Title: 14/15 PSI - Statistical Mechanics - Lecture 4

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Abstract:

$$G_{ij} = \langle \sigma_i \sigma_j \rangle - \langle \sigma_i \rangle \langle \sigma_j \rangle \; ; \quad \varphi_i = \frac{1}{\sqrt{N}} \sum_k \varphi_k e^{i\vec{k}}$$

$$\sum_l \left[\delta_{il} - \frac{1}{T} J_{il} \right] G_{lj} = \delta_{ij}$$

Diagonalize by Fourier transform.

Periodic boundary condition

$$\varphi(\vec{r}_i) \equiv \varphi_i = \varphi(\vec{r}_i + L\vec{\lambda})$$

L - size of the system, $\vec{\lambda} = \hat{x}, \hat{y}, \hat{z}$

$\sum \varphi_k e^{i\vec{k}\cdot\vec{r}_i}$

conditions.

$+L\vec{\lambda})$

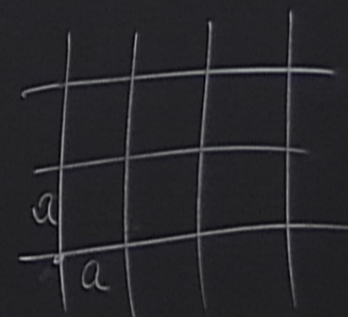
$, \vec{\lambda} = \hat{x}, \hat{y}, \hat{z}, \ldots$

$$e^{i\vec{k}\cdot\vec{r}_i} = e^{i\vec{k}\cdot(\vec{r}_i + L\vec{\lambda})}$$

$$e^{i\vec{k}\cdot\vec{\lambda}L} = \underline{1} \; ; \quad \vec{k}\cdot\vec{\lambda}\,L = 2\pi n_\lambda \, , \quad n_\lambda = 0, \pm 1, \pm 2, \ldots$$

$$K_\lambda = \frac{2\pi n_\lambda}{L}$$

$$\vec{r}_i = \sum_{\vec{\lambda}} m_\lambda a \vec{\lambda} \; ; \quad a - \text{lattice constant.}$$



$$K_\lambda \to K_\lambda + \frac{2\pi n_\lambda}{a}$$

$$\vec{K}\cdot\vec{r_i} = \sum_\lambda K_\lambda \cdot m_{i\lambda} a \longrightarrow$$

$$\to \sum_\lambda \left(K_\lambda + \frac{2\pi n_\lambda}{a}\right) m_{i\lambda} a =$$

