Itinerant magnetism of metals
Bloch theory of electron liquid

\[ V(r) = \frac{1}{4\pi\varepsilon_0} \frac{1}{r} = \frac{1}{V} \sum_{q \neq 0} e^{i q \cdot r} \frac{e^2}{\varepsilon_0 q^2} \]

\[ H = \sum_{k \sigma} \epsilon_k a_{k \sigma}^{\dagger} a_{k \sigma} + \frac{1}{2V} \sum_{q \neq 0} \sum_{k_1 k_2 \sigma_1 \sigma_2} \frac{e^2}{\varepsilon_0 q^2} \sum_{k_1 k_2 \sigma_1 \sigma_2} a_{k_1 + q, \sigma_1}^{\dagger} a_{k_2 - q, \sigma_2}^{\dagger} a_{k_2 \sigma_2} a_{k_1 \sigma_1} =: H_0 + H_c \]

\[ \langle \psi | H | \psi \rangle = \langle \psi | H_0 | \psi \rangle + \langle \psi | H_c | \psi \rangle \]

\[ = \sum_{k \sigma} \epsilon_k n_{k \sigma} - \frac{1}{2V} \sum_{k_1 k_2 \neq k_2} \sum_{\sigma} \frac{e^2}{\varepsilon_0 |k_1 - k_2|^2} n_{k_1 \sigma} n_{k_2 \sigma} \]

\[ n_{k \sigma} := \langle \psi | a_{k \sigma}^{\dagger} a_{k \sigma} | \psi \rangle \in \{ 0, 1 \} \]

\[ \langle \psi | H_0 | \psi \rangle = \frac{V}{10\pi^2 2m} \sum_{\sigma} k_{F \sigma}^5 = \frac{V}{10\pi^2 2m} \frac{6\pi}{5} \left( \frac{9\pi}{2} \right)^{1/3} \sum_{\sigma} n_{\sigma}^{5/3} \]

\[ n_{\sigma} = k_{F \sigma}^3 / 6\pi^2 \text{ so that } k_{F \sigma} = (6\pi^2 n_{\sigma})^{1/3} \]

\[ \langle \psi | H_c | \psi \rangle = -\frac{Ve^2}{16\pi^4 \varepsilon_0} \sum_{\sigma} \int_{k_{F \sigma}} \int_{k_{F \sigma}} \int_{k_{F \sigma}} \int_{k_{F \sigma}} \int_0^\pi d\theta \sin \theta \frac{1}{k_1^2 + k_2^2 - 2k_1 k_2 \cos \theta} \]

\[ = -\frac{Ve^2}{32\pi^4 \varepsilon_0} \sum_{\sigma} k_{F \sigma}^4 = \frac{Ve^2}{32\pi^4 \varepsilon_0} \sum_{\sigma} k_{F \sigma}^4 \]

\[ \frac{1}{V} \langle \psi | H | \psi \rangle = \frac{\hbar^2}{2m} \frac{6\pi}{5} \left( \frac{9\pi}{2} \right)^{1/3} \left[ n_{\uparrow}^{5/3} + n_{\downarrow}^{5/3} \right] - \alpha \left( n_{\uparrow}^{4/3} + n_{\downarrow}^{4/3} \right) \]

\[ =: \hbar^2 \frac{6\pi}{5} \left( \frac{9\pi}{2} \right)^{1/3} g(n_{\uparrow}) \quad \alpha := \frac{5}{12\pi^2} \left( \frac{9\pi}{2} \right)^{1/3} \frac{1}{4\pi\varepsilon_0 \hbar^2} \]
\[
n_c := \left( \frac{\alpha}{1 + 2^{-1/3}} \right)^3
\]

- for \( n > n_c \), \( g(n_\uparrow) \) has its global minimum at \( n_\uparrow = n/2 \), the electron gas is unpolarized,
- for \( n < n_c \), \( g(n_\uparrow) \) has its global minimum at \( n_\uparrow = 0 \) and \( n_\uparrow = n \), the electron gas is completely spin polarized. Note that theses minima occur at the edges of the allowed range; \( g'(n_\uparrow) \) does not vanish there. A material with complete spin polarization of the valence band is also called a half-metallic ferromagnet, since it only has electrons of spin direction at the Fermi energy.
Tight-binding (Hubbard) model

