Final Exam: Statistical Mechanics 2018/19, ICFP Master (first year)

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Introduction

Some general information:

- Starting time: 14:00 AM, finishing time: 17:00 PM

- External material is not allowed (no books, scripts, calculators, computers, smart phones etc.).

- Use only paper provided by ENS.

- Do not forget to write your name onto the cover sheet.

- Please transfer your answers from the green scratch paper (brouillon) to the white exam paper.

- Do not forget to sign the register ("feuille d'émargement").

Useful formulas, cheat sheet

Integral representation of the Dirac delta function

$$\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\lambda \exp(i\lambda x)$$

Integral representation of the Kronecker delta function

$$\delta_{j,k} = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\lambda \exp[i\lambda(j-k)]$$

Transforming sums into integrals Remember that sums over integer elements are best transformed as

$$\sum_{n=1,2,\dots} f(n) \equiv \sum_{n=1,2,\dots} \Delta_n f(n)$$

with the differential $\Delta_n = 1$. Substitutions of n then apply to Δ_n.

Eigenvalues of the harmonic trap Remember that the eigenvalues of the harmonic oscillator are

$$\hbar\omega(n + 1/2), \quad n = 0, 1, 2, \dots \tag{1}$$

You can (should) omit the $1/2$ term.

Bose distribution function Remember that this function is given by

$$\frac{e^{-\beta(E-\mu)}}{1 - e^{-\beta(E-\mu)}} = \frac{1}{e^{\beta(E-\mu)} - 1}$$

Useful one-dimensional integrals Remember that

$$\int_0^{\infty} dx\, x \frac{1}{e^x - 1} = \frac{\pi^2}{6}, \qquad \int_0^{\infty} dx\, x^2 \frac{1}{e^x - 1} = 2\zeta(3), \qquad \int_0^{\pi} d\theta e^{z\cos\theta} = \pi I_0(x) \quad \text{(mod. Bessel function)}$$

n-dimensional Gaussian integral Remember [$\mathbf{B} = (B_1, \dots, B_n)$] that for symmetric positive definite matrices A:

$$\int_{-\infty}^{\infty} dx_1 \cdots \int_{-\infty}^{\infty} dx_n \exp\left(-\frac{1}{2}\sum_{i,j=1}^{n} A_{ij}x_i x_j + \sum_{i=1}^{n} B_i x_i\right) = \sqrt{\frac{(2\pi)^n}{\det A}} \exp\left(\frac{1}{2}\mathbf{B}^T A^{-1} \mathbf{B}\right)$$

I.   BOSE–EINSTEIN CONDENSATION, DIMENSIONALITY, AND SATURATION NUMBERS

In this question, we consider the harmonic trap with $\omega = 1$ in one dimension and, in dimensions $d > 1$, the isotropic harmonic trap with $\omega_x = \omega_y (= \omega_z) = 1$. We set the mass $m = 1$ and, finally, $\hbar = 1$. We omit the term $1/2$ in eq. (1).

A.   Single-particle state, N-body state (non-interacting particles)

Consider a harmonic trap in $d = 2$ (two) dimensions, with a single particle (of mass 1).

- Write down the (single-particle) states of low energy.

  $E = 0$ and $(0,0)$ $E = 1$ and $(0,1), (1,0)$ $E = 2$ and $(0,2), (2,0), (1,1)$ Density of states: $\mathcal{N}(E) = 1$ for $E = 0, 1, 2...$ in $d = 1$, $\mathcal{N}(E) = E + 1$ for $E = 0, 1, 2...$ in $d = 2$, $\mathcal{N}(E) = (E+1)(E + 2/2$ for $E = 0, 1, 2...$ in $d = 3$,

- Then suppose you put three (non-interacting) particles into this trap. Write down the (three-particle) many-body states of low energy (the energy of an N-body state is the sum of the single-particle energies).

  Here, it is convenient to number the different single-particle states, for example $\sigma = 0 \equiv (0,0)$, $\sigma = 1 \equiv (1,0)$, $\sigma = 2 \equiv (0,1)$, $\sigma = 3 \equiv (1,1)$, etc. A three-body state is then given through a tuple $\sigma_1, \sigma_2, \sigma_3$.

- Give formal expressions for the exact partition function in terms of the 3-body states for the case of 3 distinguishable (non-interacting) particles and for the case of 3 (non-interacting) indistinguisable particles (bosonic statistics).

