MAGNETISM IN MATERIALS

Lecture 8: Itinerant Magnetism (cont.)

Ivica Zivkovic

ITINERANT MAGNETISM

- *q*-dependence
- spin-density wave
- RKKY
- Kondo effect
- Hubbard model

$$\mathcal{H} = \frac{\boldsymbol{p}^2}{2m_e} \qquad \mathcal{H}\psi_{\boldsymbol{k}\pm} = E\psi_{\boldsymbol{k}\pm} \qquad \psi_{\boldsymbol{k}\pm}(\boldsymbol{r}) = \frac{1}{\sqrt{V}} e^{i\boldsymbol{k}\boldsymbol{r}} |\pm\rangle$$

$$\mathcal{H} = \frac{\boldsymbol{p}^2}{2m_e} \qquad \mathcal{H}\psi_{\boldsymbol{k}\pm} = E\psi_{\boldsymbol{k}\pm} \qquad \psi_{\boldsymbol{k}\pm}(\boldsymbol{r}) = \frac{1}{\sqrt{V}}e^{i\boldsymbol{kr}}|\pm\rangle$$

$\xrightarrow{\mathcal{H}'_{pert}}$

$$\psi_{(\boldsymbol{k}+\boldsymbol{q})\pm}(\boldsymbol{r}) = \frac{1}{\sqrt{V}}e^{i(\boldsymbol{k}+\boldsymbol{q})\boldsymbol{r}}|\pm\rangle$$

$$\psi_{(\boldsymbol{k}-\boldsymbol{q})\pm}(\boldsymbol{r}) = \frac{1}{\sqrt{V}}e^{i(\boldsymbol{k}-\boldsymbol{q})\boldsymbol{r}}|\pm\rangle$$

spatially varying magnetic field: $\boldsymbol{H}(\boldsymbol{r}) = \boldsymbol{H}_{\boldsymbol{q}} \cos \boldsymbol{qr}$

$$\mathcal{H}'_{pert} = \pm\frac{1}{2}g\mu_0\mu_B|\boldsymbol{H}_{\boldsymbol{q}}|\cos \boldsymbol{qr}$$

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spatially varying magnetic field: $\boldsymbol{H}(\boldsymbol{r}) = \boldsymbol{H}_{\boldsymbol{q}}\cos\boldsymbol{q}\boldsymbol{r}$

$$\mathcal{H}'_{pert} = \pm\frac{1}{2}g\mu_0\mu_B|\boldsymbol{H}_{\boldsymbol{q}}|\cos\boldsymbol{q}\boldsymbol{r}$$

$$\psi_{\boldsymbol{k}\pm}(\boldsymbol{r}) = \frac{1}{\sqrt{V}}\left[e^{i\boldsymbol{k}\boldsymbol{r}} \pm \frac{1}{4}g\mu_0\mu_B|\boldsymbol{H}_{\boldsymbol{q}}|\left(\frac{e^{i(\boldsymbol{k}+\boldsymbol{q})\boldsymbol{r}}}{E_{\boldsymbol{k}+\boldsymbol{q}} - E_{\boldsymbol{k}}} + \frac{e^{i(\boldsymbol{k}-\boldsymbol{q})\boldsymbol{r}}}{E_{\boldsymbol{k}-\boldsymbol{q}} - E_{\boldsymbol{k}}}\right)\cos\boldsymbol{q}\boldsymbol{r}\right]|\pm\rangle$$

$|\boldsymbol{H}_{\boldsymbol{q}}| \ll \quad \longrightarrow$ keeping only linear terms

$$|\psi_{\boldsymbol{k}\pm}(\boldsymbol{r})|^2 = \frac{1}{V}\left[1 \pm \frac{1}{\hbar^2}m_e g\mu_0\mu_B|\boldsymbol{H}_{\boldsymbol{q}}|\left(\frac{1}{(\boldsymbol{k}+\boldsymbol{q})^2 - k^2} + \frac{1}{(\boldsymbol{k}-\boldsymbol{q})^2 - k^2}\right)\cos\boldsymbol{q}\boldsymbol{r}\right]$$

$$|\psi_{\boldsymbol{k}\pm}(\boldsymbol{r})|^2 = \frac{1}{V}\left[1 \pm \frac{1}{\hbar^2} m_e g \mu_0 \mu_B |\boldsymbol{H}_{\boldsymbol{q}}| \left(\frac{1}{(\boldsymbol{k}+\boldsymbol{q})^2 - k^2} + \frac{1}{(\boldsymbol{k}-\boldsymbol{q})^2 - k^2}\right) \cos \boldsymbol{qr}\right]$$

$$M(\boldsymbol{r}) = \frac{g\mu_0\mu_B}{2}\left(|\psi_{\boldsymbol{k}+}(\boldsymbol{r})|^2 - |\psi_{\boldsymbol{k}-}(\boldsymbol{r})|^2\right) = M_{\boldsymbol{q}} \cos \boldsymbol{qr}$$

$$M_{\boldsymbol{q}} = \frac{m_e g^2 \mu_0 \mu_B^2 |\boldsymbol{H}_{\boldsymbol{q}}|}{V\hbar^2} \int_0^{|\boldsymbol{k}|<k_F} \left(\frac{1}{(\boldsymbol{k}+\boldsymbol{q})^2 - k^2} + \frac{1}{(\boldsymbol{k}-\boldsymbol{q})^2 - k^2}\right) g(\boldsymbol{k}) d^3\boldsymbol{k}$$

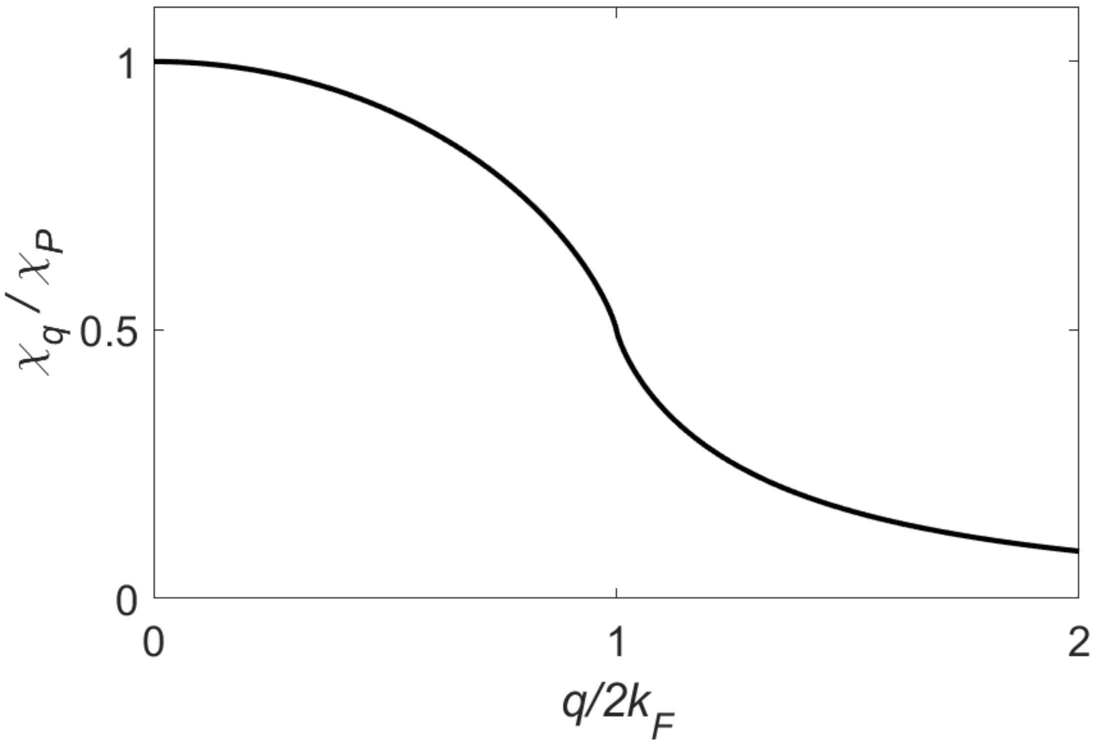
$$g(k)dk \sim k^2 dk$$

$$M_{\boldsymbol{q}} = \frac{k_F m_e g^2 \mu_0 \mu_B^2 |\boldsymbol{H}_{\boldsymbol{q}}|}{\pi^2\hbar^2} \left(1 + \frac{4k_F^2 - q^2}{4k_F q} \log\left|\frac{q+2k_F}{q-2k_F}\right|\right)$$

$$M_{\boldsymbol{q}} = \frac{k_F m_e g^2 \mu_0 \mu_B^2 \left|\boldsymbol{H}_{\boldsymbol{q}}\right|}{\pi^2 \hbar^2}\left(1 + \frac{4k_F^2 - q^2}{4k_F q}\log\left|\frac{q + 2k_F}{q - 2k_F}\right|\right)$$

$$\boldsymbol{M}_{\boldsymbol{q}} = \chi_{\boldsymbol{q}} \boldsymbol{H}_{\boldsymbol{q}} \qquad \chi_{\boldsymbol{q}} = \chi_P F\left(\frac{q}{2k_F}\right) \qquad F(x) = \frac{1}{2}\left(1 + \frac{1 - x^2}{2x}\ln\left|\frac{x+1}{x-1}\right|\right)$$

Pauli paramagnetism



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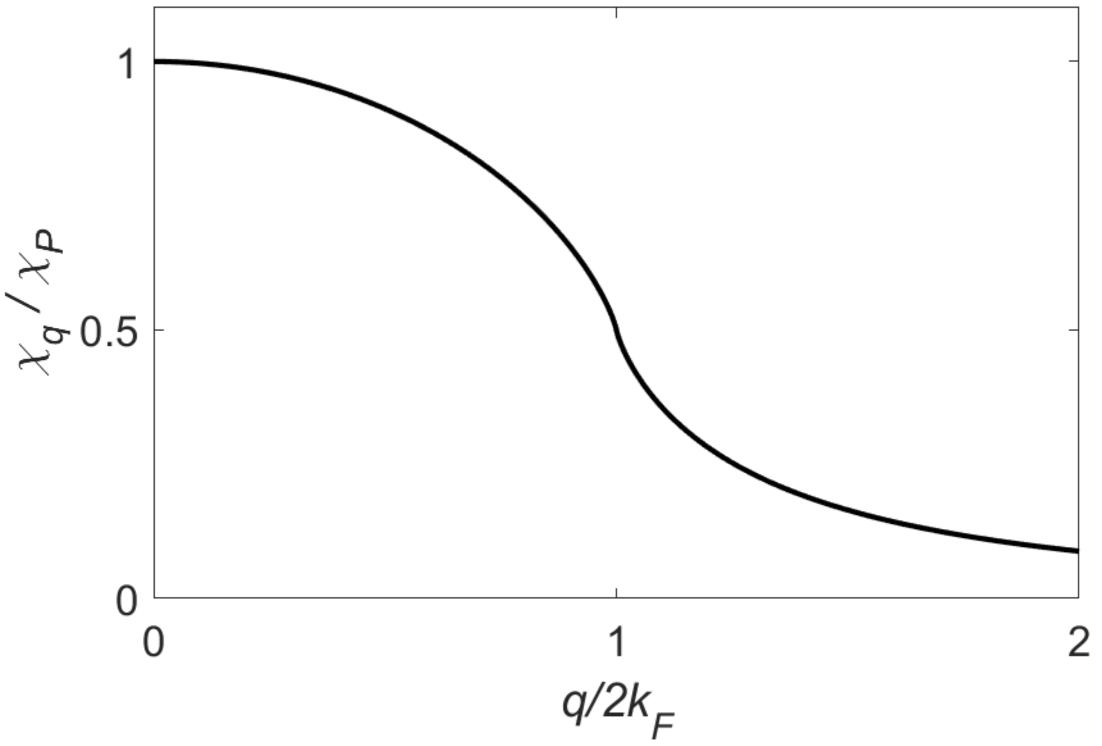