- On-site Coulomb interactions

\[ H_c \simeq \frac{1}{2} \sum \sum \sum \left\{ K_{m_1 m_2} a_{Rm_1 \sigma_1} a_{Rm_2 \sigma_2} a_{Rm_2 \sigma_2} a_{Rm_1 \sigma_1} + J_{m_1 m_2} a_{Rm_1 \sigma_1} a_{Rm_2 \sigma_2} a_{Rm_1 \sigma_1} a_{Rm_2 \sigma_2} \right\} \]

\[ K_{m_1 m_2} := \langle m_1, m_2 | \frac{e^2}{4\pi \varepsilon_0 |r_1 - r_2|} | m_2, m_1 \rangle \]
\[ = \int d^3r_1 d^3r_2 \phi_m(r_1) \phi_m(r_2) \frac{e^2}{4\pi \varepsilon_0 |r_1 - r_2|} \phi_m(r_2) \phi_m(r_1) \]

\[ J_{m_1 m_2} := \langle m_1, m_2 | \frac{e^2}{4\pi \varepsilon_0 |r_1 - r_2|} | m_1, m_2 \rangle \]

\[ = \int d^3r_1 d^3r_2 \phi_m^*(r_1) \phi_m^*(r_2) \frac{e^2}{4\pi \varepsilon_0 |r_1 - r_2|} \phi_m(r_2) \phi_m(r_1) \]

\[ \sum_{m_1 m_2} a_{Rm_1 \sigma_1} a_{Rm_2 \sigma_2} a_{Rm_2 \sigma_2} a_{Rm_1 \sigma_1} = \frac{1}{2} n_{Rm_1} n_{Rm_2} + 2 s_{Rm_1} \cdot s_{Rm_2} \]

Fact (without proof):

\[ J_{m_1 m_2} \geq 0, \quad K_{m_1 m_2} \geq J_{m_1 m_2}, \quad K_{m_1 m_2} - 1/2 J_{m_1 m_2} > 0 \]

For single orbital:

\[ H_c \simeq \frac{1}{2} \sum R \int d^3r_1 d^3r_2 \phi^*(r_1) \phi^*(r_2) \frac{e^2}{4\pi \varepsilon_0 |r_1 - r_2|} \phi(r_2) \phi(r_1) \left( a_{R \uparrow} a_{R \downarrow} a_{R \downarrow} a_{R \uparrow} + a_{R \downarrow} a_{R \uparrow} a_{R \uparrow} a_{R \downarrow} + U a_{R \uparrow} a_{R \downarrow} a_{R \downarrow} a_{R \uparrow} \right) \]

- Hubbard term

- Inter-site Coulomb interactions - negligible

\[ K_{12} = K_{R_1 R_2} \]
\[ J_{12} = J_{R_1 R_2} \]
\[ H_{\text{exc}} = - \sum_{R_1 R_2} J_{12} s_1 \cdot s_2 \]
\[ J_{12} \geq 0 \]

Comment: the Hartree (Hubbard) term dominates the on-site interaction while the Fock (exchange) term dominates the inter-site interaction.
Antiferromagnetism in the Hubbard model – Mott insulator

\[
H = -\sum_{R\sigma} t(R-R') a_{R\sigma}^\dagger a_{R\sigma} + U \sum_{R} a_{R\uparrow}^\dagger a_{R\downarrow}^\dagger a_{R\downarrow} a_{R\uparrow}

\equiv -\sum_{R\sigma} t(R-R') a_{R\sigma}^\dagger a_{R\sigma} + U \sum_{R} a_{R\uparrow}^\dagger a_{R\uparrow} a_{R\downarrow}^\dagger a_{R\downarrow}
\]

