Center for Electronic Correlations and Magnetism
University of Augsburg

Ferromagnetism in *f*-electron systems

International Conference on Heavy Electrons (ICHE2010)

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Dieter Vollhardt

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Outline:

- Ferromagnetic *f*-electron materials

- Periodic Anderson model:

  - Influence of degeneracy of the conduction band or *f*-orbital on T_C

  - Effect of binary alloy disorder on T_C

In collaboration with:

Unjong Yu (Augsburg; Gwangju, Korea)
Krzysztof Byczuk (Augsburg; Warsaw)

Magnetism in *f*-electron systems

Tsunetsugu, Sigrist, Ueda (1997)
Fulde, Thalmeier, Zwicknagl (2006)
v. Löhneysen, Rosch, Vojta, Wölfle (2007)
Si, Steglich (2010)

Antiferromagnetism at/near half filling of conduction band

CeM_2Si_2, M=Ag,Au,Pd,Rh — Grier *et al.* (1984)

$UCu_{5-x}Pd_x$ — Chau, Maple (1996); Vollmer *et al.* (2000)

Ferromagnetism

UCu_2Si_2, UCu_2Ge_2 — Chelmicki *et al.* (1985)

$CeRh_3B_2$ — Malik *et al.* (1985)

YbNiSn — Bonville *et al.* (1992)

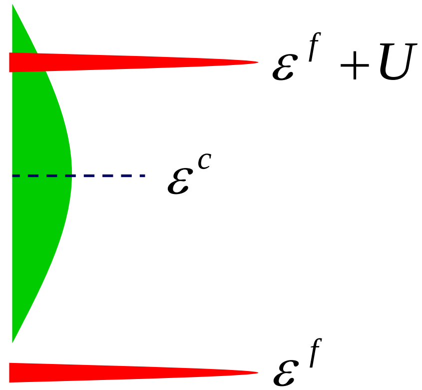
URhSi, URhGe — Tran, Troc, Andre (1998)

CeRuPO — Krellner *et al.* (2007)

$CePd_{1-x}Rh_x$ — Westerkamp *et al.* (2009)

Appropriate model: Periodic Anderson model (PAM)

$$H = \sum_{ij\sigma} t_{ij}^{c} c_{i\sigma}^{+} c_{j\sigma} + \sum_{i} \left(\varepsilon^{f} n_{i}^{f} + \varepsilon^{c} n_{i}^{c} \right) + U \sum_{i} n_{i\uparrow}^{f} n_{i\downarrow}^{f} + V \sum_{i\sigma} \left(c_{i\sigma}^{+} f_{i\sigma} + \text{H.c.} \right)$$



Ferromagnetism found away from half-filling

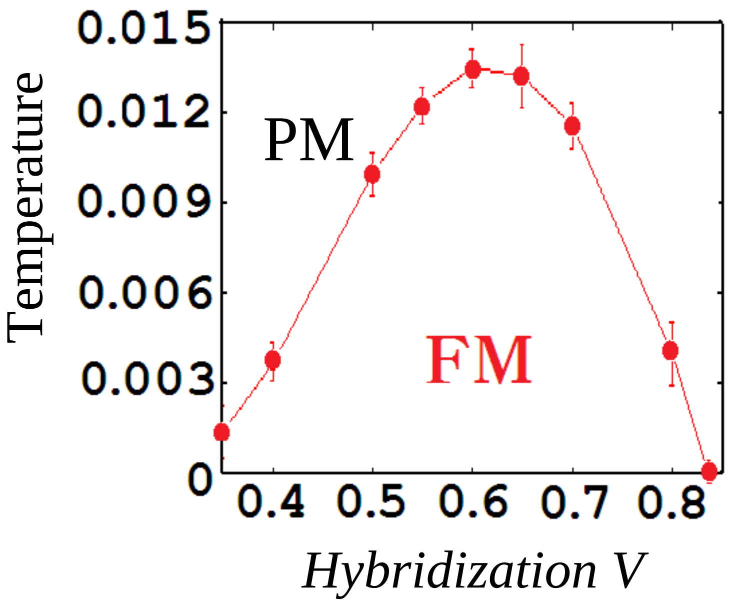
Slave-boson mean-field theory	Möller, Wölfle (1993)
Slave-fermion mean-field theory	Rasul (2000)
DMRG (d=1)	Guerrero, Noack (1996)
DMFT	Tahvildar-Zadeh, Jarrell, Freericks (1997)
	Meyer, Nolting (2000)
Exact ground states	Gulacsi, DV (2005)
Variational Monte Carlo ($CeRh_3B_2$)	Kono, Kuramoto (2006)

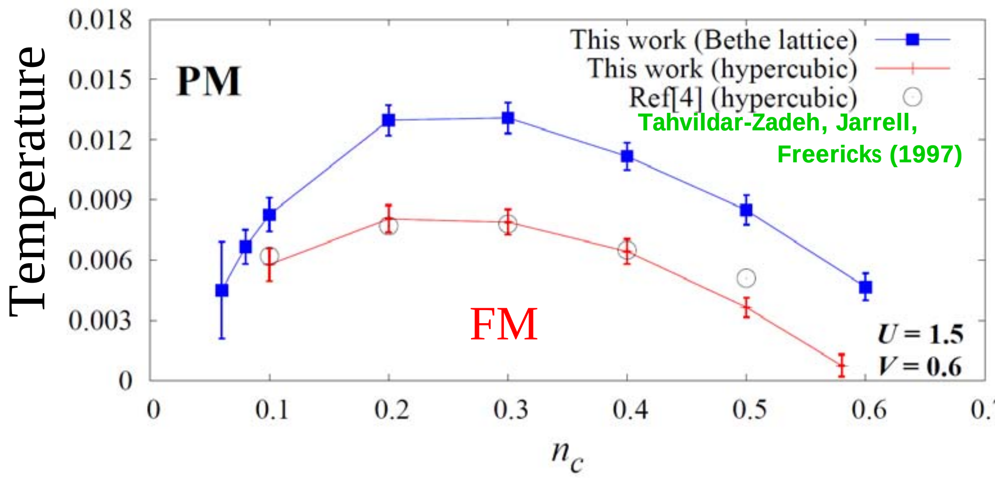
Ferromagnetism in the PAM

Dynamical mean-field theory (DMFT)

Yu, Byczuk, DV (PRB, 2008)

U=1.5, n_{tot}=1.3





Influence of orbital and band degeneracy of f- and conduction electrons on FM?

Hubbard model:
Band degeneracy greatly enhances FM due to Hund's rule coupling
PAM: ?

