Ferromagnetism and metal-insulator transitions in correlated electron systems with alloy disorder

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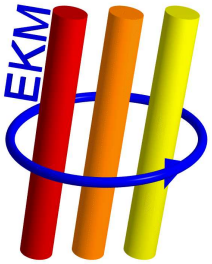
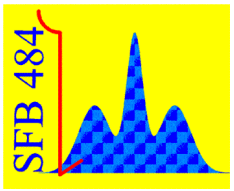


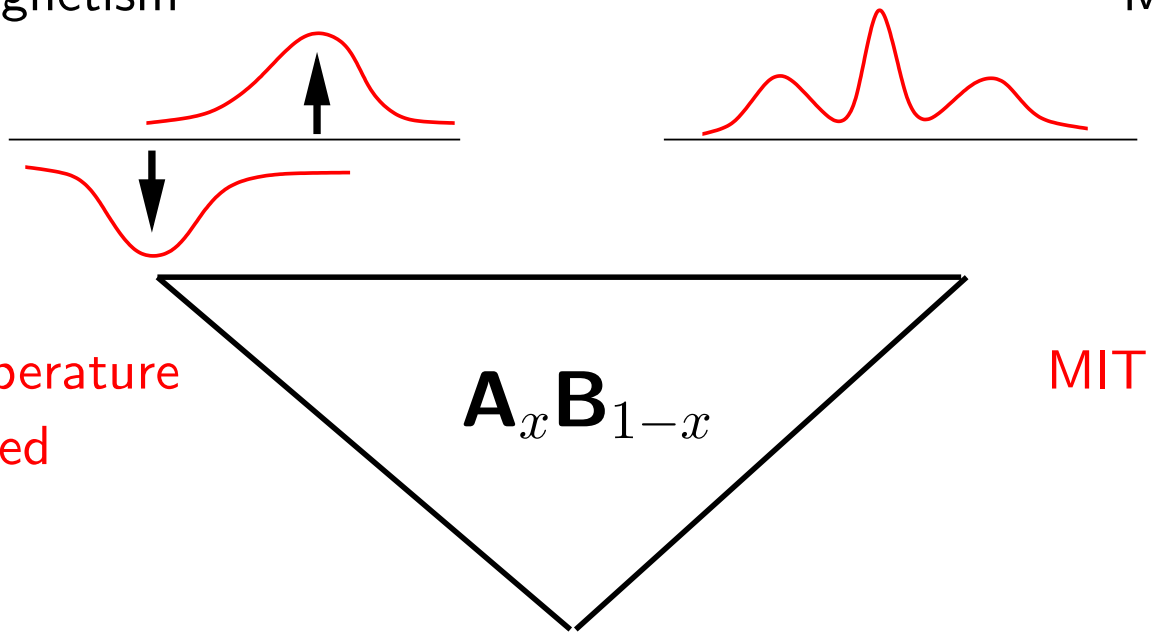


http://www.physik.uni-augsburg.de/theo3/kbyczuk/index.html

Correlations versus Binary Disorder

Itinerant ferromagnetism

Mott-Hubbard MIT



Curie temperature enhanced

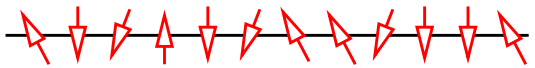
$\mathbf{A}_x\mathbf{B}_{1-x}$

MIT at non-integer densities

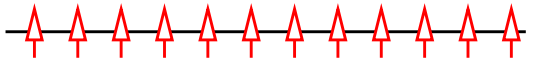
Binary alloy

K. Byczuk, M. Ulmke, D. Vollhardt, *Phys. Rev. Lett.* **90**, *196403 (2003)*
K. Byczuk, W. Hofstetter, D. Vollhardt, *Phys. Rev. B* **69**, *04512 (2004)*
K. Byczuk, M. Ulmke, *Eur. Phys. J. B* **45**, *449 (2005)*
U. Yu, K. Byczuk, D. Vollhardt, *Phys. Rev. Lett.* **100**, *246401 (2008)*

Ferromagnetism of localized vs itinerant moments

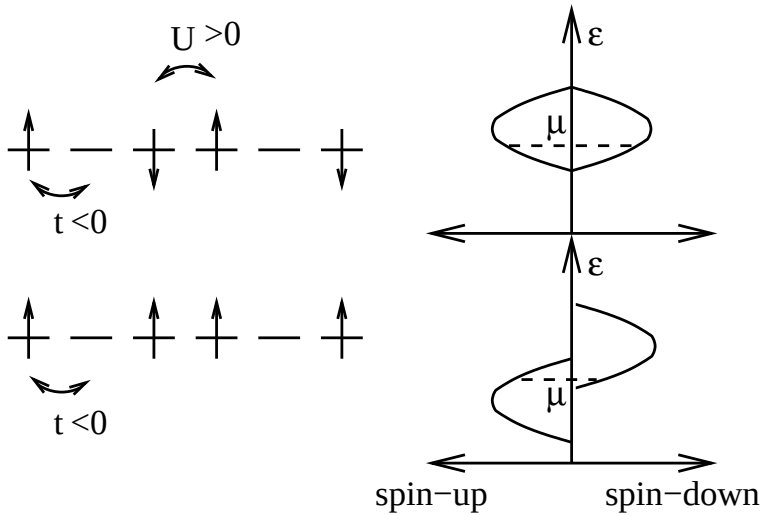


$T > T_c$



$T < T_c$

$M(T=0) = \mu_B S$



$M(T=0) < \mu_B S$

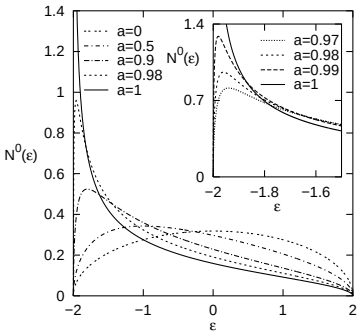
$J < 0 \rightarrow$ FM stable at $T_c > 0$

