Bose-Hubbard and rotor models

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Bose-Hubbard Hamiltonian:

$$\boxed{H_{BH} = -J_H \sum_{\langle ij \rangle} \left(a_i^+ a_j + h.c. \right) + \frac{U_H}{2} \sum_i \left(n_i - \tilde{n} \right)^2 - \mu \sum_i \left(n_i - \tilde{n} \right)}$$

large filling, truncate Hilbert space to $|\tilde{n}-1\rangle, |\tilde{n}\rangle, |\tilde{n}+1\rangle$ for each site

- introduce three bosons t_-, t_0, t_+ for each site

$$|\tilde{n}-1\rangle = t_-^+ |\underline{0}\rangle, \quad |\tilde{n}\rangle = t_0^+ |\underline{0}\rangle, \quad |\tilde{n}+1\rangle = t_+^+ |\underline{0}\rangle$$

with constraint $\sum_{\alpha=-,0,+} t_\alpha^+ t_\alpha = 1$ $\qquad \uparrow$ vacuum

- write a, a^+ in terms of t, t^+

$$a^+ = \sqrt{\tilde{n}}\, t_0^+ t_- + \sqrt{\tilde{n}+1}\, t_+^+ t_0$$

$$a = \sqrt{\tilde{n}}\, t_-^+ t_0 + \sqrt{\tilde{n}+1}\, t_0^+ t_+$$

check action on basis states

$$a^+ |\tilde{n}-1\rangle = \left(\sqrt{\tilde{n}}\, t_0^+ t_- + \sqrt{\tilde{n}+1}\, t_+^+ t_0 \right) t_-^+ |\underline{0}\rangle$$

$$= \sqrt{\tilde{n}}\, t_0^+ |0\rangle = \sqrt{\tilde{n}}\, |\tilde{n}\rangle$$

$$a^+ |\tilde{n}\rangle = \left(\sqrt{\tilde{n}}\, t_0^+ t_- + \sqrt{\tilde{n}+1}\, t_+^+ t_0 \right) t_0^+ |\underline{0}\rangle$$

$$= \sqrt{\tilde{n}+1}\, t_+^+ |0\rangle = \sqrt{\tilde{n}+1}\, |\tilde{n}+1\rangle$$

$$a|\tilde{n}\rangle = \left(\sqrt{\tilde{n}}\, t_-^+ t_0 + \sqrt{\tilde{n}+1}\, t_0^+ t_+\right) t_0^+ |\underline{0}\rangle$$

$$= \sqrt{\tilde{n}}\, t_-^+ |0\rangle = \sqrt{\tilde{n}}\, |\tilde{n}-1\rangle$$

$$a|\tilde{n}+1\rangle = \left(\sqrt{\tilde{n}}\, t_-^+ t_0 + \sqrt{\tilde{n}+1}\, t_0^+ t_+\right) t_+^+ |\underline{0}\rangle$$

$$= \sqrt{\tilde{n}+1}\, t_0^+ |0\rangle = \sqrt{\tilde{n}+1}\, |\tilde{n}\rangle$$

all OK ✓

<u>check commutator</u> $[a, a^+] = aa^+ - a^+a = 1$

because of Hilbert space truncation, this can only be tested when acting on $|\tilde{n}\rangle$ (otherwise you are taken out of truncated Hilbert space).

Formulate Hamiltonian in terms of t, t^+

$$H = -J_H \sum_{\langle ij \rangle} \Big[\left(\sqrt{\tilde{n}}\, t^+_{0i} t_{-i} + \sqrt{\tilde{n}+1}\, t^+_{+i} t_{0i} \right)\left(\sqrt{\tilde{n}}\, t^+_{-j} t_{0j} + \sqrt{\tilde{n}+1}\, t^+_{0j} t_{+j} \right) + h.c \Big]$$

$$+ \frac{U_H}{2} \sum_i \left((\tilde{n}-1) t^+_{-i} t_{-i} + \tilde{n}\, t^+_{0i} t_{0i} + (\tilde{n}+1) t^+_{+i} t_{+i} - \tilde{n} \right)^2$$

$$- \mu \sum_i \left((\tilde{n}-1) t^+_{-i} t_{-i} + \tilde{n}\, t^+_{0i} t_{0i} + (\tilde{n}+1) t^+_{+i} t_{+i} - \tilde{n} \right)$$

$\tilde{n} \gg 1$

$$H = -J_H \tilde{n} \sum_{\langle ij \rangle} \Big[\left(t^+_{0i} t_{-i} + t^+_{+i} t_{0i} \right)\left(t^+_{-j} t_{0j} + t^+_{0j} t_{+j} \right) + h.c. \Big]$$

$$+ \frac{U_H}{2} \sum_i \left(t^+_{+i} t_{+i} - t^+_{-i} t_{-i} \right)^2 - \mu \sum_i \left(t^+_{+i} t_{+i} - t^+_{-i} t_{-i} \right)$$

Define new operators

$$\left.\begin{aligned} S^z_i &= t^+_{+i} t_{+i} - t^+_{-i} t_{-i} \\ S^+_i &= \sqrt{2} \left(t^+_{0i} t_{-i} + t^+_{+i} t_{0i} \right) \\ S^-_i &= \sqrt{2} \left(t^+_{-i} t_{0i} + t^+_{0i} t_{+i} \right) \end{aligned}\right\} \text{ spin-1 algebra}$$

$$S^x_i \pm i S^y_i = S^\pm_i$$

rewrite H in terms of S

$$H = -J_H \tilde{n} \sum_{\langle ij \rangle} \left[\frac{1}{2} S_i^+ S_j^- + \frac{1}{2} S_j^+ S_i^- \right] + \frac{U_H}{2} \sum_i \left(S_i^z \right)^2 - \mu \sum_i S_i^z$$

$$\boxed{H = -J_H \tilde{n} \sum_{\langle ij \rangle} \left(S_i^x S_j^x + S_i^y S_j^y \right) + \frac{U_H}{2} \sum_i \left(S_i^z \right)^2 - \mu \sum_i S_i^z}$$

rotor model in spin representation

absorb $\tilde{n}$: $J = J_H \tilde{n}$, $U = U_H$

$$H = -J \sum_{\langle ij \rangle} \left(S_i^x S_j^x + S_i^y S_j^y \right) + \frac{U}{2} \sum_i \left(S_i^z \right)^2 - \mu \sum_i S_i^z$$

$$H = -\frac{J}{2} \sum_{\langle ij \rangle} \left(S_i^+ S_j^- + S_j^+ S_i^- \right) + \frac{U}{2} \sum_i \left(S_i^z \right)^2 - \mu \sum_i S_i^z$$

Superfluid order parameter

- in original Bose-Hubbard model

$$\psi_{BH}(\vec{x}_i) = \langle a_i \rangle \qquad \Rightarrow \text{ substitute operators}$$

$$\psi_{BH}(\vec{x}_i) = \langle \sqrt{\tilde{n}}\, t^+_{-i} t_{0i} + \sqrt{\tilde{n}+1}\, t^+_{0i} t_{+i} \rangle$$

$$\approx \sqrt{\tilde{n}}\, \langle t^+_{-i} t_{0i} + t^+_{0i} t_{+i} \rangle$$

$$= \frac{\sqrt{\tilde{n}}}{\sqrt{2}} \langle S^-_i \rangle$$

- ignore prefactor $\Rightarrow$ OP can be defined as either $\langle S^+ \rangle$ or $\langle S^- \rangle$ (one is complex conjugate of the other)

Altman/Auerbach PRL defines

$$\boxed{\psi(\vec{x}_i) = \langle S^+_i \rangle} = \langle S^x_i \rangle + i \langle S^y_i \rangle$$

- measures <u>symmetry-breaking</u> in XY plane

Quantum mean-field theory for rotor model

H in spin representation

$$\boxed{\begin{aligned} H &= -J \sum_{\langle ij \rangle} \left(S_i^x S_j^x + S_i^y S_j^y \right) + \frac{U}{2} \sum_i \left(S_i^z \right)^2 - \mu \sum_i S_i^z \\ H &= -\frac{J}{2} \sum_{\langle ij \rangle} \left(S_i^+ S_j^- + S_j^+ S_i^- \right) + \frac{U}{2} \sum_i \left(S_i^z \right)^2 - \mu \sum_i S_i^z \end{aligned}}$$

use $|\uparrow_i\rangle \; |0_i\rangle \; |\downarrow_i\rangle$ for S_i^z eigenstates

mean-field approach:

ground state has product form

$$|\Phi\rangle = \prod_i |\varphi_i\rangle$$

where $|\varphi_i\rangle$ locally interpolates between Mott insulator and superfluid

$$\boxed{|\varphi_i\rangle = \cos(\theta/2)\, |0_i\rangle + \sin(\theta/2)\, e^{i\eta} \frac{1}{\sqrt{2}} \left(|\uparrow_i\rangle + |\downarrow_i\rangle \right)}$$

θ rotates from MI to SF, η is phase variable

Note: ansatz is for particle-hole symmetric case, $\mu = 0$ (equal weights on $|\uparrow\rangle$ and $|\downarrow\rangle$)

$S^+|\uparrow\rangle = 0$, $S^+|0\rangle = \sqrt{2}\,|\uparrow\rangle$, $S^+|\downarrow\rangle = \sqrt{2}\,|0\rangle$

$S^-|\uparrow\rangle = \sqrt{2}\,|0\rangle$, $S^-|0\rangle = \sqrt{2}\,|\downarrow\rangle$, $S^-|\downarrow\rangle = 0$

Variational energy

- evaluate $\langle \Phi | H | \Phi \rangle$

Coulomb-part:

$$\langle \Phi | \frac{U}{2} \sum_i (S_i^z)^2 | \Phi \rangle = \frac{U}{2} \sum_i \langle \varphi_i | (S_i^z)^2 | \varphi_i \rangle$$

$$= \frac{U}{2} \sum_i \sin^2\left(\frac{\theta}{2}\right) \frac{1}{2} \left(\langle \uparrow_i | \uparrow_i \rangle + \langle \downarrow_i | \downarrow_i \rangle \right)$$

$$= N \frac{U}{2} \sin^2\left(\frac{\theta}{2}\right)$$

Josephson-part

$$\langle \Phi | -\frac{J}{2} \sum_{\langle ij \rangle} \left(S_i^+ S_j^- + S_j^+ S_i^- \right) | \Phi \rangle =$$

$$= -\frac{J}{2} \frac{z}{2} N \langle \varphi_i | \langle \varphi_j | \left(S_i^+ S_j^- + S_j^+ S_i^- \right) | \varphi_j \rangle | \varphi_i \rangle$$

$$= -\frac{Jz}{4} N \left[\langle \varphi_i | S_i^+ | \varphi_i \rangle \langle \varphi_j | S_j^- | \varphi_j \rangle + c.c. \right]$$

$$= -\frac{Jz}{4} N \left[\left(\cos\frac{\theta}{2} \sin\frac{\theta}{2} \left(e^{i\eta} + e^{-i\eta} \right) \right)^2 + c.c. \right]$$

$$= -\frac{Jz}{4} N \left[\left(\sin\theta \cos\eta \right)^2 + c.c. \right]$$

$$= -\frac{Jz}{2} N \sin^2\theta \cos^2\eta$$

agrees with (4)
in Altman PRL
for $\bar{n} \to \infty$, $\alpha = \frac{\pi}{2}$

- collect terms:

$$\boxed{\frac{E_0}{N} = \frac{1}{N}\langle \Phi | H | \Phi \rangle = \frac{U}{2}\sin^2\left(\frac{\theta}{2}\right) - \frac{J_z}{2}\sin^2\theta\cos^2\eta}$$

- minimize $\partial/\partial\theta\, E_0 = \frac{\partial}{\partial\eta} E_0 = 0$

$$\partial E_0/\partial\eta = 0 \quad \Rightarrow \quad \eta = 0, \pi \quad \text{minima} \quad \Rightarrow \cos^2\eta = 1$$

$$\left(\eta = \frac{\pi}{2}, \frac{3}{2}\pi \quad \text{maxima}\right)$$

$$\partial E_0/\partial\theta = \frac{\partial}{\partial\theta}\left[\frac{U}{2}\sin^2\frac{\theta}{2} - \frac{J_z}{2}\sin^2\theta\right]$$

$$= \frac{1}{2}U\sin\frac{\theta}{2}\cos\frac{\theta}{2} - J_z\sin\theta\cos\theta$$

$$= \frac{U}{4}\sin\theta - J_z\sin\theta\cos\theta = 0$$

two solutions

(i) $\sin\theta = 0 \quad \Rightarrow \quad \theta = 0, 2\pi, \ldots$ minima

$(\quad \pi, 3\pi, \ldots$ maxima$)$

(ii) $\frac{U}{4} - J_z\cos\theta = 0 \qquad \cos\theta = \frac{U}{4J_z}$

Solution exists for $U < 4J_z$

$\Rightarrow$ $\boxed{\text{MI to SF QPT at } U = 4J_z}$

Order parameter of product wave function

$$|\Phi\rangle = \prod_i |\varphi_i\rangle = \prod_i \left[\cos\left(\frac{\theta}{2}\right)|0_i\rangle + \sin\left(\frac{\theta}{2}\right) e^{i\eta} \frac{1}{\sqrt{2}}\left(|\uparrow_i\rangle + |\downarrow_i\rangle\right)\right]$$

Order parameter:

$$\Psi(\vec{x}_i) = \langle \varphi_i | S_i^+ | \varphi_i \rangle$$

$$\Psi(\vec{x}_i) = \cos\frac{\theta}{2}\sin\frac{\theta}{2}\left(e^{i\eta} + e^{-i\eta}\right) = \sin\theta\cos\eta$$

real, phase fixed

- evaluate OP for M.F. solutions of page (8)

(i) $\theta = 0, 2\pi, \ldots \qquad \eta = 0, \pi, \ldots$

$$\Psi = \sin\theta\cos\eta = 0 \quad \Rightarrow \quad \text{Mott insulator}$$

(ii) $\cos\theta = \frac{U}{4Jz} \qquad \eta = 0, \pi, \ldots$

$$\boxed{\Psi = \pm\sqrt{1 - \left(\frac{U}{4Jz}\right)^2} \neq 0} \qquad \text{Superfluid}$$

$$\Psi = \pm\sqrt{1 - \left(\frac{U}{U_c}\right)^2} = \sqrt{\frac{U_c^2 - U^2}{U_c^2}} \approx \sqrt{\frac{2(U_c - U)}{U_c^2}}$$

$$\sim (U_c - U)^{1/2} \quad \Rightarrow \quad \beta = \frac{1}{2} \quad \text{as expected}$$

Phase of the order parameter

- Order parameter of mean-field wave function from page 6 (or page 9) was <u>real</u>

<u>Question:</u> Where is the OP phase that corresponds to the $U(1)$ or $O(2)$ symmetry?

- Use wave function with additional phase between $|\uparrow\rangle$ and $|\downarrow\rangle$

$$|\Phi\rangle = \prod_i |\varphi_i\rangle = \prod_i \left[\cos\left(\frac{\theta}{2}\right)|0_i\rangle + \sin\left(\frac{\theta}{2}\right) e^{i\eta} \frac{1}{\sqrt{2}}\left(e^{i\varphi}|\uparrow_i\rangle + e^{-i\varphi}|\downarrow_i\rangle\right)\right]$$

- <u>variational energy</u>

$$\langle\Phi| \frac{U}{2}\sum_i (S_i^z)^2 |\Phi\rangle = \frac{U}{2}\sum_i \langle\varphi_i|(S_i^z)^2|\varphi_i\rangle$$

$$= \frac{U}{2}\sum_i \sin^2\left(\frac{\theta}{2}\right) = N\frac{U}{2}\sin^2\left(\frac{\theta}{2}\right) \qquad \underline{\text{as before}}$$

$$\langle\Phi| -\frac{J}{2}\sum_{\langle ij\rangle}\left(S_i^+S_j^- + S_j^+S_i^-\right)|\Phi\rangle = -\frac{Jz}{4}N\langle\varphi_i|\langle\varphi_j|\left(S_i^+S_j^- + S_j^+S_i^-\right)|\varphi_j\rangle|\varphi_i\rangle$$

$$= -\frac{Jz}{4}N\left[\langle\varphi_i|S_i^+|\varphi_i\rangle\langle\varphi_j|S_j^-|\varphi_j\rangle + c.c.\right]$$

$$= -\frac{Jz}{4}N\left[\cos\frac{\theta}{2}\sin\frac{\theta}{2}\left(e^{-i\eta-i\varphi} + e^{i\eta-i\varphi}\right)\cos\frac{\theta}{2}\sin\frac{\theta}{2}\left(e^{i\eta+i\varphi} + e^{-i\eta+i\varphi}\right) + c.c.\right]$$

$$= -\frac{Jz}{4}N\cos^2\frac{\theta}{2}\sin^2\frac{\theta}{2}\left[e^{-i\varphi}2\cos\eta\, e^{i\varphi}2\cos\eta + c.c.\right]$$

$$= -\frac{Jz}{2}N\sin^2\theta\cos^2\eta \qquad \underline{\text{as before}}$$

Variational energy does not depend on φ !