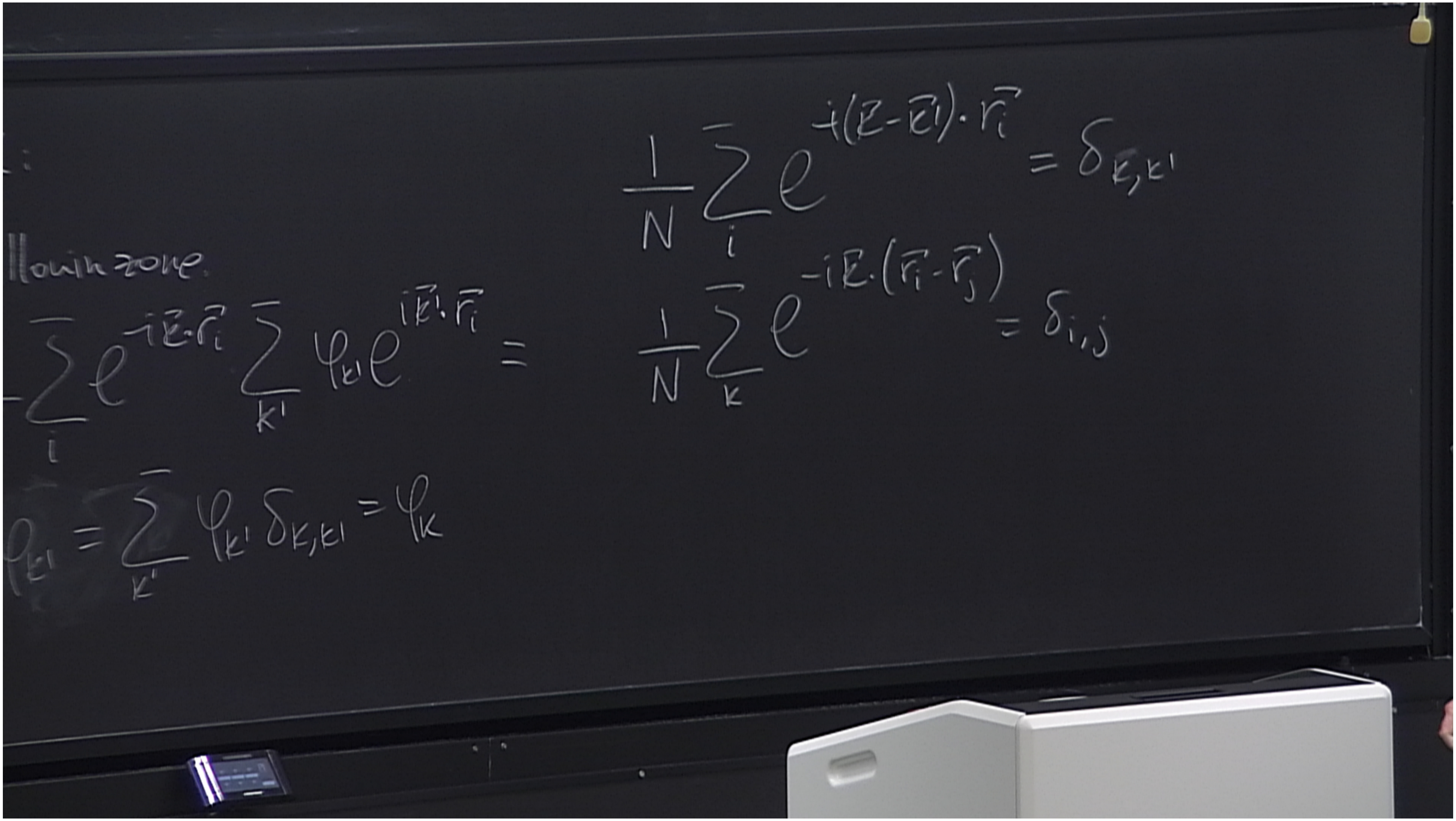
$$= \sum_\lambda K_\lambda m_{i\lambda} a + \sum_\lambda 2\pi n_\lambda m_{i\lambda}$$

Restrict K_λ to the interval:

$$-\frac{\pi}{a} \le K_\lambda \le \frac{\pi}{a} \text{ - first Brillouin zone}$$

$$\varphi_k = \frac{1}{\sqrt{N}} \sum_i \varphi_i e^{-i\vec{k}\cdot\vec{r_i}} = \frac{1}{N} \sum_i e^{-i\vec{k}\cdot\vec{r_i}} \sum_{k'} \varphi_{k'} e^{i\vec{k'}\cdot\vec{r_i}} =$$

$$= \frac{1}{N} \sum_{k'} \sum_i e^{-i(\vec{k}-\vec{k'})\cdot\vec{r_i}} \varphi_{k'} = \sum_{k'} \varphi_{k'} \delta_{k,k'} = \varphi_k$$



llouin zone.
$\sum_i e^{-i\vec{k}\cdot\vec{r}_i}\sum_{k'}\varphi_{k'}e^{i\vec{k}'\cdot\vec{r}_i} =$
$\varphi_{k'} = \sum_{k'}\varphi_{k'}\delta_{k,k'} = \varphi_k$
$\frac{1}{N}\sum_i e^{i(\vec{k}-\vec{k}')\cdot\vec{r}_i} = \delta_{k,k'}$
$\frac{1}{N}\sum_k e^{-i\vec{k}\cdot(\vec{r}_i-\vec{r}_j)} = \delta_{i,j}$

$$G_{ij} = \frac{1}{N}\sum_{q} G(\bar{q})\, e^{i\vec{q}\cdot(\vec{r}_i - \vec{r}_j)} \quad ; \quad J_{ij}$$

