Lecture 2: Study of Fluctuations.

From the results deduced previously relating the missing long-range order in $D=1$, one realizes that the emergence possibilities of qualitative changes in many-body systems depend on quite general quantities like the dimension D. At the moment one has information only about $D=1$: so we would like to understand $D>1$, furthermore, we would like to properly understand what is the clear physical reason for the observed behavior. But we realize that the Landau's manner to approach the problem cannot be extended to $D>1$ (for example in $D=2$, the $D=1$ touching points become arbitrary shape modifying touching closed curves). So we need something else for the study. This is the reason why we start to analyze the effect of fluctuations.

I. Fluctuations in the thermodynamic potential

Let us have X_i, $i=\overline{1,n}$ local vectorial quantities of the system described by the thermodynamic potential Φ (for example lattice site positions). Since the system's behavior will depend on the set $\{X_i\}$ one has

$$\Phi = \Phi(X_1, X_2, \dots X_n) \tag{20}$$

Now let X_i^e = the value of X_i at equilibrium, and let us denote by X_i the actual value of the parameter under discussion. In this case, a local fluctuation measured relative to the equilibrium value becomes

$$y_i = \Delta X_i^e = X_i - X_i^e \tag{21}$$

Now we fix the origine of the X_i variable to X_i^o, and we measure the fluctuation relative to X_i^o. In this case the local fluctuation becomes y_i (y_i bar):

$$y_i = \Delta X_i = X_i - X_i^o = \underbrace{(X_i - X_i^e)}_{y_i} - \underbrace{(X_i^o - X_i^e)}_{\langle y_i \rangle} = y_i - \langle y_i \rangle \tag{22}$$

where $\langle y_i \rangle$ represents the average of the local fluctuation y_i measured from the origine.

The thermodynamic potential at equilibrium becomes

$$\Phi_o = \Phi_o(X_1^e, X_2^e, \dots X_n^e), \tag{23}$$

and if we introduce fluctuations in the system, relatively close to the equilibrium state, the modification in Φ becomes

$$\Delta\Phi = \Phi - \Phi_o = \frac{1}{2}\sum_{ij} p_{ij}\, y_i\, y_j = \frac{1}{2}\sum_{ij} p_{ij}\,(y_i - \langle y_i \rangle)(y_j - \langle y_j \rangle) \tag{24}$$

We consider anisotropic system, so the matrix p_{ij} is symmetric, $1/2$ emerges because the double sum is not restricted, the first order term is missing because Φ_o is a minimum of Φ (in the taylor expansion of Φ the first order terms = first order derivatives are zero), and

we stopped in Eq(24) the expression at second order (neglecting higher orders) because we are now interested only in the leading terms.

II The average of a product of fluctuations.

Since in Eq(24) (and other further quantities) averages occur, we are now interested to calculate average values. A fluctuation $\Delta\Phi$ appears usually with a probability density $w = A\exp\left[-\frac{\Delta\Phi}{k_BT}\right]$. I note that since $\Delta\Phi$ is bilinear in the random variables y_i, and a bilinear form always can be transformed in a quadratic expression by a linear transformation, it means that w follows in fact a normal (i.e. Gaussian) distribution. Furthermore the average value (arithmetic mean) of independent random variables (with well defined expected value and variance — namely $\langle(x-\langle x\rangle)^2\rangle$ —) and a sufficiently large number of iterates, given by the central limit theorem, will be normally distributed. Hence, considering y_i independent variables, the w expression is rather acceptable. and highly

Now if w is given, the average of an arbitrary quantity M becomes

$$\langle M\rangle = \int w M\, d\tau \;;\quad d\tau = dy_1 dy_2 \dots dy_n \tag{25}$$

Using Eq(25) for y_j, one finds

$$\langle y_j\rangle = A\int y_j\, e^{-\frac{\Delta\Phi}{k_BT}}\, d\tau \;;\quad \text{where } A \text{ is a normalisation constant} \tag{26}$$

In the following step one calculates the derivative of Eq.(25) in function of $\langle y_k\rangle$, and one finds:

$$\delta_{jk} = A\int y_j\left[\frac{\partial}{\partial\langle y_k\rangle} e^{-\frac{\Delta\Phi}{k_BT}}\right] dy_1 \dots dy_n \tag{27}$$

Calculating the derivative in the right hand side, we find:

$$\frac{\partial}{\partial\langle y_k\rangle} e^{-\frac{\Delta\Phi}{k_BT}} = \frac{\partial}{\partial\langle y_k\rangle} e^{-\frac{1}{2k_BT}\sum_{i,\ell}\beta_{i\ell}(y_i-\langle y_i\rangle)(y_\ell-\langle y_\ell\rangle)} =$$

$$= 2\left(-\frac{1}{2k_BT}\right)(-1)\left(\sum_i \beta_{ik}(y_i-\langle y_i\rangle)\right) e^{-\frac{\Delta\Phi}{k_BT}}, \tag{28}$$

where only the $i=k$ and $\ell=k$ cases provide contributions, and since $\beta_{ij}=\beta_{ji}$, the result will be 2 times the value for the $\ell=k$ case.

