WiSe 2006 12/14/06

Prof. Dr. E. Frey
Dr. T. Franosch

Lehrstuhl für Statistische Physik
Biologische Physik & Weiche Materie
Arnold-Sommerfeld-Zentrum für Theoretische Physik
Department für Physik

Ludwig Maximilians Universität

T VI: Soft Matter and Biological Physics
(Prof. E. Frey)

Problem set 8

Problem 8.1 *Wick's theorem*
The joint probability distribution for N gaussian variables $\{\varphi_i\}_{i=1,\ldots,N}$ reads

$$P[\varphi] = \frac{1}{\sqrt{(2\pi)^N \det A}} \exp\left(-\frac{1}{2}\,\varphi^T \cdot A^{-1} \cdot \varphi\right),$$

with some real positive definite symmetric matrix A and the shorthand notation $\varphi^T \cdot A^{-1} \cdot \varphi = \sum_{i=1}^N \sum_{j=1}^N \varphi_i (A^{-1})_{ij} \varphi_j$ has been introduced.

1. Convince yourself that P is properly normalized.
2. Prove the following relation for the *generating functional*
$$Z[j] = \langle \exp\left(j^T \cdot \varphi\right)\rangle = \exp\left(\frac{1}{2}\, j^T \cdot A \cdot j\right).$$
3. Correlation functions are then readily obtain by taking appropriate derivatives
$$\langle \varphi_{i_1} \ldots \varphi_{i_{2n}} \rangle = \left.\frac{\partial^{2n}}{\partial j_{i_1} \ldots \partial j_{i_{2n}}}\right|_{j=0} Z[j]\,.$$
Evaluate explicitly the two- and four-point correlation functions $\langle \varphi_{i_1}\varphi_{i_2}\rangle, \langle \varphi_{i_1}\varphi_{i_2}\varphi_{i_3}\varphi_{i_4}\rangle$.
4. Prove that all only non-vanishing correlation functions contain an even number of random variables. Furthermore show that higher order correlation function can be related to two-point function via
$$\langle \varphi_{i_1} \ldots \varphi_{i_{2n}} \rangle = \langle \varphi_{i_1}\varphi_{i_2}\rangle \langle \varphi_{i_3}\varphi_{i_4}\rangle \ldots \langle \varphi_{i_{2n-1}}\varphi_{i_{2n}}\rangle + \text{ permutations}\,.$$

Problem 8.2 *cubic anisotropy*
Consider the modified Landau-Ginzburg Hamiltonian

$$\beta\mathcal{H} = \bar{\mathcal{H}} = \int \mathrm{d}^d x \left\{ \sum_{i=1}^{M} \left[\frac{c}{2}\left(\vec{\nabla}\varphi_i\right)^2 + \frac{r}{2}\varphi_i^2\right] + u(\sum_{i=1}^{M}\varphi_i^2)^2 + v\sum_{i=1}^{M}\varphi_i^4 \right\}$$

for an M-component vector $\varphi_i(\vec{x}), i = 1, \ldots M$. The term $v\sum_{i=1}^M \varphi_i^4$ generates a *cubic anisotropy.*

1. Mean-field theory:

(a) The anisotropy breaks roatiational symmetry. Find the optimal direction for a fixed magnitude $\sum_{i=1}^{M} \varphi_i^2$ for $v > 0$ and for $v < 0$? What is the degeneracy of the easy magnetization axes in each direction?

(b) Provide conditions for the stability of the mean-field solution in the u–v plane.

(c) In general higher order terms, e.g. $w \left(\sum_{i=1}^{M} \varphi_i^2\right)^3$ with $w > 0$, ensure stability in the regions not allowed from part b). Sketch a phase diagram in the r–v plane for fixed $u > 0$ and indicate the ordered phases and nature of the phase transitions.

(d) Are there any Goldstone modes in the ordered phases?

2. ϵ-expansion: Perform a perturbation expansion up to second order, and inspect the resulting diagrams.

(a) Show that the first order correction yields recursion relations

$$\begin{aligned}
\frac{\mathrm{d}r}{\mathrm{d}\ell} &= (d + 2\zeta)r + 4A[u(M+2) + 3v] + \mathcal{O}(u^2, uvv^2, \ldots)\,, \\
\frac{\mathrm{d}c}{\mathrm{d}\ell} &= (d - 2 + 2\zeta)c + \mathcal{O}(u^2, uv, v^2, \ldots)\,,
\end{aligned}$$

where

$$A = \int_p^{>} \frac{1}{r + cp^2} = \frac{1}{c} K_d \Lambda^{d-2} \mathrm{d}\ell + \mathcal{O}(r)$$

Assume that the non-trivial fixed point are $\mathcal{O}(\epsilon)$ where $\epsilon = 4 - d$ to conclude that

$$\zeta = \frac{2-d}{2} + \mathcal{O}(\epsilon^2)\,.$$

The parameter c may then kept fixed at unity, $c = 1$.