If we didn't have translational symmetry:

$$J(\bar{q}) =$$

$$G_{ij} = \frac{1}{N}\sum_{q,q'} G(\bar{q},\bar{q}')\, e^{i\vec{q}\cdot\vec{r}_i}\, e^{i\vec{q}'\cdot\vec{r}_j}$$

$$J_{ij} = \frac{1}{N}\sum_{q} J(\bar{q})\, e^{i\bar{q}\cdot(\bar{r}_i - \bar{r}_j)}$$

$$J(\bar{q}) = \frac{1}{N}\sum_{ij} J_{ij}\, e^{-i\bar{q}\cdot(\bar{r}_i - \bar{r}_j)}$$

$$\left(1 - \frac{J(\bar{q})}{T}\right) G(\bar{q}) = 1$$

$e^{i\vec{q}\cdot(\vec{r}_i-\vec{r}_j)}$

$$G(\vec{q}) = \frac{1}{1-\frac{J(\vec{q})}{T}}$$

$\cdot(\vec{r}_i-\vec{r}_j)$

$$J(\vec{q}) = \frac{1}{N}\sum_{ij} J_{ij}\, e^{-i\vec{q}\cdot(\vec{r}_i - \vec{r}_j)}$$

$$J(\vec{q}) \simeq \frac{1}{N}\sum_{ij} J_{ij}$$

Interested in behavior of G_{ij} at long distances.

$K = \frac{2\pi}{\lambda}$ long distances = small wavevectors.

$|\vec{r}_i - \vec{r}_j| \gg a$; $q \ll \frac{1}{a}$; $qa \ll 1$

vees.

evectors.

$$J(\vec{q}) = \frac{1}{N}\sum_{ij} J_{ij}\left[1 - \cancelto{0}{i\vec{q}\cdot(\vec{r}_i - \vec{r}_j)} - \frac{1}{2}\left(\vec{q}\cdot(\vec{r}_i - \vec{r}_j)\right)^2 + \cdots\right] =$$

$$J_{ij} = J_{ji}\ ; \quad = \overbrace{\frac{1}{N}\sum_{ij} J_{ij}}^{J} - \frac{1}{2N}\sum_{ij} J_{ij}\left[\vec{q}\cdot(\vec{r}_i - \vec{r}_j)\right]^2 =$$

$$= J - \frac{1}{2N}\sum_{ij} J_{ij}\sum_{\lambda,\lambda'} q_\lambda (\vec{r}_i - \vec{r}_j)_\lambda\, q_{\lambda'} (\vec{r}_i - \vec{r}_j)_{\lambda'}$$

$$\vec{q}) = \frac{1}{N}\sum_{ij} J_{ij}\left[1 - i\,\cancel{\vec{q}\cdot(\vec{r}_i - \vec{r}_j)}^{\,0} - \frac{1}{2}\left(\vec{q}\cdot(\vec{r}_i - \vec{r}_j)\right)^2 + \cdots\right] =$$

$$J_{ij} = J_{ji}\,; \quad = \overbrace{\frac{1}{N}\sum_{ij} J_{ij}}^{J} - \frac{1}{2N}\sum_{ij} J_{ij}\left[\vec{q}\cdot(\vec{r}_i - \vec{r}_j)\right]^2 =$$

