

Correlation function for Ornstein-Zernike

Define Fourier transforms:

$$\left\{ \begin{array}{l} \text{cont.} \quad \phi(x) = \int \frac{d^d k}{(2\pi)^d} e^{ikx} \hat{\phi}(k) \\ \text{discrete} \quad \phi(x) = \frac{1}{L^d} \sum_k e^{ikx} \hat{\phi}_k \end{array} \right.$$

This implies:

$$\left\{ \begin{array}{l} \delta(x) = \int \frac{d^d k}{(2\pi)^d} e^{ikx} \\ \delta(x) = \frac{1}{L^d} \sum_k e^{ikx} \end{array} \right.$$

Or: $\delta(\vec{k}) = \int \frac{d^d x}{(2\pi)^d} e^{ikx}$, $\delta_{k,0} = \frac{1}{L^d} \int d^d x e^{ikx}$

is the Kronecker delta.

• We have: $D(k) = \frac{L^d}{(2\pi)^d}$ as the density of states in k .

So that

$$\sum_k F(k) \rightarrow \left(\frac{L}{2\pi} \right)^d \int d^d k F$$

$$\text{or } \lim_{L \rightarrow \infty} \frac{1}{L^d} \sum_k F(k) = \int \frac{d^d k}{(2\pi)^d} F(k) \text{ for any function } F(k).$$

$$\begin{aligned} \Delta k &= \frac{2\pi}{L} \\ \sum_k F(k) &= \sum_k \frac{L}{(2\pi)^d} F(k) \\ &= \sum_k F(k) \Delta k \\ &\approx \frac{L^d}{(2\pi)^d} \int F(k) d^d k \end{aligned}$$

We now have: $E = \int d^d x \left[\frac{k}{2} (\partial \phi)^2 + \frac{r}{2} \phi^2 \right] \quad T > T_c$

$$E = \int d^d x \left[\frac{k}{2} (\nabla \phi)^2 + |r| \phi^2 \right] \quad T < T_c$$

and we wish to calculate the correlation function

$$C(x) = \langle \phi(0) / \phi(x) \rangle$$

We conduct the calculation in Fourier space:

$$\begin{aligned}
 \int d^d x \frac{K}{2} (\nabla \psi)^2 &= \frac{K}{2} \int d^d x \left[\frac{\partial}{\partial x} \int \frac{d^d k}{(2\pi)^d} e^{i\vec{k}\cdot\vec{x}} \hat{\psi}(\vec{k}) \right]^2 = \\
 &= \frac{K}{2} \int d^d x \int \frac{d^d k}{(2\pi)^d} \int \frac{d^d k'}{(2\pi)^d} (i\vec{k}) \cdot (i\vec{k}') \hat{\psi}(\vec{k}) \hat{\psi}(\vec{k}') e^{i(\vec{k}+\vec{k}')\cdot\vec{x}} = \\
 &= \frac{K}{2} \int \frac{d^d k}{(2\pi)^d} \int \frac{d^d k'}{(2\pi)^d} (-\vec{k} \cdot \vec{k}') \hat{\psi}(\vec{k}) \hat{\psi}(\vec{k}') \underbrace{\int d^d x e^{i(\vec{k}+\vec{k}')\cdot\vec{x}}}_{(2\pi)^d \delta(\vec{k}+\vec{k}')} = \\
 &= \frac{K}{2} \int \frac{d^d k}{(2\pi)^d} |\vec{k}|^2 \hat{\psi}(\vec{k}) \hat{\psi}(-\vec{k}) = \\
 &= \frac{K}{2} \int \frac{d^d k}{(2\pi)^d} k^2 |\hat{\psi}(\vec{k})|^2
 \end{aligned}$$

A similar calculation can be conducted with $\frac{r}{2} \psi^2$ leading to:

$$E = \int \frac{d^d k}{(2\pi)^d} \left(\frac{K}{2} k^2 + \frac{r}{2} \right) |\hat{\psi}(\vec{k})|^2 \quad \text{in the continuum case}$$

$$E = \frac{1}{L^d} \sum_{\vec{k}} \left(\frac{K}{2} k^2 + \frac{r}{2} \right) |\hat{\psi}_{\vec{k}}|^2 \quad \text{in the discrete case.}$$

In order to compute the partition function, we have to sum over all states. Now: $\psi(\vec{x})$ is real, whereas $\hat{\psi}$ is complex ($\hat{\psi}^*(\vec{k}) = \hat{\psi}(-\vec{k})$) so we only need to sum over half the spectrum of independent modes (otherwise we will count every state twice).

$$\sum_{\text{states}} \rightarrow \prod_x \int d\psi(x) = \int \prod_{\vec{k}} d\hat{\psi}_{\vec{k}}$$

and since $\hat{\psi}_{\vec{k}}$ is complex $d\hat{\psi}_{\vec{k}} = d\hat{\psi}_{\vec{k}}^{\text{real}} d\hat{\psi}_{\vec{k}}^{\text{imag}}$

