2022.7.6 Lecture 13

10:25 – 11:55

Lecture on

Magnetic Properties of Materials

磁性 (Magnetism)

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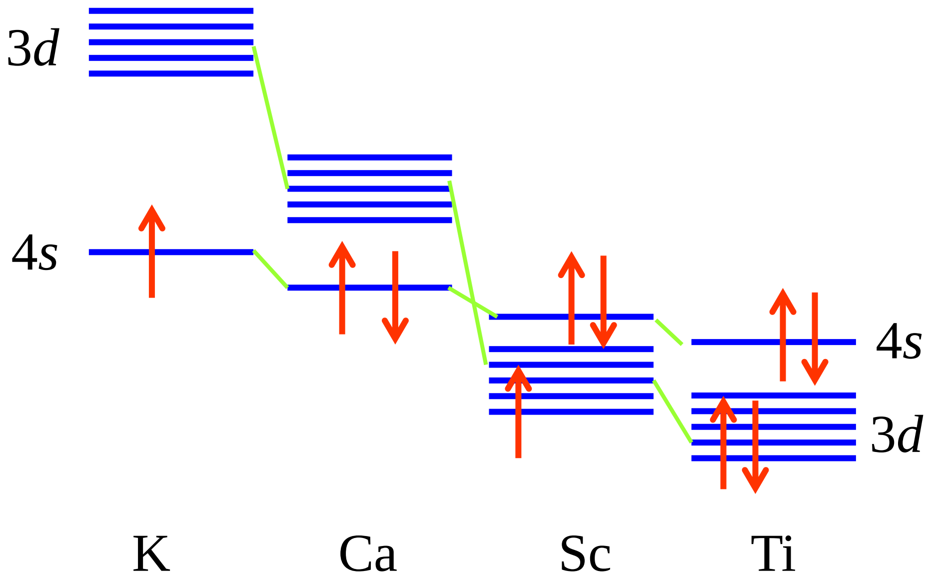
Chapter 6 Magnetism of Itinerant Electron Systems

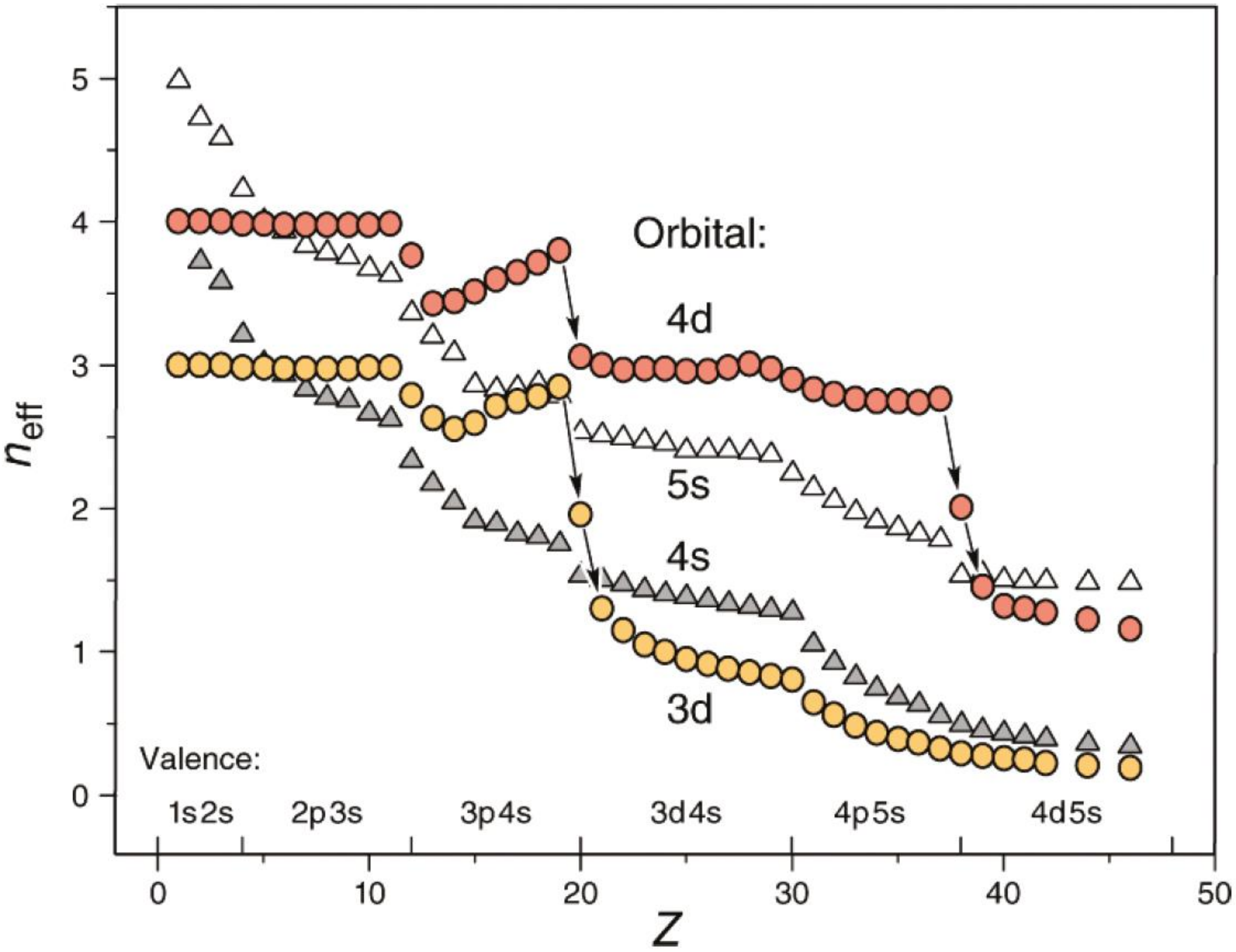
- Ferromagnetism in Electron gas
  - Hartree-Fock approximation
  - Diffusion Monte-Carlo calculation
- Hubbard model: mean field theory
  - Hartree-Fock approximation: Stoner criterion
  - Magnetic susceptibility
- Magnetism in 3*d* transition metals
  - Slater-Pauling's curve
  - Density of states by APW method

Outline

- Magnetism in 3*d* transition metals
  - Slater-Pauling's curve
  - Density of states by APW method
- Kubo formula (linear response)
- Fluctuation dissipation theorem
- Random phase approximation (RPA)

3*d* and 4*s* electrons in isolated transition metal atoms

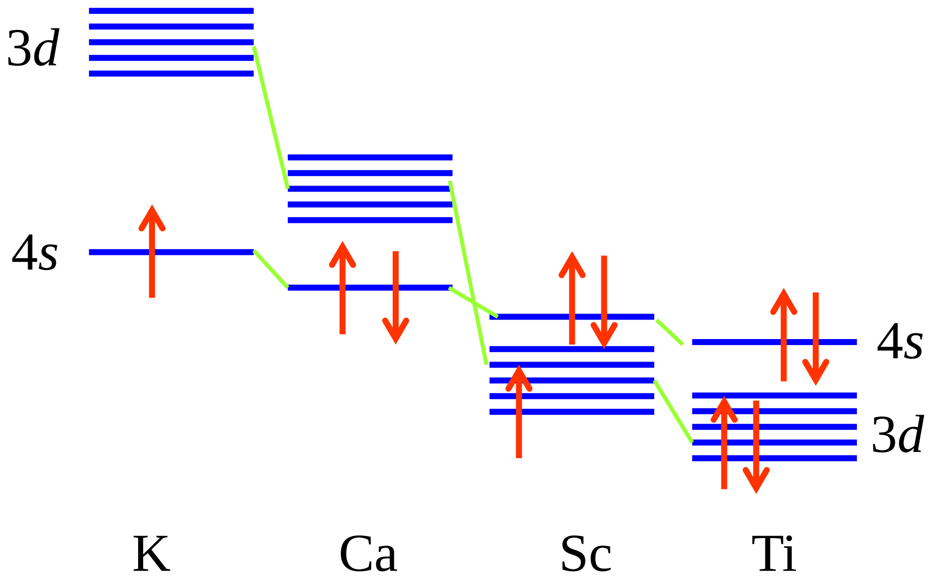


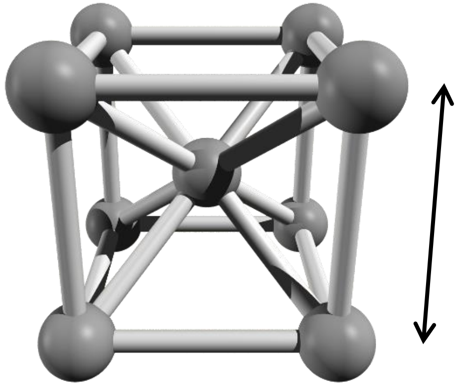


Radial wavefunction

$$\begin{cases} |4s\rangle \propto R_{40}(r) \propto \exp\left(-\dfrac{r}{4a_{\mathrm{B}}}\right) \\ |3d\rangle \propto R_{32}(r) \propto \left(\dfrac{r}{r_{\mathrm{B}}}\right)^2 \exp\left(-\dfrac{r}{3a_{\mathrm{B}}}\right) \end{cases}$$