The lattice has inversion symmetry

$$-\frac{1}{2N}\sum_{ij} J_{ij}\sum_{\lambda,\lambda'} q_\lambda (\vec{r}_i - \vec{r}_j)_\lambda\, q_{\lambda'} (\vec{r}_i - \vec{r}_j)_{\lambda'} = J - \frac{1}{2N}\sum_{ij} J_{ij}\sum_{\lambda} q_\lambda^2 (\vec{r}_i - \vec{r}_j)_\lambda^2$$

$$\frac{1}{N}\sum_{ij} J_{ij}\left[1 - i\cancel{\vec{q}\cdot(\vec{r}_i-\vec{r}_j)}^{\,0} - \frac{1}{2}\left(\vec{q}\cdot(\vec{r}_i-\vec{r}_j)\right)^2 + \cdots\right] =$$

$$= J_{ji}\ ; \quad = \overbrace{\frac{1}{N}\sum_{ij} J_{ij}}^{J} - \frac{1}{2N}\sum_{ij} J_{ij}\left[\vec{q}\cdot(\vec{r}_i-\vec{r}_j)\right]^2 =$$

The lattice has inversion symmetry

$$\frac{}{N}\sum_{ij} J_{ij}\sum_{\lambda,\lambda'} q_\lambda(\vec{r}_i-\vec{r}_j)_\lambda\, q_{\lambda'}(\vec{r}_i-\vec{r}_j)_{\lambda'} = J - \frac{1}{2N}\sum_{ij} J_{ij}\sum_{\lambda} q_\lambda^2(\vec{r}_i-\vec{r}_j)_\lambda^2 =$$

$$\cancel{\vec{q}\cdot(\vec{r}_i-\vec{r}_j)}^{\,\to 0} - \frac{1}{2}\left(\vec{q}\cdot(\vec{r}_i-\vec{r}_j)\right)^2 + \dots \Big] = \qquad q^2 = \sum_\lambda q_\lambda^2$$

$$J$$

$$J_{ij} - \frac{1}{2N}\sum_{ij} J_{ij}\left[\vec{q}\cdot(\vec{r}_i-\vec{r}_j)\right]^2 =$$

The lattice has inversion symmetry.

$$q_\lambda(\vec{r}_i-\vec{r}_j)_\lambda\, q_{\lambda'}(\vec{r}_i-\vec{r}_j)_{\lambda'} = J - \frac{1}{2N}\sum_{ij} J_{ij}\sum_\lambda q_\lambda^2(\vec{r}_i-\vec{r}_j)_\lambda^2 =$$

$$J(\vec{q}) = J - \frac{1}{2Nd}\sum_{ij} J_{ij}\, q^2 |\vec{r}_i - \vec{r}_j|^2 \;;\quad J(\vec{q}) = J -$$

$$K = \frac{1}{Nd}\sum_{ij} J_{ij} |\vec{r}_i - \vec{r}_j|^2$$

$$\ldots_i - \vec{r}_j|^2 \; ; \; J(\vec{q}) = J - \frac{1}{2} K q^2$$

$$; \quad G(\vec{q}) = \frac{1}{1 - \frac{1}{T} J(\vec{q})} = \frac{1}{1 - \frac{J}{T} + \frac{K}{2T} q^2} = \frac{T}{T - T_c + \frac{1}{2} K q^2}$$

$$\dim\left[\frac{T - T_c}{K}\right] = \frac{1}{L^2}$$

$$\ldots \vec{r}_i - \vec{r}_j|^2 \; ; \quad J(\vec{q}) = J - \frac{1}{2} K q^2$$

$$G(\vec{q}) = \frac{1}{1 - \frac{1}{T} J(\vec{q})} = \frac{1}{1 - \frac{J}{T} + \frac{K}{2T} q^2} = \frac{T}{T - T_c + \frac{1}{2} K q^2}$$

$$\dim\left[\frac{T - T_c}{K}\right] = \frac{1}{L^2}$$

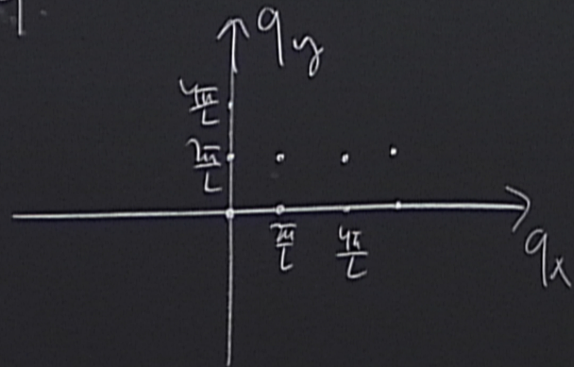
$$G(\vec{r}) = \frac{1}{N}\sum_{\vec{q}} G(\vec{q})\, e^{i\vec{q}\cdot\vec{r}}$$