FM stable if $U \gtrsim |t|$

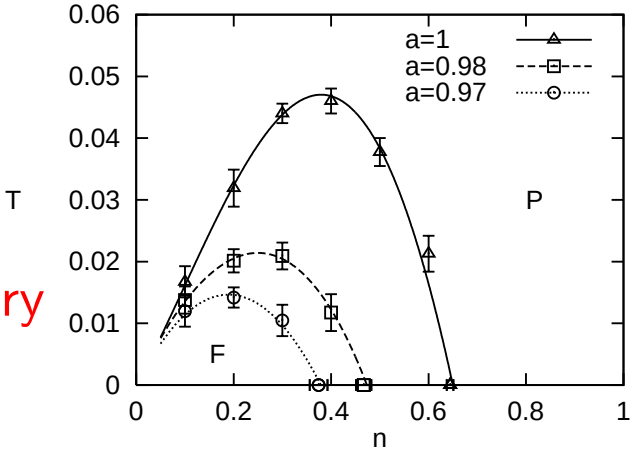
Itenerant ferromagnetism - intermediate coupling problem !!!

Routes to FM in one-band Hubbard (DMFT)

$$H = \sum t_{ij} a^{\dagger}_{i\sigma} a_{j\sigma} + U \sum n_{i\uparrow} n_{i\downarrow}$$

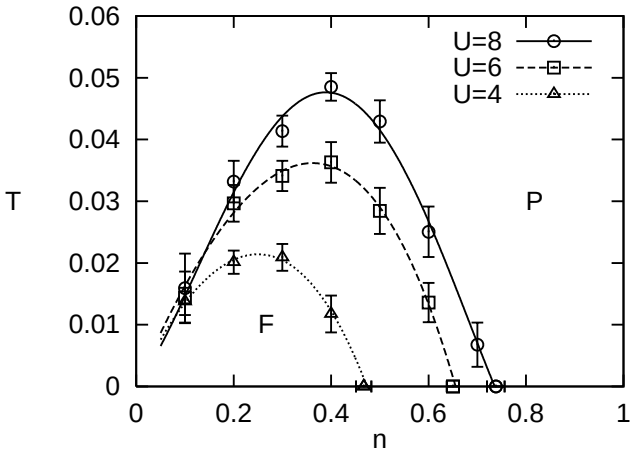


DOS asymmetry



$U = 4$

Interaction



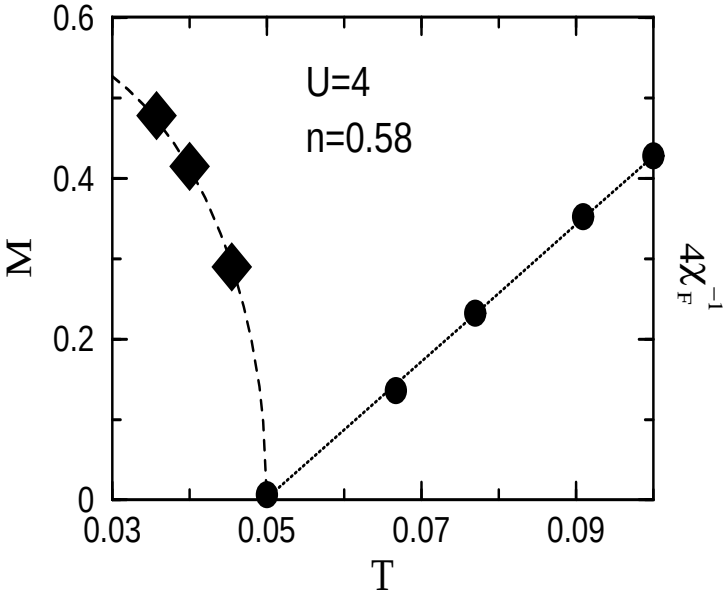
$a = 0.98$

J. Wahle et al., Phys. Rev. B 58, 12749 (1998)

DOS asymmetry and strong interaction needed for itinerant FM

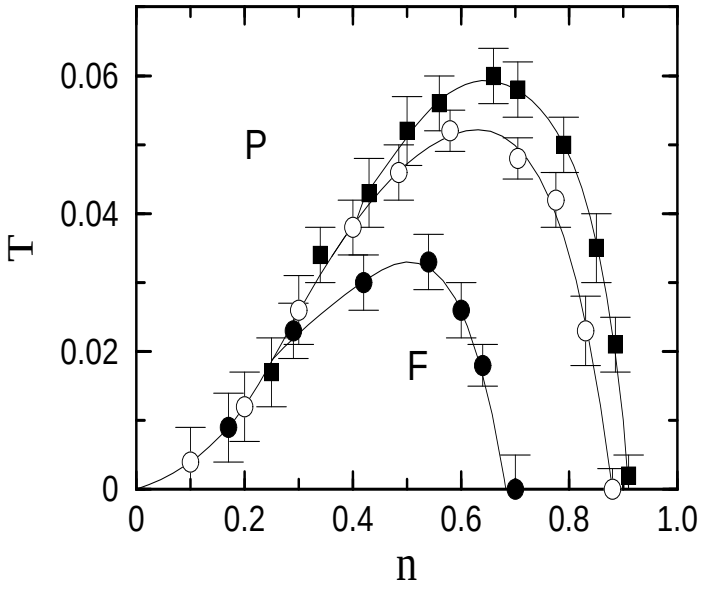
FCC FM in one-band Hubbard (DMFT)

$$N^0_{d\to\infty}(\epsilon) = \frac{\exp[-\frac{1+\sqrt{2}\epsilon}{2}]}{\sqrt{\pi(1+\sqrt{2}\epsilon)}}$$

