

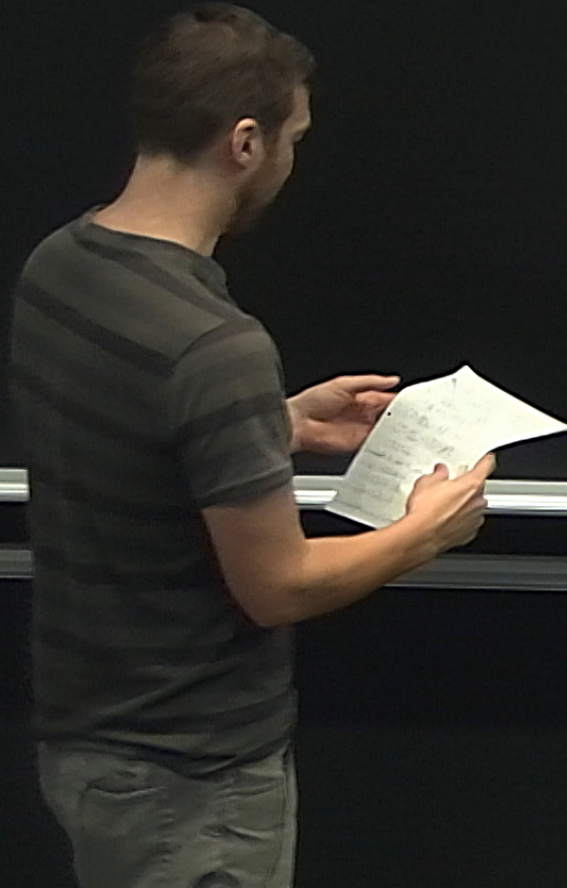
Title: 2016/2017 Statistical Mechanics 2 - Roger Melko - Lecture 5

Date: Jan 18, 2017 10:30 AM

URL: <http://pirsa.org/17010051>

Abstract:

MFT gives $G_{ij} = -T \frac{\partial^2 F}{\partial B_i \partial B_j} \Big|_{B=0} = T \frac{\partial m_i}{\partial B_j} \Big|_{B=0}$



CAUTION
Do not touch the board or the chalkboard eraser.
If you need to use the board, please contact the instructor.

$$= \left[\frac{1}{T} \sum_k \mathcal{J}_{ij} G_{kj} + \delta_{ij} \right] [1 - m^2]$$

Today: let's calculate G_{ij} above T_c where $M=0$

$$= \left[\frac{1}{T} \sum_{\ell} J_{\ell} G_{\ell j} + \delta_{ij} \right] [1 - m^2]$$

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$$T > T_c, \quad G_{ij} = \left[\frac{1}{T} \sum_{\ell} J_{i\ell} G_{\ell j} + \delta_{ij} \right]$$

$$G_{ij} - \frac{1}{T} \sum_{\ell} J_{i\ell} G_{\ell j} = \delta_{ij}$$

$$\sum_{\ell} \left[\delta_{i\ell} - \frac{1}{T} J_{i\ell} \right] G_{\ell j} = \delta_{ij}$$

Solve this equation
using Fourier
transform.

Introduce the lattice F.T.

$$T > T_c, \quad G_{ij} = \left[\frac{1}{T} \sum_l J_{le} G_{lij} + \delta_{ij} \right]$$

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$$\psi_i = \frac{1}{N} \sum_k \psi_k e^{i \vec{k} \cdot \vec{r}_i}$$

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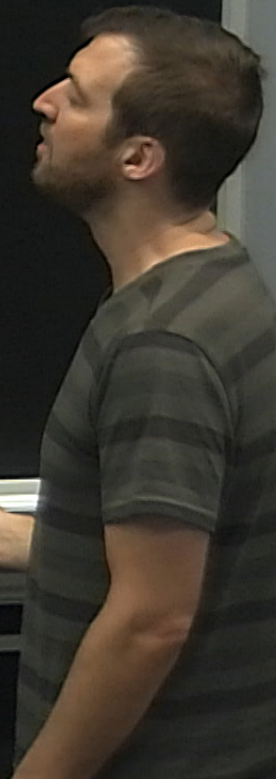
assume Periodic Boundary
conditions

$$\psi(\vec{r}_i) \equiv \psi_i = \psi(\vec{r}_i + L\vec{a})$$

where L is the length of the crystal
vectors along the lattice directions.