OP of generalized wave function

$$|\Phi\rangle = \prod_i |\varphi_i\rangle = \prod_i \left[\cos\left(\frac{\theta}{2}\right)|0_i\rangle + \sin\left(\frac{\theta}{2}\right) e^{i\eta} \frac{1}{\sqrt{2}}\left(e^{i\varphi}|\uparrow_i\rangle + e^{-i\varphi}|\downarrow_i\rangle\right)\right]$$

$$\psi(\vec{x}_i) = \langle \varphi_i | S_i^+ | \varphi_i \rangle$$

$$= \cos\frac{\theta}{2}\sin\frac{\theta}{2}\left(e^{-i\eta - i\varphi} + e^{i\eta - i\varphi}\right) = \sin\theta \cos\eta \, e^{-i\varphi}$$

$\Rightarrow$ complex OP, i.e. φ represents OP phase

- Goldstone mode corresponds to slow variations of φ
- Higgs mode corresponds to slow variation of θ

Order parameter and OP magnitude in mean-field theory

$$|\Phi\rangle = \prod_i |\varphi_i\rangle = \prod_i \left[\cos\left(\frac{\theta}{2}\right)|0_i\rangle + \sin\left(\frac{\theta}{2}\right)\frac{1}{\sqrt{2}}\left(e^{i\varphi}|\Uparrow_i\rangle + e^{-i\varphi}|\Downarrow_i\rangle\right)\right]$$

local OP:

$$\langle\psi_i\rangle = \langle\varphi_i|S_i^+|\varphi_i\rangle = 2\cos\frac{\theta}{2}\sin\frac{\theta}{2}\,e^{-i\varphi}$$

$$\boxed{\langle\psi_i\rangle = \sin\theta\, e^{-i\varphi}} \qquad = \langle S_i^x\rangle + i\langle S_i^y\rangle$$

local OP magnitude

$$\langle|\psi_i^2|\rangle = \langle\varphi_i|S_i^{x2} + S_i^{y2}|\varphi_i\rangle = \frac{1}{2}\langle\varphi_i|S_i^+S_i^- + S_i^-S_i^+|\varphi_i\rangle$$

use $S_x^2 + S_y^2 = S^2 - S^{z2}$ (here $S^2 = S(S+1) = 2$)

$$\langle\varphi_i|S_i^{z2}|\varphi_i\rangle = \frac{1}{2}\sin^2\frac{\theta}{2}\,(1+1) = \sin^2\frac{\theta}{2}$$

$$\langle|\psi_i^2|\rangle = 2 - \sin^2\frac{\theta}{2}$$

$$\boxed{\langle|\psi_i|^2\rangle = \frac{3}{2} + \frac{1}{2}\cos\theta}$$

$\cos\theta = 1 - 2\sin^2\frac{\theta}{2}$

$\sin^2\frac{\theta}{2} = \frac{1}{2}(1-\cos\theta)$

insulator: $\theta = 0$ $\quad \langle\psi_i\rangle = 0$, $\langle|\psi_i|^2\rangle = 2$

superfluid $\cos\theta = \frac{U}{4Jz} = \frac{U}{U_c}$ $\quad \langle\psi\rangle = \sqrt{1-(U/U_c)^2}\, e^{i\varphi}$

$$\langle|\psi^2|\rangle = \frac{3}{2} + \frac{1}{2}\frac{U}{4Jz}$$

Excitations of mean-field ground state

- consider excitations about m.f. state

$$|\Phi\rangle = \prod_i |\varphi_i\rangle = \prod_i \left[\cos\left(\frac{\theta}{2}\right)|0_i\rangle + \sin\left(\frac{\theta}{2}\right)\frac{1}{\sqrt{2}}\left(|\Uparrow_i\rangle + |\Downarrow_i\rangle\right)\right]$$

(fixing the phases η and φ at zero)

- canonical transformation (rotation) from bosons t_{0i}, t_{+i}, t_{-i} to $b_{0i}, b_{\alpha i}, b_{\varphi i}$

$$\boxed{\begin{aligned} b_{0i} &= \cos\left(\frac{\theta}{2}\right) t_{0i} + \sin\left(\frac{\theta}{2}\right)\frac{1}{\sqrt{2}}\left(t_{+i} + t_{-i}\right) \\ b_{\alpha i} &= \sin\left(\frac{\theta}{2}\right) t_{0i} - \cos\left(\frac{\theta}{2}\right)\frac{1}{\sqrt{2}}\left(t_{+i} + t_{-i}\right) \\ b_{\varphi i} &= \frac{1}{\sqrt{2}}\left(t_{+i} - t_{-i}\right) \end{aligned}}$$

b_{0i}^{+} creates mean-field ground state

$b_{\alpha i}^{+}$ and $b_{\varphi i}^{+}$ create two states orthogonal to m.f. ground state

$b_{\alpha i} \sim \frac{\partial}{\partial\theta} b_{0i}$ $\Rightarrow$ amplitude mode

$b_{\varphi i} \sim \frac{\partial}{\partial\varphi} b_{0i}$ $\Rightarrow$ Goldstone mode (if we had kept φ-phase in b_{0i})

- <u>local constraint</u>

$$b_{0i}^{+} b_{0i} + b_{\alpha i}^{+} b_{\alpha i} + b_{\varphi i}^{+} b_{\varphi i} = 1$$

Transformation matrix

$$
M = \begin{pmatrix} \cos\frac{\theta}{2} & \frac{1}{\sqrt{2}}\sin\frac{\theta}{2} & \frac{1}{\sqrt{2}}\sin\theta/2 \\ \sin\frac{\theta}{2} & -\frac{1}{\sqrt{2}}\cos\frac{\theta}{2} & -\frac{1}{\sqrt{2}}\cos\frac{\theta}{2} \\ 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix}
$$

- check unitarity

$$
M^{+}M = \begin{pmatrix} C & S & 0 \\ \frac{1}{\sqrt{2}}S & -\frac{1}{\sqrt{2}}C & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}}S & -\frac{1}{\sqrt{2}}C & -\frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} C & \frac{1}{\sqrt{2}}S & \frac{1}{\sqrt{2}}S \\ S & -\frac{1}{\sqrt{2}}C & -\frac{1}{\sqrt{2}}C \\ 0 & 1/\sqrt{2} & -1/\sqrt{2} \end{pmatrix} =
$$

$$
= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \Rightarrow \quad \underset{\text{unitary}}{M}
$$

- unitary transformation

$$
b_\alpha = \sum_j M_{\alpha j}\, t_j \qquad\qquad t_j = \sum_\alpha M^{T}_{j\alpha}\, b_\alpha
$$

preserves boson commutation relations!

Construct H in new basis

local basis states

$$|g_i\rangle = \cos\frac{\theta}{2}|0_i\rangle + \sin\frac{\theta}{2}\frac{1}{\sqrt{2}}\left(|1_i\rangle + |-1_i\rangle\right)$$

$$|\theta_i\rangle = +\sin\frac{\theta}{2}|0_i\rangle - \cos\frac{\theta}{2}\frac{1}{\sqrt{2}}\left(|1_i\rangle + |-1_i\rangle\right)$$

$$|\varphi_i\rangle = \frac{1}{\sqrt{2}}\left(|1_i\rangle - |-1_i\rangle\right)$$

$$\left(S_i^z\right)^2|g_i\rangle = \sin\frac{\theta}{2}\frac{1}{\sqrt{2}}\left(|1_i\rangle + |-1\rangle_i\right)$$

$$= \sin\frac{\theta}{2}\left(\sin\frac{\theta}{2}|g_i\rangle - \cos\frac{\theta}{2}|\theta_i\rangle\right)$$

$$= \sin^2\frac{\theta}{2}|g_i\rangle - \sin\frac{\theta}{2}\cos\frac{\theta}{2}|\theta_i\rangle$$

$$\left(S_i^z\right)^2|\theta_i\rangle = -\cos\frac{\theta}{2}\frac{1}{\sqrt{2}}\left(|1_i\rangle + |-1_i\rangle\right)$$

$$= -\cos\frac{\theta}{2}\left(\sin\frac{\theta}{2}|g_i\rangle - \cos\frac{\theta}{2}|\theta_i\rangle\right)$$

$$= -\sin\frac{\theta}{2}\cos\frac{\theta}{2}|g_i\rangle + \cos^2\frac{\theta}{2}|\theta_i\rangle$$

$$\left(S_i^z\right)^2|\varphi_i\rangle = \frac{1}{\sqrt{2}}\left(|1_i\rangle - |-1_i\rangle\right) = |\varphi_i\rangle$$

- Operator formulation

$$\left(S_i^z\right)^2 = \sin^2\frac{\theta}{2}\, b^+_{0i} b_{0i} + \cos^2\frac{\theta}{2}\, b^+_{\theta i} b_{\theta i} + b^+_{\varphi i} b_{\varphi i}$$

$$+ \sin\frac{\theta}{2}\cos\frac{\theta}{2}\left(b^+_{\theta i} b_{0i} + b^+_{0i} b_{\theta i}\right)$$

eliminate $b^+_{0i} b_{0i}$ using constraint $\sum_{0,\theta,\varphi} b^+ b = 1$,

$$\left(S_i^z\right)^2 = \sin^2\frac{\theta}{2} + \left(\cos^2\frac{\theta}{2} - \sin^2\frac{\theta}{2}\right) b^+_{\theta i} b_{\theta i} + \left(1 - \sin^2\frac{\theta}{2}\right) b^+_{\varphi i} b_{\varphi i}$$

$$- \sin\frac{\theta}{2}\cos\frac{\theta}{2}\left(b^+_{\theta i} b_{0i} + b^+_{0i} b_{\theta i}\right)$$

$$\boxed{\begin{aligned}\left(S_i^z\right)^2 &= \tfrac{1}{2}\left(1 - \cos\theta\right) + \cos\theta\, b^+_{\theta i} b_{\theta i} + \tfrac{1}{2}\left(1 + \cos\theta\right) b^+_{\varphi i} b_{\varphi i} \\ &\quad - \tfrac{1}{2}\sin\theta\left(b^+_{\theta i} b_{0i} + b^+_{0i} b_{\theta i}\right)\end{aligned}}$$

drop terms in 2nd line as they correspond to correction to MF GS

$$S_i^+ |g_i\rangle = \sqrt{2}\left(\cos\frac{\theta}{2}|1_i\rangle + \sin\frac{\theta}{2}|0_i\rangle\right)$$

$$= \cos\frac{\theta}{2}\left(\sin\frac{\theta}{2}|g_i\rangle - \cos\frac{\theta}{2}|\theta_i\rangle + |\varphi_i\rangle\right)$$

$$+ \sin\frac{\theta}{2}\left(\cos\frac{\theta}{2}|g_i\rangle + \sin\frac{\theta}{2}|\theta_i\rangle\right)$$

$$= \sin\theta\,|g_i\rangle - \cos\theta\,|\theta_i\rangle + \cos\frac{\theta}{2}|\varphi_i\rangle$$

$$S_i^+ |\theta_i\rangle = \sqrt{2}\sin\frac{\theta}{2}|1_i\rangle - \cos\frac{\theta}{2}|0_i\rangle$$

$$= \sin\frac{\theta}{2}\left(\sin\frac{\theta}{2}|g_i\rangle - \cos\frac{\theta}{2}|\theta_i\rangle + |\varphi_i\rangle\right)$$

$$- \cos\frac{\theta}{2}\left(\cos\frac{\theta}{2}|g_i\rangle + \sin\frac{\theta}{2}|\theta_i\rangle\right)$$

$$= -\cos\theta\,|g_i\rangle - \sin\theta\,|\theta_i\rangle + \sin\frac{\theta}{2}|\varphi_i\rangle$$

$$S_i^+ |\varphi_i\rangle = -\frac{1}{\sqrt{2}}|0_i\rangle = -\left(\cos\frac{\theta}{2}|g_i\rangle + \sin\frac{\theta}{2}|\theta_i\rangle\right)$$

<u>operator formulation</u>

$$S_i^+ = \sin\theta\, b^+_{0i} b_{0i} - \cos\theta\, b^+_{\theta i} b_{0i} + \cos\frac{\theta}{2}\, b^+_{\varphi i} b_{0i}$$

$$- \sin\theta\, b^+_{\theta i} b_{\theta i} - \cos\theta\, b^+_{0i} b_{\theta i} + \sin\frac{\theta}{2}\, b^+_{\varphi i} b_{\theta i}$$

$$- \cos\theta/2\, b^+_{0i} b_{\varphi i} - \sin\frac{\theta}{2}\, b^+_{\theta i} b_{\varphi i}$$

Detour: calculate S^x, S^y

$$S^{\pm} = S^x \pm i S^y \qquad S^x = \frac{1}{2}\left(S^+ + S^-\right)$$
$$S^y = \frac{1}{2i}\left(S^+ - S^-\right)$$

$$\begin{aligned}
2S^x = \;& \sin\theta\, b_0^+ b_0 - \cos\theta\, b_\theta^+ b_0 + \cos\tfrac{\theta}{2}\, \cancel{b_\varphi^+ b_0} \\
& - \sin\theta\, b_\theta^+ b_\theta - \cos\theta\, b_0^+ b_\theta + \sin\tfrac{\theta}{2}\, \cancel{b_\varphi^+ b_\theta} \\
& - \cos\tfrac{\theta}{2}\, \cancel{b_0^+ b_\varphi} - \sin\tfrac{\theta}{2}\, \cancel{b_\theta^+ b_\varphi} \\
& + \sin\theta\, b_0^+ b_0 - \cos\theta\, b_0^+ b_\theta + \cos\tfrac{\theta}{2}\, \cancel{b_0^+ b_\varphi} \\
& - \sin\theta\, b_\theta^+ b_\theta - \cos\theta\, b_\theta^+ b_0 + \sin\tfrac{\theta}{2}\, \cancel{b_\theta^+ b_\varphi} \\
& - \cos\tfrac{\theta}{2}\, \cancel{b_\varphi^+ b_0} - \sin\tfrac{\theta}{2}\, \cancel{b_\varphi^+ b_\theta}
\end{aligned}$$

$$\boxed{S^x = \sin\theta\, b_0^+ b_0 - \sin\theta\, b_\theta^+ b_\theta - \cos\theta\left(b_\theta^+ b_0 + b_0^+ b_\theta\right)}$$

analogously

$$2iS^y = 2\cos\tfrac{\theta}{2}\left(b_\varphi^+ b_0 - b_0^+ b_\varphi\right) + 2\sin\tfrac{\theta}{2}\left(b_\varphi^+ b_\theta - b_\theta^+ b_\varphi\right)$$

$$\boxed{S^y = i\cos\tfrac{\theta}{2}\left(b_0^+ b_\varphi - b_\varphi^+ b_0\right) + i\sin\tfrac{\theta}{2}\left(b_\theta^+ b_\varphi - b_\varphi^+ b_\theta\right)}$$

16 b

$$S^{x2} = \left[\sin\theta\, b_0^+ b_0 - \sin\theta\, b_\theta^+ b_\theta - \cos\theta \left(b_\theta^+ b_0 + b_0^+ b_\theta \right) \right]^2$$

$$= \sin^2\theta\, b_0^+ b_0 + \sin^2\theta\, b_\theta^+ b_\theta$$
$$+ \cos^2\theta \left(b_\theta^+ b_0 + b_0^+ b_\theta \right)^2$$

$$- \sin^2\theta \left(b_0^+ b_0 b_\theta^+ b_\theta + b_\theta^+ b_\theta b_0^+ b_0 \right) \leftarrow \text{vanishes due to constraint}$$

$$- \sin\theta\cos\theta \left(b_0^+ b_0 \left(b_\theta^+ b_0 + b_0^+ b_\theta \right) + \left(b_\theta^+ b_0 + b_0^+ b_\theta \right) b_0^+ b_0 \right)$$
$$+ \sin\theta\cos\theta \left(b_\theta^+ b_\theta (\sim) + (\sim) b_\theta^+ b_\theta \right)$$

$$= \sin^2\theta\, b_0^+ b_0 + \sin^2\theta\, b_\theta^+ b_\theta$$
$$+ \cos^2\theta \left(b_\theta^+ b_0 b_0^+ b_\theta + b_0^+ b_\theta b_\theta^+ b_0 \right)$$
$$\cancel{- \sin\theta\cos\theta \left(b_\theta^+ b_0 + b_0^+ b_\theta \right)}$$
$$\cancel{+ \sin\theta\cos\theta \left(\sim \right)}$$

$$\boxed{S^{x2} = b_0^+ b_0 + b_\theta^+ b_\theta}$$

Constraint $\quad b_0^+ b_0 + b_\theta^+ b_\theta + b_\varphi^+ b_\varphi = 1$, restricts boson numbers to 0 or 1

$$S^{y2} = -\cos^2\frac{\theta}{2}\left(b_0^+ b_\varphi - b_\varphi^+ b_0\right)\left(b_0^+ b_\varphi - b_\varphi^+ b_0\right)$$

$$-\sin^2\frac{\theta}{2}\left(b_\theta^+ b_\varphi - b_\varphi^+ b_\theta\right)\left(b_\theta^+ b_\varphi - b_\varphi^+ b_\theta\right)$$

$$-\sin\frac{\theta}{2}\cos\frac{\theta}{2}\left(b_0^+ b_\varphi - b_\varphi^+ b_0\right)\left(b_\theta^+ b_\varphi - b_\varphi^+ b_\theta\right)$$

$$-\sin\frac{\theta}{2}\cos\frac{\theta}{2}\left(b_\theta^+ b_\varphi - b_\varphi^+ b_\theta\right)\left(b_0^+ b_\varphi - b_\varphi^+ b_0\right)$$

$$= -\cos^2\frac{\theta}{2}\left(-b_\varphi^+ b_\varphi - b_0^+ b_0\right)$$

$$-\sin^2\frac{\theta}{2}\left(-b_\theta^+ b_\theta - b_\varphi^+ b_\varphi\right)$$

$$-\sin\frac{\theta}{2}\cos\frac{\theta}{2}\left(-b_0^+ b_\theta - b_\theta^+ b_0\right)$$

$$\boxed{\begin{aligned} S^{y2} = {} & b_\varphi^+ b_\varphi + \cos^2\frac{\theta}{2}\, b_0^+ b_0 + \sin^2\frac{\theta}{2}\, b_\theta^+ b_\theta \\ & + \sin\frac{\theta}{2}\cos\frac{\theta}{2}\left(b_0^+ b_\theta + b_\theta^+ b_0\right) \end{aligned}}$$

$$S^{x2} + S^{y2} = \overbrace{b_0^+ b_0 + b_\theta^+ b_\theta + b_\varphi^+ b_\varphi}^{1 \ (\text{constraint})}$$

$$+ \cos^2\frac{\theta}{2}\, b_0^+ b_0 + \sin^2\frac{\theta}{2}\, b_\theta^+ b_\theta$$

$$+ \sin\frac{\theta}{2}\cos\frac{\theta}{2}\left(b_0^+ b_\theta + b_\theta^+ b_0\right)$$

use $\sin\frac{\theta}{2}\cos\frac{\theta}{2} = \frac{1}{2}\sin\theta$

$\cos^2\frac{\theta}{2} = \frac{1}{2}(1+\cos\theta)$ $\qquad \sin^2\frac{\theta}{2} = \frac{1}{2}(1-\cos\theta)$

$$S^{x2} + S^{y2} = 1 + \tfrac{1}{2}(1+\cos\theta)\, b_0^+ b_0 + \tfrac{1}{2}(1-\cos\theta)\, b_\theta^+ b_\theta$$
$$+ \tfrac{1}{2}\sin\theta \left(b_0^+ b_\theta + b_\theta^+ b_0 \right)$$