Toy model - dimer

\[
H = -t \sum_{\sigma} (a_{1\sigma}^\dagger a_{2\sigma} + a_{2\sigma}^\dagger a_{1\sigma}) - \mu \sum_{\sigma} (a_{1\sigma}^\dagger a_{1\sigma} + a_{2\sigma}^\dagger a_{2\sigma}) + U \sum_{i=1,2} a_{i\uparrow}^\dagger a_{i\uparrow} a_{i\downarrow}^\dagger a_{i\downarrow}
\]

\[\{|\uparrow\downarrow, 0\rangle, |0, \uparrow\downarrow\rangle, |\uparrow, \downarrow\rangle, |\downarrow, \uparrow\rangle, |\uparrow, \uparrow\rangle, |\downarrow, \downarrow\rangle\}\]

by transforming from \(|\uparrow, \downarrow\rangle, |\downarrow, \uparrow\rangle\) onto \((|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle)/\sqrt{2}, (|\uparrow, \downarrow\rangle + |\downarrow, \uparrow\rangle)/\sqrt{2}\),

\[
H' = \begin{pmatrix}
U & 0 & t & -t & 0 & 0 \\
0 & U & t & -t & 0 & 0 \\
t & t & 0 & 0 & 0 & 0 \\
-t & -t & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}
\]

\[
H'' = \begin{pmatrix}
U & 0 & \sqrt{2}t & 0 & 0 & 0 \\
0 & U & \sqrt{2}t & 0 & 0 & 0 \\
\sqrt{2}t & \sqrt{2}t & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}
\]

The eigenergies of \(U, \frac{U \pm \sqrt{U^2 + 16t^2}}{2}\) are zero, while other eigenergies are \(U, \frac{U \pm \sqrt{U^2 + 16t^2}}{2}\).

For \(|t|/U \rightarrow \infty\), the lowest energy state is singlet \(\frac{U - \sqrt{U^2 + 16t^2}}{2} \approx -\frac{4t^2}{U} < 0\) \(|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle)/\sqrt{2}\).
Conclusions:
- The system becomes insulating due to the on-site coupling despite of incompletely-filled conduction band!
- In the ground state, ions are half-filled; \( n_{i\uparrow} + n_{i\downarrow} \equiv n_{i} = 1 \) for all sites \( i \) and the Mott insulator is antiferromagnetically ordered with \( S=1/2 \).

\[ H_{\text{eff}} = -J \sum_{(ij)} s_i \cdot s_j \]

\[ J = -\frac{4t^2}{U} \quad \text{for} \quad U \gg t. \]

The name „kinetic exchange” follows from lowering the kinetic exchange of antiparallel spins in the singlet state relative to that of triplet states.

Note: More accurate **t-J model** of the Mott phase does not completely neglect hoping while it includes the contribution to \( J \)-constant from the intersite (direct) exchange (the later can be positive or negative).
Stoner mean-field approach to the Hubbard model

\[ H = - \sum_{ij} t_{ij} a^\dagger_{i\sigma} a_{j\sigma} + U \sum_i a^\dagger_{i\uparrow} a^\dagger_{i\downarrow} a_{i\downarrow} a_{i\uparrow} = - \sum_{ij} t_{ij} a^\dagger_{i\sigma} a_{j\sigma} + \frac{U}{2} \sum_{i\sigma_1\sigma_2} a^\dagger_{i\sigma_1} a^\dagger_{i\sigma_2} a_{i\sigma_2} a_{i\sigma_1} \]

\[ H = \sum_{k\sigma} \epsilon_k a^\dagger_{k\sigma} a_{k\sigma} + \frac{U}{2N} \sum_{k_1k_2q\neq 0} \sum_{\sigma_1\sigma_2} a^\dagger_{k_1+q,\sigma_1} a^\dagger_{k_2-q,\sigma_2} a_{k_2\sigma_2} a_{k_1\sigma_1}. \]

The \( q = 0 \) term has been omitted since it is canceled by the interaction of the electrons with the average potential of the nuclei.

