Lecture 3: The study of correlations.

We know already that the strong fluctuations destroy the tendencies for ordering, but we do not know precisely what is the mathematical object on which they act in fact. We also know that the long-range order is defined by correlation functions. Because of these reasons we start to analyze correlations, and try to understand how fluctuations modify them.

I. Expressing correlations: A.) Introduction:

We are placed at $T \neq 0$, as before $y(\vec{r})$ denotes a local thermal fluctuation, and $X(\vec{r})$ a characteristic density specific for the system as previously. Let us denote by $X_o(\vec{r})$ the equilibrium value of the specific density. If now we act on it, and make it to fluctuate, obtaining by this the actual value $X(\vec{r})$, mathematically this effect can be described as a shift in the argument.

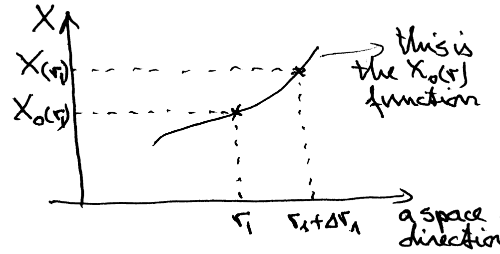

Fig 9.

$$X(\vec{r}_1) = X_o(\vec{r}_1 + \Delta\vec{r}_1) \qquad (71)$$

Denoting $\Delta\vec{r}_1 = -\vec{y}(\vec{r}_1)$, where $\vec{y}(\vec{r}_1)$ can be considered as a local fluctuation, one finds:

$$\langle X(\vec{r}_1) X(\vec{r}_2)\rangle = \langle X_o(\vec{r}_1 - \vec{y}(\vec{r}_1)) X_o(\vec{r}_2 - \vec{y}(\vec{r}_2))\rangle \qquad (72).$$

Because the Fourier transformation helps the mathematical description, on turns below to see how (72) looks like in Fourier components language.

B.) About Fourier components:

As usually one has

$$(72) \quad X_o(\vec{r}) = \sum_{\vec{k}} X_{\vec{k}} e^{i\vec{k}\cdot\vec{r}} = \bar{X} + \sum_{\vec{k}\neq 0} X_{\vec{k}} e^{i\vec{k}\cdot\vec{r}} \; ; \; \bar{X} = \langle X_o\rangle = \langle X\rangle$$

So the first observation is that $\bar{X}$ is the average of X_o, and this is exactly the $X_{\vec{k}=0}$ component. Indeed, since the system is homogenous, an $\vec{r}$ dependent probability density must be $\vec{r}$ independent (constant), then (const $= \frac{1}{V}$):

$$(73): \langle X_o\rangle = \bar{X} = \frac{1}{V}\int d^3r \, X_o(\vec{r}) = \frac{1}{V}\int d^3r \left[\sum_{\vec{k}} X_{\vec{k}} e^{i\vec{k}\cdot\vec{r}}\right] = \sum_{\vec{k}} X_{\vec{k}} \underbrace{\left[\frac{1}{V}\int e^{i\vec{k}\cdot\vec{r}} d^3r\right]}_{\delta_{\vec{k},0}} = X_{\vec{k}=0}.$$

Furthermore a translation in argument randomly made not modifies an uniformous space average, i.e $\langle X_o\rangle = \langle X\rangle$ based on Eq. (71). Hence one obtains ($y(\vec{r}_i) \equiv y_i$):

$$(74): X_o(\vec{r}_1 - \vec{y}_1) = \bar{X} + \sum_{\vec{k}\neq 0} X_{\vec{k}} e^{i\vec{k}(\vec{r}_1 - \vec{y}_1)}$$

Now if we introduce (74) in (72) and multiply $X_0(\vec{r}_1-\vec{y}_1)X_0(\vec{r}_2-\vec{y}_2)$ in the average, one obtains averages with a single $\sum_{\vec{k}\neq 0}$ as well and these vanish. Indeed:

(75) $\left\langle \sum_{\vec{k}\neq 0} X_{\vec{k}} e^{i\vec{k}\cdot\vec{r}} \right\rangle = \left\langle X_0(\vec{r}) - \bar{X} \right\rangle = \left\langle X_0 - \langle X_0\rangle \right\rangle = \langle X_0\rangle - \langle X_0\rangle = 0$

Consequently:

$$\langle X(\vec{r}_1)X(\vec{r}_2)\rangle = \bar{X}^2 + \left\langle \sum_{\vec{k}_1,\vec{k}_2\neq 0} X(\vec{k}_1)X(\vec{k}_2)\, e^{i\vec{k}_1(\vec{r}_1-\vec{y}_1)+i\vec{k}_2(\vec{r}_2-\vec{y}_2)} \right\rangle =$$

(76)
$$= \bar{X}^2 + \sum_{\vec{k}_1\neq 0}\sum_{\vec{k}_2\neq 0} X(\vec{k}_1)X(\vec{k}_2) \left\langle e^{i\vec{k}_1(\vec{r}_1-\vec{y}_1)} e^{i\vec{k}_2(\vec{r}_2-\vec{y}_2)} \right\rangle$$

