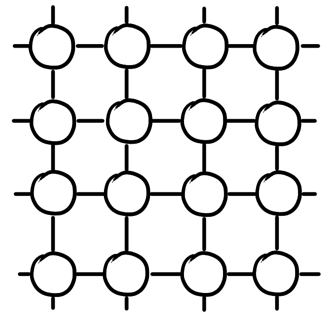
Hubbard model and collective magnetic phenomena

① Model & basic picture

- single-band Hubbard model
  - designed as the simplest model to capture electron correlations
  - lattice model with the four-state local basis



$\bigcirc = |\rangle$ $\quad$ $(\uparrow) = c^{+}_{R\uparrow}|\rangle$ $\quad$ $(\downarrow) = c^{+}_{R\downarrow}|\rangle$ $\quad$ $(\uparrow\downarrow) = c^{+}_{R\uparrow}c^{+}_{R\downarrow}|\rangle$

1) single-electron part – hopping of electrons on a given lattice

$$H_{TB} = -t\sum_{R}\sum_{\delta}\sum_{\sigma}\hat{c}^{+}_{R+\delta\,\sigma}\hat{c}_{R\sigma} \longrightarrow \text{bare dispersion } \varepsilon_k = -2t(\cos k_x + \cos k_y) \text{ etc.}$$

2) intraionic Coulomb repulsion – energy U penalizing double occupation of orbitals

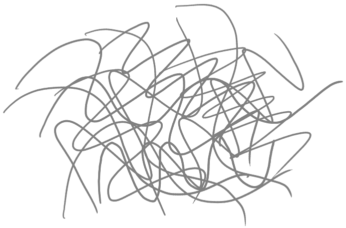
$$H_{Coul} = U\sum_{R} n_{R\uparrow}n_{R\downarrow} \longrightarrow \text{correlated behavior of electrons}$$

- Full model Hamiltonian

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

kinetic energy

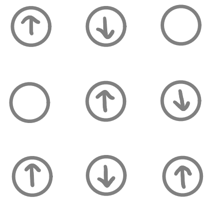
diagonalized by Bloch waves



$$|GS\rangle = \prod_{\varepsilon_k < E_F} \hat{c}^+_{k\sigma} |\,\rangle$$

Coulomb repulsion

diagonalized by localized states



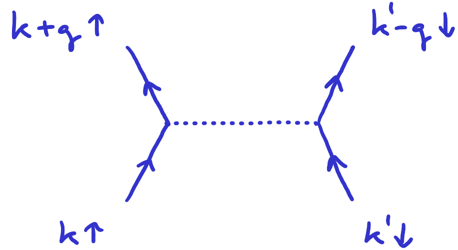
$$\prod \hat{c}^+_{R\sigma} |\,\rangle$$

occupied sites & σ

→ competition: delocalized × localized → transition: metal / Mott insulator

- Bloch basis representation of U term

$$H_{coul} = \frac{1}{N} U \sum_{kk'q} \hat{c}^+_{k+q\uparrow} \hat{c}^+_{k'-q\downarrow} \hat{c}_{k'\downarrow} \hat{c}_{k\uparrow}$$



local interaction – constant matrix element

② Mean-field solution and Stoner criterion

- rearangements in the interaction

  Fourier component of ↑ or ↓ electron density $\hat{n}_{q\sigma} = \frac{1}{N} \sum_k c^\dagger_{k\sigma} c_{k+q\sigma}$

  interaction $H_{Coul} = U N \sum_q \hat{n}_{q\uparrow} \hat{n}_{-q\downarrow}$

  site occupancy $\hat{n}_{R\sigma} = \sum_q e^{iqR} \hat{n}_{q\sigma}$

→ tendency to develop nonzero $\langle n_{q\uparrow} \rangle$ & $\langle n_{-q\downarrow} \rangle$ to optimize the Coulomb energy

1) non zero q : $\langle n_{q\uparrow} \rangle$ and $\langle n_{-q\downarrow} \rangle$ of opposite sign → AF like modulation

2) zero q : $\langle n_{q=0\uparrow} \rangle$ and $\langle n_{q=0\downarrow} \rangle$ split around $\frac{1}{2} n$ → FM band polarization

- decided by the dispersion ε_k and band filling

- treatments - mean-field decoupling - non-zero $\langle n_{q\sigma} \rangle$ reduces total energy
  - magnetic ordering signalled by diverging spin susceptibility $\chi(q, \omega \to 0)$

- mean-field decoupling

$$(\hat{A}-\langle A\rangle)(\hat{B}-\langle B\rangle) = \hat{A}\hat{B} - \hat{A}\langle B\rangle - \langle A\rangle\hat{B} + \langle A\rangle\langle B\rangle \approx 0$$

deviations from the averages small

$\rightarrow$ $\hat{A}\hat{B}$ replaced by $\hat{A}\langle B\rangle + \langle A\rangle\hat{B} - \langle A\rangle\langle B\rangle$

$$H_{MF} = \sum_{k\sigma}(\varepsilon_k-\mu)c^+_{k\sigma}c_{k\sigma} + UN\sum_q\left(\hat{n}_{q\uparrow}\langle n_{-q\downarrow}\rangle + \langle n_{q\uparrow}\rangle\hat{n}_{-q\downarrow} - \langle n_{q\uparrow}\rangle\langle n_{-q\downarrow}\rangle\right)$$

- FM case - only $q=0$ averages nonzero: $\langle n_{q=0,\sigma}\rangle = \frac{1}{N}\sum_k\langle c^+_{k\sigma}c_{k\sigma}\rangle = \langle n_{R\sigma}\rangle = \langle n_\sigma\rangle$

corresponds to local occupancy

1) $\langle n_\uparrow\rangle$ and $\langle n_\downarrow\rangle$ differ $\rightarrow$ FM ordered moment

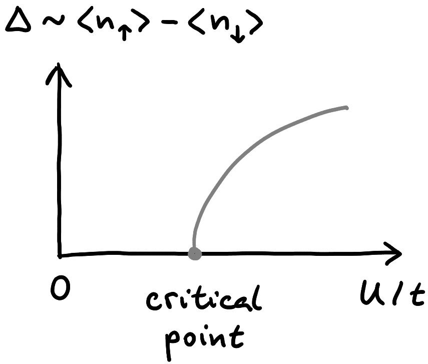
2) Fixed occupancy $n = \langle n_\uparrow\rangle + \langle n_\downarrow\rangle$

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

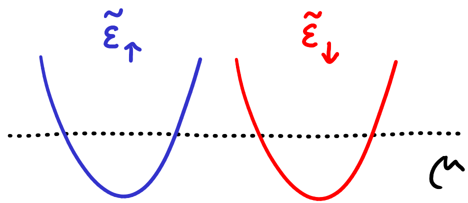
$\rightarrow$ Free-electron Hamiltonians with spin-dependent band shift