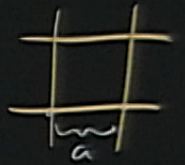
$$\Rightarrow e^{i\vec{k} \cdot \vec{r}_i} = e^{i\vec{k} \cdot (\vec{r}_i + L\hat{x})}$$

$$\Rightarrow \vec{k} \cdot \hat{x} = k_x = \frac{2\pi n_x}{L}$$



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

$$\Rightarrow \vec{k} \cdot \vec{a} = k_x = \frac{2\pi n_x}{L} \quad \text{and } n_x \text{ is an integer}$$



where $\vec{r}_i = \sum_{\vec{a}} l_i \vec{a}$ where $\left\{ \begin{array}{l} a \text{ is the lattice "constant"} \\ \text{and } l_i \text{ is an integer.} \end{array} \right.$

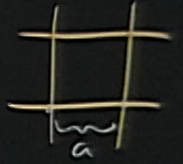
vectors along the lattice directions.

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

$$\Rightarrow \vec{k} \cdot \vec{\lambda} = k_{\lambda} = \frac{2\pi n_{\lambda}}{L} \quad \text{and } n_{\lambda} \text{ is an integer}$$

where $\vec{r}_i = \sum_{\vec{\lambda}} l_i a \vec{\lambda}$ where $\left\{ \begin{array}{l} a \text{ is the lattice "constant"} \\ \text{and } l_i \text{ is an integer.} \end{array} \right.$

This means that k_{λ} can be restricted to the first BZ



Since $k_x \rightarrow k_x + \frac{2\pi n}{a}$ doesn't change $\vec{k} \cdot \vec{r}_i$

CAUTION

DO NOT TOUCH THE BOARD
OR THE BOARDER
OR THE BOARDER

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Now define the F.T. for G_{ij} , J_j (use \vec{q} for momentum)

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

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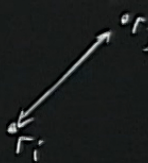
$$J_{ij} = \frac{1}{N} \sum_{\vec{q}} J(\vec{q}) e^{i\vec{q} \cdot (\vec{r}_i - \vec{r}_j)}$$


$$G_{ij} - \frac{1}{T} \sum_{\ell} J_{\ell} G_{\ell j} = \delta_{ij} \quad \text{sub in the above expressions.}$$

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CAUTION
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IF YOU HAVE ANY QUESTIONS
PLEASE ASK THE LECTURER

$$\frac{1}{N} \sum_{\vec{q}} G(\vec{q}) e^{i\vec{q} \cdot (\vec{r}_i - \vec{r}_j)} = \frac{1}{T} \sum_{\ell} \frac{1}{N} \sum_{\vec{q}'} \sum_{\vec{q}''} J(\vec{q}') e^{i\vec{q}'' \cdot (\vec{r}_i - \vec{r}_j)}$$

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$$\begin{aligned}
 \frac{1}{N} \sum_{\vec{q}} G(\vec{q}) e^{i\vec{q} \cdot (\vec{r}_i - \vec{r}_j)} &= \frac{1}{T} \sum_{\ell} \frac{1}{N^2} \sum_{\vec{q}'} \sum_{\vec{q}''} J(\vec{q}') e^{i\vec{q}' \cdot (\vec{r}_i - \vec{r}_\ell)} G(\vec{q}'') \\
 &= \frac{1}{N} \sum_{\vec{q}} e^{i\vec{q} \cdot (\vec{r}_i - \vec{r}_j)}
 \end{aligned}$$