3*d* and 4*s* electrons in isolated transition metal atoms





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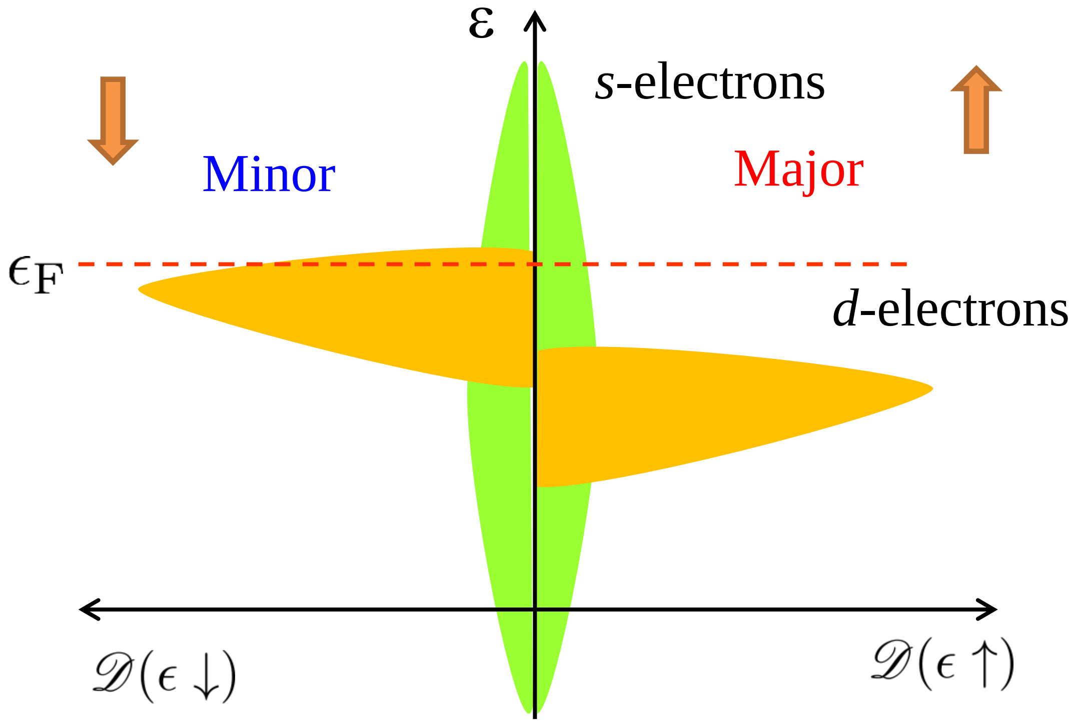
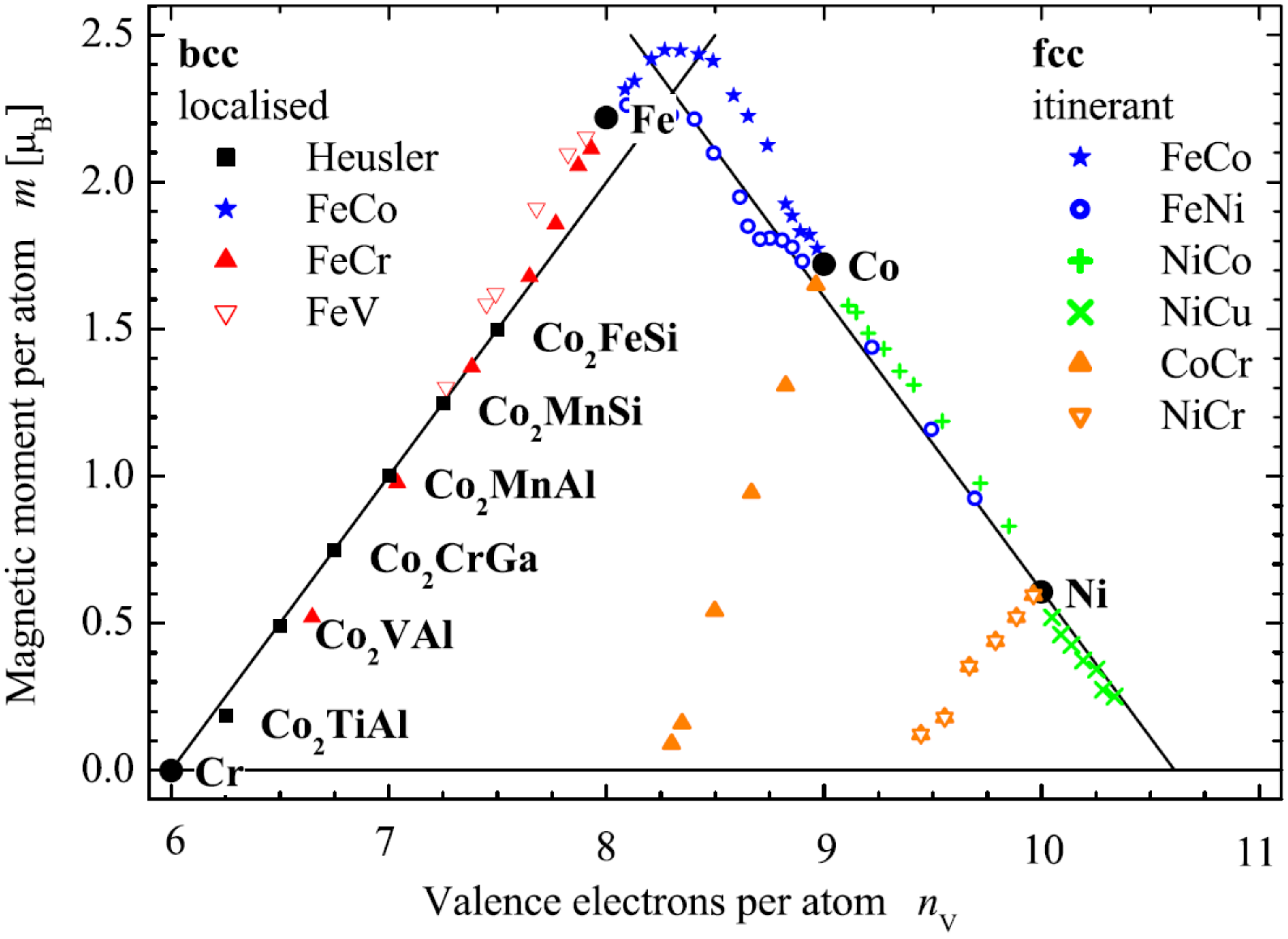
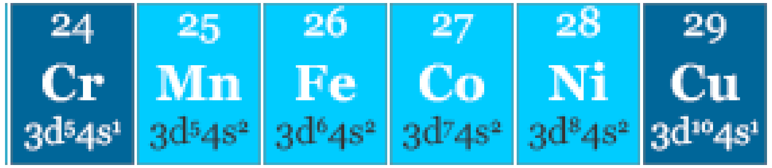


Magnetism of 3*d* transition metals: Slater-Pauling's curve



Balke et al., Sci. Technol. Adv. Mater. **9**, 014102 (2008).



Slater-Pauling's curve

Experimental data are in line.

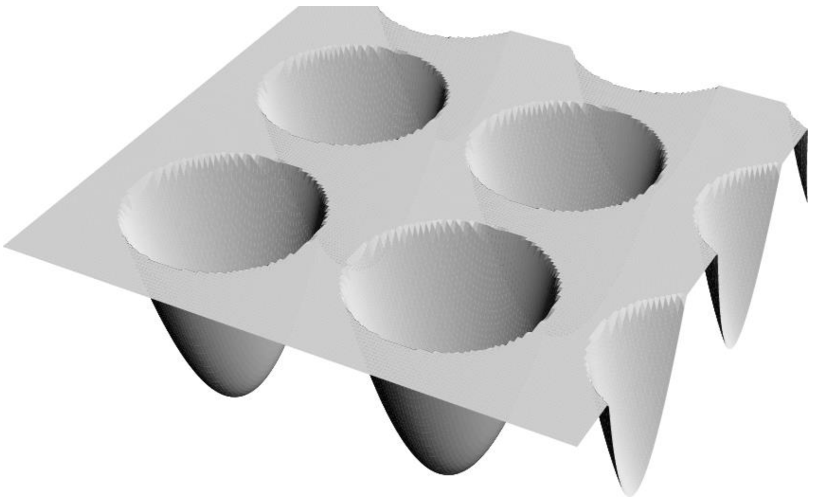
The gradient is ± 1 !