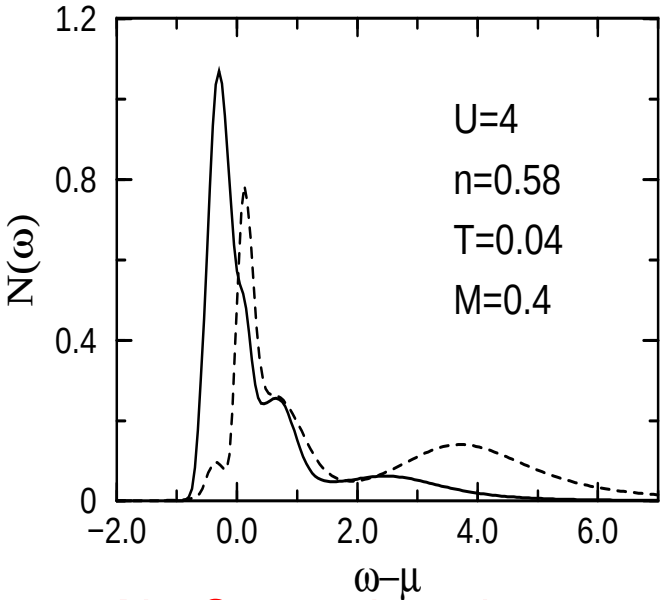


M. Ulmke, Eur. Phys. J. B 1, 301 (1998)

Curie-Weiss behavior within DMFT



$U = 2, 4, 5$



No Stoner but dynamical band splitting

K.B. and D. Vollahrdt, Phys. Rev. B 65, 134433 (2002)

FM in binary alloy itinerant electrons

Hubbard Hamiltonian with binary local disorder

$$H = \sum_{ij,\sigma} t_{ij} \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + \sum_{i\sigma} \epsilon_i \hat{n}_{i\sigma} + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

where ϵ is random variable with bimodal PDF

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

Physical observables averaged arithmetically

$$\langle \cdots \rangle_{\text{dis}} = \int d\epsilon P(\epsilon)(\cdots)$$

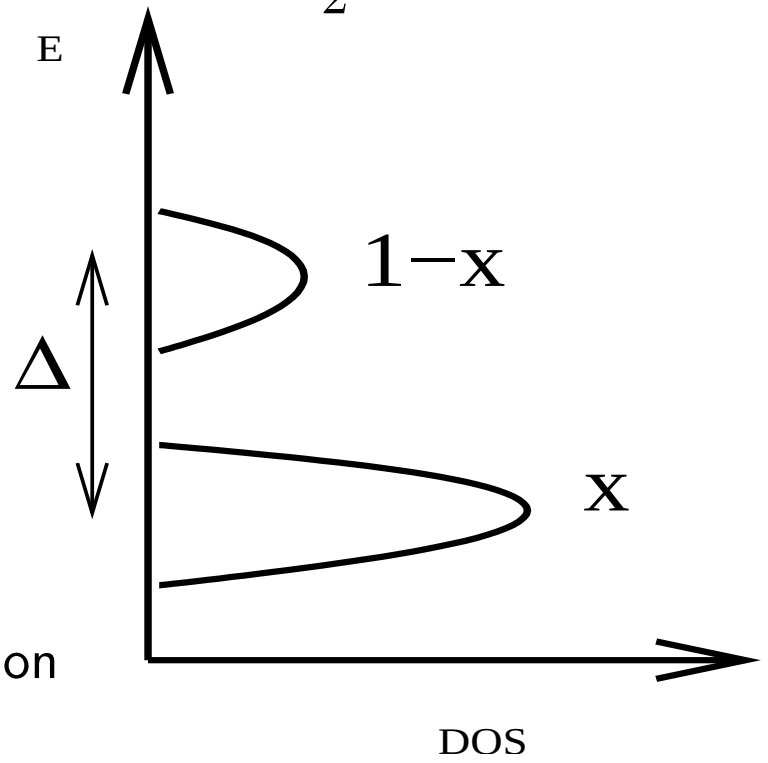
Disorder strength: $\delta = x(1-x)\Delta$

Alloy Band Splitting

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

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

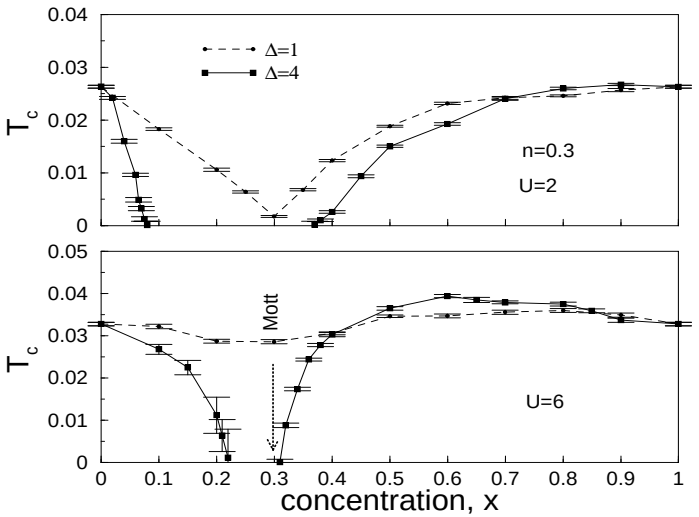
$H = \sum_i \epsilon_i + t \sum_{ij} a_i^\dagger a_j$