Ferromagnetism in the PAM:
I. Influence of band and orbital degeneracy

Multi-orbital periodic Anderson model

$$H = \sum_{\langle ij \rangle m\sigma} t_m^c c_{im\sigma}^+ c_{jm\sigma} + \sum_{im} \varepsilon_m^f n_{im}^f + \sum_{im} \varepsilon_m^c n_{im}^c + U \sum_{im} n_{im\uparrow}^f n_{im\downarrow}^f$$

$$+ \sum_{i\sigma_1\sigma_2} \sum_{m_1<m_2} \left(U' - \delta_{\sigma_1\sigma_2} F \right) n_{im_1\sigma_1}^f n_{im_2\sigma_2}^f + V \sum_{i\sigma} \sum_{m_1 m_2} \left(c_{im_1\sigma}^+ f_{im_2\sigma} + \text{H.c.} \right)$$

orbital index $m = 1, 2, \cdots, D^{c,f}$ for c, f - electrons

U : intra-orbital Coulomb interaction

U' : inter-orbital Coulomb interaction

F : Hund's rule coupling

Calculation details

Yu, Byczuk, DV (PRB, 2008)

- Degenerate bands: $t_m^c = t^c\,,\quad \varepsilon_m^c = \varepsilon^c\,,\quad \varepsilon_m^f = \varepsilon^f$

- DOS: $N(\varepsilon) = (1/2\pi)\sqrt{4-\varepsilon^2}$; band-width $= 4t^c$ (energy unit)

- Parameters: $U = 1.5,\ V = 0.6,\ U' = 1.1,\ F = 0.2$

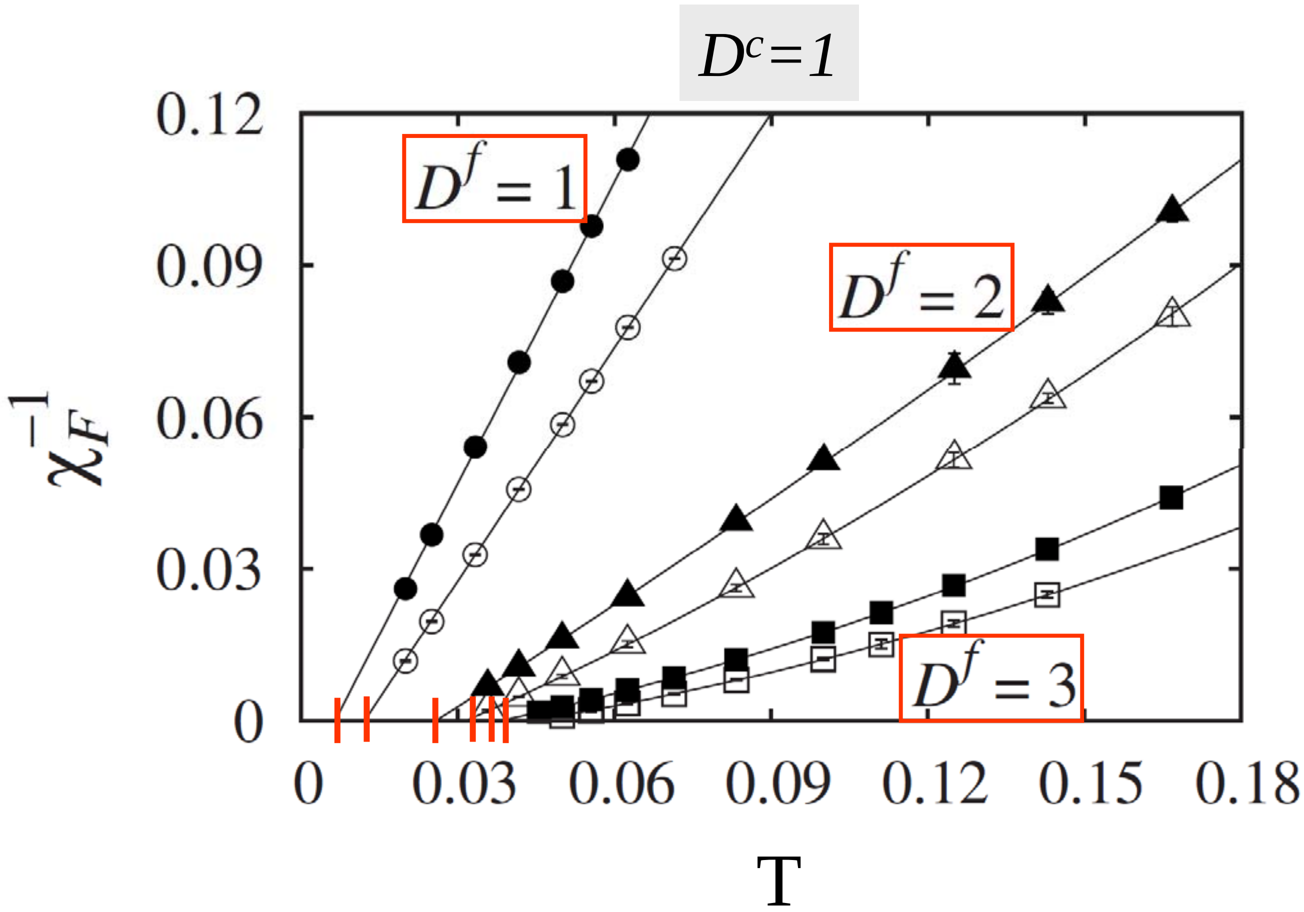
$$\mu = \varepsilon^f + U/2 + (D^f - 1)(U' - F/2)$$

→ f-level ~ half filled → formation of local moments

- Calculational method: Dynamical mean-field theory (DMFT) +QMC

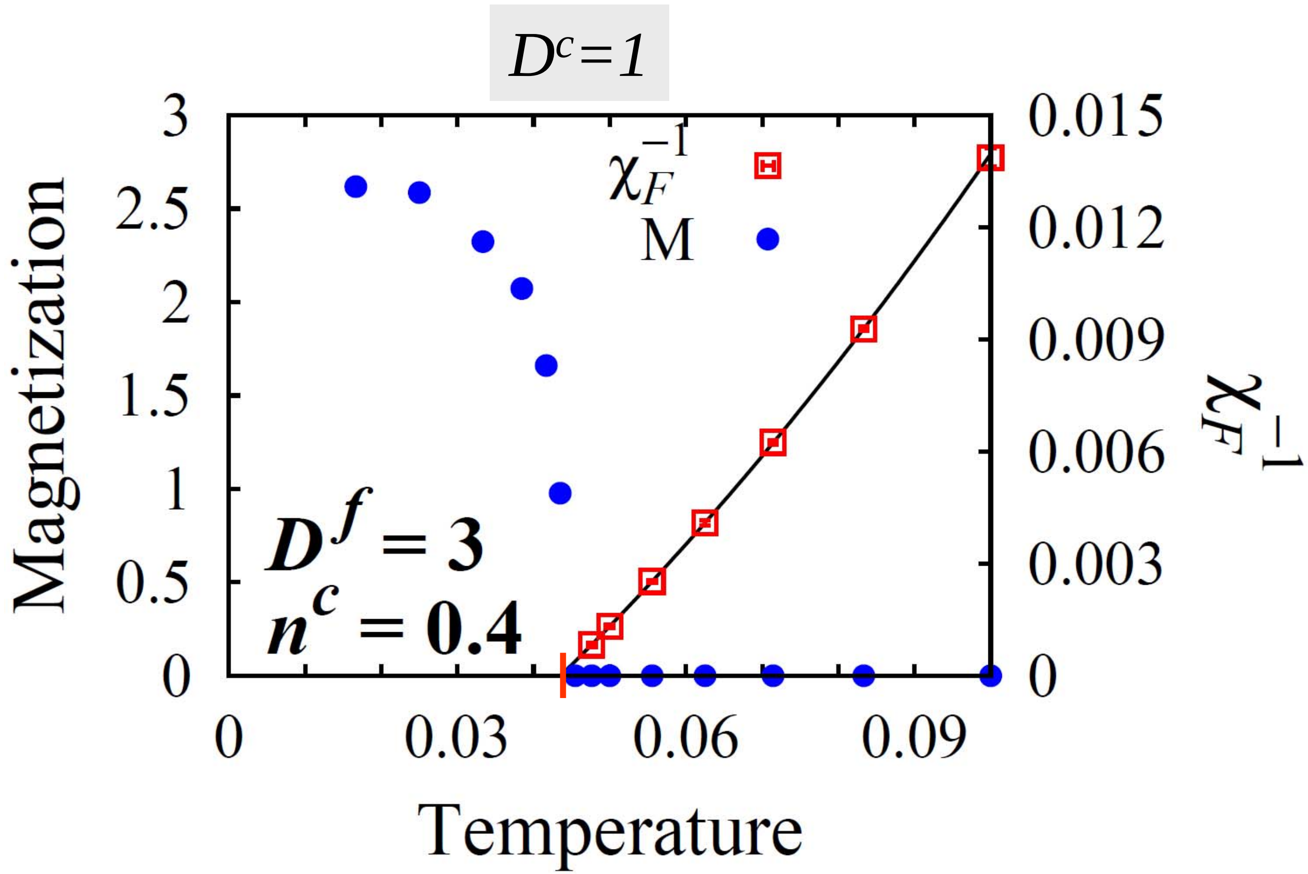
Determination of T_c

Yu, Byczuk, DV (PRB, 2008)