\[ H \simeq H_{\text{Stoner}} := \sum_{k\sigma} \epsilon_k a^\dagger_{k\sigma} a_{k\sigma} - \frac{U}{2N} \sum_{k_1k_2} \sum_{\sigma} \left( n_{k_2\sigma} a^\dagger_{k_1\sigma} a_{k_1\sigma} + n_{k_1\sigma} a^\dagger_{k_2\sigma} a_{k_2\sigma} - n_{k_1} n_{k_2} \right) \]

\[ n_{k\sigma} := \langle a^\dagger_{k\sigma} a_{k\sigma} \rangle \]

\[ H_{\text{Stoner}} = \sum_{k\sigma} \epsilon_k a^\dagger_{k\sigma} a_{k\sigma} - \frac{U}{2N} (N_\uparrow - N_\downarrow) \sum_k (a^\dagger_{k\uparrow} a_{k\uparrow} - a^\dagger_{k\downarrow} a_{k\downarrow}) + \frac{U}{4N} (N_\uparrow - N_\downarrow)^2 - \frac{U}{4N} N_e^2 \]

\[ N_\sigma := \sum_k n_{k\sigma} \]

\[ N_e := N_\uparrow + N_\downarrow \]

\[ k_B \theta := \frac{N_e}{2N} U. \]
Stoner criterion of ferromagnetism

\[ E = \langle H_{\text{Stoner}} \rangle = N \int_{-\infty}^{E_F} d\epsilon \epsilon D\left(\epsilon + k_B\theta \frac{N_\uparrow - N_\downarrow}{N_e}\right) + N \int_{-\infty}^{E_F} d\epsilon \epsilon D\left(\epsilon - k_B\theta \frac{N_\uparrow - N_\downarrow}{N_e}\right) + \frac{k_B\theta}{2N_e}(N_\uparrow - N_\downarrow)^2 - \frac{k_B\theta}{2}N_e, \]

Hybrid: Fermi gas with on-site interactions

\[ D(\epsilon) = \frac{m^{3/2}}{(\sqrt{2}\pi^2\hbar^3)}\sqrt{\epsilon} \Theta(\epsilon) \]

\[ \frac{E}{N_e} = \frac{3}{5} \frac{E\text{para}}{2} \left[ (1 + \zeta)^{5/3} + (1 - \zeta)^{5/3} \right] - \frac{k_B\theta}{2} \zeta^2 - \frac{k_B\theta}{2} \]

\[ 0 = \frac{\partial}{\partial \zeta} \frac{E}{N_e} = \frac{E\text{para}}{2} \left[ (1 + \zeta)^{2/3} + (1 - \zeta)^{2/3} \right] - k_B\theta\zeta \]

\[ \frac{k_B\theta}{E\text{para}} \zeta = \frac{(1 + \zeta)^{2/3} - (1 - \zeta)^{2/3}}{2} \]

1. for \( k_B\theta/E\text{para} < 2/3 \): no intersection for \( \zeta \neq 0 \), the only solution is \( \zeta = 0 \), non-magnetic state,
2. \( 2/3 < k_B\theta/E\text{para} < 1/2^{1/3} \): intersection for \( 0 < |\zeta| < 1 \), partially polarized ferromagnetic state,
3. for \( k_B\theta/E\text{para} > 1/2^{1/3} \): One can see from \( E/N_e \) that the energy has a minimum at the edge \( |\zeta| = 1 \); the derivative does not vanish there. This is a completely polarized ferromagnetic state, i.e., only spin-up electrons are present.

Stoner criterion of ferromagnetism

(it leads to while not contradicting Mott-insulator condition)
There are examples for all three cases in real compounds:

1. Platinum belongs to the first case—the local Coulomb interaction is rather strong but not strong enough to cause ferromagnetism.

2. The ferromagnetic transition metals iron, cobalt, and nickel belong to this case. One has to keep in mind that the underlying Hubbard model is a caricature of real materials, though.