From (27-28) we find

$$\delta_{jk} = \frac{1}{k_BT}\int y_j\left(\sum_i \beta_{ik}(y_i-\langle y_i\rangle)\right)\underbrace{\left(Ae^{-\frac{\Delta\Phi}{k_BT}}\right)}_{w} d\tau$$

$$= \frac{1}{k_BT}\sum_i\left[\int y_j y_i\, w\, d\tau - \left(\int y_j w\, d\tau\right)\langle y_i\rangle\right]\beta_{ik}. \tag{29}$$

Equation (29) gives :

(30) $\delta_{jk} = \frac{1}{K_B T} \sum_i \left[\langle y_j y_i \rangle - \langle y_j \rangle \langle y_i \rangle \right] \beta_{ik}$;

But now one realizes that the origine of a system of coordinates can be taken everywhere. Hence one chooses $X_i^0 = X_i^e$, i.e $\langle y_i \rangle = 0, \forall i$, and using the Einstein convention (two repeated index represent a sumation over that index, we find

(31) $K_B T \delta_{jk} = \sum_i \langle y_j y_i \rangle \beta_{ik} = \langle y_j y_i \rangle \beta_{ik}$

On the right side of (31) one has a matrix product between the matrix $\langle \tilde{y_j y_i} \rangle$, and the matrix $\tilde{\beta}_{ij}$, while in the left hand side one has the unity matrix $\tilde{\delta}_{ij}$. The obtained result than can be written as (tilde denotes here the matrix):

(32) $\langle \tilde{y_i y_j} \rangle = K_B T \frac{\tilde{\delta}_{ij}}{\tilde{\beta}_{ij}}$; or, taking into account that precisely a matrix division is present on the right hand side, usually is written:

(33) $\langle y_i y_j \rangle = K_B T \frac{\delta_{ij}}{\beta_{ij}}$; So the central result of this paragraph is as follows:

> For $\Delta\Phi = \frac{1}{2} \sum_{ij} \beta_{ij} y_i y_j$, hence $w = A \exp\left[-\frac{1}{2K_B T} \sum_{ij} \beta_{ij} y_i y_j \right]$
> one has $\langle y_i y_j \rangle = K_B T \frac{\delta_{ij}}{\beta_{ij}}$

The obtained result has the importace to give the expectation value of a product of two local fluctuations directly from the value of $\Delta\Phi$ (taking β_{ij} from there)

III $\Delta\Phi$ expressed in κ-space.

One started the calculations in $\vec{r}$ space (direct geometrical space), and now one continues it in $\vec{\kappa}$ space (the reciprocal space). The use of the Fourier transformed variable has several advantages. For example a differential equation in $\vec{r}$ variable becomes algebraic equation in $\vec{\kappa}$ variable, etc.

In order to turn in $\vec{\kappa}$ space, we first transform the discret position $\vec{r}_i$ (specifying y_i) in a continuous variable $\vec{r}$, hence X_i becomes now $X(\vec{r})$, and the local fluctuation y_i turns in $y(\vec{r}) = \Delta X(\vec{r})$. One thinks about $X(\vec{r})$ as an arbitrary characteristic density function of the system (e.g. mass density, charge density, magnetic moment density...) In such situation one has also a thermodynamic potential density $\bar{\Phi}(\vec{r})$, and the true thermodynamic potential becomes $\Phi = \int \bar{\Phi}(r)\, dV$.

In such conditions the variation of the thermodynamic potential given by fluctuations becomes

(34) $$\Delta\Phi = \int(\bar{\Phi} - \bar{\Phi}_0)dV$$

where $\bar{\Phi}_0$ corresponds to the equilibrium value of $X(\vec{r}) = X^0(\vec{r})$, while $\bar{\Phi}$ corresponds to the actual value of $X(\vec{r})$. Following the expression $\Delta\Phi = \frac{1}{2}\sum_{ij} \beta_{ij} y_i y_j$ used previously, similarly now one has for densities $\Delta\bar{\Phi} = \bar{\Phi} - \bar{\Phi}_0$, where

$$\bar{\Phi} = \bar{\Phi}_0 + \frac{1}{2}\sum_{\alpha\beta} y_\alpha(\vec{r}_1) y_\beta(\vec{r}_2) \frac{\partial^2\bar{\Phi}}{\partial y_\alpha(\vec{r}_1)\partial y_\beta(\vec{r}_2)} \quad ; \quad (35)$$

where we stop the Taylor expression at second order because we are interested in the leading contributions, furthermore the first order terms are missing from (35) because we are placed around a minimum ($\bar{\Phi}_0$), and hence $\partial\bar{\Phi}/\partial y_\alpha = 0$. We note that in (35), the indices α, β denote the vector components of the "vectorial" fluctuation $y(\vec{r})$ (by considering it for generality, a vector). Now one expands the $y_\alpha(\vec{r})$ function in Fourier sum:

(36) $$y_\alpha(\vec{r}) = \sum_{\vec{k}} y_{\alpha\vec{k}} e^{i\vec{k}\cdot\vec{r}} \quad ,$$

and one denotes $\varphi_{\alpha\beta}(\vec{r}_1,\vec{r}_2) = \dfrac{\partial^2\bar{\Phi}}{\partial y_\alpha(\vec{r}_1)\partial y_\beta(\vec{r}_2)}$, obtaining from (35)

