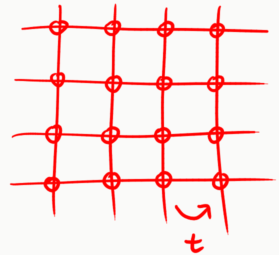
Hubbard model - itinerant magnetism

MUNI SCI
Department of Condensed Matter Physics

- single-band Hubbard model

1) hopping of electrons on the lattice



$$H_{TB} = -t \, \frac{1}{2} \sum_{R\delta} \sum_{\sigma} c^{\dagger}_{R+\delta,\sigma} c_{R\sigma} \quad \text{(tight-binding approx.)}$$

$\longrightarrow$ band dispersion such as $\varepsilon_k = -2t(\cos k_x a + \cos k_y a)$

2) intraionic Coulomb repulsion - penalty U for doubly occupied orbitals

$\uparrow\downarrow$ U

$$H_{Coul} = U \sum_{R} n_{R\uparrow} n_{R\downarrow}$$

$\longrightarrow$ correlated behavior of electrons

full model Hamiltonian

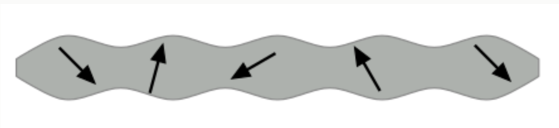
$$H = \sum_{k\sigma} (\varepsilon_k - \mu) c^{\dagger}_{k\sigma} c_{k\sigma} + U \sum_{R} n_{R\uparrow} n_{R\downarrow}$$

- itinerant vs localized limit

1) kinetic energy – characterized by the bandwidth $W \sim t$

2) Coulomb repulsion – characterized by Hubbard parameter U

$W \gg U$ – correlated metal



→ itinerant magnetism

(Stoner picture)

$W \ll U$ – Mott insulator

→ magnetism with localized moments

(for the spring course FK120)

magnetic order

- high enough DOS at E_F combined with U leads to spin polarization of the bands (FM) or spin density wave (AF)

magnetic order

- alignment of local moments by virtue of effective interactions

- conversion of the on-site Coulomb term into momentum representation

$$c_{R\sigma} = \frac{1}{\sqrt{N}} \sum_k e^{ikR} c_{k\sigma}$$

lattice FT

$$c_{k\sigma} = \frac{1}{\sqrt{N}} \sum_R e^{-ikR} c_{R\sigma}$$

maintains normalized fermionic anticommutation relations

$$\{c_{R\sigma}, c^+_{R'\sigma'}\} = \delta_{RR'}\delta_{\sigma\sigma'}$$

$$\{c_{k\sigma}, c^+_{k'\sigma'}\} = \delta_{kk'}\delta_{\sigma\sigma'}$$

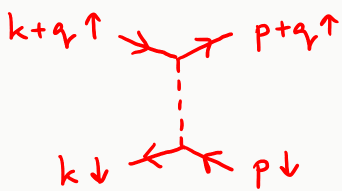
local electron density

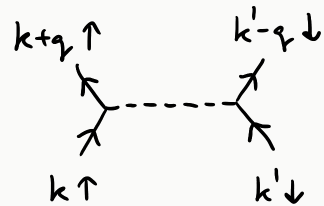
$$n_{R\sigma} = \sum_q e^{iqR} n_{q\sigma} \quad \text{with} \quad n_{q\sigma} = \frac{1}{N}\sum_R e^{-iqR} n_{R\sigma} = \frac{1}{N}\sum_k c^+_{k\sigma} c_{k+q\sigma}$$

interaction

$$H_{Coul} = U \sum_R n_{R\uparrow} n_{R\downarrow} = UN \sum_q n_{-q\uparrow} n_{q\downarrow} = \frac{U}{N} \sum_{kk'q} c^+_{k+q\uparrow} c_{k\uparrow} c^+_{k'-q\downarrow} c_{k'\downarrow}$$

$$= \frac{U}{N} \sum_{kpq} c^+_{p+q\uparrow} c_{k+q\uparrow} c^+_{k\downarrow} c_{p\downarrow}$$





① mean-field treatment - FM state with magnetization along z

$\langle n_{q\sigma} \rangle = \frac{1}{N} \sum_k \langle c^+_{k\sigma} c_{k+q\sigma} \rangle$ is nonzero only for $q=0$ and differs for $\sigma = \uparrow, \downarrow$

homogeneous $\langle n_{R\sigma} \rangle = \langle n_\sigma \rangle = \langle n_{q=0,\sigma} \rangle = \frac{1}{N} \sum_k \langle c^+_{k\sigma} c_{k\sigma} \rangle$

occupancy condition $\langle n_\uparrow \rangle + \langle n_\downarrow \rangle = n$ (electrons per site)

- MF decoupling

$$(A - \langle A \rangle)(B - \langle B \rangle) \approx 0 \rightarrow AB \approx A \langle B \rangle + \langle A \rangle B - \langle A \rangle \langle B \rangle$$

$$U N \sum_q n_{-q\uparrow} n_{q\uparrow} \approx U N \sum_q \left(n_{-q\uparrow} \langle n_{q\downarrow} \rangle + \langle n_{-q\uparrow} \rangle n_{q\downarrow} \right) + \text{const.}$$

$$\rightarrow H_{MF} = \sum_k (\underbrace{\varepsilon_k + U \langle n_\downarrow \rangle}_{\tilde{\varepsilon}_{k\uparrow}} - \mu) c^+_{k\uparrow} c_{k\uparrow} + \sum_k (\underbrace{\varepsilon_k + U \langle n_\uparrow \rangle}_{\tilde{\varepsilon}_{k\downarrow}} - \mu) c^+_{k\downarrow} c_{k\downarrow}$$

Free-electron Hamiltonian with spin-dependent band shift

k-independent gap $\tilde{\varepsilon}_{k\downarrow} - \tilde{\varepsilon}_{k\uparrow} = U\left(\langle n_\uparrow\rangle - \langle n_\downarrow\rangle\right) = \Delta$

occupations given by Fermi-Dirac statistics

$$\langle c_{k\sigma}^{+} c_{k\sigma}\rangle = n_F(\tilde{\varepsilon}_{k\sigma}) = \frac{1}{e^{\beta(\tilde{\varepsilon}_{k\sigma}-\mu)}+1}$$

selfconsistent set of equations

$$\left.\begin{aligned}\langle n_\uparrow\rangle &= \frac{1}{N}\sum_k \frac{1}{e^{\beta(\varepsilon_k + U\langle n_\downarrow\rangle - \mu)}+1}\\ \langle n_\downarrow\rangle &= \frac{1}{N}\sum_k \frac{1}{e^{\beta(\varepsilon_k + U\langle n_\uparrow\rangle - \mu)}+1}\end{aligned}\right\}$$

together with

$$\langle n_\uparrow\rangle + \langle n_\downarrow\rangle = n$$

gives

$\langle n_\uparrow\rangle, \langle n_\downarrow\rangle, \mu$

- existence of FM solution (Stoner criterion)

by combining $\langle n_\uparrow \rangle + \langle n_\downarrow \rangle = n$ and $U(\langle n_\uparrow\rangle - \langle n_\downarrow\rangle) = \Delta$:

± 1

$$\langle n_\uparrow \rangle = \frac{1}{2} n + \frac{\Delta}{2U} \qquad \langle n_\downarrow \rangle = \frac{1}{2} n - \frac{\Delta}{2U} \qquad \rightarrow \qquad \langle n_\sigma \rangle = \frac{1}{2} n + \frac{\Delta}{2U}\sigma$$