In order to compute $C(x)$ we define $\langle \hat{\psi}(k) \hat{\psi}(k') \rangle$.

$$\langle \hat{\psi}(k) \hat{\psi}(k') \rangle = \int d^d x \int d^d x' e^{-ikx} e^{-ik'x'} \langle \psi(x) \psi(x') \rangle$$

if translational
invariance holds

$$\stackrel{\downarrow}{=} \int d^d x \int d^d x' e^{-ikx} e^{-ik'x'} C(x-x') \quad \text{define } y = x-x'$$

$$y' = \frac{1}{2}(x+x')$$

$$\text{and } d^d x d^d x' = d^d y d^d y'$$

$$\langle \hat{\psi}(k) \hat{\psi}(k') \rangle = \int d^d y d^d y' e^{-i(k+k') \cdot \frac{y}{2}} G(y).$$

$$\begin{aligned} \text{or } x &= y' + \frac{1}{2}y \\ x' &= y' - \frac{1}{2}y \end{aligned}$$

$$\underbrace{\int d^d y' e^{-i(k+k') \cdot y'}}_{(2\pi)^d \delta(k+k')}$$

$$\begin{aligned} \Rightarrow \langle \hat{\psi}(k) \hat{\psi}(k') \rangle &= \int d^d y e^{-iky} G(y) (2\pi)^d \delta(k+k') \\ &= \underbrace{\int d^d y e^{-iky} G(y)}_{\hat{G}(k)} (2\pi)^d \delta(k+k') \end{aligned}$$

$$\begin{aligned} \Rightarrow \langle \hat{\psi}(k) \hat{\psi}(k') \rangle &= \hat{G}(k) (2\pi)^d \delta(k+k') \quad \text{continuous} \\ &= G_k L^d \delta_{k+k',0} \quad \text{discrete.} \end{aligned}$$

$\Rightarrow$ the only terms we need to calculate in Fourier space is:

$$\langle \hat{\psi}_k \hat{\psi}_{-k} \rangle = \langle |\hat{\psi}_k|^2 \rangle.$$

By definition:

$$\langle |\hat{\psi}_k|^2 \rangle = \frac{1}{L^d} \int d^d x' |\psi_{k'}|^2 e^{-\frac{1}{k_B T L^d} \sum_{k''} \left(\frac{K}{2} k''^2 + \frac{r}{2} \right) |\psi_{k''}|^2}$$

$$\frac{1}{L^d} \int d^d x' |\psi_{k'}|^2 e^{-\frac{1}{k_B T L^d} \sum_{k''} \left(\frac{K}{2} k''^2 + \frac{r}{2} \right) |\psi_{k''}|^2}$$

All products in numerator and denominator cancel except for k .

$$\langle |\hat{\psi}_k|^2 \rangle = \frac{\int d\hat{\psi}_k |\hat{\psi}_k|^2 e^{-\frac{2}{k_B T L^d} \left(\frac{k}{2} k^2 + \frac{r}{2} \right) |\hat{\psi}_k|^2}}{\int d\hat{\psi}_k e^{-\frac{2}{k_B T L^d} \left(\frac{k}{2} k^2 + \frac{r}{2} \right) |\hat{\psi}_k|^2}}$$

→ the factor of two in the exponent comes from $\psi_k \psi_k + \psi_k \psi_k$ both contributing to the sum. This is unrelated to the π' restriction. For any of the unrestricted k 's, we have two terms in the sum.

The integrals that are left are Gaussian. With $\hat{h}_k = R e^{i\theta}$

$$\text{so that } \langle |\hat{\psi}_k|^2 \rangle = \frac{\int_0^\infty R dR R^2 e^{-R^2/a}}{\int_0^\infty R dR e^{-R^2/a}} \quad \text{with } a = L^d k_B T \frac{k^2}{2} + \frac{r}{2}$$

The integral leads to: $\langle |\hat{\psi}_k|^2 \rangle = a$

$$\Rightarrow \boxed{\langle |\hat{\psi}_k|^2 \rangle = \frac{k_B T L^d}{\frac{k^2}{2} + \frac{r}{2}}}$$

or $\boxed{G_k = \frac{k_B T}{\frac{k^2}{2} + \frac{r}{2}}}$ as the Fourier transform of the correlation function

Below the critical point:

$$c(r) = \langle \Delta \psi(0) \Delta \psi(r) \rangle = \langle \psi(0) \psi(r) \rangle - \frac{|r|}{u}$$

and a similar calculation leads to:

$$\boxed{G_k(r) = \frac{k_B T}{k^2 + 2|r|} - \frac{|r|}{u} (2\pi)^d \delta(k)}$$