

6CCP3212 Statistical Mechanics Homework 5

Lecturer: Prof. Eugene A. Lim

<https://nms.kcl.ac.uk/eugene.lim/teach/statmech/sm.html>

1) In the lectures, we argue that the critical limit of a BEC $T \rightarrow T_{\text{crit}}$, at fixed V , the mean number of particles and the mean energy are given by

$$\langle N_{\text{crit}} \rangle = \int_0^\infty \frac{4\sqrt{2}\pi V}{(2\pi\hbar)^3} m^{3/2} \frac{E^{1/2}}{e^{\beta E} - 1} dE, \quad (1)$$

and

$$\langle E \rangle = \int_0^\infty \frac{4\sqrt{2}\pi V}{(2\pi\hbar)^3} m^{3/2} \frac{E^{3/2}}{e^{\beta E} - 1} dE \quad (2)$$

Compute the integrals, and show that they are

$$\langle N_{\text{crit}} \rangle = 2.612 \frac{V}{\lambda^3} \quad (3)$$

and

$$\langle E \rangle = 1.783 \frac{4\sqrt{2}\pi V}{(2\pi\hbar)^3} m^{3/2} (k_b T)^{5/2} \quad (4)$$

where

$$\lambda = \sqrt{\frac{2\pi\hbar^2}{mk_b T}}, \quad (5)$$

is the thermal de Broglie wavelength.

2) Consider the Van der Waals equation of state for fixed N

$$Nk_b T = \left(P + \frac{N^2}{V^2} a \right) (V - Nb) . \quad (6)$$

(i) Express the pressure P as a function of V and T .

(ii) The critical conditions are given by $(\partial P / \partial V)_T = 0$ and $(\partial^2 P / \partial V^2)_T = 0$. Find P_c , T_c and V_c as a function of a , b and N .

(iii) From Problem Set 1 Q6, you have shown that

$$\left(\frac{\partial E}{\partial V} \right)_T = -P + T \left(\frac{\partial P}{\partial T} \right)_V . \quad (7)$$

Using the Van der Waals equation, and the fact that C_V^{id} for an ideal gas is given by $C_V^{\text{id}} = (3/2)Nk_b$, show that the energy for a Van der Waals gas is

$$E = \frac{3}{2}Nk_b T - \frac{aN^2}{V} . \quad (8)$$

Hence show that at the critical point T_c , the specific heat C_V for the Van der Waals gas does not scale with T , i.e.

$$C_V \propto (T - T_c)^\alpha, \quad \alpha = 0 . \quad (9)$$

(Note you can directly derive the above relation using the results of Problem Set 1 Q3 too.)

(iv) In Problem Set 1 Q4, you were given the isothermal compressibility of a gas as

$$K_T \equiv -\frac{1}{V} \left(\frac{\partial V}{\partial P} \right)_T . \quad (10)$$

Show, at the critical point T_C and V_C , the isothermal compressibility of the Van der Waals gas scales as

$$\kappa \propto (T - T_C)^{-1} . \quad (11)$$

(*Hint*: Recall that at the critical point $(\partial P/\partial V)_T = 0$.)

3) (Landau Model of 1st Order Phase Transition). Consider the following Landau Functional

$$F = F_0(T) + a(T - T_C)m^2 + \frac{1}{2}bm^4 + \frac{1}{3}cm^6 , \quad (12)$$

where m is the order parameter and, $a > 0$, $b < 0$ and $c > 0$ are real constants.

(i) Find the minima of F , and show that there are five solutions given by

$$m = 0 , \quad m^2 = \frac{-b \pm \sqrt{b^2 - 4a(T - T_C)c}}{2c} . \quad (13)$$

(ii) Consider the case $T < T_C$, how many of the above solutions are real and stable? Sketch F in this regime.

(iii) Consider the case when $T > T_C$. Show that there are only one stable solution when $T > T_*$ where

$$T_* = \frac{b^2}{4ac} + T_C . \quad (14)$$

In the regime where $T_C < T < T_*$, show that there exist three real and stable solutions given by

$$m = 0 , \quad m = \pm \sqrt{\frac{-b + \sqrt{b^2 - 4a(T - T_C)c}}{2c}} . \quad (15)$$

Sketch both of these cases.

(iv) Consider a system described by this Landau functional F . We start at temperature $T > T_*$, and gradually cool the system down. What happens at T_* ? What happens at T_C ? Calculate the jump in the order parameter m when a phase transition occurs.

(v) Conversely, if we start at temperature $T < T_C$, and gradually heat the system up. What happens at T_C ? What happens at T_* ? Similarly, calculate the jump in the order parameter m when a phase transition occurs.

(vi) Calculate the latent heat for the two transitions described in (iv) and (v), and show that it is $L = (abT_C)/c$ for the former and $L = (abT_C)/2c$ for the latter.