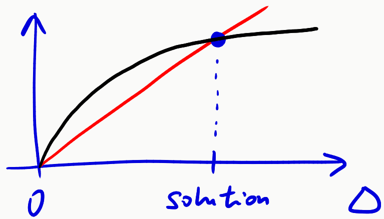
onset of FM state characterized by small Δ $\rightarrow$ expansion in $\langle n_\sigma\rangle$ equations

$$\langle n_\sigma \rangle = \frac{1}{N}\sum_k \frac{1}{e^{\beta(\varepsilon_k - \mu + U\langle n_{-\sigma}\rangle)} + 1} = \frac{1}{N}\sum_k n_F(\varepsilon_k + U\langle n_{-\sigma}\rangle)$$

$$\approx \frac{1}{N}\sum_k n_F(\varepsilon_k + \tfrac{1}{2}Un) - \frac{1}{N}\sum_k \frac{\partial n_F}{\partial \varepsilon}\bigg|_{\varepsilon_k + \frac{1}{2}Un} \frac{\Delta}{2}\sigma + \mathcal{O}(\Delta^2)$$

$\rightarrow$ Δ - equation:
$$- U\Delta \frac{1}{N}\sum_k \underbrace{\frac{\partial n_F}{\partial \varepsilon}\bigg|_{\varepsilon_k + \frac{1}{2}Un}}_{\text{negative}} + \mathcal{O}(\Delta^3) = \Delta$$

graphical solution



$$\underbrace{\alpha}_{\substack{\text{initial slope}\\ -\frac{U}{N}\sum_k \frac{\partial n_F}{\partial \varepsilon}\Big|_{\varepsilon_k+\frac{1}{2}Un}}}\Delta + \underbrace{\mathcal{O}(\Delta^3)}_{\substack{\text{saturation}\\ \text{effect}}} = \Delta$$

to have $\Delta \neq 0$ solution, we need $\alpha > 1$

using $-\frac{\partial n_F}{\partial \varepsilon} \xrightarrow{T=0} \delta(\varepsilon - E_F)$: $\quad \alpha = U \underbrace{\frac{1}{N}\sum_k \delta\left(\varepsilon_k + \frac{1}{2}Un - E_F\right)}_{\text{density of states at the Fermi level } \mathcal{N}(E_F)}$

hence

$U\mathcal{N}(E_F) > 1$ to get FM state (Stoner criterion)

- Example – cubic lattice

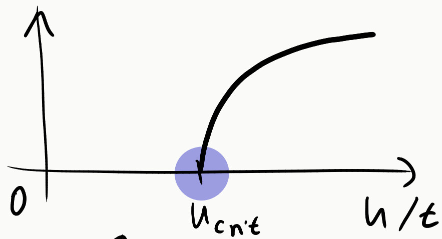
NN hopping amplitude

band dispersion in TB approximation $\varepsilon_k = -2t(\cos k_x + \cos k_y + \cos k_z)$

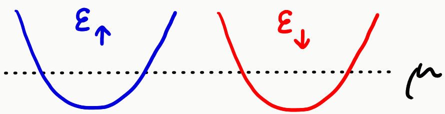
when the electron occupation n is low, ε_k can be approximated by a parabolic band

shifted $\varepsilon_k \approx +t\,k^2 \longrightarrow$ density of states $\mathcal{N}(\varepsilon) \sim \sqrt{\varepsilon}$

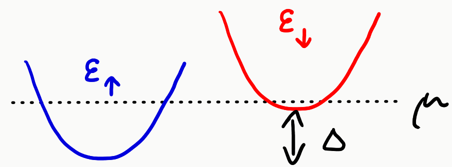
$\Delta \sim \langle n_\uparrow \rangle - \langle n_\downarrow \rangle$

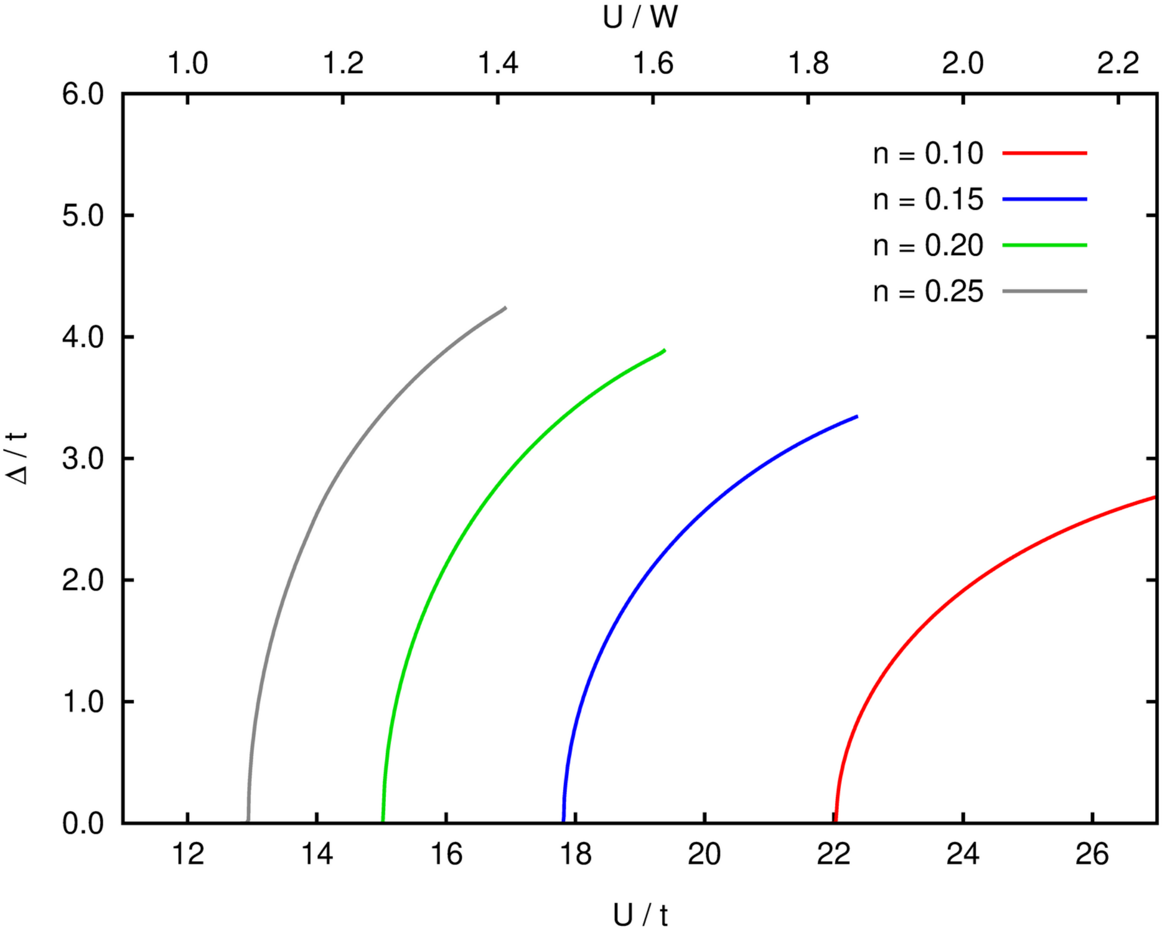


non-polarized bands



spin-polarized bands




U / W
1.0
1.2
1.4
1.6
1.8
2.0
2.2
6.0
5.0
4.0
3.0
2.0
1.0
0.0
Δ / t
n = 0.10
n = 0.15
n = 0.20
n = 0.25
12
14
16
18
20
22
24
26
U / t

② GF approach equivalent to MF – generalized HF scheme

- spin susceptibility

$$\chi_{\alpha\beta}(q,E) = \frac{i}{\hbar}\int_{-\infty}^{\infty} e^{\frac{i}{\hbar}(E+i0^+)t}\langle[\hat{S}^\alpha_q(t),\hat{S}^\beta_{-q}]\rangle\,dt \quad \text{with} \quad \hat{S}^\alpha_q = \frac{1}{\sqrt{N}}\sum_R e^{-iqR}\hat{S}^\alpha_R$$