Landau diamagnetism

$$\chi_{\boldsymbol{q}} = -\frac{1}{3}\chi_P G\left(\frac{q}{2k_F}\right)$$

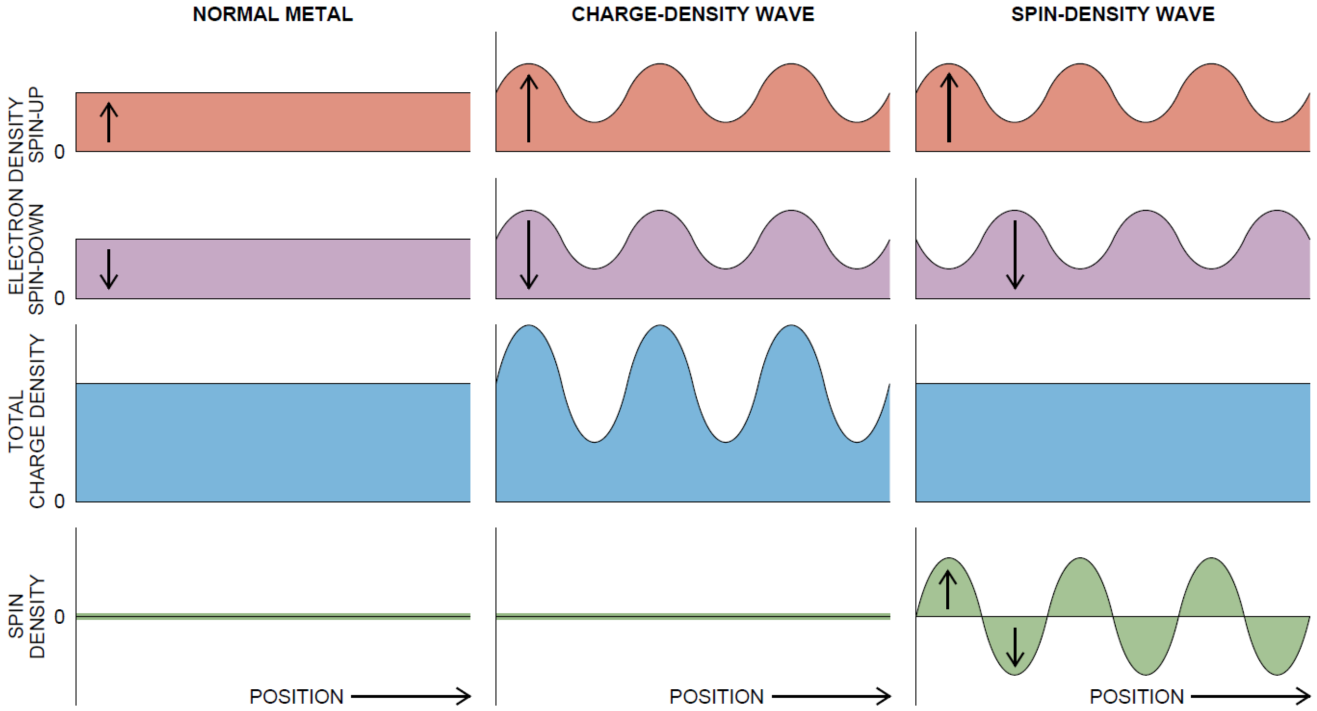
❖ Stoner criterion with *q*-dependence

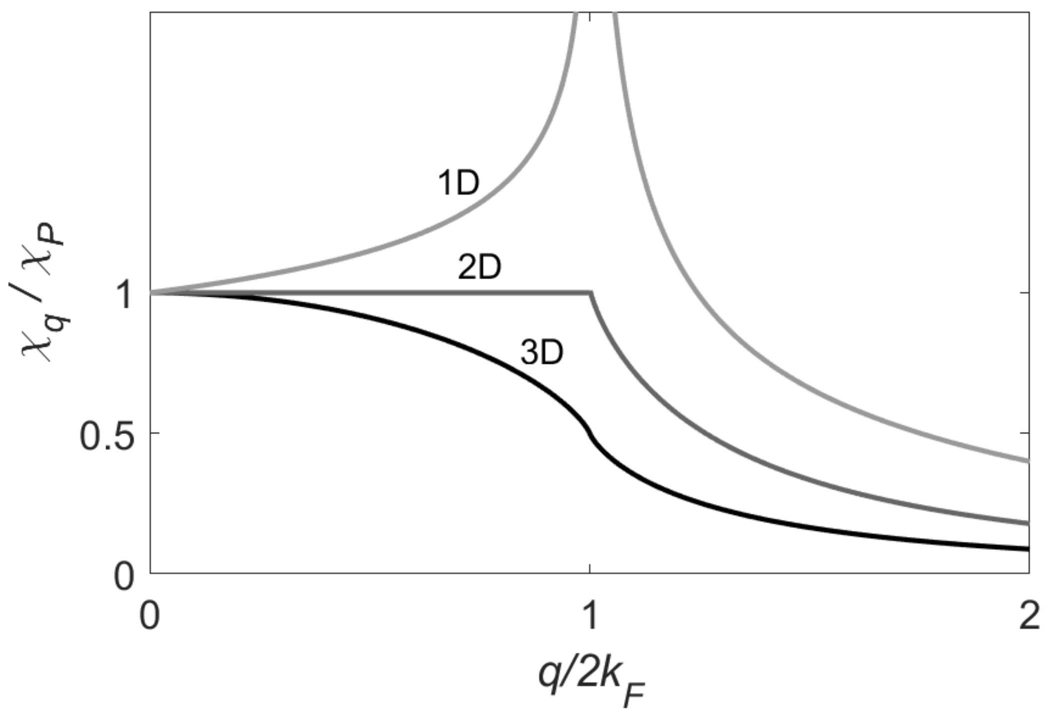
$$\chi_{\boldsymbol{q}} = \chi_{\boldsymbol{q}}^0 = \chi_P F\left(\frac{q}{2k_F}\right) \longrightarrow \frac{\chi_{\boldsymbol{q}}^0}{1 - \frac{1}{\mu_0 \mu_B^2} U \chi_{\boldsymbol{q}}^0}$$

- Stoner criterion with *q*-dependence

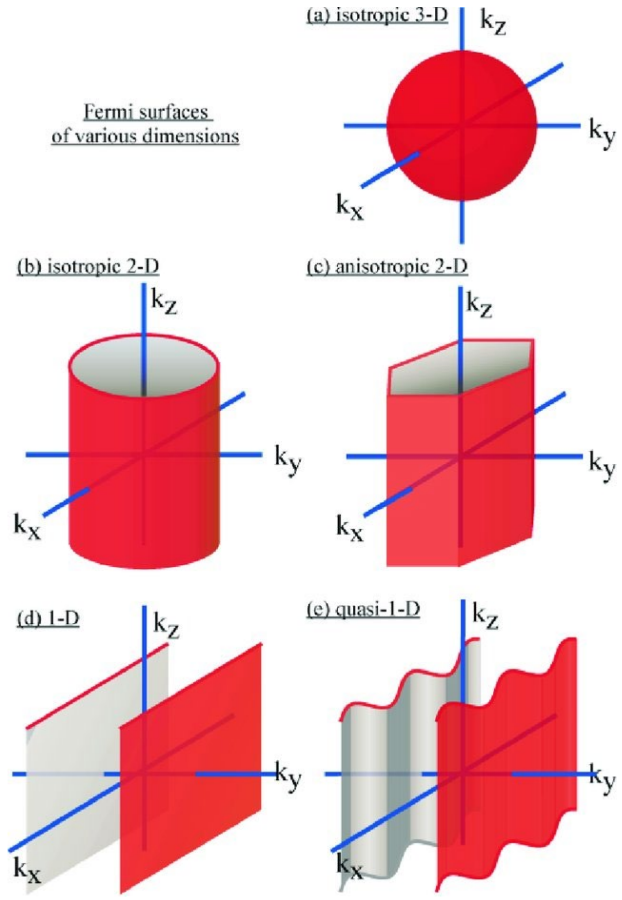
$$\chi_{\boldsymbol{q}} = \chi_{\boldsymbol{q}}^{0} = \chi_P F\left(\frac{q}{2k_F}\right) \longrightarrow \frac{\chi_{\boldsymbol{q}}^{0}}{1 - \frac{1}{\mu_0 \mu_B^2} U \chi_{\boldsymbol{q}}^{0}}$$

Scientific American 270, 50 (1994)

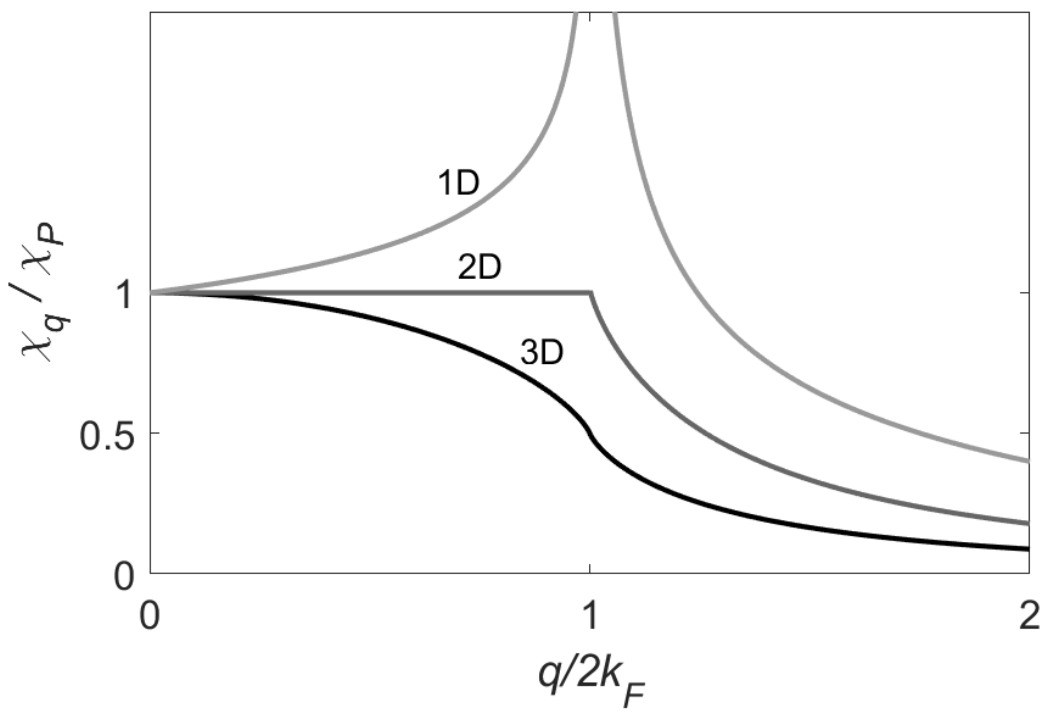




1D: Kohn anomaly (gap at the Fermi surface)