Abrupt change around Fe

APW method to calculate DOS

$$\mathscr{H}\phi(\boldsymbol{r}) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{r})\right]\phi(\boldsymbol{r}) = E\phi(\boldsymbol{r})$$

Muffin-tin potential: $V(\boldsymbol{r}) = \begin{cases} V_{\mathrm{a}}(r) \ \ (\text{spherical}) & (r < r_{\mathrm{c}}) \\ V_{\mathrm{o}} \ (= V_{\mathrm{a}}(r_{\mathrm{c}}):\ \text{const.}) & (r \geq r_{\mathrm{c}}) \end{cases}$



Muffin-tin potential

Hartree: $V_{\mathrm{d}}(\boldsymbol{r}) = \sum_i \langle\phi_i(\boldsymbol{r}')| \frac{e^2}{|\boldsymbol{r}-\boldsymbol{r}'|} |\phi_i(\boldsymbol{r}')\rangle$

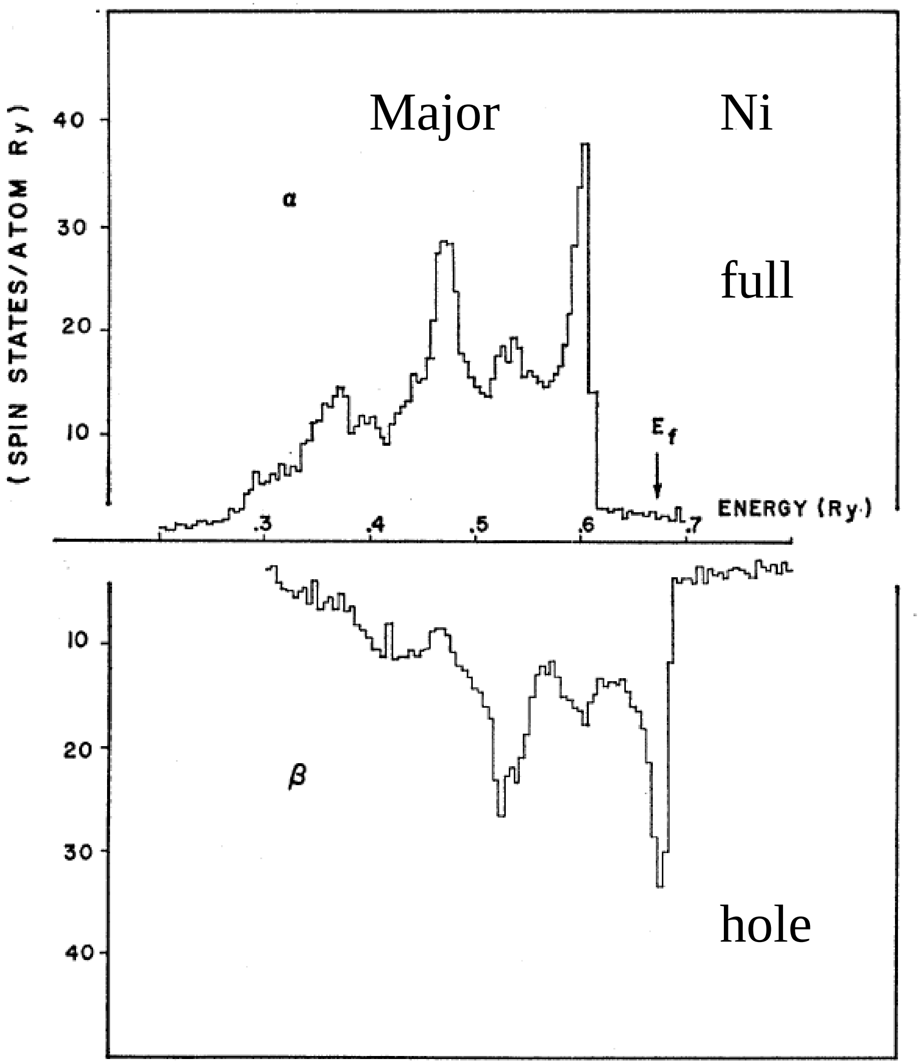
Exchange: $V_{\mathrm{ex}\uparrow} = -3e^2\left(\frac{3}{4\pi}\right)^{1/3} \rho_{\uparrow}(\boldsymbol{r})^{1/3}$

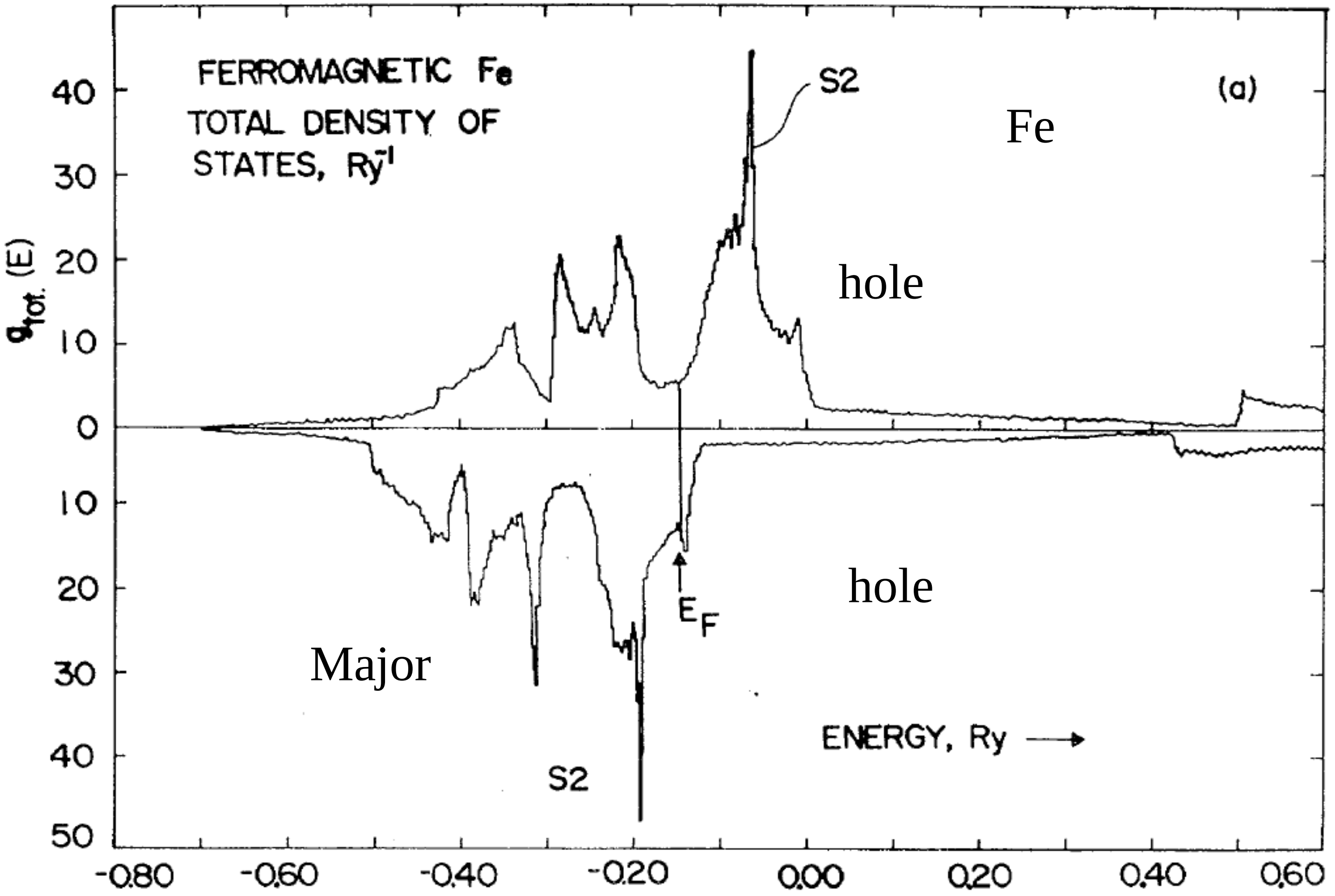
Variational wavefunction: $\Phi_{\mathrm{vr}}(\boldsymbol{r}) = \begin{cases} \sum_{l,m} A_{lm}R_l(r)Y_l^m(\theta,\varphi) & r < r_{\mathrm{c}}, \\ \sum_{n=0}^{N} B_n \exp[i(\boldsymbol{k}+\boldsymbol{K}_n)\cdot\boldsymbol{r}] & r > r_{\mathrm{c}} \end{cases}$