$e^{i\vec{q}'' \cdot (\vec{r}_j - \vec{r}_\ell)}$

$$N \sum_{\vec{q}}$$

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

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

Here I've used

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

Similarly note:

$$\delta_{\vec{q}' \vec{q}''} = \frac{1}{N} \sum_{\vec{r}_l} e^{-i(\vec{q}' - \vec{q}'') \cdot \vec{r}_l}$$

CAUTION

$$\frac{1}{N} \sum_{\vec{q}} G(\vec{q}) e^{i\vec{q} \cdot (\vec{r}_i - \vec{r}_j)} = \frac{1}{T} \sum_{\ell} \frac{1}{N^2} \sum_{\vec{q}'} \sum_{\vec{q}''} J(\vec{q}') e^{i\vec{q}' \cdot \vec{r}_i} G(\vec{q}'') e^{i\vec{q}'' \cdot (\vec{r}_j - \vec{r}_\ell)}$$

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

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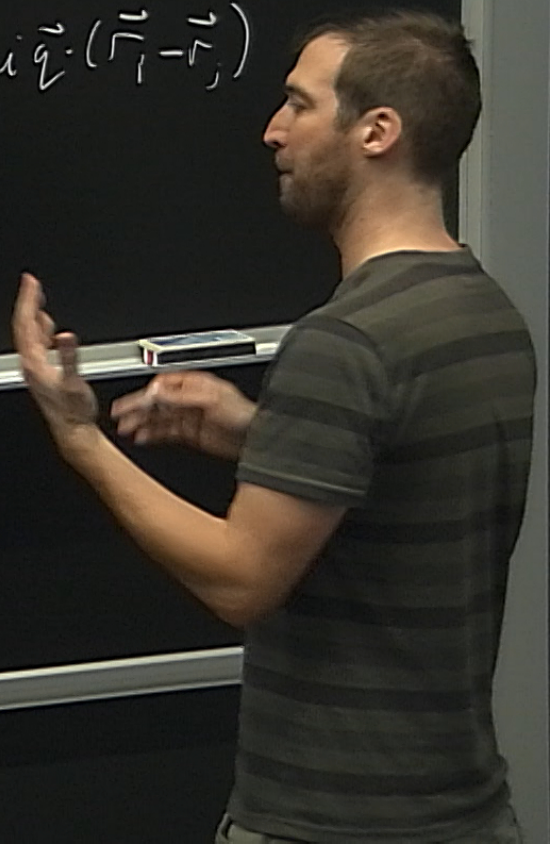
Similarly note: $\delta_{\vec{q}'\vec{q}''} = \frac{1}{N} \sum_{\ell} e^{-i(\vec{q}' - \vec{q}'') \cdot \vec{r}_\ell}$

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Therefore

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



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Therefore

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

Equate all the terms inside $\sum_{\vec{q}}$ to get

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

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

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We are interested in G_{ij} at large distances $|\vec{r}_i - \vec{r}_j| \gg R$

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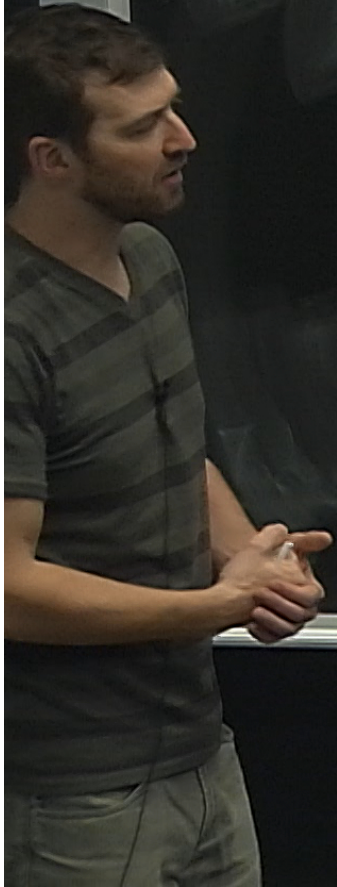
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where R is the "effective range" of interactions J_{ij} (eg. $R \sim a$)

Long distances mean small q . So we will expand the exponential in a Taylor series.