J.Phys.Condens.Matter 19, 19 (2007)



1D: Kohn anomaly (gap at the Fermi surface)

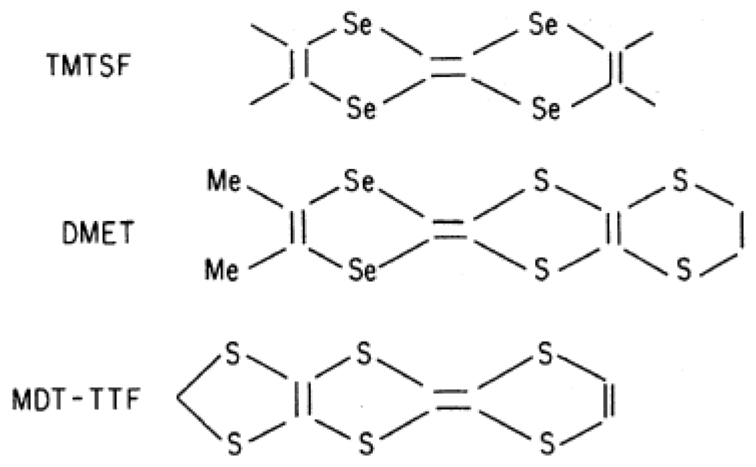
	pairing	total spin	total momentum	broken symmetry	collective excitations
singlet SC	e^--e^-	0	0	gauge	gapped
triplet SC	e^--e^-	1	0	gauge	?
CDW	e^--h^+	0	$2k_F$	translation	phasons amplitudons
SDW	e^--h^+	1	$2k_F$	translation	phasons magnons

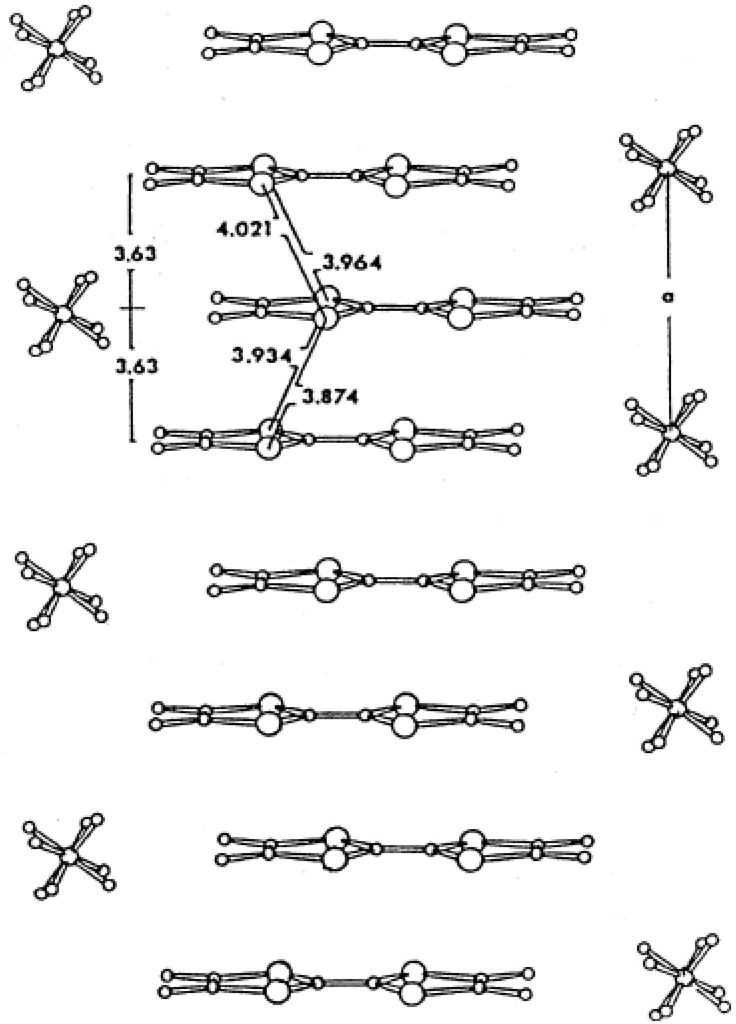
BCS

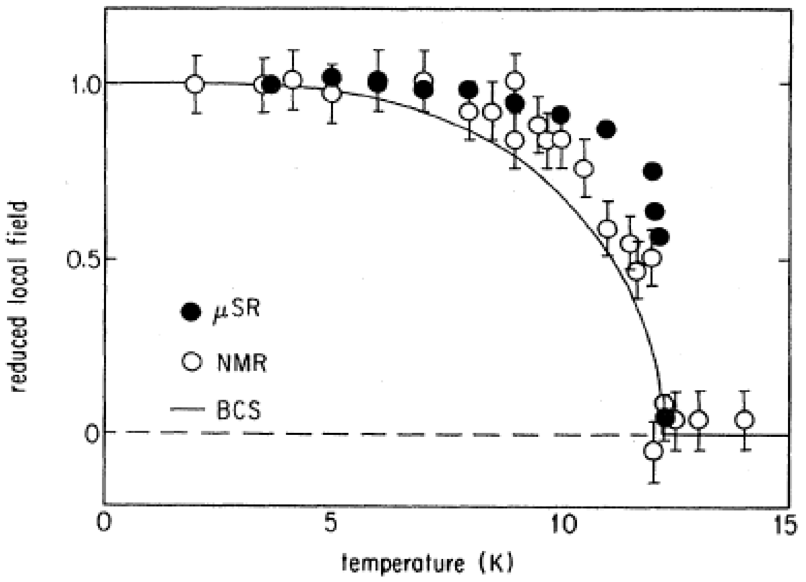
$$\Delta_{T=0} = 2E_F e^{-\frac{1}{Ug(E)}}$$

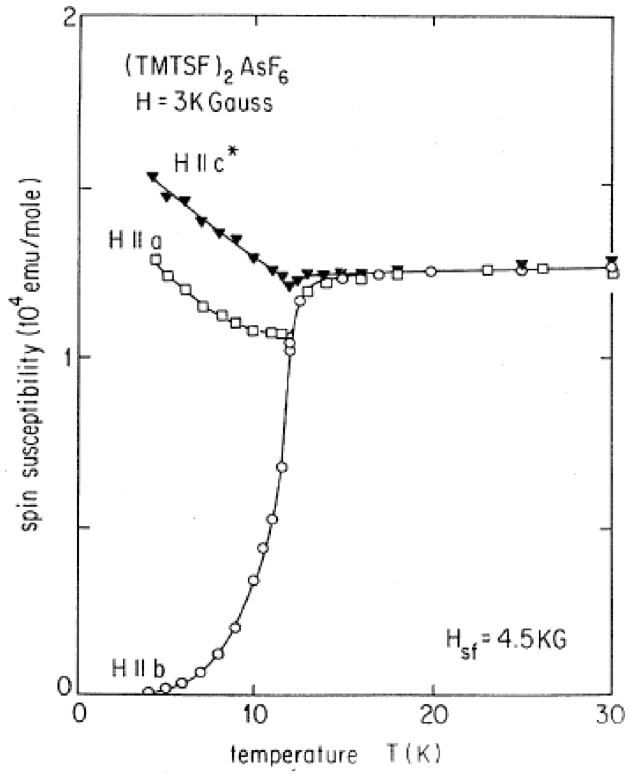
$$2\Delta = 3.52 k_B T_C$$

Rev.Mod.Phys. 66, 1 (1994)