  For 3 distinguishable particles, we have

  $$Z = \sum_{\sigma_1} \sum_{\sigma_2} \sum_{\sigma_3} \exp\left\{-\beta\left[E(\sigma_1) + E(\sigma_2) + E(\sigma_3)\right]\right\} = \left[\sum_{\sigma} \exp\left(-\beta E(\sigma)\right)\right]^3$$

  For 3 indistinguishable particles, we have

  $$Z = \sum_{\sigma_1} \sum_{\sigma_2 \geq \sigma_1} \sum_{\sigma_3 \geq \sigma_2} \exp\left\{-\beta\left[E(\sigma_1) + E(\sigma_2) + E(\sigma_3)\right]\right\}$$

B.   Chemical potential

We now consider different statistical ensembles.

- Following what we did in the lecture and in the homework, explain how one goes from the bosonic canonic partition function (as a function of N and the inverse temperature β) of Section I A to the grand canonic partition function, in terms of a chemical potential μ and β. (Hint: Look at the "Useful" formulas.)

  We can write the partition function through occupation levels $n_0, n_1, \ldots$ for the single-particle states $\sigma = 0, \sigma = 1, \ldots$. The correct number of particles is imposed through a Kronecker delta function. One then finds that the partition function is given through

  $$Z_N(\beta) = \int_{-\pi}^{\pi} \frac{d\lambda}{2\pi} \prod_{\sigma} \left[\sum_{n_\sigma} e^{n_\sigma(-\beta E_\sigma + i\lambda)}\right]$$

- Write down the grand-canonical partition function, quite generally, for ideal bosons, in terms of the density of states $\mathcal{N}(E)$. Explain your formula for the grand-canonical partition function. (Attention: make sure that all the signs and prefactors are OK.) What is the density of states in the harmonic trap in $d = 1$, and of the isotropic harmonic trap, in $d = 2$, and $d = 3$?

The grand-canonical partition function treats each single-particle state as independently occupied. The statistical weight of an N-body state is the product over all single-particle states of their probabilities. For each of these states, the total statistical weight is the sum of the weights to put $0, 1, 2, \ldots$ particles, that is $1 + e^{-\beta(E-\mu)} + e^{-2\beta(E-\mu)} + \cdots = 1/(1 - e^{-\beta(E-\mu)})$. Therefore

$$Z(\beta, \mu) = \prod_{\sigma} \frac{1}{1 - \exp\left[-\beta(E_\sigma - \mu)\right]} \tag{2}$$

which can be written as

$$Z(\beta, \mu) = \prod_{E=0,1,2,\ldots} \left[\frac{1}{1 - \exp\left[-\beta(E - \mu)\right]}\right]^{\mathcal{N}(E)} \tag{3}$$

The density of state for the harmonic oscillators is:

$$\mathcal{N}(E) = \begin{cases} 1 & \text{for } d = 1 \\ E + 1 & \text{for } d = 2 \\ (E+1)(E+2)/2 & \text{for } d = 3 \end{cases}$$

C. Ideal Bosons and saturation numbers

As discussed in lectures and homeworks, we can describe the Bose–Einstein phase transition in terms of the saturation number (the mean maximum number of particles in excited states).

- Formally express the saturation number in a harmonic trap in terms of the densities of states $\mathcal{N}(E)$. Connect the saturation number to the phenomenon of Bose–Einstein condensation.

  To compute the saturation number, we put $\mu = 0$. It cannot get any bigger.

  $$\langle N_{\text{sat}} \rangle = \sum_{E>0} \mathcal{N}(E) \frac{1}{\exp(\beta E) - 1}.$$

  (The total number $\langle N \rangle$ is the same expression, but summed over all states.) The saturation number gives the maximum number of particles that can be put into the excited states. If we add more particles, they must necessarily go into the ground state, that is, into the condensate.

- Explain why, in the harmonic trap in $1d$, and in the isotropic harmonic trap in $d > 1$, the study of Bose-Einstein condensation for large particle numbers $\langle N \rangle$ takes place at high temperature. Write the high-temperature limit of the saturation number as an integral (rather than a sum over energies E). (Hint: take a look at the "Useful" formulas for the transition from sums to integrals.)