Matsubara counterpart $\chi_{\alpha\beta}(q,i\nu) = \frac{1}{\hbar}\int_0^{\hbar\beta} e^{i\nu\frac{\tau}{\hbar}}\langle T\{\hat{S}^\alpha_q(\tau)\,\hat{S}^\beta_{-q}\}\rangle\,d\tau$

energy

1) For an isotropic system $\chi_{\alpha\beta} = \chi\,\delta_{\alpha\beta}$ → single susceptibility

2) For a FM/AF system with (staggered) magnetization along z axis

transverse susceptibility χ_{-+} – derived from $S^{\mp} = S^x \mp i S^y$

longitudinal susceptibility χ_{zz} → $\chi_{xx} = \chi_{yy} = \frac{1}{4}(\chi_{-+} + \chi_{+-})$

- equation of motion approach for χ_{-+}

$$\chi_{-+}(q,\tau) = \frac{1}{\hbar}\left\langle T\left\{S_q^-(\tau)\, S_{-q}^+\right\}\right\rangle = \frac{1}{\hbar}\left[\left\langle S_q^-(\tau)\, S_{-q}^+\right\rangle \theta(\tau) + \left\langle S_{-q}^+ S_q^-(\tau)\right\rangle \theta(-\tau)\right]$$

τ- derivative :

$$\hbar \frac{\partial}{\partial \tau}\chi_{-+}(q,\tau) = \left\langle \left[S_q^-, S_{-q}^+\right]\right\rangle \delta(\tau) + \left\langle \frac{\partial S_q^-(\tau)}{\partial \tau} S_{-q}^+\right\rangle \theta(\tau) + \left\langle S_{-q}^+ \frac{\partial S_q^-(\tau)}{\partial \tau}\right\rangle \theta(-\tau)$$

$$\frac{\partial S_q^-}{\partial \tau} = -\frac{1}{\hbar}\left[S_q^-, H\right]$$

Final equation for χ_{-+}

$$\hbar \frac{\partial}{\partial \tau}\chi_{-+}(q,\tau) = \left\langle \left[S_q^-, S_{-q}^+\right]\right\rangle \delta(\tau) - \frac{1}{\hbar}\left\langle T\left\{\left[S_q^-, H\right](\tau)\, S_{-q}^+\right\}\right\rangle$$

$$\hat{S}_q^- = \frac{1}{\sqrt{N}}\sum_R e^{-iqR} c_{R\downarrow}^+ c_{R\uparrow} = \frac{1}{\sqrt{N}}\sum_k c_{k\downarrow}^+ c_{k+q\uparrow}$$

$\longrightarrow$ take the elementary contribution $c_{k\downarrow}^+ c_{k+q\uparrow}$

1) commutator of spin operators

$$\langle [S^-_q, S^+_{-q}] \rangle = \frac{1}{N} \sum_{kk'} \Big[\langle c^+_{k\downarrow} \underbrace{c_{k+q\uparrow}\, c^+_{k'+q\uparrow}}_{1-\hat{n}_{k+q\uparrow}} c_{k'\downarrow} \rangle - \langle c^+_{k'+q\uparrow} c_{k'\downarrow} \underbrace{c^+_{k\downarrow}\, c_{k+q\uparrow}}_{1-\hat{n}_{k\downarrow}} \rangle \Big] \delta_{kk'}$$

$$= \frac{1}{N} \sum_{k} \langle c^+_{k\downarrow} c_{k\downarrow} \rangle - \langle c^+_{k+q\uparrow} c_{k+q\uparrow} \rangle - \cancel{\langle n_{k\downarrow} n_{k+q\uparrow} \rangle} + \cancel{\langle n_{k+q\uparrow} n_{k\downarrow} \rangle} = \langle n_\downarrow \rangle - \langle n_\uparrow \rangle$$

from S^-_q

$$H = H_{TB} + H_{Coul} = \sum_{k\sigma} (\varepsilon_k - \mu)\, c^+_{k\sigma} c_{k\sigma} + \frac{U}{N} \sum_{kpq} c^+_{p+q\uparrow} c_{k+q\uparrow}\, c^+_{k\downarrow} c_{p\downarrow}$$

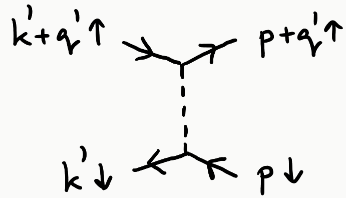
2) commutator with the band term

$$\Big[c^+_{k\downarrow} c_{k+q\uparrow} \,,\, \sum_{k\sigma} (\varepsilon_k - \mu)\, c^+_{k\sigma} c_{k\sigma} \Big] = (\varepsilon_k - \mu) \big[c^+_{k\downarrow} c_{k+q\uparrow} \,,\, c^+_{k\downarrow} c_{k\downarrow} \big]$$

$$+ (\varepsilon_{k+q} - \mu) \big[c^+_{k\downarrow} c_{k+q\uparrow} \,,\, c^+_{k+q\uparrow} c_{k+q\uparrow} \big]$$

$$= -(\varepsilon_k - \mu)\, c^+_{k\downarrow} c_{k+q\uparrow} + (\varepsilon_{k+q} - \mu)\, c^+_{k\downarrow} c_{k+q\uparrow} = (\varepsilon_{k+q} - \varepsilon_k)\, c^+_{k\downarrow} c_{k+q\uparrow}$$

3) commutator with the Hubbard term



$$\left[c^{+}_{k\downarrow} c_{k+q\uparrow} \, , \; \frac{U}{N} \sum_{k'pq'} c^{+}_{p+q'\uparrow} c_{k'+q'\uparrow} c^{+}_{k'\downarrow} c_{p\downarrow} \right] =$$

$$\frac{U}{N} \sum_{k'pq'} \Big(c^{+}_{k\downarrow} \underbrace{c_{k+q\uparrow} \, c^{+}_{p+q'\uparrow}}_{\delta_{k+q,p+q'} - c^{+}c} c_{k'+q'\uparrow} c^{+}_{k'\downarrow} c_{p\downarrow} - c^{+}_{p+q'\uparrow} c_{k'+q'\uparrow} c^{+}_{k'\downarrow} \underbrace{c_{p\downarrow} \, c^{+}_{k\downarrow}}_{\delta_{pk} - c^{+}c} c_{k+q\uparrow} \Big)$$

$\rightarrow p = k+q-q'$ $\qquad\qquad$ $\rightarrow p = k$

after three additional exchanges in both terms (no δ this time)

$$\frac{U}{N} \sum_{k'q'} \Big(c^{+}_{k\downarrow} c_{k'+q'\uparrow} c^{+}_{k'\downarrow} c_{k+q-q'\downarrow} - c^{+}_{k+q'\uparrow} c_{k'+q'\uparrow} c^{+}_{k'\downarrow} c_{k+q\uparrow}$$

$$+ \sum_{p} c^{+}_{p+q'\uparrow} c_{k'+q'\uparrow} c^{+}_{k\downarrow} c_{k+q\uparrow} c^{+}_{k'\downarrow} c_{p\downarrow} - c^{+}_{p+q'\uparrow} c_{k'+q'\uparrow} c^{+}_{k\downarrow} c_{k+q\uparrow} c^{+}_{k'\downarrow} c_{p\downarrow} \Big)$$

cancellation

Summary of the intermediate results

$$\hbar \frac{\partial}{\partial \tau} \chi_{-+}(q,\tau) = \langle [S^-_q, S^+_{-q}] \rangle \, \delta(\tau) - \frac{1}{\hbar} \left\langle T\left\{ [S^-_q, H](\tau)\, S^+_{-q} \right\} \right\rangle$$