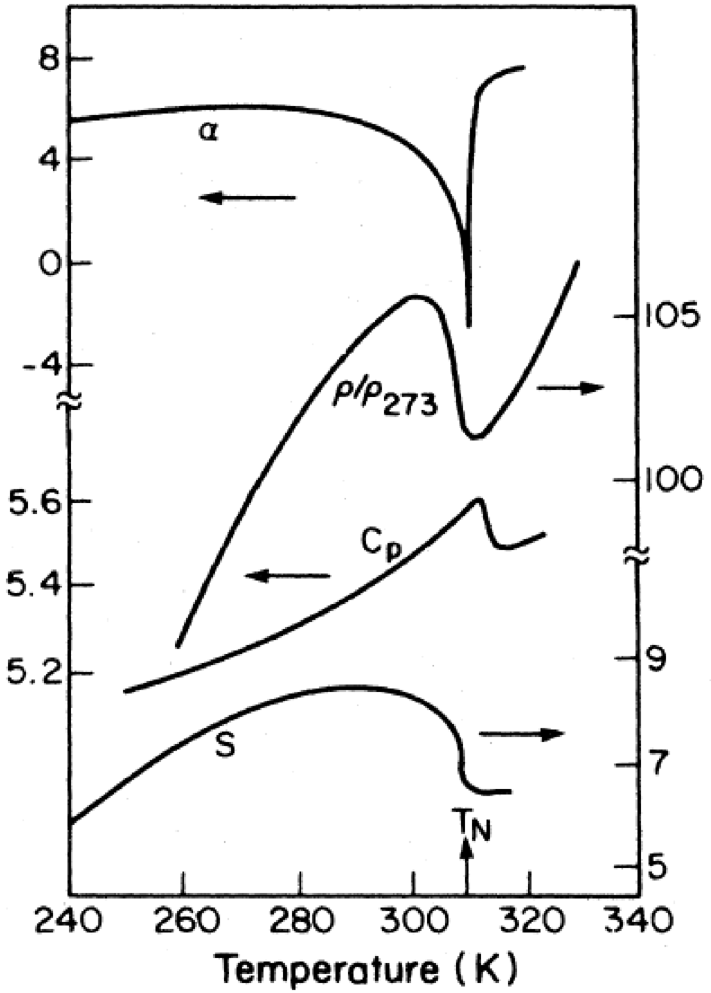


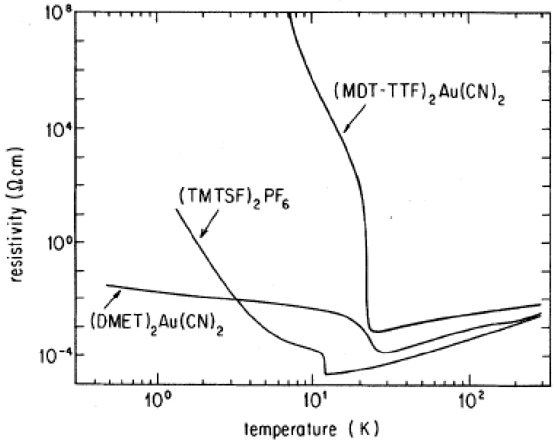


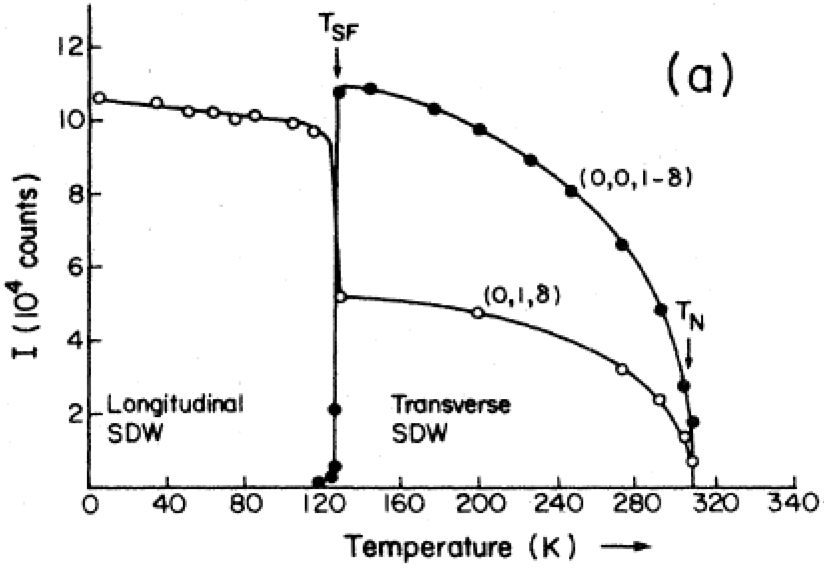
chromium: T_{SDW} = 310K

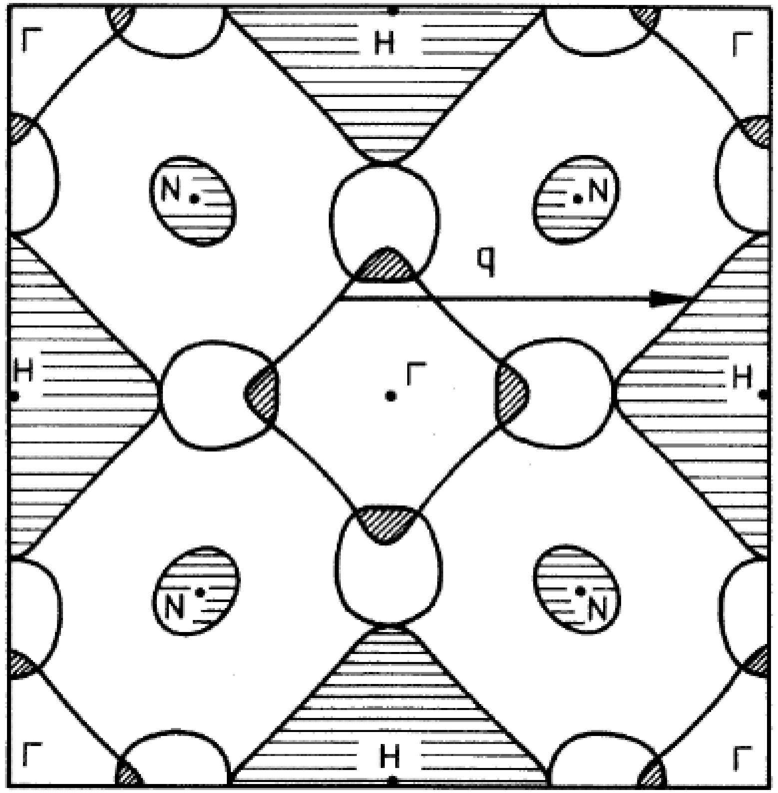
PRB 23, 4977 (1981)

Rev.Mod.Phys. 60, 209 (1988)







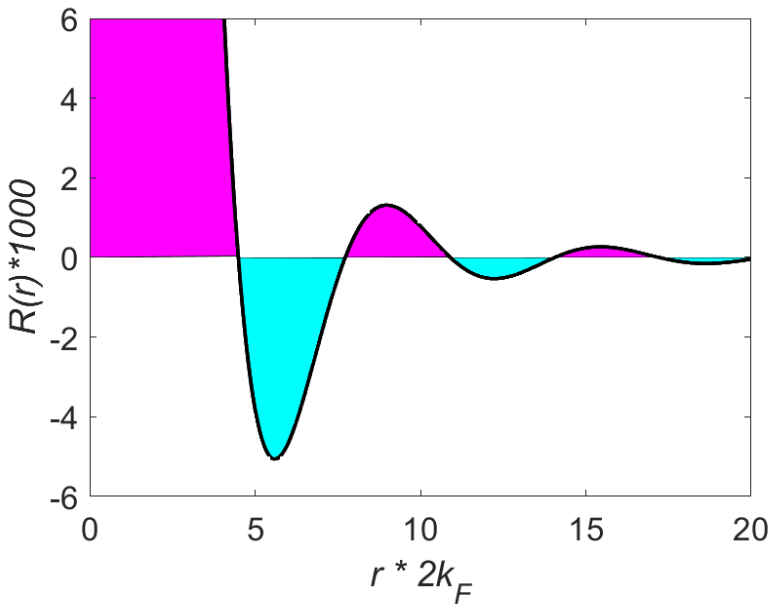


- Ruderman-Kittel-Kasuya-Yosida interaction
- response to a delta-function perturbation (nuclear moments, impurities)
- limited at high q/small distances

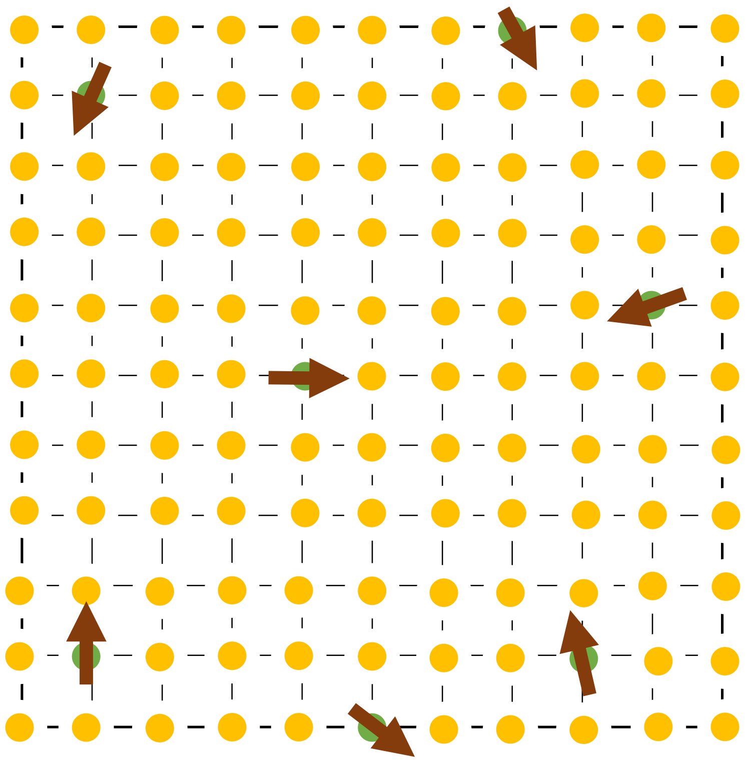
$$\boldsymbol{H}(\boldsymbol{r}) = \boldsymbol{H}\delta(\boldsymbol{r})$$

$$\chi(\boldsymbol{r}) = \frac{1}{(2\pi)^3}\int \chi_{\boldsymbol{q}} e^{i\boldsymbol{q}\boldsymbol{r}} d^3\boldsymbol{q} \sim \chi_P R(2rk_F)$$

$$R(x) = \frac{-x\cos x + \sin x}{x^4}$$



- charge channel $\rightarrow$ Friedel oscillations



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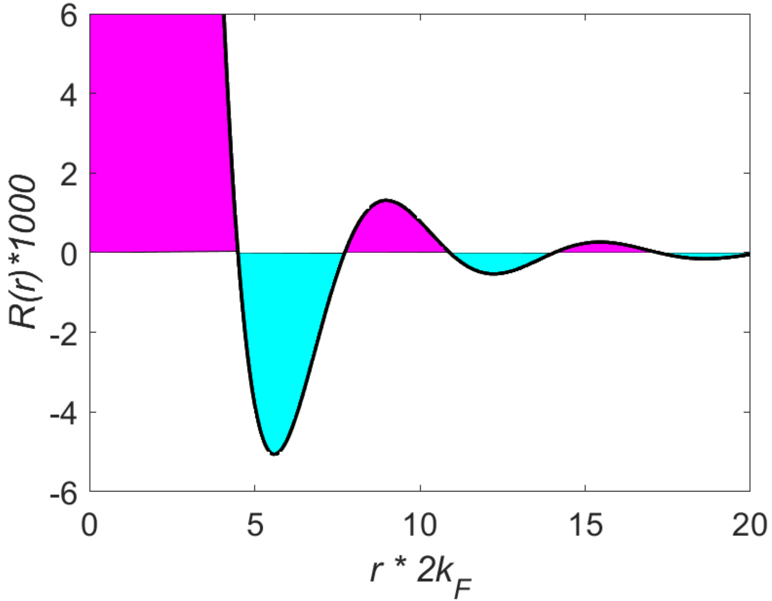


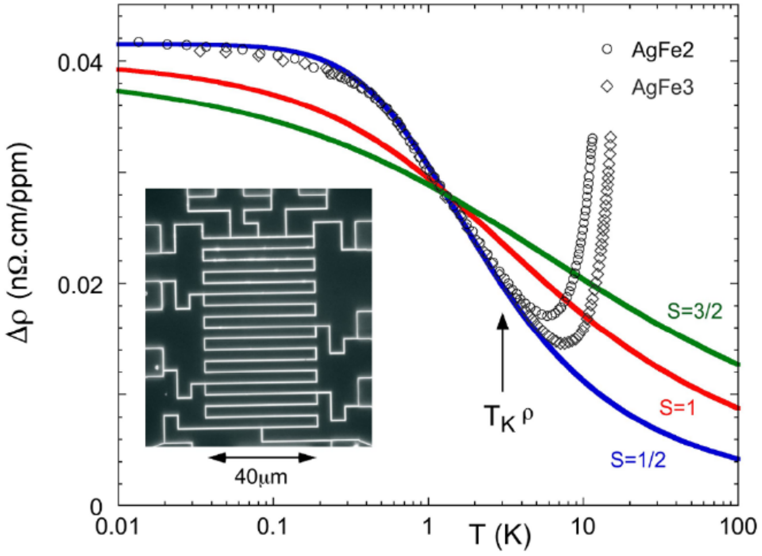
- charge channel → Friedel oscillations

typical resistivity of metals: $\rho(T) = \rho_0 + AT^2 + \rho_{ph}$

1934: resistance minimum in gold

1964: Kondo effect ~ log(T)

PRL 97, 226804 (2006)