⇓

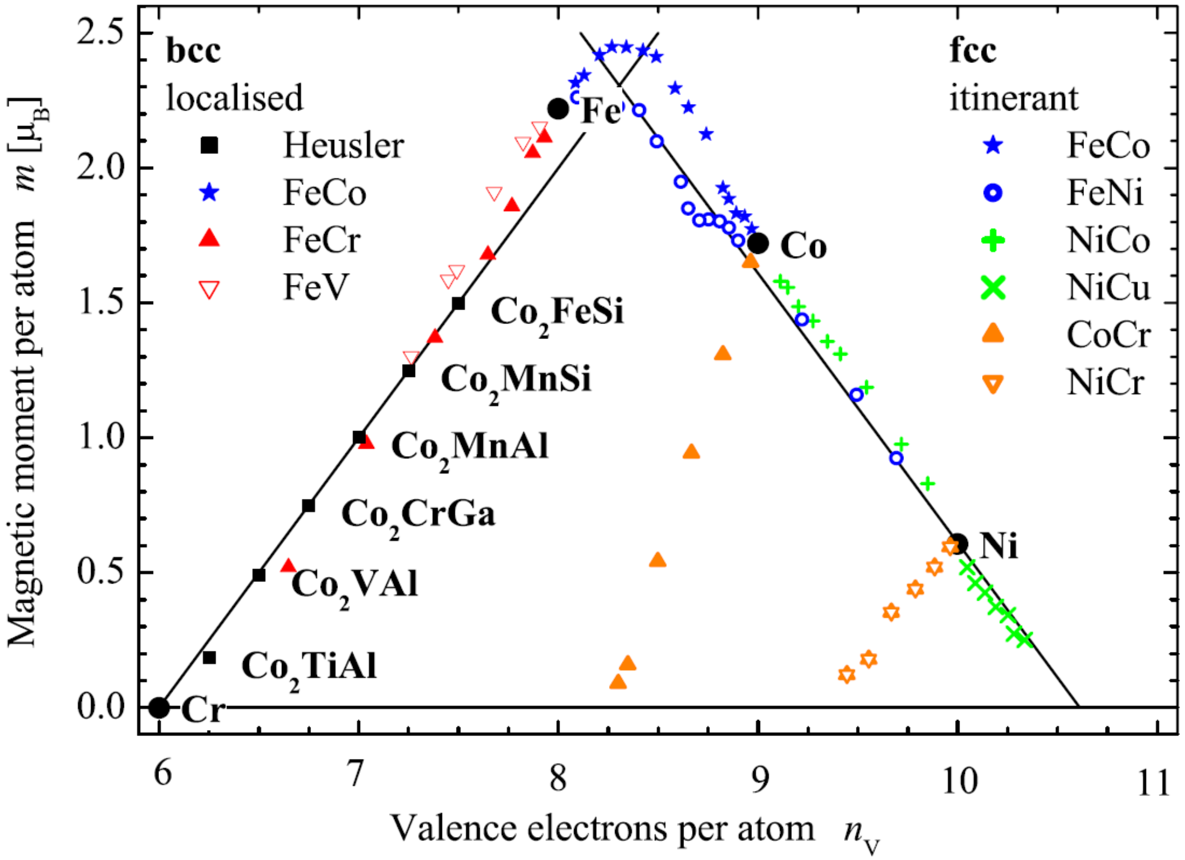
Iteration for convergence for each ***k***

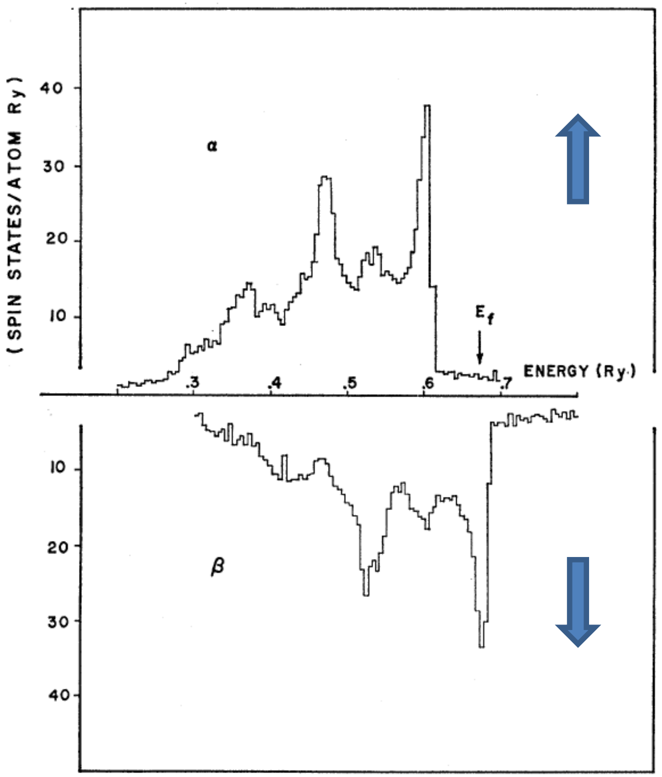
Density of states in Ni and Fe





Explanation of Slater-Pauling's curve (1)