$$\langle [c^+_{k\downarrow} c_{k+q\uparrow}, S^+_{-q}] \rangle = \frac{1}{\sqrt{N}} \left(\langle c^+_{k\downarrow} c_{k\downarrow} \rangle - \langle c^+_{k+q\uparrow} c_{k+q\uparrow} \rangle \right)$$

$$[c^+_{k\downarrow} c_{k+q\uparrow}, H_{TB}] = (\varepsilon_{k+q} - \varepsilon_k)\, c^+_{k\downarrow} c_{k+q\uparrow}$$

$$[c^+_{k\downarrow} c_{k+q\uparrow}, H_{Coul}] = \frac{U}{N} \sum_{k'q'} \left(c^+_{k\downarrow} c_{k'+q'\uparrow} c^+_{k'\downarrow} c_{k+q-q'\downarrow} - c^+_{k+q'\uparrow} c_{k'+q'\uparrow} c^+_{k'\downarrow} c_{k+q\uparrow} \right)$$

by collecting all the terms

$[S,S]\delta$ $\quad$ $[S, H_{TB}]$ $\quad$ $[S, H_{Coul}]$

$$\hbar \frac{\partial}{\partial \tau} \frac{1}{\hbar} \left\langle T\left\{ \underbrace{c^+_{k\downarrow} c_{k+q\uparrow}}_{}(\tau)\, S^+_{-q} \right\} \right\rangle =$$

$$\frac{1}{\sqrt{N}} \left(\langle n_{k\downarrow} \rangle - \langle n_{k+q\uparrow} \rangle \right) \delta(\tau) - (\varepsilon_{k+q} - \varepsilon_k) \frac{1}{\hbar} \left\langle T\left\{ \underbrace{c^+_{k\downarrow} c_{k+q\uparrow}}_{}(\tau)\, S^+_{-q} \right\} \right\rangle +$$

$$- \frac{U}{N} \sum_{k'q'} \frac{1}{\hbar} \left\langle T\left\{ \left(\underbrace{c^+_{k\downarrow} c_{k'+q'\uparrow} c^+_{k'\downarrow} c_{k+q-q'\downarrow}}_{} - \underbrace{c^+_{k+q'\uparrow} c_{k'+q'\uparrow} c^+_{k'\downarrow} c_{k+q\uparrow}}_{} \right)(\tau)\, S^+_{-q} \right\} \right\rangle$$

decoupling of the term arising from $[S, H_{coul}]$ within

- generalized Hartree-Fock approximation

$$-\frac{U}{N}\sum_{k'q'}\frac{1}{\hbar}\left\langle T\left\{\left(c^+_{k\downarrow}c_{k'+q'\uparrow}c^+_{k'\downarrow}c_{k+q-q'\downarrow} - c^+_{k+q'\uparrow}c_{k'+q'\uparrow}c^+_{k'\downarrow}c_{k+q\uparrow}\right)(\tau)\; S^+_{-q}\right\}\right\rangle$$

① $\langle n_{k\downarrow}\rangle\,\delta_{k,k+q-q'}$

② $\langle n_{k'\downarrow}\rangle\,\delta_{k',k+q-q'}$

③ $\langle n_{k+q'\uparrow}\rangle\,\delta_{k+q',k'+q'}$

④ $\langle n_{k+q\uparrow}\rangle\,\delta_{k+q',k+q}$

$$-\frac{U}{N}\sum_{k'}\frac{1}{\hbar}\left\langle T\left\{\left(\overset{①}{-\langle n_{k\downarrow}\rangle c^+_{k'\downarrow}c_{k'+q\uparrow}} + \overset{④}{\langle n_{k+q\uparrow}\rangle c^+_{k'\downarrow}c_{k'+q\uparrow}}\right)(\tau)\; S^+_{-q}\right\}\right\rangle$$

$$-\frac{U}{N}\sum_{k'}\frac{1}{\hbar}\left\langle T\left\{\left(\langle n_{k'\downarrow}\rangle c^+_{k\downarrow}c_{k+q\uparrow}\right)(\tau)\; S^+_{-q}\right\}\right\rangle \quad ②$$

$$+\frac{U}{N}\sum_{q'}\frac{1}{\hbar}\left\langle T\left\{\left(\langle n_{k+q'\uparrow}\rangle c^+_{k\downarrow}c_{k+q\uparrow}\right)(\tau)\; S^+_{-q}\right\}\right\rangle \quad ③$$

denote $\chi_{-+}(k,q,\tau) = \frac{1}{\sqrt{N}}\frac{1}{\hbar}\langle T\{\underbrace{c^+_{k\downarrow}c_{k+q\uparrow}}(\tau)\,S^+_{-q}\}\rangle \rightarrow \chi_{-+}(q,\tau) = \sum_k \chi_{-+}(k,q,\tau)$

EOM can be summarized as

$$\hbar\frac{\partial}{\partial\tau}\chi_{-+}(k,q,\tau) = \frac{1}{N}\left(\langle n_{k\downarrow}\rangle - \langle n_{k+q\uparrow}\rangle\right)\delta(\tau)$$

$$-(\varepsilon_{k+q}-\varepsilon_k)\,\chi_{-+}(k,q,\tau) - \frac{U}{N}\Big(\sum_{k'}\langle n_{k'\downarrow}\rangle - \sum_{q'}\langle n_{k+q'\uparrow}\rangle\Big)\chi_{-+}(k,q,\tau)$$

2 3

$$-\frac{U}{N}\sum_{k'}\left(\langle n_{k+q\uparrow}\rangle - \langle n_{k\downarrow}\rangle\right)\chi_{-+}(k',q,\tau)$$

4 1

introduce again $\tilde{\varepsilon}_{k\uparrow} = \varepsilon_k + \frac{U}{N}\sum_{k'}\langle n_{k'\downarrow}\rangle = \varepsilon_k + U\langle n_\downarrow\rangle$ and $\tilde{\varepsilon}_{k\downarrow} = \ldots$

$$\left[\hbar\frac{\partial}{\partial\tau} - (\tilde{\varepsilon}_{k\downarrow} - \tilde{\varepsilon}_{k+q\uparrow})\right]\chi_{-+}(k,q,\tau) =$$

$$-\frac{1}{N}\left(\langle n_{k+q\uparrow}\rangle - \langle n_{k\downarrow}\rangle\right)\left[\delta(\tau) + U\sum_{k'}\chi_{-+}(k',q,\tau)\right]$$

go to Matsubara representation

$$\hbar \frac{\partial}{\partial \tau} \to -i\nu \quad (\text{energy}) \qquad \chi(\tau) \to \chi(i\nu) \qquad \delta(\tau) \to 1$$

solve for k-contribution to χ_{-+}

$$\chi_{-+}(k,q,i\nu) = \frac{1}{N}\left(\langle n_{k+q\uparrow}\rangle - \langle n_{k\downarrow}\rangle\right) \frac{1 + U \sum_{k'} \chi_{-+}(k',q,i\nu)}{i\nu + (\tilde{\varepsilon}_{k\downarrow} - \tilde{\varepsilon}_{k+q\uparrow})}$$

sum over k to get the susceptibility

$$\chi_{-+}(q,i\nu) = \frac{1}{N}\sum_k \frac{\langle n_{k+q\uparrow}\rangle - \langle n_{k\downarrow}\rangle}{i\nu + (\tilde{\varepsilon}_{k\downarrow} - \tilde{\varepsilon}_{k+q\uparrow})} \left(1 + U \chi_{-+}(q,i\nu)\right)$$

final result

$$\chi_{-+}(q,i\nu) = \frac{\chi^{(0)}_{-+}(q,i\nu)}{1 - U \chi^{(0)}_{-+}(q,i\nu)} \qquad \chi^{(0)}_{-+} = \frac{1}{N}\sum_k \frac{\langle n_{k+q\uparrow}\rangle - \langle n_{k\downarrow}\rangle}{i\nu - \tilde{\varepsilon}_{k+q\uparrow} + \tilde{\varepsilon}_{k\downarrow}}$$