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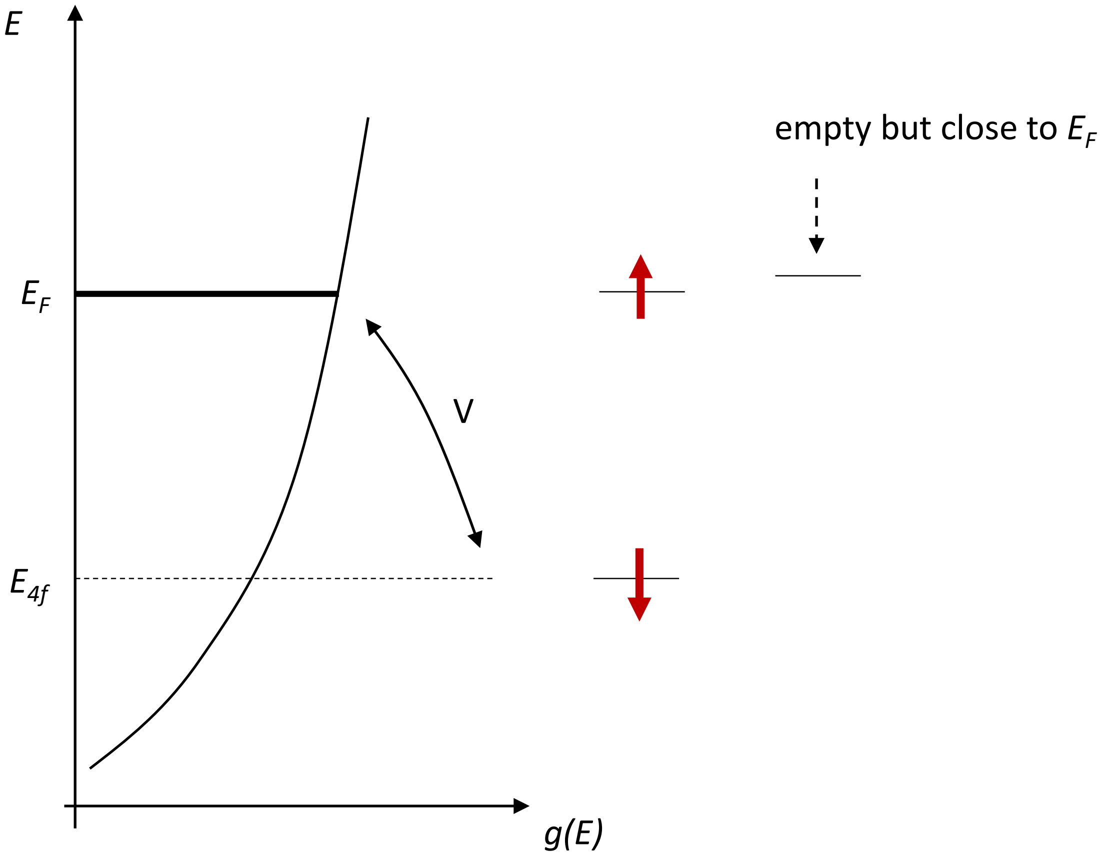

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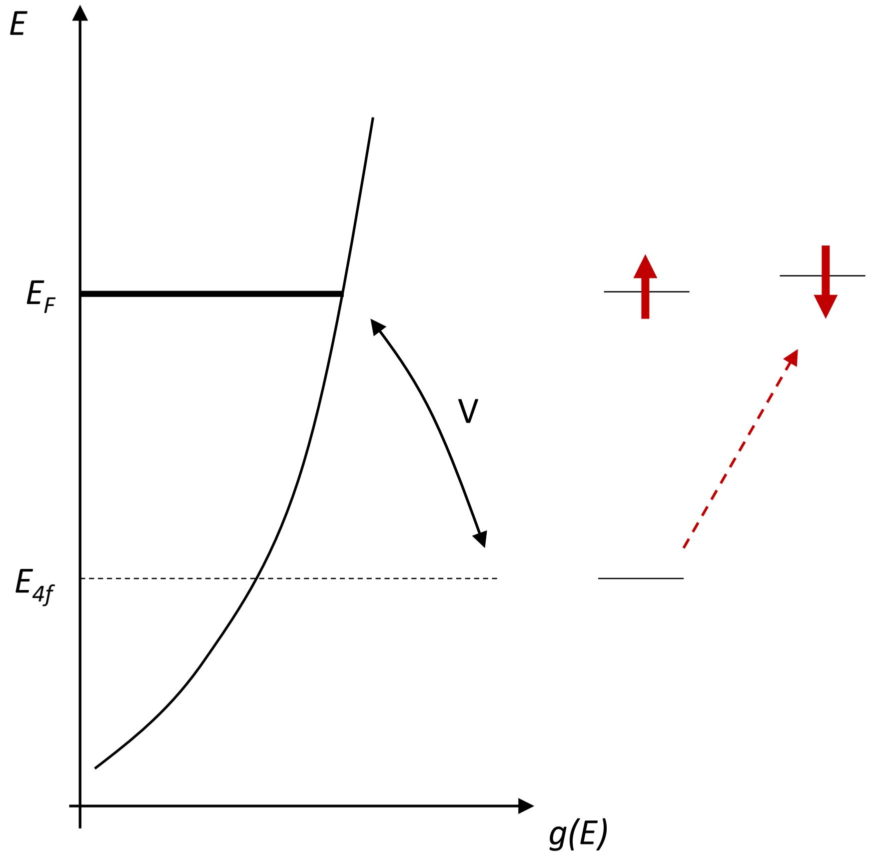

$$\sim \frac{1}{E_F - E_{4f}}$$

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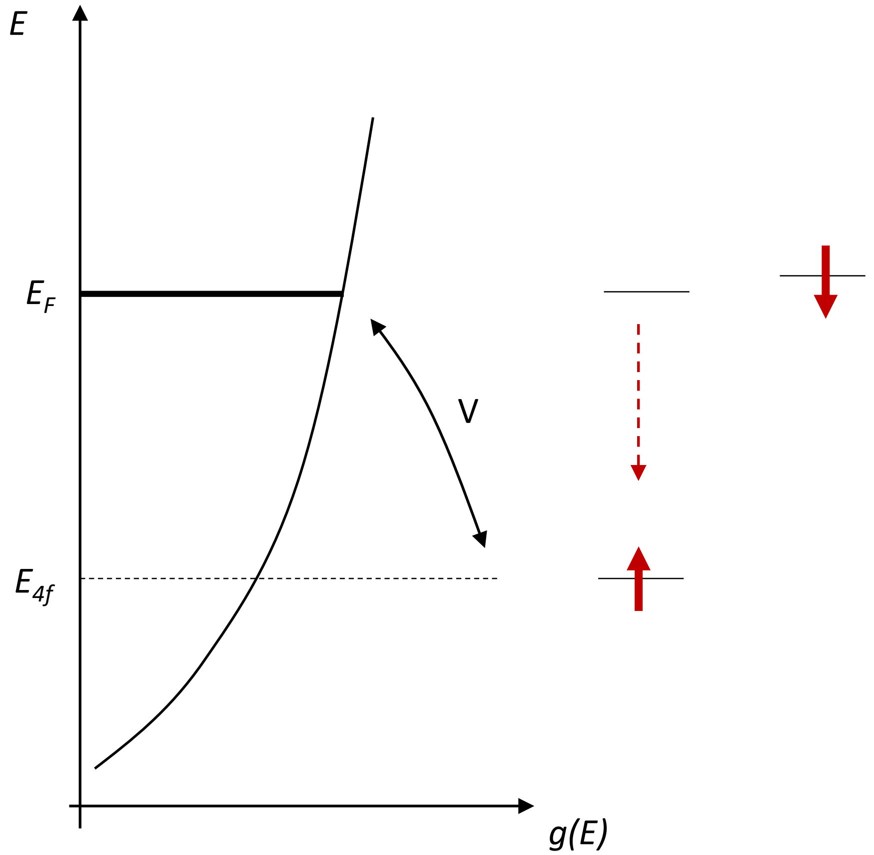

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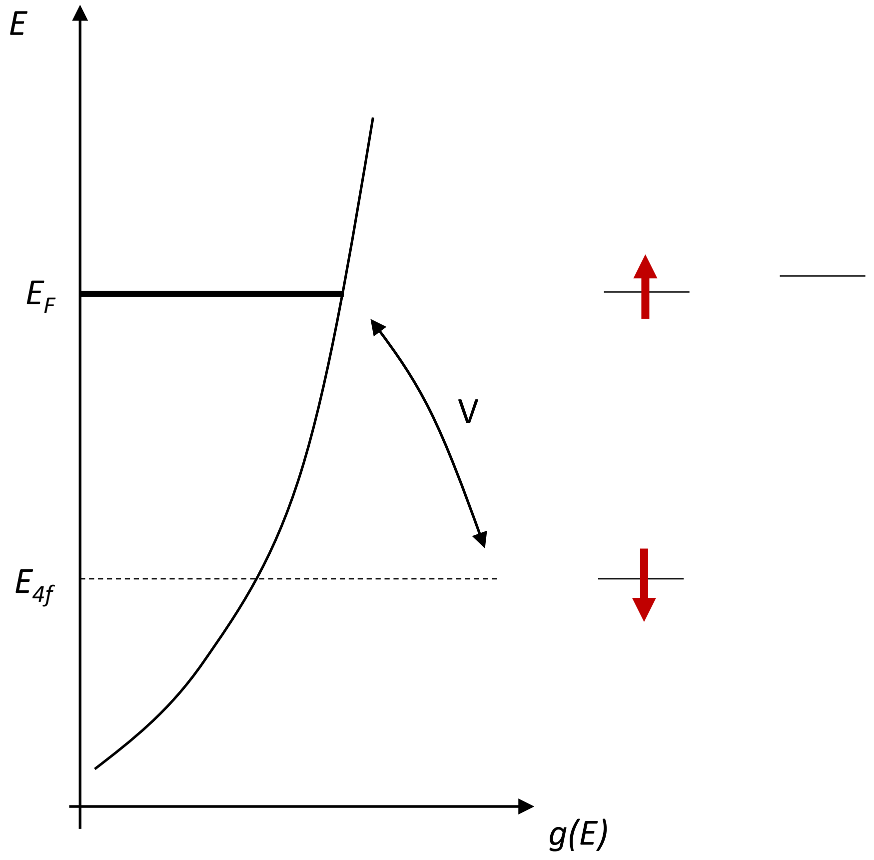

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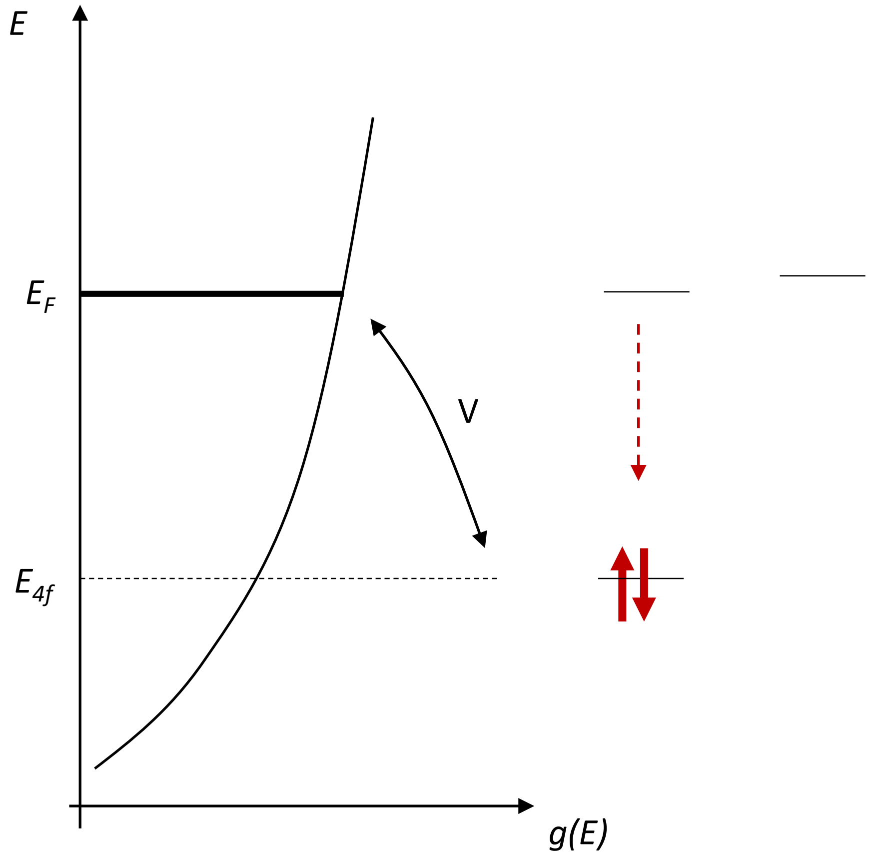