CAUTION
Do not touch the surface of the board.
Do not touch the board.
Do not touch the board.

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

In a Taylor series. (Q: does this make sense?)

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

CAUTION
Do not touch the screen or the board.
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$$\Rightarrow J(\vec{q}) = J - \frac{1}{2N} \sum_{ij} J_{ij} [\vec{q} \cdot (\vec{r}_i - \vec{r}_j)]^2 \quad \left(J = \sum_j J_{ij} \right)$$

the dot product $\vec{q} \cdot (\vec{r}_i - \vec{r}_j) = \sum_{\lambda} q_{\lambda} (r_i - r_j)_{\lambda}$

$$\sum_{ij} J_{ij} [\vec{q} \cdot (\vec{r}_i - \vec{r}_j)]^2 = \sum_{ij} J_{ij} \sum_{\lambda \lambda'} q_{\lambda} q_{\lambda'} (r_i - r_j)_{\lambda} (r_i - r_j)_{\lambda'}$$

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$$= \sum_{ij} J_{ij} \sum_{\lambda} q_{\lambda}^2 (\vec{r}_i - \vec{r}_j)_{\lambda}^2 \quad (\oplus)$$

$$= \frac{1}{d} \sum_{ij} J_{ij} |\vec{r}_i - \vec{r}_j|^2 q_r^2 \quad (d \text{ dimensions})$$

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

$$\Rightarrow J(\vec{q}) \approx J - \frac{1}{2} K q_r^2$$

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⊗ proof for

$$\sum_{ij} J_{ij} [\vec{q} \cdot (\vec{r}_i - \vec{r}_j)]^2 = \sum_{ij} J_{ij} \sum_{\lambda} \sum_{\lambda'} q_{\lambda} q_{\lambda'} (\vec{r}_i - \vec{r}_j)_{\lambda} (\vec{r}_i - \vec{r}_j)_{\lambda'}$$

Let's

$$\sum_{\lambda, \lambda'} q_{\lambda} q_{\lambda'} (\mathbf{r}_i - \mathbf{r}_{\lambda}) (\mathbf{r}_i - \mathbf{r}_{\lambda'})_{\lambda} = q_{\lambda_x}^2 (\mathbf{r}_i - \mathbf{r}_{\lambda})_x + q_{\lambda_y}^2 (\mathbf{r}_i - \mathbf{r}_{\lambda})_y$$

$$+ q_{\lambda_x} q_{\lambda_y} (\mathbf{r}_i - \mathbf{r}_{\lambda})_x (\mathbf{r}_i - \mathbf{r}_{\lambda})_y + q_{\lambda_y} q_{\lambda_x} (\mathbf{r}_i - \mathbf{r}_{\lambda})_y (\mathbf{r}_i - \mathbf{r}_{\lambda})_x$$

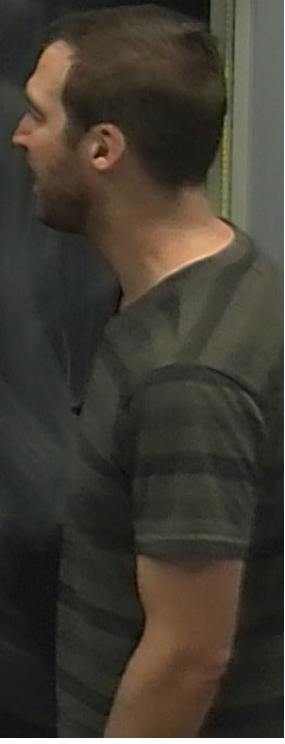
$$J_{ij} = N \sum_{\mathbf{q}} J(\mathbf{q}) e^{i\mathbf{q} \cdot (\mathbf{r}_i - \mathbf{r}_j)}$$