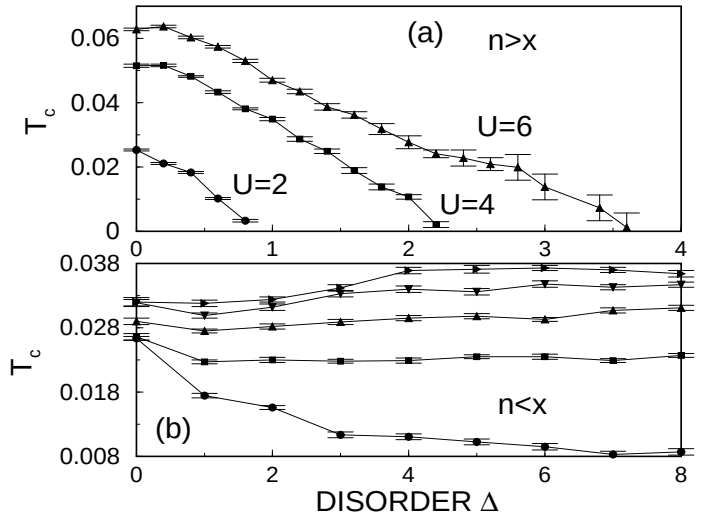


alloy band splitting for $\Delta \gtrsim W$ in any dimension

intermediate "coupling" problem !!! Nonperturbative!

Curie temperature in binary alloy correlated systems

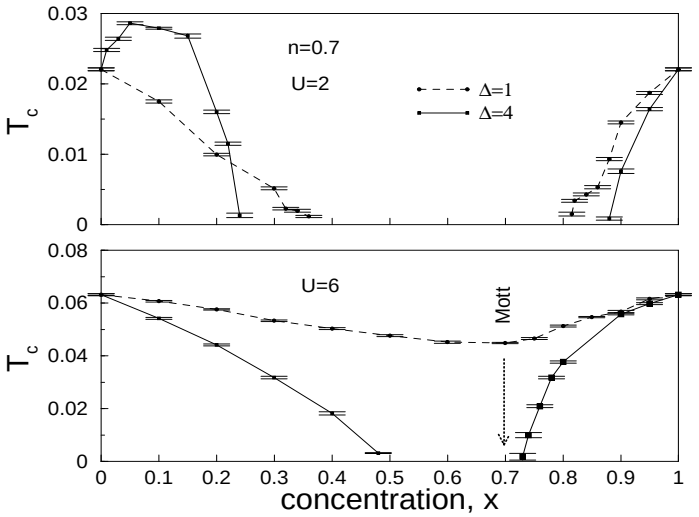


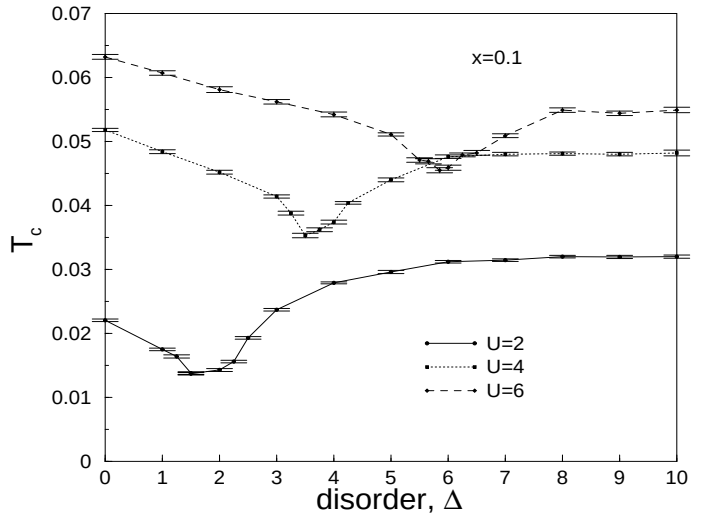


$n = 0.7,\ x = 0.5$

$n = 0.3,\ x = 0.5$

$T_c(x)$ increases !!! in some cases





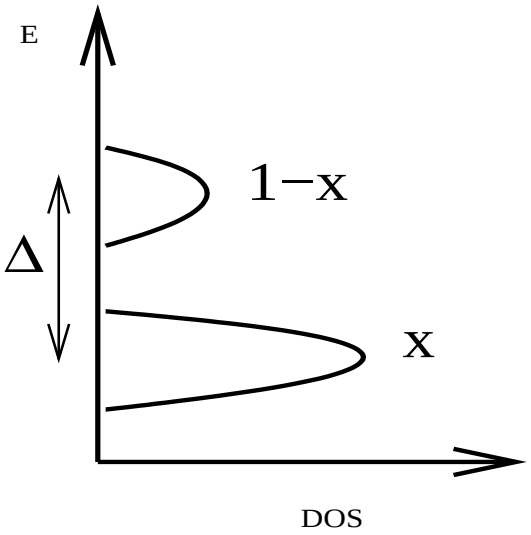
$n = 0.7,\ x = 0.1$

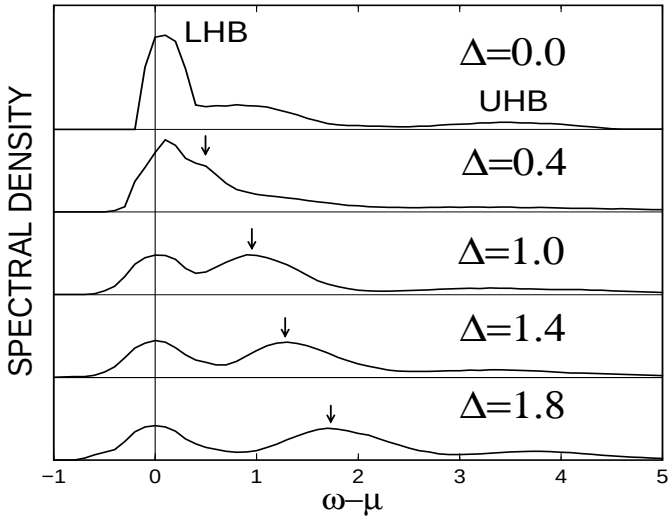
K.B., M. Ulmke, D. Vollhardt, Phys. Rev. Lett. **90**, *196403 (2003)*