Because of isotropy, only $\vec{r}_1-\vec{r}_2=\vec{r}$ dependences should remain in the correlation function, in (76) only $\vec{k}_1=-\vec{k}_2=\vec{k}$ terms remain non-vanishing, and one finds:

$$\langle X(\vec{r}_1)X(\vec{r}_2)\rangle = \bar{X}^2 + \sum_{\vec{k}\neq 0} X_{\vec{k}}^2\, e^{i\vec{k}(\vec{r}_1-\vec{r}_2)} \left\langle e^{-i\vec{k}\cdot(\vec{y}_1-\vec{y}_2)} \right\rangle =$$

(77)
$$= \bar{X}^2 + \sum_{\vec{k}\neq 0} X_{\vec{k}}^2\, e^{i\vec{k}\cdot\vec{r}} \left\langle e^{-i\vec{k}\cdot(\vec{y}_1-\vec{y}_2)} \right\rangle; \quad X_{\vec{k}} = X_{-\vec{k}};$$

Now we need an average of one expression in which the random variable appears in the exponent. Using the Einstein sum convention and denoting by x_i the random variable, the relation which we use is:

(78) $\langle e^{\alpha_i x_i}\rangle = e^{\frac{1}{2}\alpha_i\alpha_j\langle x_i x_j\rangle}$

Below one proves the equality (78)

C. Random variable in the exponent:

Let us use as in the case of the fluctuations a probability density $w = A\exp\left[\frac{1}{2}\gamma_{ij}x_i x_j\right]$ where A is a normalization constant and compairing with (24-26) of Lecture 2, one has

(79) $\gamma_{ij} = \dfrac{\beta_{ij}}{k_B T}$

One has than for an arbitrary quantity M the expression

(80) $\langle M\rangle = \int w M\, d\Gamma$; $d\Gamma = \prod_i dx_i$

and based on (33) one already knows that

(81) $\langle x_i x_j\rangle = \dfrac{1}{\gamma_{ij}}$; (in numerator one has unity matrix, in denominator matrix division.)

Based on (80) and taking $M = e^{\alpha_i x_i}$; α_i some constants, one obtains

(82) $\langle e^{\alpha_i x_i}\rangle = A\int \exp\left[\alpha_i x_i - \frac{1}{2}\gamma_{ij}x_i x_j\right] d\Gamma$

Now a linear transformation is made from x_i to x_i' via

(83) $x_i = a_{in}x_n'$ $\left(=\sum_n a_{in}x_n'\right)$; a_{in} are constants.

Hence, for the exponent in the right side of (82) one obtains

(84) $E = \alpha_i x_i - \frac{1}{2}\gamma_{ij} x_i x_j = \alpha_i a_{in} x'_n - \frac{1}{2}\gamma_{ij} a_{in} a_{jm} x'_n x'_m$

The new coefficients a_{in} we chose now such to satisfy: (a mathematical transformation is made not to complicate our job, but to simplify it):

(85) $\gamma_{ij} a_{in} a_{jm} = \delta_{nm}$

Hence we find

(86) $E = \alpha_i a_{in} x'_n - \frac{1}{2}(x'_n)^2 = -\frac{1}{2}(x'_n - \alpha_i a_{in})^2 + \frac{1}{2}\alpha_i \alpha_j a_{in} a_{jn}$

Consequently, introducing this result in (82)

(87) $\langle e^{\alpha_i x_i} \rangle = e^{+\frac{1}{2}\alpha_i \alpha_j a_{in} a_{jn}} \Big\{ \underbrace{A \int e^{-\frac{1}{2}(x'_n - \alpha_i a_{in})^2} d\Gamma}_{B} \Big\}$

The number B in (87) is 1 because (87) must hold for all α_i, so also for $\alpha_i = 0$, providing $B = \langle 1 \rangle = 1$. Now from (85) at $n = m$ we find $a_{in} a_{jn} = \frac{1}{\gamma_{ij}} = \langle x_i x_j \rangle$ where (81) has been also used. Hence we find

(88) $\langle e^{\alpha_i x_i} \rangle = \exp\left[\frac{1}{2}\alpha_i \alpha_j \langle x_i x_j \rangle\right]$

which represents exactly the equality (78). Consequently, (78) has been demonstrated.

D. The expectation value from (77)

Now one turns back to (77) and calculate $\langle e^{-i\vec{k}\cdot(\vec{y}_1 - \vec{y}_2)} \rangle$. Note that $\vec{k}\cdot(\vec{y}_1 - \vec{y}_2) = \sum_\alpha k_\alpha (y_1 - y_2)_\alpha = k_\alpha (y_1 - y_2)_\alpha$, where α represents the vector components, and at the last equality the Einstein sum convention has been used. Taking now $x_i \to (y_1 - y_2)_\alpha$; $\alpha_i \to k_\alpha(-i)$ we obtain:

(89) $\langle e^{-i\vec{k}\cdot(\vec{y}_1 - \vec{y}_2)} \rangle = \langle e^{-ik_\alpha(y_1 - y_2)_\alpha} \rangle = e^{-\frac{1}{2}k_\alpha k_\beta \langle (y_1 - y_2)_\alpha (y_1 - y_2)_\beta \rangle}$