  The saturation number increases with the temperature ($\exp(\beta E) \to 1$ for $\beta \to 0$. The expression for the saturation number is

  $$\langle N_{\text{sat}} \rangle = \sum_{E>0} \Delta_E \frac{1}{\exp(\beta E) - 1}$$

  taking $\beta E = x$, so that $dE = dx/\beta$, we reach

  $$= \frac{1}{\beta} \int_0^\infty dx \frac{1}{\exp(x) - 1}$$

- Study the integral you just obtained (for $d = 1$) in the limit $\langle N \rangle \to \infty$. (Hint: study what happens at what corresponds to small energies.) What does this imply for the phenomenon of Bose–Einstein condensation in a one-dimensional trap?

  The above integral diverges logarithmically at small x, as the integrand goes like $1/x$ at small x. The consequence is that the energy levels are never saturated and that there is no Bose–Einstein condensation in a one-dimensional harmonic trap.

D. Ideal Bosons in isotropic two- and three-dimensional harmonic traps

- Compute the saturation number for the isotropic harmonic trap in $d = 2$ in the limit $N \to \infty$. (Hint: See the "Useful" formulas for integrals, if needed.) Determine the Bose–Einstein condensation temperature T_c and the condensate fraction for large $\langle N \rangle$ below T_c.

  In $d = 2$, we have

  $$\langle N_{\text{sat}} \rangle = \frac{1}{\beta^2} \int_0^\infty dx\, x \frac{1}{\exp(x) - 1} = \frac{\pi^2}{6}(k_B T)^2 \tag{4}$$

  The saturation number is finite (and it grows with temperature). The Bose–Einstein-condensation temperature is when $\langle N_{\text{sat}} \rangle = \langle N \rangle$. This gives $k_B T_c = \sqrt{6 \langle N \rangle}/\pi$. To get the condensate fraction, we put $\langle N_{\text{sat}} \rangle + \langle N_0 \rangle = N$. This gives for $T < T_c$:

  $$\frac{N_0}{N} = 1 - \frac{\langle N_{\text{sat}} \rangle}{\langle N \rangle} = 1 - \left(\frac{T}{T_c}\right)^2 \quad \text{for } T < T_c, \text{ in } d = 2$$

- Obtain the critical temperature T_c for Bose–Einstein condensation and the condensate fraction below T_c for a three-dimensional isotropic harmonic trap. (Hint: See the "Useful" formulas, if needed.)

  In $d = 3$, as discussed in the lecture, we have

  $$\langle N_{\text{sat}} \rangle = \frac{1}{2\beta^3} \int_0^\infty dx\, x^2 \frac{1}{\exp(x) - 1} = \zeta(3)(k_B T)^3 \tag{5}$$

  This gives $k_B T_c = (\langle N \rangle / \zeta(3))^{1/3}$ and

  $$\frac{N_0}{N} = 1 - \frac{\langle N_{\text{sat}} \rangle}{\langle N \rangle} = 1 - \left(\frac{T}{T_c}\right)^3 \quad \text{for } T < T_c, \text{ in } d = 3$$

- In all of physics, the ideal Bose gas is the only system of not mutually interacting particles that features a phase transition. Can you explain why that is so?

  Two answers are possible:

  1. In terms of wave functions, the symmetrization of Bosonic wave functions introduces an effective interaction, even for non-interacting particles $\psi_{\text{Bos}}(x, y) = \psi_1(x)\psi_2(y) + \psi_1(y)\psi_2(x)$. However, it is amazing that the symmetrization does not appear in the calculation leading to the equation of states, but only influences the density of states.
  2. In terms of path integrals, the same symmetrization applies to the arguments of the diagonal density matrix.

II.   THE SPHERICAL MODEL

We consider an hypercubic lattice of length L in d dimensions (with periodic boundary conditions) with a spin σ_i on each vertex i. There are $N = L^d$ spins in the system. We consider the "spherical model" solved in 1952 by Berlin and Kac. The spherical model stands out because it can be solved in a non-zero magnetic field. Although we will not solve it up to the very end, it has a phase transition in high dimensions, but not in low dimensions, just like the Ising model.

The spherical model is defined through an energy that is similar to the one of the Ising model:

$$E = -J \sum_{(i,j)} \sigma_i \sigma_j - H \sum_{i=1}^{N} \sigma_i, \tag{6}$$

where are (i,j) are neighboring sites on the d-dimensional hypercubic lattice. However, instead of taking only the values ± 1, each spin can take on any real value $\sigma_i \in [-\infty, +\infty]$. Together, the spins $\sigma_1, \ldots, \sigma_N$ are subject only to the global constraint that

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

In the following, we write $K = \beta J$ and $h = \beta H$.