Case of Ni

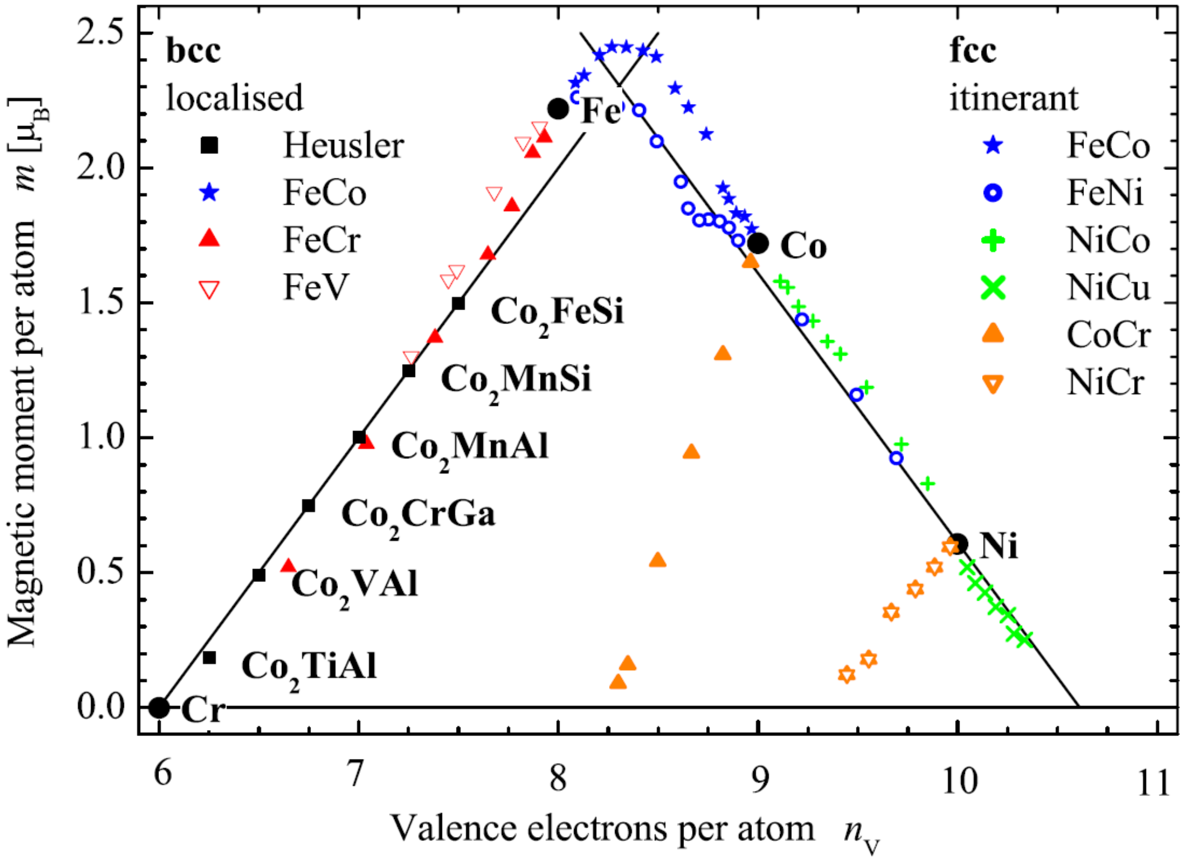
$3d\uparrow$: full 5 electrons

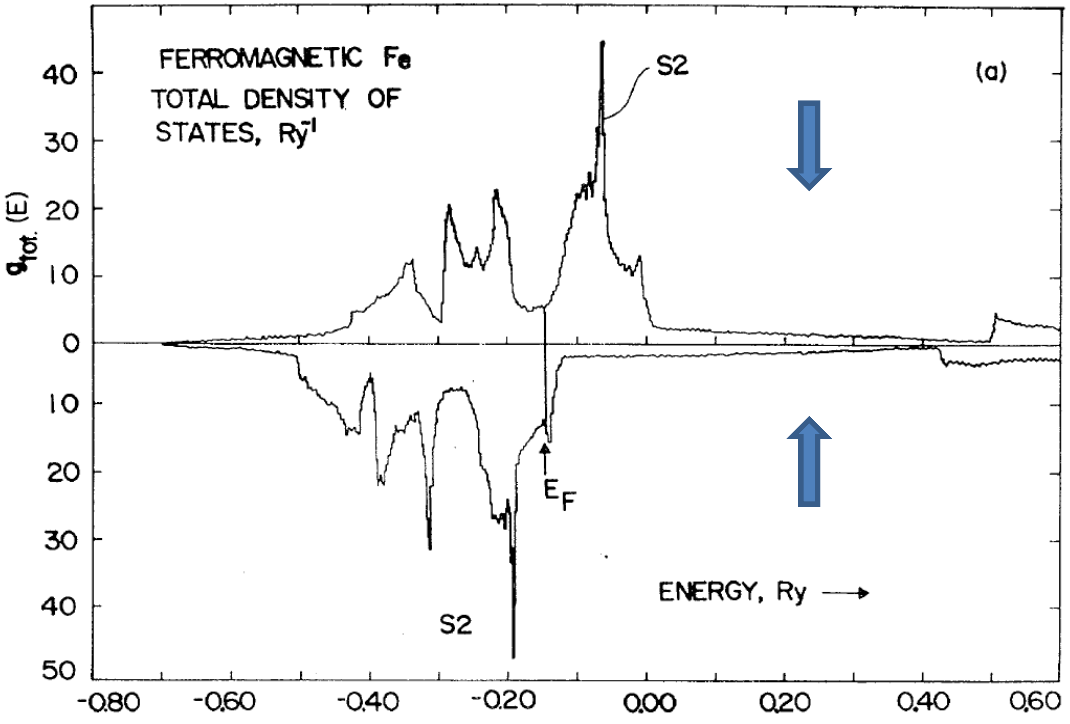
$3d\downarrow$: 4.4 electrons

Increase of electrons → filling up the holes and the magnetic moment decreases

Decrease of electrons → opening holes in $3d\downarrow$ and the magnetic moment increases

Explanation of Slater-Pauling's curve (2)





Case of Fe $3d\downarrow$: 2.5 electrons

$3d\uparrow$: 4.7 electrons (not full, hole exists)

Increase of electrons → filling up the holes in ↑ and the magnetic moment increases

After complete filling up of ↑ → filling up the holes in ↓ and the magnetic moment decreases

Magnetic susceptibility in HF approximation

Magnetic moment: $$M = \frac{g\mu_{\mathrm{B}}}{2}\sum_i [\langle n_{i\uparrow}\rangle - \langle n_{i\downarrow}\rangle] = \frac{g\mu_{\mathrm{B}}}{2}\sum_i n_{i-}$$

Magnetic susceptibility per atom: $$\chi = \frac{M}{NB} = \frac{g\mu_{\mathrm{B}}}{2}\frac{n_-}{B}$$

Electron energy in magnetic field: $$E_B = E(0) + E_2 n_-^2 - N\frac{g\mu_{\mathrm{B}}}{2}Bn_-$$

where $$E_2 = \frac{1}{2}\frac{d^2(\Delta E)}{dn_-^2}$$ with $$\Delta E = \frac{N}{4}\left[\frac{m^2}{\mathscr{D}(E_{\mathrm{F}})} - Um^2\right]$$

This should be positive for the appearance of ferromagnetism. (remember GL theory).

Then minimization of E_B should give n_- as $$\chi = \frac{(g\mu_{\mathrm{B}})^2 N}{4E_2}$$

We finally obtain $$\chi = \left(\frac{g\mu_{\mathrm{B}}}{2}\right)^2 \frac{\mathscr{D}(E_{\mathrm{F}})}{1 - U\mathscr{D}(E_{\mathrm{F}})} = \frac{\chi_{\mathrm{Pauli(a)}}}{1 - U\mathscr{D}(E_{\mathrm{F}})}$$

Stoner factor

Temperature dependence of susceptibility in HF approximation

By using the identity for degenerated Fermi gas:
$$\mu = \mu_0 \left[1 - \frac{\pi^2}{6} \frac{d\log \mathscr{D}(\mu_0)}{d\log \mu_0} \left(\frac{k_B T}{\mu_0}\right)^2 + \cdots \right]$$

we write
$$\delta\mu = -\frac{\pi^2 \mathcal{D}'_F}{6\mathcal{D}_F}(k_B T)^2 \qquad d\mathscr{D}(E)/dE|_{E=E_F} \to \mathcal{D}'_F$$

By defining
$$A = \frac{\pi^2}{6}\left(\frac{(\mathcal{D}'_F)^2}{\mathcal{D}_F} - \mathcal{D}''_F\right)$$

Susceptibility with temperature correction:
$$\chi = \left(\frac{g\mu_B}{2}\right)^2 \frac{\mathscr{D}(E_F)}{1 - U\mathscr{D}(E_F) + UA(k_B T)^2}$$

⇒
$$\chi = \frac{C}{T^2 - T_C^2}$$

This is not Curie-Weiss observed in experiments.

Kubo formula

Dynamical response to magnetic field $\mathscr{H}_0 + \underline{\mathscr{H}_{\text{ext}}(t)}$ Time-dependent perturbation

Heisenberg equation of motion $i\hbar \dfrac{\partial \rho}{\partial t} = [\mathscr{H}_0 + \mathscr{H}_{\text{ext}}(t), \rho(t)]$

Single body density matrix: $\rho(x, x') = \sum_{i=1}^{N} \varphi_{k_i}^*(x) \varphi_{k_i}(x')$

Initial condition: $t = -\infty$ $\rho(-\infty) = \rho_{\text{eq}} = \dfrac{1}{Z_0} \exp\left(-\dfrac{\mathscr{H}_0}{k_{\text{B}} T}\right)$

Unperturbed system partition function: $Z_0 = \text{Tr}[\exp(-\mathscr{H}_0 / k_{\text{B}} T)]$

Then the density matrix should satisfy (see lecture note for the calculation)

$$\rho(t) = \rho_{\text{eq}} + \frac{1}{i\hbar} \int_{-\infty}^{t} dt' [U_0(t-t') \mathscr{H}_{\text{ext}}(t') U_0^{-1}(t-t'), U_0(t-t') \rho(t') U_0^{-1}(t-t')]$$

$$= \rho_{\text{eq}} + \frac{1}{i\hbar} \int_{-\infty}^{t} dt' U_0(t-t') [\mathscr{H}_{\text{ext}}(t'), \rho(t')] U_0^{-1}(t-t')$$

where

$$U_0(t) \equiv \exp\left(\frac{\mathscr{H}_0}{i\hbar} t\right)$$

Kubo formula (2)

For linear response we can replace $\rho(t') \to \rho_{\mathrm{eq}}$ made of eigenstates of unperturbed Hamiltonian

Then we can write $$\rho(t) \simeq \rho_{\mathrm{eq}} + \frac{1}{i\hbar}\int_{-\infty}^{t} dt' [U_0(t-t')\mathscr{H}_{\mathrm{ext}}(t')U_0^{-1}(t-t'), \rho_{\mathrm{eq}}]$$

External field $\mathscr{H}_{\mathrm{ext}}(t) = -PF(t)$

Expectation value of general physical quantity Q $$\langle Q(t)\rangle = \mathrm{Tr}\{\rho(t)Q\} = \langle Q_{\mathrm{eq}}\rangle + \frac{1}{i\hbar}\int_{-\infty}^{t} dt' \, \langle [P, Q(t-t')]\rangle \, F(t')$$

where $\langle Q_{\mathrm{eq}}\rangle = \mathrm{Tr}\{\rho_{\mathrm{eq}} Q\}, \quad Q(t) = U_0(t)^{-1} Q U_0(t)$

$\langle [P, Q(t-t')]\rangle$ is a pure imaginary.

