

(a) スピンのゆらぎに対する近似理論

(b) 振幅と空間分布からながめた物質の位置

図 2.2 強磁性、反強磁性のスピンのゆらぎに対する近似理論 (a) と、スピンのゆらぎの振幅と空間分布からながめた物質の位置 (守谷の作ったものを補強)
 (1) Pd, Sc, TiBe₂, YCo₅ (3) β-Mn, Cr, V, Se₂, V, Se₃,
 (2) Sc₂In, ZrZn₂, Ni₃Al, Ni-Pt, (4) 絶縁体磁性化合物, 4f 金属,

局在モーメントモデル

乱雑位相近似 (RPA)

自己無撞着 (SCR) スピン揺らぎ理論

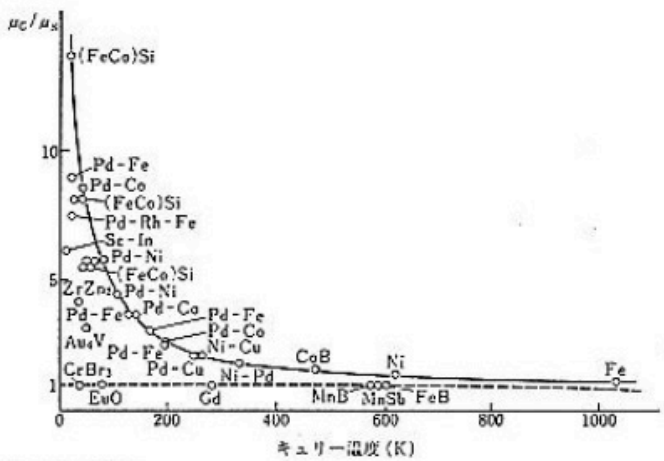
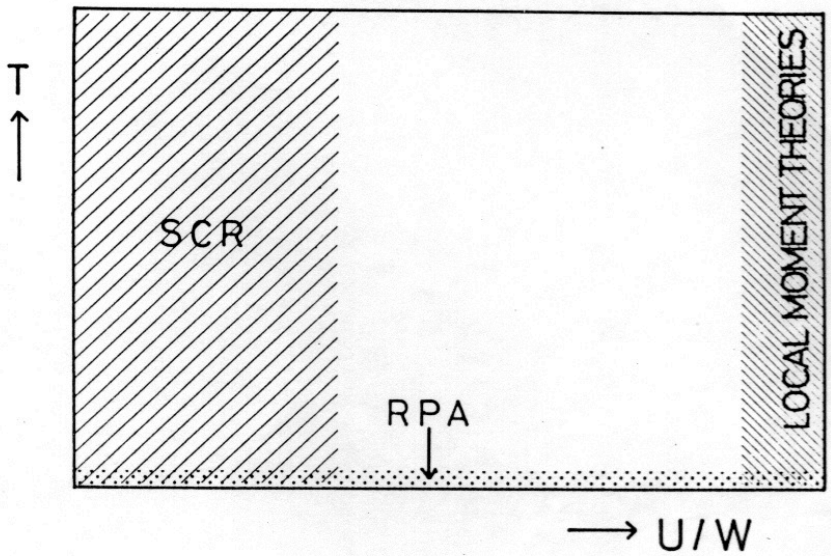
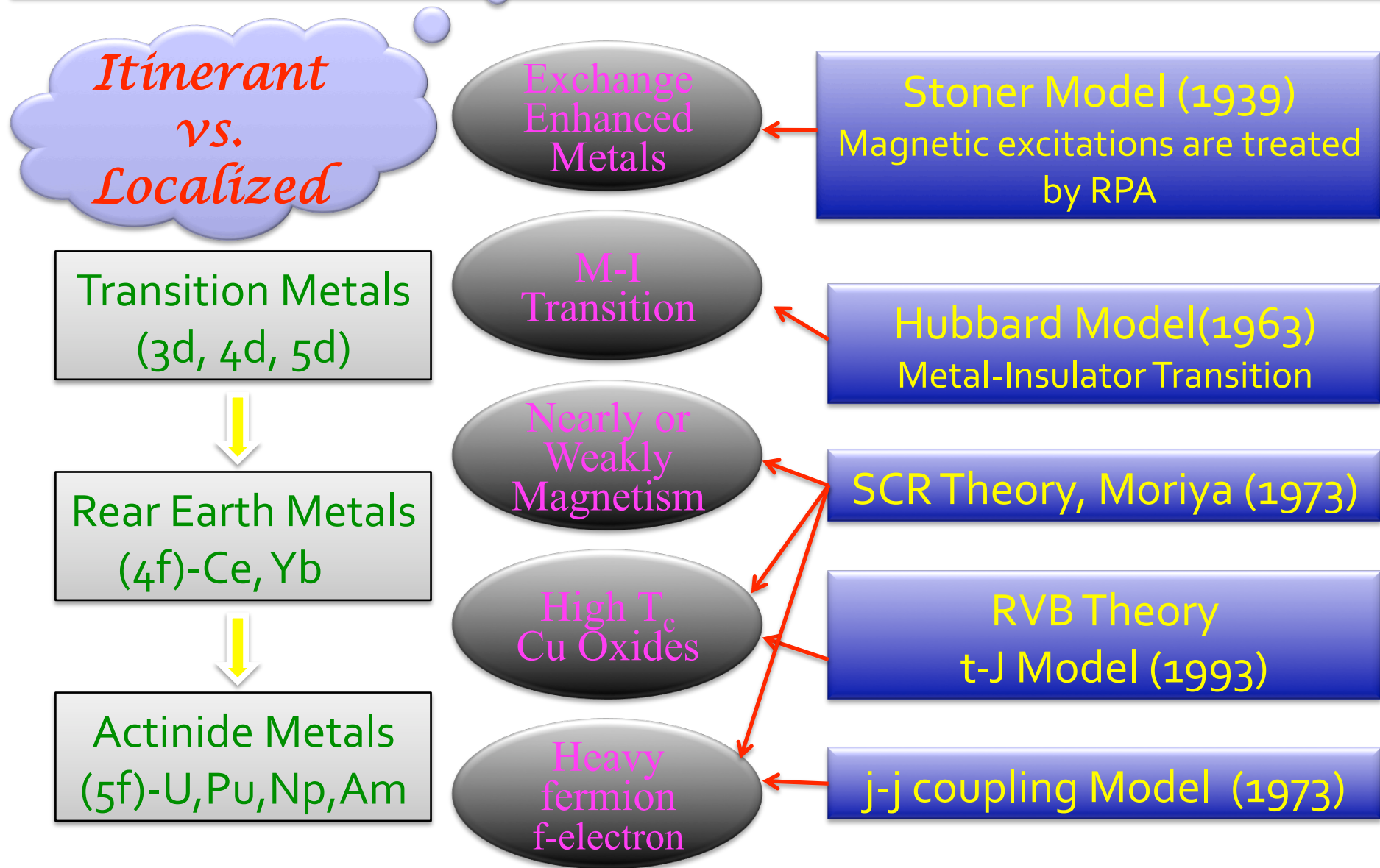