<u>check</u> $\quad S^{x2} + S^{y2} + S^{z2} = S(S+1) = 2$

$$1 + \tfrac{1}{2}(1+\cos\theta)\, b_0^+ b_0 + \tfrac{1}{2}(1-\cos\theta)\, b_\theta^+ b_\theta + \cancel{\tfrac{1}{2}\sin\theta \left(b_0^+ b_\theta + b_\theta^+ b_0 \right)}$$
$$+ \tfrac{1}{2}(1-\cos\theta)\, b_0^+ b_0 + \tfrac{1}{2}(1+\cos\theta)\, b_\theta^+ b_\theta + b_\varphi^+ b_\varphi$$
$$\cancel{-\tfrac{1}{2}\sin\theta \left(b_0^+ b_\theta + b_\theta^+ b_0 \right)}$$

$$= 1 + b_0^+ b_0 + b_\theta^+ b_\theta + b_\varphi^+ b_\varphi = 2$$

<u>OK</u>

<u>disordered (insulating) phase</u>

$$S^{x2} = b_0^+ b_0 + b_\theta^+ b_\theta = 1 - b_\varphi^+ b_\varphi$$
$$S^{y2} = b_0^+ b_0 + b_\varphi^+ b_\varphi = 1 - b_\theta^+ b_\theta$$

$$S_i^+ S_j^- = \Big(\sin\theta\, b_{0i}^+ b_{0i} - \cos\theta\, b_{\theta i}^+ b_{0i} + \cos\tfrac{\theta}{2}\, b_{\varphi i}^+ b_{0i}$$
$$- \sin\theta\, b_{\theta i}^+ b_{\theta i} - \cos\theta\, b_{0i}^+ b_{\theta i} + \sin\tfrac{\theta}{2}\, b_{\varphi i}^+ b_{\theta i}$$
$$- \cos\tfrac{\theta}{2}\, b_{0i}^+ b_{\varphi i} - \sin\theta/2\, b_{\theta i}^+ b_{\varphi i} \Big) \times$$
$$\times \Big(\sin\theta\, b_{0j}^+ b_{0j} - \cos\theta\, b_{0j}^+ b_{\theta j} + \cos\tfrac{\theta}{2}\, b_{0j}^+ b_{\varphi j}$$
$$- \sin\theta\, b_{\theta j}^+ b_{\theta j} - \cos\theta\, b_{\theta j}^+ b_{0j} + \sin\tfrac{\theta}{2}\, b_{\theta j}^+ b_{\varphi j}$$
$$- \cos\tfrac{\theta}{2}\, b_{\varphi j}^+ b_{0j} - \sin\tfrac{\theta}{2}\, b_{\varphi j}^+ b_{\theta j} \Big)$$

- keep only terms quadratic in b_θ and b_φ

$$S_i^+ S_j^- = \sin^2\theta\, b_{0i}^+ b_{0i} b_{0j}^+ b_{0j} - \sin^2\theta\, b_{0i}^+ b_{0i} b_{\theta j}^+ b_{\theta j}$$
$$+ \sin\theta\, b_{0i}^+ b_{0i} \sin\tfrac{\theta}{2}\, b_{\theta j}^+ b_{\varphi j} - \sin\theta\, b_{0i}^+ b_{0i} \sin\tfrac{\theta}{2}\, b_{\varphi j}^+ b_{\theta j}$$
$$+ \cos^2\theta\, b_{\theta i}^+ b_{0i} b_{0j}^+ b_{\theta j} - \cos\theta \cos\tfrac{\theta}{2}\, b_{\theta i}^+ b_{0i} b_{0j}^+ b_{\varphi j}$$
$$+ \cos^2\theta\, b_{\theta i}^+ b_{0i} b_{\theta j}^+ b_{0j} + \cos\theta \cos\tfrac{\theta}{2}\, b_{\theta i}^+ b_{0i} b_{\varphi j}^+ b_{0j}$$
$$- \cos\tfrac{\theta}{2} \cos\theta\, b_{\varphi i}^+ b_{0i} b_{0j}^+ b_{\theta j} + \cos^2\tfrac{\theta}{2}\, b_{\varphi i}^+ b_{0i} b_{0j}^+ b_{\varphi j}$$
$$- \cos\tfrac{\theta}{2} \cos\theta\, b_{\varphi i}^+ b_{0i} b_{\theta j}^+ b_{0j} - \cos^2\tfrac{\theta}{2}\, b_{\varphi i}^+ b_{0i} b_{\varphi j}^+ b_{0j}$$

$$- \sin^2\theta \; b_{\theta i}^+ b_{\theta i} b_{0j}^+ b_{0j}$$

$$+ \cos^2\theta \; b_{0i}^+ b_{\theta i} b_{0j}^+ b_{\theta j} - \cos\theta \cos\frac{\theta}{2} \, b_{0i} b_{\theta i} b_{0j}^+ b_{\varphi j}$$

$$+ \cos^2\theta \; b_{0i}^+ b_{\theta i} b_{\theta j}^+ b_{0j} + \cos\theta \cos\frac{\theta}{2} \, b_{0i}^+ b_{\theta i} b_{\varphi j}^+ b_{0j}$$

$$+ \sin\theta \sin\theta/2 \; b_{\varphi i}^+ b_{\theta i} b_{0j}^+ b_{0j}$$

$$+ \cos\frac{\theta}{2} \cos\theta \; b_{0i}^+ b_{\varphi i} b_{0j}^+ b_{\theta j} - \left(\cos\frac{\theta}{2}\right)^2 b_{0i}^+ b_{\varphi i} b_{0j}^+ b_{\varphi j}$$

$$+ \cos\frac{\theta}{2} \cos\theta \; b_{0i}^+ b_{\varphi i} b_{\theta j}^+ b_{0j} + \cos^2\frac{\theta}{2} \, b_{0i}^+ b_{\varphi i} b_{\varphi j}^+ b_{0j}$$

$$- \sin\frac{\theta}{2} \sin\theta \; b_{\theta i}^+ b_{\varphi i} b_{0j}^+ b_{0j}$$

Simplify:

$$S_i^+ S_j^- = \sin^2\theta\left(1 - b^+_{i\theta} b_{i\theta} - b^+_{i\varphi} b_{i\varphi} - b^+_{j\theta} b_{j\theta} - b^+_{j\varphi} b_{j\varphi}\right)$$

$$- \sin^2\theta\, b^+_{\theta j} b_{\theta j} + \sin\theta \sin\frac{\theta}{2}\left(\cancel{b^+_{\theta j} b_{\varphi j}} - \cancel{b^+_{\varphi j} b_{\theta j}}\right)$$

cancel with terms in $S_j^+ S_i$

$$+ \cos^2\theta\, b^+_{\theta i} b_{\theta j} - \cos\theta\cos\frac{\theta}{2}\, \cancel{b^+_{\theta i} b_{\varphi j}}$$

cancel with terms in $S_j^+ S_i$

$$+ \cos^2\theta\, b^+_{\theta i} b^+_{\theta j} + \cos\theta \cos\frac{\theta}{2}\, \cancel{b^+_{\theta i} b^+_{\varphi j}}$$

$$- \cos\frac{\theta}{2}\cos\theta\, \cancel{b^+_{\varphi i} b_{\theta j}} + \cos^2\frac{\theta}{2}\, b^+_{\varphi i} b_{\varphi j}$$

$$- \cos\frac{\theta}{2}\cos\theta\, \cancel{b^+_{\varphi i} b^+_{\theta j}} - \cos^2\frac{\theta}{2}\, b^+_{\varphi i} b^+_{\varphi j}$$

$$- \sin^2\theta\, b^+_{\theta i} b_{\theta i}$$

$$+ \cos^2\theta\, b_{\theta i} b_{\theta j} - \cos\theta\cos\frac{\theta}{2}\, \cancel{b_{\theta i} b_{\varphi j}}$$

$$+ \cos^2\theta\, b_{\theta i} b^+_{\theta j} + \cos\theta\cos\frac{\theta}{2}\, \cancel{b_{\theta i} b^+_{\varphi j}}$$

$$+ \sin\theta \sin\theta/2\, \cancel{b^+_{\varphi i} b_{\theta i}}$$

$$+ \cos\frac{\theta}{2}\cos\theta\, \cancel{b_{\varphi i} b_{\theta j}} - \cos^2\frac{\theta}{2}\, b_{\varphi i} b_{\varphi j}$$

$$+ \cos\theta/2 \cos\theta\, \cancel{b_{\varphi i} b^+_{\theta j}} + \cos^2\frac{\theta}{2}\, b_{\varphi i} b^+_{\varphi j}$$

$$- \sin\frac{\theta}{2}\sin\theta\, \cancel{b^+_{\theta i} b_{\varphi i}}$$

this eliminates all couplings between Higgs and Goldstone bosons, as expected

Simplify further

$$S_i^+ S_j + S_j^+ S_i = h_{ij}^{\theta} + h_{ij}^{\phi} + 2\sin^2\theta$$

$$\boxed{\begin{aligned} h_{ij}^{\theta} = & -4\sin^2\theta \left(b_{i\theta}^+ b_{i\theta} + b_{j\theta}^+ b_{j\theta} \right) \\ & + 2\cos^2\theta \left(b_{i\theta}^+ b_{j\theta} + b_{j\theta}^+ b_{i\theta} \right) \\ & + 2\cos^2\theta \left(b_{i\theta}^+ b_{j\theta}^+ + b_{i\theta} b_{j\theta} \right) \end{aligned}}$$

$$\boxed{\begin{aligned} h_{ij}^{\phi} = & -2\sin^2\theta \left(b_{i\varphi}^+ b_{i\varphi} + b_{j\varphi}^+ b_{j\varphi} \right) \\ & + (1+\cos\theta)\left(b_{i\varphi}^+ b_{j\varphi} + b_{j\varphi}^+ b_{i\varphi} \right) \\ & - (1+\cos\theta)\left(b_{i\varphi}^+ b_{j\varphi}^+ + b_{i\varphi} b_{j\varphi} \right) \end{aligned}}$$

- these expressions agree with Eqs 24, 25 in Pekker et al PRB 86, 144527 (2012)

Insert into full Hamiltonian

$$H = -\frac{J}{2}\sum_{\langle ij\rangle}\left(S_i^+ S_j^- + S_j^+ S_i^-\right) + \frac{u}{2}\sum_i \left(S_i^t\right)^2$$

$$H = \frac{u}{2}\sum_i \frac{1}{2}(1-\cos\theta) - \frac{J}{2}\sum_{\langle ij\rangle} 2\sin^2\theta$$

$$+ H_\theta + H_\varphi \quad (\text{Higgs} + \text{Goldstone parts})$$

$$H_\theta = \frac{u}{2}\sum_i \cos\theta\, b_{\theta i}^+ b_{\theta i} - \frac{J}{2}\sum_{\langle ij\rangle}\Big(-4\sin^2\theta\left(b_{i\theta}^+ b_{i\theta} + b_{j\theta}^+ b_{j\theta}\right)$$

$$+ 2\cos^2\theta\left(b_{i\theta}^+ b_{j\theta} + b_{j\theta}^+ b_{i\theta}\right) + 2\cos^2\theta\left(b_{i\theta}^+ b_{j\theta}^+ + b_{i\theta} b_{j\theta}\right)\Big)$$

$$\boxed{\begin{aligned} H_\theta = &\sum_i \left(\frac{u}{2}\cos\theta + 2Jz\sin^2\theta\right) b_{i\theta}^+ b_{i\theta} \\ &- \sum_{\langle ij\rangle} J\cos^2\theta\left(b_{i\theta}^+ b_{j\theta} + b_{j\theta}^+ b_{i\theta} + b_{i\theta}^+ b_{j\theta}^+ + b_{i\theta} b_{j\theta}\right)\end{aligned}}$$

$$H_\varphi = \frac{U}{2}\sum_i \frac{1}{2}(1+\cos\theta)\, b_{i\varphi}^+ b_{i\varphi} - \frac{J}{2}\sum_{\langle ij\rangle}\Big[-2\sin^2\theta\left(b_{i\varphi}^+ b_{i\varphi} + b_{j\varphi}^+ b_{j\varphi}\right)$$

$$+ (1+\cos\theta)\left(b_{i\varphi}^+ b_{j\varphi} + b_{j\varphi}^+ b_{i\varphi}\right) - (1+\cos\theta)\left(b_{i\varphi}^+ b_{j\varphi}^+ + b_{i\varphi} b_{j\varphi}\right)\Big]$$

$$\boxed{\begin{aligned} H_\varphi = &\sum_i \left(\frac{U}{4}(1+\cos\theta) + Jz\sin^2\theta\right) b_{i\varphi}^+ b_{i\varphi} \\ &- \sum_{\langle ij\rangle} \frac{J}{2}(1+\cos\theta)\left(b_{i\varphi}^+ b_{j\varphi} + b_{j\varphi}^+ b_{i\varphi} - b_{i\varphi}^+ b_{j\varphi}^+ - b_{i\varphi} b_{j\varphi}\right)\end{aligned}}$$

<u>Check:</u> in disordered phase (insulator) both modes are indistinguishable $\Rightarrow$ must have identical Hamiltonian

set $\theta = 0$ for insulator

$$H_\theta = \sum_i \frac{U}{2} b_{i\theta}^+ b_{i\theta} - \sum_{\langle ij\rangle} J\left(b_{i\theta}^+ b_{j\theta} + b_{j\theta}^+ b_{i\theta} + b_{i\theta}^+ b_{j\theta}^+ + b_{i\theta} b_{j\theta}\right)$$

$$H_\varphi = \sum_i \frac{U}{2} b_{i\varphi}^+ b_{i\varphi} - \sum_{\langle ij\rangle} J\left(b_{i\varphi}^+ b_{j\varphi} + b_{j\varphi}^+ b_{i\varphi} - b_{i\varphi}^+ b_{j\varphi}^+ - b_{i\varphi} b_{j\varphi}\right)$$

- at first glance, there seems to be <u>sign difference</u> in anomalous terms (as in Pekker et al paper) but can be transformed away by

$b \to ib$, $b^+ \to -ib^+$ (has to do with phase of $b_{0i} b_{0j}$)

Fourier transformation

$$a_{k\theta} = \frac{1}{\sqrt{N}} \sum_j b_{j\theta}\, e^{i\vec{k}\cdot\vec{r}}$$
$$a^+_{k\theta} = \frac{1}{\sqrt{N}} \sum_j b^+_{j\theta}\, e^{-i\vec{k}\cdot\vec{r}}$$

analogously for Goldstone mode

$$\boxed{\begin{aligned} H_\theta = &\sum_k \left(\frac{U}{2}\cos\theta + 2Jz\sin^2\theta - J\cos^2\theta\, \varepsilon_k \right) a^+_{k\theta} a_{k\theta} \\ &+ \sum_k -J\cos^2\theta \frac{1}{2}\varepsilon(k) \left(a^+_{k\theta} a^+_{-k\theta} + a_{k\theta} a_{-k\theta} \right) \end{aligned}}$$

$$\varepsilon_k = 2\cos k_x + 2\cos k_y$$ for square lattice $(z=4)$

$$\boxed{\begin{aligned} H_\varphi = &\sum_k \left(\frac{U}{4}(1+\cos\theta) + Jz\sin^2\theta - \frac{J}{2}(1+\cos\theta)\, \varepsilon_k \right) a^+_{k\varphi} a_{k\varphi} \\ &+ \sum_k + \frac{J}{2}(1+\cos\theta) \frac{1}{2}\varepsilon(k) \left(a^+_{k\varphi} a^+_{-k\varphi} + a_{k\varphi} a_{-k\varphi} \right) \end{aligned}}$$

$\llcorner$ or $-$ (see page 22)