Field with frequency ω $F(t) = F_0 \cos(\omega t) = \mathrm{Re}[F_0 e^{-i\omega t}]$

Definition of susceptibility $\chi(\omega)$ $\Delta Q(t) = \langle Q(t)\rangle - \langle Q_{\mathrm{eq}}\rangle = \mathrm{Re}[\chi(\omega) F_0 e^{-i\omega t}]$

We can equalize this with $$\Delta Q(t) = \frac{1}{i\hbar}\int_{-\infty}^{t} dt' \, \langle [P, Q(t-t')]\rangle \, \mathrm{Re}[F_0 e^{-i\omega t'}]$$

Kubo formula (3)

Definition of susceptibility $\chi(\omega)$ $\Delta Q(t) = \langle Q(t) \rangle - \langle Q_{\text{eq}} \rangle = \text{Re}[\chi(\omega) F_0 e^{-i\omega t}]$

We can equalize this with $\Delta Q(t) = \frac{1}{i\hbar} \int_{-\infty}^{t} dt' \, \langle [P, Q(t-t')] \rangle \, \text{Re}[F_0 e^{-i\omega t'}]$

The first equation → $\text{Re}[\chi(\omega) F_0 e^{-i\omega t}] = \frac{F_0}{2} [\chi^*(\omega) e^{i\omega t} + \chi(\omega) e^{-i\omega t}]$

The second equation → $\frac{F_0}{2i\hbar} \left\{ \left[\int_0^{\infty} d\tau \, \langle [P, Q(\tau)] \rangle \, e^{-i\omega\tau} \right] e^{i\omega t} + \left[\int_0^{\infty} d\tau \, \langle [P, Q(\tau)] \rangle \, e^{i\omega\tau} \right] e^{-i\omega t} \right\}$

$\tau = t - t'$

Kubo formula $\chi_{QP}(\omega) = \frac{i}{\hbar} \int_0^{\infty} \langle [Q(\tau), P] \rangle \, e^{i\omega\tau} d\tau$

Fluctuation-dissipation theorem

Green's function $G^{\pm}_{QP}(t) = \mp\frac{i}{\hbar}\theta(\pm t)\left\langle [Q(t), P] \right\rangle$ (+: retarded, –: advanced)

$$\theta(t) = \begin{cases} 1 & (t \geq 0) \\ 0 & (t < 0) \end{cases}$$ Heaviside function

Kubo formula is re-written as: $\chi_{QP}(\omega) = -\mathcal{G}^{+}_{QP}(\omega) = -\mathscr{F}_{\omega}\{G^{+}_{QP}(t)\}$

Fourier transform to ω-space

$$\mathcal{S}_{QP}(\omega) = \int_{-\infty}^{\infty} dt \left\langle Q(t), P \right\rangle e^{i\omega t}$$

Correlation function

Fluctuation-dissipation theorem:

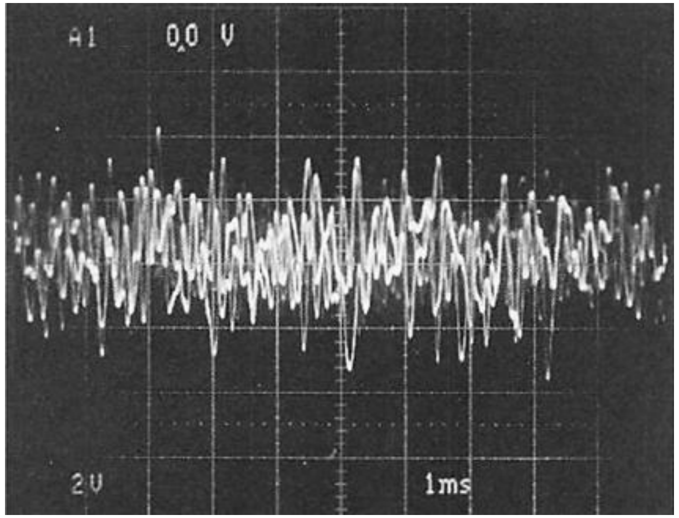
$$\mathcal{S}_{QP}(\omega) = \frac{i}{1 - e{-}\beta\hbar\omega}[\mathcal{G}^{+}_{QP}(\omega) - \mathcal{G}^{-}_{QP}(\omega)]$$

See the lecture note for the calculation

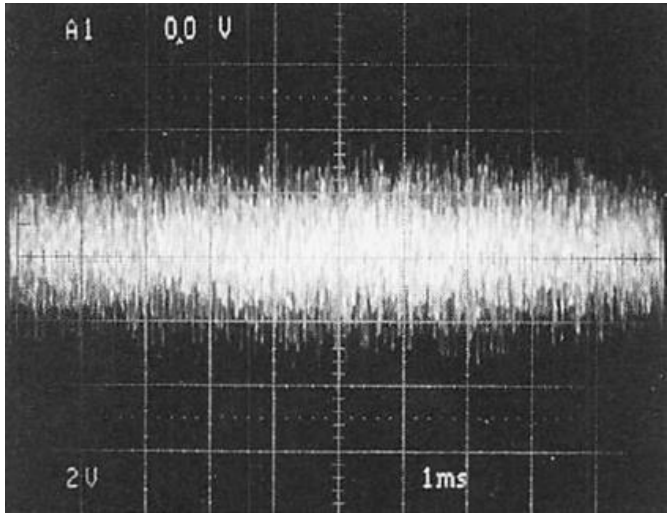
Example of fluctuation-dissipation theorem

$$G_{\rm v}(\omega) = 4k_{\rm B}T{\rm Re}[Z(i\omega)]$$
$$= 4k_{\rm B}TR$$

Johnson-Nyquist noise
Thermal noise



Low pass 5 kHz



100 kHz

Random phase approximation (RPA)

External magnetic field: $\boldsymbol{B}(\boldsymbol{r},t)=\boldsymbol{B}(\boldsymbol{q},\omega)e^{i(\boldsymbol{q}\cdot\boldsymbol{r}-\omega t)}$

Hubbard model: $\mathscr{H}=\sum_{i,j,s} t_{ij}c^{\dagger}_{is}c_{js}+U\sum_{i}^{N}\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$

Local magnetization (in unit $-g\mu_{\mathrm{B}}$): $\boldsymbol{S}(\boldsymbol{r})=\frac{1}{2}\sum_{i}\sum_{\alpha,\beta}\delta(\boldsymbol{r}-\boldsymbol{r}_i)c^{\dagger}_{i\alpha}\boldsymbol{\sigma}_{\alpha\beta}c_{i\beta}$ $\quad\boldsymbol{\sigma}=(\sigma_x,\sigma_y,\sigma_z)$

Perturbation Hamiltonian: $\mathscr{H}_{\mathrm{ext}}(t)=g\mu_{\mathrm{B}}\int\boldsymbol{B}(\boldsymbol{r},t)\cdot\boldsymbol{S}(\boldsymbol{r})d^3\boldsymbol{r}=g\mu_{\mathrm{B}}\boldsymbol{S}_{-\boldsymbol{q}}\cdot\boldsymbol{B}(\boldsymbol{q},\omega)e^{-i\omega t}$

Magnetization in q-space

$$\left.\begin{aligned}
S_{\boldsymbol{q}+}&=S_{\boldsymbol{q}x}+iS_{\boldsymbol{q}y}=\sum_{\boldsymbol{k}}a^{\dagger}_{\boldsymbol{k}\uparrow}a_{\boldsymbol{k}+\boldsymbol{q}\downarrow},\\
S_{\boldsymbol{q}-}&=S_{\boldsymbol{q}x}-iS_{\boldsymbol{q}y}=\sum_{\boldsymbol{k}}a^{\dagger}_{\boldsymbol{k}\downarrow}a_{\boldsymbol{k}+\boldsymbol{q}\uparrow},\\
S_{\boldsymbol{q}z}&=(1/2)\sum_{\boldsymbol{k}}(a^{\dagger}_{\boldsymbol{k}\uparrow}a_{\boldsymbol{k}+\boldsymbol{q}\uparrow}-a^{\dagger}_{\boldsymbol{k}\downarrow}a_{\boldsymbol{k}+\boldsymbol{q}\downarrow}).
\end{aligned}\right\}$$