Introducing the notation:

(90) $X_{\alpha\beta}(\vec{r}) = \langle (y_1 - y_2)_\alpha (y_1 - y_2)_\beta \rangle$; $y_{1,2} = y(\vec{r}_{1,2})$; $\vec{r} = \vec{r}_1 - \vec{r}_2$,

the needed correlation function from (77) becomes

(91) $\langle X(\vec{r}_1) X(\vec{r}_2) \rangle = \overline{X}^2 + \sum_{\vec{k} \neq 0} X^2_{\vec{k}} e^{i\vec{k}\cdot\vec{r}} e^{-\frac{1}{2}k_\alpha k_\beta X_{\alpha\beta}(\vec{r})}$

Now is seen that in order to calculate the needed correlation function we must first calculate $X_{\alpha\beta}(\vec{r})$. This we do in the following paragraph. $X_{\alpha\beta}$ must depend on $\vec{r}$ because of the isotropy.

E. Study of $\chi_{\alpha\beta}(\vec r)$.

From (90) we finds:

$$\chi_{\alpha\beta}(\vec r) = \langle (y_1 - y_2)_\alpha (y_1 - y_2)_\beta \rangle = [\langle y_{1\alpha} y_{1\beta}\rangle + \langle y_{2\alpha} y_{2\beta}\rangle] - [\langle y_{1\alpha} y_{2\beta}\rangle + \langle y_{2\alpha} y_{1\beta}\rangle]$$

(92) $= 2[\langle y_{1\alpha} y_{1\beta}\rangle - \langle y_{1\alpha} y_{2\beta}\rangle]$; because of the homogenity and isotropy.

Taking the Fourier components:

(93) $y_{1\alpha} = \sum_{\vec K_1} y_{\vec K_1,\alpha} e^{i\vec K_1\cdot\vec r_1}$; $y^*_{1\beta} = \sum_{\vec K_2} y^*_{K_2,\beta} e^{-i\vec K_2\cdot\vec r_1} = \sum_{\vec K_2} y_{K_2,\beta} e^{-i\vec K_2\cdot\vec r_1} = y_{1\beta}$

because of homogenity and isotropy y_α and $y_{K\alpha}$ are both real.

Hence

(94) $\langle y_{1\alpha} y_{1\beta}\rangle = \sum_{\vec K_1,\vec K_2} e^{i\vec K_1\vec r_1} e^{-i\vec K_2\vec r_1} \langle y_{\vec K_1\alpha} y_{\vec K_2\beta}\rangle$; But now from (57) of Lecture 2 one has

(95) $\langle y_{\vec K_1\alpha} y_{\vec K_2\beta}\rangle = \frac{K_BT}{A_{\alpha\beta}} \frac{\delta_{\vec K_1,\vec K_2}\delta_{\alpha\beta}}{K_1^2}$; which introduced in (94) and using the $\vec K = \vec K_1 = \vec K_2$ notation gives

(96) $\langle y_{1\alpha} y_{1\beta}\rangle = K_BT \frac{\delta_{\alpha\beta}}{A_{\alpha\beta}} \sum_{\vec K} \frac{1}{K^2} = K_BT \frac{\delta_{\alpha\beta}}{A_{\alpha\beta}} \int \frac{d^DK}{(2\pi)^D} \frac{1}{K^2}$; Se (62-63).

From the another hand, and similarly

(97) $\langle y_{1\alpha} y_{2\beta}\rangle = \sum_{\vec K_1,\vec K_2} e^{i\vec K_1\cdot\vec r_1 - i\vec K_2\cdot\vec r_2} \langle y_{\vec K_1\alpha} y_{\vec K_2\beta}\rangle$, where using (95) we find

(98) $\langle y_{1\alpha} y_{2\beta}\rangle = K_BT \frac{\delta_{\alpha\beta}}{A_{\alpha\beta}} \sum_{\vec K} e^{i\vec K\cdot\vec r} \frac{1}{K^2} = K_BT \frac{\delta_{\alpha\beta}}{A_{\alpha\beta}} \int \frac{d^DK}{(2\pi)^D} \frac{\cos\vec K\cdot\vec r + i\sin\vec K\cdot\vec r}{K^2}$;

Because $\vec K$ has a symmetric domain ($\vec K$ and $-\vec K$ as well), the $\sin\vec K\cdot\vec r$ term represents an odd function integrated on a symmetric domain, hence this term vanishes, and we finally obtain:

(99) $\langle y_{1\alpha} y_{2\beta}\rangle = K_BT \frac{\delta_{\alpha\beta}}{A_{\alpha\beta}} \int \frac{d^DK}{(2\pi)^D} \frac{\cos\vec K\cdot\vec r}{K^2}$;

Using now (92), (96), (98) we find

$$\boxed{(100)\quad \chi_{\alpha\beta}(\vec r) = 2K_BT \frac{\delta_{\alpha\beta}}{A_{\alpha\beta}} \int \frac{d^DK}{(2\pi)^D} \frac{(1-\cos\vec K\cdot\vec r)}{K^2}};$$