Volume of $\frac{(2\pi)^3}{L^3}$ per single value of $\vec{q}$

$$\frac{1}{N}\sum_{q} \longrightarrow \frac{1}{N}\int \frac{d^3q}{\frac{(2\pi)^3}{L^3}}$$

$d=3$

$$q_x = \frac{2\pi n_x}{L}$$



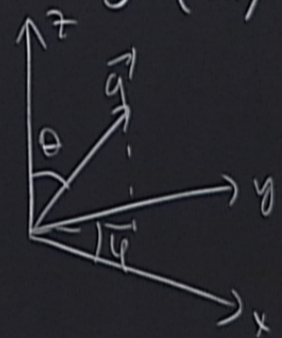
Volume of $\dfrac{(2\pi)^3}{L^3}$ per single value of $\vec{q}$.

$$\frac{1}{N}\sum_{\vec{q}} \longrightarrow \frac{1}{N}\int \frac{d^3q}{\frac{(2\pi)^3}{L^3}} = \frac{L^3}{N}\int \frac{d^3q}{(2\pi)^3} = a^3 \int \frac{d^3q}{(2\pi)^3}$$

q_x

per single value of $\vec{q}$

$$\frac{1}{N}\int \frac{d^3q}{\frac{(2\pi)^3}{L^3}} = \frac{L^3}{N}\int \frac{d^3q}{(2\pi)^3} = a^3 \int \frac{d^3q}{(2\pi)^3}$$



$$G(\vec{r}) = a^3 \int \frac{d^3q}{(2\pi)^3} G(\vec{q})\, e^{i\vec{q}\cdot\vec{r}}$$

Use spherical coordinates with z-axis along $\vec{r}$.

$$d^3q = d\varphi\, d\theta \sin\theta\, dq \cdot q^2$$

$$G(\vec{r}) = \frac{a^3}{8\pi^3}\int_0^{2\pi} d\varphi \int_0^{\pi} d\theta \sin\theta \int_0^{\infty} dq \cdot q^2\, G(q)\, e^{iqr\cos\theta} =$$

$$= \frac{a^3}{4\pi^2}\int_0^{\infty} dq \cdot q^2\, G(q) \int_{-1}^{1} d(\cos\theta)\, e^{iqr\cos\theta} = \frac{a^3}{4\pi^2}\int_0^{\infty} dq \cdot q^2\, G(q)\, \frac{1}{iqr}\left(e^{iqr} - e^{-iqr}\right)$$

$$q) e^{iqr\cos\theta} =$$

$$= \frac{a^3}{4\pi^2} \int_0^\infty dq\, q^2 G(q) \frac{1}{iqr} \left(e^{iqr} - e^{-iqr} \right) = \frac{a^3}{2\pi^2} \int_0^\infty dq\, q^2 G(q) \frac{\sin(qr)}{qr}$$

$$G(r) = \frac{a^3}{2\pi^2 r}\int_0^\infty dq \cdot q \frac{\sin(qr)\, T}{T - T_c + \frac{1}{2}\kappa q^2} = \frac{a^3 T}{\pi^2 r \kappa}\int_0^\infty dq \cdot q \frac{\sin(qr)}{\left(q - i\sqrt{2\frac{T-T_c}{\kappa}}\right)\left(q + i\sqrt{2\frac{T-T_c}{\kappa}}\right)}$$

