Spatial Correlations

Correlation between spin i and j

$$G(x_i, x_j) := \langle (s_i - \langle s_i \rangle)(s_j - \langle s_j \rangle) \rangle$$

$$= \langle s_i s_j \rangle - \langle s_i \rangle \langle s_j \rangle$$

Write the partition function

$$Z(\{h_i\}) = \sum_{\{s_i\}} e^{-\beta \mathcal{H} + \beta \sum_i h_i s_i}$$

with the <u>bookkeeping fields h_i</u>

We recover the original partition function $Z = \sum_{\{s_i\}} e^{-\beta \mathcal{H}}$ by setting all $h_i \equiv 0$

It is understood that this will be done at the end of all calculations

We find

$$\langle s_i \rangle = \frac{1}{Z} \sum_{\{s_j\}} s_i \, e^{-\beta \mathcal{H} + \beta \sum_j h_j s_j} = \frac{1}{\beta Z} \frac{\partial Z}{\partial h_j}$$

$$\langle s_i \rangle = \frac{1}{\beta} \frac{\partial \ln Z}{\partial h_i} = -\frac{\partial F}{\partial h_i}$$

$$\langle s_i s_j \rangle = \frac{1}{\beta^2 Z} \frac{\partial^2 Z}{\partial h_i \partial h_j}$$

such that

$$G(\underline{r}_i, \underline{r}_j) = \frac{1}{\beta^2 Z} \frac{\partial^2 Z}{\partial h_i \partial h_j} - \frac{1}{\beta^2} \frac{1}{Z} \frac{\partial Z}{\partial h_i} \frac{1}{Z} \frac{\partial Z}{\partial h_j}$$

We usually assume the system to be homogeneous, then

$$G(\underline{r}_i, \underline{r}_j) = G(\underline{r}_i - \underline{r}_j)$$

For widely separated points

$$|\underline{r}_i - \underline{r}_j| \to \infty$$

we assume the spins to become uncorrelated

$$\langle s_i s_j \rangle \to \langle s_i \rangle \langle s_j \rangle$$

and thus

$$G(r \to \infty) \to 0$$

Consider a fluid of N particles in a volume V. Its density field $\rho(\underline{r})$ is normalized such that

$$\int_V \rho(\underline{r})\, d^d r = N$$

Define the correlation function

$$G(\underline{r}_1-\underline{r}_2) = \frac{1}{\rho^2}\left[\langle \rho(\underline{r}_1)\rho(\underline{r}_2)\rangle - \rho^2\right]$$

where $\rho = N/V$ is the mean density

We can also add bookkeeping fields to the Landau free energy functional

$$\mathcal{F}[M] \to \mathcal{F}[M] + \int d\underline{r}\, h(\underline{r}) M(\underline{r})$$

and we have

$$Z[h] = \int \mathcal{D}[M(\underline{r})]\, e^{-\beta \mathcal{F}[M] + \beta \int d\underline{r}\, h(\underline{r}) M(\underline{r})}$$

Define the functional derivative of a functional $F[M]$ as

$$\frac{\delta F}{\delta M(\underline{r}')} := \lim_{\varepsilon\to 0} \frac{F[M(\underline{r}) + \varepsilon\delta(\underline{r}-\underline{r}')] - F[M(\underline{r})]}{\varepsilon}$$

in the usual way.
What we need from functional calculus is

$$\frac{\delta}{\delta M(\underline{r})} \int d\underline{r}' M^n(\underline{r}') = n M^{n-1}(\underline{r})$$

$$\frac{\delta}{\delta M(\underline{r})} \int d\underline{r}' M(\underline{r}') = 1$$

$$\frac{\delta}{\delta M(\underline{r})} M(\underline{r}') = \delta(\underline{r}-\underline{r}')$$

$$\frac{\delta}{\delta M(\underline{r})} \int d\underline{r}' \frac{1}{2}(\nabla M(\underline{r}'))^2 = -\nabla^2 M(\underline{r})$$

up to surface terms

Response Functions

Consider we have the free energy $F = F[h]$ including the bookkeeping fields $h(\underline{r})$ which we find from minimizing the Landau free energy $\mathcal{Z}[M,h]$, i.e.