図 2.3 常磁性モーメント μ_c と強磁性飽和磁気モーメント μ_s の比 μ_c/μ_s とキュリー温度 T_c との関係。 $\mu_s = M/N_c(\mu_B)$, μ_c はキュリー定数 $C = N_c \mu_B \times \mu_c (\mu_c + 1) / 3k$ より求めている (文献 16) を補強した



Conceptional Research Stream of the Magnetism in Metals



遍歴電子磁性理論：Stonerモデル→RPA近似→SCR理論

$$S^+ = c_{\uparrow}^{\dagger} c_{\downarrow}, \quad S^- = c_{\downarrow}^{\dagger} c_{\uparrow}, \quad S^z = \frac{1}{2} (c_{\uparrow}^{\dagger} c_{\uparrow} - c_{\downarrow}^{\dagger} c_{\downarrow}).$$

$$\langle S^2 \rangle = \frac{3}{2} n - \frac{3}{4} n^2 - \frac{3}{4} \langle \delta n^2 \rangle$$

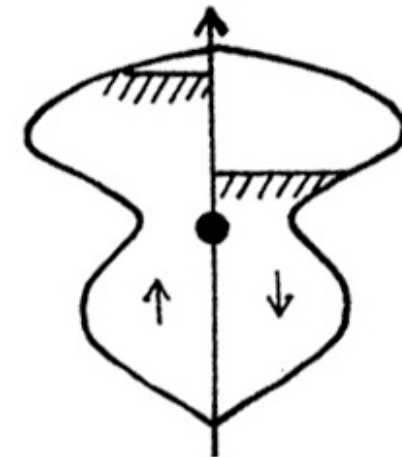
Landau展開

$$F(M) = \left(\frac{1}{2\chi_0} - I \right) M^2 + \frac{1}{4} g M^4 - Mh$$

$$\chi(q, \omega) = \frac{2\chi_0(q, \omega)}{1 + I\chi_0(q, \omega)}$$

$$\langle S^2 \rangle = \text{const} - O((k_B T/W)^2)$$

$$S^+ = \sum_{\mu=1,2} c_{\mu\uparrow}^{\dagger} c_{\mu\downarrow}, \quad S^- = \sum_{\mu=1,2} c_{\mu\downarrow}^{\dagger} c_{\mu\uparrow}$$



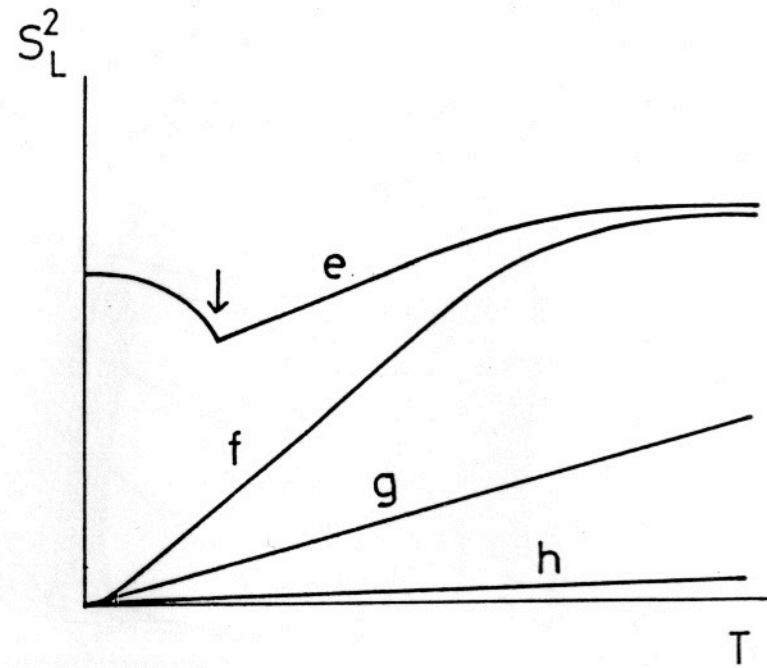
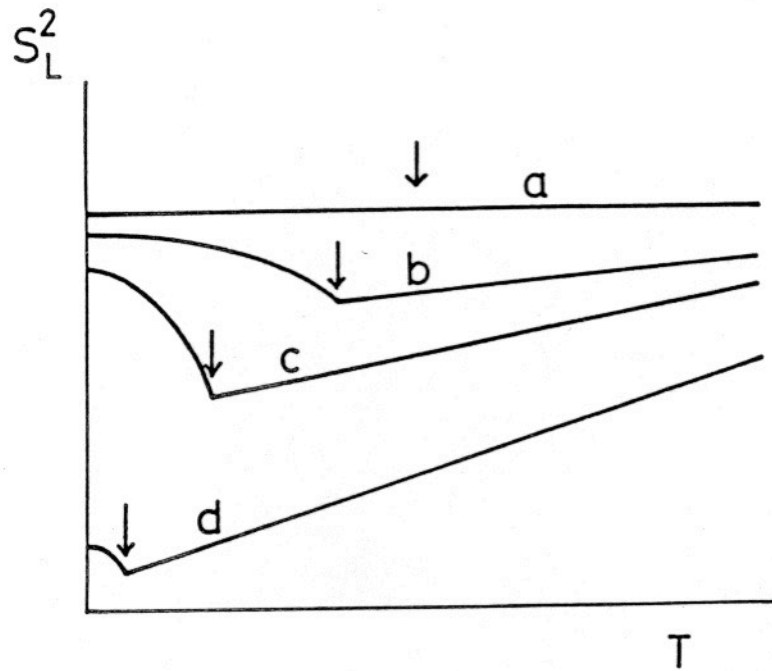
$$S^z = \sum_{\mu=1,2} \frac{1}{2} (c_{\mu\uparrow}^{\dagger} c_{\mu\uparrow} - c_{\mu\downarrow}^{\dagger} c_{\mu\downarrow})$$