$$\frac{\sin(qr)}{\left(q - i\underbrace{\sqrt{2\frac{T-T_c}{K}}}_{\frac{1}{\xi}}\right)\left(q + i\underbrace{\sqrt{2\frac{T-T_c}{K}}}_{\frac{1}{\xi}}\right)} = \frac{a^3 T}{2i\pi^2 r K}\int_0^\infty dq \cdot q \,\frac{e^{iqr} - e^{-iqr}}{\left(q-\frac{i}{\xi}\right)\left(q+\frac{i}{\xi}\right)}$$

$$\frac{\sin(qr)}{\left(q - i\underbrace{\sqrt{2\frac{T-T_c}{\kappa}}}_{\frac{1}{\xi}}\right)\left(q + i\underbrace{\sqrt{2\frac{T-T_c}{\kappa}}}_{\frac{1}{\xi}}\right)} = \frac{a^3 T}{2i\pi^2 r \kappa}\int_0^\infty dq\, q\, \frac{e^{iqr} - e^{-iqr}}{\left(q - \frac{i}{\xi}\right)\left(q + \frac{i}{\xi}\right)} =$$

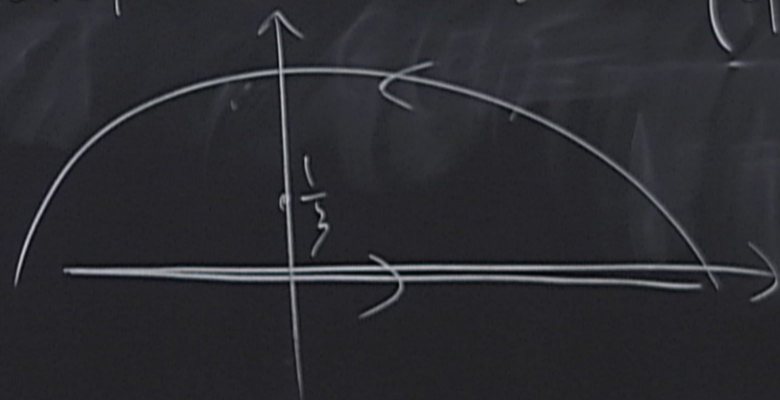
$$= \frac{a^3 T}{2\pi \kappa r} e^{-\frac{r}{\xi}} \quad , \quad \xi = \sqrt{\frac{\kappa}{2(T-T_c)}}$$

$$\frac{\sin(qr)}{\Big(q - i\underbrace{\sqrt{2\tfrac{T-T_c}{K}}}_{\frac{1}{\xi}}\Big)\Big(q + i\underbrace{\sqrt{2\tfrac{T-T_c}{K}}}_{\frac{1}{\xi}}\Big)} = \frac{a^3 T}{2i\pi^2 r K}\int_0^\infty dq\, q\,\frac{e^{iqr}-e^{-iqr}}{\left(q-\frac{i}{\xi}\right)\left(q+\frac{i}{\xi}\right)} =$$

$$= \frac{a^3 T}{2\pi K r}\, e^{-\frac{r}{\xi}}, \quad \xi = \sqrt{\frac{K}{2(T-T_c)}}$$

$$\frac{\;}{r}\int_0^\infty dq\cdot q\,\frac{\sin(qr)\,T}{T-T_c+\frac{1}{2}Kq^2} = \frac{a^3 T}{\pi^2 r K}\int_0^\infty dq\cdot q\,\frac{\sin(qr)}{\Big(q-i\underbrace{\sqrt{2\frac{T-T_c}{K}}}_{\frac{1}{\xi}}\Big)\Big(q+i\underbrace{\sqrt{2\frac{T-T_c}{K}}}_{\frac{1}{\xi}}\Big)} = \frac{a}{2i}$$