3. The compounds CrO₂ and EuB₆ are completely polarized ferromagnetic metals.
Susceptibility and excitations
Susceptibility of Pauli paramagnet

The single-particle energy

\[ e_{\sigma} = \frac{\hbar^2 k^2}{2m} + \sigma \frac{g \mu_B B}{2} \quad \text{with } \sigma = \uparrow, \downarrow = \pm 1 \]

and the magnetization

\[ M = -\frac{g \mu_B}{2V} \sum_{\sigma} n_F (e_{\sigma} - \mu) \]

lead to the static susceptibility

\[ \chi = \frac{\partial M}{\partial B} \bigg|_{B=0} = -\frac{g \mu_B}{2V} \sum_{\sigma} n_F \left( \frac{\hbar^2 k^2}{2m} - \mu \right) \sigma \frac{g \mu_B}{2} = -\frac{g^2 \mu_B^2}{4V} \sum_{k} n_F \left( \frac{\hbar^2 k^2}{2m} - \mu \right) \]

\[ = -\frac{g^2 \mu_B^2}{2} \int d\epsilon D(\epsilon) n_F (\epsilon - \mu) \quad D(\epsilon) = \frac{1}{V} \sum_k \delta(\epsilon - \hbar^2 k^2/2m) \]

and, with \( n_F (\epsilon) \approx -\delta(\epsilon) \) (\( T \to 0 \)), to

"Dynamic susceptibility" is found via including just one Fourier mode of the field, that leads to the single-particle states

For \( q \neq 0 \), the first order correction

\[ |k\sigma(1)\rangle = \sum_{k\sigma^{'}} \frac{1}{\Sigma_{k\sigma} - \Sigma_{k\sigma^{'}}} |k\sigma^{'}, k\sigma\rangle = \sigma \frac{g \mu_B B_q}{2} \frac{m}{\hbar^2} \sum_{k} \left( \frac{|k\sigma^{'})|}{2m} \cos q \cdot r \right) \]

\[ = \sigma \frac{g \mu_B B_q}{2} \frac{m}{\hbar^2} \sum_{k} \left( \frac{|k\sigma^{'})|}{2m} \cos q \cdot r \right) \]

provides the non-zero magnetization

\[ M_q = M(q, \omega = 0) = -\frac{g \mu_B}{2V} \sum_{k \sigma} \langle k \sigma | + \langle 1 \rangle | k \sigma \rangle \rangle \cos q \cdot r \langle k \sigma | + \langle 1 \rangle | k \sigma \rangle \rangle n_F (e_{\sigma} - \mu) \]

\[ \approx \frac{g^2 \mu_B^2 B_q}{2V} \frac{m}{\hbar^2} \sum_{k} \left( \frac{1}{q^2 + 2k \cdot q - q^2} \right) n_F (e_{\sigma} - \mu) = \frac{g^2 \mu_B^2 B_q}{2V} \frac{m}{\hbar^2} \int_{-\infty}^{\infty} dk \left( \frac{1}{q^2 + 2k \cdot q - q^2} \right) \ln \left( \frac{2k + q}{2k - q} \right) \]

which leads to the \( \omega \to 0 \) limit of the dynamic susceptibility

\[ \chi_q = \frac{M_q}{B_q} = \frac{g^2 \mu_B^2 m k_f}{8\pi^2} f \left( \frac{q}{2k_f} \right) = \frac{1}{2} \chi_{\text{Pauli}} f \left( \frac{q}{2k_f} \right) \quad f(x) = 1 + \frac{1 - x^2}{2x} \ln \left| \frac{1 + x}{1 - x} \right| \]
Static susceptibility of Stoner magnet