$$\langle S_L^2 \rangle = \frac{3k_B T}{N_0} \sum_q \chi_q = \frac{3k_B T}{N_0} \sum_{q, \omega} \frac{\text{Im} \chi(q, \omega)}{\omega}$$

Spin Fluctuations

$$\frac{1}{\chi} = \frac{(1-\alpha)}{\chi_0} + \frac{5}{3} g N_0^2 S_L(T)^2$$

$$= \left[4N_0 I^2 S_L(T_C)^2 / 3T_C T_0 \right] (T - T_C)$$



スピンの揺らぎ

$$\langle S^2 \rangle = \frac{3}{N_0^2} \sum_q \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \coth\left(\frac{\beta\omega}{2}\right) \times \text{Im} \chi(q, \omega).$$

$$\langle S^2 \rangle = \langle S^2 \rangle_T + \langle S^2 \rangle_{\text{Z.P.}}$$

$$\langle S^2 \rangle_T = \frac{6}{N_0^2} \sum_q \int_0^{\infty} \frac{d\omega}{\pi} n(\omega) \text{Im} \chi(q, \omega),$$

$$\langle S^2 \rangle_{\text{Z.P.}} = \frac{3}{N_0^2} \sum_q \int_0^{\infty} \frac{d\omega}{\pi} \text{Im} \chi(q, \omega),$$

$$\coth \frac{\beta\omega}{2} = \text{sgn}(\omega)(1 + 2n(|\omega|)),$$

$$(n(\omega) = (e^{\beta\omega} - 1)^{-1}). \quad n(\omega) = \frac{1}{e^{\beta\omega} - 1}, \quad \beta = \frac{1}{k_B T}$$

$$\frac{1}{\chi} = \frac{(1-\alpha)}{\chi_0} + \frac{5}{3} g N_0^2 S_L(T)^2$$

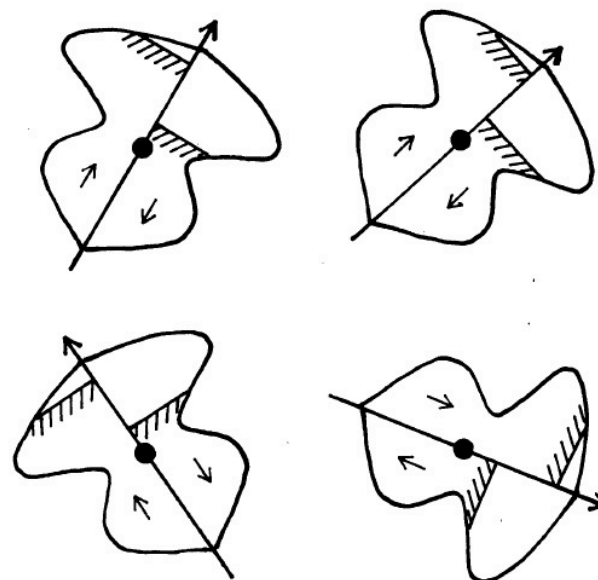
$$m^2 = m_{\parallel}^2 + m_{\perp}^2 = S_L^2 - (M/N_0)^2$$

$$\frac{3k_B T}{N_0} \sum_q \text{Re} \chi(q, 0) = \langle S^2 \rangle = S(S+1)$$

$$\text{Re} \chi(q, 0) = \frac{1}{\pi} \int_{-\infty}^{\infty} d\omega \frac{\text{Im} \chi(q, \omega)}{\omega}$$

$$\left[-\frac{(\alpha-1)}{\chi_0} + \frac{5}{3} g N_0^2 \bar{m}^2 \right] M + g M^3 = h$$

$$\bar{m}^2 = \frac{3}{5} (3m_{\parallel}^2 + 2m_{\perp}^2)$$



SCR理論 The Self-Consistent Renormalization (SCR) Theory of Spin Fluctuations

The dynamical susceptibility:

$$\chi^+(q\omega) = \frac{\chi_0^+(q\omega)}{1 - I\chi_0^+(q\omega) + \lambda(q\omega)}, \quad (T > T_C)$$