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

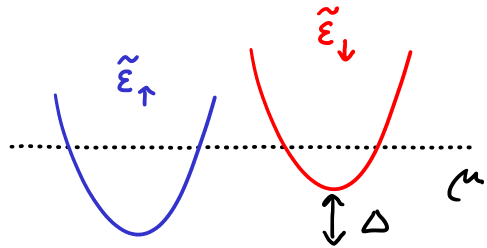
- qualitative picture



non-polarized bands



spin-polarized bands



- selfconsistent solution

band occupation given by Fermi-Dirac $\langle c^{+}_{k\sigma} c_{k\sigma} \rangle = n_F(\tilde{\varepsilon}_{k\sigma}) = \dfrac{1}{e^{\beta \tilde{\varepsilon}_{k\sigma}} + 1}$

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

together with $\langle n_\uparrow \rangle + \langle n_\downarrow \rangle = n$ gives $\langle n_\uparrow \rangle, \langle n_\downarrow \rangle, \mu$ as functions of T

- existence of FM solution

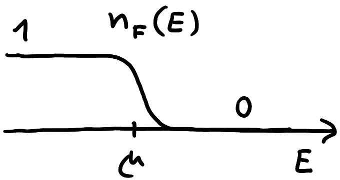
$$\left.\begin{aligned} \langle n_\uparrow\rangle + \langle n_\downarrow\rangle &= n \\ U(\langle n_\uparrow\rangle - \langle n_\downarrow\rangle) &= \Delta \end{aligned}\right\} \quad \langle n_\sigma\rangle = \frac{n}{2} + \sigma\frac{\Delta}{2U} \qquad \sigma = \pm 1$$

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

$$\langle n_\sigma\rangle = \frac{1}{N}\sum_k n_F(\varepsilon_k + U\langle n_{-\sigma}\rangle) \approx \frac{1}{N}\sum_k n_F\left(\varepsilon_k + U\frac{n}{2} - \sigma\frac{\Delta}{2U}\right)$$

$$\approx \frac{1}{N}\sum_k \left[n_F\left(\varepsilon_k + U\frac{n}{2}\right) - \left.\frac{\partial n_F}{\partial \varepsilon}\right|_{\varepsilon_k + U\frac{n}{2}} \sigma\frac{\Delta}{2U}\right] + \mathcal{O}(\Delta^2)$$

$$\Delta = U(\langle n_\uparrow\rangle - \langle n_\downarrow\rangle) = U \underbrace{\frac{1}{N}\sum_k -\left.\frac{\partial n_F}{\partial \varepsilon}\right|_{\varepsilon_k + U\frac{n}{2}}}_{\approx \frac{1}{N}\sum_k \delta(\varepsilon_k + U\frac{n}{2} - \mu)} \Delta + \mathcal{O}(\Delta^3)$$

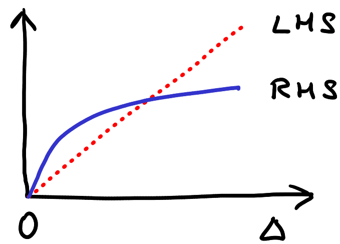


$$\approx \frac{1}{N}\sum_k \delta\left(\varepsilon_k + U\frac{n}{2} - \mu\right) =$$ density of states at Fermi level $\mathcal{N}(E_F)$

$$\Delta = U\mathcal{N}(E_F)\,\Delta + \mathcal{O}(\Delta^3)$$

initial linear slope — saturation

graphical solution:



$\rightarrow$ Finite Δ = FM state if $U\mathcal{N}(E_F) > 1$ (Stoner criterion)

Example:

cubic lattice with

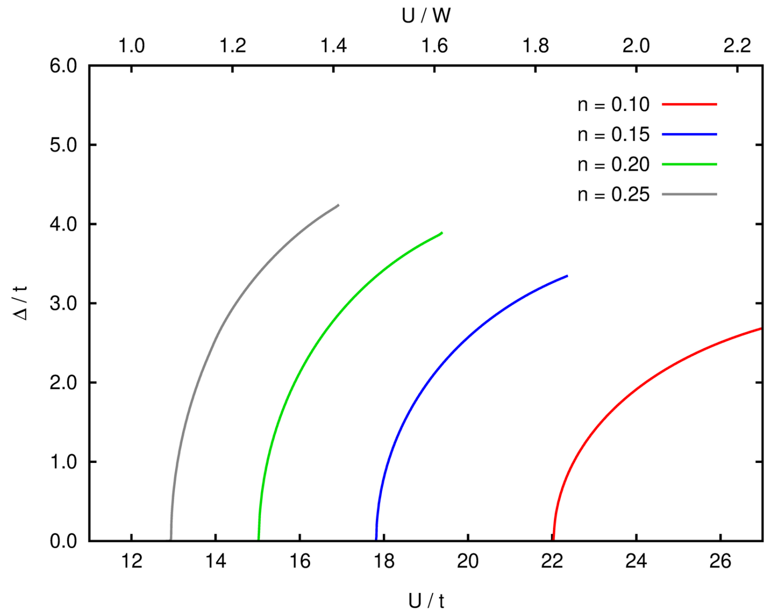
$$\varepsilon_k = -2t\,(\cos k_x + \cos k_y + \cos k_z)$$

low electron occupation

$\rightarrow$ bottom of the band relevant

$$\varepsilon_k \approx \varepsilon_0 + t k^2$$

$$\mathcal{N}(E_F) \sim \sqrt{E_F} \sim k_F \sim n^{\frac{1}{3}}$$



3 Equation of motion approach to the spin susceptibility

- spin susceptibility

$$\chi_{\alpha\beta}(q,E) = \frac{i}{\hbar}\int_{-\infty}^{\infty} \langle [\hat{S}_q^\alpha(t), \hat{S}_{-q}^\beta(0)] \rangle \,\vartheta(t)\, e^{\frac{i}{\hbar}(E+i0^+)t}\, dt \qquad \hat{S}_q^\alpha = \frac{1}{\sqrt{N}}\sum_R e^{-iqR}\,\hat{S}_R^\alpha$$

Matsubara counterpart $\chi_{\alpha\beta}(q,i\nu) = \frac{1}{\hbar}\int_0^{\hbar\beta} \langle T\{\hat{S}_q^\alpha(\tau), \hat{S}_{-q}^\beta(0)\}\rangle\, e^{i\nu\frac{\tau}{\hbar}}\, d\tau$

- symmetry of the susceptibility tensor

spin-isotropic system without magnetic ordering: $\chi_{\alpha\beta} = \delta_{\alpha\beta}\,\chi$