The single-particle energy in the mean-field approximation

\[ \epsilon_{k\sigma} = \epsilon_k - \sigma k_B \theta \zeta + \sigma \frac{g \mu_B B}{2} \]

and the magnetization

\[ M = -\frac{g \mu_B}{2V} \sum_{k\sigma} \sigma n_F (\epsilon_{k\sigma} - \mu) \]

lead, via the substitution

\[ \zeta = -\frac{2V}{g \mu_B} \frac{X_B}{N_e} \]

to the self-consistent susceptibility equation

\[ \chi = \frac{\partial M}{\partial B} \bigg|_{B=0} = -\frac{g \mu_B}{2V} \sum_{k\sigma} \sigma n_F \left( \frac{\hbar^2 k^2}{2m} - \mu \right) \sigma \frac{g \mu_B}{2} \left( 1 + \frac{k_B \theta}{N_e} \frac{4V}{g^2 \mu_B^2} \chi \right) \]

\[ = \chi_{\text{Pauli}} \left( 1 + \frac{k_B \theta}{N_e} \frac{4V}{g^2 \mu_B^2} \chi \right) = \chi_{\text{Pauli}} \left( 1 + \frac{2V}{N} \frac{U}{g^2 \mu_B^2} \chi \right) \]

Its solution is

\[ \chi = \frac{\chi_{\text{Pauli}}}{1 - \frac{2V}{N} \frac{U}{g^2 \mu_B^2}} \]
Stoner excitations and dynamic susceptibility of ferromagnet

Within the mean-field--random-phase approximation, the excitation energy is equal to

\[ \varepsilon_{k+q} - \varepsilon_k + 2k_B \theta \zeta = \frac{\hbar^2}{m} k \cdot q + \frac{\hbar^2 q^2}{2m} + 2k_B \theta \zeta \]

Proof:

\[
\begin{align*}
H_{\text{Stoner}} a_{k+q,\uparrow}^\dagger a_{k,\uparrow} |GS\rangle &= (E_{\text{GS}} + \varepsilon_{k+q} - \varepsilon_k + 2k_B \theta \zeta) a_{k+q,\uparrow}^\dagger a_{k,\uparrow} |GS\rangle \\
H_{\text{Stoner}} a_{k+q,\downarrow}^\dagger a_{k,\downarrow} |GS\rangle &= [H_{\text{Stoner}}, a_{k+q,\downarrow}^\dagger a_{k,\downarrow}] + E_{\text{GS}} a_{k+q,\downarrow}^\dagger a_{k,\downarrow} |GS\rangle \\
[H_{\text{Stoner}}, a_{k+q,\downarrow}^\dagger a_{k,\downarrow}] &= \sum_{k'} \left\{ (\varepsilon_{k'} - k_B \theta \zeta) \left[ a_{k',\uparrow}^\dagger a_{k',\uparrow}, a_{k+q,\downarrow}^\dagger a_{k,\downarrow} \right] + (\varepsilon_{k'} + k_B \theta \zeta) \left[ a_{k',\downarrow}^\dagger a_{k',\downarrow}, a_{k+q,\uparrow}^\dagger a_{k,\uparrow} \right] \right\} \\
&= (\varepsilon_k + k_B \theta \zeta) a_{k+q,\uparrow}^\dagger a_{k,\uparrow}
\end{align*}
\]

The distribution functions for particles of plus or minus spin are different (the bands are considerably shifted, even at zero external field)

Random-phase approximation (RPA) is the assumption of negligibility of the field-fluctuations (field-oscillations) contribution to the single-particle energies
Let the effective field contain the „molecular“ (mean-field) part and the time dependence of the driving field is included via

\[ \zeta_g = - \frac{2V}{g \mu_B} \frac{\chi_1 B_q}{N_e} \]

\[ \cos q \cdot r \rightarrow \cos (q \cdot r + \omega t) \]

Within the RPA approximation we modify the calculation of the dynamic susceptibility of the Pauli paramagnet

\[
|k\sigma|^{(1)} = \left( -\sigma k_B \theta \zeta_g + \sigma \frac{g \mu_B B_q}{2} \right) \frac{m}{\hbar^2} \left( \frac{|k+q,\sigma|}{-2\omega \frac{m}{\hbar} - 2k \cdot q - q^2 - 2k_B \theta \zeta_g \frac{m}{\hbar^2}} + \frac{|k-q,\sigma|}{2\omega \frac{m}{\hbar} + 2k \cdot q - q^2 - 2k_B \theta \zeta_g \frac{m}{\hbar^2}} \right)
\]