The long wave approximation:

$$\frac{\chi_0^+(q\omega)}{\chi_0^+(0,0)} = 1 - Aq^2 - B\left(\frac{\omega}{q}\right)^2 + iC\omega q + \dots$$

$$\lambda(q\omega) = \left(\frac{5\alpha}{2\pi\rho}\right)(1+\delta)F_1 \sum_q \int_0^\infty d\omega \frac{1}{e^{\omega/T} - 1} \cdot \frac{C\omega/q}{(\delta + Aq^2)^2 + (C\omega q)^2}$$

$$\delta = \frac{\chi_0}{\alpha\chi} = \frac{1 - \alpha + \lambda}{\alpha}$$

$$\lambda(q\omega) \approx \lambda(0,0) = \frac{5}{3}\chi_0 g N_0^2 S_L(T)^2 = \frac{5}{3} \frac{\chi_0}{N_0} \bar{F}_1 S(T)_L^2$$

$$\frac{1}{\chi} = \frac{(1-\alpha)}{\chi_0} + \frac{5}{3} g N_0^2 S_L(T)^2 = \left[4N_0 I^2 S_L(T_C)^2 / 3T_C T_0\right](T - T_C)$$

Stoner Enhancement Factor: $\frac{1}{1-\alpha} \quad \alpha = I\rho$

I: the intra-atomic exchange interaction,
 ρ : the density of states at the Fermi level.

Landau Expansion of Free Energy:

$$F(M) = \frac{1-\alpha}{2\chi_0} M^2 + \frac{1}{4} \bar{F}_1 M^4 + \dots - 2\mu_B H \cdot M$$

$$\bar{F}_1 M^2 = \frac{2\mu_B H}{M} + \frac{2(\alpha-1)}{\rho}$$

Arrott Plots:

$$\bar{F}_1 [M(T,H)^2 - M(T,0)^2] = 2\mu_B \frac{H}{M(T,H)}, \quad p_s = 2M(0,0)$$

$$\left[-\frac{(\alpha-1)}{\chi_0} + \frac{5}{3} g N_0^2 \bar{m}^2 \right] M + g M^3 = h$$

$$m^2 = m_{//}^2 + m_{\perp}^2 = S_L^2 - (M/N_0)^2$$

$$\bar{m}^2 = \frac{3}{5} (3m_{//}^2 + 2m_{\perp}^2)$$

SCR理論

$$\text{Im}\chi(q,\omega) = \frac{\chi(0,0)}{1+q^2/\kappa^2} \frac{\Gamma_q \omega}{\omega^2 + \Gamma_q^2}$$

$$\Gamma_q = \Gamma_0 q (\kappa^2 + q^2) \quad \chi(0)\kappa^2 = \frac{N_0}{2\bar{A}}$$

$$\begin{aligned} \langle S^2 \rangle_{\text{Z.P.}} &= \frac{3}{\pi} \frac{v_0}{(2\pi)^3} \frac{1}{2\bar{A}} \int d^3q \frac{1}{\kappa^2 + q^2} \int_0^{\omega_c(q)} d\omega \frac{\omega \Gamma_q}{\omega^2 + \Gamma_q^2}, \\ &= \frac{3}{\pi} \frac{v_0}{(2\pi)^3} \frac{\Gamma_0}{2\bar{A}} \int d^3q \frac{q}{2} [\log \{ \omega_c(q)^2 + \Gamma_q^2 \} - 2 \log \Gamma_q], \end{aligned}$$

$$\langle S^2 \rangle_{\text{Z.P.}} = \frac{9T_0}{2T_A} \int_0^1 dx x^3 \{ \log (f(x)^2 + (x^2 + y)^2) - 2 \log (x^2 + y) \}$$

$$\langle S^2 \rangle_{\text{T}} = \frac{9T_0}{T_A} \eta^4 \int_0^{1/\eta} dz z^3 \left\{ \log u - \frac{1}{2u} - \psi(u) \right\}$$

$$\begin{aligned} u &= z(y/\eta^2 + z^2)/t, \\ \eta^3 &= T_C/T_0, \end{aligned}$$

$$\log u - \frac{1}{2u} - \psi(u) = 2 \int_0^\infty \frac{t dt}{\exp 2\pi t - 1} \cdot \frac{1}{t^2 + u^2}$$

$$\chi(q,\omega) = \frac{\chi_0(q,\omega)}{1 - I\chi_0(q,\omega) + \lambda(q,\omega)}$$

$$\lambda(q,\omega) \rightarrow \lambda(0,0) = \frac{5}{3} \chi_0 g N_0 S_L(T)^2 = \frac{5}{3} \frac{\chi_0}{N_0} \bar{F}_1 S_L(T)^2$$

$$\left[-\frac{(\alpha-1)}{\chi_0} + \frac{5}{3} g N_0^2 \bar{m}^2 \right] M + g M^3 = h$$

$$x = q/q_B, \quad (q_B = (6\pi^2/v_0)^{1/3}),$$

$$f(x) = \omega_c(q)/\Gamma_0 q q_B^2,$$

$$T_0 = \Gamma_0 q_B^3 / 2\pi,$$

$$T_A = \bar{A} q_B^2,$$

$$y = \kappa^2 / q_B^2.$$

$$\frac{1}{\chi} = \frac{(1-\alpha)}{\chi_0} + \frac{5}{3} g N_0^2 S_L(T)^2$$

スピンの揺らぎの高橋理論

$$\frac{1}{2} Z(y) = -c_{4/3}(\eta^*)^4 + \eta^4 \int_0^{1/\eta} dz z^3 \times \left\{ \log u - \frac{1}{2u} - \psi(u) \right\}.$$