FM/AF order with magnetization ∥ z developed – still isotropic in xy plane

$$\chi_{xx} = \chi_{yy} \text{ (transverse)} \quad \neq \quad \chi_{zz} \text{ (longitudinal)}$$

transverse components captured by

$$\chi_{-+} = \frac{1}{\hbar}\langle T\{S^-(\tau)\,S^+(0)\}\rangle = \frac{1}{\hbar}\langle T\{[S^x(\tau) - iS^y(\tau)]\,[S^x(0)+iS^y(0)]\}\rangle = \chi_{xx}+\chi_{yy}$$

- general equation of motion

def.: $\chi_{AB}(\tau) = \frac{1}{\hbar}\langle T\{\hat{A}(\tau)\,\hat{B}(0)\}\rangle$ $\qquad$ $\hat{A},\hat{B}$ – bosonic operators

EOM: $\frac{\partial}{\partial\tau}\chi_{AB} = ?\,\delta(\tau) + ?\,\langle T\{\frac{\partial\hat{A}(\tau)}{\partial\tau}\,\hat{B}(0)\}\rangle = ?\,\delta(\tau) + ?\,\langle T\{[\hat{A},\hat{H}]_\tau\,\hat{B}(0)\}\rangle$

derivation

$$\chi_{AB}(\tau) = \frac{1}{\hbar}\langle T\{\hat{A}(\tau)\hat{B}(0)\}\rangle = \frac{1}{\hbar}\left[\langle\hat{A}(\tau)\hat{B}(0)\rangle\vartheta(\tau) + \langle\hat{B}(0)\hat{A}(\tau)\rangle\vartheta(-\tau)\right]$$

$$\hbar\frac{\partial}{\partial\tau}\chi_{AB}(\tau) = \langle\hat{A}(\tau)\hat{B}(0)\rangle\delta(\tau) - \langle\hat{B}(0)\hat{A}(\tau)\rangle\delta(\tau)$$
$$+ \langle\frac{\partial\hat{A}(\tau)}{\partial\tau}\hat{B}(0)\rangle\vartheta(\tau) + \langle\hat{B}(0)\frac{\partial\hat{A}(\tau)}{\partial\tau}\rangle\vartheta(-\tau)$$

$$= \langle[\hat{A},\hat{B}]\rangle\delta(\tau) + \langle T\{\frac{\partial\hat{A}(\tau)}{\partial\tau}\hat{B}(0)\}\rangle$$

operator EOM

$$\frac{\partial\hat{A}(\tau)}{\partial\tau} = -\frac{1}{\hbar}[\hat{A},\hat{H}]_\tau$$

$$= \langle[\hat{A},\hat{B}]\rangle\delta(\tau) - \frac{1}{\hbar}\langle T\{[\hat{A},\hat{H}]_\tau\hat{B}(0)\}\rangle$$

- application to χ_{-+}

$$\hbar \frac{\partial}{\partial\tau}\chi_{-+}(q,\tau) = \underbrace{\langle[\hat{S}^-_q,\hat{S}^+_{-q}]\rangle \delta(\tau)}_{1} - \frac{1}{\hbar}\langle T\{[\hat{S}^-_q, \underbrace{\hat{H}_{TB}}_{2} + \underbrace{\hat{H}_{coul}}_{3}]_\tau \hat{S}^+_{-q}(0)\}\rangle$$

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

1) $\langle[\hat{S}^-_q,\hat{S}^+_{-q}]\rangle =$

shortcut: $= \frac{1}{N}\sum_{RR'} e^{-iqR}e^{iqR'}\langle\underbrace{[S^-_R,S^+_{R'}]}_{-2S^z_R\,\delta_{RR'}}\rangle = \frac{1}{N}\sum_R\langle -2S^z_R\rangle = \langle n_\downarrow\rangle - \langle n_\uparrow\rangle$

pedestrian:

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

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

$$= \frac{1}{N}\sum_k\left(\langle n_{k\downarrow}\rangle - \cancel{\langle n_{k\downarrow}n_{k+q\uparrow}\rangle} - \langle n_{k+q\uparrow}\rangle + \cancel{\langle n_{k+q\uparrow}n_{k\downarrow}\rangle}\right) = \langle n_\downarrow\rangle - \langle n_\uparrow\rangle$$

$$\hat{H} = \sum_{k\sigma} (\varepsilon_k - \mu)\, \hat{c}^{+}_{k\sigma} \hat{c}_{k\sigma} + \frac{1}{N} U \sum_{kk'q} \hat{c}^{+}_{k+q\uparrow} \hat{c}^{+}_{k'-q\downarrow} \hat{c}_{k'\downarrow} \hat{c}_{k\uparrow} \qquad \hat{S}^{-}_{q} = \frac{1}{\sqrt{N}} \sum_{k} \hat{c}^{+}_{k\downarrow} \hat{c}_{k+q\uparrow}$$

2) commutator of $c^{+}_{k\downarrow} c_{k+q\uparrow}$ with $\hat{H}_{TB}$

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

$$+ (\varepsilon_{k+q} - \mu) \Big[c^{+}_{k\downarrow} c_{k+q\uparrow}, c^{+}_{k+q\uparrow} c_{k+q\uparrow}\Big] \qquad k+q = k',\ \sigma = \uparrow$$

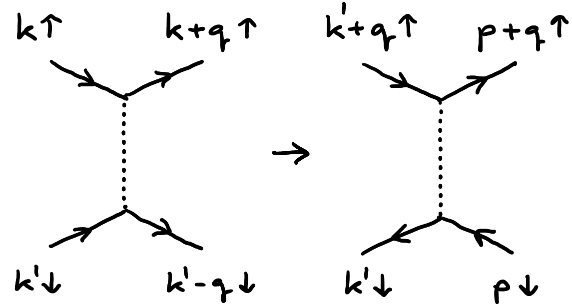
$$\Big[c^{+}_{k\downarrow} c_{k+q\uparrow}, c^{+}_{k\downarrow} c_{k\downarrow}\Big] = \underbrace{c^{+}_{k\downarrow} c_{k+q\uparrow} c^{+}_{k\downarrow}}_{0} c_{k\downarrow} - \cancel{c^{+}_{k\downarrow} c_{k\downarrow}}\, c^{+}_{k\downarrow} c_{k+q\uparrow} = - c^{+}_{k\downarrow} c_{k+q\uparrow}$$

$$\Big[c^{+}_{k\downarrow} c_{k+q\uparrow}, c^{+}_{k+q\uparrow} c_{k+q\uparrow}\Big] = c^{+}_{k\downarrow} c_{k+q\uparrow} \cancel{c^{+}_{k+q\uparrow} c_{k+q\uparrow}} - c^{+}_{k+q\uparrow} \underbrace{c_{k+q\uparrow} c^{+}_{k\downarrow} c_{k+q\uparrow}}_{0} = c^{+}_{k\downarrow} c_{k+q\uparrow}$$

$$\rightarrow \quad \Big[\hat{S}^{-}_{q}, \hat{H}_{TB}\Big] = \frac{1}{\sqrt{N}} \sum_{k} (\varepsilon_{k+q} - \varepsilon_k)\, c^{+}_{k\downarrow} c_{k+q\uparrow}$$

similar structure to $\hat{S}^{-}_{q}$ itself

3) commutator of $c^+_{k\downarrow} c_{k+q\uparrow}$ with H_{Coul}



$$\Big[\underbrace{c^+_{k\downarrow} c_{k+q\uparrow}}_{\text{e-h pair with } \uparrow\downarrow \text{ and q-shift}} ,\ \frac{1}{N} U \sum_{pk'q'} c^+_{p+q'\uparrow} c^+_{k'\downarrow} c_{p\downarrow} c_{k'+q'\uparrow} \Big]$$

$$c^+_{p+q'\uparrow} c_{k'+q'\uparrow} c^+_{k'\downarrow} c_{p\downarrow}$$

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

$$\delta_{k+q,p+q'} - c^+_{p+q'\uparrow} c_{k+q\uparrow} \qquad\qquad \delta_{pk} - c^+_{k\downarrow} c_{p\downarrow}$$