Bogoliubov transformation

2×2 Hamiltonian for a_k, a_{-k}

$$H = \frac{1}{2} \left(a_k^+, a_{-k} \right) \begin{pmatrix} \alpha_k & \beta_k \\ \beta_k^* & \alpha_k \end{pmatrix} \begin{pmatrix} a_k \\ a_{-k}^+ \end{pmatrix}$$

with

$$\left.\begin{aligned} \alpha_k &= \frac{U}{2} \cos\theta + 2Jz \sin^2\theta - J\cos^2\theta \, \varepsilon_k \\ \beta_k &= -J\cos^2\theta \, \varepsilon_k \end{aligned}\right\} \text{ Higgs } \theta$$

or

$$\left.\begin{aligned} \alpha_k &= \frac{U}{4}(1+\cos\theta) + Jz\sin^2\theta - \frac{J}{2}(1+\cos\theta)\,\varepsilon_k \\ \beta_k &= \frac{J}{2}(1+\cos\theta)\,\varepsilon_k \end{aligned}\right\} \text{ Goldstone } \varphi$$

diagonalized by bosonic Bogoliubov transformation

$$\boxed{H = \frac{1}{2} \sum_k \gamma_k^+ \gamma_k \, E_k \qquad \text{with } E_k = \sqrt{\alpha_k^2 - \beta_k^2}}$$

see next 3 pages (24a to c)

Detour: bosonic Bogoliubov transformation

- two bosons a, b with

$$H = \alpha\left(a^+a + b^+b\right) + \beta\left(a^+b^+ + ab\right) \qquad (\alpha, \beta \text{ real})$$

$$= \left(a^+, b\right)\begin{pmatrix}\alpha & \beta \\ \beta & \alpha\end{pmatrix}\begin{pmatrix}a \\ b^+\end{pmatrix} \quad (\text{up to constant})$$

- new bosons γ, δ with

$$a = u\gamma + v\delta^+ \qquad a^+ = u\gamma^+ + v\delta$$

$$b^+ = v\gamma + u\delta^+ \qquad b = v\gamma^+ + u\delta \qquad (u, v \text{ real})$$

- check bosonic commutator

$$[a, a^+] = [u\gamma + v\delta^+, u\gamma^+ + v\delta] = u^2 - v^2 = 1$$

- insert into Hamiltonian

$$H = \alpha\left[(u\gamma^+ + v\delta)(u\gamma + v\delta^+) + (v\gamma + u\delta^+)(v\gamma^+ + u\delta)\right]$$

$$+ \beta\left[(u\gamma^+ + v\delta)(v\gamma + u\delta^+) + (u\gamma + v\delta^+)(v\gamma^+ + u\delta)\right]$$

$$= \gamma^+\gamma\left(\alpha u^2 + \alpha v^2 + 2\beta uv\right) + \delta^+\delta\left(\alpha u^2 + \alpha v^2 + 2\beta uv\right)$$

$$+ \gamma^+\delta^+\left(2\alpha uv + \beta u^2 + \beta v^2\right) + \gamma\delta\left(2\alpha uv + \beta u^2 + \beta v^2\right)$$

$$H = \left(\alpha u^2 + \alpha v^2 + 2\beta uv\right)\left(\gamma^+\gamma + \delta^+\delta\right)$$

$$+ \left(2\alpha uv + \beta u^2 + \beta v^2\right)\left(\gamma^+\delta^+ + \gamma\delta\right)$$

- off-diagonal terms (anomalous terms) must vanish

$$2\alpha uv + \beta(u^2+v^2) = 0 \qquad \underline{u, v \text{ opposite signs}}$$

$$4\alpha^2 u^2 v^2 = \beta^2(u^2+v^2)^2 \qquad \text{use} \quad u^2 = 1+v^2$$

$$4\alpha^2 v^2(1+v^2) = \beta^2(1+2v^2)^2$$

$$(4\alpha^2 - 4\beta^2)v^4 + (4\alpha^2 - 4\beta^2)v^2 - \beta^2 = 0$$

$$v^4 + v^2 - \frac{\beta^2}{4(\alpha^2-\beta^2)} = 0$$

$$v^2 = -\frac{1}{2} + \sqrt{\frac{1}{4} + \frac{\beta^2}{4(\alpha^2-\beta^2)}} = -\frac{1}{2} + \sqrt{\frac{\alpha^2}{4(\alpha^2-\beta^2)}}$$

$$v^2 = \frac{1}{2}\left(\frac{\alpha}{\sqrt{\alpha^2-\beta^2}} - 1\right) \qquad u^2 = \frac{1}{2}\left(\frac{\alpha}{\sqrt{\alpha^2-\beta^2}} + 1\right)$$

$$uv = -\frac{1}{2}\sqrt{\left(\frac{\alpha}{\sqrt{\alpha^2-\beta^2}} - 1\right)\left(\frac{\alpha}{\sqrt{\alpha^2-\beta^2}} + 1\right)} = -\frac{1}{2}\sqrt{\frac{\alpha^2}{\alpha^2-\beta^2} - 1}$$

$$= -\frac{1}{2}\frac{\beta}{\sqrt{\alpha^2-\beta^2}}$$

Insert into Hamiltonian

$$H = (\alpha u^2 + \alpha v^2 + 2\beta uv)(\gamma^+\gamma + \delta^+\delta)$$

$$= \left(\frac{\alpha^2}{\sqrt{\alpha^2-\beta^2}} - \frac{\beta^2}{\sqrt{\alpha^2-\beta^2}}\right)(\gamma^+\gamma + \delta^+\delta)$$

$$\boxed{H = \sqrt{\alpha^2-\beta^2}\,(\gamma^+\gamma + \delta^+\delta)}$$

ground state properties in terms of old bosons a, b

$$\boxed{\begin{aligned} a &= u\gamma + v\delta^+ & \gamma &= ua - vb^+ \\ b &= v\gamma^+ + u\delta & \delta &= -va^+ + ub \end{aligned}}$$

$$\langle GS | a | GS \rangle = \langle GS | u\gamma + v\delta^+ | GS \rangle = 0$$

$$\langle GS | b | GS \rangle = \langle GS | v\gamma^+ + u\delta | GS \rangle = 0$$

BUT

$$\langle GS | a^+ a | GS \rangle = \langle GS | (u\gamma^+ + v\delta)(u\gamma + v\delta^+) | GS \rangle$$

$$= v^2 = \frac{1}{2}\left(\frac{\alpha}{\sqrt{\alpha^2-\beta^2}} - 1\right)$$

$$\langle GS | a^+ a | GS \rangle > 0 \qquad \text{if} \qquad \beta^2 \neq 0$$

diverges for $\alpha = \beta$ $\Rightarrow$ BE condensation

Note: $|GS\rangle$ contains fluctuations of a, b bosons

$$\langle GS | b^+ b | GS \rangle = \langle GS | (v\gamma + u\delta^+)(v\gamma^+ + u\delta) | GS \rangle$$

$$= v^2 = \frac{1}{2}\left(\frac{\alpha}{\sqrt{\alpha^2-\beta^2}} - 1\right)$$

- explicit expression for $|GS\rangle$ in terms of a, b

<u>ansatz</u> $\quad |GS\rangle = e^{\lambda a^+ b^+} |0_{ab}\rangle$

$\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad \uparrow$ a, b vacuum

$|GS\rangle$ has to fulfill $\quad \gamma|GS\rangle = \delta|GS\rangle = 0$

$$\gamma|GS\rangle = (u a - v b^+) e^{\lambda a^+ b^+} |0_{ab}\rangle$$

$$b^+ e^{\lambda a^+ b^+} = e^{\lambda a^+ b^+} b^+$$

$$a\, e^{\lambda a^+ b^+} = e^{\lambda a^+ b^+} \underbrace{e^{-\lambda a^+ b^+} a\, e^{\lambda a^+ b^+}}$$

use Baker-Hausdorff theorem

$$e^{-Q} P e^{Q} = P + [P, Q] + \frac{1}{2}[[P,Q],Q] + \ldots$$

$$= e^{\lambda a^+ b^+}\left(a + [a, \lambda a^+ b^+] + \frac{1}{2}[[a, \lambda a^+ b^+], \lambda a^+ b^+]\right)$$

$$= e^{\lambda a^+ b^+}(a + \lambda b^+ + 0)$$

$$\gamma|GS\rangle = e^{\lambda a^+ b^+}\left(u a + u\lambda b^+ - v b^+\right)|0_{ab}\rangle \overset{!}{=} 0$$

$$u\lambda = v \quad \Rightarrow \quad \lambda = \frac{v}{u}$$

$$\boxed{|GS\rangle = e^{\frac{v}{u} a^+ b^+} |0_{ab}\rangle}$$

Higgs mode:

$$E_{k\theta} = \sqrt{\alpha_{k\theta}^2 - \beta_{k\theta}^2}$$

$$\boxed{E_{k\theta}^2 = \left(\frac{U}{2}\cos\theta + 2Jz\sin^2\theta - J\cos^2\theta\,\varepsilon_k\right)^2 - J^2\cos^4\theta\,\varepsilon_k^2}$$

- Higgs mass $m_\theta = E_{k\theta}\big|_{k=0}$

use $\varepsilon_k = 2\cos k_x + 2\cos k_y = 4$ for $k=0$

$z = 4$ for square lattice

$$\boxed{m_\theta^2 = \left(\frac{U}{2}\cos\theta + 8J\sin\theta^2 - 4J\cos^2\theta\right)^2 - 16J^2\cos^4\theta}$$

<u>insulating</u> (disordered) phase $\theta = 0$

$$m_\theta^2 = \left(\frac{U}{2} - 4J\right)^2 - 16J^2$$

at criticality: $U_c = 4Jz = 16J$

$$m_\theta^2 = (8J - 4J)^2 - 16J^2 = 0$$

as it should be!

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<u>Ordered phase</u> $\cos\theta = \frac{u}{4Jz} = \frac{u}{16J}$

$$m_\theta^2 = \left(\frac{u}{2}\frac{u}{16J} + 8J\left(1 - \frac{u^2}{256J^2}\right) - 4J\frac{u^2}{256J^2}\right)^2 - 16J^2\left(\frac{u}{16J}\right)^4$$

$$= \left(\frac{u^2}{J}\left(\frac{1}{32} - \frac{1}{32} - \frac{1}{64}\right) + 8J\right)^2 - \frac{1}{64^2}\frac{u^4}{J^2}$$

$$= \left(-\frac{1}{64}\frac{u^2}{J} + 8J\right)^2 - \left(\frac{1}{64}\frac{u^2}{J}\right)^2$$

$$m_\theta^2 = 64J^2 - \frac{1}{4}u^2$$

vanishes at criticality $u_c = 16J$,

positive for $u < u_c$, i.e. in superfluid

Goldstone mode

$$\mathcal{E}_{k\varphi} = \sqrt{\alpha_{k\varphi}^2 - \beta_{k\varphi}^2}$$

$$\boxed{\mathcal{E}_{k\varphi}^2 = \left(\frac{U}{4}(1+\cos\theta) + Jz\sin^2\theta - \frac{J}{2}(1+\cos\theta)\,\varepsilon_k \right)^2 - \frac{J^2}{4}(1+\cos\theta)^2 \varepsilon_k^2}$$

- Goldstone mass $m_\varphi = \mathcal{E}_{k\varphi}\big|_{\varphi=0}$

$$\boxed{m_\varphi^2 = \left(\frac{U}{4}(1+\cos\theta) + 4J\sin^2\theta - 2J(1+\cos\theta) \right)^2 - 4J^2(1+\cos\theta)^2}$$

insulating phase, $\theta = 0$

$$m_\varphi^2 = \left(\frac{U}{2} - 4J \right)^2 - 16J^2$$

identical to Higgs as it should be in disordered phase

at criticality $U_c = 16J$

$$m_\varphi^2 = (8J - 4J)^2 - 16J^2 = 0$$

✓

Ordered phase: $\cos\theta = \frac{u}{16J}$

$$m_\varphi^2 = \left(\frac{u}{4}\left(1+\frac{u}{16J}\right) + 4J\left(1-\frac{u^2}{256J^2}\right) - 2J\left(1+\frac{u}{16J}\right)\right)^2 - 4J^2\left(1+\frac{u}{16J}\right)^2$$

$$= \left(\frac{u}{4} + \cancel{\frac{u^2}{64J}} + 4J - \cancel{\frac{1}{64}\frac{u^2}{J}} - 2J + \frac{1}{8}u \right)^2 - 4J^2\left(1+\frac{u}{16J}\right)^2$$

$$= \left(\frac{u}{8} + 2J\right)^2 - 4J^2\left(1+\frac{u}{16J}\right)^2$$

$$= 4J^2\left(1+\frac{u}{16J}\right)^2 - 4J^2\left(1+\frac{u}{16J}\right)^2 = 0$$

Goldstone mass vanishes everywhere in ordered phase, as it should!

Alternative method for analyzing effective Hamiltonians

Go to *first* quantization, find eigenmodes

- effective Higgs Hamiltonian

$$H = \sum_i \left(\frac{U}{2} \cos\theta + 2Jz \sin^2\theta \right) b^+_{i\theta} b_{i\theta} - \sum_{\langle ij \rangle} J \cos^2\theta \left(b^+_{i\theta} + b_{i\theta} \right) \left(b^+_{j\theta} + b_{j\theta} \right)$$

- go to first quantization: ($m = \hbar = 1$)

$$b^+ + b = \sqrt{2\omega}\, x \quad , \quad \omega b^+ b = \frac{p^2}{2} + \frac{1}{2}\omega^2 x^2$$

<u>Here:</u>

$$\omega = \frac{U}{2}\cos\theta + 2Jz \sin^2\theta$$

$$b^+ + b = \left(U\cos\theta + 4Jz\sin^2\theta \right)^{\frac{1}{2}} x$$

- rewrite H

$$H_\theta = \sum_i \left(\frac{p_i^2}{2} + \frac{1}{2} \left(\frac{U}{2}\cos\theta + 2Jz\sin^2\theta \right)^2 x_i^2 \right)$$

$$- \sum_{\langle ij \rangle} J\cos^2\theta \left(U\cos\theta + 4Jz\sin^2\theta \right) x_i x_j$$

- Fourier transformation $\quad \tilde{x}_k = \frac{1}{\sqrt{N}} \sum_j e^{ikj} x_j$

$$H_\theta = \sum_k \frac{\tilde{p}_k^2}{2} + \frac{1}{2} \sum_k \tilde{x}_k \tilde{x}_{-k} \Bigg(\left(\frac{U}{2}\cos\theta + 2Jz\sin^2\theta \right)^2 -$$

$$- J\cos^2\theta \left(U\cos\theta + 4Jz\sin^2\theta \right) \varepsilon_k \Bigg)$$

$$\varepsilon_k = 2\cos k_x + 2\cos k_y$$

Read off the eigenmode frequencies

$$\boxed{E_{k\theta}^2 = \left(\frac{U}{2}\cos\theta + 2Jz\sin^2\theta\right)^2 - 2J\cos^2\theta\left(\frac{U}{2}\cos\theta + 2Jz\sin^2\theta\right)\varepsilon_k}$$

This agrees with $E_{k\theta}^2$ from the Bogoliubov transformation on page 25!

This method avoids the Bogoliubov transformation, maybe easier in disordered case ?!