$$c_{4/3}(\eta^*)^4 = \frac{T_A}{9T_0} \{ \langle S^2 \rangle - \langle S^2 \rangle_{Z.P.}(T_C) \}$$

$$(\eta^*)^4 = \frac{\eta^4}{c_{4/3}} \int_0^{1/\eta} dz z^3 \left\{ \log z^3 - \frac{1}{2z^3} - \psi(z^3) \right\},$$

$$c_{4/3} = \int_0^\infty dz z^3 \left\{ \log z^3 - \frac{1}{2z^3} - \psi(z^3) \right\},$$

$$= \frac{1}{3^{3/2}} \frac{1}{(2\pi)^{1/3}} \Gamma(4/3) \zeta(4/3) = 0.3353 \dots$$

$$p_s^2/4 \cong \frac{15cT_0}{T_A} \eta^4 = \frac{15cT_0}{T_A} \left(\frac{T_C}{T_0} \right)^{4/3}$$

$$\langle S^2 \rangle - \langle S^2 \rangle_{Z.P.} = \langle S^2 \rangle_T$$

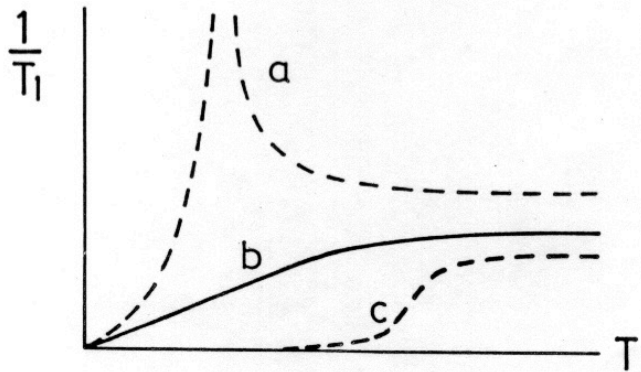
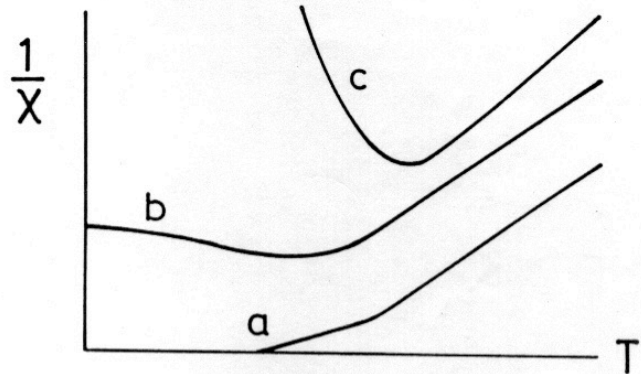
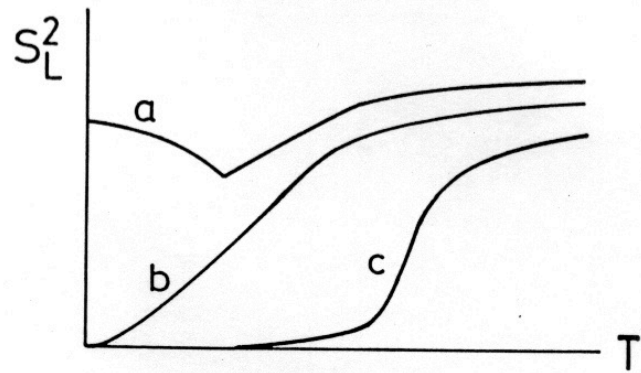
$$\langle S^2 \rangle_{Z.P.}(T_C) - \langle S^2 \rangle_{Z.P.}(T)$$

$$= -\{ \langle S^2 \rangle - \langle S^2 \rangle_{Z.P.}(T_C) \} + \langle S^2 \rangle_T(T)$$

$$\langle S^2 \rangle = \langle S^2 \rangle_T + \langle S^2 \rangle_{Z.P.} = \text{一定}$$