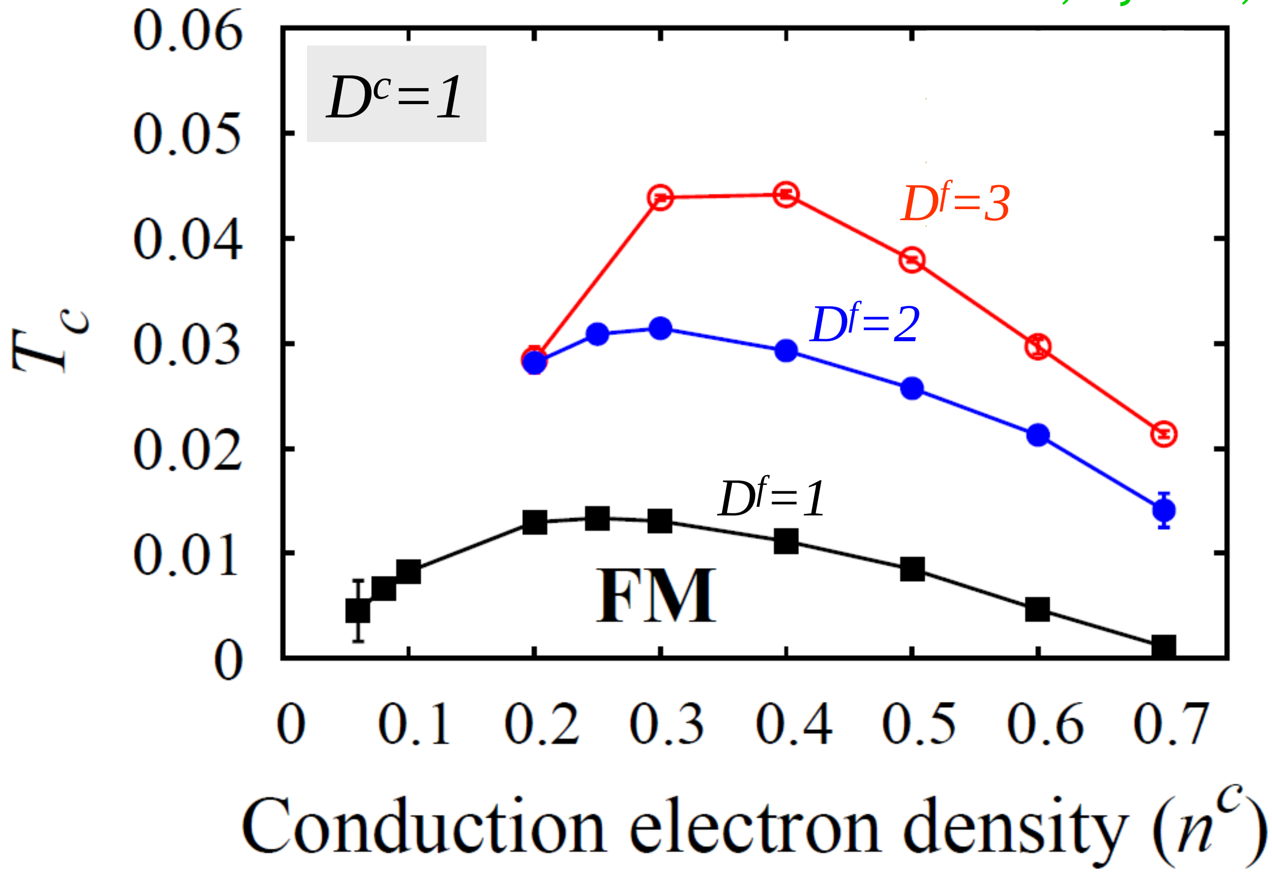
Determination of T_c

Yu, Byczuk, DV (PRB, 2008)



Magnetic phase diagram for different *f*-level degeneracy D^f

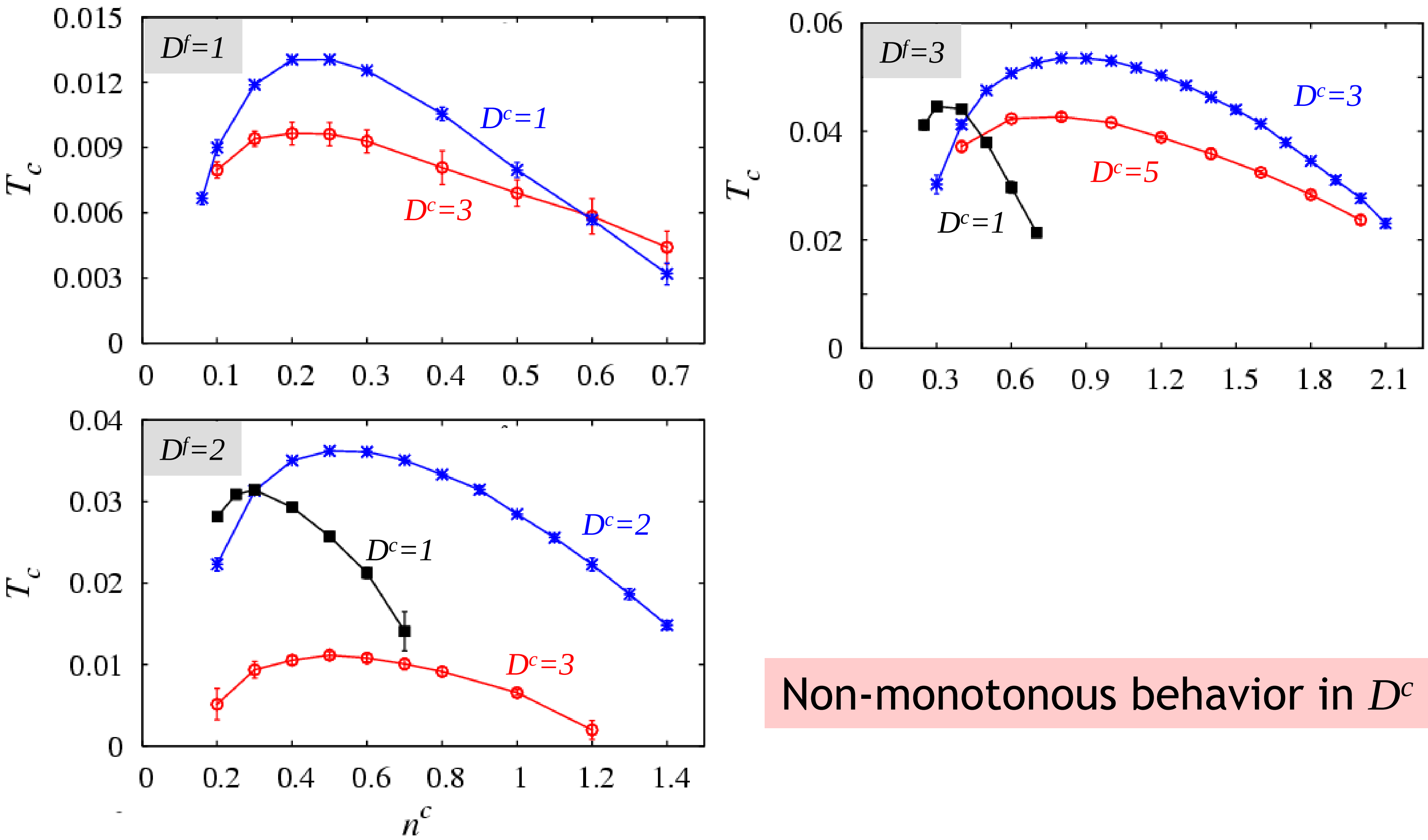
Yu, Byczuk, DV (PRB, 2008)