A.   Partition function, using Dirac delta function

Formally write the partition function of the model using a Dirac delta function.

$$Z_N = \frac{1}{2\pi} \int_{-\infty}^{\infty} \ldots \int_{-\infty}^{\infty} d\sigma_1 \ldots d\sigma_N \exp\left(K \sum_{(i,j)} \sigma_i \sigma_j + h \sum_i \sigma_i \right) \delta\left(\sum_i \sigma_i^2 - N \right)$$

With the constraint $aN - a\sum_i \sigma_i^2 = 0$ for all a. Therefore, adding such a term does not change the energy.

B.   Partition function, using the integral representation of the Dirac delta function

Note that we can modify the energy in eq. (6) by adding a term $E \to E + aN - a\sum_i \sigma_i^2$ without affecting the partition function. From now on we will keep this term.

We denote $\sigma = (\sigma_1, \sigma_2, \ldots, \sigma_N)$ (an N-dimensional column vector). Use the integral representation of the Dirac delta function to show that the partition function can be written as:

$$Z_N = \frac{1}{2\pi} \int_{-\infty}^{\infty} \ldots \int_{-\infty}^{\infty} d\sigma \int_{-\infty}^{\infty} ds \exp\left(-\sigma^T V \sigma + \overline{h}^T \sigma + (a + is)N \right)$$

(Hint: Take a look at the "Useful" formulas.) Find the expressions for V and $\overline{h}$.

first we write the partition function as :

$$Z_N = \int_{-\infty}^{\infty} \ldots \int_{-\infty}^{\infty} d\sigma_1 \ldots d\sigma_N \int_{-\infty}^{\infty} ds \exp\left(K \sum_{(i,j)} \sigma_i \sigma_j + h \sum_i \sigma_i + (aN - a\sum_i \sigma_i^2) \right) \delta\left(\sum_i \sigma_i^2 - N \right)$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} \ldots \int_{-\infty}^{\infty} d\sigma_1 \ldots d\sigma_N \exp\left(K \sum_{(i,j)} \sigma_i \sigma_j + h \sum_i \sigma_i + (aN - a\sum_i \sigma_i^2) \right) \int_{-\infty}^{+\infty} ds \, e^{is(\sum_i \sigma_i^2 - N)}$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} \ldots \int_{-\infty}^{\infty} d\sigma_1 \ldots d\sigma_N \int_{-\infty}^{\infty} ds \exp\left(K \sum_{(i,j)} \sigma_i \sigma_j + h \sum_i \sigma_i + (a + is)N - (a + is)\sum_i \sigma_i^2 \right)$$

Clearly $\bar{h} = (h, \ldots, h)$.

V is such that $\sigma^T V \sigma = \sum_{jl} \sigma_j V_{jl} \sigma_l = (a + is) \sum_j \sigma_j^2 - K \sum_{(i,j)} \sigma_i \sigma_j$. So $V_{ii} = (a + is)$ and $V_{ij} = -K$ if sites i and j are neighbors.

C. Partition function, from Gaussian integral

Show that Z_N can be rewritten as:

$$Z_N = \frac{1}{2} \pi^{\frac{N}{2}-1} \int_{-\infty}^{\infty} ds \, [\det V]^{-\frac{1}{2}} \exp\left\{ (a + is) N + \frac{1}{4} \bar{h}^T V^{-1} \bar{h} \right\}$$

(Hint: again take a look at the "Useful" formulas.)

Because of the periodic boundary conditions of the hypercubic lattice, one can show that the eigenvalues of V are $\lambda(\omega_1, \ldots, \omega_d) = a + is - K (\cos\omega_1 + \ldots + \cos\omega_d)$ where each ω_j can take value in $\left\{ 0, \frac{2\pi}{L}, \frac{4\pi}{L}, \ldots, \frac{2\pi(L-1)}{L} \right\}$.