Lindhard function (up to some factor)

③ Diagrammatic treatment of the Hubbard interaction

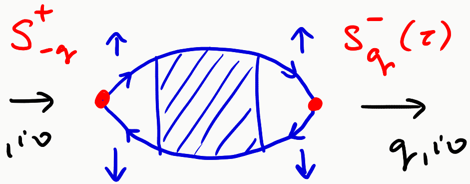
$$\chi_{-+}(q, i\nu) = \frac{1}{\hbar} \int_0^{\hbar\beta} e^{i\nu\frac{\tau}{\hbar}} \langle T\{\hat{S}^-_q(\tau)\,\hat{S}^+_{-q}\}\rangle \, d\tau$$

$i\nu$: energy

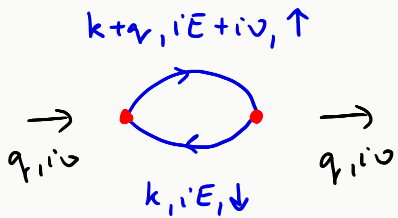
$$\hat{S}^+_{-q} = \frac{1}{\sqrt{N}} \sum_k c^+_{k+q\uparrow} c_{k\downarrow}$$

$$\hat{S}^-_{q} = \frac{1}{\sqrt{N}} \sum_k c^+_{k\downarrow} c_{k+q\uparrow}$$

corresponding diagram

$\chi_{-+} =$ 

• lowest order ~ Lindhard function

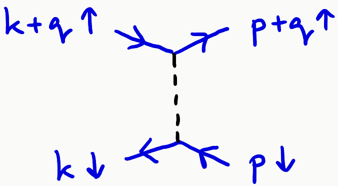


From spin vertices •

$$\chi^{(0)}_{-+}(q, i\nu) = (-1)\left(\frac{1}{\sqrt{N}}\right)^2 \sum_k \frac{1}{\beta} \sum_{iE} \mathcal{G}_0(k+q, iE+i\nu)\,\mathcal{G}_0(k, iE)$$

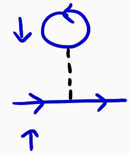
$$= \frac{1}{N} \sum_k \frac{n_F(\varepsilon_{k+q\uparrow}) - n_F(\varepsilon_{k\downarrow})}{i\nu - \varepsilon_{k+q\uparrow} + \varepsilon_{k\downarrow}} = -\frac{1}{N} P$$

- inclusion of the Hubbard interaction term



$$\frac{U}{N} \sum_{kpq} c^{+}_{p+q\uparrow} c_{k+q\uparrow} c^{+}_{k\downarrow} c_{p\downarrow}$$

1) Hartree-like selfenergy

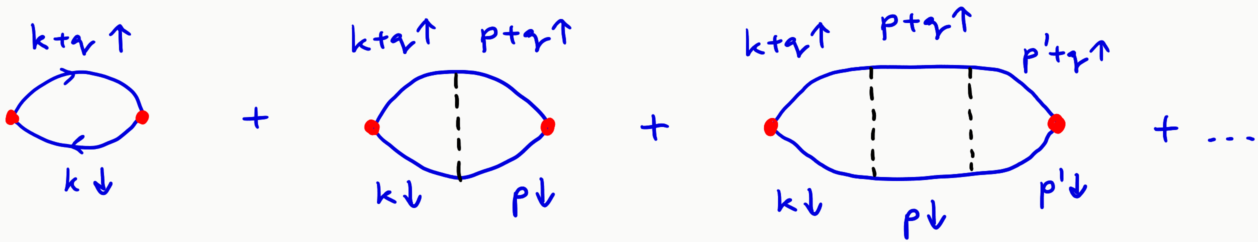


leads to $\varepsilon_k \to \tilde{\varepsilon}_{k\sigma}$

$$\tilde{\varepsilon}_{k\sigma} = \varepsilon_k + U \langle n_{-\sigma} \rangle$$

2) RPA-like series for χ_{-+}

$\chi_{-+} =$



$$\chi_{-+} = (-1)\frac{1}{\sqrt{N}} P \frac{1}{\sqrt{N}} + (-1)\frac{1}{\sqrt{N}} P \left(-\frac{U}{N}\right) P \frac{1}{\sqrt{N}} + (-1)\frac{1}{\sqrt{N}} P \left(-\frac{U}{N}\right) P \left(-\frac{U}{N}\right) P \frac{1}{\sqrt{N}} +$$

$$= (-1)\frac{1}{N} \frac{P}{1 + \frac{U}{N} P} = \frac{\chi^{(0)}_{-+}}{1 - U \chi^{(0)}_{-+}}$$

④ Example – Hubbard model on a cubic lattice

- spin susceptibility in a paramagnetic state ($U < U_{crit}$)

$$\chi^{(0)}_{-+}(q, i\nu) = \frac{1}{N} \sum_k \frac{\langle n_{k+q\uparrow} \rangle - \langle n_{k\downarrow} \rangle}{i\nu - \tilde{\varepsilon}_{k+q\uparrow} + \tilde{\varepsilon}_{k\downarrow}} = \frac{1}{N} \sum_k \frac{n_F(\varepsilon_{k+q}) - n_F(\varepsilon_k)}{i\nu - \varepsilon_{k+q} + \varepsilon_k}$$

$$\chi_{-+} = \frac{\chi^{(0)}_{-+}}{1 - U \chi^{(0)}_{-+}}$$

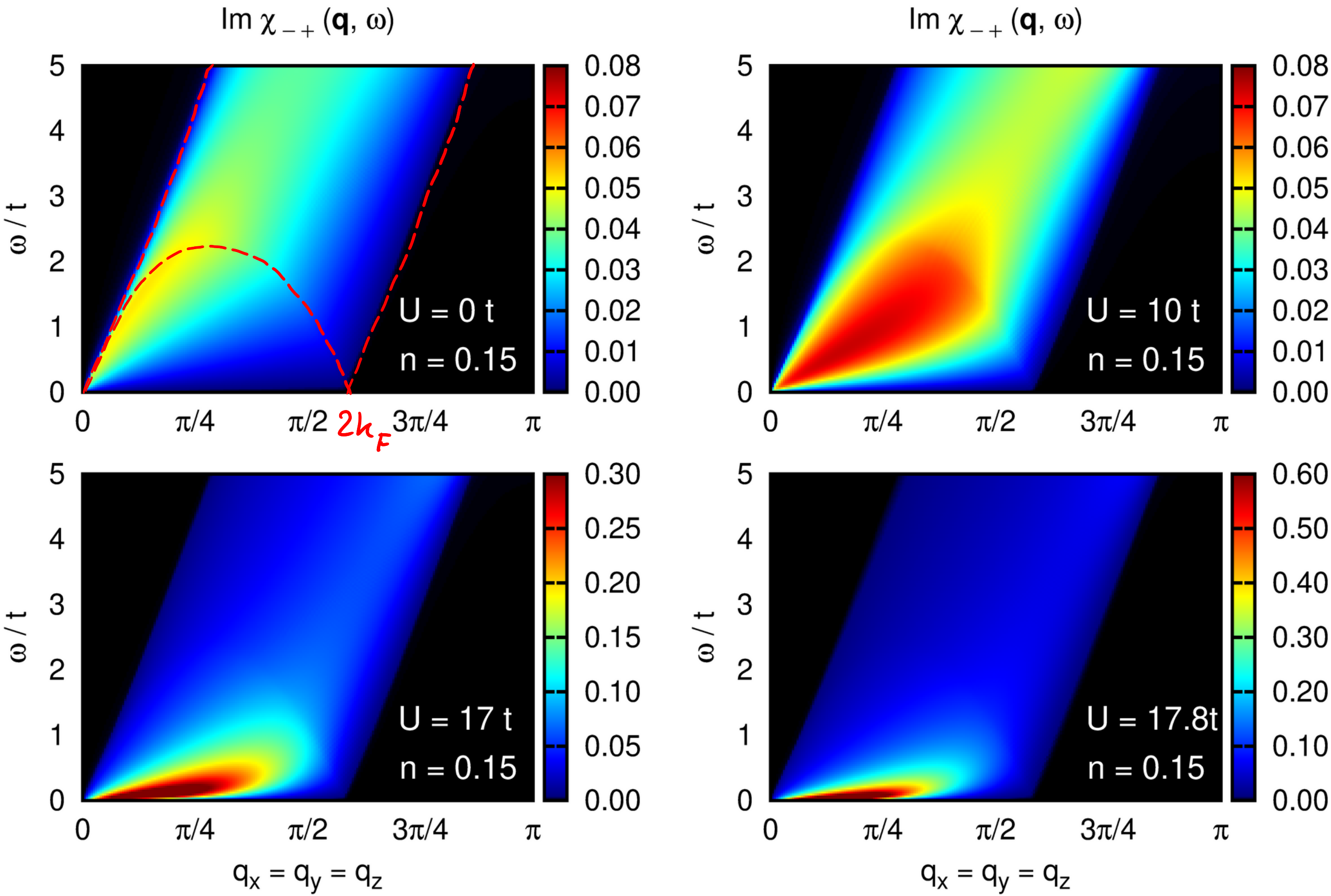
potential divergence for strong enough U