$$\sim \frac{1}{E_{4f} - E_F + U_f}$$

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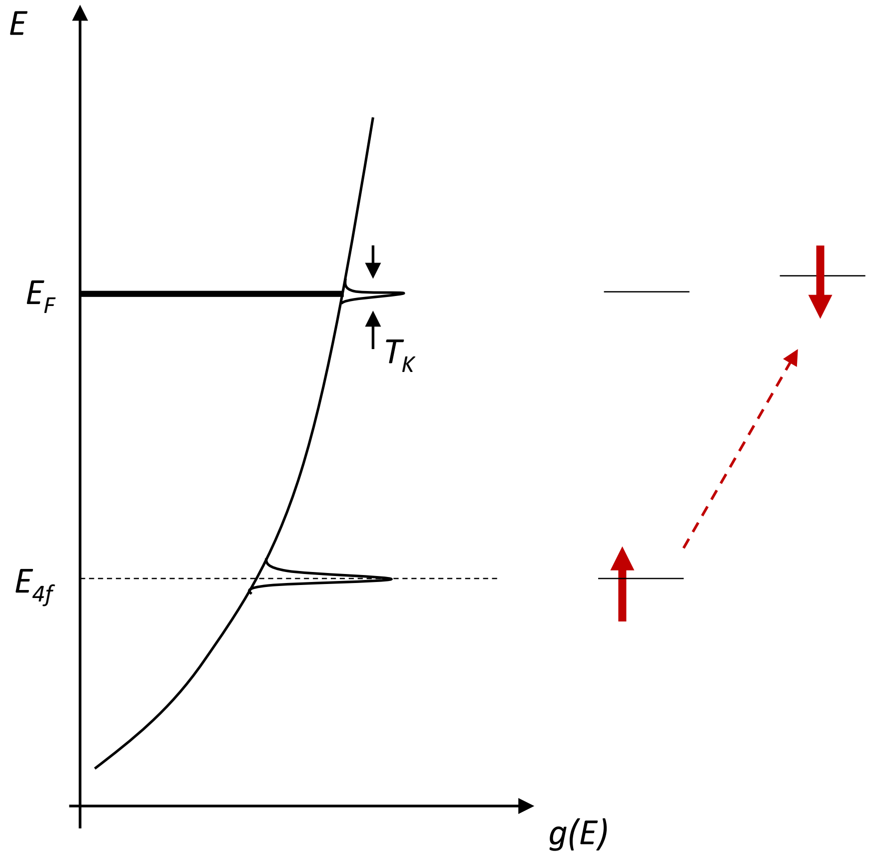


$$\sim \frac{1}{E_{4f} - E_F + U_f}$$

$$J = \frac{2V^2 U}{(E_F - E_{4f})(E_{4f} - E_F + U_f)}$$

$$\mathcal{H} = J\boldsymbol{\sigma}\boldsymbol{S}$$

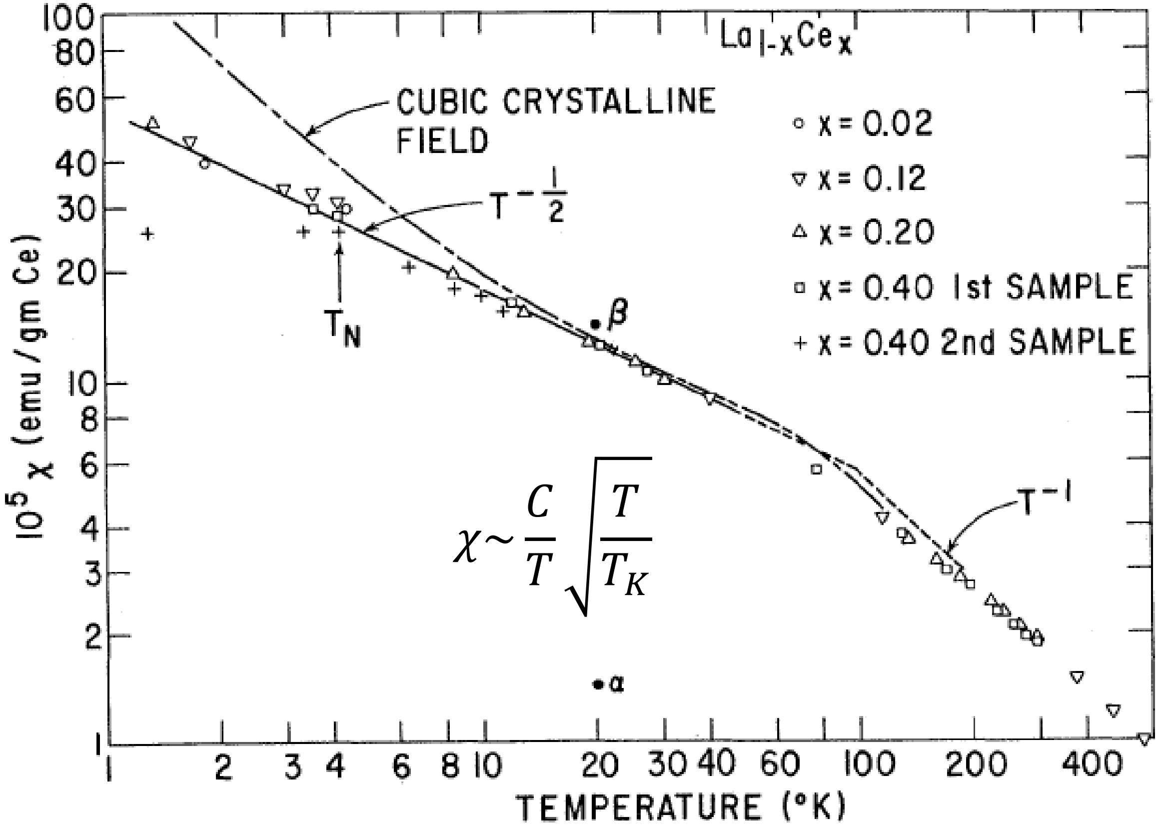
$$T_K \sim E_F e^{-\frac{1}{|J| g(E_F)}}$$

Kondo temperature

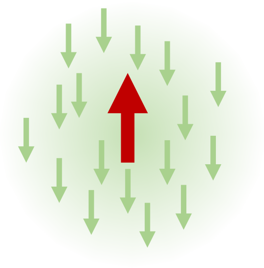
not a phase transition!

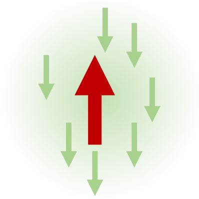
❖ low concentration of impurities

PRL 20, 1348 (1968)



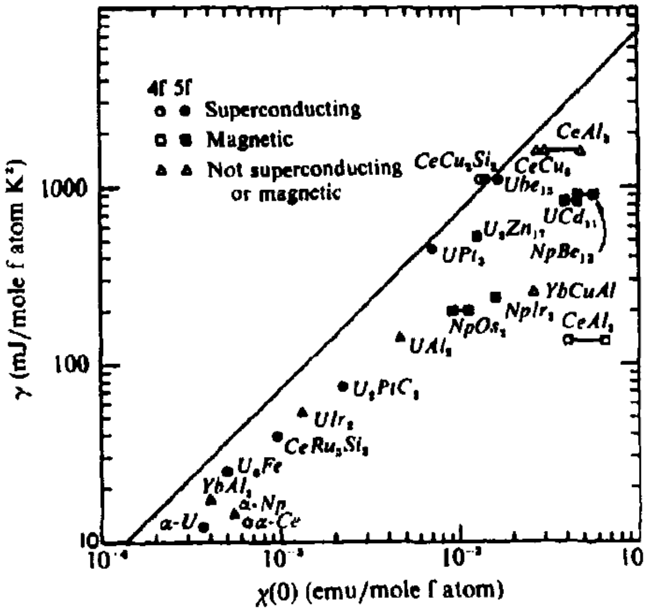
$$\chi \sim \frac{C}{T}\sqrt{\frac{T}{T_K}}$$



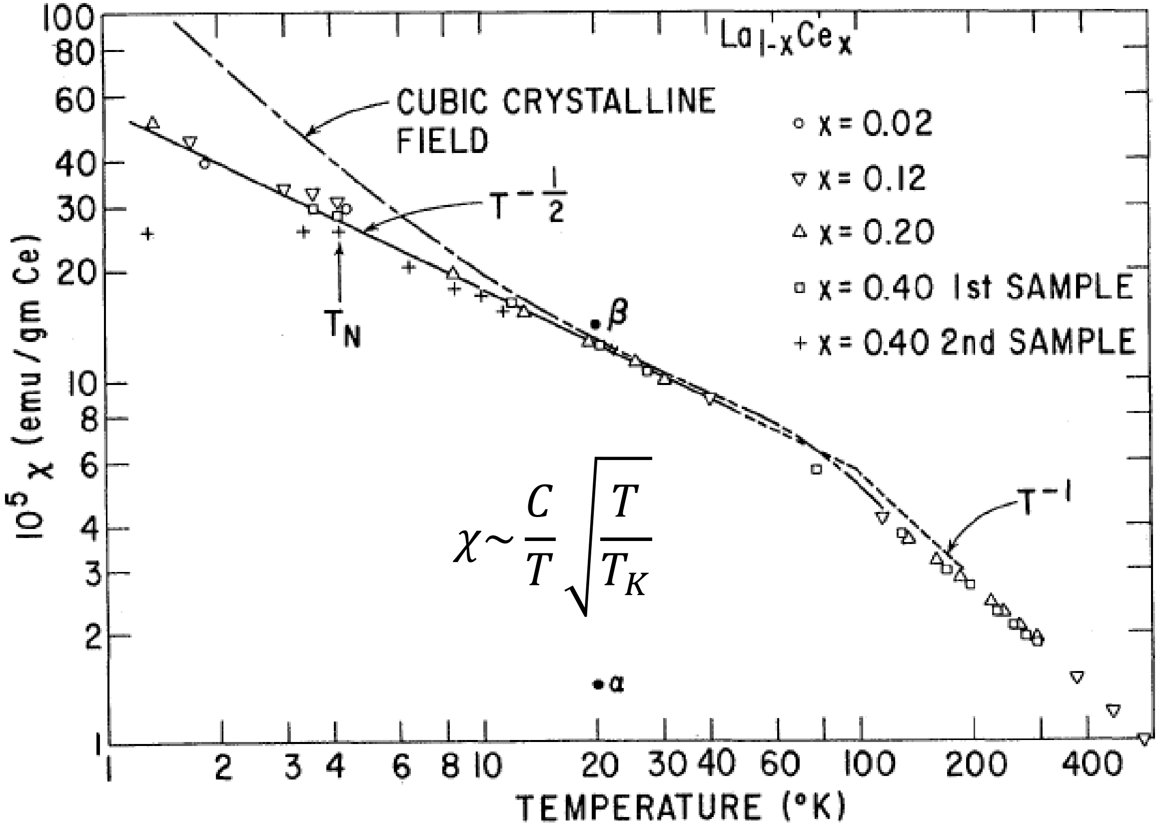


$$\chi = \frac{C}{T}$$

- low concentration of impurities

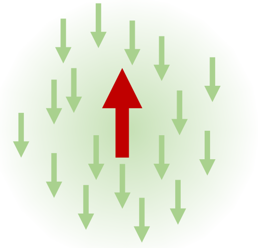


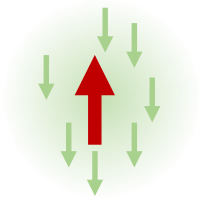
PRL 20, 1348 (1968)