(b) The second order perturbation yields the recursion relation for the couplings. Using the results derived so far show that

$$\begin{aligned}
\frac{\mathrm{d}u}{\mathrm{d}\ell} &= \epsilon u - 4u^2(M+8)K_4 - 24uvK_4 + \mathcal{O}(\epsilon^3)\,, \\
\frac{\mathrm{d}v}{\mathrm{d}\ell} &= \epsilon v - 36v^2K_4 - 48uvK_4 + \mathcal{O}(\epsilon^3)\,.
\end{aligned}$$

(c) Find all fixed points in the u–v plane, and draw the flow patterns for $M < 4$ and $M > 4$. Discuss the relevance of the cubic anisotropy term near the stable fixed point in each case. Calculate the exponent ν at the stable fixed point for the cases $M < 4$ and $M > 4$.

(d) Is the region of stability in the u–v plane calculated within mean-field approximation enhance or diminished by inclusion of fluctuations? Since in reality higher order terms will be present, what does this imply about say the nature of the phase transition for a small negative v and $M > 4$.

(e) Sketch schematic phase diagrams in the r–v plane for $M > 4, M < 4$ and $u > 0$, identifying the ordered phases. Are there Goldstone modes in any of these phases close to the phase transition?

Solution 8.1

Gaussian variables

$$P[\varphi] = \frac{1}{\sqrt{(2\pi)^N \det A}} \exp\left(-\frac{1}{2}\,\varphi^T \cdot A^{-1} \cdot \varphi\right)\,,$$

1. Normalization. Since A is real symmetric positive definite, there is a rotation matrix R, i.e. $R \cdot R^T = R^T \cdot R = \mathbb{I}$, such that

$$R \cdot A \cdot R^T = D = \text{diag}\,[\lambda_1, \ldots, \lambda_N]$$

where all eigenvalues are real and positive $\lambda_i > 0$. In particular, $\det A = \det D = \prod_{i=1}^N \lambda_i$. Consequently

$$D^{-1} = (R^T \cdot A \cdot R)^{-1} = R^{-1} \cdot A^{-1} \cdot (R^T)^{-1} = R^T \cdot A^{-1} \cdot R$$

Then substitution $\varphi = R \cdot \psi$ leaves the measure invariant, since $|\det R| = 1$,

$$\begin{aligned}
\int [\mathrm{d}\varphi] P[\varphi] &= \frac{1}{\sqrt{(2\pi)^N \det A}} \int [\mathrm{d}\varphi] \exp\left(-\frac{1}{2}\,\varphi^T \cdot A^{-1} \cdot \varphi\right) \\
&= \frac{1}{\sqrt{(2\pi)^N \det A}} \int [\mathrm{d}R \cdot \psi] \exp\left(-\frac{1}{2}\,(R \cdot \psi)^T \cdot A^{-1} \cdot R \cdot \psi\right) \\
&= \frac{1}{\sqrt{(2\pi)^N \det D}} \int [\mathrm{d}\psi] \exp\left(-\frac{1}{2}\,\psi^T \cdot D^{-1} \cdot \psi\right) \\
&= \prod_{i=1}^N \int \frac{\mathrm{d}\psi_i}{\sqrt{2\pi\lambda_i}} \mathrm{e}^{-\psi_i^2/2\lambda_i} = 1
\end{aligned}$$

2. The generating functional

$$\begin{aligned}
Z[j] &= \langle \exp\left(j^T \cdot \varphi\right) \rangle \\
&= \int [\mathrm{d}\varphi]\ P[\varphi]\ \exp\left(j^T \cdot \varphi\right) \\
&= \frac{1}{\sqrt{(2\pi)^N\ \det A}} \int [\mathrm{d}\varphi] \exp\left(-\frac{1}{2}\,\varphi^T \cdot A^{-1} \cdot \varphi + \frac{1}{2} j^T \cdot \varphi + \frac{1}{2} \varphi^T \cdot j\right) \\
&= \frac{1}{\sqrt{(2\pi)^N\ \det A}} \int [\mathrm{d}\varphi] \exp\left(-\frac{1}{2}\,(\varphi^T - j^T \cdot A) \cdot A^{-1} \cdot (\varphi - A \cdot j) + \frac{1}{2}\, j^T \cdot A \cdot j\right) \qquad \text{note: } A = A^T \\
&= \frac{1}{\sqrt{(2\pi)^N\ \det A}} \int [\mathrm{d}\tilde\varphi] \exp\left(-\frac{1}{2}\,(\tilde\varphi^T \cdot A^{-1} \cdot \tilde\varphi + \frac{1}{2}\, j^T \cdot A \cdot j\right) \qquad \text{substitute } \tilde\varphi = \varphi - A \cdot j \\
&= Z[0] \exp\left(\frac{1}{2}\, j^T \cdot A \cdot j\right)
\end{aligned}$$