In the limit of large L, show that $\log(\det V)$ can be written as :

$$\log(\det V) = N \left[\log(K) + g(z) \right]$$

with $z = \frac{a + is - Kd}{K}$. What is the expression for $g(z)$?

$$\log(\det V) = \log\left(\Pi_{\omega_1} \ldots \Pi_{\omega_d} \lambda(\omega_1, \ldots, \omega_d) \right) = \sum_{\omega_1} \ldots \sum_{\omega_d} \log\left[\lambda(\omega_1, \ldots, \omega_d) \right]$$

$$= \frac{N}{(2\pi)^d} \int_0^{2\pi} \ldots \int_0^{2\pi} d\omega_1 \ldots d\omega_d \log(a + is - K (\cos\omega_1 + \ldots + \cos\omega_d))$$

$$= \frac{N}{(2\pi)^d} \left(\log(K)(2\pi)^d + \int_0^{2\pi} \ldots \int_0^{2\pi} d\omega_1 \ldots d\omega_d \log\left(\frac{a + is - Kd}{K} + d - \cos\omega_1 - \ldots - \cos\omega_d \right) \right)$$

$$= N \left(\log(K) + g(z) \right)$$

with $z = \frac{a + is - Kd}{K}$ and

$$g(z) = \frac{1}{(2\pi)^d} \int_0^{2\pi} \ldots \int_0^{2\pi} d\omega_1 \ldots d\omega_d \log\left(z + d - \cos\omega_1 - \ldots - \cos\omega_d \right)$$

D. Partition function, as a one-dimensional complex integral

Using the fact that $\bar{h}$ is the eigenvector associated with the smallest eigenvalue of V, show that : $\bar{h}^T V^{-1} \bar{h} = \frac{Nh^2}{Kz}$.

We can rewrite Z_N as:

$$Z_N = \frac{K}{2\pi i} \left(\frac{\pi}{K} \right)^{\frac{N}{2}} \int_{c-i\infty}^{c+i\infty} dz \, e^{N\phi(z)}.$$

What are the expressions for c and of $\phi(z)$?

$\bar{h}$ is the eigenvector associated with the smallest eigenvalue of V. The smallest eigenvalue of V is obtained when $\omega_1 = \ldots = \omega_N = 0$, therefore : $\lambda_{min} = a + is - Kd = Kz$. Clearly: $\bar{h}^T V^{-1} \bar{h} = (Kz)^{-1} \bar{h}^T \bar{h} = \frac{Nh^2}{Kz}$.

If we go back to expression (IIC) and use the formula for $\det(V)$ and for $\bar{h}^T V^{-1} \bar{h}$ that we've computed we get

$$Z_N = \frac{1}{2} \pi^{\frac{N}{2}-1} \int_{-\infty}^{\infty} ds \, K^{-\frac{N}{2}} e^{-\frac{g(z(s))N}{2}(a+is)N + \frac{Nh^2}{4Kz(s)}}$$

we change variable from s to $z = \frac{a + is - Kd}{K}$ and get :

$$Z_N = \frac{K}{2\pi i} \left(\frac{\pi}{K} \right)^{\frac{N}{2}} \int_{\frac{a-Kd}{K}-i\infty}^{\frac{a-Kd}{K}+i\infty} dz \, e^{N\left(Kz + Kd - \frac{g(z)}{2} + \frac{h^2}{4Kz} \right)}$$

Hence: $c = \frac{a - Kd}{K}$ and $\phi(z) = Kz + Kd - \frac{g(z)}{2} + \frac{h^2}{4Kz}$.

This expression of Z_N actually does not depend on the choice of c as long as $Re(z)$ is positive. One can show that $\lim_{z \to 0} \phi(z) = \lim_{z \to +\infty} \phi(z) = +\infty$ and that $\phi''(z) > 0$. Therefore, ϕ has a minimum on the real axis which we call z_0. We choose the arbitrary constant c to be z_0.

E. Free energy, magnetization, equation of state

The free energy per site is $f = -\frac{1}{\beta} \lim_{N \to \infty} N^{-1} \log(Z_N)$. Express f as a function of K and $\phi(z_0)$ (Hint: Remember that we are in the $N \to \infty$ limit. You can use a saddle-point integration.)

directly we have:

$$f = -\frac{1}{\beta} \lim_{N \to \infty} \left(-\frac{1}{2} \log \left(\frac{K}{\pi} \right) + N^{-1} \log \left(\int_{z_0 - i\infty}^{z_0 + i\infty} dz e^{N\phi(z)} \right) \right)$$

We now use the saddle-point method to get $N^{-1} \log \left[\int_{z_0 - i\infty}^{z_0 + i\infty} dz e^{N\phi(z)} \right] \to \log [\phi(z_0)]$ when $N \to \infty$. We end up with : $f = -\frac{1}{\beta} \left(-\frac{1}{2} \log \left(\frac{K}{\pi} \right) + \phi(z_0) \right)$

Show that the magnetization is given by $M = -\partial_H f$. Find the expression of M (as a function of J, H and z_0.