Transformation of boson creation and destruction operators in 1st-quantized version

$$x_j = \frac{1}{\sqrt{2\omega}} (b_j^+ + b_j) \qquad p_j = i\sqrt{\frac{\omega}{2}} (b_j^+ - b_j)$$

- Fourier transformation

$$\tilde{x}_k = \frac{1}{\sqrt{N}} \sum_j x_j e^{ikj} = \frac{1}{\sqrt{2\omega}} \sum_j (b_j^+ + b_j) e^{ikj}$$

$$\tilde{x}_k = \frac{1}{\sqrt{2\omega}} (a_k + a_{-k}^+)$$

$$\tilde{p}_k = i\sqrt{\frac{\omega}{2}} (a_{-k}^+ - a_k)$$

- after diagonalization in 1st quantization, define new bosons

$$\gamma_k = \sqrt{\frac{E_k}{2}} \left(\tilde{x}_k + \frac{i}{E_k} \tilde{p}_k \right)$$

$$= \frac{1}{2}\sqrt{\frac{E_k}{\omega}} (a_k + a_{-k}^+) + \frac{i}{2}\sqrt{\frac{\omega}{E_k}}\, i (a_{-k}^+ - a_k)$$

$$\boxed{\gamma_k = \frac{1}{2}\left(\sqrt{\frac{E_k}{\omega}} + \sqrt{\frac{\omega}{E_k}} \right) a_k + \frac{1}{2}\left(\sqrt{\frac{E_k}{\omega}} - \sqrt{\frac{\omega}{E_k}} \right) a_{-k}^+}$$

takes form of Bogoliubov transformation

$$\gamma_k = u_k a_k - v_k a_{-k}^+$$

$\Rightarrow$ check coefficients

$$u_k^2 = \frac{1}{4}\left(\sqrt{\frac{E_k}{\omega}} + \sqrt{\frac{\omega}{E_k}}\right)^2$$

<u>Higgs case:</u> $\omega = \frac{u}{2}\cos\theta + 2Jz\sin^2\theta = \alpha_k - \beta_k$ (page 24)

$$E_k^2 = \left(\frac{u}{2}\cos\theta + 2Jz\sin^2\theta\right)^2 - 2J\cos^2\theta\,\varepsilon_k\left(\frac{u}{2}\cos\theta + 2Jz\sin^2\theta\right)$$

$$= \alpha_k^2 - \beta_k^2$$

$$u_k^2 = \frac{1}{4}\left(\frac{E_k}{\omega} + \frac{\omega}{E_k} + 2\right) = \frac{1}{4}\left(\frac{\sqrt{\alpha_k^2-\beta_k^2}}{\alpha_k-\beta_k} + \frac{\alpha_k-\beta_k}{\sqrt{\alpha_k^2-\beta_k^2}} + 2\right)$$

$$= \frac{1}{4}\left(\sqrt{\frac{\alpha_k+\beta_k}{\alpha_k-\beta_k}} + \sqrt{\frac{\alpha_k-\beta_k}{\alpha_k+\beta_k}} + 2\right) = \frac{1}{4}\left(\frac{\alpha_k+\beta_k+\alpha_k-\beta_k}{\sqrt{\alpha_k^2-\beta_k^2}} + 2\right)$$

$$= \frac{1}{2}\left(\frac{\alpha_k}{\sqrt{\alpha_k^2-\beta_k^2}} + 1\right)$$

as in Bogoliubov case (page 243)

$$v_k^2 = \frac{1}{4}\left(\frac{E_k}{\omega} + \frac{\omega}{E_k} - 2\right) = \frac{1}{2}\left(\frac{\alpha_k}{\sqrt{\alpha_k^2-\beta_k^2}} - 1\right)$$

$$u_k v_k = \frac{1}{2}\left(\sqrt{\frac{E_k}{\omega}} + \sqrt{\frac{\omega}{E_k}}\right)\left(-\frac{1}{2}\right)\left(\sqrt{\frac{E_k}{\omega}} - \sqrt{\frac{\omega}{E_k}}\right)$$

$$= -\frac{1}{4}\left(\frac{E_k}{\omega} - \frac{\omega}{E_k}\right) = -\frac{1}{2}\frac{\beta_k}{\sqrt{\alpha_k^2-\beta_k^2}}$$

reproduces Bogolibov transformation

Order parameter and OP magnitude in mean-field + Gaussian fluctuations

- rewrite $\langle \psi_i \rangle$ and $\langle |\psi_i|^2 \rangle$ in terms of excitation Hamiltonian

- Order parameter

$$\langle \psi_i \rangle = \langle GS | S_i^+ | GS \rangle$$

- from page 16 : S_i^+ in terms of b-bosons

$$S_i^+ = \sin\theta \left(1 - b_{\theta i}^+ b_{\theta i} - b_{\varphi i}^+ b_{\varphi i}\right) - \sin\theta \, b_{\theta i}^+ b_{\theta i}$$
$$- \cos\theta \, b_{\theta i}^+ + \cos\tfrac{\theta}{2} \, b_{\varphi i}^+$$
$$- \cos\theta \, b_{\theta i} - \cos\tfrac{\theta}{2} \, b_{\varphi i}$$
$$+ \sin\tfrac{\theta}{2} \, b_{\varphi i}^+ b_{\theta i} - \sin\tfrac{\theta}{2} \, b_{\theta i}^+ b_{\varphi i}$$

- from page 24d

$$\langle GS | b | GS \rangle = \langle GS | b^+ | GS \rangle = 0$$

$$\langle GS | S_i^+ | GS \rangle = \underbrace{\sin\theta}_{\text{mean-field value}} \underbrace{- \sin\theta \langle GS | 2 b_{\theta i}^+ b_{\theta i} + b_{\varphi i}^+ b_{\varphi i} | GS \rangle}_{\text{quantum fluctuations reduce OP}}$$

- evaluate fluctuation terms (see page 24d)

$$b_i^+ b_i = \frac{1}{N} \sum_k b_k^+ b_k$$

$$\langle GS | b_k^+ b_k | GS \rangle = V_k^2 = \frac{1}{2} \left(\frac{\alpha_k}{\sqrt{\alpha_k^2 - \beta_k^2}} - 1 \right)$$

Insert into OP

$$\boxed{\langle \Psi_i \rangle = \sin\theta - 2\sin\theta \frac{1}{N} \sum_k V_{k\theta}^2 - \sin\theta \frac{1}{N} \sum_k V_{k\varphi}^2}$$

MF fluctuation - corrections

- Order parameter magnitude

$$\langle |\Psi_i|^2 \rangle = \langle GS | (S_i^x)^2 + (S_i^y)^2 | GS \rangle = \langle GS | 2 - (S_i^z)^2 | GS \rangle$$

from page 15 $(S_i^z)^2$ in terms of b-bosons

$$(S_i^z)^2 = \frac{1}{2}(1-\cos\theta) + \cos\theta \; b_{\theta i}^+ b_{\theta i} + \frac{1}{2}(1+\cos\theta) \, b_{\varphi i}^+ b_{\varphi i}$$
$$- \frac{1}{2}\sin\theta \left(b_{\theta i}^+ + b_{\theta i} \right)$$

from page 24a: $\langle GS | b | GS \rangle = \langle GS | b^+ | GS \rangle = 0$

$$\langle GS | (S_i^z)^2 | GS \rangle = \frac{1}{2}(1-\cos\theta)$$
$$+ \langle GS | \cos\theta \, b_{\theta i}^+ b_{\theta i} | GS \rangle$$
$$+ \langle GS | \frac{1}{2}(1+\cos\theta) b_{\varphi i}^+ b_{\varphi i} | GS \rangle$$

from Bogoliubov transformation

$$\langle GS | b_{\theta i}^+ b_{\theta i} | GS \rangle = \frac{1}{N} \sum_k V_{k\theta}^2$$
$$\langle GS | b_{\varphi i}^+ b_{\varphi i} | GS \rangle = \frac{1}{N} \sum_k V_{k\varphi}^2$$

$$\boxed{\langle GS | (S_i^z)^2 | GS \rangle = \frac{1}{2}(1-\cos\theta) + \cos\theta \frac{1}{N} \sum_k V_{k\theta}^2 + \frac{1}{2}(1+\cos\theta) \frac{1}{N} \sum_k V_{k\varphi}^2}$$

c.f. eq (A8) in Pekker et al PRB 86, 144527 (2012)

$$\langle |\psi_n^i|^2 \rangle = \langle GS | 2 - (S_n^{iz})^2 | GS \rangle$$

$$\boxed{\langle |\psi_n^i|^2 \rangle = \frac{3}{2} + \frac{1}{2}\cos\Theta - \cos\Theta \frac{1}{N} \sum_k V_{k\Theta}^2 - \frac{1}{2}(1 + \cos\Theta) \frac{1}{N} \sum_k V_{k\varphi}^2}$$

Scalar susceptibility

- goal: compute Green's function of order parameter magnitude

- recall: local OP magnitude (on site j)

$$|\psi_j|^2 = (S_j^x)^2 + (S_j^y)^2 = S(S+1) - (S_j^z)^2 = 2 - (S_j^z)^2$$

- express $(S_j^z)^2$ in terms of b-bosons (page 15)

$$|\psi_j|^2 = \frac{3}{2} + \frac{1}{2}\cos\theta - \cos\theta\, b^\dagger_{\theta j} b_{\theta j} - \frac{1}{2}(1+\cos\theta)\, b^\dagger_{\varphi j} b_{\varphi j}$$
$$+ \frac{1}{2}\sin\theta\,(b^\dagger_{\theta j} + b_{\theta j})$$

(note: $|\psi_j|^2$ has nonzero expectation value
$\Rightarrow$ construct connected correlation / Green's function)

Retarded scalar Green's function

$$\boxed{G_{jn}(t) = -i\Theta(t)\, \langle GS|\,[\,|\psi_j(t)|^2, |\psi_n(0)|^2\,]\,|GS\rangle}$$

(note: commutator automatically removes additive constants $\Rightarrow$ only connected part survives)

- insert representation of $|\psi|^2$ in terms of $b, b^\dagger$, keep only terms up to quadratic order in $b, b^\dagger$

$$\boxed{G_{jn}(t) = -i\,\theta(t)\,\frac{1}{4}\sin^2\theta \left\langle GS \right| \left[b^+_{\theta j}(t) + b_{\theta j}(t),\, b^+_{\theta n}(0) + b_{\theta n}(0) \right] \left| GS \right\rangle}$$

all other terms either cancel under commutator or are of higher order in b, b^+

- Note: $G_{jn}(t) \sim \sin^2\theta \Rightarrow$ vanishes in disordered (insulating) phase
  - Why? Also observed in Pekker et al PRB 86, 144527 (2012)
  - Can be fixed by going to higher order in G and in Hamiltonian, leads to coupling between Higgs and Goldstone modes

- Fourier transformation of b-bosons (see page 23)

$$\left.\begin{aligned} b_{\theta j} &= \frac{1}{\sqrt{N}} \sum_k e^{-ikj} a_{\theta k} \\ b^+_{\theta j} &= \frac{1}{\sqrt{N}} \sum_k e^{ikj} a^+_{\theta k} \end{aligned}\right\} \qquad \begin{aligned} &b^+_{\theta j} + b_{\theta j} = \\ &\frac{1}{\sqrt{N}} \sum_k e^{ikj} \left(a^+_{\theta k} + a_{\theta -k} \right) \end{aligned}$$

- Fourier transform Green's function, use translational invariance

$$\tilde{G}_k(t) = \frac{1}{N} \sum_j \sum_m e^{ikm}\, G_{j,j+m}(t)$$

$$= \frac{1}{N} \sum_j \sum_m e^{ikm} (-i)\,\theta(t) \frac{1}{4} \sin^2\theta \; \frac{1}{N} \sum_{q_1 q_2} e^{iq_1 j + iq_2 (j+m)} \times$$

$$\times \left\langle GS \right| \left[a^+_{\theta q_1}(t) + a_{\theta -q_1}(t),\, a^+_{\theta q_2}(0) + a_{\theta -q_2}(0) \right] \left| GS \right\rangle$$

Simplify sums over phase factors

$$\frac{1}{N^2}\sum_{jm}\sum_{q_1 q_2} e^{ikm}\, e^{iq_1 j + iq_2(j+m)} \qquad \text{j-sum}$$

$$= \frac{1}{N}\sum_{m}\sum_{q_1 q_2} e^{ikm}\, e^{-iq_1 m}\; \delta_{q_1,-q_2} \qquad \text{m-sum}$$

$$= \sum_{q_1 q_2} \delta_{k,q_1}\, \delta_{q_1,-q_2}$$

$$\boxed{\tilde{G}_k(t) = -i\,\Theta(t)\,\frac{1}{4}\sin^2\theta\,\langle GS|\left[a^+_{\theta k}(t) + a_{\theta -k}(t),\, a^+_{\theta -k}(0) + a_{\theta k}(0)\right]|GS\rangle}$$

- now express $a_{\theta k}$, $a^+_{\theta k}$ in terms of Bogoliubov bosons γ, γ^+ (page 24)

$$a_k = u_k \gamma_k + v_k \gamma^+_{-k} \qquad u_k, v_k \text{ \underline{even} in } k$$

$$a^+_{-k} = v_k \gamma_k + u_k \gamma^+_{-k}$$

$$a^+_k + a_{-k} = u_k \gamma^+_k + v_k \gamma_{-k} + u_k \gamma_{-k} + v_k \gamma^+_k$$

$$\boxed{a^+_k + a_{-k} = (u_k + v_k)(\gamma^+_k + \gamma_{-k})}$$

insert into Green's function

$$\boxed{\begin{aligned}\tilde{G}_k(t) = -i\,\theta(t)\,\tfrac{1}{4}\sin^2\theta\,(u_k+v_k)^2 \;\times\\ \times \langle GS|\left[\gamma^+_{\theta k}(t)+\gamma_{\theta -k}(t),\ \gamma^+_{\theta -k}(0)+\gamma_{\theta k}(0)\right]|GS\rangle\end{aligned}}$$

- since the since the Bogoliubov Hamiltonian has the simple form $H = \frac{1}{2}\sum_k E_{k\theta}\,\gamma^+_{k\theta}\gamma_{k\theta}$, eigenstates have fixed numbers of γ-bosons

$\Rightarrow$ keep only $\gamma^+\gamma$ and $\gamma\gamma^+$ terms

$$\tilde{G}_k(t) = -i\,\theta(t)\,\tfrac{1}{4}\sin^2\theta\,(u_k+v_k)^2\Big(\langle GS|\left[\gamma^+_{\theta k}(t),\gamma_{\theta k}(0)\right]|GS\rangle + \langle GS|\left[\gamma_{\theta -k}(t),\gamma^+_{\theta -k}(0)\right]|GS\rangle\Big)$$

- expand commutators, keep only terms $\gamma\gamma^+$ terms because GS is γ-vacuum

$$\boxed{\tilde{G}_k(t) = -i\,\theta(t)\,\tfrac{1}{4}\sin^2\theta\,(u_k+v_k)^2\,\langle GS|-\gamma_{\theta k}(0)\gamma^+_{\theta k}(t)+\gamma_{\theta -k}(t)\gamma^+_{\theta -k}(0)|GS\rangle}$$

use $\hat{A}(t) = e^{i\hat{H}t}\,\hat{A}\,e^{-i\hat{H}t}$

$$\langle GS|-\gamma_{\theta k}(0)\gamma^+_{\theta k}(t)|GS\rangle = -e^{iE_{k\theta}t}$$

$$\langle GS|\gamma_{\theta -k}(t)\gamma^+_{\theta -k}(0)|GS\rangle = e^{-iE_{k\theta}t}$$

$$\tilde{G}_k(t) = -i\,\Theta(t)\,\frac{1}{4}\sin^2\theta\,(U_k+V_k)^2\left(-e^{iE_{k\theta}t} + e^{-iE_{k\theta}t}\right)$$

Fourier transform in time

$$\tilde{G}_k(\omega) = \int_{-\infty}^{\infty} dt\; e^{i(\omega+i\delta)t}\,\tilde{G}_k(t)$$

$$= -i\,\frac{1}{4}\sin^2\theta\,(U_k+V_k)^2\int_0^{\infty} dt\; e^{i(\omega+i\delta)t}\left(-e^{iE_{k\theta}t} + e^{-iE_{k\theta}t}\right)$$

$$= -i\frac{1}{4}\sin^2\theta\,(u_k+V_k)^2\left(\frac{1}{i(\omega+i\delta)+iE_{k\theta}} - \frac{1}{i(\omega+i\delta)-iE_{k\theta}}\right)$$

$$\boxed{\tilde{G}_k(\omega) = \frac{\frac{1}{4}\sin^2\theta\,(u_k+V_k)^2}{\omega+i\delta-E_{k\theta}} - \frac{\frac{1}{4}\sin^2\theta\,(u_k+V_k)^2}{\omega+i\delta+E_{k\theta}}}$$

spectral density $A(\omega)$ defined via

$$\tilde{G}(\omega) = \int_{-\infty}^{\infty} dx\,\frac{A(x)}{\omega+i\delta-x}$$

$$\boxed{A_k(\omega) = \frac{1}{4}\sin^2\theta\,(U_k+V_k)^2\Big(\delta(\omega-E_{k\theta}) - \delta(\omega+E_{k\theta})\Big)}$$

δ-peaks at the Bogoliubov eigenfrequencies, odd in ω as expected

Order parameter susceptibility

recall: local OP $\langle \psi_i \rangle = \langle GS | S_i^+ | GS \rangle$

order is in x-y plane of spin space

in mean-field theory $\langle \psi_i \rangle = \sin\theta \, e^{i\varphi}$

$S_i^+ = S_i^x + i S_i^y \Rightarrow S_i^x$ and S_i^y give x, y components of OP

- in our fluctuation expansion in terms of b-bosons, we set $\varphi = 0 \Rightarrow$ order in x-direction

- construct longitudinal and transverse dynamic susceptibilities

$$\boxed{\begin{aligned} \chi_{ij}^{\parallel}(t) &= -i\theta(t) \langle GS | [S_i^x(t), S_j^x(0)] | GS \rangle \\ \chi_{ij}^{\perp}(t) &= -i\theta(t) \langle GS | [S_i^y(t), S_j^y(0)] | GS \rangle \end{aligned}}$$

recall (page 31)

$$\begin{aligned} S_i^+ = {} & \sin\theta(1 - b_{\theta i}^+ b_{\theta i} - b_{\varphi i}^+ b_{\varphi i}) - \sin\theta \, b_{\theta i}^+ b_{\theta i} - \cos\theta \, b_{\theta i}^+ \\ & + \cos\frac{\theta}{2} b_{\varphi i}^+ - \cos\theta \, b_{\theta i} - \cos\frac{\theta}{2} b_{\varphi i} \\ & + \sin\frac{\theta}{2} b_{\varphi i}^+ b_{\theta i} - \sin\frac{\theta}{2} b_{\theta i}^+ b_{\varphi i} \end{aligned}$$

$$S_i^{\pm} = S_i^x \pm i S_i^y$$

$$S_i^x = \frac{1}{2}\left(S_i^+ + S_i^-\right) \qquad S_i^y = \frac{1}{2i}\left(S_i^+ - S_i^-\right)$$

$$S_i^x = \sin\theta - 2\sin\theta\, b_{\theta i}^+ b_{\theta i} - \sin\theta\, b_{\varphi i}^+ b_{\varphi i}$$
$$- \cos\theta\left(b_{\theta i}^+ + b_{\theta i}\right)$$

$$S_i^y = \frac{1}{i}\left(\cos\frac{\theta}{2}\left(b_{\varphi i}^+ - b_{\varphi i}\right) + \sin\frac{\theta}{2}\left(b_{\varphi i}^+ b_{\theta i} - b_{\theta i}^+ b_{\varphi i}\right)\right)$$