$$= \frac{a}{2}$$



$$G(r) \sim \frac{e^{-\frac{r}{\xi}}}{r^{d-2}}$$

a

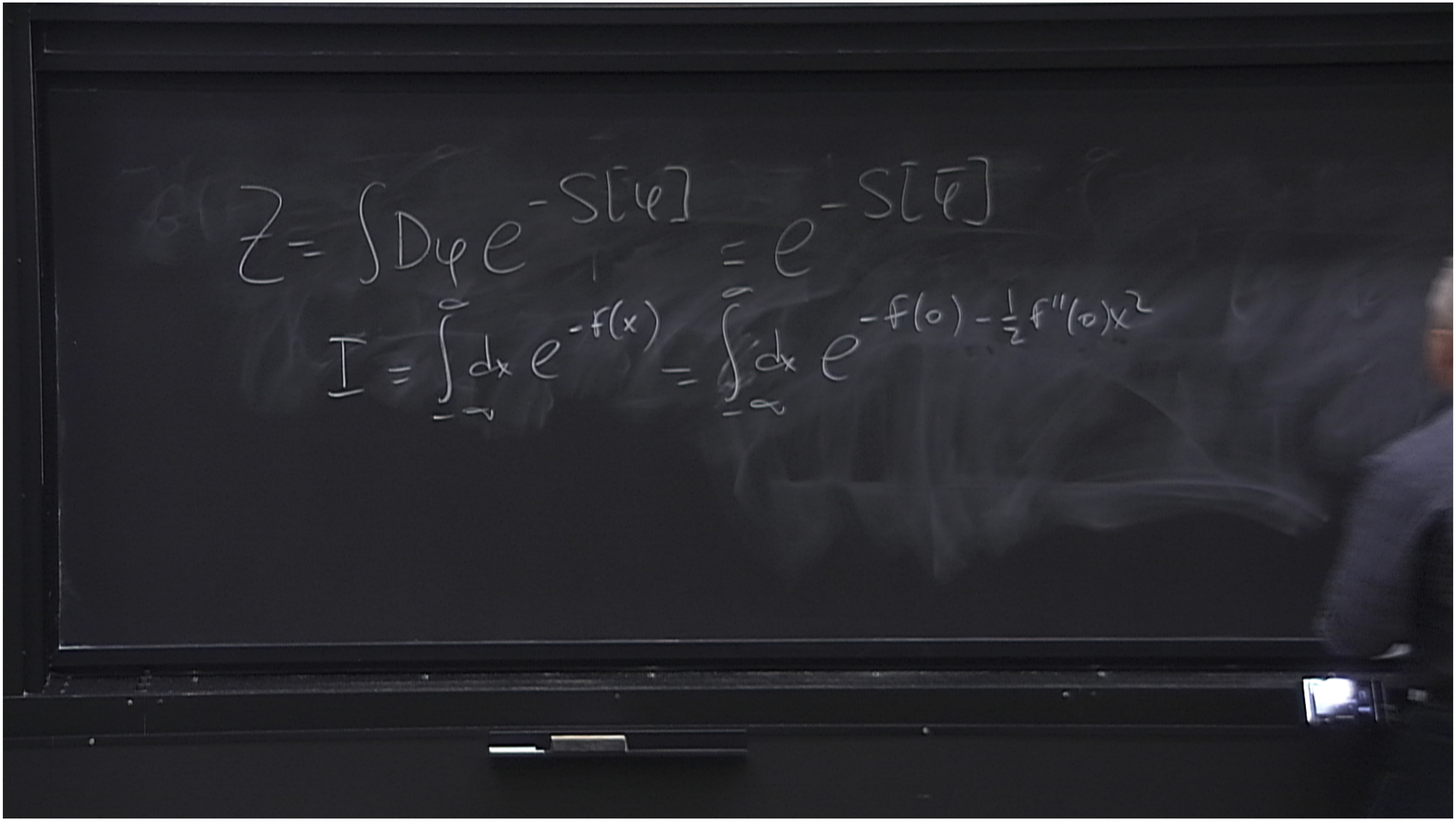
$$G_{ij} = \langle \sigma_i \sigma_j \rangle - \underbrace{\langle \sigma_i \rangle \langle \sigma_j \rangle}_{M^2}$$

$$\xi \sim \frac{1}{\sqrt{T-T_c}} \sim |t|^{-\nu}$$

At $T = T_c$

$$G(r) \sim \frac{1}{r^{d-2}}$$ - scale invariant.