Now, before using (100) in (91) several observations must be underlined concerning $\chi_{\alpha\beta}(\vec r)$ in (100).

i) The expression under the integral is no more divergent at $K\to 0$. Indeed, the Taylor expression of $\cos x$ for $x\to 0$ is $\cos x = 1 - \frac{x^2}{2} + \dots$, hence at $K\to 0$ a K^2 appears in nominator which cancells the denominator. So if the primitive function of the integral is $F(\vec K,\vec r)$; i.e

(101) $\int \frac{d^DK}{(2\pi)^D} \frac{1-\cos\vec K\cdot\vec r}{K^2} = F(\vec K,\vec r)\Big|$ taken between $\vec K$ integration limits; one has

(102) $\lim_{\vec K\to 0} F(\vec K,\vec r) = \text{finite}$

ii) In the opposite limit, for $\kappa \to \kappa_{max}$; $\kappa = |\vec{\kappa}|$; $\kappa \gg 1$, the cosinus function (because of his large argument) is strongly oscillating, hence cancells out under the integral. Then

$$(103) \quad \lim_{\kappa \to \kappa_{max}} F(\vec{\kappa}, \vec{r}) = \text{the primitive function of } \frac{d^D\kappa}{(2\pi)^D} \cdot \frac{1}{\kappa^2};$$

iii) Note that $\chi_{\alpha\beta}(\vec{r})$ collects practically the fluctuation effects via (100) and introduce them in the correlation function (91). This is the mathematical way in which the fluctuations act on the correlation function.

F. Dimension dependence.

Now one analizes (100) in (91) in its dimension dependence.

a.) Case D=1: in this case $\vec{\kappa}$ and $\vec{r}$ are one the same line: $\vec{\kappa}\cdot\vec{r} = \kappa r$, and because $d^D\kappa = d\kappa$ in this case, and in (100) the following integral emerges: (we use a variable transformation from κ to $\kappa r = x$):

$$(104) \quad \int_0^{\kappa_{max}} \frac{d\kappa}{2\pi} \frac{1-\cos\kappa r}{\kappa^2} = r \int_0^{r\kappa_{max}} \frac{dx}{2\pi} \frac{(1-\cos x)}{x^2} = \frac{r}{2\pi} \Big[\underbrace{-\frac{1-\cos x}{x} + si(x)}_{F(\kappa, r) \text{ function}} \Big] \Bigg|_0^{r\kappa_{max} \to \infty}$$

where $si(x) = -\int_x^{\infty} \frac{\sin t}{t} dt$ is the sinusintegral function, were $si(0) = -\frac{\pi}{2}$; (Taken from Gradstein-Rijik); $\frac{1-\cos x}{x}\Big|_0^{\infty} = 0$,

and $si(x)\Big|_0^{\infty} = \underbrace{si(\infty)}_{=0} - si(0) = \frac{\pi}{2}$; hence in this case

$$(105) \quad \int_0^{\kappa_{max} \to \infty} \frac{d\kappa}{2\pi} \frac{1-\cos\kappa r}{\kappa^2} = \frac{r}{4}; \Rightarrow \boxed{\chi_{\alpha\beta}(r) = \kappa_B T r \frac{\delta_{\alpha\beta}}{2A_{\alpha\beta}}}$$

Because Einstein convention is present in (91) one obtains, and D=1 hence only $\alpha = 1$ exists

$$(106) \quad e^{-\frac{1}{2}\kappa_\alpha \kappa_\beta \chi_{\alpha\beta}} = \exp\left[-\frac{\kappa_B T r}{2} \cdot \frac{\kappa^2}{A_{11}}\right]; \text{ where } A_{11} = \text{const}.$$

From (91) one has

$$(107) \quad \langle X(\vec{r}_1) X(\vec{r}_2) \rangle - \bar{X}^2 = \Gamma(\vec{r}) = \sum_{\vec{\kappa} \neq 0} X_{\vec{\kappa}}^2 e^{i\vec{\kappa}\cdot\vec{r}} \cdot \exp\left[-\frac{\kappa_B T \kappa^2}{2A_{11}} \cdot r\right]$$

when the true physical correlation function is $\Gamma(\vec{r})$ (one must extract the trivial, always present $\langle x \rangle^2$ term from it). Now $\vec{\kappa}$ has in fact discrete values so (because $\vec{\kappa} = 0$ is excluded) one takes the smallest nonzero $\vec{\kappa} = \vec{\kappa}_s$. The other terms are exponentially smaller because

$$(108): \quad e^{-Cx_1^2} + e^{-Cx_2^2} \underset{x_2 > x_1}{=} e^{-Cx_1^2}\left[1 + e^{-C(x_2^2 - x_1^2)}\right]$$

where the second term is exponentially smaller than 1. Hence in leading term:

$$(109) \quad \boxed{\Gamma(r) = X_{\kappa_s}^2 e^{-C\cdot r} e^{i\kappa_s r}; \quad C = \frac{\kappa_B T \kappa_s^2}{2A_{11}}}$$

(all suppositions of fluctuation treatement are here: short-range interactions and thermodyn. limit.)