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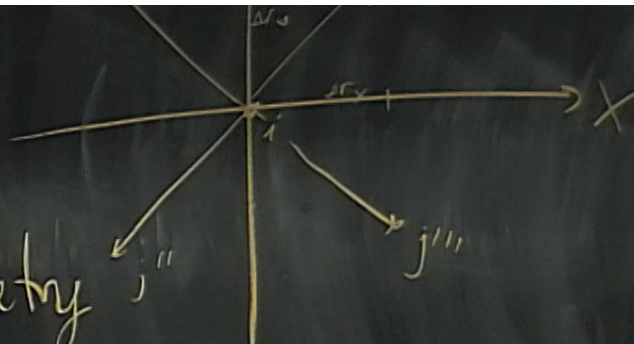
$$+ q_l q_y (r_l, r_x) (r_l, r_y) + q_y q_x (r_l, r_x) (r_l, r_y)$$

We need

$$\sum_j J_{ij} (\vec{r}_i - \vec{r}_j)_x (\vec{r}_i - \vec{r}_j)_y = 0$$



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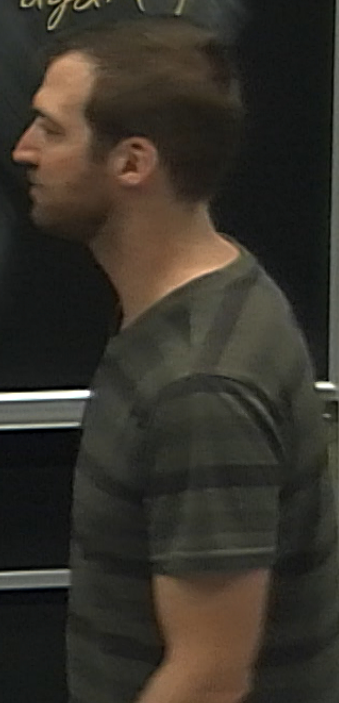


True if you have "inversion" symmetry "j"

$\Rightarrow \sum_{ij} J_{ij} \sum_{\lambda} q_{\lambda}^2 (\vec{r}_i - \vec{r}_j)_{\lambda}^2$ generally. (check $d=x,y$ again)

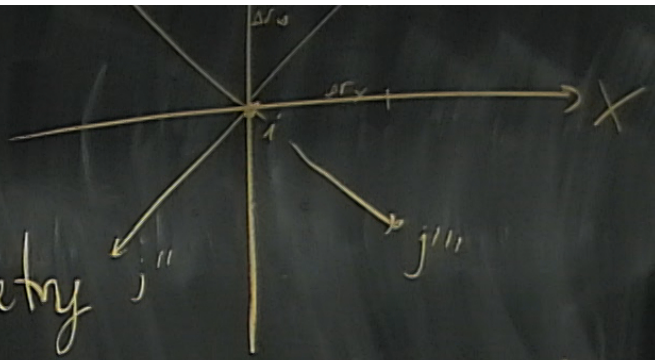
$$= \sum_{ij} J_{ij} \left[(\vec{r}_i - \vec{r}_j)_x^2 q_x^2 + q_y^2 (\vec{r}_i - \vec{r}_j)_y^2 \right]$$