- happens at $U = U_{crit}$, $\omega = 0$, and ordering $q = Q$

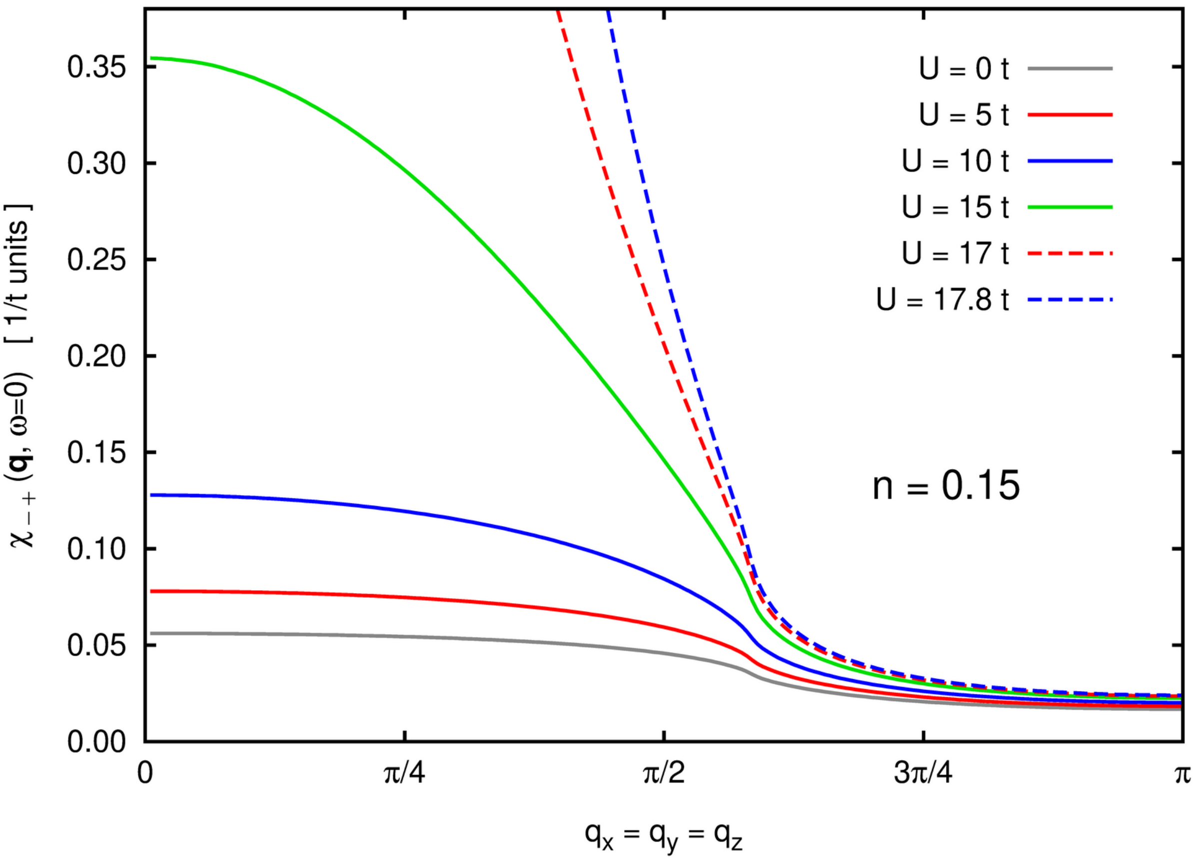
onset of ferromagnetism for U_{crit}: $1 - U_{crit} \chi^{(0)}_{-+}(q \to 0, \omega = 0) = 0$

$$\chi^{(0)}_{-+}(q \to 0, \omega = 0) = \lim_{q \to 0} \frac{1}{N} \sum_k \frac{n_F(\varepsilon_{k+q}) - n_F(\varepsilon_k)}{-\varepsilon_{k+q} + \varepsilon_k} = \frac{1}{N} \sum_k -\frac{\partial n_F}{\partial \varepsilon} = \mathcal{N}(E_F)$$

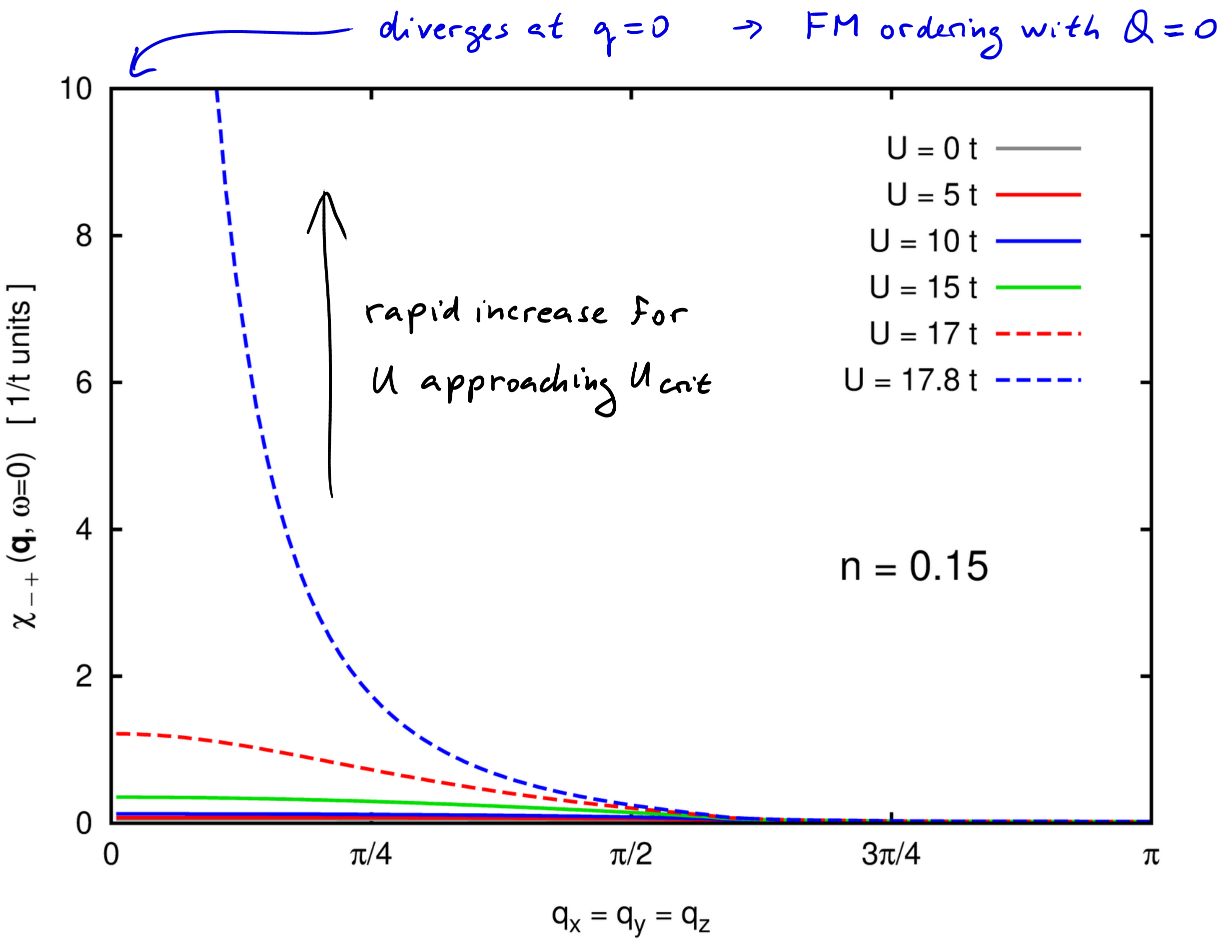
$\longrightarrow \quad 1 = U_{crit} \mathcal{N}(E_F)$ (identical condition to Stoner criterion)