which means that the correlation functions are exponentially decreasing in D=1. This is why long range order $\Gamma(\vec{r})|_{\vec{r} \to \infty} \neq 0$ does not exists in D=1. $e^{i\kappa_s r}$ oscillates, but the amplitude exponentially decreases.

b.) Case D=2: One has $d^2k = k\,dk\,d\varphi$; φ is the angle between the fixed $\vec r$ direction and $\vec k$ (see Fig 10). The integral from (100) now becomes:

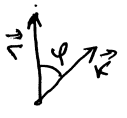

Fig 10

$$I_2 = \frac{1}{(2\pi)^2}\int_0^{2\pi} d\varphi \int_0^{K_{max}} \frac{k\,dk}{k^2}\left(1-\cos[k\cdot r\cos\varphi]\right) = \int \frac{d^2k}{(2\pi)^2}\,\frac{1-\cos\vec k\cdot\vec r}{k^2}; \quad (110).$$

We further have $\int_0^{2\pi}\cos(z\cos x)\,dx = 4\int_0^{\pi/2}\cos(z\cos x)\,dx = \frac{\pi}{2}\cdot 4J_0(z)$ (Gradstein – Rijic)

Hence from (110)

$$I_2 = \frac{1}{2\pi}\int_0^{K_{max}}\frac{dk}{k} - \frac{1}{(2\pi)^2}\int_0^{K_{max}}\frac{dk}{k}\,2\pi J_0(kr) = \frac{1}{2\pi}\int_0^{K_{max}}\frac{dk}{k}\left(1-J_0(kr)\right); \quad (111)$$

Note that the $J_0(z) = \sum_{n=0}^{\infty}(-1)^n\left(\frac{z}{2}\right)^{2n}\frac{1}{n!\,\Gamma(n+1)}$ Bessel function with the definition $J_0(z) = \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{iz\sin\theta}\,d\theta$ has $J_0(0)=1$ value and one has

(112) $$J_0(z) = 1 - \frac{z^2}{4}\frac{1}{(1!)^2} + \left(\frac{z^2}{4}\right)^2\frac{1}{(2!)^2} - \left(\frac{z^2}{4}\right)^3\frac{1}{(3!)^2} + \dots \quad \text{at } z\to 0$$

Effectuating the $x=kr$ change in variables, one obtains (from (100), (111))

(113) $\chi_{\alpha\beta}(\vec r) = 2K_BT\,\frac{\delta_{\alpha\beta}}{A_{\alpha\beta}}\,I_2$; $I_2 = \frac{1}{2\pi}\int_0^{rK_{max}}\frac{dx}{x}\left(1-J_0(x)\right)$; Let be $F(x)$ the primitive function of the integral in I_2, namely

(114) $I_2 = \frac{1}{2\pi}\int_0^{rK_{max}}\frac{1-J_0(x)}{x}\,dx = \frac{1}{2\pi}F(x)\Big|_0^{rK_{max}}$; For $x\to 0$, $F(x)$ is the primitive function of $\frac{x}{4}$ (see (112)) so

(115) $\lim_{x\to 0}F(x) \cong \frac{x^2}{8}$; (see (102))

For $x\gg 1$, see (103), $F(x)$ approximates the primitive function of $\frac{1}{x}$ ($J_0(x)$ strongly oscillates so cancells out). Hence $F(x)\sim\ln x$, that is

(116) $F(x)\Big|_{x\gg 1} \propto \ln x$; Using the second equality of (114) we find

(117) $I_2 = \frac{1}{2\pi}F(x)\Big|_0^{rK_{max}} = \frac{1}{2\pi}\left[\ln(rK_{max}) - 0\right] = \frac{1}{2\pi}\ln(r\cdot K_{max})$; $r=|\vec r|$

Then using (113) one finds:

(118) $$\boxed{\chi_{\alpha\beta}(\vec r) = \frac{K_BT}{\pi}\,\frac{\delta_{\alpha\beta}}{A_{\alpha\beta}}\,\ln(r\cdot K_{max}); \quad r=|\vec r|}$$

Introducing this result in (91) we obtain

(119) $$\Gamma(\vec r) = \sum_{\vec k\neq 0} X_{\vec k}^2\, e^{i\vec k\cdot\vec r}\exp\left[-\frac{1}{2}\sum_{\alpha=1,2}k_\alpha^2\,\frac{K_BT}{\pi A_{\alpha\alpha}}\ln(r\cdot K_{max})\right]$$

Because of the isotropy $A_{11}=A_{22}$ can be considered, $\sum_{\alpha=1,2}\frac{k_\alpha^2}{A_{\alpha\alpha}} = \frac{k^2}{A_{11}}$, so

(120) $$\Gamma(\vec r) = \sum_{\vec k\neq 0} X_{\vec k}^2\, e^{i\vec k\cdot\vec r}\exp\left[-\frac{1}{2}\frac{k^2}{A_{11}}\frac{K_BT}{\pi}\ln(r\cdot K_{max})\right]$$

Using again the $\vec{k}=\vec{k}_s$ component only from the $\vec{k}$-sum of (120) since the other terms are exponentially smaller, we find the leading term in (120) as

