shown to be a valuable tool for describing the **rich phase diagram** of the ^{3}He-^{4}He mixture, even at a mean-field level.
- We propopsed an alternative derivation of the mean-field equations, starting from the direct substitution of the probability distribution, when the original work proposed a **variational approach**.
- We solved numerically the mean-field equations, and apply a **Maxwell construction** to fix the unphysical features of the mean-field model.
- We pointed out the **theoretical relevance** of the Blume-Emery-Griffiths, and the Blume-Capel model, that are applied widely in statistical mechanics.

Thanks for the attention!

Relevant references

[1] M. Blume. “Theory of the First-Order Magnetic Phase Change in UO_2”. In: *Physical Review* 141.2 (1966), p. 517.

[2] M. Blume, V. J. Emery, and R. B. Griffiths. “Ising model for the λ transition and phase separation in He3-He4 mixtures”. In: *Physical review A* 4.3 (1971), p. 1071.

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[7] R. B. Griffiths. “Thermodynamics near the two-fluid critical mixing point in He3-He4”. In: *Physical Review Letters* 24.13 (1970), p. 715.

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