\[
M(q,\omega) \approx -\frac{g \mu_B}{2V} \sum_{k\sigma} (|k\sigma| + |(k\sigma)|) \sigma \cos q \cdot r (|k\sigma| + |k\sigma|^{(1)}) n_F(\epsilon_k - \mu)
\]

\[
= \left( k_B \theta \frac{4V}{g^2 \mu_B^2} \frac{\chi(q,\omega)}{N_e} + 1 \right) \chi_0(q,\omega) B(q,\omega) = \chi(q,\omega) B(q,\omega)
\]

\[
\chi(q,\omega) = \frac{\chi_0(q,\omega)}{1 - k_B \theta \frac{4V}{g^2 \mu_B^2} \frac{\chi_0(q,\omega)}{N_e}} = \frac{\chi_0(q,\omega)}{1 - \frac{2V}{N} \frac{U}{g^2 \mu_B^2} \chi_0(q,\omega)} := \chi_{\text{RPA}}(q,\omega)
\]

relates to the spin-wave poles, for \( \omega \ll \epsilon_F, \ q \ll q_F, \ 2\omega/\sqrt{q_F} \ll 1 \), of the dispersion \( \hbar \omega_q = Dq^2 - O(q^4) \),

\[
D = \frac{U}{3N} \sum_k \left\{ f_k^+ \frac{f_k^+}{4k_B \theta \zeta} \nabla_k^2 \epsilon_k - \frac{f_k^+ - f_k^+}{(2k_B \theta \zeta)^2} \nabla_k^2 \epsilon_k \right\}^2
\]

(Izuyama, Kubo, 1964)
Excitations in the itinerant ferromagnet

- Spin waves: the flip of an electron spin is connected to the creation of the electron-hole pair (exciton) that prevents change of the electron band
- Stoner excitations: the flip of an electron spin is accompanied by change of the band, however, with change of the electron wavevector as well
The band picture - summary

\[ M = \mu_B (N_\uparrow - N_\downarrow) = 2\mu_B \rho(E_F) \delta \varepsilon \]

Decrease of magnetic energy: \[ E_M = Un_\uparrow n_\downarrow = U \frac{N^2}{4} - U \rho(E_F)^2 (\delta \varepsilon)^2 \]

Increase of kinetic energy: \[ \Delta E_C = \rho(E_F) (\delta \varepsilon)^2 \]

Zeeman energy: \[ E_Z = -\overrightarrow{M} \cdot \overrightarrow{B} = -2\mu_B \rho(E_F) B \delta \varepsilon \]

\[ \Delta E_{total} = \left( \frac{M}{2\mu_B \rho(E_F)} \right)^2 \rho(E_F)(1 - U \rho(E_F)) - MB \]

Resulting magnetic moment: \[ M = \frac{2\mu_B^2 \rho(E_F)}{1 - U \rho(E_F)} B \]

Susceptibility: \[ \chi = \frac{X_{\text{Pauli}}}{1 - U \rho(E_F)} \]

Here \( \rho(\mu) = \frac{V}{N} D(\mu) \) is the genuine density of states. Hence, the susceptibility is calculated per lattice cell.
Motivation from chromium: the „antiferromagnetic“ state \( T_N = 311\text{K} \) of Cr exists despite lack of localized magnetic momenta (purely-itinerant antiferromagnet) and without superexchange interactions (typical for antiferromagnetic Mott-insulator phase). Additionally, in the „antiferromagnetic“ state of Cr, 4% of the Fermi surface is truncated by an energy gap.

Explanation on the basis of 1D case

When the Fermi surface is not spherical, the paramagnetic susceptibility can be singular at \( q = 2k_F \). This results in an instability of the paramagnetic state!