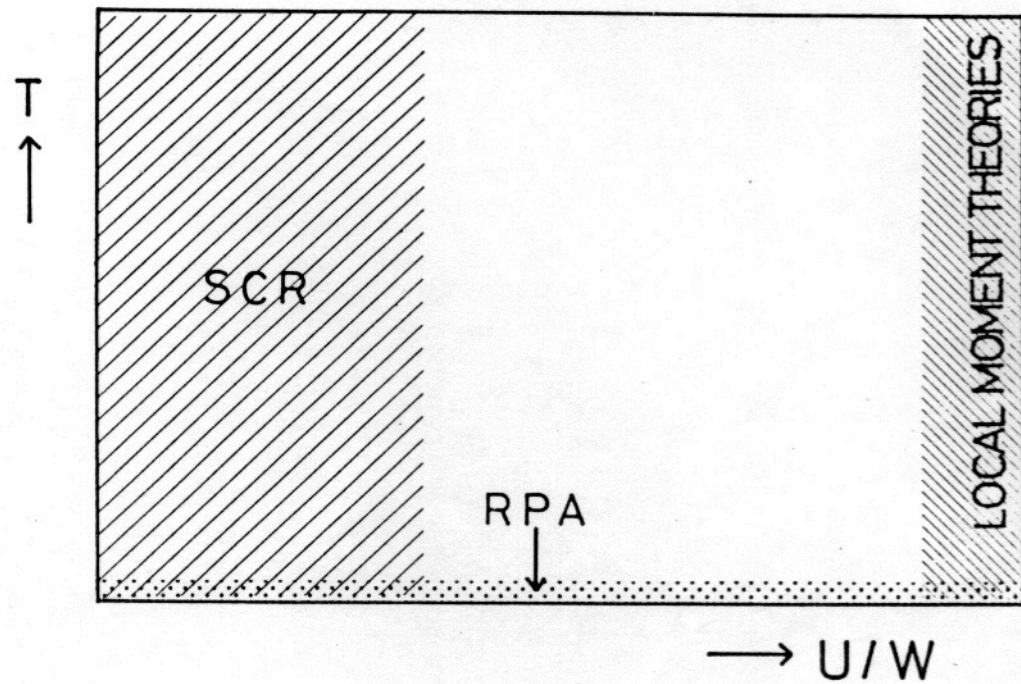
Y.Takahashi,
JPSJ 55 (1986) 3553

$$\bar{F}_1 = \frac{4k_B T_A^2}{15T_0}$$



$$\frac{1}{\chi} = \frac{(1-\alpha)}{\chi_0} + \frac{5}{3} g N_0^2 S_L (T)^2$$

$$= \left[4 N_0 I^2 S_L (T_C)^2 / 3 T_C T_0 \right] (T - T_C)$$

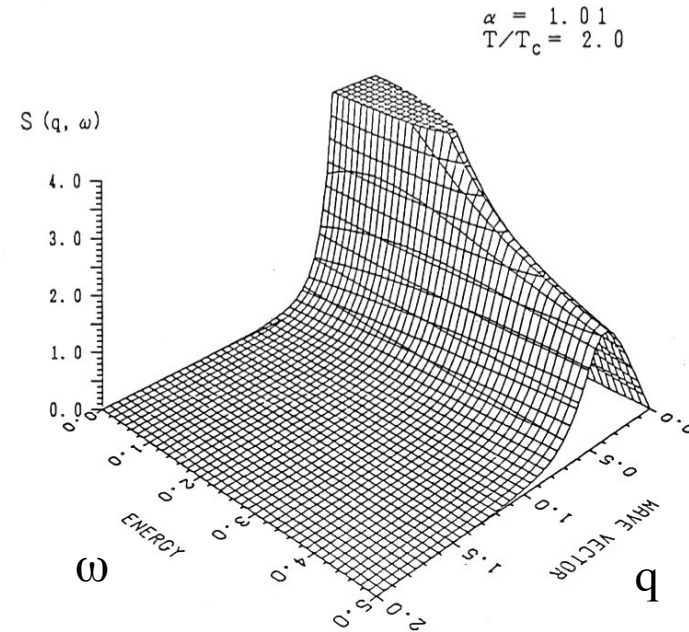


- **The Self-Consistent Renormalization (SCR) Theory of Spin Fluctuations**

$$\text{Im}\chi(q,\omega) = \frac{\chi(0,0)}{1 + q^2/\kappa^2} \cdot \frac{\omega\Gamma_q}{\omega^2 + \Gamma_q^2}$$

$$\Gamma_q = \Gamma_0 q(\kappa^2 + q^2), \quad \Gamma_0 = A/C$$

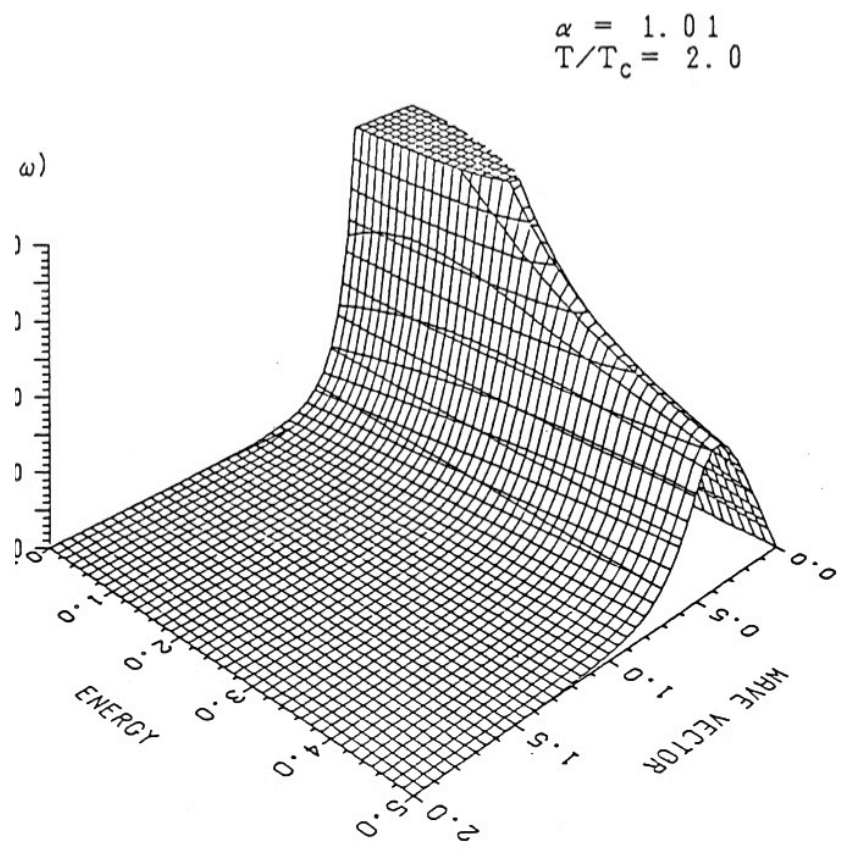
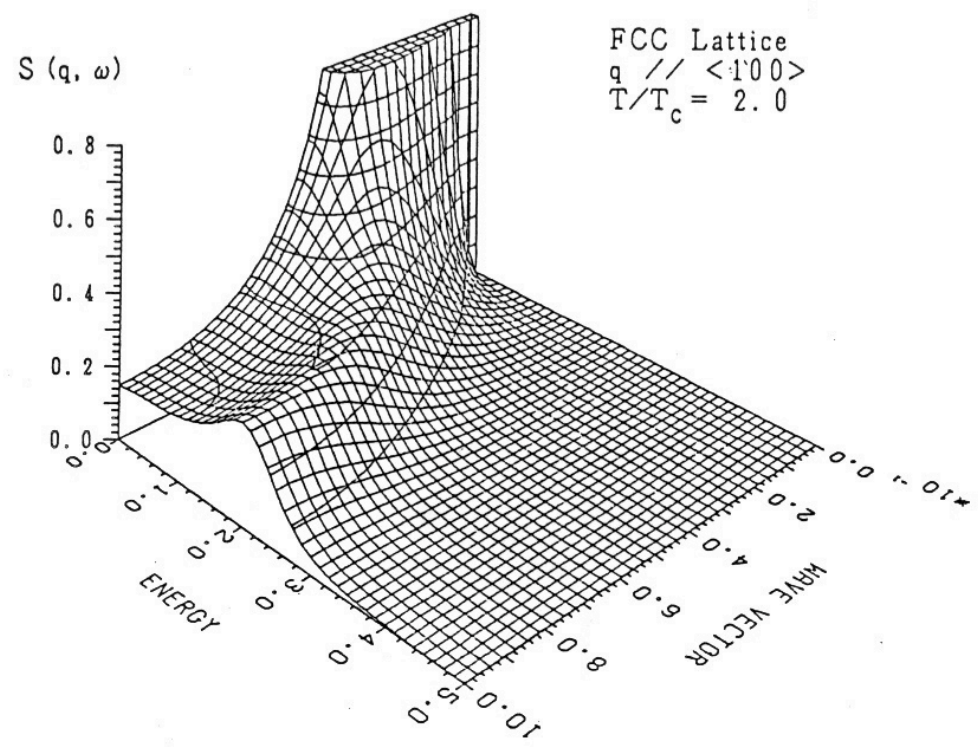
$$\kappa^2 = \frac{1}{2\bar{A}} \cdot \frac{N_0}{\chi}, \quad \bar{A} = AN_0/\rho$$