(121) $\Gamma(\vec{r}) = X^2_{\vec{k}_s}\, e^{i\vec{k}_s\cdot\vec{r}} \exp\left[-C\cdot T \ln(r\cdot k_{max})\right]$; $C = \dfrac{k_B k_s^2}{2\pi A_{11}} = \text{const}$

Since $\exp[-a\ln x] = \exp[\ln(x^{-a})] = \dfrac{1}{x^a}$; $x = r\cdot k_{max}$; $a = CT$ one finds the leading term in the correlation function in $D=2$ as

(122) $\Gamma(\vec{r}) = X^2_{\vec{k}_s}\, e^{i\vec{k}_s\cdot\vec{r}} \dfrac{1}{(r\cdot k_{max})^{C\cdot T}} \sim \dfrac{1}{r^{C\cdot T}}\, e^{i\vec{k}_s\cdot\vec{r}}$,

So the amplitude decreases again to zero for $r\to\infty$, as a consequence, long-range order is not present, but the decrease is now polynomial not exponential (all presumptions used at the study of fluctuations are present: short-range interactions, thermodinamic limit $n>1$ i.e. characteristic dynamical variable with more than 1 component). So again in $D=2$

(123) $\lim\limits_{\vec{r}\to\infty}\Gamma(\vec{r}) = 0$, but the decrease is polinomial not exponential. So increasing D, the decrease to zero vehemence of $\Gamma(\vec{r})$ is not so accentuated.

c) Case $D=3$: Now $d^3k = k^2\sin\theta\, d\theta\, d\varphi\, dk$ and $(\vec{k}\cdot\vec{r} = kr\cos\theta)$

(124): $\chi_{\alpha\beta}(\vec{r}) = 2k_BT \dfrac{\delta_{\alpha\beta}}{A_{\alpha\beta}} \underbrace{\int_0^{2\pi} d\varphi \int_0^{\pi} d\theta \int_0^{k_{max}} dk \left[\dfrac{1-\cos\vec{k}\cdot\vec{r}}{(2\pi)^3}\right]}_{\text{finite } = C_3} = 2k_BT \dfrac{\delta_{\alpha\beta}}{A_{\alpha\beta}} C_3$; i.e. no r dependence

Indeed, since k is not present in the denominator, for small k $\cos\vec{k}\cdot\vec{r} = 1 - \frac{1}{2}(kr\cos\theta)^2 + \ldots\ldots$ (see for θ the Fig 11), hence since $\int_0^{2\pi} d\varphi = 2\pi$ and $\int_0^{\pi}\cos^2\theta\, d\theta = \frac{\pi}{2}$, from the integral in (124) it remains:

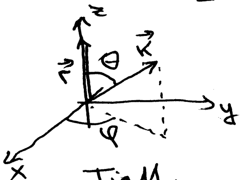

Fig 11.

$C_3 = 2\pi\cdot\dfrac{\pi}{2}\cdot\dfrac{1}{(2\pi)^3}\dfrac{r^2}{2}\int k^2 dk$, $k\to 0$, so the primitive function at $k\to 0$, $F(r,k)\sim\dfrac{k^3}{3}$, i.e

(125): $F(r,k)\sim\dfrac{k^3}{2}$; for $k\to 0$. (see also (102))

In the opposite limit, for $k\to\infty$, see (103), $F(r,k)$ becomes the primitive function of

$C_3 = 2\pi\cdot\pi\dfrac{1}{(2\pi)^3}\int dk$; $k\to\infty$, hence $F(r,k) = \dfrac{1}{4\pi}k$, i.e

(126): $F(r,k) \cong \dfrac{k}{4\pi}$; for $k\gg 1$. As a consequence:

(127): $\boxed{\chi_{\alpha\beta}(\vec{r}) = 2k_BT\dfrac{\delta_{\alpha\beta}}{A_{\alpha\beta}} F(r,k)\Big|_0^{k_{max}} = 2k_BT\dfrac{k_{max}}{4\pi}\dfrac{\delta_{\alpha\beta}}{A_{\alpha\beta}}}$
which not contains r dependence

This means that $\Gamma(\vec{r})\big|_{\vec{r}\to\infty} \neq 0$ (which must be understood that there are not present obligatory constrains to drive $\Gamma(\vec{r})$ to zero when $\vec{r}$ increases). Consequently $D \geq 3$ is the true world of the long-range order.

d. Case $D \geq 4$. The behavior of $\Gamma(\vec{r})$ remains similar, and in $D \to \infty$ limit the description becomes of mean-field type in short-range interactions are present. This is because the number of nearest neighbors increases (e.g. in cubic type of systems the number of nearest-neighbors in $D=1$ is 2, in $D=2$ is 4, in $D=3$ is 6, ... etc.), so practically the nearest-neighbors create the „mean-field" with which one-particle interacts, and this mean field better and better approximates the sum of the real interactions.

Continuous Phase Transitions.

I. Basic characteristics:

We have defined already the continuous phase transitions: these are the transitions which are accompanied by a change in symmetry (symmetry breaking), and in the Ehrenfest's classification are named of II. order. Let us see below what are the direct consequences simply, of the symmetry change which emerges at the phase transition.

a.) Continuous phase transitions do not have critical points.