z_0 is a minimum of ϕ, then $\phi'(z_0) = 0$ which gives us that $K - \frac{h^2}{4Kz_0^2} = \frac{g'(z_0)}{2}$
We differentiate the expression of f and use the previous equation to get:

$$M = \frac{h}{2Kz_0} + \phi'(z_0) \frac{dz_O}{dh}$$

Then once again we remember that $\phi'(z_0) = 0$ to get $M = \frac{h}{2Kz_0} = \frac{H}{2Jz_0}$

Use this result for M to write the exact equation of state (i.e. the relation between M, H and T) of the spherical model. (Hint: This expression will involve the function g.)

from $M \frac{H}{2Jz_0}$ and $K - \frac{h^2}{4Kz_0^2} = \frac{g'(z_0)}{2}$, one obtains:

$$2J(1 - M^2) = k_B T g' \left(\frac{H}{2M} \right)$$

III.   THE XY MODEL, AND ITS HARMONIC APPROXIMATION

In this question, we consider the XY model described by the hamiltonian

$$H = -J \sum_{\langle i,j \rangle} \mathbf{S}_i \mathbf{S}_j = -J \sum_{\langle i,j \rangle} \cos{(\phi_i - \phi_j)} \tag{7}$$

where $\mathbf{S}_i$ and $\mathbf{S}_j$ are classical spins in the eponymous (that is, name-giving) XY plane with $|\mathbf{S}_i| = 1$.

A.   One-dimensional XY model, exact treatment

Compute the partition function and the free energy per particle of the one-dimensional XY model (N spins with free boundary conditions). (Hint: check out the "Useful" formulas). What does the temperature behavior of the free-energy per particle establish about the phase behavior of the model?

The one-dimensional XY model is described through the $N-1$ relative angles between particles and an overall rotation. One finds:

$$Z = 2\pi \int d\phi_{12} e^{\beta J \cos \phi_{12}} \cdots \int d\phi_{N-1,N} e^{\beta J \cos \phi_{N-1,N}} = 2\pi \left[2\pi I_0(\beta J) \right]^{N-1}$$

For $N \to \infty$, the free energy per particle is

$$f = -\frac{1}{\beta} \log \left[2\pi I_0(\beta J) \right]$$

There is no phase transition.

B.   Two-dimensional XY model (harmonic approximation)

Explain in what consists the harmonic approximation of the XY model, and what are its fundamental properties in dimensions $d = 1$, $d = 2$, and $d > 2$. Discuss the correlations of $\phi(x)$ and $\phi(y)$ and the spin correlation function $\langle \cos{[\phi(x) - \phi(y)]} \rangle$. Discuss the behavior at low temperature and at high temperature.

The harmonic model replaces the $\cos(\phi_i - \phi_j)$ by $1 - \frac{1}{2}(\phi_i - \phi_j)^2$ There is no phase transition in this model, but the spin correlation function decays differently in $d = 1$ (exponential) $d = 2$ (algebraic) and $d = 3$ (constant).

C.   Kosterlitz–Thouless picture of the phase behavior in the two-dimensional XY model

Explain the basic insight of Kosterlitz and Thouless (1973) concerning the physics of the low- and high-temperature phases in the XY model. Discuss both the low-temperature and at high-temperature behavior.

Kosterlitz and Thouless explained the pertinence of vortex and anti-vortex excitations. A single vortex has energy $\sim J_R \log L$, but its entropy is also in the logarithm of the system size. The entropy and the energy do not depend on temperature, but because of $F = E - TS$, the free energy does. At low temperature, the free energy for creating a single vortex goes to infinite, at high temperature it goes to $-\infty$. A pair of vortices has finite energy, so it is always stable. Kosterlitz and Thouless described the phase transition in the XY model as a vortex-antivortex unbinding.

D.   Fröhlich and Spencer and the nature of the phase transition

As discussed in the lecture, Fröhlich and Spencer essentially proved that at low temperatures, the harmonic approximation of the XY model is OK. Explain what this means, and explain why this (while establishing the existence of the low-temperature phase), does not establish the existence of a Kosterlitz–Thouless phase transition. Discuss other possible scenarios in this model.

At low temperature, vortices and antivortices are thus effectively bound. The KT argument gives a temperature of unbinding through entropic effects. This is however relevant only if at this temperature, the vortices and antivortices are still bound. A first-order phase transition can have interfered before.