RPA: susceptibility

Kubo formula $$\chi_{QP}(\omega) = \frac{i}{\hbar}\int_0^\infty \langle [Q(\tau), P]\rangle\, e^{i\omega\tau} d\tau$$

Correspondence $$P \to g\mu_{\mathrm{B}} \boldsymbol{S}_{-\boldsymbol{q}} \qquad Q \to g\mu_{\mathrm{B}} \boldsymbol{S}_{\boldsymbol{q}}$$

Susceptibility $$\chi_{zz}(\boldsymbol{q}, \omega) = (g\mu_{\mathrm{B}})^2 \frac{i}{\hbar}\int_0^\infty dt\, \langle [S_{\boldsymbol{q}z}(t), S_{-\boldsymbol{q}z}]\rangle\, e^{i\omega t}$$

$$\chi_{+-}(\boldsymbol{q}, \omega) = (g\mu_{\mathrm{B}})^2 \frac{i}{\hbar}\int_0^\infty dt\, \langle [S_{\boldsymbol{q}+}, S_{-\boldsymbol{q}-}]\rangle\, e^{i\omega t}$$

To calculate above, let us consider a Green's function $$G^{+}_{\boldsymbol{kq}}(t) = -i\theta(t)\, \langle [a^\dagger_{\boldsymbol{k}\uparrow}(t) a_{\boldsymbol{k}+\boldsymbol{q}\downarrow}(t), S_{-\boldsymbol{q}-}]\rangle$$

$$i\hbar\frac{\partial G_{\boldsymbol{kq}}}{\partial t} = -i\theta(t)\, \langle [e^{i\mathscr{H}t/\hbar}[a^\dagger_{\boldsymbol{k}\uparrow} a_{\boldsymbol{k}+\boldsymbol{q}\downarrow}, \mathscr{H}] e^{-i\mathscr{H}t/\hbar}, S_{-\boldsymbol{q}-}]\rangle + \delta(t)\hbar\, \langle [a^\dagger_{\boldsymbol{k}\uparrow}(t) a_{\boldsymbol{k}+\boldsymbol{q}\downarrow}(t), S_{-\boldsymbol{q}-}]\rangle$$

RPA: susceptibility (2)

Hubbard Hamiltonian $\mathscr{H} = \mathscr{H}_\mathrm{k} + \mathscr{H}_\mathrm{int}$

$$[a^\dagger_{\boldsymbol{k}\uparrow} a_{\boldsymbol{k}+\boldsymbol{q}\downarrow}, S_{-\boldsymbol{q}-}] = \sum_{\boldsymbol{k}'} [a^\dagger_{\boldsymbol{k}\uparrow} a_{\boldsymbol{k}+\boldsymbol{q}\downarrow}, a^\dagger_{\boldsymbol{k}'+\boldsymbol{q}\downarrow} a_{\boldsymbol{k}'\uparrow}]$$

$$= a^\dagger_{\boldsymbol{k}\uparrow} a_{\boldsymbol{k}\uparrow} - a^\dagger_{\boldsymbol{k}+\boldsymbol{q}\downarrow} a_{\boldsymbol{k}+\boldsymbol{q}\downarrow},$$

$$[a^\dagger_{\boldsymbol{k}\uparrow} a_{\boldsymbol{k}+\boldsymbol{q}\downarrow}, \mathscr{H}_\mathrm{k}] = (\epsilon_{\boldsymbol{k}+\boldsymbol{q}} - \epsilon_{\boldsymbol{k}}) a^\dagger_{\boldsymbol{k}\uparrow} a_{\boldsymbol{k}+\boldsymbol{q}\downarrow},$$

$$[a^\dagger_{\boldsymbol{k}\uparrow} a_{\boldsymbol{k}+\boldsymbol{q}\downarrow}, \mathscr{H}_\mathrm{int}] = (U/N) \sum_{\boldsymbol{k}_1, \boldsymbol{k}_2, \boldsymbol{p}} [a^\dagger_{\boldsymbol{k}\uparrow} a_{\boldsymbol{k}+\boldsymbol{q}\downarrow}, a^\dagger_{\boldsymbol{k}_1+\boldsymbol{p}\uparrow} a^\dagger_{\boldsymbol{k}_2-\boldsymbol{p}\downarrow} a_{\boldsymbol{k}_2\downarrow} a_{\boldsymbol{k}_1\uparrow}]$$

$$= -(U/N) \left[\sum_{\boldsymbol{k}_1, \boldsymbol{p}} a^\dagger_{\boldsymbol{k}\uparrow} a^\dagger_{\boldsymbol{k}_1+\boldsymbol{p}\uparrow} a_{\boldsymbol{k}+\boldsymbol{q}+\boldsymbol{p}\downarrow} a_{\boldsymbol{k}_1\uparrow} + \sum_{\boldsymbol{k}_2, \boldsymbol{p}} a^\dagger_{\boldsymbol{k}+\boldsymbol{p}\uparrow} a^\dagger_{\boldsymbol{k}_2-\boldsymbol{q}\downarrow} a_{\boldsymbol{k}_2\downarrow} a_{\boldsymbol{k}+\boldsymbol{q}\downarrow} \right].$$

Mean field approximation

$$- \sum_{\boldsymbol{p}} a^\dagger_{\boldsymbol{k}+\boldsymbol{p}\uparrow} a_{\boldsymbol{k}+\boldsymbol{q}+\boldsymbol{p}\downarrow} \langle a^\dagger_{\boldsymbol{k}\uparrow} a_{\boldsymbol{k}\uparrow} \rangle + \sum_{\boldsymbol{k}_1} a^\dagger_{\boldsymbol{k}\uparrow} a_{\boldsymbol{k}+\boldsymbol{q}\downarrow} \langle a^\dagger_{\boldsymbol{k}_1\uparrow} a_{\boldsymbol{k}_1\uparrow} \rangle$$

Random phase approximation (RPA)

$$- \sum_{\boldsymbol{k}_2} a^\dagger_{\boldsymbol{k}\uparrow} a_{\boldsymbol{k}+\boldsymbol{q}\downarrow} \langle a^\dagger_{\boldsymbol{k}_2\downarrow} a_{\boldsymbol{k}_2\downarrow} \rangle + \sum_{\boldsymbol{p}} a^\dagger_{\boldsymbol{k}+\boldsymbol{p}\uparrow} a_{\boldsymbol{k}+\boldsymbol{q}+\boldsymbol{p}\downarrow} \langle a^\dagger_{\boldsymbol{k}+\boldsymbol{q}\downarrow} a_{\boldsymbol{k}+\boldsymbol{q}\downarrow} \rangle$$

RPA: susceptibility (3)

In paramagnetic state:

$$i\hbar\frac{\partial G_{\boldsymbol{kq}}}{\partial t} = (\epsilon_{\boldsymbol{k}+\boldsymbol{q}} - \epsilon_{\boldsymbol{k}})G_{\boldsymbol{kq}}(t) - (U/N)(\langle a^{\dagger}_{\boldsymbol{k}\uparrow}a_{\boldsymbol{k}\uparrow}\rangle - \langle a^{\dagger}_{\boldsymbol{k}+\boldsymbol{q}\downarrow}a_{\boldsymbol{k}+\boldsymbol{q}\downarrow}\rangle)\sum_{\boldsymbol{p}} G_{(\boldsymbol{k}+\boldsymbol{p})\boldsymbol{q}}(t) + (\langle a^{\dagger}_{\boldsymbol{k}\uparrow}a_{\boldsymbol{k}\uparrow}\rangle - \langle a^{\dagger}_{\boldsymbol{k}+\boldsymbol{q}\downarrow}a_{\boldsymbol{k}+\boldsymbol{q}\downarrow}\rangle)\delta(t)$$

Fourier transformation:

$$\mathcal{G}_{\boldsymbol{kq}}(\omega) = \frac{f_{\boldsymbol{k}\uparrow} - f_{\boldsymbol{k}+\boldsymbol{q}\downarrow}}{\hbar\omega + \epsilon_{\boldsymbol{k}} - \epsilon_{\boldsymbol{k}+\boldsymbol{q}}}\left[1 - \frac{U}{N}\sum_{\boldsymbol{p}}\mathcal{G}_{\boldsymbol{pq}}(\omega)\right]$$

$f_{\boldsymbol{k}s} = \langle a^{\dagger}_{\boldsymbol{k}s}a_{\boldsymbol{k}s}\rangle$

Fermi distribution function

Summation on ***k***

$$\chi_{+-}(\boldsymbol{q},\omega) = N(g\mu_{\mathrm{B}})^2\frac{2\chi^{(0)}(\boldsymbol{q},\omega)}{1 - 2U\chi^{(0)}(\boldsymbol{q},\omega)}$$