(37) $$\bar{\Phi} = \bar{\Phi}_0 + \frac{1}{2}\sum_{\alpha\beta}\sum_{\vec{k}_1,\vec{k}_2} y_\alpha(\vec{k}_1) y_\beta(\vec{k}_2) e^{i\vec{k}_1\cdot\vec{r}_1 + i\vec{k}_2\vec{r}_2} \varphi_{\alpha\beta}(\vec{r}_1,\vec{r}_2) .$$

But one considers a homogeneous and isotropic system, hence all dependences in geometrical positions must be given by $\vec{r} = \vec{r}_1 - \vec{r}_2$. This means that from the $\vec{k}_2$ sum only $\vec{k}_2 = -\vec{k}_1$ survives, and $\varphi_{\alpha\beta}(\vec{r})$ emerges. Only one $\vec{k}$ vector sum remains ($\vec{k} = \vec{k}_1$), and one obtains

(38) $$\bar{\Phi} = \bar{\Phi}_0 + \frac{1}{2}\sum_{\alpha\beta}\sum_{\vec{k}} y_{\alpha\vec{k}} y_{\beta,-\vec{k}} e^{i\vec{k}\cdot\vec{r}} \varphi_{\alpha\beta}(\vec{r}) .$$

Introducing (38) in (34) one finds

(39) $$\Delta\Phi = \int(\bar{\Phi} - \bar{\Phi}_0)d^3r = \frac{1}{2}\sum_{\alpha\beta}\sum_{\vec{k}} y_{\alpha\vec{k}} y_{\beta,-\vec{k}} \varphi_{\alpha\beta}(\vec{k}) \text{ , where}$$

(40) $$\varphi_{\alpha\beta}(\vec{k}) = \int e^{i\vec{k}\cdot\vec{r}} \varphi_{\alpha\beta}(\vec{r})\, d^3r .$$

At this moment we must observe some important properties of the Fourier components $y_{\alpha\vec{k}}$, namely:

i) since $y_\alpha(\vec{r})$ is real (is a physical fluctuation in the density $X(\vec{r})$):

(41) $$y_\alpha(\vec{r}) = \sum_{\vec{k}} y_{\alpha\vec{k}} e^{i\vec{k}\cdot\vec{r}}$$
$$y^*_\alpha(\vec{r}) = \sum_{\vec{k}} y^*_{\alpha\vec{k}} e^{-i\vec{k}\cdot\vec{r}} = \sum_{\vec{k}} y^*_{\alpha,-\vec{k}} e^{i\vec{k}\cdot\vec{r}} \quad (\vec{k}\to -\vec{k} \text{ since the } \vec{k} \text{ domain is symmetric})$$

Consequently, since $y_\alpha(\vec{r}) = y^*_\alpha(\vec{r}) \Rightarrow$ $$y_{\alpha\vec{k}} = y^*_{\alpha,-\vec{k}} \quad ; \quad (42)$$

ii) the system is also isotropic, i.e. $\gamma_\alpha(\vec{r}) = \gamma_\alpha(-\vec{r})$, hence

(43)
$$\gamma_\alpha(\vec{r}) = \sum_{\vec{k}} \gamma_{\alpha\vec{k}}\, e^{i\vec{k}\cdot\vec{r}} ;$$
$$\gamma_\alpha(-\vec{r}) = \sum_{\vec{k}} \gamma_{\alpha\vec{k}}\, e^{-i\vec{k}\cdot\vec{r}} \underset{\vec{k}\to-\vec{k}}{=} \sum_{\vec{k}} \gamma_{\alpha,-\vec{k}}\, e^{i\vec{k}\cdot\vec{r}} ;$$

Consequently, since $\gamma_\alpha(\vec{r}) = \gamma_\alpha(-\vec{r}) \Rightarrow \gamma_{\alpha,\vec{k}} = \gamma_{\alpha,-\vec{k}}$; (44)

Hence one finides for real and isotropic system that also the Fourier components are real and isotropic.

(45): $\gamma_{\alpha\vec{k}} = \gamma_{\alpha,-\vec{k}} = \gamma^*_{\alpha,-\vec{k}}$

Using (45) and (39), we obtain for $\Delta\mathcal{O}$ in $\vec{k}$ space the expression:

(46) $$\boxed{\Delta\mathcal{O} = \frac{1}{2}\sum_{\alpha\beta}\sum_{\vec{k}} \gamma_{\alpha\vec{k}}\gamma_{\beta\vec{k}}\varphi_{\alpha\beta}(\vec{k})}$$

At this point an observation must be underlined. We will use (46) also by applying the deduced result in (33). But the deduction of (33) needs at least a double index (i, and j). The double index nature of (46) is preserved by α,β (i.e. the components of the vector $\gamma(\vec{r})$). Consequently, if the chacteristic dynamical variable of the system has only 1 component (e.g. is Ising spin), the relation (33) cannot be used in the context of (46).