$\nu = \frac{1}{2}$ - correlation length critical exponent.


$Z = \int D\varphi\, e^{-S[\varphi]} \approx e^{-S[\bar{\varphi}]}$
$I = \int_{-\infty}^{\infty} dx\, e^{-f(x)} \approx \int_{-\infty}^{\infty} dx\, e^{-f(0) - \frac{1}{2} f''(0) x^2}$

Expand $S[\varphi]$ around $\varphi = \bar{\varphi}$

$$S[\varphi] \simeq S[\bar{\varphi}] + \frac{1}{2}\sum_{ij} \left.\frac{\partial^2 S}{\partial\varphi_i \partial\varphi_j}\right|_{\bar{\varphi}} \delta\varphi_i\, \delta\varphi_j$$

$$\delta\varphi_i = \varphi_i - \bar{\varphi}$$

$\bar{\varphi}]$

$(0) - \frac{1}{2} f''(0) x^2$

Expand $S[\varphi]$ around $\varphi = \bar{\varphi}$

$$S[\varphi] \simeq S[\bar{\varphi}] + \frac{1}{2} \sum_{ij} \left. \frac{\partial^2 S}{\partial \varphi_i \partial \varphi_j} \right|_{\bar{\varphi}} \delta\varphi_i \, \delta\varphi_j$$

$$\delta\varphi_i = \varphi_i - \bar{\varphi}$$

$$S[\varphi] = \frac{1}{2T} \sum_{ij} \varphi_i J^{-1}_{ij} \varphi_j - \sum_i \ln\left[2\cosh\left(\frac{\varphi_i}{T}\right)\right]$$

$\bar{\varphi}]$

$(0) - \frac{1}{2} f''(0) x^2$

Expand $S[\varphi]$ around $\varphi = \bar{\varphi}$

$$S[\varphi] \simeq S[\bar{\varphi}] + \frac{1}{2} \sum_{ij} \frac{\partial^2 S}{\partial \varphi_i \partial \varphi_j}\Big|_{\bar{\varphi}} \delta\varphi_i \, \delta\varphi_j$$

$$\delta\varphi_i = \varphi_i - \bar{\varphi}$$

$$S[\varphi] = \frac{1}{2T} \sum_{ij} \varphi_i J^{-1}_{ij} \varphi_j - \sum_i \ln\left[2\cosh\left(\frac{\varphi_i}{T}\right)\right], \quad \varphi_i = \bar{\varphi} + \delta\varphi_i$$

$$S[\varphi] = \frac{1}{2T} \sum_{ij} \left(\bar{\varphi} + \delta\varphi_i\right) J^{-1}_{ij} \left(\bar{\varphi} + \delta\varphi_j\right) - \sum_i \ln\left[2\cosh\left(\frac{\bar{\varphi} + \delta}{T}\right.\right.$$

$$\ldots\cosh\left(\frac{\bar{\varphi}+\delta\varphi_i}{T}\right)\Big] = S[\bar{\varphi}] + \frac{1}{T}\sum_{ij} J^{-1}_{ij}\,\bar{\varphi}\,\delta\varphi_i - \frac{1}{T}\sum_i \tanh\left(\frac{\bar{\varphi}}{T}\right)\delta\varphi_i$$

$$+\delta\varphi_j) - \sum_i \ln\left[2\cosh\left(\frac{\bar{\varphi}+\delta\varphi_i}{T}\right)\right]\Big] = S[\bar{\varphi}] + \frac{1}{T}\sum_{ij} J_{ij}^{-1}\,\bar{\varphi}\,\delta\varphi_i \, -$$

$$-\frac{1}{2}\sum_i \left[1-\tanh^2\left(\frac{\bar{\varphi}}{T}\right)\right]\left(\frac{\delta\varphi_i}{T}\right)^2 + \frac{1}{2T}\sum_{ij}\delta\varphi_i\, J_{ij}^{-1}\,\delta\varphi_j$$