Susceptibility of non-interacting system:

$$\chi^{(0)}(\boldsymbol{q},\omega) = \frac{1}{2N}\sum_{\boldsymbol{k}}\frac{f_{\boldsymbol{k}+\boldsymbol{q}\downarrow} - f_{\boldsymbol{k}\uparrow}}{\hbar\omega + \epsilon_{\boldsymbol{k}} - \epsilon_{\boldsymbol{k}+\boldsymbol{q}}}$$

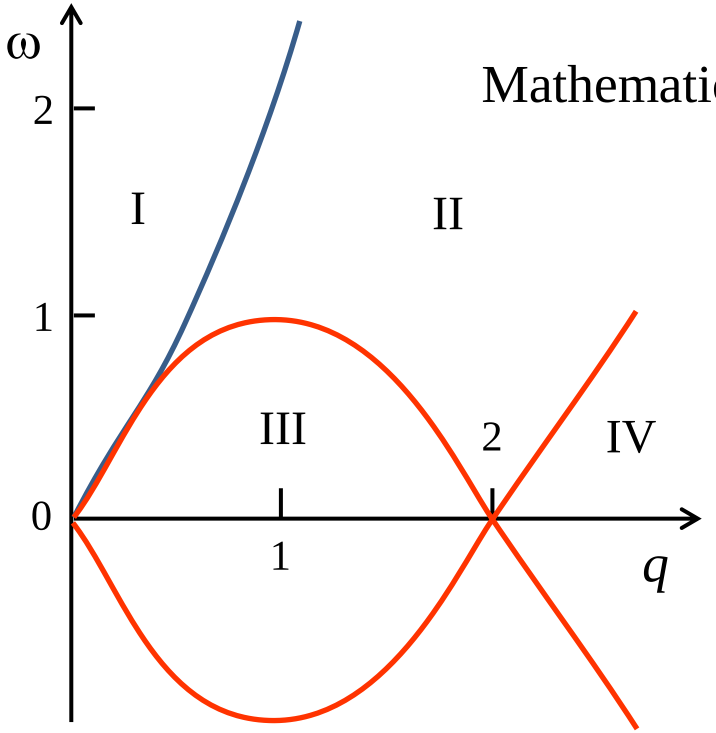
unit $(g\mu_{\mathrm{B}})^2$

Susceptibility of non-interacting system

$\hbar \to 1$ Wavenumber unit: k_F Energy unit: E_F

$$\frac{1}{2N}\sum_{\boldsymbol{k}} \frac{f_{\boldsymbol{k}}}{\omega + \epsilon_{\boldsymbol{k}-\boldsymbol{q}} - \epsilon_{\boldsymbol{k}}} = \frac{1}{2}\rho(\epsilon_{\mathrm{F}}) \int_0^1 k^2 dk \int_{-1}^{1} \frac{d(\cos\theta)}{\omega + q^2 - 2kq\cos\theta}$$

$$= \frac{1}{2}\rho(\epsilon_{\mathrm{F}}) \int_0^1 k^2 dk \frac{1}{2kq} \log \frac{\omega + q^2 + 2kq}{\omega + q^2 - 2kq}$$



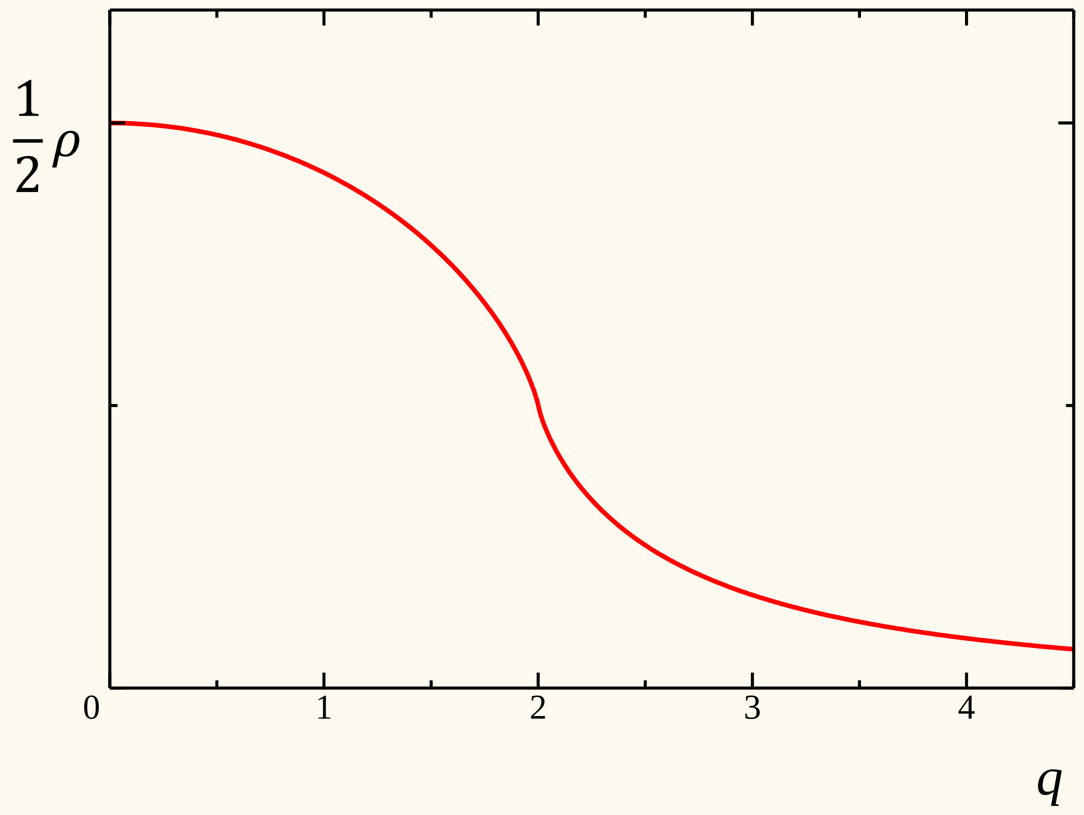
Mathematical identity: $$\int x \log(ax+b)dx = \frac{1}{2}\left[x^2 - \left(\frac{b}{a}\right)^2\right]\log(ax+b) - \frac{x^2}{4} + \frac{b}{2a}x$$

$$\chi^{(0)}(q,\omega) = \frac{\rho(\epsilon_{\mathrm{F}})}{2}\frac{1}{2q}\left\{\frac{1}{2}\left[1 - \left(\frac{\omega+q^2}{2q}\right)^2\right]\log\frac{\omega+q^2+2q}{\omega+q^2-2q} + \frac{\omega+q^2}{2q}\right.$$
$$\left. -\frac{1}{2}\left[1 - \left(\frac{-\omega+q^2}{2q}\right)^2\right]\log\frac{-\omega+q^2-2q}{\omega+q^2+2q} + \frac{-\omega+q^2}{2q}\right\}$$

Boundary of Kohn anomaly: $\omega = \pm(q^2 \pm 2q)$

Kohn anomaly, Stoner condition, SDW

$\mathrm{Re}[\chi^{(0)}(q,0)]$



In region III

$$\mathrm{Im}[\chi^{(0)}(q,\omega)] = \frac{\rho(\epsilon_F)}{2}\frac{\pi}{4}\frac{\omega}{q}$$

$$\mathrm{Re}[\chi^{(0)}(q,0)] = \frac{\rho(\epsilon_F)}{2}\frac{1}{2q}\left\{\left(1-\frac{q^2}{4}\right)\log\left|\frac{2+q}{2-q}\right| + q\right\}$$

$$\rightarrow \frac{\rho(\epsilon_F)}{2} \quad (q \rightarrow 0)$$

$$\chi_{+-}(\boldsymbol{q},\omega) = N(g\mu_B)^2 \frac{2\chi^{(0)}(\boldsymbol{q},\omega)}{1-2U\chi^{(0)}(\boldsymbol{q},\omega)}$$

$$U\chi^{(0)}(\boldsymbol{q}_{max},0) \geq \frac{1}{2}$$ Magnetic order

$\boldsymbol{q}_{max} = 0$ Stoner condition

$\boldsymbol{q}_{max} \neq 0$ Spin density wave (SDW)

Summary

- Magnetism in 3*d* transition metals
  - Slater-Pauling’s curve
  - Density of states by APW method
- Kubo formula (linear response)
- Fluctuation dissipation theorem
- Random phase approximation (RPA)