III. The leading contribution in $\varphi_{\alpha\beta}(\vec{k})$:

In what will follows we are interested to deduce the leading contributions in $\varphi_{\alpha\beta}(\vec{k})$

i) The $\vec{k}\to 0$ limit: It is known that $\vec{k}\to 0$ corresponds to $\vec{r}\to\infty$ in Fourier transformed variables. But because long-range forces are considered missing $\varphi_{\alpha\beta}(\vec{r})$ for $|\vec{r}|\gg 1$ is zero. Consequently

(47) $$\lim_{|\vec{k}|\to 0} \varphi_{\alpha\beta}(\vec{k}) = 0$$

This means that if we use a Taylor expansion for $\varphi_{\alpha\beta}(\vec{k})$ as

(48) $$\varphi_{\alpha\beta}(\vec{k}) = a_0 + a_1\vec{k} + a_2\vec{k}^2 + \dots ,$$ then one has

(49) $$a_0 = 0 ;$$

ii) Linear $\vec{k}$ terms in $\varphi_{\alpha\beta}(\vec{k})$: From (40) linear $\vec{k}$ terms in $\varphi_{\alpha\beta}(\vec{k})$ arise from the $i\vec{k}\cdot\vec{r}$ term of the Taylor expansion of $e^{i\vec{k}\cdot\vec{r}} = 1 + i\vec{k}\cdot\vec{r} + \frac{1}{2}(i\vec{k}\cdot\vec{r})^2 + \dots$ This means that the coefficient a_1 in (48) is $a_1 \sim \int \vec{r}\,\varphi_{\alpha\beta}(\vec{r})\,d^3\vec{r}$. But given by the isotropy, $\varphi_{\alpha\beta}(\vec{r}) = \varphi_{\alpha\beta}(-\vec{r})$, hence a_1 is given by an integral over an odd function ($f(\vec{r}) = -f(-\vec{r})$) taken over an symmetric interval (domain $\vec{r}$), consequently: $a_1 = 0$; (50).

iii) κ^2 term in $\varphi_{\alpha\beta}(\vec{\kappa})$. Since $\varphi_{\alpha\beta}(\vec{\kappa}) = \int e^{i\vec{\kappa}\cdot\vec{r}} \varphi_{\alpha\beta}(\vec{r})\, d^3r$, see (40), κ^2 contribution in $\varphi_{\alpha\beta}(\vec{\kappa})$ is obtained from the $\frac{1}{2}(i\vec{\kappa}\cdot\vec{r})^2$ contribution of the Taylor expansion of $e^{i\vec{\kappa}\cdot\vec{r}}$. This provides the

(51) $$\int \tfrac{1}{2}(i\vec{\kappa}\cdot\vec{r})\varphi_{\alpha\beta}(\vec{r})\, d^3r = -\frac{1}{2}\int [\kappa_x^2 x^2 + \kappa_y^2 y^2 + \kappa_z^2 z^2]\varphi_{\alpha\beta}(\vec{r})\, dx\, dy\, dz$$

contribution in $\varphi_{\alpha\beta}(\vec{\kappa})$. Because of the isotropy the contributions in different $\vec{\kappa}$ directions must be the same, we obtain

(52) $$\varphi_{\alpha\beta}(\vec{\kappa}) = \underbrace{(\kappa_x^2+\kappa_y^2+\kappa_z^2)}_{\kappa^2}\Big[\underbrace{-\frac{1}{2}\int x^2 \varphi_{\alpha\beta}(\vec{r})\, dV}_{A_{\alpha\beta}}\Big] + \text{higher } \kappa \text{ orders}$$

Because $\varphi_{\alpha\beta}(\vec{r})\big|_{\vec{r}\to\infty} \to 0$, the coefficient $A_{\alpha\beta}$ is finite, and we obtain the leading contribution in $\varphi_{\alpha\beta}(\vec{\kappa})$ as:

(53) $$\boxed{\varphi_{\alpha\beta}(\vec{\kappa}) = \kappa^2 A_{\alpha\beta}}$$

which fixes the leading order contributions in $\varphi_{\alpha\beta}(\vec{\kappa})$ for small $\vec{\kappa}$ values, where $A_{\alpha\beta}$ is a finite coefficient.

The result in (53) can be written as

(54) $$\varphi_{\alpha\beta}(\vec{\kappa}_1,\vec{\kappa}_2) = \delta_{\vec{\kappa}_1,\vec{\kappa}_2}\varphi_{\alpha\beta}(\vec{\kappa}_1);\quad \varphi_{\alpha\beta}(\vec{\kappa}_1) = \kappa_1^2 A_{\alpha\beta};$$

which introduced in (46) gives

(55) $$\boxed{\Delta\phi = \frac{1}{2}\sum_{\alpha,\beta}\sum_{\vec{\kappa}_1,\vec{\kappa}_2} y_{\alpha\vec{\kappa}_1} y_{\beta\vec{\kappa}_2}\varphi_{\alpha\beta}(\vec{\kappa}_1,\vec{\kappa}_2)}$$

In this moment (33) directly can be used for (55) considering mathematically: $i=(\vec{\kappa}_1,\alpha)$; $j=(\vec{\kappa}_2,\beta)$, and one finds

(56) $$\langle y_{\alpha\vec{\kappa}_1} y_{\beta\vec{\kappa}_2}\rangle = k_B T\,\frac{\delta_{\vec{\kappa}_1,\vec{\kappa}_2}\delta_{\alpha\beta}}{\varphi_{\alpha\beta}(\vec{\kappa}_1,\vec{\kappa}_2)}$$

Now, because $\varphi_{\alpha\beta}(\vec{\kappa}_1,\vec{\kappa}_2)$ enters in the denominator of (56) we need the leading contributions of this function, taken as in (48) for small $\vec{\kappa}$ values (this are the smallest contributions in $\varphi_{\alpha\beta}(\vec{\kappa})$, but the highest contributions in (56). Exactly these contributions are expressed in (54), hence one finds

(57) $$\boxed{\langle y_{\alpha\vec{\kappa}_1} y_{\beta\vec{\kappa}_2}\rangle = \frac{k_B T}{A_{\alpha\beta}}\cdot\frac{\delta_{\vec{\kappa}_1,\vec{\kappa}_2}\delta_{\alpha\beta}}{\kappa_1^2}}$$

which is the main result of this paragraph (subsection).