Local moment, and therefore T_C, increases with *f*-level degeneracy

Magnetic phase diagram for different band degeneracy D^c

Yu, Byczuk, DV (PRB, 2008)



Non-monotonous behavior in D^c

Mean-field ansatz for T_c in the RKKY-model

Dietl *et al.* (1999)

$$T_c(U,V,\mu) = T_c^0(U,V,\mu) F^f(\mu-\varepsilon^f) F^c(\mu-\varepsilon^c)$$

Formation of local *f*-electron moments (F^f) is independent of their ordering mediated by the *c*-electron (F^c)

$$F^f(\underbrace{\mu-\varepsilon^f}_{\text{fixed}}) \propto J_{\text{eff}}^2 S(S+1) \quad \text{with} \quad J_{\text{eff}} = -\frac{8V^2}{U_{\text{eff}}}$$

$$U_{\text{eff}} = E(n_0^f+1) + E(n_0^f-1) - 2E(n_0^f)$$

Half filled *f*-level: $n_0^f = D^f,\; U_{\text{eff}} = U + (D^f-1)F$

$$\overset{S=\frac{D^f}{2}}{\Rightarrow} \quad F^f \propto \frac{(D^f/2)(D^f/2+1)}{U_{\text{eff}}^2}$$

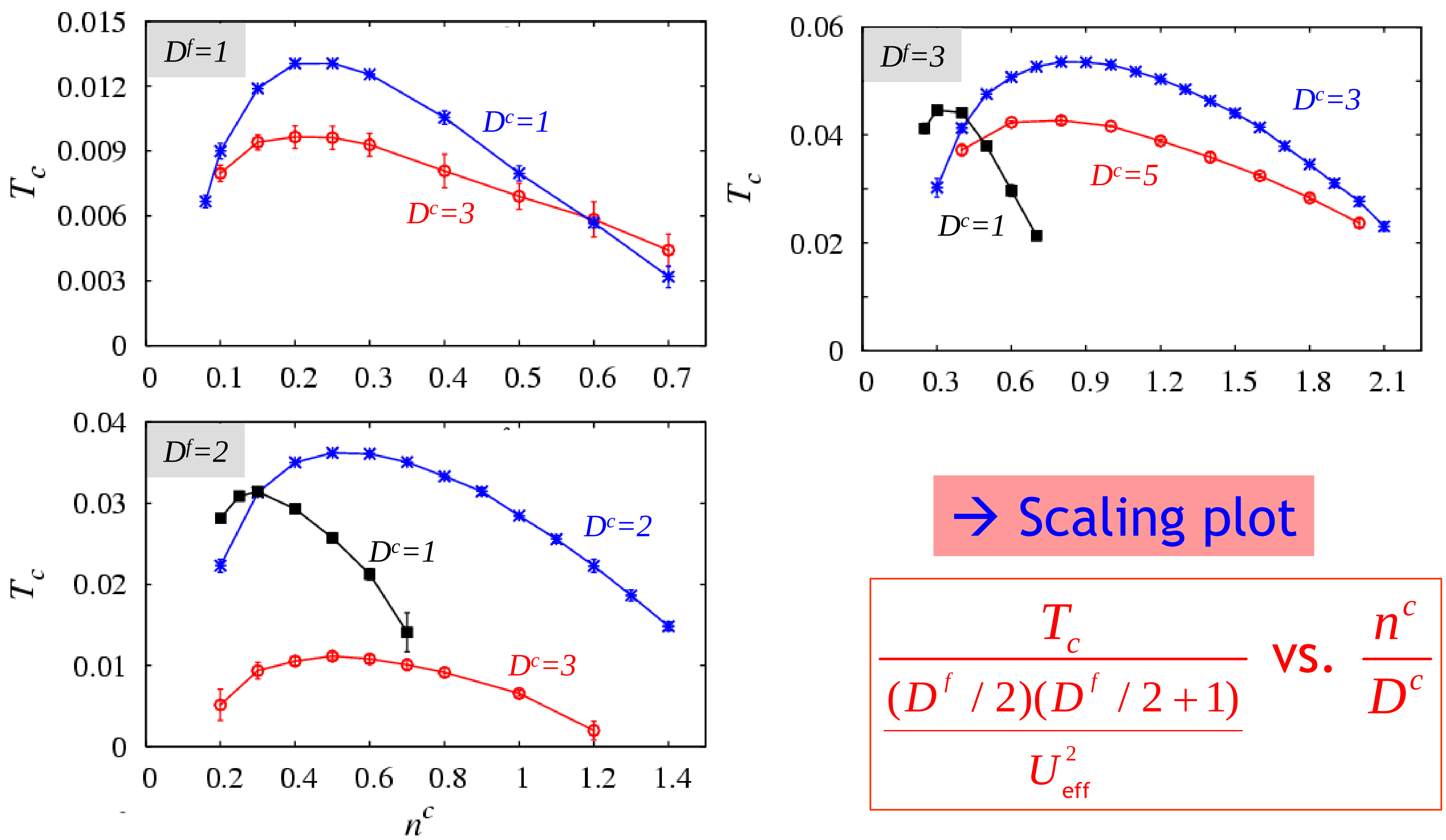
$$F^c = F^c(n_{\text{eff}}^c), \quad n_{\text{eff}}^c = \frac{n^c}{D^c}$$

→ $\dfrac{T_c}{\dfrac{(D^f/2)(D^f/2+1)}{U_{\text{eff}}^2}}$ vs. $\dfrac{n^c}{D^c}$ should be a universal curve

Yu, Byczuk, DV (PRB, 2008)

Magnetic phase diagram for different band degeneracy D^c

Yu, Byczuk, DV (PRB, 2008)