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

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

alltogether 1 + 2 + 3

1 2 two-particle propag.

$$\hbar \frac{\partial}{\partial\tau}\chi_{-+}(q,\tau) = \left(\langle n_\downarrow\rangle - \langle n_\uparrow\rangle\right)\delta(\tau) - \frac{1}{\hbar}\frac{1}{\sqrt{N}}\sum_k (\varepsilon_{k+q}-\varepsilon_k)\langle T\{c^+_{k\downarrow}(\tau)\,c_{k+q\uparrow}(\tau)\,\hat{S}^+_{-q}(0)\}\rangle$$

3 higher-order propagator

$$-\frac{1}{\hbar}\frac{1}{\sqrt{N}}\sum_k \frac{U}{N}\sum_{k'q'}\langle T\{\left(\underline{c^+_{k\downarrow}}\, c_{k'+q'\uparrow}\, c^+_{k'\downarrow}\, \underline{c_{k+q-q'\downarrow}} - \underline{c^+_{k+q'\uparrow}\, c_{k'+q'\uparrow}}\, c^+_{k'\downarrow}\, \underline{c_{k+q\uparrow}}\right)_\tau \hat{S}^+_{-q}(0)\}\rangle$$

a b c d

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

4 Decoupling of EOM - generalized Hartree-Fock scheme

b c

$$-\frac{1}{\hbar}\frac{1}{\sqrt{N}}\sum_k \frac{U}{N}\Big[\langle T\{\Big[\sum_{k'}\langle n_{k'\downarrow}\rangle\, c^+_{k\downarrow}c_{k+q\uparrow} - \sum_{q'}\langle n_{k+q'\uparrow}\rangle\, c^+_{k\downarrow}c_{k+q\uparrow}$$

$$-\sum_{k'}\langle n_{k\downarrow}\rangle\, c^+_{k'\downarrow}c_{k'+q\uparrow} + \sum_{k'}\langle n_{k+q\uparrow}\rangle\, c^+_{k'\downarrow}c_{k'+q\uparrow}\Big]_\tau \hat{S}^+_{-q}(0)\}\rangle$$

a d

alltogether 1+2+3 after decoupling

$$\hbar \frac{\partial}{\partial \tau} \frac{1}{\hbar} \frac{1}{\sqrt{N}} \sum_k \langle T\{(c^+_{k\downarrow} c_{k+q\uparrow})_\tau \hat{S}^+_{-q}(0)\}\rangle \qquad \hbar \frac{\partial}{\partial \tau} \chi_{-+}(q,\tau)$$

$$= \frac{1}{N} \sum_k (\langle n_{k\downarrow}\rangle - \langle n_{k+q\uparrow}\rangle)\, \delta(\tau) \qquad 1 \quad \text{(q-shift kept for convenience)}$$

$$- \frac{1}{\hbar} \frac{1}{\sqrt{N}} \sum_k (\varepsilon_{k+q} - \varepsilon_k) \langle T\{c^+_{k\downarrow}(\tau) c_{k+q\uparrow}(\tau) \hat{S}^+_{-q}(0)\}\rangle \qquad 2$$

$$- \frac{1}{\hbar} \frac{1}{\sqrt{N}} \sum_k (U\langle n_\downarrow\rangle - U\langle n_\uparrow\rangle) \langle T\{c^+_{k\downarrow}(\tau) c_{k+q\uparrow}(\tau) \hat{S}^+_{-q}(0)\}\rangle \qquad 3b \quad 3c$$

$$- U \frac{1}{N} \sum_k (\langle n_{k\downarrow}\rangle - \langle n_{k+q\uparrow}\rangle) \left[- \frac{1}{\hbar} \frac{1}{\sqrt{N}} \sum_{k'} \langle T\{c^+_{k'\downarrow}(\tau) c_{k'+q\uparrow}(\tau) \hat{S}^+_{-q}(0)\}\rangle \right] \qquad 3a \quad 3d$$

denote $\chi_{-+}(k,q,\tau) = \frac{1}{\hbar} \frac{1}{\sqrt{N}} \langle T\{c^+_{k\downarrow}(\tau) c_{k+q\uparrow} \hat{S}^+_{-q}(0)\}\rangle$ $\qquad \chi_{-+}(q,\tau) = \sum_k \chi_{-+}(k,q,\tau)$

$$\hbar \frac{\partial}{\partial \tau} \chi_{-+}(k,q,\tau) = - \left[(\varepsilon_{k+q} + U\langle n_\downarrow\rangle) - (\varepsilon_k + U\langle n_\uparrow\rangle) \right] \chi_{-+}(k,q,\tau) \qquad 2 \quad 3b \quad 3c$$

$$+ \frac{1}{N} (\langle n_{k\downarrow}\rangle - \langle n_{k+q\uparrow}\rangle) \left[\delta(\tau) + U \sum_{k'} \chi_{-+}(k',q,\tau) \right] \qquad 1 \quad 3a \quad 3d$$

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

$$\left[\hbar\frac{\partial}{\partial\tau} + (\tilde{\varepsilon}_{k+q\uparrow} - \tilde{\varepsilon}_{k\downarrow})\right]\chi_{-+}(k,q,\tau) = \frac{1}{N}\left(\langle n_{k\downarrow}\rangle - \langle n_{k+q\uparrow}\rangle\right)\left[\delta(\tau) + U\overbrace{\sum_{k'}\chi_{-+}(k',q,\tau)}^{\chi_{-+}(q,\tau)}\right]$$

- in Matsubara representation: $\chi_{-+}(\tau) \to \chi_{-+}(i\nu)$ $\quad \hbar\frac{\partial}{\partial\tau} \to -i\nu$ $\quad \delta(\tau) \to 1$ *

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

extract $\chi_{-+}(k,q,i\nu)$ and sum over k to get $\chi_{-+}(q,i\nu)$:

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

Lindhard function $\chi^{(0)}_{-+}(q,i\nu)$

- Final result

$$\chi_{-+} = \chi^{(0)}_{-+}(1 + U\chi_{-+}) \to \chi_{-+}(q,i\nu) = \frac{\chi^{(0)}_{-+}(q,i\nu)}{1 - U\chi^{(0)}_{-+}(q,i\nu)}$$

enhances $\chi^{(0)}_{-+}$

leads to divergence at U_{crit}

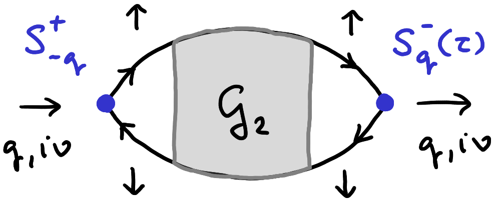
(5) Diagrammatic evaluation of the spin susceptibility

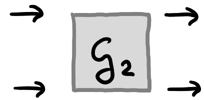
$$\chi_{-+}(q,i\nu) = \frac{1}{\hbar}\int_0^{\hbar\beta} \langle T\{\hat{S}^-_q(\tau)\,\hat{S}^+_{-q}(0)\}\rangle\, e^{i\nu\frac{\tau}{\hbar}}\, d\tau$$

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

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

corresponding diagram

$\chi_{-+} =$ 

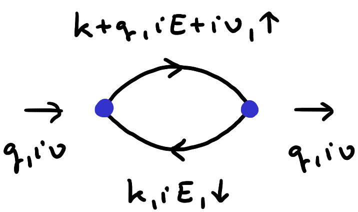


two-particle propagator

- lowest order – Lindhard function

From spin vertices

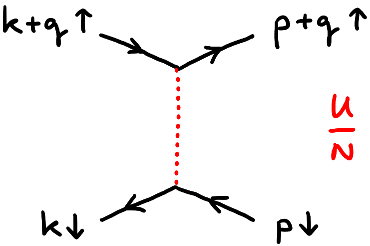
$$\chi^{(0)}_{-+}(q,i\nu) = (-1)\left(\frac{1}{\sqrt{N}}\right)^2 \sum_k \frac{1}{\beta}\sum_{iE} \mathcal{G}_0(k+q, iE+i\nu)\,\mathcal{G}_0(k, iE)$$

$\chi^{(0)}_{-+} =$ 

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

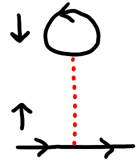
bubble w/o (-1)

- 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 selfenergy

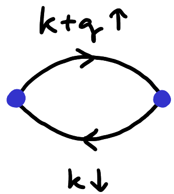


leads to $\varepsilon_k \to \tilde{\varepsilon}_{k\sigma}$

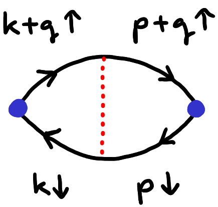
$$\tilde{\varepsilon}_{k\sigma} = \varepsilon_k + \Sigma_H$$
$$= \varepsilon_k + U\langle n_{-\sigma}\rangle$$

2) RPA-like series for χ_{-+}

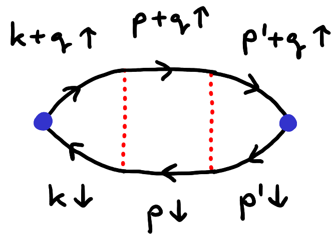
$\chi_{-+} =$



$+$



$+$



$+ \;\dots$

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

$$= (-1)\frac{1}{\sqrt{N}^{2}}\frac{P}{1+\frac{U}{N}P} = \frac{\chi^{(0)}_{-+}}{1-U\chi^{(0)}_{-+}}$$

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

⑥ Application – Hubbard model on a cubic lattice

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

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

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

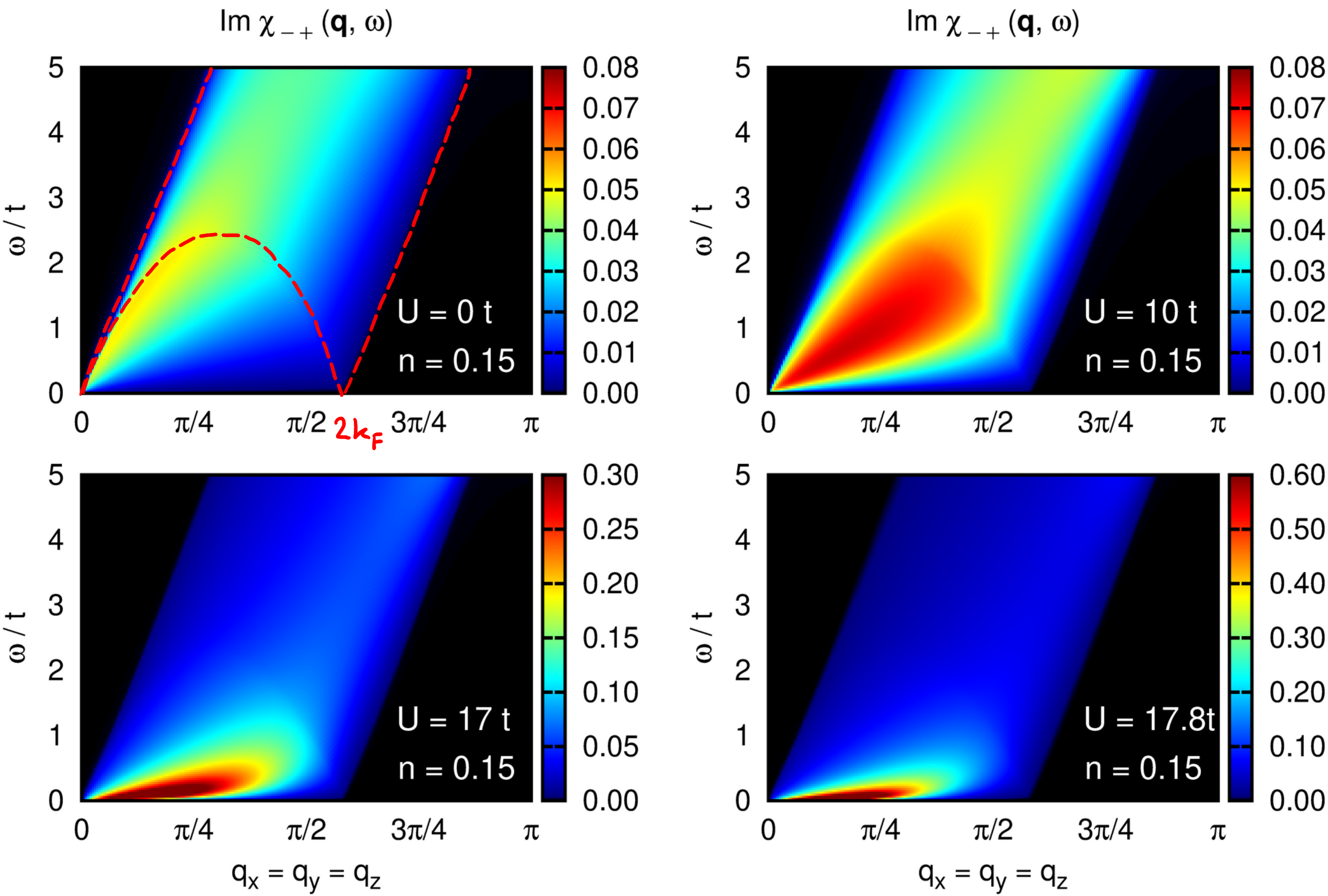
potential divergence for strong enough U