IV The average of the square of local fluctuations.

Based on the mathematical background presented above, we would like to calculate how big the local fluctuations are in the system. Since $\langle y(\vec{r})\rangle$ is meaningless because even if $|y(\vec{r})|$ is big, given by sign alternations $\langle y(\vec{r})\rangle$ can be zero, one calculates below $\langle y^2(\vec{r})\rangle$. One has

$$(58)\quad \langle y^2(\vec{r})\rangle = \sum_\alpha \langle y_\alpha(\vec{r}) y_\alpha(\vec{r})\rangle = \sum_\alpha \langle y_\alpha(\vec{r}) y_\alpha^*(\vec{r})\rangle$$

because $y_\alpha(\vec{r}) = y_\alpha^*(\vec{r})$ is real. Now

$$(59)\quad y_\alpha(\vec{r}) = \sum_{\vec{k}} y_{\alpha\vec{k}} e^{i\vec{k}\cdot\vec{r}}\ ;\ y_\alpha^*(\vec{r}) = \sum_{\vec{k}} y_{\alpha\vec{k}}^* e^{-i\vec{k}\cdot\vec{r}} = \sum_{\vec{k}} y_{\alpha\vec{k}} e^{-i\vec{k}\cdot\vec{r}}$$

because $y_{\alpha\vec{k}} = y_{\alpha\vec{k}}^*$ is also real (isotropic and homogeneous system). Hence, using (58-59) one has

$$(60)\quad \langle y^2(\vec{r})\rangle = \sum_\alpha \sum_{\vec{k}_1,\vec{k}_2} \langle y_{\alpha\vec{k}_1} y_{\alpha\vec{k}_2}\rangle e^{i\vec{r}(\vec{k}_1-\vec{k}_2)}$$

But now, using (57), $\langle y_{\alpha\vec{k}_1} y_{\alpha\vec{k}_2}\rangle = \frac{K_B T}{A_{\alpha\alpha}} \frac{\delta_{\vec{k}_1,\vec{k}_2}}{k_1^2}$, and $e^{i\vec{r}(\vec{k}_1-\vec{k}_2)}\big|_{\vec{k}_1=\vec{k}_2} = 1$ one finds

$$(61)\quad \langle y^2(\vec{r})\rangle = K_B T \sum_\alpha \frac{1}{A_{\alpha\alpha}} \sum_{\vec{k}} \frac{1}{k^2}\ ;\ A = \sum_\alpha \frac{1}{A_{\alpha\alpha}} = \text{constant, one has}$$

$$(62)\quad \langle y^2(\vec{r})\rangle = A K_B T \sum_{\vec{k}} \frac{1}{k^2}\ ;$$

Now because $\sum_{\vec{k}} \to \int \frac{d^D k}{(2\pi)^D}$, where D = the dimension, where we continuized the $\vec{k}$ variable, one obtains

$$\boxed{(63)\quad \langle y^2(\vec{r})\rangle = A K_B T \int \frac{d^D k}{(2\pi)^D} \frac{1}{k^2}\ ;}$$

At this stage one observes that

i) The fluctuations we analyze are thermal. Indeed, if $T=0$ then everything is erased, and we find $\langle y^2(\vec{r})\rangle = 0$.

ii) $$\int d^D k = f_D \int_0^{k_{max}} k^{D-1} dk\ ;\quad (64)$$

Indeed $k_{max} \sim \frac{1}{a}$ where a is the particle diameter, and f_D is a D dependent constant. To see this: here $k = |\vec{k}|$,

$D=1$, $d^1k = dk$; $f_D = 1$;

$D=2$, $d^2k = k\,dk\,d\varphi \to 2\pi k\,dk$; $f_D = 2\pi$;

$D=3$, $d^3k = k^2 \sin\theta\, d\theta\, d\varphi\, dk \to 4\pi k^2 dk$; $f_D = 4\pi$;

$\vdots$

So one obtains

$$\boxed{(64)\ ;\ \langle y^2(\vec{r})\rangle = A f_D K_B T \int_0^{k_{max}} k^{D-3} dk}$$

Using (64), a dimension dependent analysis can be made about the magnitude of the average of the square of local fluctuations:

$$D=1: \int_0^{K_m} \frac{dK}{K^2} = -\frac{1}{K}\Big|_0^{K_m} = \frac{1}{\varepsilon}\Big|_{\varepsilon\to 0} - \frac{1}{K_m} \sim \lim_{\varepsilon\to 0}\frac{1}{\varepsilon}\,;\ \text{polynomial divergence}$$

$$(65)\quad D=2: \int_0^{K_m} \frac{dK}{K} = \ln K\Big|_{\varepsilon\to 0}^{K_m} = \ln\frac{K_m}{\varepsilon}\Big|_{\varepsilon\to 0}\,;\ \text{logaritmic divergence}$$

$$D=3: \int_0^{K_m} dK = K\Big|_0^{K_m} = K_m\,;\ \text{divergence is not present.}$$

IV.1 <u>The $D=1$ case</u>: now one understands why long-range order is missing from $D=1$ (in conditions underlined in Lecture 1). The reason is that local thermal fluctuations polynomially diverge and destroy the ordering tendencies.