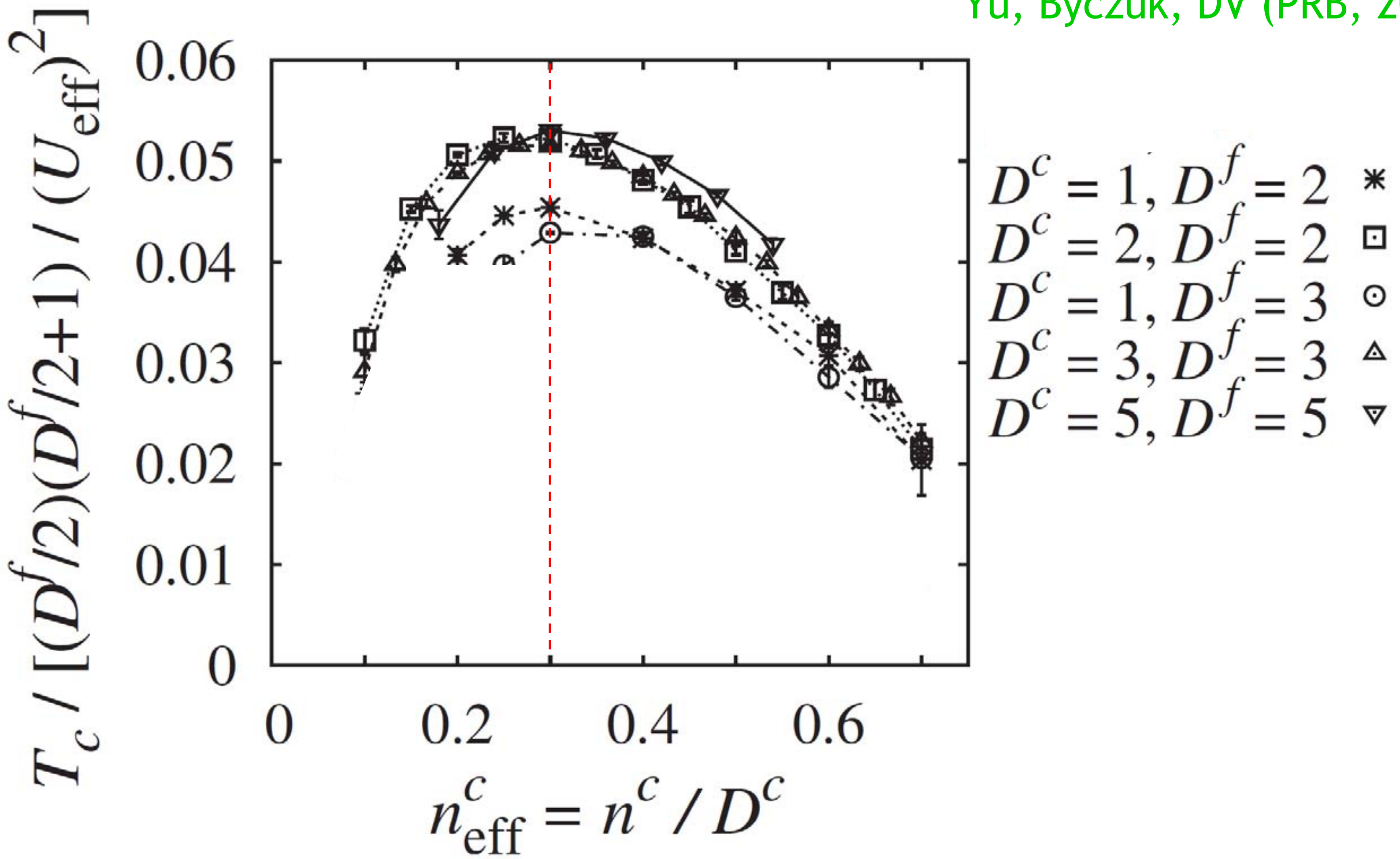


→ Scaling plot

$$\frac{T_c}{\dfrac{(D^f/2)(D^f/2+1)}{U_{\text{eff}}^2}} \quad \text{vs.} \quad \frac{n^c}{D^c}$$

Scaling plot

Yu, Byczuk, DV (PRB, 2008)



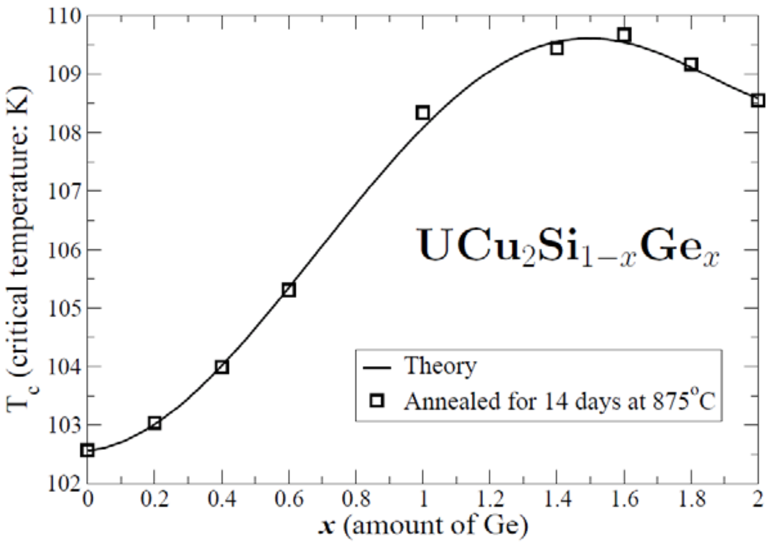
$T_c^{\max}$ at $n^c_{\mathrm{eff}} \approx 0.3$

Ferromagnetism in the PAM:
II. Influence of disorder

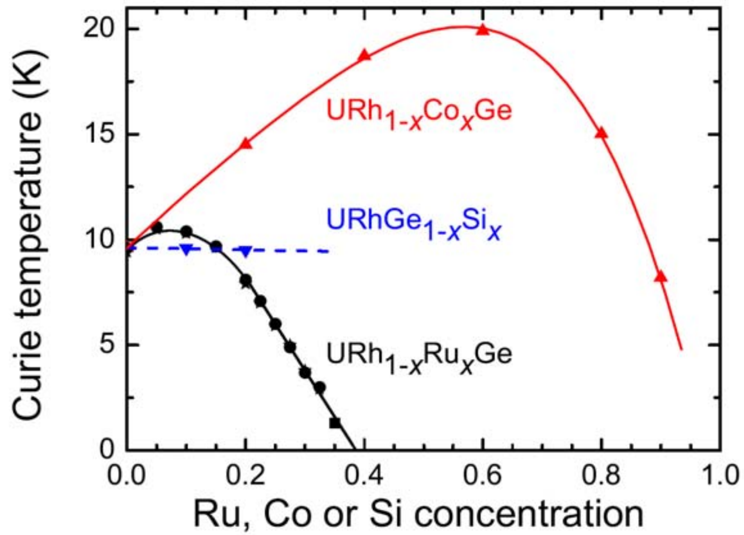
Alloying of f-electron materials introduces disorder

→ in general, reduction of T_c

But:



Silva Neto *et al.* (2003)



Sakarya *et al*. (2008)

→ Alloying can enhance ferromagnetism

PAM with disorder

$$H=\sum_{ij\sigma} t_{ij}^{c} c_{i\sigma}^{+} c_{j\sigma} + \sum_{i}\left(\varepsilon^{f} n_{i}^{f} + \varepsilon^{c} n_{i}^{c}\right) + U\sum_{i} n_{i\uparrow}^{f} n_{i\downarrow}^{f} + V\sum_{i\sigma}\left(c_{i\sigma}^{+} f_{i\sigma} + \text{H.c.}\right)$$

$\varepsilon^{f}, \varepsilon^{c}$: random variables (binary alloy disorder)

Yoshimori, Kasai (1986)
Schlottmann (1992)
Miranda, Dobrosavljevic, Kotliar (1997)
Meyer (2002)
Grenzebach, Anders, Czycholl, Pruschke (2008)

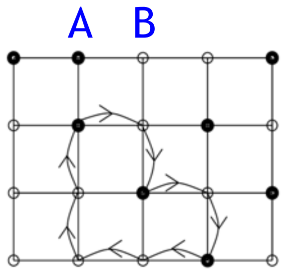
Effects of binary alloy disorder in the conduction electrons?