$$\chi \sim \frac{C}{T}\sqrt{\frac{T}{T_K}}$$

- singlet
- large effective mass

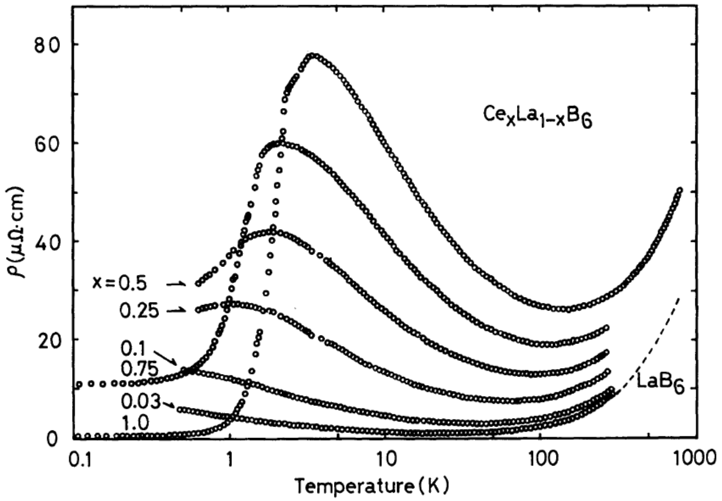




$$\chi = \frac{C}{T}$$

- concentration $\to$ 1

JPSJ 54, 1923 (1985)



$$\left.\begin{array}{l} T_K \sim E_F e^{-\frac{1}{|J| g(E_F)}} \\[2em] T_{RKKY} \sim \dfrac{J^2}{E_F} \dfrac{\cos(2k_F r)}{r^3} \end{array}\right\} f\left(E_F - E_{4f}\right)$$

Khomskii (2014)

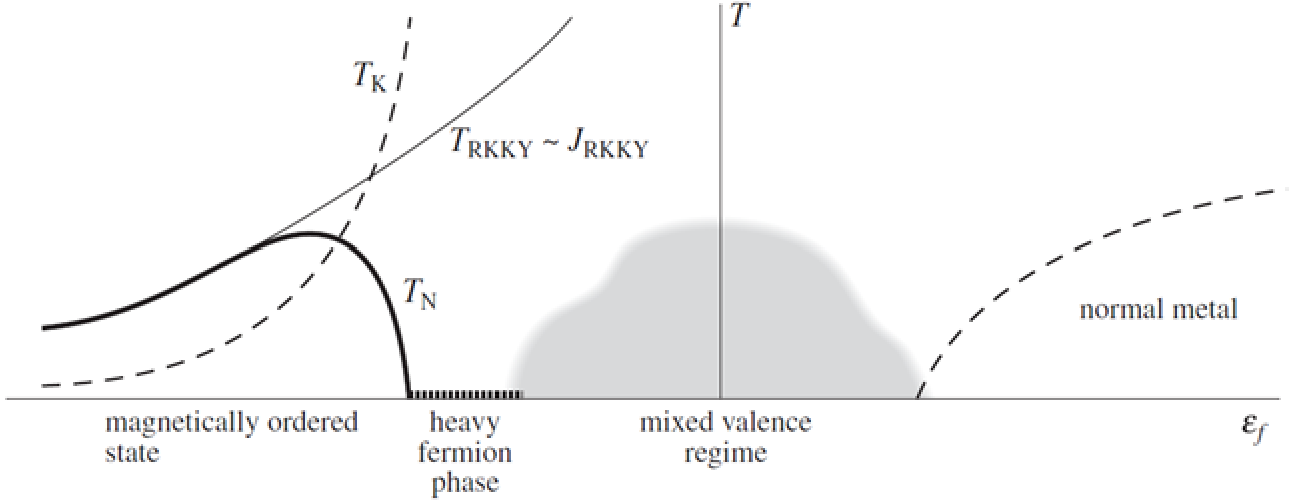
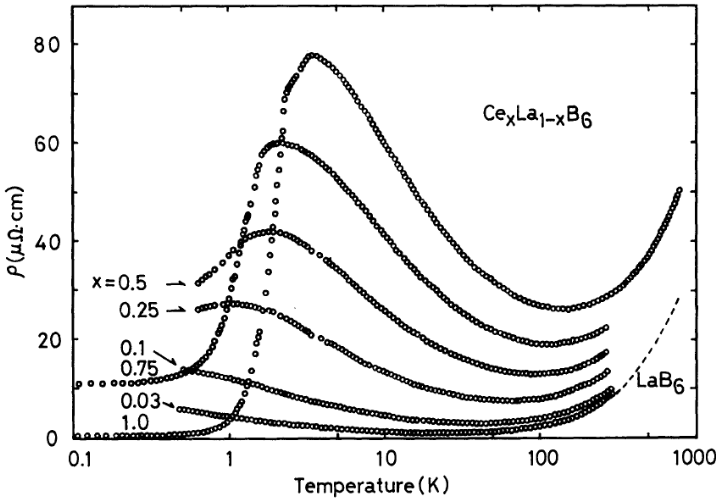


image source: wikimedia.org

- concentration $\rightarrow 1$

JPSJ 54, 1923 (1985)

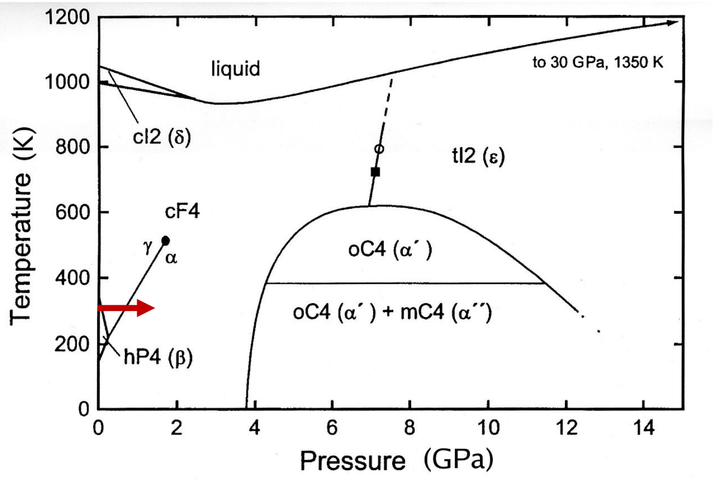


$$T_K \sim E_F e^{-\frac{1}{|J|g(E_F)}}$$

$$T_{RKKY} \sim \frac{J^2}{E_F}\frac{\cos(2k_F r)}{r^3}$$

$$f(E_F - E_{4f})$$

Cerium:



volume collapse due to 4f electron becoming delocalized

Khomskii (2014)

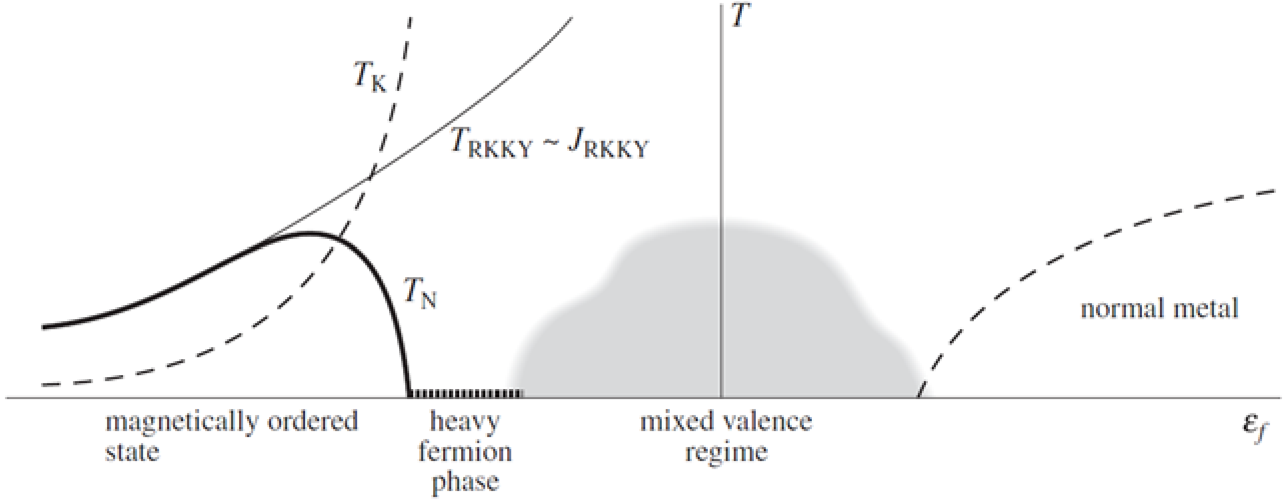
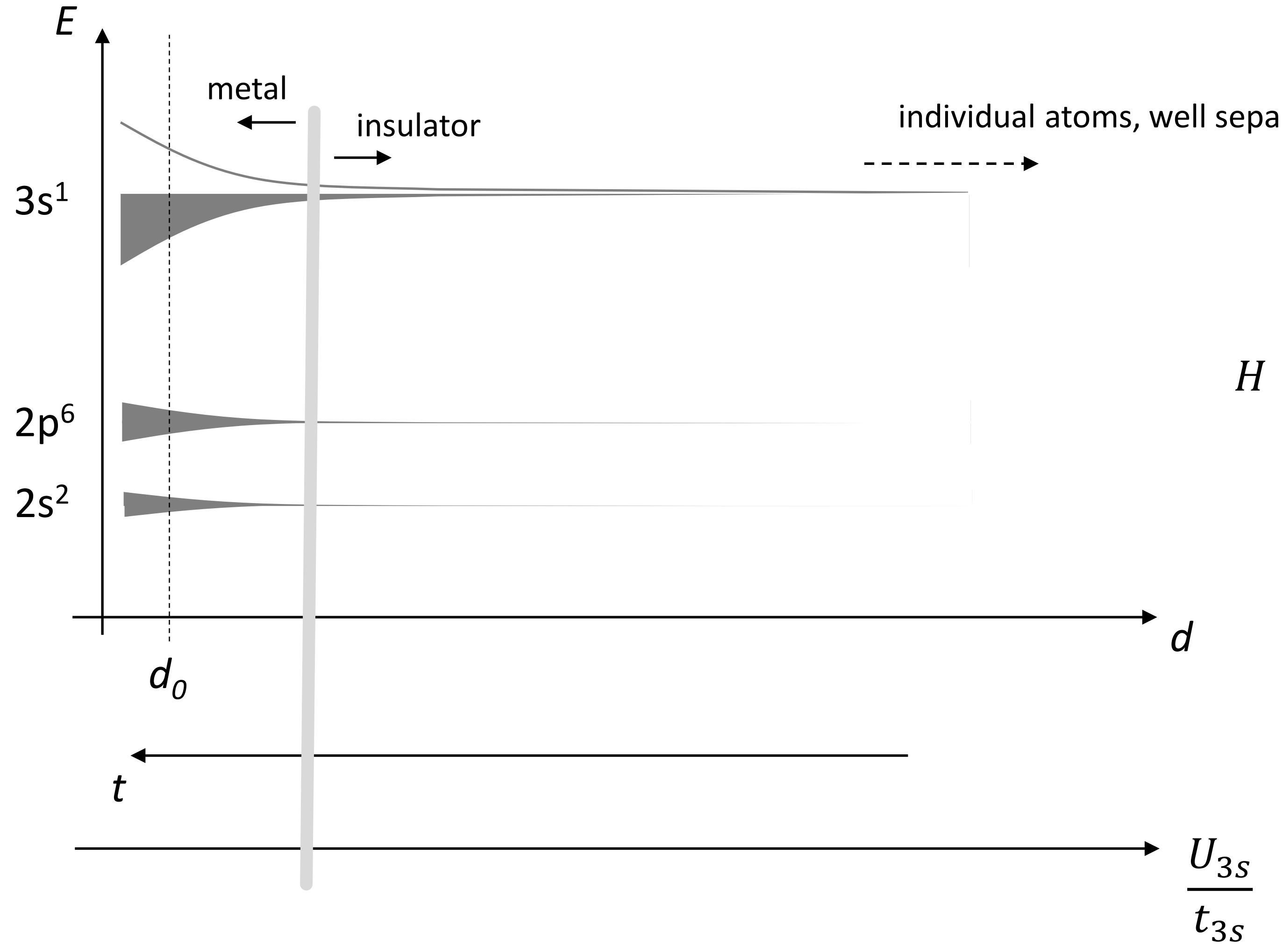
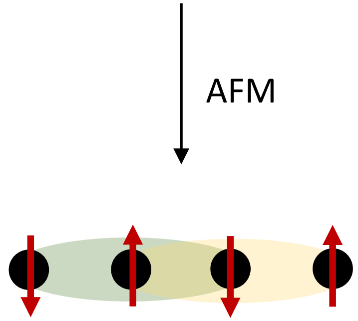