=



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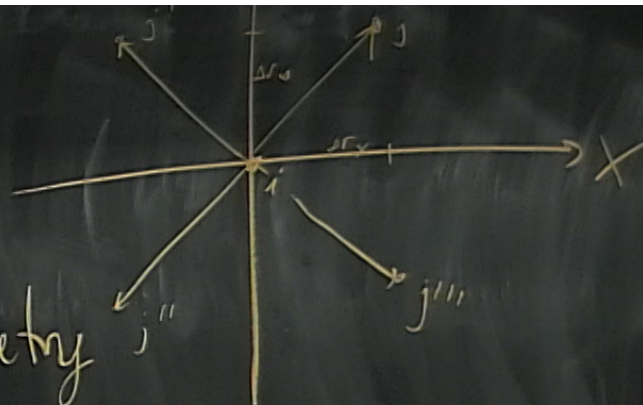
$$\Rightarrow \sum_{i,j} J_{ij} \sum_{\lambda} q_{\lambda}^2 (\vec{r}_i - \vec{r}_j)_{\lambda}^2 \text{ generally. (check } d=x,y \text{ again)}$$

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$$= \frac{1}{d} \sum_{i,j} J_{ij} |\vec{r}_i - \vec{r}_j|^2 q^2 \quad (\text{check})$$

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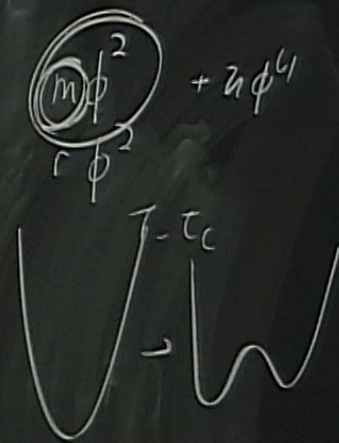
$$= \frac{1}{d} \sum_{ij} J_{ij} |\vec{r}_i - \vec{r}_j|^2 q^2 \quad (\text{check})$$

d-dim hypercube.

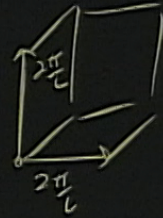
Then: $G(\vec{q}) = \frac{1}{1 - \frac{1}{T}(J - \frac{1}{2}Kq^2)} = \frac{1}{1 - \frac{J}{T} + \frac{1}{2T}q^2}$

Recall that in MFT $T_c = J$

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

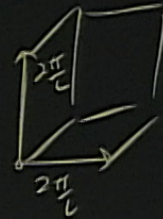


Note: to take the continuum limit of a lattice sum
→ recip. Lattice spacing is $\frac{2\pi}{L}$ in every direction



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→ Volume V_0 per lattice site, $V_0 \rightarrow 0$ in the cont

→ Total volume has to be fixed

(tot vol $\sim V = L^3$)

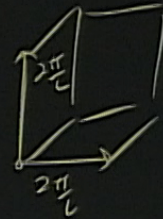
$$V_0 \sum_{\vec{q}} = \int d\vec{q}$$

(3d)

$$\sum_{\vec{q}} \rightarrow \frac{L^3}{(2\pi)^3}$$

Note: to take the continuum limit of a lattice sum

→ recip. Lattice spacing is $\frac{2\pi}{L}$ in every direction



→ Volume V_0 per lattice site, $V_0 \rightarrow 0$ in the continuum

→ Total volume has to be fixed

(total volume $V = L^3$)

$$V_0 \sum_{\vec{q}} = \int d\vec{q}$$

$$\text{and } \frac{L^3}{N} = a^3$$

(3d)

$$\sum_{\vec{q}} \rightarrow \frac{L^3}{(2\pi)^3} \int d\vec{q}$$

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

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

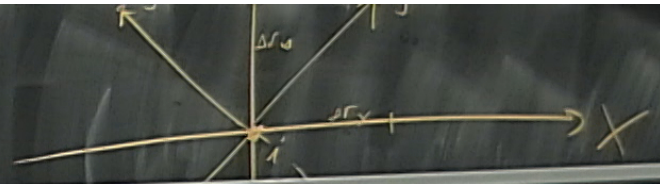
$$G(\vec{r}) = \frac{a^3 T}{\pi^2 r K} \int_0^{\infty} \frac{dq \cdot q \cdot \sin(qr)}{\left(q - i\sqrt{2\frac{T-T_c}{K}}\right)\left(q + i\sqrt{2\frac{T-T_c}{K}}\right)}$$