K.B., M. Ulmke, Eur. Phys. J. B **45**, *449 (2005)*

Is there an alloy band splitting at $U > 0$?

$U = 4,\ n = 0.3,\ x = 0.5,\ T = 0.071$, MEM





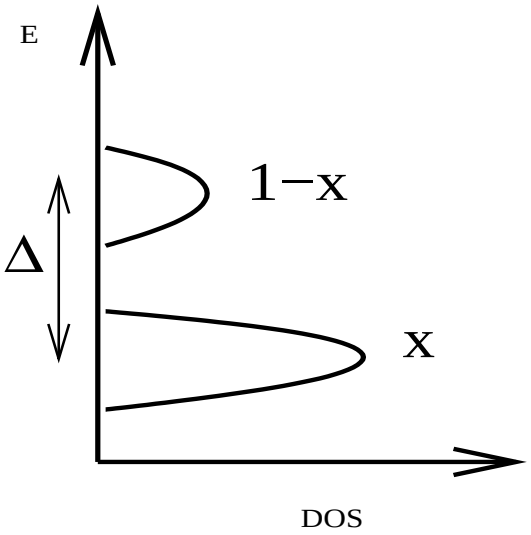
Subtle interplay between Δ and U increases T_c!

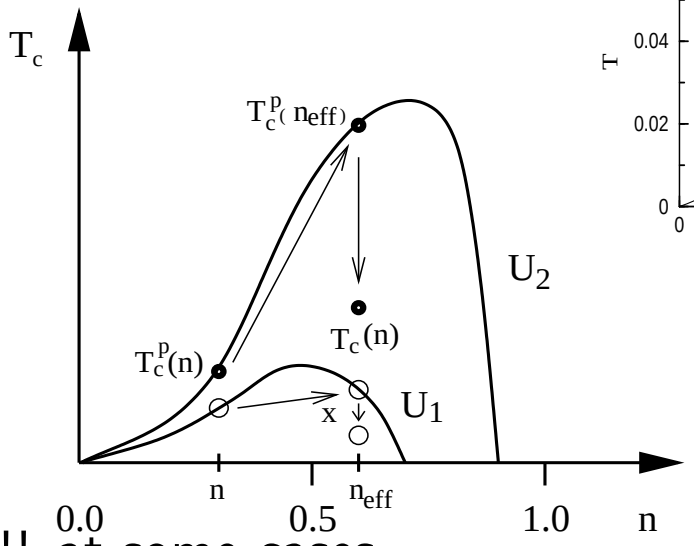
K.B., M. Ulmke, D. Vollhardt, Phys. Rev. Lett. **90**, *196403 (2003)*

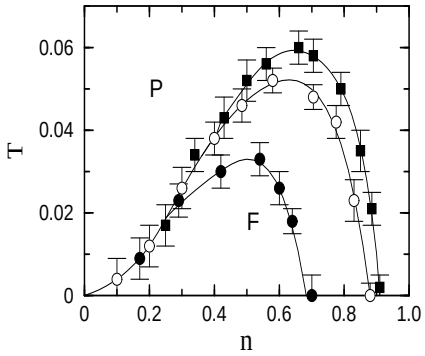
Why is Curie temperature enhanced?