Im χ−+ (q, ω)
Im χ−+ (q, ω)
ω / t
U = 0 t
n = 0.15
2k_F
U = 10 t
n = 0.15
U = 17 t
n = 0.15
U = 17.8t
n = 0.15
0 π/4 π/2 3π/4 π
qx = qy = qz
qx = qy = qz



$\chi_{-+}(\mathbf{q}, \omega=0)$ [1/t units]
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35
0
π/4
π/2
3π/4
π
$q_x = q_y = q_z$
U = 0 t
U = 5 t
U = 10 t
U = 15 t
U = 17 t
U = 17.8 t
n = 0.15



diverges at q = 0 → FM ordering with Q = 0
rapid increase for U approaching U crit
U = 0 t
U = 5 t
U = 10 t
U = 15 t
U = 17 t
U = 17.8 t
n = 0.15
χ−+(q, ω=0) [1/t units]
qx = qy = qz
0
π/4
π/2
3π/4
π
10
8
6
4
2
0

- Ferromagnetic metal $(U > U_{crit})$

$$\chi^{(0)}_{-+}(q, i\nu) = \frac{1}{N}\sum_k \frac{\langle n_{k+q\uparrow}\rangle - \langle n_{k\downarrow}\rangle}{i\nu - \tilde{\varepsilon}_{k+q\uparrow} + \tilde{\varepsilon}_{k\downarrow}} = \frac{1}{N}\sum_k \frac{n_F(\tilde{\varepsilon}_{k+q\uparrow}) - n_F(\tilde{\varepsilon}_{k\downarrow})}{i\nu - \varepsilon_{k+q} + \varepsilon_k + \Delta}$$

$$\tilde{\varepsilon}_{k\uparrow} = \varepsilon_k + U\langle n_\downarrow\rangle \qquad\qquad \Delta = U(\langle n_\uparrow\rangle - \langle n_\downarrow\rangle)$$

$q \to 0$ limit:

$$\chi^{(0)}_{-+}(q\to 0, \omega) = \frac{\frac{1}{N}\sum_k (\langle n_{k\uparrow}\rangle - \langle n_{k\downarrow}\rangle)}{\omega + \Delta} = \frac{\langle n_\uparrow\rangle - \langle n_\downarrow\rangle}{\omega + \Delta} = \frac{\Delta/U}{\omega + \Delta}$$

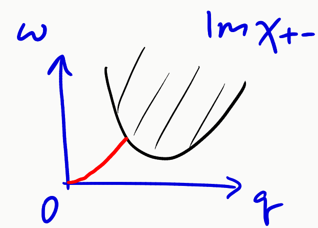
$$\chi_{-+}(q\to 0) = \frac{\Delta/U}{\omega}$$

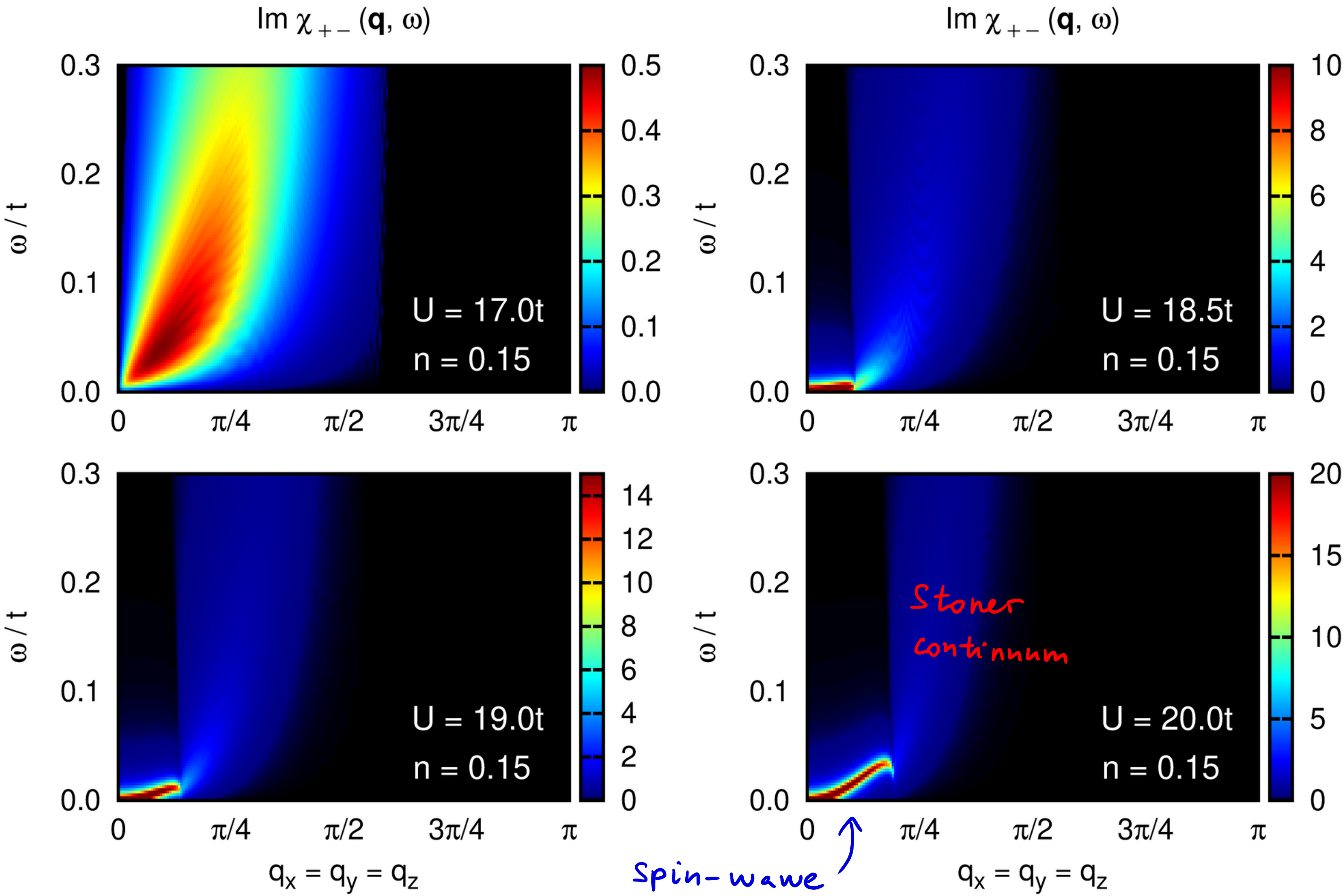
zero-energy pole

more appropriate quantity for $\langle n_\uparrow\rangle > \langle n_\downarrow\rangle$ $(\Delta > 0)$