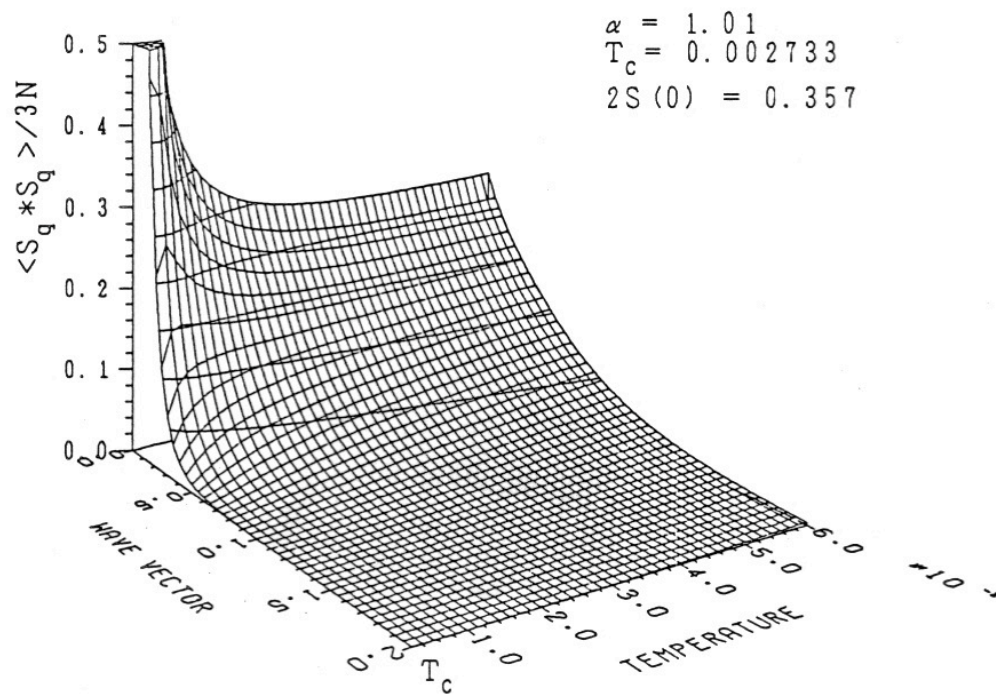
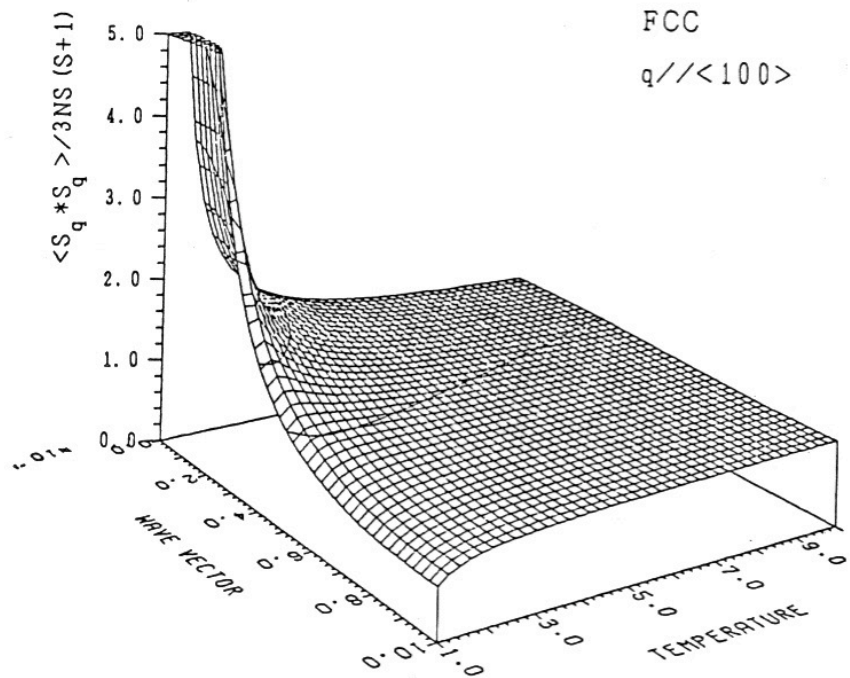