4) (Exact solution of the Ising Model in 1-dimension). In this problem, we solve the Ising Model in 1D exactly. Ising solved this problem as a PhD student in 1925, but here we will follow a more general method first devised by Kramers and Wannier in 1941. The energy or Hamiltonian of the Ising model is given by

$$E = -\mu H \sum_i^N s_i - J \sum_{j, (n.n.)}^N J_{ij} s_i s_j \quad (16)$$

where the spins are

$$s_i = \begin{cases} +1 & , \quad \text{for spin up } \uparrow \\ -1 & , \quad \text{for spin down } \downarrow \end{cases} \quad (17)$$

The key idea of the Kramers-Wannier method is to note that we can “wrap around” the a long line of N nodes, by identifying the end points, such that $s_{N+1} \equiv s_1$, and then take $N \rightarrow \infty$, as shown in Fig. 1. This is called the *Ising chain*. In this form, the energy can be written in the *symmetric form* as

$$E = -\frac{1}{2}\mu H \sum_i^N (s_i + s_{i+1}) - \sum_{j, (n.n.)}^N J_{ij} s_i s_j . \quad (18)$$

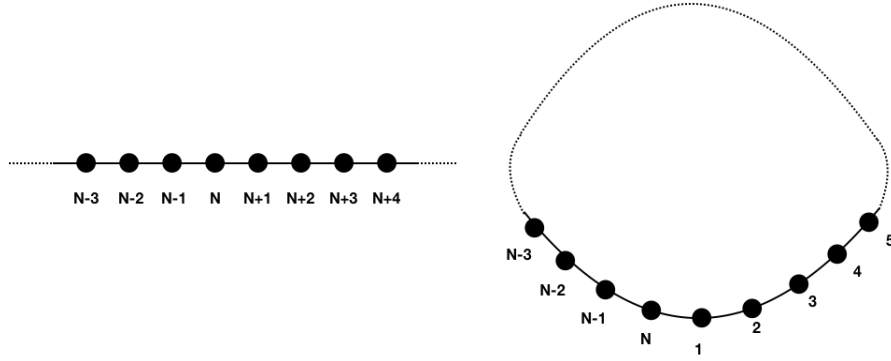


Figure 1: (Q4) An infinitely long 1D line of nodes (left) can be “wrapped around” to itself to make an Ising Chain (right).

(i) Show that the partition function for the Ising chain is given by

$$Z_{1D} = \sum_{s_i=\pm 1} \cdots \sum_{s_N=\pm 1} \prod_{i=1}^N \exp \left[\beta J s_i s_{i+1} + \frac{\beta \mu H}{2} (s_i + s_{i+1}) \right]. \quad (19)$$

(ii) Now consider the term, for any i ,

$$T(s_i, s_{i+1}) \equiv \exp \left[\beta J s_i s_{i+1} + \frac{\beta \mu H}{2} (s_i + s_{i+1}) \right]. \quad (20)$$

Since $s_i = \pm 1$ and $s_{i+1} = \pm 1$, there are *four* possible values for T . Write down these four possible values $T_{++} = T(s_i = 1, s_{i+1} = 1)$, $T_{-+} = T(s_i = -1, s_{i+1} = 1)$, $T_{+-} = T(s_i = 1, s_{i+1} = -1)$, and $T_{--} = T(s_i = -1, s_{i+1} = -1)$. We can collect all these four possibilities as a 2×2 matrix

$$T = \begin{pmatrix} T_{++} & T_{-+} \\ T_{+-} & T_{--} \end{pmatrix}. \quad (21)$$

(iii) For each i , the coefficients of the matrix T depends on the s_i and s_{i+1} , which are summed over in the partition function. We can also think of T as a *transfer matrix*, whose values depend on “input” s_{i+1} and “output” s_i (you can also think of both as “inputs” if you like), and borrow the notation of quantum mechanics to write

$$\langle s_i | T | s_{i+1} \rangle \equiv \exp \left[\beta J s_i s_{i+1} + \frac{\beta \mu H}{2} (s_i + s_{i+1}) \right]. \quad (22)$$

Show that the partition function in (i) can then be written as

$$Z_{1D} = \sum_{s_i=\pm 1} \cdots \sum_{s_N=\pm 1} \langle s_1 | T | s_2 \rangle \langle s_2 | T | s_3 \rangle \cdots \langle s_i | T | s_{i+1} \rangle \cdots \langle s_{i=N} | T | s_1 \rangle. \quad (23)$$

(iv) Solve the partition function in (iii), and show that it is

$$Z_{1D} = \text{Tr}(T^N). \quad (24)$$

(*Hint*: This is a standard linear algebra trick of “completing the set” which you have learned in quantum mechanics. Recall that in quantum mechanics, the wave function for two operators A and B can be expressed as $\langle \psi | AB | \phi \rangle = \sum_i \langle \psi | A | i \rangle \langle i | B | \phi \rangle$ by inserting a complete set of eigenmodes $\mathbf{1} = \sum_i | i \rangle \langle i |$.)

(v) Recalling that the trace of any invertible matrix M is the sum of its eigenvalues, show that the eigenvalues for T is given by

$$\lambda_{\pm} = e^{\beta J} \left[\cosh(\beta \mu H) \pm \sqrt{e^{-4\beta J} + \sinh^2(\beta \mu H)} \right]. \quad (25)$$

Hence argue that the partition function is given by

$$Z_{1D} = \lambda_+^N + \lambda_-^N , \tag{26}$$

as we have asserted in the lectures.