Since by normalization $Z[0] = 1$,

$$Z[j] = \exp\left(\frac{1}{2}\, j^T \cdot A \cdot j\right)$$

3. Correlation functions are then readily obtain by taking appropriate derivatives

$$\langle \varphi_{i_1} \ldots \varphi_{i_{2n}} \rangle = \left.\frac{\partial^{2n}}{\partial j_{i_1} \ldots \partial j_{i_{2n}}}\right|_{j=0} Z[j]$$

Obvious by construction.

The two-point correlation function

$$\langle \varphi_{i_1} \varphi_{i_2} \rangle = \left.\frac{\partial^2}{\partial j_{i_1} \partial j_{i_2}}\right|_{j=0} Z[j]$$

$$
\begin{aligned}
&= \left.\frac{\partial^2}{\partial j_{i_1}\partial j_{i_2}}\right|_{j=0} \exp\left(\frac{1}{2}\sum_{k,l} j_k A_{kl} j_l\right) \\
&= \left.\frac{\partial}{\partial j_{i_2}}\right|_{j=0} A_{i_1 l} j_l \exp\left(\frac{1}{2}\sum_{k,l} j_k A_{kl} j_l\right) \\
\langle \varphi_{i_1}\varphi_{i_2}\rangle &= A_{i_1 i_2}
\end{aligned}
$$

Similarly

$$
\begin{aligned}
\langle \varphi_{i_1}\varphi_{i_2}\varphi_{i_3}\varphi_{i_4}\rangle &= \left.\frac{\partial^4}{\partial j_{i_1}\partial j_{i_2}\partial j_{i_3}\partial j_{i_4}}\right|_{j=0} \exp\left(\frac{1}{2}\sum_{k,l} j_k A_{kl} j_l\right) \qquad \text{expand exponential} \\
&= \frac{\partial^4}{\partial j_{i_1}\partial j_{i_2}\partial j_{i_3}\partial j_{i_4}} \frac{1}{2!}\left(\frac{1}{2}\sum_{k,l} j_k A_{kl} j_l\right)^2 \\
&= \frac{\partial^3}{\partial j_{i_2}\partial j_{i_3}\partial j_{i_4}} \left(\sum_l A_{i_1 l} j_l\right)\left(\frac{1}{2}\sum_{m,n} j_m A_{mn} j_n\right) \\
&= \frac{\partial^2}{\partial j_{i_3}\partial j_{i_4}} \left[A_{i_1 i_2}\left(\frac{1}{2}\sum_{m,n} j_m A_{mn} j_n\right) + \left(\sum_l A_{i_1 l} j_l\right)\left(\sum_n A_{i_2 n} j_n\right)\right] \\
&= \frac{\partial}{\partial j_{i_4}} \left[A_{i_1 i_2}\sum_n A_{i_3 n} j_n + A_{i_1 i_3}\sum_n A_{i_2 n} j_n + \left(\sum_l A_{i_1 l} j_l\right) A_{i_2 i_3}\right] \\
&= A_{i_1 i_2}A_{i_3 i_4} + A_{i_1 i_3}A_{i_2 i_4} + A_{i_1 i_4}A_{i_2 i_3} \\
\langle \varphi_{i_1}\varphi_{i_2}\varphi_{i_3}\varphi_{i_4}\rangle &= \langle \varphi_{i_1}\varphi_{i_2}\rangle\langle \varphi_{i_3}\varphi_{i_4}\rangle + \langle \varphi_{i_1}\varphi_{i_3}\rangle\langle \varphi_{i_2}\varphi_{i_4}\rangle + \langle \varphi_{i_1}\varphi_{i_4}\rangle\langle \varphi_{i_2}\varphi_{i_3}\rangle
\end{aligned}
$$

4. The general case is known as Wick's theorem in quantum field theory or gaussian moment theorem in probability theory.

a) Since the Taylor expansion of $Z[j] = \exp(\frac{1}{2}\, j^T \cdot A \cdot j)$ is even in j only even-number correlation function are non-vanishing.

b) For the $2n$-point correlation function, only a single term of the Taylor expanded exponential survives

$$
\langle \varphi_{i_1}\varphi_{i_2}\dots\varphi_{i_{2n-1}}\varphi_{i_{2n}}\rangle = \frac{\partial^{2n}}{\partial j_{i_1}\dots\partial j_{i_{2n}}}\frac{1}{n!}\left(\frac{1}{2}\, j^T \cdot A \cdot j\right)^n
$$

Differentiating the polynomial yields $(2n)!$ terms, each being of the desired form but with a prefactor of $1/2^n n!$. However this factor is canceled since this is precisely the combinatorial factor of how many times a particular contraction occurs.