$$\frac{\delta \mathcal{Z}}{\delta M}[\bar{M},0] \stackrel{!}{=} 0$$

and then evaluating

$$\mathcal{Z}[\bar{M},h] \equiv F[h]$$

In analogy to $\langle s_i \rangle = -\frac{\partial F}{\partial h_i}$ we find

$$\langle M(\underline{r}) \rangle = -\frac{\delta F}{\delta h(\underline{r})}$$

More intuitively: If we change $h(\underline{r})$ by a small amount $\delta h(\underline{r})$

the free energy changes by

$$\delta F = -\int d\underline{r} \langle M(\underline{r})\rangle \delta h(\underline{r})$$

We can introduce a generalized susceptibility

$$\chi(\underline{r}_1,\underline{r}_2) = \frac{\delta\langle M(\underline{r}_1)\rangle}{\delta h(\underline{r}_2)} = -\frac{\delta^2 F}{\delta h(\underline{r}_1)\delta h(\underline{r}_2)}$$

which can be read as

$$\delta\langle M(\underline{r}_1)\rangle = \int d\underline{r}_2 \chi(\underline{r}_1,\underline{r}_2)\delta h(\underline{r}_2)$$

i.e. the response function χ desribes how the magnetization $\langle M(\underline{r})\rangle$ responds to a small change in the field $\delta h(\underline{r})$

Because the response is assumed to be linear in δh, this is an instance of

linear response theory

Interestingly we have

$$\chi(\underline{r}_1, \underline{r}_2) = -\frac{\delta^2 F}{\delta h(\underline{r}_1)\delta h(\underline{r}_2)}$$

$$= k_B T \left[\frac{1}{Z} \frac{\delta^2 Z}{\delta h(\underline{r}_1)\delta h(\underline{r}_2)} - \frac{1}{Z}\frac{\delta Z}{\delta h(\underline{r}_1)} \frac{1}{Z}\frac{\delta Z}{\delta h(\underline{r}_2)} \right]$$

$$= \frac{1}{k_B T} \left[\langle M(\underline{r}_1) M(\underline{r}_2) \rangle - \langle M(\underline{r}_1)\rangle \langle M(\underline{r}_2) \rangle \right]$$

$$=: \frac{1}{k_B T} G(\underline{r}_1, \underline{r}_2)$$

where $G(\underline{r}_1, \underline{r}_2)$ is the natural continuum generalization of our two-point spin-correlation function $G(\underline{r}_i, \underline{r}_j) = \langle s_i s_j \rangle - \langle s_i \rangle \langle s_j \rangle$

The relation

$$k_B T \chi(\underline{r}_1, \underline{r}_2) = G(\underline{r}_1, \underline{r}_2)$$

between the correlation function G and the response function is a central result of linear response theory

For a homogeneous system we can also consider the correlation- and response functions in the Fourier domain, $\tilde{\chi}(\underline{k})$, $\tilde{G}(\underline{k})$.
The original susceptibility is then

$$\frac{\partial M}{\partial H} \equiv \chi = \tilde{\chi}(\underline{k}=0)$$

and with $\tilde{\chi}(0) = \int d\underline{r}\, \chi(\underline{r})$
we obtain a sum rule

$$\chi = \beta \int d\underline{r}\, G(\underline{r})$$

The correlation function from Landau Theory

We start from

$$\mathcal{F} = \int d\underline{r} \left[At\, M^2(\underline{r}) + B\, M^4(\underline{r}) - H(\underline{r}) M(\underline{r}) + \kappa \left(\nabla M(\underline{r})\right)^2 \right]$$