$n < 2x \rightarrow n_{\text{eff}} = \frac{n}{x}$

$T_c = xT_c^p(n_{\text{eff}})$





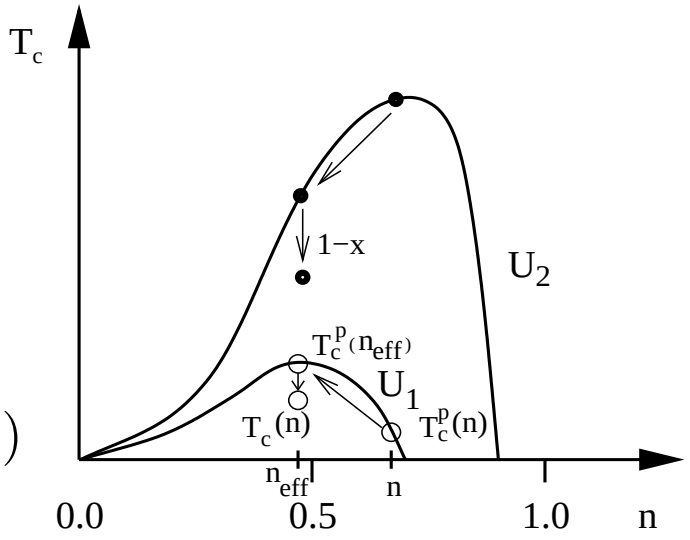


$T_c(x)$ increases !!! at some cases

Good for large U

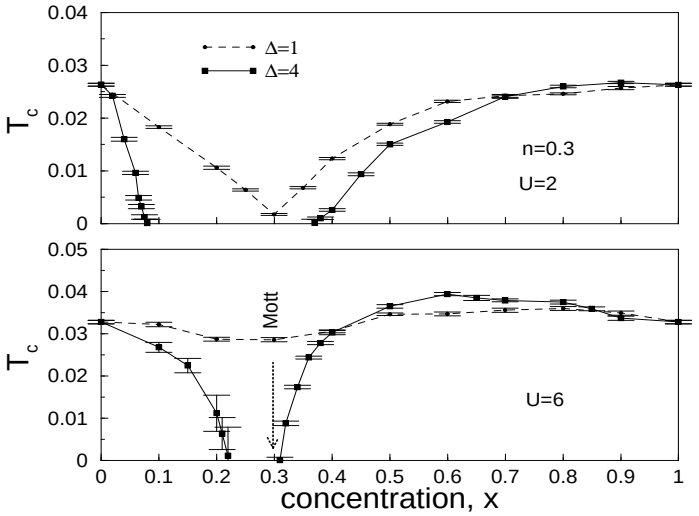
$n > 2x \rightarrow n_{\text{eff}} = \frac{n-2x}{1-x}$

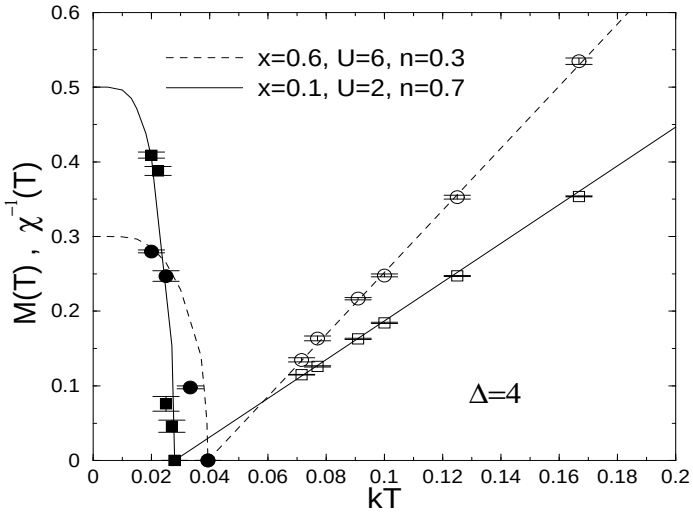
$T_c = (1-x)T_c^p(n_{\text{eff}})$



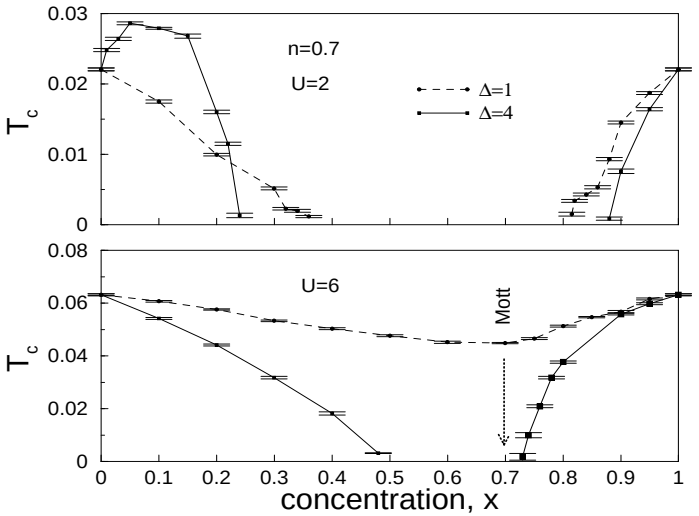
Good for small U

Magnetization and Curie-Weiss law





If $\Delta \gg W$ and $n < 2x \rightarrow M_s = n$ but $n > 2x \rightarrow M_s = n - 2x$

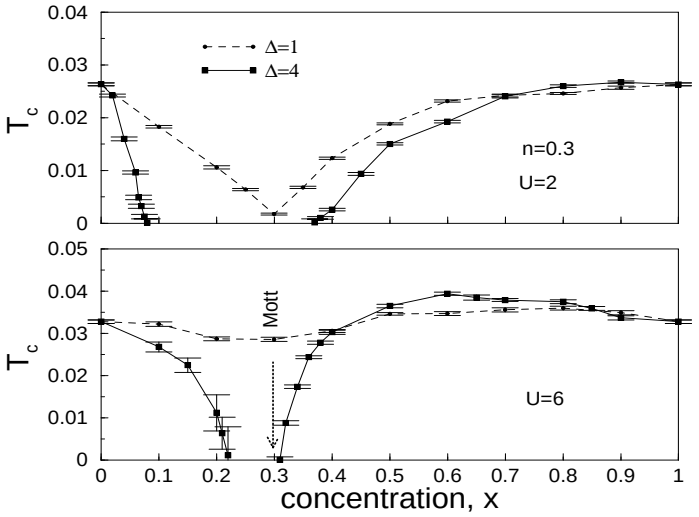


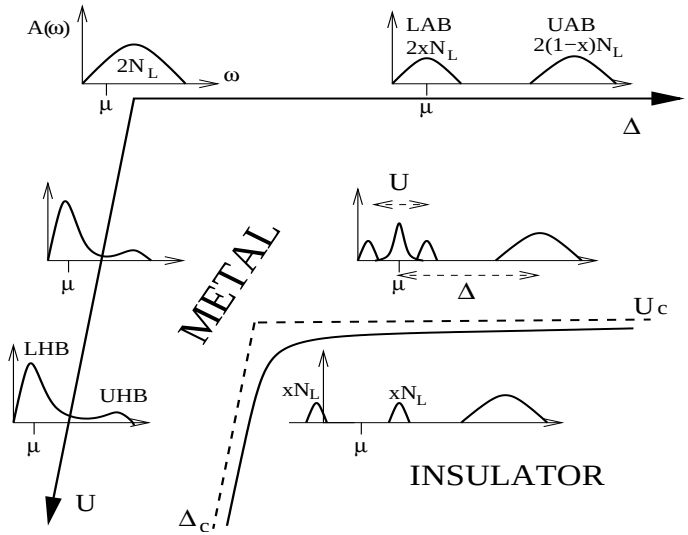
$$\frac{M(T)}{M_s} = \tanh[\frac{T_c M(T)}{T M_s}]$$