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

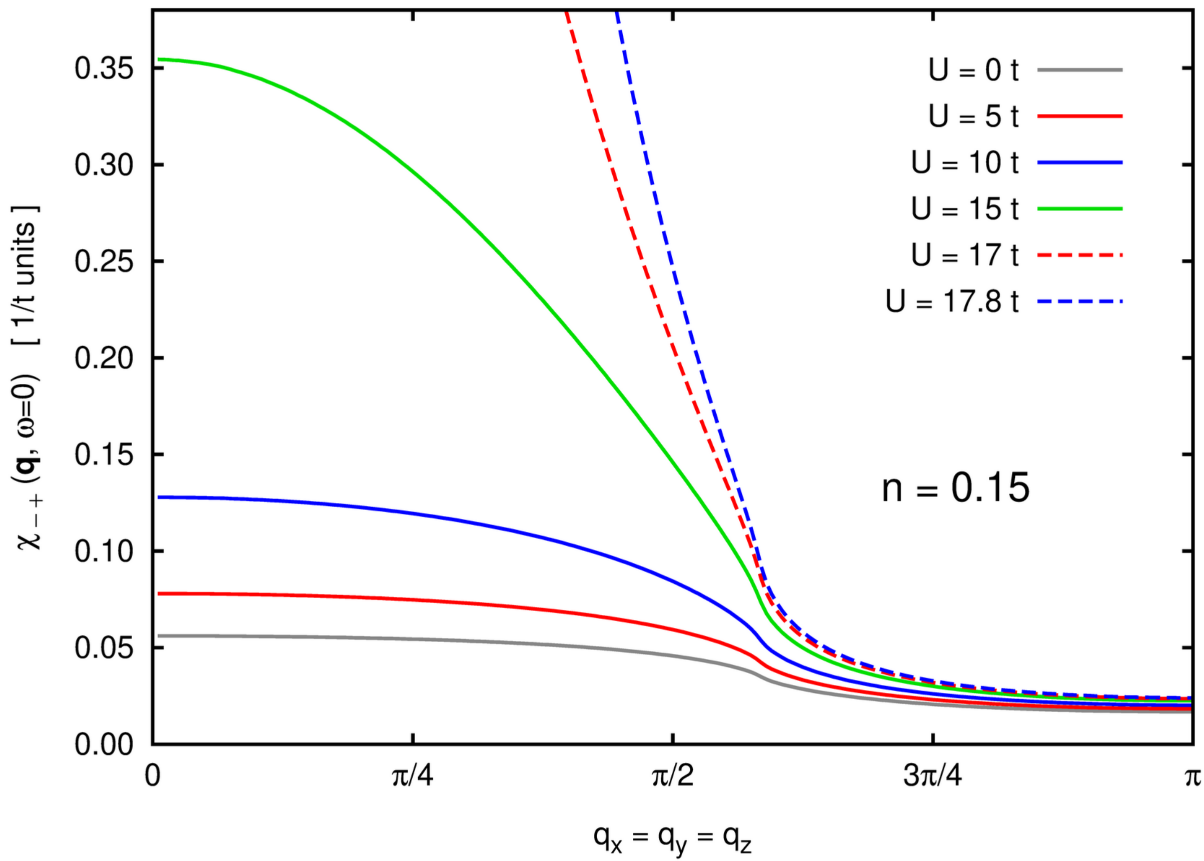
- onset of ferromagnetism for U_{crit}: $1 - U_{crit}\,\chi^{(0)}_{-+}(q\to 0, \omega = 0) = 0$

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

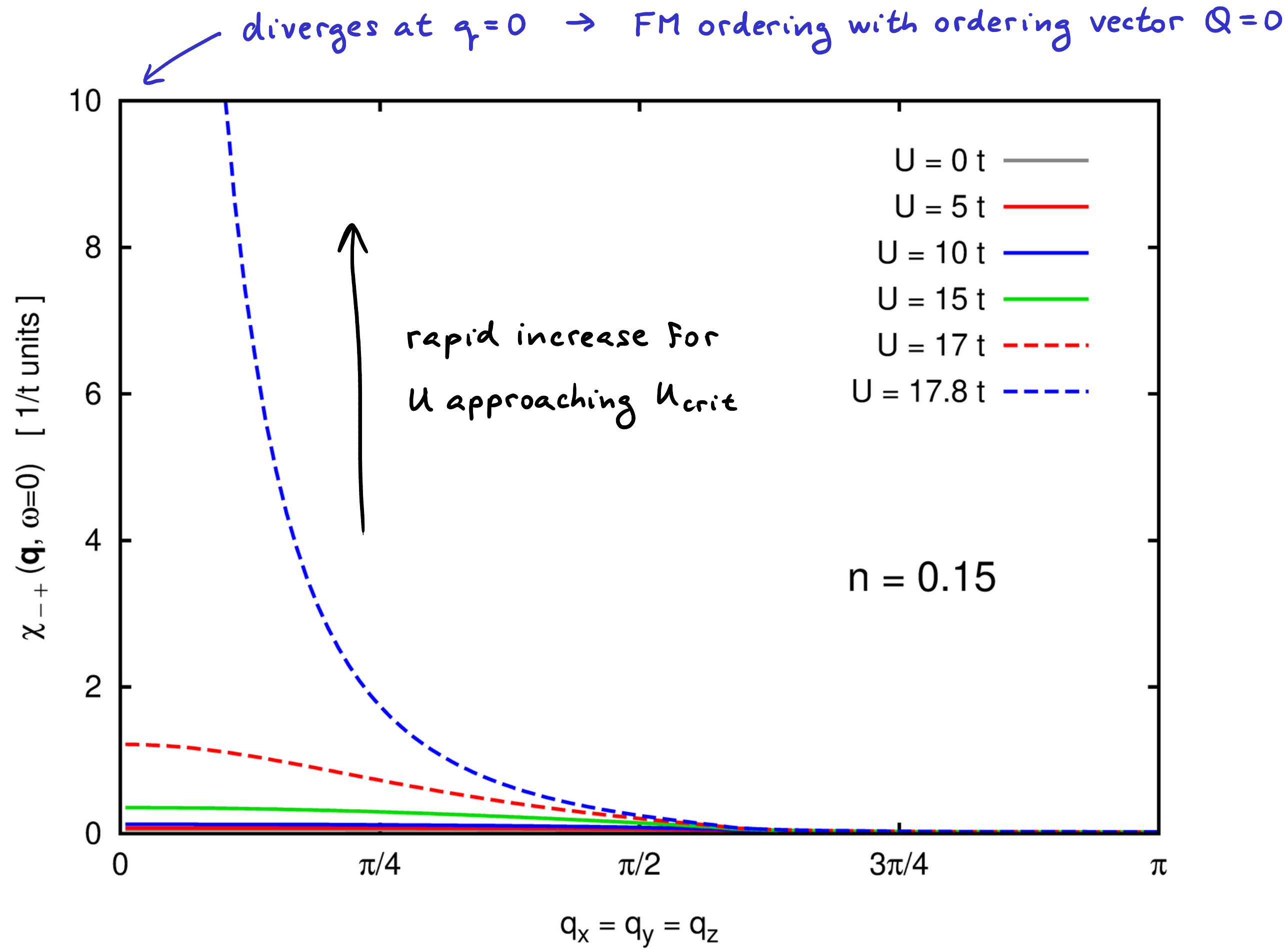
$\rightarrow \quad 1 - U_{crit}\,\mathcal{N}(E_F) = 0$ – identical requirement as in the Stoner criterion