Longitudinal susceptibility

expand to quadratic order in b, constant terms drop out under commutator

$$\boxed{\chi_{jn}^{\parallel}(t) = -i\Theta(t)\cos^2\theta \left\langle GS\right| \left[b_{\theta j}^+(t) + b_{\theta j}(t),\, b_{\theta n}^+(0) + b_{\theta n}(0)\right] \left|GS\right\rangle}$$

$$\boxed{\chi_{jn}^{\perp}(t) = -i\Theta(t)\left(-\cos^2\frac{\theta}{2}\right) \left\langle GS\right| \left[b_{\varphi j}^+(t) - b_{\varphi j}(t),\, b_{\varphi n}^+(0) - b_{\varphi n}(0)\right] \left|GS\right\rangle}$$

- can be turned into + by rotating $b \to ib$ (see page 22)

- Same structure as scalar susceptibility but different prefactor

- in Mott insulator phase, $\theta = 0$, $\chi^{\parallel}$ and $\chi^{\perp}$ become identical as they should

Inhomogeneous mean-field theory for disordered rotor model

H in spin representation

$$\boxed{H = -\frac{1}{2}\sum_{\langle ij\rangle} J_{ij}\left(S_i^+ S_j^- + S_j^+ S_i^-\right) + \frac{1}{2}\sum_i U_i \left(S_i^z\right)^2 - \sum_i \mu_i S_i^z}$$

mean-field wave function

$$|\Phi\rangle = \prod_i |\varphi_i\rangle$$

$$|\varphi_i\rangle = \cos\left(\frac{\theta_i}{2}\right)|0_i\rangle + \sin\left(\frac{\theta_i}{2}\right)\frac{1}{\sqrt{2}}\left(e^{i\varphi_i}|\uparrow_i\rangle + e^{-i\varphi_i}|\downarrow_i\rangle\right)$$

<u>Note</u>: - θ_i rotates from MI to SF

- φ_i is SF OP phase

- ansatz is for particle-hole symmetric case, $\mu_i \equiv 0$

Variational energy

$$E_0 = \langle \Phi | H | \Phi \rangle$$

Coulomb part

$$\langle \bar{\Phi} | \frac{1}{2} \sum_i U_i (S_i^z)^2 | \bar{\Phi} \rangle = \frac{1}{2} \sum_i U_i \langle \varphi_i | (S_i^z)^2 | \varphi_i \rangle$$

$$= \frac{1}{2} \sum_i U_i \, \frac{1}{2} \sin^2\left(\frac{\theta_i}{2}\right) \left[\langle \uparrow_i | \uparrow_i \rangle + \langle \downarrow_i | \downarrow_i \rangle \right]$$

$$= \frac{1}{2} \sum_i U_i \, \sin^2\left(\frac{\theta_i}{2}\right)$$

Josephson part

$$\langle \Phi | -\frac{1}{2} \sum_{\langle ij \rangle} J_{ij} \left(S_i^+ S_j^- + S_j^+ S_i^- \right) | \bar{\Phi} \rangle =$$

$$= -\frac{1}{2} \sum_{\langle ij \rangle} J_{ij} \langle \varphi_i | \langle \varphi_j | \left(S_i^+ S_j^- + S_j^+ S_i^- \right) | \varphi_j \rangle | \varphi_i \rangle$$

$$= -\frac{1}{2} \sum_{\langle ij \rangle} J_{ij} \left[\langle \varphi_i | S_i^+ | \varphi_i \rangle \langle \varphi_j | S_j^- | \varphi_j \rangle + h.c \right]$$

$$= -\frac{1}{2} \sum_{\langle ij \rangle} J_{ij} \Big[\sin\left(\frac{\theta_i}{2}\right) \cos\left(\frac{\theta_i}{2}\right) \left(e^{-i\varphi_i} + e^{-i\varphi_i} \right) \times$$
$$\sin\left(\frac{\theta_j}{2}\right) \cos\frac{\theta_j}{2} \left(e^{i\varphi_j} + e^{i\varphi_j} \right) + c.c. \Big]$$

$$= -\frac{1}{2} \sum_{\langle ij \rangle} J_{ij} \quad \sin\theta_i \, \sin\theta_j \, e^{-i(\varphi_i - \varphi_j)} \quad + c.c.$$

$$= - \sum_{\langle ij \rangle} J_{ij} \quad \sin\theta_i \sin\theta_j \quad \cos(\varphi_i - \varphi_j)$$

Collect terms

$$E_0 = \langle \Psi | H | \Psi \rangle$$

$$\boxed{E_0 = \frac{1}{2} \sum_i U_i \sin^2\left(\frac{\theta_i}{2}\right) - \sum_{\langle ij \rangle} J_{ij} \sin\theta_i \sin\theta_j \cos(\varphi_i - \varphi_j)}$$

Minimize E_0 : $\quad \frac{\partial E_0}{\partial \theta_i} = 0 \quad , \quad \frac{\partial E_0}{\partial \varphi_i} = 0$

$$\frac{\partial E_0}{\partial \varphi_i} = - \sum_j{}' J_{ij} \sin\theta_i \sin\theta_j \sin(\varphi_i - \varphi_j) = 0$$

fulfilled for $\varphi_i \equiv$ const $\Rightarrow$ uniform phase

$$\frac{\partial E_0}{\partial \theta_i} = \frac{1}{2} U_i \sin\frac{\theta_i}{2} \cos\frac{\theta_i}{2} - \sum_j{}' J_{ij} \cos\theta_i \sin\theta_j \qquad (\varphi_i \equiv \text{const})$$

$$= \boxed{\frac{U_i}{4} \sin\theta_i - \sum_j{}' J_{ij} \sin\theta_j \cos\theta_i = 0}$$

(i) insulating solution $\quad \sin\theta_i \equiv 0 \quad\quad \theta_i = 0, 2\pi$

(ii) superfluid solution $\quad \sin\theta_i \neq 0$

for small U_i / large J_{ij}

Construct effective Hamiltonian for excitations

start from pages 14 to 16 of the clean notes

- the local basis states are

$$|g_i\rangle = \cos\frac{\theta_i}{2}|0_i\rangle + \sin\frac{\theta_i}{2}\frac{1}{\sqrt{2}}\left(|1_i\rangle + |-1_i\rangle\right)$$

$$|\theta_i\rangle = \sin\frac{\theta_i}{2}|0_i\rangle - \cos\frac{\theta_i}{2}\frac{1}{\sqrt{2}}\left(|1_i\rangle + |-1_i\rangle\right)$$

$$|\varphi_i\rangle = \frac{1}{\sqrt{2}}\left(|1_i\rangle - |-1_i\rangle\right)$$

Note that in the disordered case, the angle θ_i depends on the site. The order parameter phase is still uniform and set to zero, as before.

$$\left(S_i^z\right)^2 = \cos\theta_i\, b_{\theta i}^+ b_{\theta i} + \frac{1}{2}\left(1+\cos\theta_i\right) b_{\varphi i}^+ b_{\varphi i} + \frac{1}{2}\left(1-\cos\theta_i\right)$$

$$\boxed{\left(S_i^z\right)^2 = \cos\theta_i\, b_{\theta i}^+ b_{\theta i} + \cos^2\frac{\theta_i}{2}\, b_{\varphi i}^+ b_{\varphi i} + \sin^2\frac{\theta_i}{2}}$$

b-linear terms dropped

$$\boxed{\begin{aligned} S_i^+ = {} & \sin\theta_i\, b_{0i}^+ b_{0i} - \cos\theta_i\, b_{\theta i}^+ b_{0i} + \cos\frac{\theta_i}{2}\, b_{\varphi i}^+ b_{0i} \\ & - \sin\theta_i\, b_{\theta i}^+ b_{\theta i} - \cos\theta_i\, b_{0i}^+ b_{\theta i} + \sin\frac{\theta_i}{2}\, b_{\varphi i}^+ b_{\theta i} \\ & - \cos\frac{\theta_i}{2}\, b_{0i}^+ b_{\varphi i} - \sin\frac{\theta_i}{2}\, b_{\theta i}^+ b_{\varphi i} \end{aligned}}$$

$$
\begin{aligned}
S_i^+ S_j^- = \Big(& \sin\theta_i\, b_{0i}^+ b_{0i} - \cos\theta_i\, b_{\theta i}^+ b_{0i} + \cos\tfrac{\theta_i}{2}\, b_{\varphi i}^+ b_{0i} \\
& - \sin\theta_i\, b_{\theta i}^+ b_{\theta i} - \cos\theta_i\, b_{0i}^+ b_{\theta i} + \sin\tfrac{\theta_i}{2}\, b_{\varphi i}^+ b_{\theta i} \\
& - \cos\tfrac{\theta_i}{2}\, b_{0i}^+ b_{\varphi i} - \sin\tfrac{\theta_i}{2}\, b_{\theta i}^+ b_{\varphi i} \Big) \times \\
\times \Big(& \sin\theta_j\, b_{0j}^+ b_{0j} - \cos\theta_j\, b_{0j}^+ b_{\theta j} + \cos\tfrac{\theta_j}{2}\, b_{0j}^+ b_{\varphi j} \\
& - \sin\theta_j\, b_{\theta j}^+ b_{\theta j} - \cos\theta_j\, b_{\theta j}^+ b_{0j} + \sin\tfrac{\theta_j}{2}\, b_{\theta j}^+ b_{\varphi j} \\
& - \cos\tfrac{\theta_j}{2}\, b_{\varphi j}^+ b_{0j} - \sin\tfrac{\theta_j}{2}\, b_{\varphi j}^+ b_{\theta j} \Big)
\end{aligned}
$$

Keep only terms quadratic in b_θ and b_φ

$$
\begin{aligned}
S_i^+ S_j^- = \; & \sin\theta_i \sin\theta_j \left(-b_{\theta i}^+ b_{\theta i} - b_{\varphi i}^+ b_{\varphi i} - b_{\theta j}^+ b_{\theta j} - b_{\varphi j}^+ b_{\varphi j} \right) \\
& - \sin\theta_i \sin\theta_j\, b_{\theta j}^+ b_{\theta j} + \sin\theta_i \sin\tfrac{\theta_j}{2} \left(b_{\theta j}^+ b_{\varphi j} - b_{\varphi j}^+ b_{\theta j} \right) \\
& + \cos\theta_i \cos\theta_j\, b_{\theta i}^+ b_{\theta j} - \cos\theta_i \cos\tfrac{\theta_j}{2}\, b_{\theta i}^+ b_{\varphi j} \\
& + \cos\theta_i \cos\theta_j\, b_{\theta i}^+ b_{\theta j}^+ + \cos\theta_i \cos\tfrac{\theta_j}{2}\, b_{\theta i}^+ b_{\varphi j}^+ \\
& - \cos\tfrac{\theta_i}{2} \cos\theta_j\, b_{\varphi i}^+ b_{\theta j} + \cos\tfrac{\theta_i}{2} \cos\tfrac{\theta_j}{2}\, b_{\varphi i}^+ b_{\varphi j} \\
& - \cos\tfrac{\theta_i}{2} \cos\theta_j\, b_{\varphi i}^+ b_{\theta j}^+ - \cos\tfrac{\theta_i}{2} \cos\tfrac{\theta_j}{2}\, b_{\varphi i}^+ b_{\varphi j}^+ \\
& - \sin\theta_i \sin\theta_j\, b_{\theta i}^+ b_{\theta i} \\
& + \cos\theta_i \cos\theta_j\, b_{\theta i} b_{\theta j} - \cos\theta_i \cos\tfrac{\theta_j}{2}\, b_{\theta i} b_{\varphi j} \\
& + \cos\theta_i \cos\theta_j\, b_{\theta i} b_{\theta j}^+ + \cos\theta_i \cos\tfrac{\theta_j}{2}\, b_{\theta i} b_{\varphi j}^+ \\
& + \sin\tfrac{\theta_i}{2} \sin\theta_j\, b_{\varphi i}^+ b_{\theta i} \\
& + \cos\tfrac{\theta_i}{2} \cos\theta_j\, b_{\varphi i} b_{\theta j} - \cos\tfrac{\theta_i}{2} \cos\tfrac{\theta_j}{2}\, b_{\varphi i} b_{\varphi j} \\
& + \cos\tfrac{\theta_i}{2} \cos\theta_j\, b_{\varphi i} b_{\theta j}^+ + \cos\tfrac{\theta_i}{2} \cos\tfrac{\theta_j}{2}\, b_{\varphi i} b_{\varphi j}^+ \\
& - \sin\tfrac{\theta_i}{2} \sin\theta_j\, b_{\theta i}^+ b_{\varphi i}
\end{aligned}
$$

Cancel with $S_j^+ S_i^-$ terms

$$S_i^+ S_j^- + S_j^+ S_i^- =$$

$$- 4 \sin\theta_i \sin\theta_j \left(b_{\theta i}^+ b_{\theta i} + b_{\theta j}^+ b_{\theta j} \right)$$
$$+ 2 \cos\theta_i \cos\theta_j \left(b_{\theta i}^+ b_{\theta j} + b_{\theta j}^+ b_{\theta i} \right)$$
$$+ 2 \cos\theta_i \cos\theta_j \left(b_{\theta i}^+ b_{\theta j}^+ + b_{\theta i} b_{\theta j} \right)$$

$$- 2 \sin\theta_i \sin\theta_j \left(b_{\varphi i}^+ b_{\varphi i} + b_{\varphi j}^+ b_{\varphi j} \right)$$
$$+ 2 \cos\frac{\theta_i}{2} \cos\frac{\theta_j}{2} \left(b_{\varphi i}^+ b_{\varphi j} + b_{\varphi j}^+ b_{\varphi i} \right)$$
$$- 2 \cos\frac{\theta_i}{2} \cos\frac{\theta_j}{2} \left(b_{\varphi i}^+ b_{\varphi j}^+ + b_{\varphi i} b_{\varphi j} \right)$$

$\leftarrow$ sign can be flipped by $b \to ib$

these reduce to the clean expressions on page 20 of the clean notes for $\theta_i = \theta_j$

Insert into full disordered Hamiltonian

$$H = -\frac{1}{2}\sum_{\langle ij\rangle} J_{ij}\left(S_i^+ S_j^- + S_j^+ S_i^-\right) + \frac{1}{2}\sum_i U_i \left(S_i^z\right)^2$$

$$H = H_\theta + H_\varphi + \text{const}$$

$$H_\theta = \frac{1}{2}\sum_i U_i \cos\theta_i \, b_{\theta i}^+ b_{\theta i}$$

$$-\frac{1}{2}\sum_{\langle ij\rangle} J_{ij}\Big[-4\sin\theta_i \sin\theta_j \left(b_{\theta i}^+ b_{\theta i} + b_{\theta j}^+ b_{\theta j}\right)$$

$$+2\cos\theta_i \cos\theta_j \left(b_{\theta i}^+ + b_{\theta i}\right)\left(b_{\theta j}^+ + b_{\theta j}\right)\Big]$$

$$\boxed{\begin{aligned} H_\theta = &\sum_i \Big(\frac{1}{2}U_i \cos\theta_i + 2{\sum_{j(i)}}' J_{ij}\sin\theta_i \sin\theta_j\Big) b_{\theta i}^+ b_{\theta i} \\ &-\sum_{\langle ij\rangle} J_{ij}\cos\theta_i \cos\theta_j \left(b_{\theta i}^+ + b_{\theta i}\right)\left(b_{\theta j}^+ + b_{\theta j}\right) \end{aligned}}$$

${\sum_{j(i)}}' \hat{=}$ sum over all neighbors of i

analogously

$$\boxed{\begin{aligned} H_\varphi = &\sum_i \Big(\frac{1}{2}U_i \cos^2\frac{\theta_i}{2} + {\sum_{j(i)}}' J_{ij}\sin\theta_i \sin\theta_j\Big) b_{\varphi i}^+ b_{\varphi i} \\ &-\sum_{\langle ij\rangle} J_{ij}\cos\frac{\theta_i}{2}\cos\frac{\theta_j}{2} \left(b_{\varphi i}^+ + b_{\varphi i}\right)\left(b_{\varphi j}^+ + b_{\varphi j}\right) \end{aligned}}$$

$\uparrow$ sign flipped using $b \to ib$

Transform H into first quantization

$m = \hbar = 1$

$b + b^+ = \sqrt{2\omega}\, x \quad , \quad \omega b^+ b = \frac{p^2}{2} + \frac{1}{2}\omega^2 x^2$

for H_θ

$$\omega_i = \frac{1}{2} h_i \cos\theta_i + 2 \sum_{j(i)}{}' J_{ij} \sin\theta_i \sin\theta_j$$

rewrite H_θ

$$\boxed{H_\theta = \sum_i \left(\frac{p_i^2}{2} + \frac{1}{2}\omega_i^2 x_i^2 \right) - \sum_{\langle ij \rangle} J_{ij} \cos\theta_i \cos\theta_j \, 2\sqrt{\omega_i \omega_j}\, x_i x_j}$$

Simple system of coupled harmonic oscillator

find eigenmodes by diagonaliting

$$\boxed{M_{ij} = \omega_i^2 \delta_{ij} - J_{ij} \cos\theta_i \cos\theta_j \, 2\sqrt{\omega_i \omega_j}}$$