For example, take the term $A_{i_1 i_2}A_{i_3 i_4}\dots A_{i_{2n-1}i_{2n}}$. For the first derivative $\partial/\partial j_{i_1}$, I can pick any of the n factors, additionally I have the freedom to pick first or the second j. To obtain the desired contraction, there is no choice for $\partial/\partial j_{i_2}$. For the derivative $\partial/\partial j_{i_3}$ there is the remaining choice of $(n-1)$ factors, with residual freedom of factor 2, etc. Thus each particular contraction is produced exactly $2^n n!$ times cancelling the prefactor.

It is important to realize that the total number of terms does not change even if some of the indices are the same

$$
\begin{aligned}
\langle \varphi_1\varphi_2\varphi_2\varphi_4\rangle &= \langle \varphi_1\varphi_2\rangle\langle \varphi_2\varphi_4\rangle + \langle \varphi_1\varphi_2\rangle\langle \varphi_2\varphi_4\rangle + \langle \varphi_1\varphi_4\rangle\langle \varphi_2\varphi_2\rangle \\
&= 2\langle \varphi_1\varphi_2\rangle\langle \varphi_2\varphi_4\rangle + \langle \varphi_1\varphi_4\rangle\langle \varphi_2^2\rangle
\end{aligned}
$$

Solution 8.2

The cubic anisotropy is breaks the rotational symmetry

$$
\bar{\mathcal{H}} = \int \mathrm{d}^d x \left\{\sum_{i=1}^M \left[\frac{c}{2}\left(\vec{\nabla}\varphi_i\right)^2 + \frac{r}{2}\varphi_i^2\right] + u(\sum_{i=1}^M \varphi_i^2)^2 + v\sum_{i=1}^M \varphi_i^4\right]
$$

A question one would like to answer with this model is whether the fluctuations can restore the full symmetry. We shall see that this may actually be the case

1. Mean-field theory: First we assume that $\varphi_i(\vec{x}) = const.$ is spatially homogeneous.

a) For fixed magnitude $\sum_{i=1}^{M} \varphi_i^2 = m^2$, the first two terms are independent of the direction of φ_i in the M-dimensional order parameter-space. Hence we have to minimize the anistropy term only. With a Lagrange parameter

$$\frac{\partial}{\partial \varphi_k} \left[v \sum_{i=1}^{M} \bar{\varphi}_i^4 - \lambda \left(\sum_{i=1}^{M} \bar{\varphi}_i^2 - m^2 \right) \right] = 4v\bar{\varphi}_k^3 - 2\lambda \bar{\varphi}_k = 0$$

Thus $\varphi_i = \pm\lambda/2v$ or zero for each component. For $v > 0$ the minimum correspond to aligning the magnetization diagonally along the cubic axis

$$\bar{\varphi} = \frac{m}{\sqrt{M}}(\pm 1, \pm 1, \ldots, \pm 1)$$

Obviously, there are 2^M equivalent minima.

For $v < 0$ it is favorable to maximize the alignment.

$$\bar{\varphi} = m(\pm 1, 0, \ldots, 0)$$

with a $2M$ equivalent minima.

b) The mean-field function for $v > 0$ then yields

$$\mathcal{H}_{\mathrm{MF}} = V \left[\frac{r}{2} m^2 + (u + v/M) m^4 \right] \qquad \text{stable for } u + v/M > 0$$

For $v < 0$

$$\mathcal{H}_{\mathrm{MF}} = V \left[\frac{r}{2} m^2 + (u + v) m^4 \right] \qquad \text{stable for } u + v > 0$$

Phase diagram in the r–v plane.

c) First, $v < 0$. Take the 1-direction as the ordered one with

$$m^2 = -r/2(u + v),$$

To quadratic order in the transverse fields

$$\bar{\mathcal{H}} = \int \mathrm{d}^d x \left\{ \sum_{i=2}^{M} \left[\frac{c}{2} \left(\vec{\nabla} \varphi_i \right)^2 + \frac{r}{2} \varphi_i^2 \right] + u m^2 \sum_{i=2}^{M} \varphi_i^2 \right]$$

Hence

$$\langle \varphi_2(\vec{q}_1) \varphi_2(\vec{q}_2) \rangle = (2\pi)^d \delta(\vec{q}_1 + \vec{q}_2) \frac{1}{r + cq^2 + 2um^2} = \frac{1}{r + cq^2 - ur/(u + v)} = \frac{1}{cq^2 + v|r|/(u + v)}$$

which implies massive modes. A similar consideration holds for $v > 0$.