$$= \frac{a^3 T}{\pi^2 r K} \frac{1}{2} \int_{-\infty}^{\infty} dq \cdot q \cdot \frac{\left(\frac{1}{2i}\right) (e^{iqr} - e^{-iqr})}{\left(q - i\sqrt{2\frac{T-T_c}{K}}\right)\left(q + i\sqrt{2\frac{T-T_c}{K}}\right)}$$

Use contour integration

$$\int_{-\infty}^{\infty} \frac{z e^{-iz}}{(z^2 + a)} dz = i\pi e^{-\sqrt{a}}$$

$$\sum_j J_{ij} (\vec{r}_i - \vec{r}_j)_x (\vec{r}_i - \vec{r}_j)_y$$



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

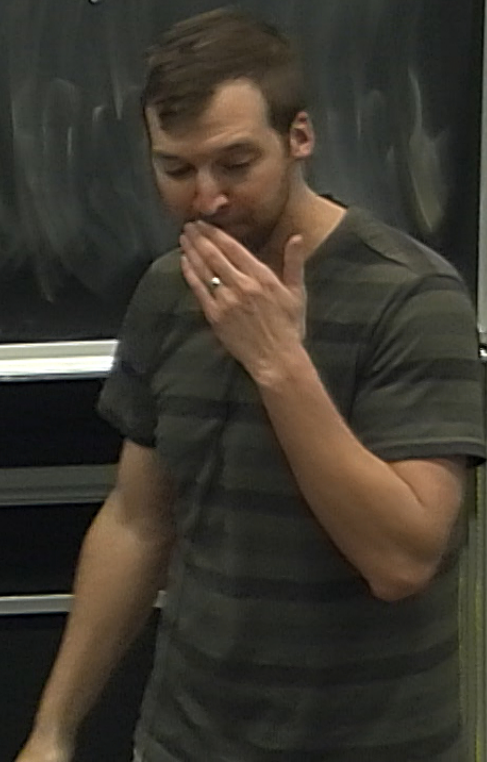
Then $G(r) = \frac{a}{2\pi Kr} e^{-\sqrt{d} r/\xi}$

Define the correlation length $\xi = \sqrt{\frac{K}{2(T-T_c)}}$

So that $G(r) \propto \frac{e^{-r/\xi}}{r}$ $d=3$ only.

Define the correlation length $\xi = \sqrt{\frac{1}{2(T-T_c)}}$

So that $G(r) \propto \frac{e^{-r/\xi}}{r}$ $d=3$ only.