- **Quantitative aspects** (The spin fluctuation parameters)

$$p_s, \quad \bar{F}_1, \quad T_0 = \Gamma_0 q_B^3 / 2\pi, \quad T_A = \bar{A} q_B^2 \quad : \text{Takahashi\& Moriya (1985)}$$

$$\left(q_B = \left(\frac{6\pi^2}{v_0} \right)^{1/3}, \quad v_0 = \text{the volume per magnetic atom} \right)$$





The SCR theory \Leftrightarrow Experiments

<The Curie temperature, T_C >

$$p_s^2/4 \cong \frac{15cT_0}{T_A} \eta^4 = \frac{15cT_0}{T_A} \left(\frac{T_C}{T_0} \right)^{4/3} \quad c = \frac{1}{3^{3/2}} (2\pi)^{-1/3} \Gamma(4/3) \zeta(4/3) = 0.3353 \dots$$

<Reduced Susceptibility, y >

$$y = \frac{N_0}{2T_A \eta^2} \chi^{-1} \cong \frac{\bar{F}_1 p_s^2}{8T_A \eta^2} \left\{ -1 + \frac{1}{c} \int_0^{1/\eta} dz z^3 \left[\ln u - \frac{1}{2u} - \psi(u) \right] \right\}$$

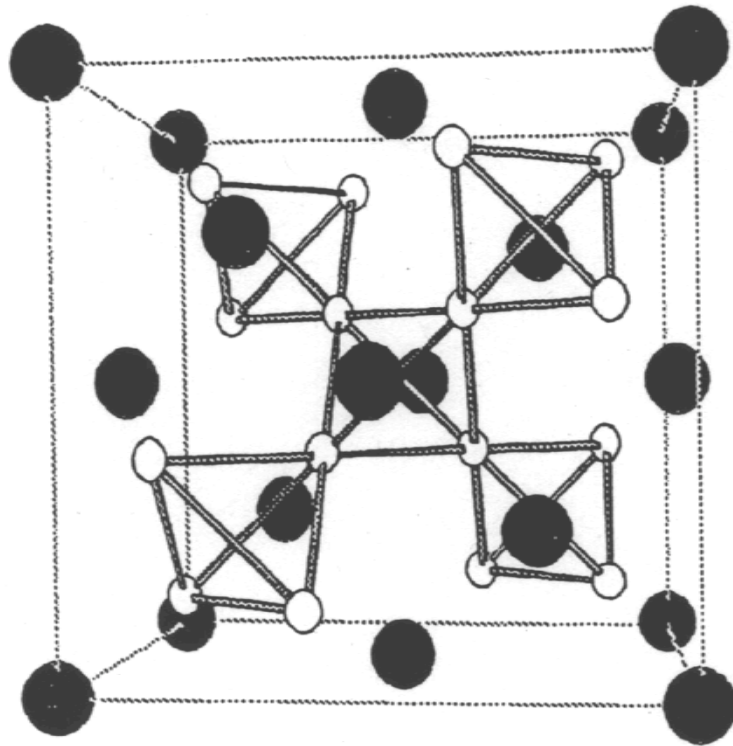
$$u = z(y + z^2)/t, \quad t = T/T_C, \quad \eta = (T_C/T_0)^{1/3}, \quad \psi: \text{digamma function}$$

$$\frac{1}{\chi} = \frac{(1-\alpha)}{\chi_0} + \frac{5}{3} g N_0^2 S_L(T)^2 = \frac{4N_0 I^2 S_L(T_C)^2 / T_0}{3T_C^2 (t-1)} \quad \chi = \frac{N_0 p_{eff}^2}{3k_B T_C (t^{4/3} - 1)} \quad (T_C \text{近傍})$$

<NMR, T_1 >

$$\frac{1}{T_1} = \gamma_N^2 A_{hf}^2 T \frac{\chi}{4\pi^2 \mu_B \Gamma_0}, \quad T_0 = \frac{\Gamma_0 q_B^3}{2\pi}$$

YCo₂の結晶構造



- Y 8a ダイヤモンド格子
- Co 16d パイロクロア格子
(正四面体が3次的に頂点を共有)

立方晶C15ラーベス構造

RCo₂の遍歴電子磁性

RCo₂ (R=Rare Earth)はRの種類によって様々なCoの遍歴電子磁性

- Rが非磁性 : 交換増強されたパウリ常磁性
- Rが軽希土類金属 : 遍歴電子強磁性
- Rが重希土類金属 : フェリ磁性

•これらのCoの遍歴電子磁性はCo間の強い交換相互作用に起因

•Rに磁性があるときはRがつくる分子場が寄与！

•Yは非磁性なのでYCo₂は交換増強されたパウリ常磁性

Y(Co-Fe)₂→強磁性→非磁性元素の置換で強磁性出現を！