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
q_x = q_y = q_z
0.00 0.01 0.02 0.03 0.04 0.05 0.06 0.07 0.08
0.00 0.05 0.10 0.15 0.20 0.25 0.30
0.00 0.10 0.20 0.30 0.40 0.50 0.60



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


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

- spin susceptibility in ferromagnetic metallic state ($U > U_{crit}$)

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

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

$q \to 0$ limit:

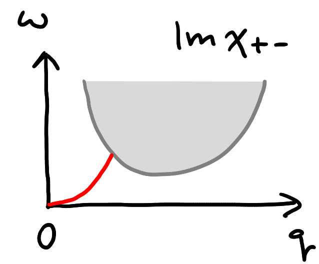
$$\chi^{(0)}_{-+}(q\to 0, \omega) = \frac{\frac{1}{N}\sum_k (\langle n_{k\uparrow}\rangle - \langle n_{k\downarrow}\rangle)}{\omega + \Delta} = \frac{\langle n_\uparrow\rangle - \langle n_\downarrow\rangle}{\omega + \Delta} = \frac{\Delta/U}{\omega + \Delta} \to \chi_{-+}(q\to 0) = \frac{\Delta/U}{\omega}$$

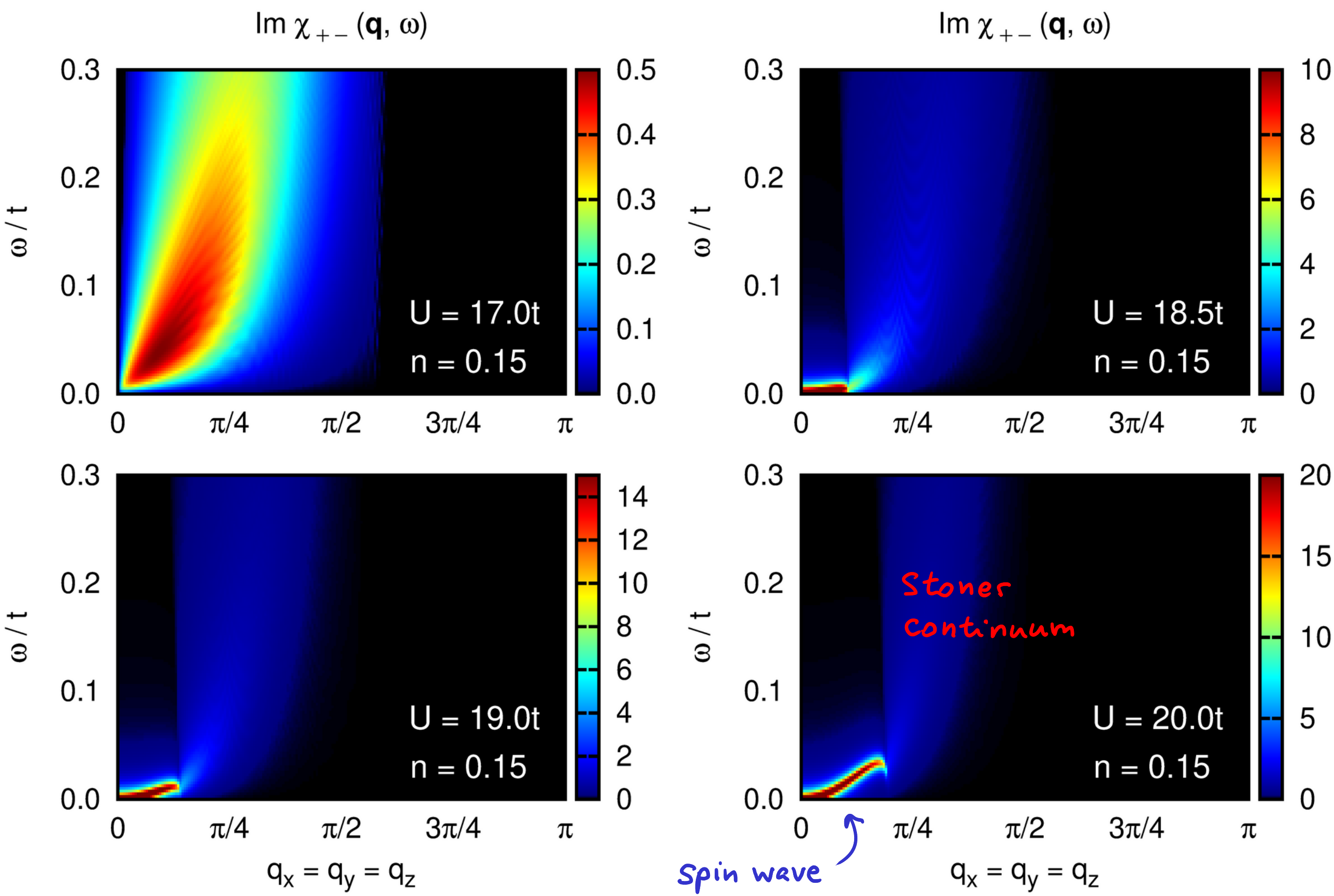
zero-frequency pole

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

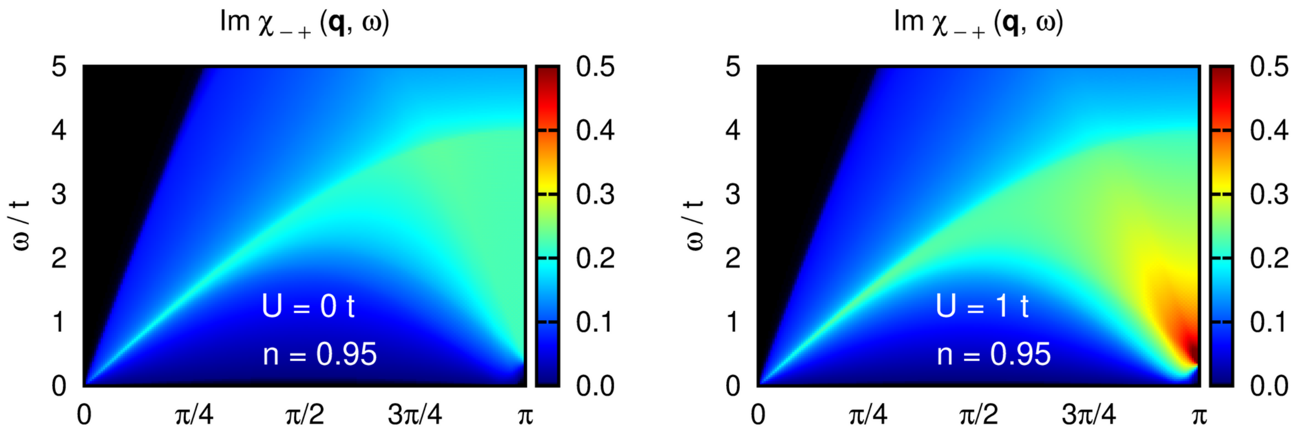
$$\chi_{+-} = \frac{\chi^{(0)}_{+-}}{1 - U\chi^{(0)}_{+-}}$$

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

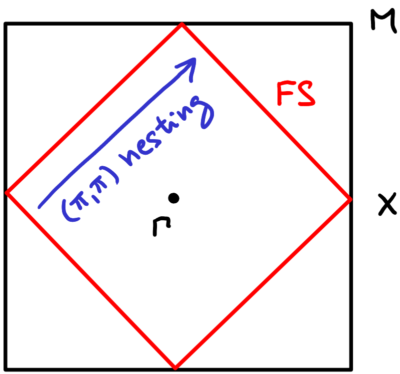


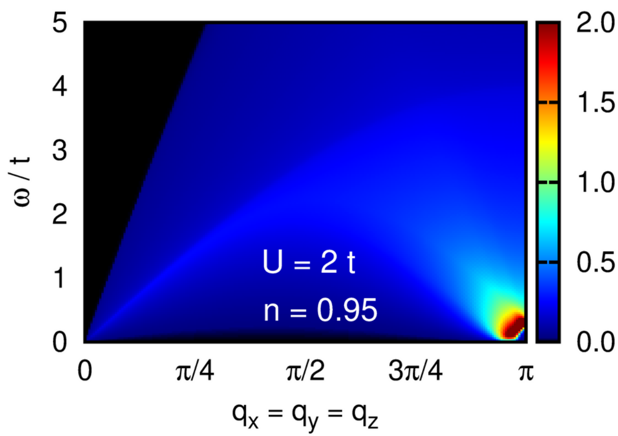

Im χ+− (q, ω)
Im χ+− (q, ω)
ω / t
U = 17.0t
n = 0.15
U = 18.5t
n = 0.15
U = 19.0t
n = 0.15
U = 20.0t
n = 0.15
Stoner continuum
spin wave
qx = qy = qz
qx = qy = qz

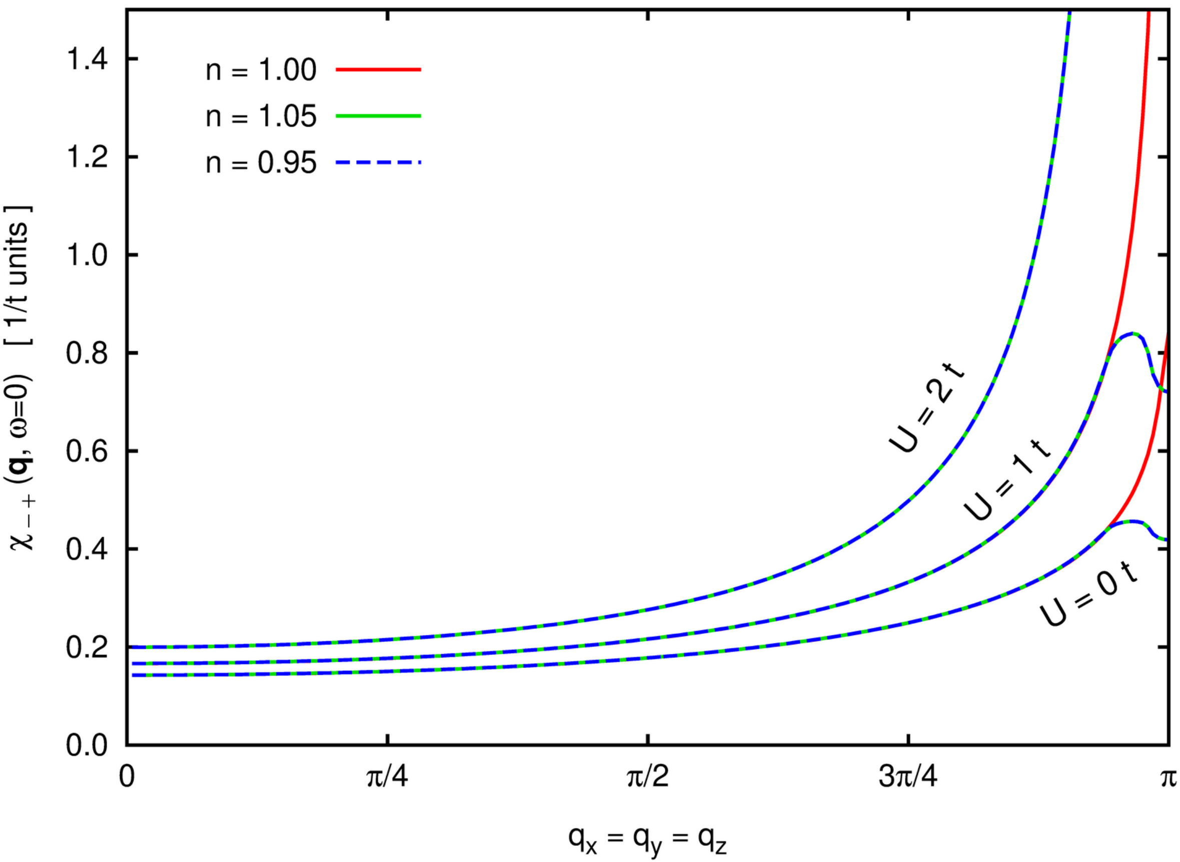
• tendency toward AF ordering near the half-filled case



2D TB case with n=1






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