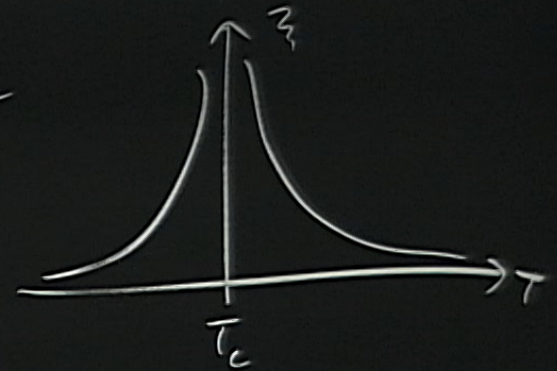
H.W. #2: in d
dimensions

$$G(r) \propto \frac{e^{-r/\xi}}{r^{(d-2)/2}} \quad \text{⑦ assign}$$

So the correlation length diverges at T_c

$$\text{as } \xi \sim (T - T_c)^{-\nu}$$

$$\text{and } \nu = \frac{1}{2} \text{ in MFT}$$

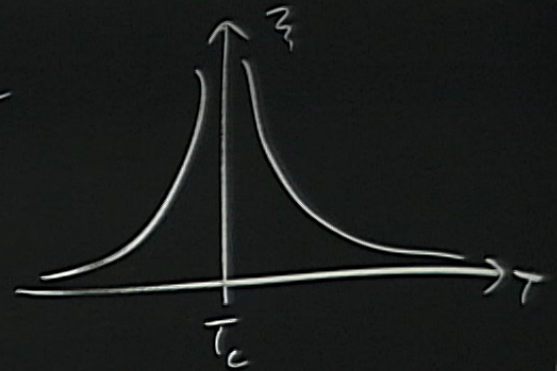


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(note $\xi \rightarrow \infty$ at T_c gives us "criticality" at a continuous transition. For First-order this is not true)

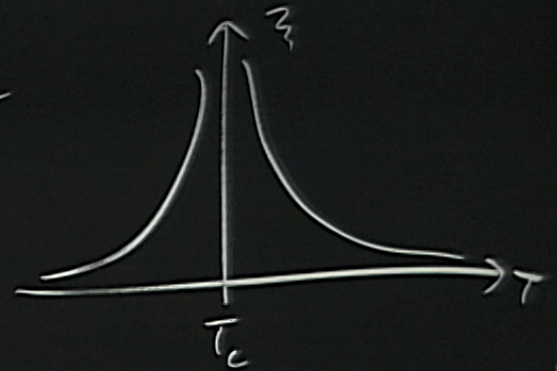


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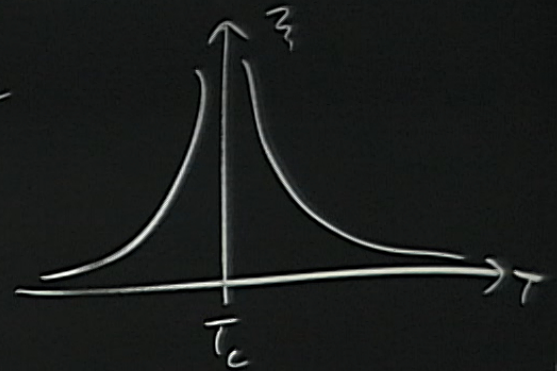
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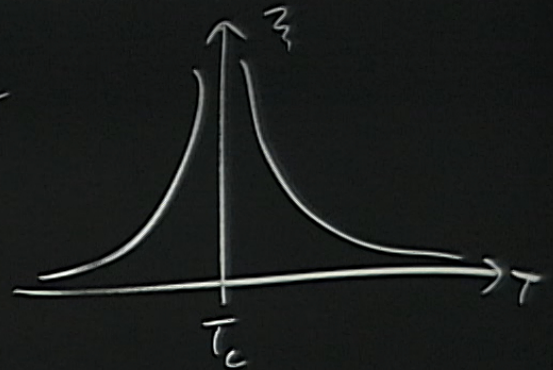
ξ is a measure of length



So the correlation length diverges at T_c

$$\text{as } \xi \sim (T - T_c)^{-\nu}$$

$$\text{and } \nu = \frac{1}{2} \text{ in MFT}$$



(note $\xi \rightarrow \infty$ at T_c gives us "criticality" at a continuous transition. For First-order this is not true)

ξ is a measure of length over which two particles are correlated with probability 1.

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

$$= \frac{a^3 T}{\pi^2 r K} \frac{1}{2} \int_{-\infty}^{\infty} dq \, q \frac{\left(\frac{1}{2i}\right) (e^{iqr} - e^{-iqr})}{\left(q - i\sqrt{2\frac{T-T_c}{K}}\right)\left(q + i\sqrt{2\frac{T-T_c}{K}}\right)}$$

Use contour integration

$$\int_{-\infty}^{\infty} \frac{z e^{iz}}{(z^2 + a)} dz = \pm i\pi e^{-\sqrt{a}}$$