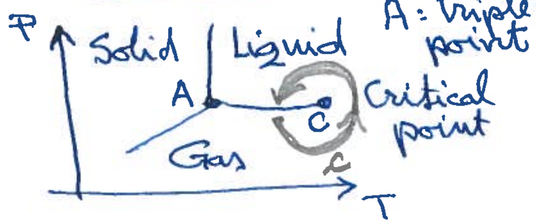

Fig 12.

The critical point C shown in a 1 component real gas phase diagram (see Fig 12) is the point where the phase separation line A–C terminates. Now following the curve c, is possible to move from one side of the line A–C to the opposite side of the same curve without crossing a phase transition line, i.e. remaining in the same quality. But different symmetries represent different qualities. Consequently, the curve A–C cannot be a continuous transition line, i.e. continuous transition phase separation line cannot have critical points.

b.) We know that in reality, the A–C curve denotes a first order transition line. Since first order transition curves have critical point, that it means that often the first order phase transition lines delimit two phases which only quantitatively differ (and not qualitatively). If this is the case the first order transition line is called „proper" first order transition curve.

There are however exceptions. To understand them we need the order parameter notion. This will be analyzed in details later on, but in order to make you understand non-proper first order phase transitions, I note the following aspects relating the order parameter: i) For each continuous phase transition, starting from the fact that symmetry breaking emerges, an order parameter can be defined which has 3 main properties: a) $\Delta = 0$ in the disordered phase, b.) $\Delta \neq 0$ in the ordered phase, and c) crossing the continuous phase transition line, Δ (the order parameter) increases from zero to non-zero values continuously. ii) The temperature dependence of Δ for continuous phase transitions is as shown in

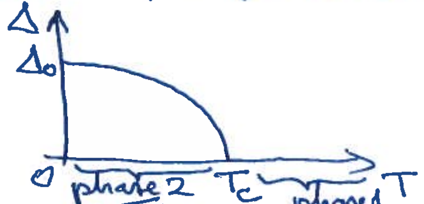

Fig 13.

If Δ behaves as shown in Fig 13, the transition at T_c is continuous (i.e. second order in the Ehrenfests classification. Hence in this case the 2 delimited phases have different symmetries (here phase 1, and phase 2 in Fig 13) so they qualitatively differ. However, sometimes, we find Δ behaviors as shown in Fig 14. In this case, because the order parameter notion can be introduced, phase 1 and phase 2 have different symmetries, so qualitatively differ. But at T_c, Δ becomes nonzero non-continuously by a jump. Since at the transition non-continuity appears, the transition is no more continuous (i.e. second order) but becomes of first order. This is the non-proper first order transition.

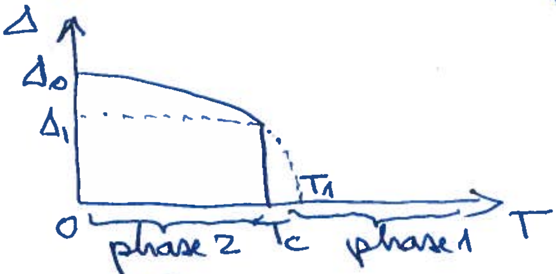

Fig 14.

The reason is as follows: usually at fixed T one has a $\Phi(\Delta \neq 0)$ and a $\Phi(\Delta = 0)$ value, furthermore, we have also an equation for $\Delta = \Delta(T)$. What happens in Fig 14 is that the $\Delta = \Delta(T)$ equation allows $\Delta \neq 0$ solutions for $T \in (T_c, T_1)$ region, but here $\Phi(\Delta=0) < \Phi(\Delta \neq 0)$ so phase 1 will be present. At T_c, the $\Phi(\Delta \neq 0)$ becomes smaller than $\Phi(\Delta = 0)$, the $\Delta = \Delta(T)$ equation allows here $\Delta_1 > 0$ solution, hence starting from this point the ordered phase appears but with nonzero and higher than zero $\Delta = \Delta_1$. In such cases a crossing point between $\Phi(\Delta=0)$ and $\Phi(\Delta \neq 0)$ appears. Since a cusp point appears in the Φ plots at $T = T_c$, the first derivatives of Φ differ in the left and right sides of T_c, i.e. the transition is of first order. This is non-proper first order phase transition because delimits two phases with different symmetries.

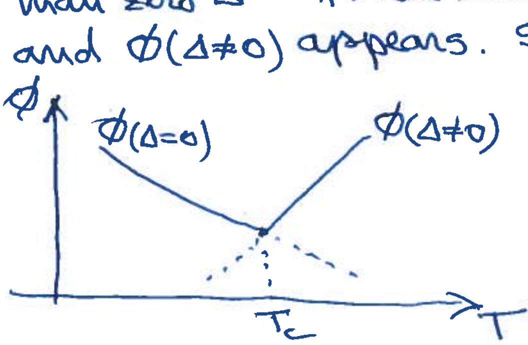

Fig 15.

c.) One the two sides of the phase transition line (continu-ous transition is present) well defined symmetries are present characteristic for phase 1 and phase 2, and differe[nt]. Consequently the extrapolation of ϕ_1 in the phase [2] (and vice versa) is not related to a real physical phase, because ϕ_1 is connected to the symmetry 1 but in the phase 2, symmetry $2 \neq$ symmetry 1 is present. Consequently, at continuous phase tran-sitions phenomenon like overheating cannot appear (i.e. phase 1 cannot exist as a metastable state in the domain 2). But overheati[ng] is present at the first oder phase transitions (e.g. the steam was overheated in the old steam locomotives.)