$\chi(T) = \frac{C}{T - T_c}$, where $C \approx M_s$

$\frac{C_1}{C_2} = 0.623$ close to $\frac{3}{5}$

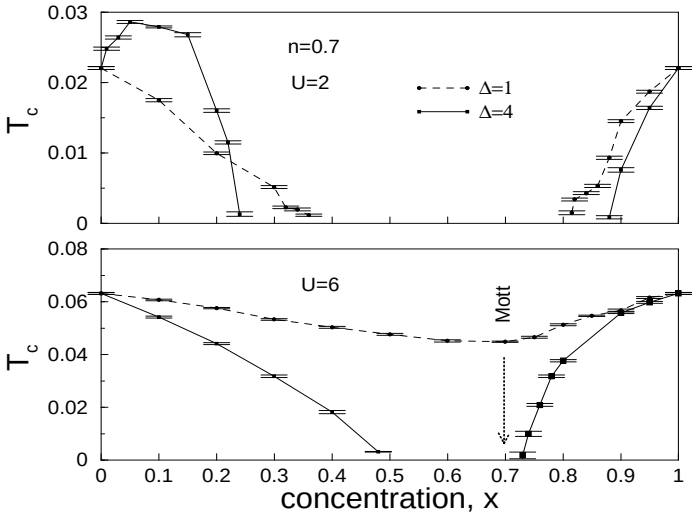
Mott-Hubbard metal-insulator transition

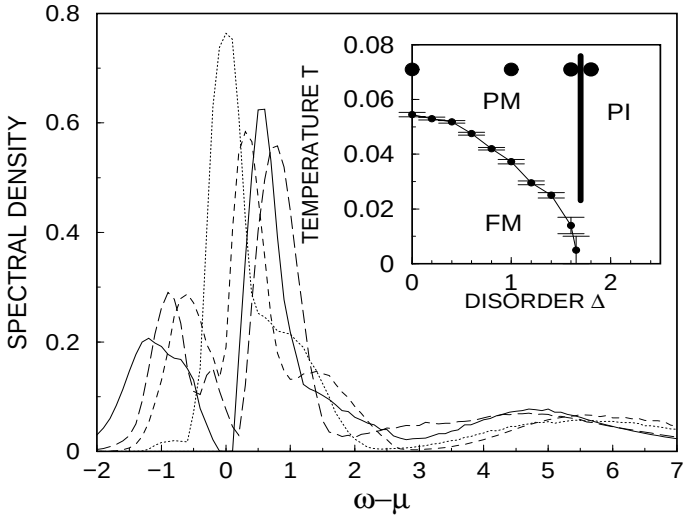




If $n = x$ (or $1 + x$) Mott-Hubbard MIT occures for $\Delta > \sqrt{x}$ and $U > 6\sqrt{x}$

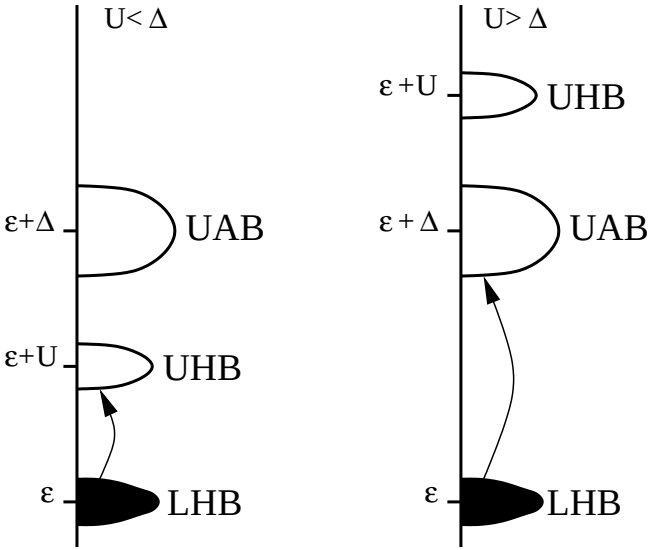
$U = 6,\ x = 0.5,\ n = 0.5,\ T = 0.071$, MEM