$$\chi_{+-} = \frac{\chi^{(0)}_{+-}}{1 - U\chi^{(0)}_{+-}}$$

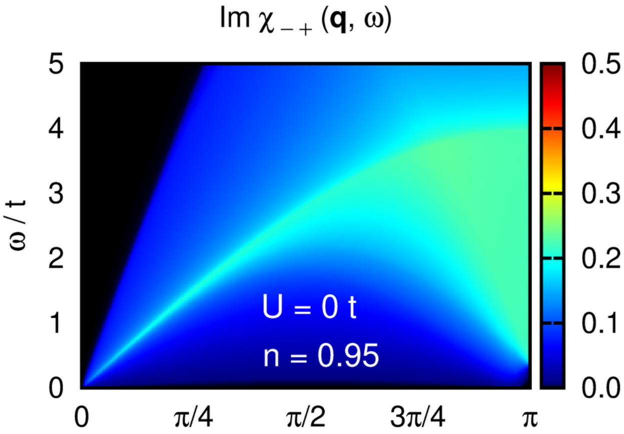
produces non-damped spin-wave below Stoner continuum with a quadratic dispersion $\omega_q \sim q^2$

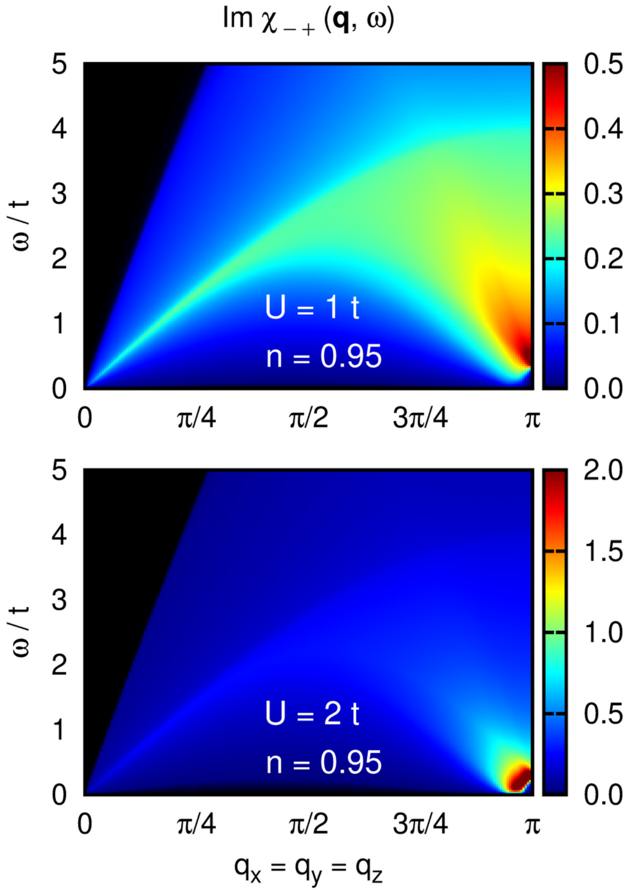




Im χ+− (q, ω)
Im χ+− (q, ω)
ω / t
ω / t
q_x = q_y = q_z
q_x = q_y = q_z
U = 17.0t
n = 0.15
U = 18.5t
n = 0.15
U = 19.0t
n = 0.15
U = 20.0t
n = 0.15
Stoner continuum
Spin-wawe

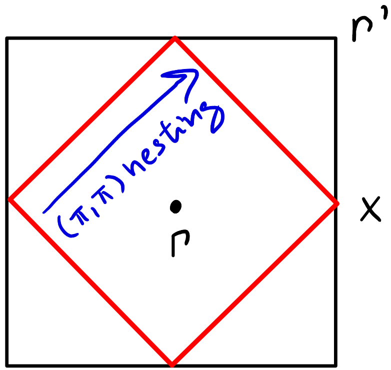
- tendency toward AF ordering for half-filled case

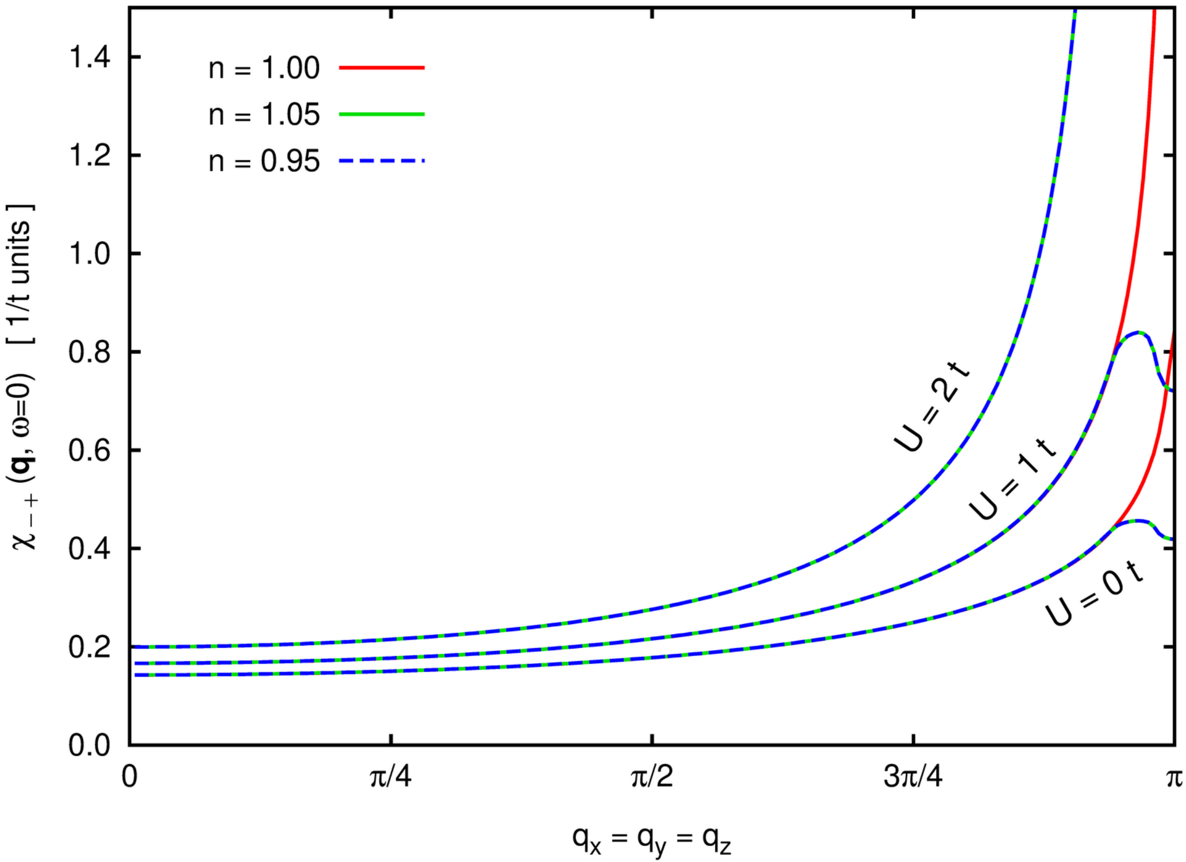




2D case

with $n = 1$





n = 1.00
n = 1.05
n = 0.95
U = 2 t
U = 1 t
U = 0 t
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0
π/4
π/2
3π/4
π
χ−+ (q, ω=0) [1/t units]
qx = qy = qz