M_{ij} is symmetric matrix

Note: $\sum_{\langle ij \rangle}$ goes over each pair once, thus extra factor $1/2$ for symmetric matrix M

eigenvalues and eigenvectors of M_{ij}

$$M_{ij} V_{j\nu} = E_\nu^2 V_{i\nu}$$

- E_ν^2 is eigenvalue $V_{j\nu}$ is corresponding eigenvector number ν (normalized)

- in eigenbasis of M, H_θ takes the form

$$H_\theta = \sum_\nu \frac{p_\nu^2}{2} + \frac{1}{2} E_\nu^2 x_\nu^2$$

$$\boxed{H_\theta = \sum_\nu E_\nu d_\nu^+ d_\nu}$$

c.f. clean case

$$M_{ij} = \omega^2 \delta_{ij} - 2\omega \cos^2\theta \, J_{ij} \qquad \omega = \frac{U}{2}\cos\theta + 2Jz\sin^2\theta$$

eigenvalues (via Fourier transformation)

$$E_k^2 = \left(\frac{U}{2}\cos\theta + 2Jz\sin^2\theta\right)^2 - 2J\cos^2\theta\left(\frac{U}{2} + 2Jz\sin^2\theta\right)\varepsilon_k$$

$$\varepsilon_k = 2\cos k_x + 2\cos k_y$$

as before

transformation between d and b bosons

$$x_j = \underline{V}_{j\nu}\, \tilde{x}_\nu \qquad\qquad \tilde{x}_\nu = x_j\, \underline{V}_{j\nu}$$

$$p_j = \underline{V}_{j\nu}\, \tilde{p}_\nu \qquad\qquad \tilde{p}_\nu = p_j\, V_{j\nu}$$

$$d_\nu = \sqrt{\frac{E_\nu}{2}} \left(\tilde{x}_\nu + \frac{i}{E_\nu} \tilde{p}_\nu \right)$$

$$= \sqrt{\frac{E_\nu}{2}} \sum_j \underline{V}_{j\nu} \left(x_j + \frac{i}{E_\nu} p_j \right)$$

<u>use</u> $x_j = \frac{1}{\sqrt{2\omega_j}} \left(b_j^+ + b_j \right)$, $p_j = \sqrt{\frac{\omega_j}{2}}\, i \left(b_j^+ - b_j \right)$

$$d_\nu = \sqrt{\frac{E_\nu}{2}} \sum_j \underline{V}_{j\nu} \left(\frac{1}{\sqrt{2\omega_j}} \left(b_j^+ + b_j \right) + \frac{i}{E_\nu} \sqrt{\frac{\omega_j}{2}}\, i \left(b_j^+ - b_j \right) \right)$$

$$\boxed{\begin{aligned} d_\nu &= \frac{1}{2} \sum_j \underline{V}_{j\nu} \left[\left(\sqrt{\frac{E_\nu}{\omega_j}} - \sqrt{\frac{\omega_j}{E_\nu}} \right) b_j^+ + \left(\sqrt{\frac{E_\nu}{\omega_j}} + \sqrt{\frac{\omega_j}{E_\nu}} \right) b_j \right] \\ d_\nu^+ &= \frac{1}{2} \sum_j V_{j\nu} \left[\left(\sqrt{\frac{E_\nu}{\omega_j}} - \sqrt{\frac{\omega_j}{E_\nu}} \right) d_j + \left(\sqrt{\frac{E_\nu}{\omega_j}} + \sqrt{\frac{\omega_j}{E_\nu}} \right) b_j^+ \right] \end{aligned}}$$

Check commutator

$$[d_\nu, d_\nu^+] = \frac{1}{4} \sum_{jk} \underline{V}_{j\nu} \underline{V}_{k\nu} \times$$

$$\times \Bigg[\left(\sqrt{\frac{E_\nu}{\omega_j}} - \sqrt{\frac{\omega_j}{E_\nu}} \right) b_j^+ + \left(\sqrt{\frac{E_\nu}{\omega_j}} + \sqrt{\frac{\omega_j}{E_\nu}} \right) b_j \; ,$$

$$\left(\sqrt{\frac{E_\nu}{\omega_k}} - \sqrt{\frac{\omega_k}{E_\nu}} \right) b_k + \left(\sqrt{\frac{E_\nu}{\omega_k}} + \sqrt{\frac{\omega_k}{E_\nu}} \right) b_k^+ \Bigg]$$

only $j = k$ contributes

$$[d_\nu, d_\nu^+] = \frac{1}{4} \sum_j \underline{V}_{j\nu} \underline{V}_{j\nu} \Bigg[\left(\sqrt{\frac{E_\nu}{\omega_j}} - \sqrt{\frac{\omega_j}{E_\nu}} \right)^2 (-1) + \left(\sqrt{\frac{E_\nu}{\omega_j}} + \sqrt{\frac{\omega_j}{E_\nu}} \right)^2 (+1) \Bigg]$$

mixed terms survive

$$= \frac{1}{4} \sum_j \underline{V}_{j\nu} \underline{V}_{j\nu} \quad 4 \quad = \quad 1$$

analogously

$$[d_\nu, d_\mu^+] = 0$$

back transformation (b in terms of d)

$$b_j = \sqrt{\frac{\omega_j}{2}} \left(X_j + \frac{i}{\omega_j} P_j \right)$$

$$= \sqrt{\frac{\omega_j}{2}} \sum_\nu \underline{V}_{j\nu} \left(\tilde{X}_\nu + \frac{i}{\omega_j} \tilde{P}_\nu \right)$$

use $\quad \tilde{X}_\nu = \frac{1}{\sqrt{2E_\nu}} \left(d_\nu^+ + d_\nu \right) \quad , \quad \tilde{P}_\nu = \sqrt{\frac{E_\nu}{2}}\, i \left(d_\nu^+ - d_\nu \right)$

$$\boxed{\begin{aligned} b_j &= \frac{1}{2} \sum_\nu \underline{V}_{j\nu} \left[\left(\sqrt{\frac{\omega_j}{E_\nu}} - \sqrt{\frac{E_\nu}{\omega_j}} \right) d_\nu^+ + \left(\sqrt{\frac{\omega_j}{E_\nu}} + \sqrt{\frac{E_\nu}{\omega_j}} \right) d_\nu \right] \\ b_j^+ &= \frac{1}{2} \sum_\nu \underline{V}_{j\nu} \left[\left(\sqrt{\frac{\omega_j}{E_\nu}} - \sqrt{\frac{E_\nu}{\omega_j}} \right) d_\nu + \left(\sqrt{\frac{\omega_j}{E_\nu}} + \sqrt{\frac{E_\nu}{\omega_j}} \right) d_\nu^+ \right] \end{aligned}}$$

Define matrices $\quad R_{j\nu} = \sqrt{\frac{E_\nu}{\omega_j}}\, \underline{V}_{j\nu} \quad , \quad L_{j\nu} = \sqrt{\frac{\omega_j}{E_\nu}}\, \underline{V}_{j\nu}$

$$b_j = \frac{1}{2} \sum_\nu \left[\left(L_{j\nu} - R_{j\nu} \right) d_\nu^+ + \left(L_{j\nu} + R_{j\nu} \right) d_\nu \right]$$
$$b_j^+ = \frac{1}{2} \sum_\nu \left[\left(L_{j\nu} - R_{j\nu} \right) d_\nu + \left(L_{j\nu} + R_{j\nu} \right) d_\nu^+ \right]$$

vector form

$$\boxed{\begin{pmatrix} \vec{b} \\ \vec{b}^+ \end{pmatrix} = \frac{1}{2} \begin{pmatrix} \underline{L} + \underline{R} & \underline{L} - \underline{R} \\ \underline{L} - \underline{R} & \underline{L} + \underline{R} \end{pmatrix} \begin{pmatrix} \vec{d} \\ \vec{d}^+ \end{pmatrix}}$$

$$\begin{pmatrix} \vec{d} \\ \vec{d}^+ \end{pmatrix} = \frac{1}{2} \begin{pmatrix} \underline{R}^T + \underline{L}^T & \underline{R}^T - \underline{L}^T \\ \underline{R}^T - \underline{L}^T & \underline{R}^T + \underline{L}^T \end{pmatrix} \begin{pmatrix} \vec{b} \\ \vec{b}^+ \end{pmatrix}$$

as in Jose's notes

OP and OP magnitude in mean-field + Gaussian fluctuations

Order parameter

$$\langle \psi_i \rangle = \langle GS | S_i^+ | GS \rangle$$

from page 4

$$S_i^+ = \sin\theta_i \left(1 - b_{\theta i}^+ b_{\theta i} - b_{\varphi i}^+ b_{\varphi i}\right) - \sin\theta_i\, b_{\theta i}^+ b_{\theta i}$$
$$- \cos\theta_i\, b_{\theta i}^+ + \cos\frac{\theta_i}{2}\, b_{\varphi i}^+ - \cos\theta_i\, b_{\theta i} + \sin\frac{\theta_i}{2}\, b_{\varphi i}^+ b_{\theta i}$$
$$- \cos\frac{\theta_i}{2}\, b_{\varphi i} - \sin\frac{\theta_i}{2}\, b_{i\theta}^+ b_{\varphi i}^+$$

from page 12, 13 : $\langle GS | b | GS \rangle = \langle GS | b^+ | GS \rangle = 0$

$$\boxed{\langle \psi_i \rangle = \langle GS | S_i^+ | GS \rangle = \sin\theta_i - \sin\theta_i \langle GS | 2 b_{\theta i}^+ b_{\theta i} + b_{\varphi i}^+ b_{\varphi i} | GS \rangle}$$

mean-field

Gaussian fluctuations, reduce OP

- fluctuation corrections can be calculated by expressing b, b^+ in terms of Bogoliubov bosons d, d^+

$$\begin{pmatrix} \vec{b} \\ \vec{b}^+ \end{pmatrix} = \frac{1}{2} \begin{pmatrix} \underline{L} + \underline{R} & \underline{L} - \underline{R} \\ \underline{L} - \underline{R} & \underline{L} + \underline{R} \end{pmatrix} \begin{pmatrix} \vec{d} \\ \vec{d}^+ \end{pmatrix}$$

$$\langle GS | b^\dagger_{\theta i} b_{\theta i} | GS \rangle = \langle GS | \tfrac{1}{2} \sum_\nu (L_{i\nu} - R_{i\nu}) d_\nu \, \tfrac{1}{2} (L_{i\mu} - R_{i\mu}) d^\dagger_\mu | GS \rangle$$

$$= \frac{1}{4} \sum_\nu (L_{i\nu} - R_{i\nu})^2$$

and analogously for $\langle GS | b^\dagger_{\varphi i} b_{\varphi i} | GS \rangle$

<u>to check: treat clean case as special case of general formula</u>

in clean case we had (page 24)

$$a_k = u_k \gamma_k + v_k \gamma^\dagger_{-k}$$

$$b_j = \frac{1}{\sqrt{N}} \sum_k e^{-ikj} a_k = \frac{1}{\sqrt{N}} \sum_k e^{ikj} (u_k \gamma_k + v_k \gamma^\dagger_{-k})$$

$$\Rightarrow \quad \frac{1}{2}(L_{jk} + R_{jk}) = \frac{1}{\sqrt{N}} e^{ikj} u_k$$

$$\frac{1}{2}(L_{jk} - R_{jk}) = \frac{1}{\sqrt{N}} e^{-ikj} v_k$$

$$\langle GS | b^\dagger_j b_j | GS \rangle = \frac{1}{4} \sum_k |L_{jk} - R_{jk}|^2 = \frac{1}{N} \sum_k v_k^2$$

need to use $|L_{jk} - R_{jk}|^2$ because FT is not real

(as on page 32)

Order parameter magnitude

$$\langle |\psi_i|^2 \rangle = \langle GS | (S_i^x)^2 + (S_i^y)^2 | GS \rangle = \langle GS | 2 - (S_i^z)^2 | GS \rangle$$

$$(S_i^z)^2 = \frac{1}{2}(1-\cos\theta_i) + \cos\theta_i \, b_{\theta i}^+ b_{\theta i} + \frac{1}{2}(1+\cos\theta_i) \, b_{\varphi i}^+ b_{\varphi i}$$

$$-\frac{1}{2}\sin\theta_i \left(b_{\theta i}^+ + b_{\theta i} \right)$$

page 33 or $\boxed{4}$

use $\langle GS | b | GS \rangle = \langle GS | b^+ | GS \rangle = 0$

$$\boxed{\begin{aligned} \langle |\psi_i|^2 \rangle = \frac{3}{2} + \frac{1}{2}\cos\theta_i &- \cos\theta_i \langle GS | b_{\theta i}^+ b_{\theta i} | GS \rangle \\ &- \frac{1}{2}(1+\cos\theta_i) \langle GS | b_{\varphi i}^+ b_{\varphi i} | GS \rangle \end{aligned}}$$

mean field — Gaussian fluctuations

fluctuation corrections can be calculated as on page $\boxed{15}$ by expressing b, b^+ in terms of Bogoliubov bosons

$$\langle GS | b_i^+ b_i | GS \rangle = \frac{1}{4} \sum_\nu (L_{i\nu} - R_{i\nu})^2$$

Scalar susceptibility

(Green's function of order parameter magnitude)

- local OP magnitude, see page 16

$$|\psi_j|^2 = 2 - (S_j^z)^2 = \frac{3}{2} + \frac{1}{2}\cos\theta_j - \cos\theta_j\, b_{\theta j}^+ b_{\theta j} - \frac{1}{2}(1+\cos\theta_j)\, b_{\varphi j}^+ b_{\varphi j}$$
$$+ \frac{1}{2}\sin\theta_j \left(b_{\theta j}^+ + b_{\theta j} \right)$$

- retarded Green's function

$$\boxed{G_{jn}(t) = -i\Theta(t) \langle GS | \left[|\psi_j(t)|^2 , |\psi_n(0)|^2 \right] | GS \rangle}$$

expand to quadratic order in b, b^+ (commutator removes constant pieces)

$$\boxed{G_{jn}(t) = -i\Theta(t) \frac{1}{4} \sin\theta_j \sin\theta_n \langle GS | \left[b_{\theta j}^+(t) + b_{\theta j}(t) , b_{\theta n}^+(0) + b_{\theta n}(0) \right] | GS \rangle}$$

now express b, b^+ in terms of Bogoliubov bosons d, d^+, using page 12

$$\begin{pmatrix} \vec{b} \\ b^+ \end{pmatrix} = \frac{1}{2} \begin{pmatrix} \underline{L} + \underline{R} & \underline{L} - \underline{R} \\ \underline{L} - \underline{R} & \underline{L} + \underline{R} \end{pmatrix} \begin{pmatrix} \vec{d} \\ \vec{d}^+ \end{pmatrix}$$

$$\vec{b} = \frac{1}{2}\left(\underline{L}+\underline{R}\right)\vec{d} + \frac{1}{2}\left(\underline{L}-\underline{R}\right)\vec{d}^{+}$$

$$\vec{b}^{+} = \frac{1}{2}\left(\underline{L}-\underline{R}\right)\vec{d} + \frac{1}{2}\left(\underline{L}+\underline{R}\right)\vec{d}^{+}$$

$$\vec{b}+\vec{b}^{+} = \underline{L}\,\vec{d} + \underline{L}\,\vec{d}^{+} = \underline{L}\left(\vec{d}+\vec{d}^{+}\right)$$

$$b_j + b_j^{+} = \sum_{\nu} L_{j\nu}\left(d_\nu + d_\nu^{+}\right) = \sum_{\nu} \sqrt{\frac{\omega_j}{E_\nu}}\, V_{j\nu}\left(d_\nu + d_\nu^{+}\right)$$

<u>insert into Green's function</u>

$$G_{jn}(t) = -i\,\Theta(t)\,\frac{1}{4}\sin\theta_j \sin\theta_n \sum_{\mu,\nu} L_{j\mu} L_{n\nu} \;\times$$

$$\times \langle GS | \left[d^{+}_{\theta\mu}(t) + d_{\theta\mu}(t),\; d^{+}_{\theta\nu}(0) + d_{\theta\nu}(0) \right] | GS \rangle$$

- expand commutator, keep only $d\,d^{+}$ terms for <u>same</u> state

$$\langle GS | [\ldots,\ldots] | GS \rangle = \delta_{\mu\nu} \langle GS | - d_{\theta\nu}(0)\, d^{+}_{\theta\nu}(t) + d_{\theta\nu}(t)\, d^{+}_{\theta\nu}(0) | GS \rangle$$

use $\quad \hat{A}(t) = e^{i\hat{H}t}\,\hat{A}\,e^{-i\hat{H}t}$

$$\langle GS | - d_{\theta\nu}(0)\, d^{+}_{\theta\nu}(t) | GS \rangle = -e^{iE_\nu t}$$

$$\langle GS | d_{\theta\nu}(t)\, d^{+}_{\theta\nu}(0) | GS \rangle = e^{-iE_\nu t}$$

$$\boxed{G_{jn}(t) = -i\,\Theta(t)\,\frac{1}{4}\sin\theta_j \sin\theta_n \sum_{\nu} L_{j\nu} L_{n\nu}\left(-e^{iE_\nu t} + e^{-iE_\nu t}\right)}$$

Fourier transformation in time

$$\tilde{G}_{jn}(\omega) = \int_{-\infty}^{\infty} dt \quad e^{i(\omega+i\delta)t} \; G_{jn}(t)$$

$$= -i\tfrac{1}{4}\sin\theta_j \sin\theta_n \sum_\nu L_{j\nu} L_{n\nu} \times$$

$$\times \int_0^\infty dt \; e^{i(\omega+i\delta)t} \left(-e^{iE_\nu t} + e^{-iE_\nu t}\right)$$