Please note that $K\to 0$ (i.e. long wavelength) fluctuations cause the divergence and destroy the ordering tendencies ($\vec{K}$ as wave vector is $|\vec{K}|=\frac{2\pi}{\lambda}$).

IV.2 <u>The $D=2$ case</u>: Local thermal fluctuations also diverge, but the strength of the divergence is smaller: is only a logaritmical divergence. Please note:

i) The divergence occurs again at $K\to 0$, so again long wavelength fluctuations destroy the ordering tendencies.

ii) With the increase of the dimensionality D, the strength of the divergence decreases, and (in the presented case) disappears at $D=3$

iii) See the observation below Eq(46): the deduction is not valid when the characteristic dynamical variable of the system has only 1 component (e.g. Ising spin.), $n=1$; ($n=$ nr. of components of the dynamical variable.)

Now we are able to formulate our results in a rigorous manner relating the emergence of qualitative changes in 2D. Note that short range interaction (see III.L on pg 5.), and thermodinamic limit (Eq(33)) are further required:

B) In $D=2$, long range order is missing if we have short-range interactions, the number of components of the dynamical variable is higher than 1, and the many-body system at $T\neq 0$ is taken in the thermodynamic limit.

The fact that the long-range order is missing is only intuitively present in the deduction, since it was made through $\langle y(\vec{r}_1)y(\vec{r}_2)\rangle$, see (33). A rigorous demonstration will be made in the next lecture.

Examples illustrating the law B:

a) Ising $D=2$, $n=1$ case given by the Onsager's solution we know that is phase transition in the system.

b.) In $D=2$, $n=2$ there is a Kosterlitz-Thouless-Berezinskij phase transition in the system. But the ordering is not long-range order, is a topological order.

c.) If one has a week localization providing an insulating state (localization of carriers on closed curves). If we are not placed in the thermodynamic limit and the extension of the system is small such that the length of the system in one direction is smaller than the average extension of the closed curves, the system becomes conducting, so phase transition can occur.

d.) The Kac model with long-range interaction (1963):

$$U(r) = \begin{cases} \infty ; & r<r_0 \\ -\kappa e^{-\kappa r} ; & r>r_0 \end{cases}$$

in the $\kappa \to 0$ limit gives phase transition even in $D=1$

e.) I underline another aspect here namely: the here studied systems were buil up from points. But it is possible to buil up systems from geometric profiles: e.g. benzene hexagons, which are extremely stable profiles. (providing for example graphene). The ordering in systems build up from dots, and ordering in systems with stable profiles is different.

iii) The $D=3$ case. This is the first dimensionality where local thermal fluctuations not diverge. This is the genuine domain of the long-range order.

iv) Increasing D: The fluctuations become more and more unimportant. Since fluctuations and correlation effects (as you are going to see further on) go hand in hand, for $D \to \infty$, since correlation effects become negligible, the behavior becomes of mean-field type.

Lower and upper critical dimension

Exceeding now the frame of the long range order, for any type of ordering, by increasing D, fluctuations decrease. In low dimensions they are huge, destroy the ordering tendencies, but by increasing D, the ordering can appear.

Now let us fix an arbitrary kind of order. The lowest D where it appears is called the lower critical dimension of the studied ordering. For example for the standard Ising model the lowest critical dimension is 2. ($D_c=2$)

Now if we increase D, we rich a value where the transition to the studied ordering becomes of mean-field type (i.e. can be described by mean field.) This is the upper critical dimension Du. For exemple in the standard Ising model case it is known that in D=5 the transition is of mean-field type (see G. Parisi et al. Phys. Rev B54, R3698 (1996)), so Du = 4 or 5.

Fig. 6

As a consequence the genuine existence region for a given ordering (with its own properties) is placed in between: $D \in [De, Du]$.

The notion of continuous phase transitions.

In order to put together de obtained restrictions relating the forbidments of the long rauge order in D=1,2, notions, we need information relating continuous phase transitions (which will be analysed in details in the following lectures.)

Let us concentrate on the second order phase transitions In this case Φ and Φ' are continuous so completely smooth function (note that in quantum mechanics for exaimple the smooth nature of Ψ is preserved by the continuous nature of Ψ and Ψ', since in this case even the cusp points are missing from the plot of the function). This means that during a phase transition Φ remains continuous and even a cusp point is missing during the qualitative change in the system. Than the following question arises: what is changing then during a such kind of transition?

First, such type of phase transitions during which Φ is a completely smooth are called continuous transitions.