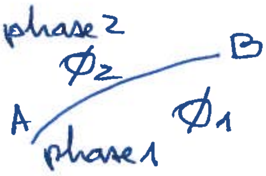

Fig 16.

d.) On the two sides of a continuous phase transition curve cannot apper arbitrary symmetries. Inded, phase 1 (let us conside[r] it the disordered, i.e. the high symmetr[y] phase) remains invariant under differe[nt] symmetry transformations which togeth[er] form the group G_1. Similarly phase 2 from its symmetry transformations constructed has its own group G_2. Now G_2 differs from G_1 because even if it has the symmetry transformations from G_1, but some symmetry transformations (those broken at the transition) are missing. Consequently, G_2 must be a subgroup of G_1

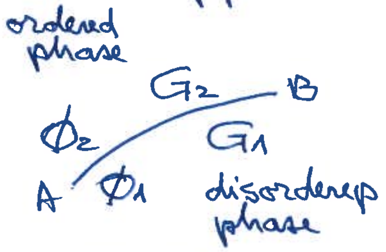

Fig 17. G_2 is a subgroup of G_1.

e.) Let us tace a 1 component system with its triple point C, and suppose two phase separation lines, say δ_1 (line A-C), and δ_2 (line C-B) are continuous phase transitions. If for example phase 1 has the highest symmetry, than the group G_1 has the highest number of elements (i.e. highest degree; degree of a group = number of elements of the group). Now during the transition to the phase 2, $\{g_2\}$ elements are lost, and we obtain the $G_2 \subset G_1$ group of phase 2. At the transition to the phase 3 (different from phase 2), the $\{g_3\}$ elements of G_1 are lost, and we recover the $G_3 \subset G_1$ group of the phase 3. But because $\{g_2\} \neq \{g_3\}$ it means that G_2 and G_3 cannot be in group-subgroup relation. That is: the line δ_3 cannot be continuous phase transition. So we learnt that a 1 comp[o]nent system has maximum a triple point. Now we know that in the triple point cannot enter 3 continuous phase transition (i.e. second order phase transition) lines. They can be 2 II. order + 1 I. order, 1 II. ord[er] + 2 I. order, or all three I. order (as in the case of real gases.)

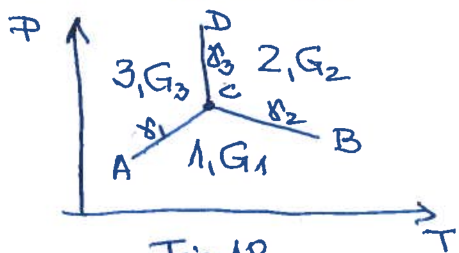

Fig 18.

f.) The name: critical point of a continuous transition

According to point e), for 1 component systems, in a triple point only 2 second order lines can enter. It can happen than (as exemplified in Fig 19) that the second order phase transition line B–A terminates in the point A. [It can also happen that the curve AD is outside of the plane of the figure, so cannot be seen in the surface of the paper sheet] Such points where at first view (and not in reality) a continuous transition line terminai are called to be the critical points of a continuous (i.e II. order) transition.

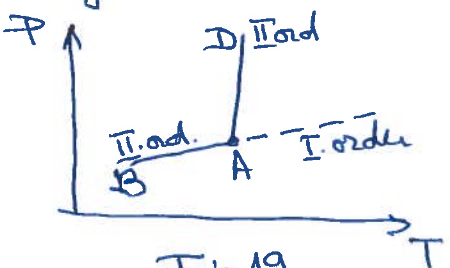

Fig 19.

g.) For multicomponent systems which admit quadratic point is possible: i) to have all curves entering in A as continuous transitions; ii) it can also happ that all lines in Fig 20 to be I. order phase transition lines, but the A point to represent a continuous transition.
The quadratic points are also named in the literature „tetracritical" points.

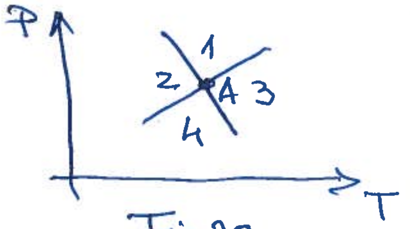

Fig 20

e.) At continuous transition from mathematical point of view must exist a parameter (i.e. a function) which denotes the ordered phase ($\Delta \neq 0$), is zero in disordered phase ($\Delta = 0$), and since the phase transition is continuous, Δ increases from zero to nonzero values continuously. This function is called „order parameter" or Landau order parameter. To Δ will be dedicated the next lecture.