Note: this ω differs from the ω_j in Bogoliubov transformation

$$\tilde{G}_{jn}(\omega) = -i\tfrac{1}{4}\sin\theta_j \sin\theta_n \sum_\nu L_{j\nu} L_{n\nu} \left(\frac{1}{i(\omega+i\delta)+E_\nu} - \frac{1}{i(\omega+i\delta)-E_\nu} \right)$$

$$\boxed{\tilde{G}_{jn}(\omega) = \sum_\nu \frac{\frac{1}{4}\sin\theta_j \sin\theta_n L_{j\nu} L_{n\nu}}{\omega+i\delta-E_\nu} - \sum_\nu \frac{\frac{1}{4}\sin\theta_j \theta_n \quad L_{j\nu} L_{n\nu}}{\omega+i\delta+E_\nu}}$$

Spectral density $A(\omega)$ defined via

$$\tilde{G}(\omega) = \int_{-\infty}^{\infty} dx \, \frac{A(x)}{\omega+i\delta-x}$$

$$\boxed{A_{jn}(\omega) = \tfrac{1}{4}\sin\theta_j \sin\theta_n \sum_\nu L_{j\nu} L_{n\nu} \Big(\delta(\omega-E_\nu) - \delta(\omega+E_\nu) \Big)}$$

δ-peaks at the Bogoliubov eigenfrequencies, odd in ω as expected to test, treat clean case as special case of general formula

from page 15 : $$b_j = \frac{1}{\sqrt{N}} \sum_k e^{ikj} \left(u_k \gamma_k + v_k \gamma_{-k}^+ \right)$$

$$b_j^+ = \frac{1}{\sqrt{N}} \sum_k e^{-ikj} \left(u_k \gamma_k^+ + v_k \gamma_{-k} \right)$$

$$= \frac{1}{\sqrt{N}} \sum_k e^{ikj} \left(u_k \gamma_{-k}^+ + v_k \gamma_k \right)$$

$$b_j + b_j^+ = \frac{1}{\sqrt{N}} \sum_k (u_k + v_k) \, (\gamma_k + \gamma_{-k})^+ \, e^{ikj}$$

thus, $L_{jk} = \frac{1}{\sqrt{N}} (u_k + v_k) \, e^{ikj}$ ← note: not real

careful !!

$$A_{jn}(\omega) = \frac{1}{4} \sin^2\theta \; \frac{1}{N} \sum_k (u_k + v_k)^2 \, e^{ik(j-n)} \left(\delta(\omega - E_k) - \delta(\omega + E_k) \right)$$

Fourier transformation in space

$$A_q(\omega) = \frac{1}{N} \sum_{jm} A_{j\,j+m}(\omega) \, e^{iqm} =$$

$$= \frac{1}{4} \sin^2\theta \; \frac{1}{N^2} \sum_{jmk} e^{iqm} \, e^{-ikm} \, (u_k + v_k)^2 \left(\delta(\omega - E_k) - \delta(\omega + E_k) \right)$$

$$A_q(\omega) = \frac{1}{4} \sin^2\theta \; (u_q + v_q)^2 \left(\delta(\omega - E_q) - \delta(\omega + E_q) \right)$$

Same result as on page 39 ✓

Scalar susceptibility to 4th order in b, b^+

- up to 2nd order in b, b^+, scalar susceptibility vanishes in Mott phase because it is proportional to $\sin^2\theta$

$\Rightarrow$ include terms up to fourth order in b, b^+

(see also Pekker et al PRB 86, 144527 (2012))

<u>recall</u>: retarded scalar Green's function

$$\boxed{G_{jn}(t) = -i\,\Theta(t)\,\langle GS|\left[|\Psi_j(t)|^2, |\Psi_n(0)|^2\right]|GS\rangle}$$

with

$$|\Psi_j|^2 = \frac{3}{2} + \frac{1}{2}\cos\theta_j - \cos\theta_j\, b_{\theta j}^+ b_{\theta j} - \frac{1}{2}(1+\cos\theta_j)\, b_{\varphi j}^+ b_{\varphi j}$$

$$+\frac{1}{2}\sin\theta_j\left(b_{\theta j}^+ + b_{\theta j}\right)$$

- as b, b^+ are linear combinations of d, d^+ only terms with <u>even</u> number of b, b^+ survive
- constant terms vanish under commutator

$$\boxed{G_{jn}(t) = G_{jn}^{(2)}(t) + G_{jn}^{(4)}(t)}$$

$$G_{jn}^{(2)}(t) = -i\,\Theta(t)\,\frac{1}{4}\sin\theta_j\sin\theta_n\,\langle GS|\left[b_{\theta j}^+(t) + b_{\theta j}(t),\, b_{\theta n}^+(0) + b_{\theta n}(0)\right]|GS\rangle$$

2nd-order term as calculated on pages $\boxed{17}$ - $\boxed{20}$

4th-order contribution

$$\boxed{\begin{aligned} G^{(4)}_{jn}(t) = &-i\Theta(t)\cos\theta_j\cos\theta_n \langle GS|\left[b^+_{\theta j}(t) b_{\theta j}(t), b^+_{\theta n}(0) b_{\theta n}(0)\right]|GS\rangle \\ &-i\Theta(t)\tfrac{1}{4}(1+\cos\theta_j)(1+\cos\theta_n)\langle GS|\left[b^+_{\varphi j}(t) b_{\varphi j}(t), b^+_{\varphi n}(0) b_{\varphi n}(0)\right]|GS\rangle \end{aligned}}$$

no terms that mix b_θ, b_φ as they always commute

Note: Hamiltonian stays quadratic in b, b^+ (see Pekker paper)

- Apply Wicks theorem (quadratic Hamiltonian)

$$\langle GS| A_1 \dots A_{2n} |GS\rangle = \sum_P \langle A_{i_1} A_{j_1}\rangle \dots \langle A_{i_n} A_{j_n}\rangle$$

with $i_\# < j_\#$ (*).
P permutation of $1..2n$ into $i_1, j_1, \dots, i_n, j_n$

A_i are linear combinations of eigenstates d, d^+

(*) this means one can "commute" operators to construct contractions but not inside a contraction

- now treat Higgs and Goldstone parts separately

$$G^{(4,4)}_{jn}(t) = -i\,\theta(t)\cos\theta_j\cos\theta_n\Big[\langle GS|\, b^+_{\theta j}(t)\, b_{\theta j}(t)\, b^+_{\theta n}(0)\, b_{\theta n}(0)\,|GS\rangle$$

$$- \langle GS|\, b^+_{\theta n}(0)\, b_{\theta n}(0)\, b^+_{\theta j}(t)\, b_{\theta j}(t)\,|GS\rangle\Big]$$

$$= -i\,\theta(t)\cos\theta_j\cos\theta_n \times$$

$$\Big[\cancel{\langle b^+_{\theta j}(t) b_{\theta j}(t)\rangle\langle b^+_{\theta n}(0) b_{\theta n}(0)\rangle} + \langle b^+_{\theta j}(t) b^+_{\theta n}(0)\rangle\langle b_{\theta j}(t) b_{\theta n}(0)\rangle$$

$$+ \langle b^+_{\theta j}(t) b_{\theta n}(0)\rangle\langle b_{\theta j}(t) b^+_{\theta n}(0)\rangle - \cancel{\langle b^+_{\theta n}(0) b_{\theta n}(0)\rangle\langle b^+_{\theta j}(t) b_{\theta j}(t)\rangle}$$

$$- \langle b^+_{\theta n}(0) b^+_{\theta j}(t)\rangle\langle b_{\theta n}(0) b_{\theta j}(t)\rangle - \langle b^+_{\theta n}(0) b_{\theta j}(t)\rangle\langle b_{\theta n}(0) b^+_{\theta j}(t)\rangle\Big]$$

- expand b, b^+ in terms of eigenstates of Bogoliubov Hamiltonian, d, d^+

$$\boxed{\begin{aligned} \vec{b} &= \tfrac{1}{2}(\underline{L}+\underline{R})\,\vec{d} + \tfrac{1}{2}(\underline{L}-\underline{R})\,\vec{d}^{\,+} \\ \vec{b}^{\,+} &= \tfrac{1}{2}(\underline{L}-\underline{R})\,\vec{d} + \tfrac{1}{2}(\underline{L}+\underline{R})\,\vec{d}^{\,+} \end{aligned}}$$

- as we are evaluating expectation values in GS (d-vacuum), keep only d^+ for right operator in $\langle\ldots\rangle$ and only d for left operator in $\langle\ldots\rangle$

$$\langle b^+_{\theta j}(t)\, b^+_{\theta n}(0)\rangle = \frac{1}{4}\sum_{\mu\nu}(L_{j\mu}-R_{j\mu})(L_{n\nu}+R_{n\nu})\langle d_\mu(t)\, d_\nu(0)\rangle$$

$$= \frac{1}{4}\sum_{\nu}(L_{j\nu}-R_{j\nu})(L_{n\nu}+R_{n\nu})\quad e^{-iE_\nu t}$$

$$\langle b_{\theta j}(t)\, b_{\theta n}(0)\rangle = \frac{1}{4}\sum_{\nu}(L_{j\nu}+R_{j\nu})(L_{n\nu}-R_{n\nu})\quad e^{-iE_\nu t}$$

$$\langle b^+_{\theta j}(t)\, b_{\theta n}(0)\rangle = \frac{1}{4}\sum_{\nu}(L_{j\nu}-R_{j\nu})(L_{n\nu}-R_{n\nu})\quad e^{-iE_\nu t}$$

$$\langle b_{\theta j}(t)\, b^+_{\theta n}(0)\rangle = \frac{1}{4}\sum_{\nu}(L_{j\nu}+R_{j\nu})(L_{n\nu}+R_{n\nu})\quad e^{-iE_\nu t}$$

$$\langle b^+_{\theta n}(0)\, b^+_{\theta j}(t)\rangle = \frac{1}{4}\sum_{\nu}(L_{n\nu}-R_{n\nu})(L_{j\nu}+R_{j\nu})\quad e^{iE_\nu t}$$

$$\langle b_{\theta n}(0)\, b_{\theta j}(t)\rangle = \frac{1}{4}\sum_{\nu}(L_{n\nu}+R_{n\nu})(L_{j\nu}-R_{j\nu})\quad e^{iE_\nu t}$$

$$\langle b^+_{\theta n}(0)\, b_{\theta j}(t)\rangle = \frac{1}{4}\sum_{\nu}(L_{n\nu}-R_{n\nu})(L_{j\nu}-R_{j\nu})\quad e^{iE_\nu t}$$

$$\langle b_{\theta n}(0)\, b^+_{\theta j}(t)\rangle = \frac{1}{4}\sum_{\nu}(L_{n\nu}+R_{n\nu})(L_{j\nu}+R_{j\nu})\quad e^{iE_\nu t}$$

$$G^{(4,4)}_{jn}(t) = -i\,\theta(t)\ \cos\theta_j \cos\theta_n \times$$

$$\Big[\frac{1}{16} \sum_{\nu\mu} (L_{j\nu}-R_{j\nu})(L_{n\nu}+R_{n\nu})(L_{j\mu}+R_{j\mu})(L_{n\mu}-R_{n\mu})\, e^{-i(E_\nu-E_\mu)t}$$

$$+ \frac{1}{16} \sum_{\nu\mu} (L_{j\nu}-R_{j\nu})(L_{n\nu}-R_{n\nu})(L_{j\mu}+R_{j\mu})(L_{n\mu}+R_{n\mu})\, e^{-i(E_\nu-E_\mu)t}$$

$$- \frac{1}{16} \sum_{\nu\mu} (L_{n\nu}-R_{n\nu})(L_{j\nu}+R_{j\nu})(L_{n\mu}+R_{n\mu})(L_{j\mu}-R_{j\mu})\, e^{i(E_\nu+E_\mu)t}$$

$$- \frac{1}{16} \sum_{\nu\mu} (L_{n\nu}-R_{n\nu})(L_{j\nu}-R_{j\nu})(L_{n\mu}+R_{n\mu})(L_{j\mu}+R_{j\mu})\, e^{i(E_\nu+E_\mu)t} \Big]$$

1st and 3rd line can be combined ($\mu \leftrightarrow \nu$)
2nd and 4th line can be combined

$$G^{(4,4)}_{jn}(t) = -i\,\theta(t)\ \frac{1}{16} \cos\theta_j \cos\theta_n \times$$

$$\Big[\sum_{\mu\nu} (L_{j\nu}-R_{j\nu})(L_{n\nu}+R_{n\nu})(L_{j\mu}+R_{j\mu})(L_{n\mu}-R_{n\mu}) \left(e^{-i(E_\nu+E_\mu)t} - e^{i(E_\nu+E_\mu)t} \right)$$

$$+ \sum_{\mu\nu} (L_{j\nu}-R_{j\nu})(L_{n\nu}-R_{n\nu})(L_{j\mu}+R_{j\mu})(L_{n\mu}+R_{n\mu}) \left(e^{-i(E_\nu+E_n)t} - e^{i(E_\nu+E_n)t} \right) \Big]$$

Fourier transformation in time

$$\tilde{G}^{(4,4)}_{jn}(\omega) = \int_{-\infty}^{\infty} dt\ e^{i(\omega+i\delta)t}\, G^{(4,4)}_{jn}(t)$$

$$\int_{-\infty}^{\infty} dt\ (-i)\,\Theta(t)\ e^{i(\omega+i\delta)t}\left(e^{-i(E_\nu+E_\mu)t} - e^{i(E_\nu+E_\mu)t}\right)$$

$$= -i\int_0^{\infty} dt\ \left(e^{i(\omega+i\delta-E_\nu-E_\mu)t} - e^{i(\omega+i\delta+E_\nu+E_\mu)t}\right)$$

$$= \frac{1}{\omega+i\delta-E_\nu-E_\mu} - \frac{1}{\omega+i\delta+E_\nu+E_\mu}$$

Insert into Green's function:

$$\tilde{G}^{(4,4)}_{jn}(\omega) = \frac{1}{16}\cos\Theta_j\cos\Theta_n\sum_{\mu\nu}\left(\frac{1}{\omega+i\delta-E_\nu-E_\mu} - \frac{1}{\omega+i\delta+E_\nu+E_\mu}\right)\times$$
$$\Big[(L_{j\nu}-R_{j\nu})(L_{n\nu}+R_{n\nu})(L_{j\mu}+R_{j\mu})(L_{n\mu}-R_{n\mu}) +$$
$$+(L_{j\nu}-R_{j\nu})(L_{n\nu}-R_{n\nu})(L_{j\mu}+R_{j\mu})(L_{n\mu}+L_{n\mu})\Big]$$

Spectral density $A(\omega)$ defined via
$\tilde{G}(\omega) = \int_{-\infty}^{\infty} dx\ \frac{A(x)}{\omega+i\delta-x}$

$$\boxed{\begin{aligned} A^{(4,4)}_{jn}(\omega) = \frac{1}{16}\cos\Theta_j\cos\Theta_n\sum_{\mu\nu}\Big(\delta(\omega-E_\nu-E_\mu) - \delta(\omega+E_\nu+E_\mu)\Big)\times \\ \Big[(L_{j\nu}-R_{j\nu})(L_{n\nu}+R_{n\nu})(L_{j\mu}+R_{j\mu})(L_{n\mu}-R_{n\mu}) + \\ +(L_{j\nu}-R_{j\nu})(L_{n\nu}-R_{n\nu})(L_{j\mu}+R_{j\mu})(L_{n\mu}+R_{n\mu})\Big] \end{aligned}}$$

- δ-peaks at energies of <u>two-</u>particle Higgs excitation
- analogous contribution will arise from Goldstone part $A^{(4,G)}_{jn}(\omega)$

Simplify $R \pm L$ terms

$$(L_{j\nu} - R_{j\nu})(L_{n\nu} + R_{n\nu})(L_{j\mu} + R_{j\mu})(L_{n\mu} - R_{n\mu})$$
$$+ (L_{j\nu} - R_{j\nu})(L_{n\nu} - R_{n\nu})(L_{j\mu} + R_{j\mu})(L_{n\mu} + R_{n\mu})$$

$$= (L_{j\nu} - R_{j\nu})(L_{j\mu} + R_{j\mu})\left[(L_{n\nu} + R_{n\nu})(L_{n\mu} - R_{n\mu}) + (L_{n\nu} - R_{n\nu})(L_{n\mu} + R_{n\mu})\right]$$

$$= \left(L_{j\nu}L_{j\mu} + R_{j\nu}R_{j\mu} - R_{j\nu}L_{j\mu} + L_{j\nu}R_{j\mu}\right) \times$$
$$\left(2L_{n\nu}L_{n\mu} - 2R_{n\nu}R_{n\mu}\right)$$

Cancel under $\sum_{\mu\nu}$

$$= 2\left(L_{j\nu}L_{j\mu} - R_{j\nu}R_{j\mu}\right)\left(L_{n\nu}L_{n\mu} - R_{n\nu}R_{n\mu}\right)$$

Insert into spectral density

$$\boxed{A^{(4,\#)}_{jn}(\omega) = \frac{1}{8}\cos\theta_j \cos\theta_n \sum_{\mu,\nu}\left(L_{j\nu}L_{j\mu} - R_{j\nu}R_{j\mu}\right)\left(L_{n\nu}L_{n\mu} - R_{n\nu}R_{n\mu}\right) \times \left(\delta(\omega - E_\nu - E_\mu) - \delta(\omega + E_\nu + E_\mu)\right)}$$