Whereas the susceptibility of the Pauli paramagnet is not singular, the interaction-enhanced susceptibility (per lattice cell can be singular, and then

\[
\chi(q) = \frac{\chi_0(q)}{1 - U\chi_0(q)/2\mu_B^2}
\]

Consider 1D case;

\[
\chi_0(2k_F, T) = 2\mu_B^2 n(\varepsilon_F) \ln(\varepsilon_0/kT)
\]

with \( \varepsilon_0 \) a cutoff energy, of the order of the Fermi energy \( \varepsilon_F \).

In order to avoid the susceptibility discrepancy, the system must undergo a phase transition at the temperature

\[
k_B T_{SDW}^{MF} = \varepsilon_F \exp \left[ -\frac{1}{\lambda} \right], \quad \lambda = U n(\varepsilon_F)
\]

Note, the exponential dependence of transition temperature is typical for energy-gapped systems.
Since, below the transition point, the dominant contribution to the spin density is periodic in space with the wavevector $2k_F$, the effective (mean-field-Hubbard) Hamiltonian reads

$$H_{\text{MF}} = \sum_{k\sigma} \varepsilon_k a_{k\sigma}^\dagger a_{k\sigma} + \frac{2N}{U} |\Delta|^2 + \left\{ \sum_k \Delta e^{i\phi}(a_{k+2k_F,\uparrow}^\dagger a_{k,\uparrow} + a_{k+2k_F,\downarrow}^\dagger a_{k,\downarrow}) + \text{H.c.} \right\}$$

where

$$\Delta e^{i\phi} = \frac{U}{N} S, \quad \langle S(x) \rangle = 2|S| \cos(2k_F x + \phi) = \frac{\langle \mu \rangle}{g\mu_B}$$

Its diagonalization gives

$$H = \sum_{k,\sigma} E_k \gamma_{k\sigma}^\dagger \gamma_{k\sigma} + 2N |\Delta|^2 \frac{U}{U}, \quad E_k = \varepsilon_F + \text{sgn}(|k| - k_F) [\hbar^2 V_F^2 (|k| - k_F)^2 + |\Delta|^2]^{1/2}$$

The second term of $E_k$ relates to the ground-state energy shift

$$E = -\frac{1}{2} n(\varepsilon_F) |\Delta|^2$$

The spin-up(-down) densities are

$$\rho_{\uparrow}(x) = \rho_0 \left[ 1 + \frac{\Delta}{V_F k_F \lambda} \cos(2k_F x + \phi) \right],$$

$$\rho_{\downarrow}(x) = \rho_0 \left[ 1 + \frac{\Delta}{V_F k_F \lambda} \cos(2k_F x + \phi + \pi) \right]$$

They lead to the spin density $\rho_{\uparrow}(x) - \rho_{\downarrow}(x)$ and a constant chargé density $\rho_{\uparrow} + \rho_{\downarrow} = \rho_0$

1D model of SDW ordering is well verified with organic magnetic conductors, see G. Gruner, Rev. Mod. Phys. 66, No 1, (1994)
SDW structure of Cr

FIG. 91. Neutron diffraction peaks expected for commensurate antiferromagnetism and for the transverse and longitudinal SDW in chromium. The diagrams at (a) represent the magnetic structures $\text{AF}_0$, $\text{AF}_1$, $\text{AF}_2$ which occur in Cr. The arrows show the directions and approximate magnitudes of the magnetic moments. The resulting density in reciprocal space in the neighborhood of the point (100) is shown at (b) for each of the structures. The symbol $\bigcirc$ indicates a peak of half the intensity of peaks marked $\bullet$, bearing in mind the available spin directions for the various domains. The curves (c) show, in each case, the shape of the peaks that would occur in the neutron-diffraction pattern, in the neighborhood of the (100) position, for a polycrystalline sample (after Bacon and Cowlam, 1969).

FIG. 93. The effect of annealing on the magnetic phase diagram deduced from the experimental observations for coarse powders of Cr. The initial diagram (a) is contrasted with (b), after annealing at 600°C, and (c), after annealing at 1000°C. Diagram (c) is approaching the behavior found in single-crystal Cr, for which the phase diagram is shown at (d) (after Bacon and Cowlam, 1969).