Second, the unique property that can be changed during the continuous transition is the symmetry. Indeed if one has in 2D a system with square symmetry and smooth, continuously, and infinitely slowly, the A and B sites move infinitesimally, the symmetry suddently change in an axial symmetry.

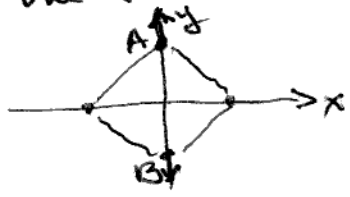

Fig. 7

Consequently, during each continuous phase transition (a second order phase transition in the Ehrenfest's notation) a given symmetry changes. This is called symmetry breaking. The high temperature phase is completely disordered and has the highest symmetry. The ordered phase has smaller symmetry (this emerges when T decreases, the symmetry breakin appears at transition).

Consequently each continuous phase transition has its symmetry breaking. E.g. at paramagnet → ferromagnet transition the full rotation symmetry is breaking; at para → antiferro transition the sublattice full rotation symmetry is breaking; at the superconducting transition the gauge symmetry is breaking; etc.

Spontaneous transitions:

The phase transitions discussed till now were all spontaneous transitions. This simply means that the qualitative change in the system is produced by the system itself and is not caused by an exterior action. Note that most transitions can be caused also by an properly chosed external field. For example on a system with magnetic moments if we apply an external magnetic field we align the moments and we produce a ferromagnetic state. But in this case the ferromagnetism not emerges via a genuine phase transition, it emerges given by an external action (external magnetic field). Such transitions are named non-spontaneous. If the phase transition under discussion is a continuous phase transition, that a spontaneous transition cause in this case a „spontaneous symmetry breaking".

The Mermin-Wagner theorem:

Now we have the sufficient background in order to discuss the Mermin-Wagner theorem. This was deduced and formulated by David Mermin, Herbert Wagner and Pierre Hohenberg in Statistical Physics, and Sidney Coleman in Field theory.

Let us consider our deduced statements A and B for continuous phase transitions. Now if we would like to formulate in common the statements A and B (i.e D=1 and D=2 together) we must elliminate the Ising case from the statement B connected to D=2. The Ising case means discrete spins which has discrete rotation symmetry, i.e the spin cannot be rotated with arbitrary angle. This means that if we consider „continuous symmetry breaking" than the statements A and B can be formulated together. This is the Mermin-Wagner theorem which looks as follows:

In $D \leq 2$, at $T \neq 0$, thermodynamic limit, and in the presence of short-range interactions in the many-body system, continuous symmetry cannot be spontaneously broken.

We already know that long wavelength ($\kappa \to 0$) fluctuation cause this. If we treat quantum mechanically the problem, the quasiparticles connected to coherent fluctuation when the continuous symmetry breaks will be bosons, and since ε monotonically increases with κ, $\kappa \to 0$ will have $\varepsilon \to 0$ meaning. So in this „language" the ordering cannot appear since the fluctuations which destroy the ordering can be generated by infinitesimally small energy values. For small κ values the $\varepsilon(\kappa)$ function in his Taylor expansion $\varepsilon(\kappa) = a_0 + a_1\kappa + a_2\kappa^2 + \dots$ (with $a_0 = 0$) will have $\varepsilon(\kappa) \sim \kappa$ leading term, and the bosons which emerge are called Goldston bosons. Since $\kappa \to 0$ gives $\varepsilon \to 0$ these are called massless bosons in field theory. The name is comming from the relativistic energy: $\varepsilon = \sqrt{(\hbar\kappa c)^2 + m_0^2 c^4}$ where m_0 is the rest mass. Acording to this, if $\kappa \to 0$ leads to $\varepsilon \to 0$, rest mass is not present, and the particle is called massless. The Goldston bosons are not rare in nature. The acustical phonons $\varepsilon \sim \kappa$ are the Goldston bosons which appear when the continuous translational symmetry of the system breaks down when the lattice is formed (this has only discrete „Bravais" translational symmetry).

Furthermore photons $\varepsilon = cp = c\hbar\kappa$ are the massless bosons (quasiparticles) of the electromagnetic field. The bosons which are the force carriers of the basic interactions are named „gauge bosons". (Maxwell theory is gauge invariant $\vec{A} \to \vec{A} + \operatorname{grad} f$; $V \to V - \frac{\partial f}{\partial t}$.) Similarly the $W^{\pm}$, Z gauge bosons mediate the weak interaction.

The Higgs Mechanism (Peter Higgs, Nobel prize 2013)

Let us now consider the case when besides a continuous symmetry, also a gauge (nonlocal gauge) symmetry is broken. This means that (in charged case) superconducting condensate appears, the energy becomes $\varepsilon = \sqrt{E^2(\kappa) + \Delta^2}$; $E(\kappa) \sim \kappa^2$, hence at $\kappa \to 0$, $\varepsilon \not\to 0$, and this means in field theory language this means that massive (with mass) particles are present: These are Cooper pairs for us, but for particle physicists these are the Higgs-bosons. If a continuous symmetry is broken (here the gauge symmetry is the continuous symmetry which breakes) Goldston bosons should appear. But if in the same time the gauge (nonlocal) symmetry is broken as well, the Goldston bosons are „eaten" by Higgs-bosons and Higgs bosons emerge. Now given by the Higgs bosons, the gauge bosons in interaction with Higgs bosons gain mass. This is the Higgs mechanism. Let us take an electromagnetic field (whose gauge boson is the photon) and act with it on a superconductor. Now the Meissner effect appears. Indeed:

The current density $\vec{J} = q n_q \vec{v}$; q = charge, n_q = carrier (charge) density, $\vec{v}$ = carrier velocity. But in the presence of the electromagnetic field the momentum $\vec{p} = m_q \vec{v} + q\vec{A}$; m_q = carrier mass, $\vec{A}$ = vector potential. From here $\vec{v} = \frac{1}{m_q}(\vec{p} - q\vec{A})$. Since for the Cooper pair (a pair of 2 electrons with $-\vec{k}$ and $+\vec{k}$ momenta (in $\hbar = 1$ units)), results $\vec{p} = 0$ for superconductor (i.e. particles building up the superconductor) and we find

(66) $\vec{J} = -\frac{q^2 n_q}{m_q}\vec{A}$. This is the London equation for superconductor.

Let us introduce it in the Maxwell equation for magnetic induction $\vec{B}$: $\nabla \times \vec{B} = \mu_0 \vec{J} + \mu_0 \varepsilon_0 \frac{\partial \vec{E}}{\partial t}$ (Ampere law) ; μ_0 = permeability, ε_0 = permitivity of the space, $\vec{E}$ = electric field which one takes constant in time, hence $\partial \vec{E}/\partial t = 0$, and with (66) one finds

(67) $\nabla \times \vec{B} = -\mu_0 \frac{q^2 n_q}{m_q}\vec{A}$; Since $\vec{B} = \nabla \times \vec{A}$, and we use the Coulomb gauge where $\nabla \cdot \vec{A} = 0$. Than we have

(68) $\nabla \times (\nabla \times \vec{A}) = -K^2 \vec{A}$; $K^2 = \mu_0 \frac{q^2 n_q}{m_q}$

$\nabla \times (\nabla \times \vec{A}) = \nabla(\underbrace{\nabla \cdot \vec{A}}_{=0}) - \nabla^2 \vec{A} = -\nabla^2 \vec{A}$, hence from (68) we obtain

(69) $\boxed{\nabla^2 \vec{A} - K^2 \vec{A} = 0}$; which as in 1D: $\frac{d^2 f}{dx^2} - K^2 f = 0$ gives the solution $f(x) = \text{const}\, e^{-Kx} = \text{const}\, e^{-\frac{x}{\lambda}}$, were $\lambda = \frac{1}{K}$ = penetration depth, from (69):

(70) $\vec{A} = \text{const} \cdot \vec{u}\, e^{-\frac{r}{\lambda}}$; $\vec{u}$ the unit vector perpendiculare to the system containing the superconductor, and $\lambda = \sqrt{\frac{m_q}{\mu_0 n_q q^2}}$, r = the distance inside the superconductor from the surface. Hence the magnetic field (here represented by $\vec{A}$) is expelled from the superconductor, which is the Meissner effect. The magnetic fields enter only at the surface, and the penetration depth is λ above.

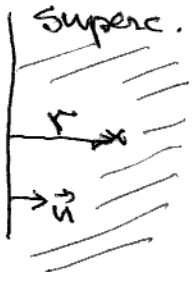

Fig 8.

But what this has to do with the photon mass?
The Maxwell equations contain in themselves that the photon mass is zero. Alexander Proca has rewritten the Maxwell equations for the case when the photon has mass. In this case in $\nabla \times \vec{B}$ equation $-\mu_\gamma^2 \vec{A}$ supplementary emerge, where $m_0 = \frac{\hbar}{c}\mu_\gamma$ is the photon mass (rest mass). In our case $\mu_\gamma = K$, hence the photon mas is

$$m_0 = \frac{\hbar}{c}\sqrt{\mu_0 \frac{q^2 n_q}{m_q}}$$

So the Higgs mechanism is in fact the process similar to the Meissner effect during which the photon in superconductor gains mass. For the first time this process has been described by Phil Anderson in Phys Rev 130, 439 (1963), and Higgs in the introduction of his paper PRL 13 (no: 16), 508-509 (1964) acknowledges this fact, mentioning that he transcribed in relativistic frame the finding of Phil Anderson.

P. W. Anderson : Phys Rev 130, 439-442 (1963)
PRL 13(9), 321-323 (1964)

Electroweak symmetry: $SU(2) \times U(1)$ gauge groups
↓
invariant under a continuous groups of local transformations

$SU(2) \times U(1)$ gauge group → 4 generátorja vam
I_1, I_2, I_3 izospin generátorai az $SU(2)$-nek
Y → az $U(1)$ generátora (hypercharge).

A szimmetriasérülés $SU(2) \times U(1)_Y \rightarrow U(1)_{em}$-be

$U(1)_{em}$ generátora $Q = \frac{Y}{2} + I_3$ → ez adja a nemsérült részét az $SU(2) \times U(1)$ gauge group-nak
(unbroken gauge groups)

Mermin-Wagner theorem at $T=0$ and $D=1$

L. Pitaevskii, S. Stringari: J. Low Temp. Phys 85(5/6) pg. 377-388 (1991)