The stationarity condition $\frac{\delta \mathcal{F}}{\delta M}[\langle M\rangle] = 0$

then reads

$$2At\langle M(\underline{r})\rangle + 4B\langle M(\underline{r})\rangle^3 - H(\underline{r}) - 2\kappa\nabla^2\langle M(\underline{r})\rangle = 0$$

We calculate the response function

$$\chi(\underline{r}_1, \underline{r}_2) = \frac{\delta\langle M(\underline{r}_1)\rangle}{\delta H(\underline{r}_2)},$$

by implicit differentiation

$$\frac{\delta^2 \mathcal{F}}{\delta[M(\underline{r}_1)]^2}\chi(\underline{r}_1, \underline{r}_2) = -\frac{\delta^2 \mathcal{F}}{\delta H(\underline{r}_2)\delta M(\underline{r}_1)}$$

$$\left[2At + 12B\langle M(\underline{r}_1)\rangle^2 - 2\kappa\nabla^2\right]\chi(\underline{r}_1, \underline{r}_2) = \delta(\underline{r}_1 - \underline{r}_2)$$

i.e., χ is a Green's function

Equivalently

$$\left[2At + 12B\langle M(\underline{r}_1)\rangle^2 - 2\kappa\nabla^2\right]G(\underline{r}_1, \underline{r}_2) = k_B T\delta(\underline{r}_1 - \underline{r}_2)$$

Approximate $\langle M(\underline{r}_1)\rangle^2 \simeq M^2$

Above T_c, we have $M = 0$ and below T_c, $M^2 = -\frac{At}{2B}$ such that we can write

$$(-\nabla^2 + \xi^{-2})\, G(\underline{r}_1, \underline{r}_2) = \frac{k_B T}{2K}\, \delta(\underline{r}_1 - \underline{r}_2)$$

with

$$\xi = \begin{cases} \sqrt{\frac{K}{At}} & \text{for } t > 0 \\ \sqrt{-\frac{K}{2At}} & \text{for } t < 0 \end{cases}$$

We will see soon that ξ is aptly called the correlation length and we observe here that it diverges at the critical point

$$\boxed{\xi \sim |t|^{-\nu}}$$

with another critical exponent $\nu = 1/2$

Let's solve the equation for $G(\underline{r})$
Assume we have a homogeneous and isotropic system such that $G = G(r)$ is a function of distance only.
In spherical coordinates we have

$$\left[-\frac{1}{r^{d-1}}\frac{\partial}{\partial r} r^{d-1}\frac{\partial}{\partial r} + \xi^{-2}\right] G(r) = \frac{k_B T}{2\kappa}\delta^d(r)$$

with $\rho := r/\xi$ we have

$$\left[-\frac{1}{\rho^{d-1}}\frac{\partial}{\partial \rho}\rho^{d-1}\frac{\partial}{\partial \rho} + 1\right] G(\rho) = \underbrace{\frac{k_B T}{2\kappa}\xi^{2-d}}_{=:c}\delta(\rho)$$

In $d=1$ we find $G(\rho) = c\,e^{-\rho}$ and for $d \geq 2$

$$G(\rho) = c\frac{1}{(2\pi)^{d/2}\rho^{\frac{d-2}{2}}} K_{\frac{d-2}{2}}(\rho)$$

where the $K_n(\rho)$ are spherical Bessel functions

Away from the critical point ξ is finite and we can look at distances $r \gg \xi$.
From the mathematical literature one obtains the asymptotic result

$$K_n(\rho) \sim \sqrt{\pi/2\rho}\, e^{-\rho} \quad \text{for } \rho \to \infty$$

and thus

$$G(r \gg \xi) \sim \frac{k_B T}{2K} \xi^{(3-d)/2} \times \frac{e^{-r/\xi}}{r^{(d-2)/2}}$$

which explains why we called ξ the correlation length
At the critical point $\xi \to \infty$ so we have to consider $r \ll \xi$.
Here we have

$$K_0(\rho) \sim -\ln \rho$$

$$K_n(\rho) \sim \rho^{-n} \quad \text{for } n > 0$$