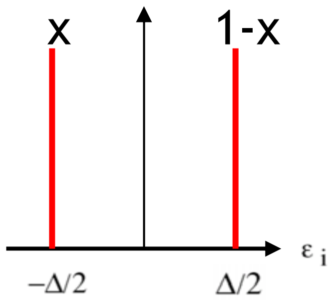
Simpler: Hubbard model

$$H = -t \sum_{\langle \mathbf{i},\mathbf{j} \rangle,\sigma} c^{\dagger}_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} + U \sum_{\mathbf{i}} n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow} + \sum_{\mathbf{i}\sigma} \varepsilon_i n_{\mathbf{i}\sigma}$$

Binary alloy disorder (alloys $A_{1-x}B_x$, *e.g.*, $Fe_{1-x}Co_x$):

$$P(\epsilon_i) = x\delta\left(\epsilon_i + \frac{\Delta}{2}\right) + (1-x)\delta\left(\epsilon_i - \frac{\Delta}{2}\right)$$





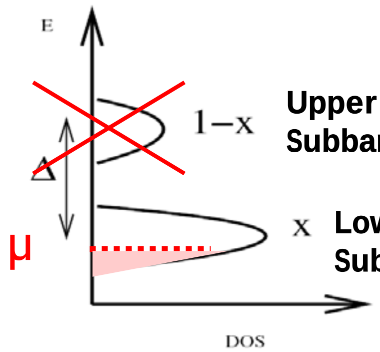
Δ: disorder strength

A,B-atoms: $N_{A,B}$
lattice sites: N_L

→ concentration $x=N_A/N_L$, $1-x=N_B/N_L$

Alloy band splitting

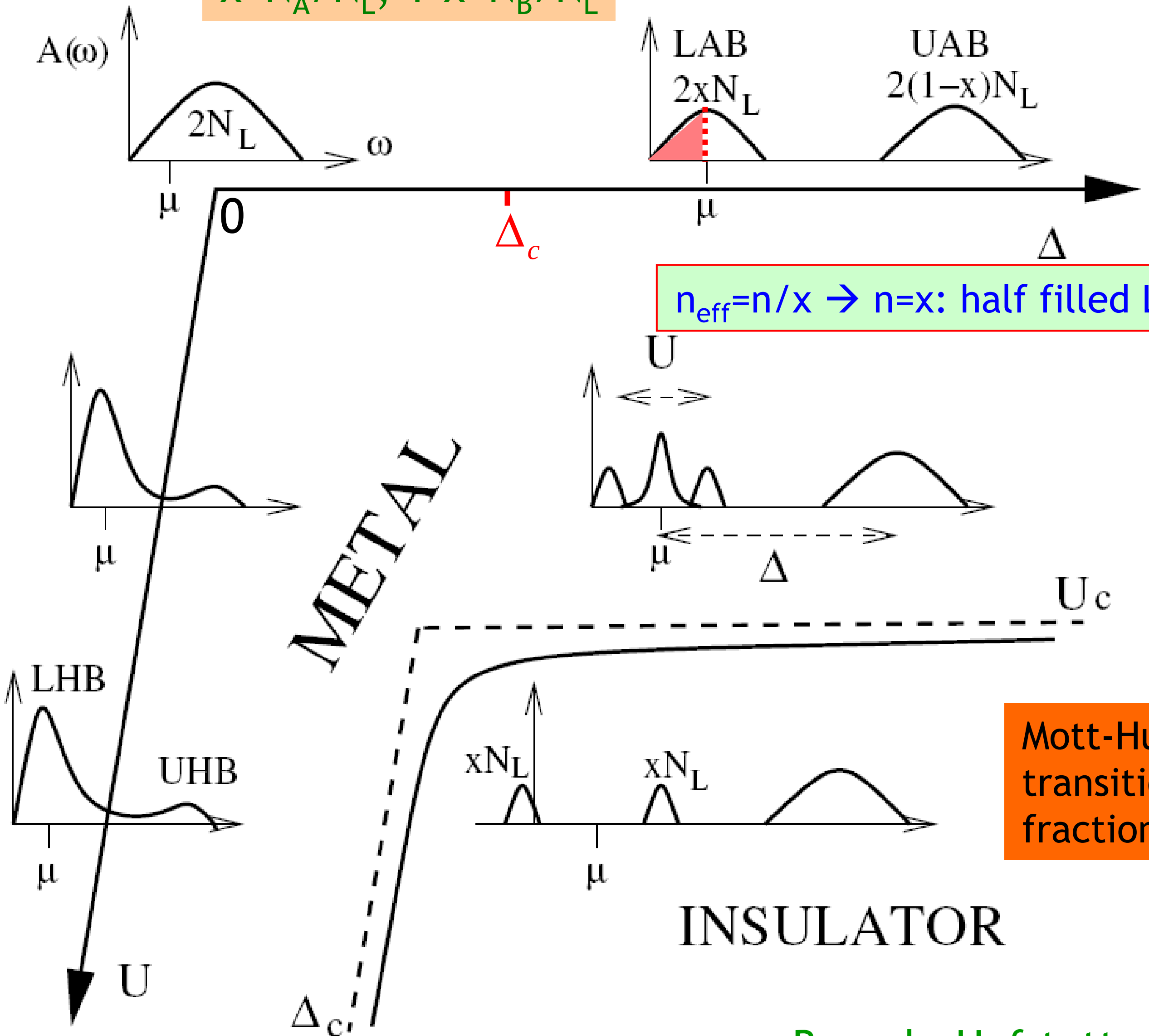
$$\Delta > \Delta_c \gg \max(|t|, U)$$



Effective filling $n_{\text{eff}} = \dfrac{n}{x}$

Mott-Hubbard transition at fractional filling

$x=N_A/N_L$, $1-x=N_B/N_L$



$n_{eff}=n/x$ → $n=x$: half filled LAB

Mott-Hubbard transition at fractional filling

Byczuk, Hofstetter, DV (2004)

Analogous effect in PAM with binary alloy disorder of c-electrons → Metal to "alloy Kondo insulator" transition at fractional filling

$$H=\sum_{ij\sigma} t^c_{ij} c^+_{i\sigma} c_{j\sigma} + \sum_i \left(\varepsilon^f_i n^f_i + \varepsilon^c_i n^c_i\right) + U\sum_i n^f_{i\uparrow} n^f_{i\downarrow} + V\sum_{i\sigma}\left(c^+_{i\sigma} f_{i\sigma} + \text{H.c.}\right)$$

$$P(\varepsilon_i) = x\delta(\varepsilon_i - \varepsilon^0) + (1-x)\delta(\varepsilon_i - \varepsilon^0 - \Delta)$$

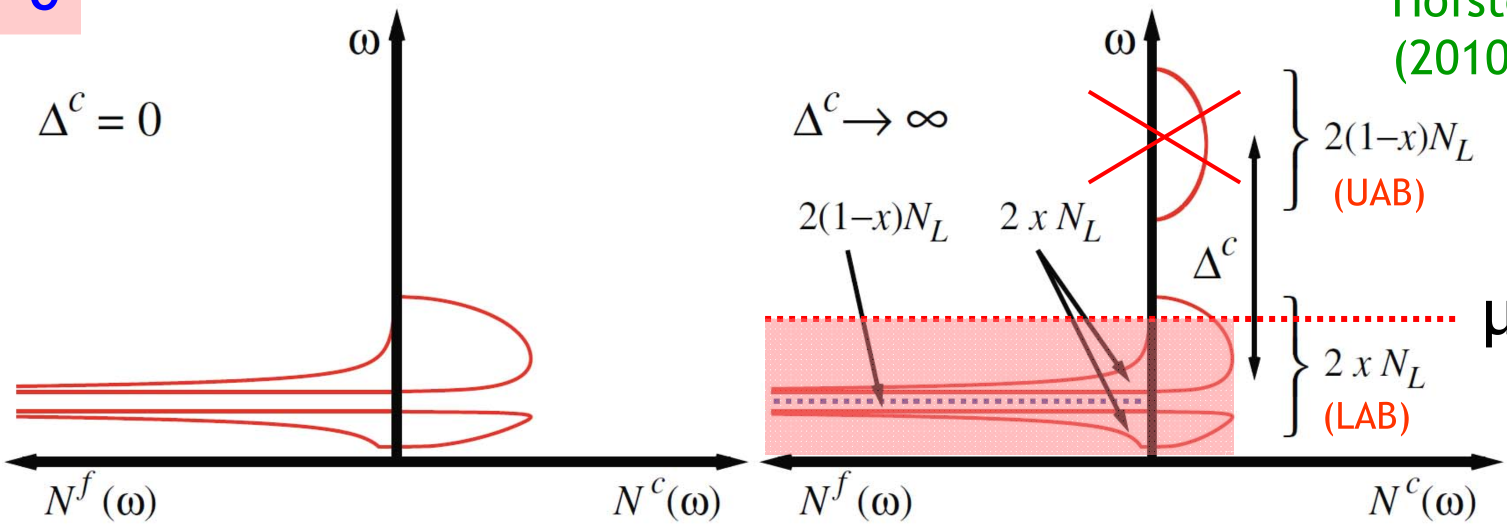
Local energies $\varepsilon_i = \varepsilon^c, \varepsilon^f$