image source: wikimedia.org

Na: $1s^2 2s^2 2p^6 3s^1$

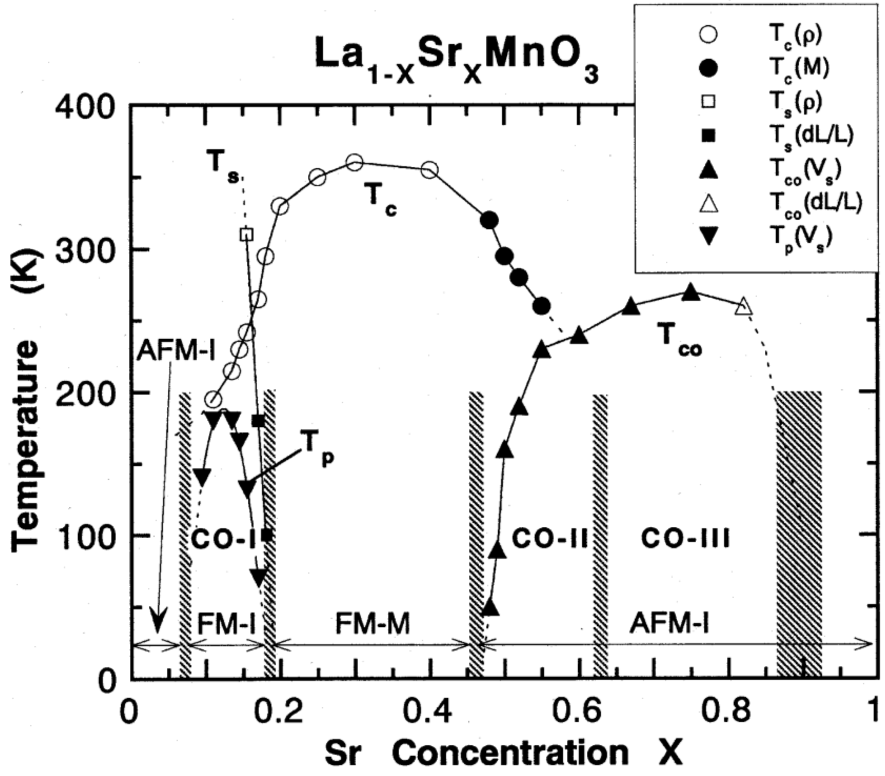


$$H = -t_{3s} \sum_{i,\sigma} \left(c_{i\sigma}^{\dagger} c_{i+1\sigma} + H.c. \right) + U_{3s} \sum_{i} n_{i\uparrow} n_{i\downarrow}$$



what happens with doping?

J. Phys. Soc. Jpn. 67, 2582 (1998)



doping $\rightarrow$ FM

$\rightarrow$ phase separation

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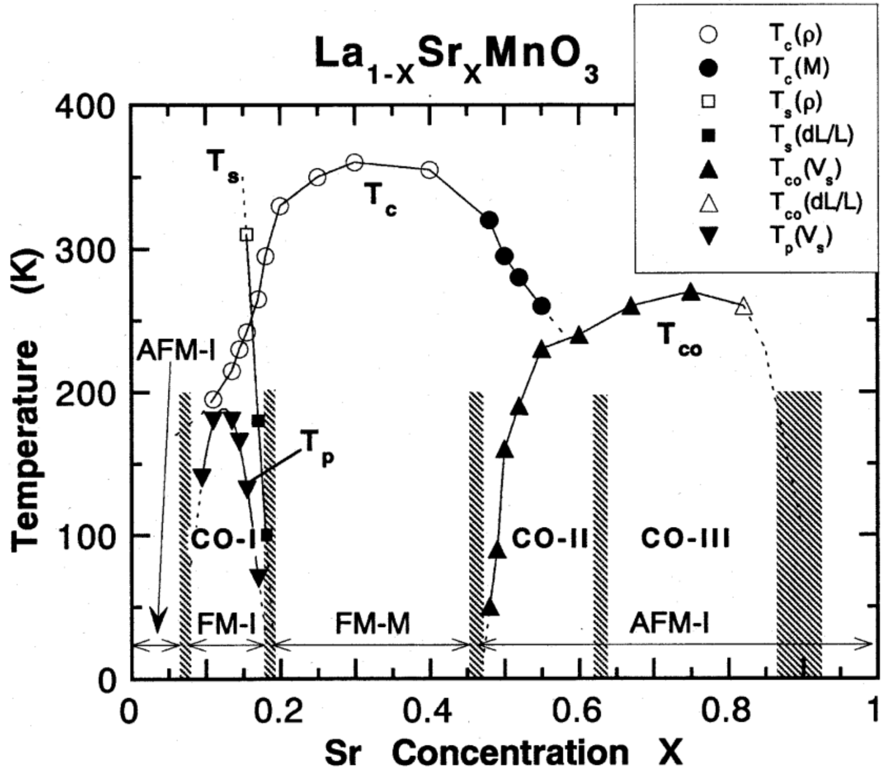

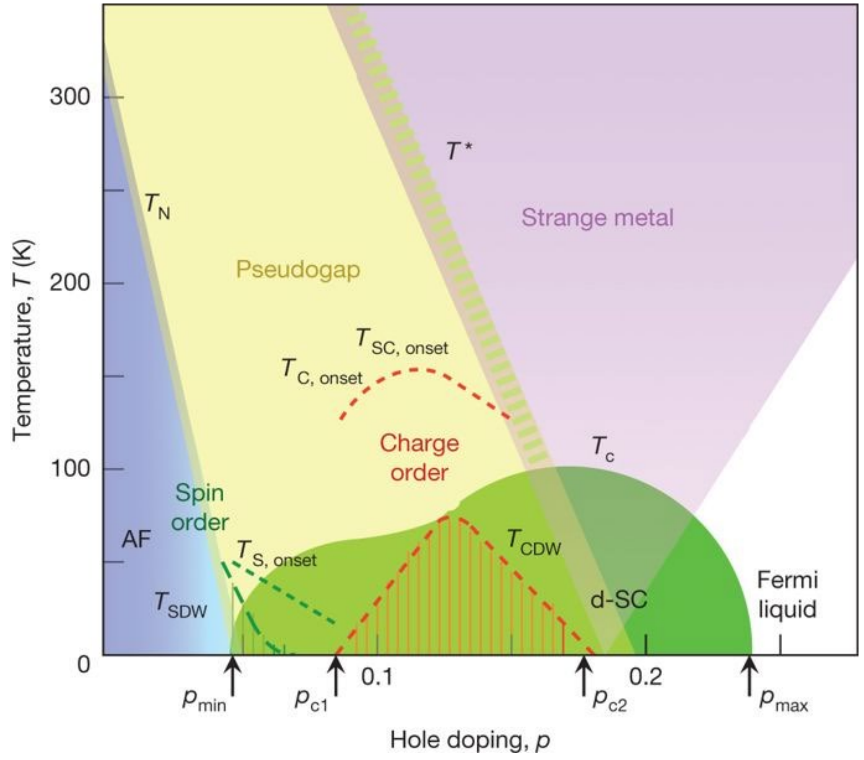

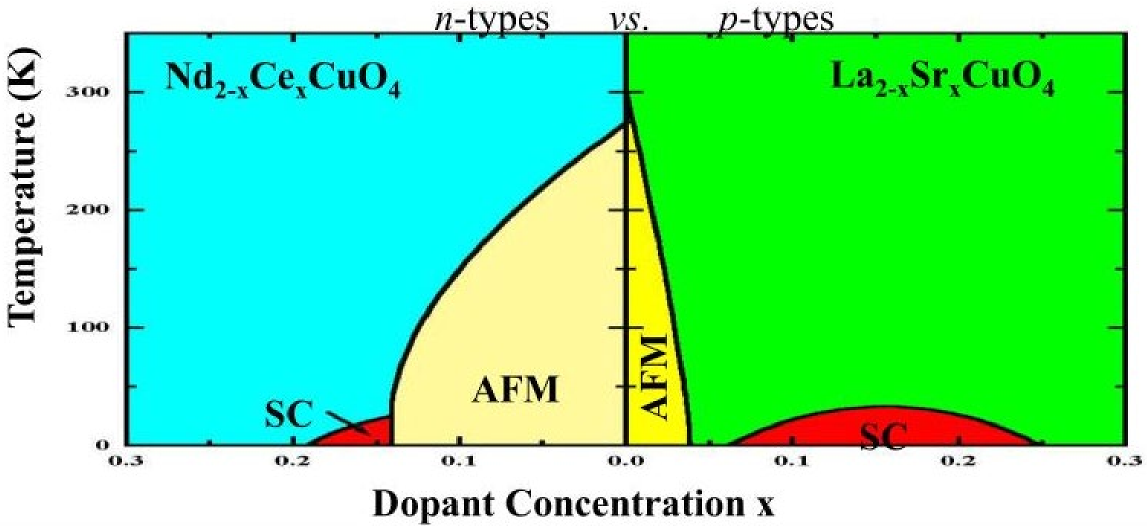

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