Energy splitting $\Delta = \Delta^c, \Delta^f$

x: alloy concentration

U=0

Byczuk, Yu, Hofstetter, DV (2010)



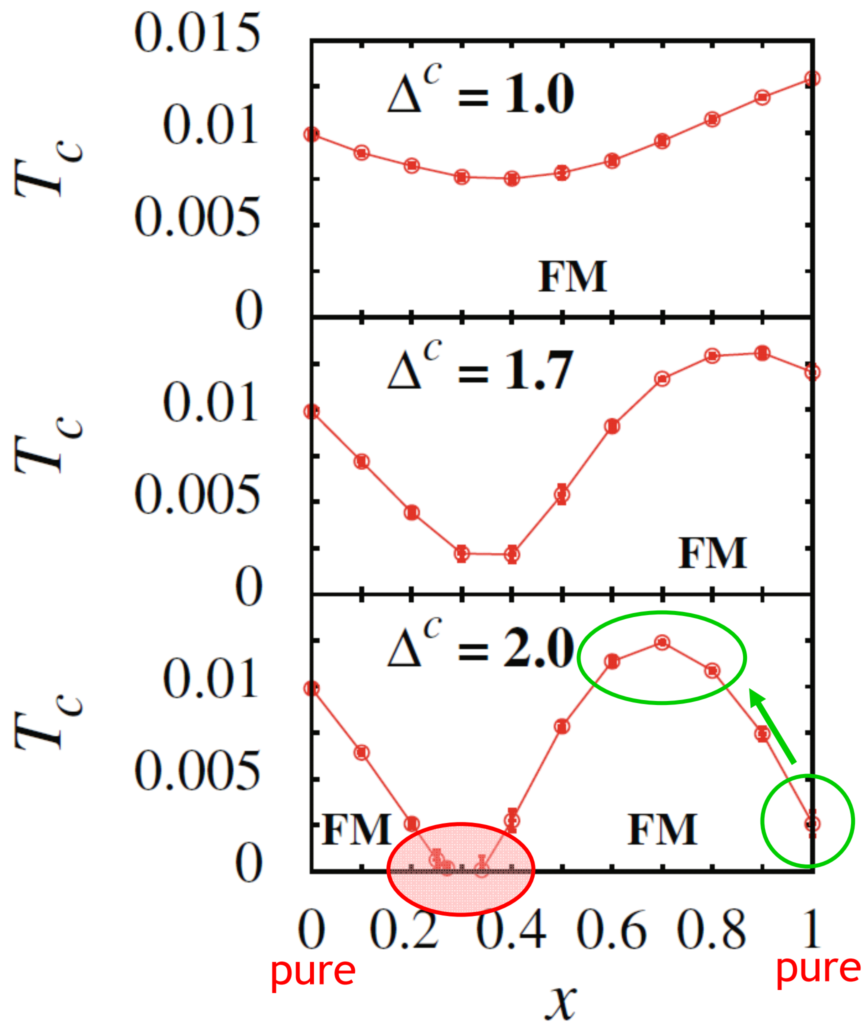
$$n^{\text{eff}}_{tot} = \frac{2n_{tot}}{1+x}$$

Disordered c-electrons

x: alloy concentration
Δ^c: disorder strength

Yu, Byczuk, DV (2008, 2010)

$U = 1.5, \quad V = 0.6$
$n_{tot} = 1.3$
$\varepsilon_0^c - \varepsilon_0^f = 3.25$



Enhancement of T_c

$T_c = 0$ at $x = 0.3$

Why ?

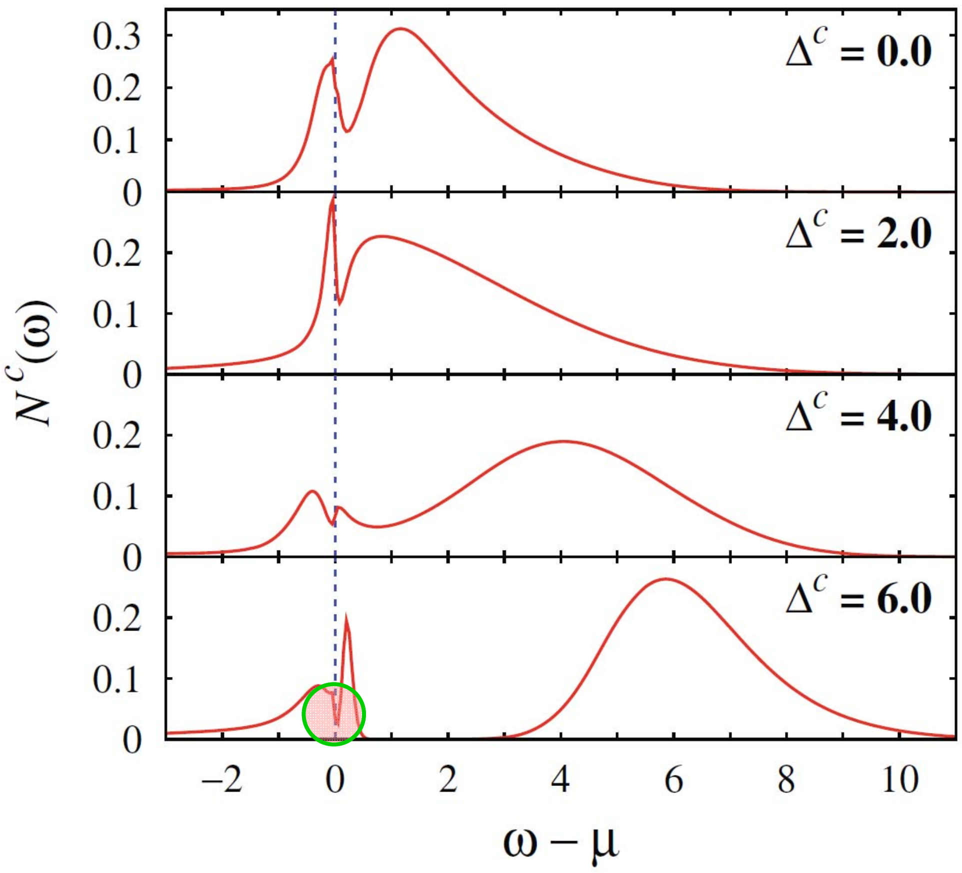
Disordered c-electrons

x: alloy concentration
Δ^c: disorder strength

Yu, Byczuk, DV (2008, 2010)

$$U = 1.5, \quad V = 0.6$$
$$n_{tot} = 1.3$$
$$\varepsilon_0^c - \varepsilon_0^f = 3.25$$

Spectral function for $x=0.3$



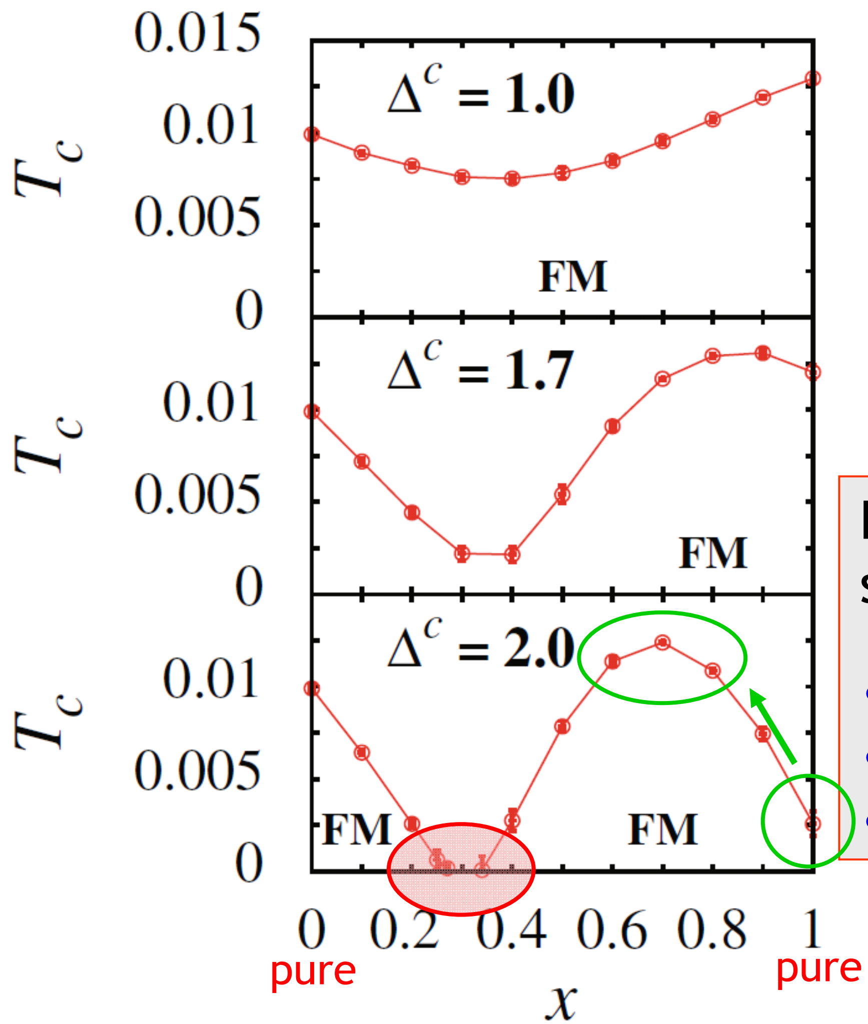
$$n_{tot}^{\text{eff}} = \frac{2n_{tot}}{1+x} \xrightarrow[n_{tot}=1.3]{x=0.3} 2$$

Half-filled lower alloy sub-band
→ alloy Kondo insulator → T_C=0

Disordered c-electrons

x: alloy concentration
Δ^c: disorder strength

Yu, Byczuk, DV (2008, 2010)



$$U = 1.5, \quad V = 0.6$$
$$n_{tot} = 1.3$$
$$\varepsilon_0^c - \varepsilon_0^f = 3.25$$

Effect of increasing energy splitting Δ^c on $T_c(x)$:

- $T_c(x=1)$ always decreases
- minimum develops at $x=n_{tot}-1>0$
- enhancement over $T_c(x=0)$, $T_c(x=1)$

$$n_{tot}^{\text{eff}} = \frac{2n_{tot}}{1+x} \xrightarrow[n_{tot}=1.3]{x=0.3} 2$$

Half-filled lower alloy sub-band
→ alloy Kondo insulator → T_C=0

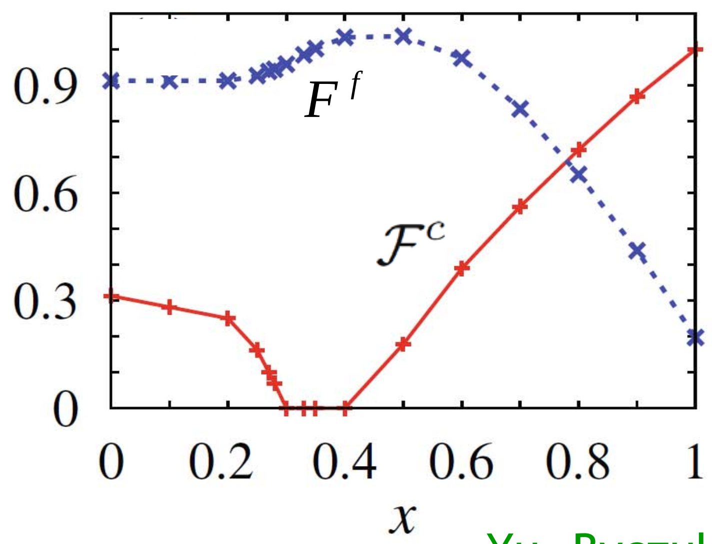
Mean-field ansatz for T_c in the RKKY-model

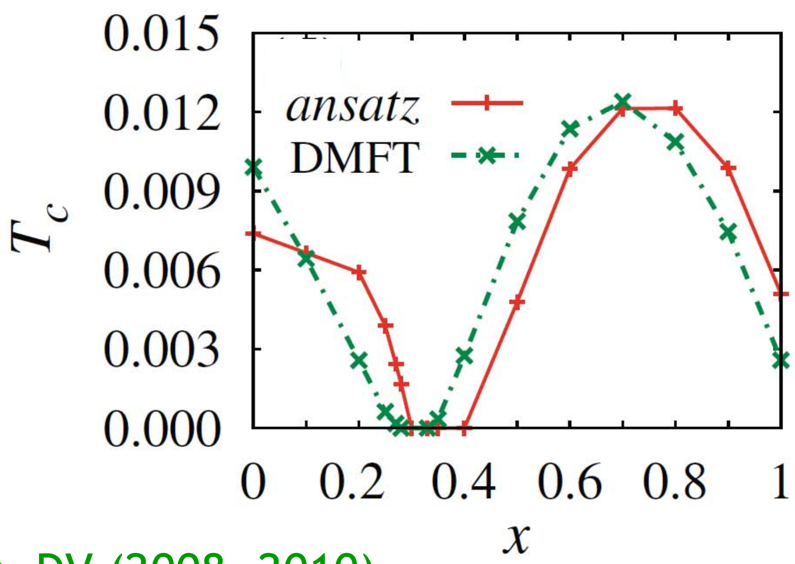
Formation of local *f*-electron moments (F^f) is independent of *c*-electron mediated ordering of those moments (F^c)

$$\boxed{T_c(U,V,\mu) = T_c^0(U,V,\mu)F^f(\mu-\varepsilon^f)F^c(\mu-\varepsilon^c)}$$

determined by DMFT for non-disordered system

$$F^c \xrightarrow[\text{disorder}]{\text{c-electron}} \mathcal{F}^c(x,\mu-\varepsilon_0^c) = xF^c(\mu-\varepsilon_0^c+\Delta^c)+(1-x)F^c(\mu-\varepsilon_0^c)$$





Yu, Byczuk, DV (2008, 2010)

Conclusion

Periodic Anderson model:

- Curie temperature T_C increases with *f*-level degeneracy

- Conduction band degeneracy can de- or increase T_C

  - Scaling $\dfrac{T_c}{\dfrac{(D^f/2)(D^f/2+1)}{U_{\text{eff}}^2}}$ vs. $\dfrac{n^c}{D^c}$ well obeyed

- Binary alloy disorder in the conduction band can lead to
  - an alloy Kondo insulator at fractional filling
  - a maximum in T_C