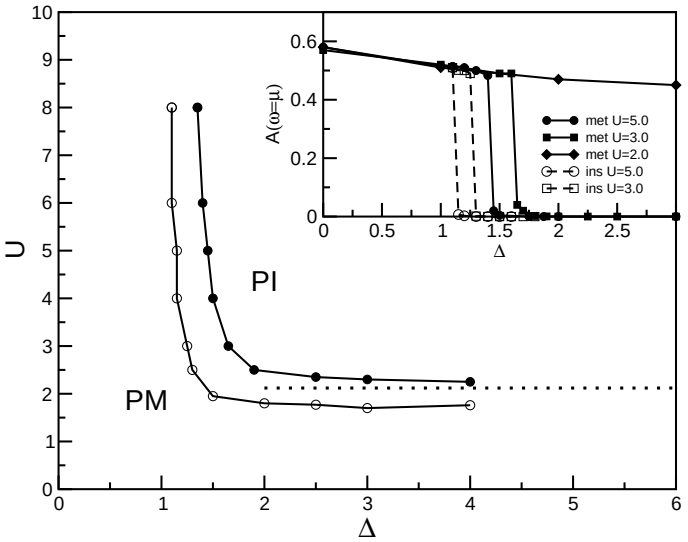
Correlated alloy insulators

- alloy Mott insulator
- alloy charge transfer insulator



alloy Mott insulator

alloy charge transfer insulator



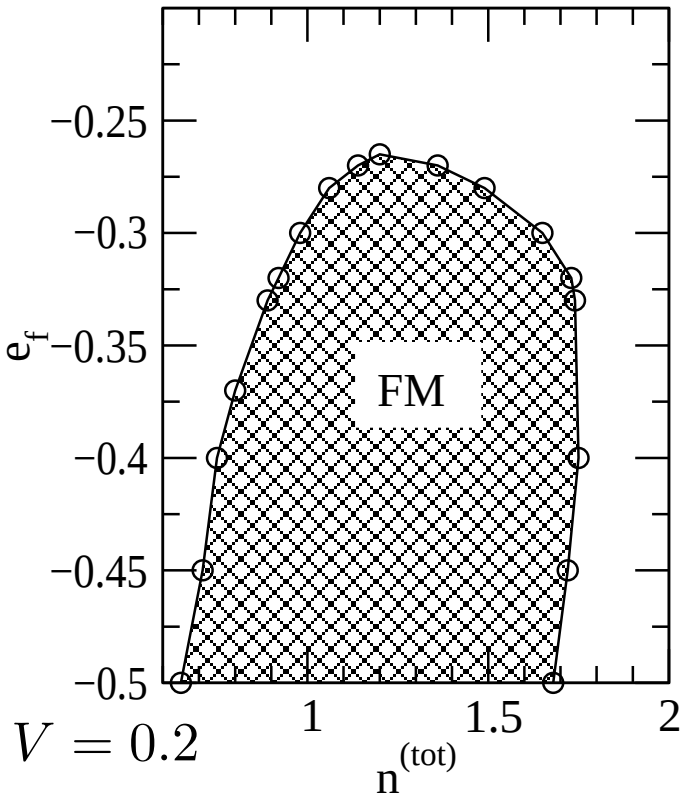
K.B., W. Hofstetter, D. Vollhardt, Phys. Rev. B **69**, *045112 (2004)*

Periodic Anderson model (DMFT)

Non-interacting itinerant electrons hybrydize with localized interacting ones

$$H = \sum_{i,j\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + \sum_{i\sigma} \left(\varepsilon^f f^\dagger_{i\sigma} f_{i\sigma} + \varepsilon^c c^\dagger_{i\sigma} c_{i\sigma} \right) + \sum_{i\sigma} \left(V c^\dagger_{i\sigma} f_{i\sigma} + V^* f^\dagger_{i\sigma} c_{i\sigma} \right) + U \sum_i n^f_{i\uparrow} n^f_{i\downarrow}$$

Ferromagnetism stable away from half-filling



$U = 4,\ V = 0.2$

Other mean-field, slave bosons studies:

R. Doradzinski, J. Spalek 1997; C.D. Batista et al. 2003; ...

Optimal FM when local moment maximized

D. Meyer, W. Nolting, Eur. Phys. J. B **18**, *382 (2000)*

Periodic Anderson model with alloy disorder

Local disorder on lattice sites:

$$H = \sum_{i,j\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + \sum_{i\sigma} \left(\varepsilon^{f}_{i} f^{\dagger}_{i\sigma} f_{i\sigma} + \varepsilon^{c}_{i} c^{\dagger}_{i\sigma} c_{i\sigma} \right) + \sum_{i\sigma} \left(V c^{\dagger}_{i\sigma} f_{i\sigma} + V^{*} f^{\dagger}_{i\sigma} c_{i\sigma} \right) + U \sum_{i} n^{f}_{i\uparrow} n^{f}_{i\downarrow}$$

with

$$P(y_i) = x\delta(y_i - y^0) + (1-x)\delta(y_i - y_0 - \Delta^y)$$

where $y_i = \varepsilon^c_i$, ε^f_i, and $\Delta^y = \Delta^c$, Δ^f

c-electron disorder
f-electron disorder

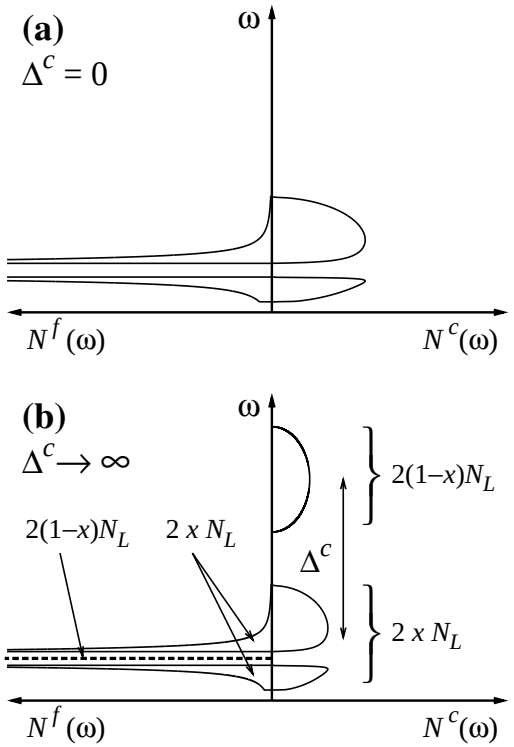
Disorder strength: $\delta^y = x(1-x)\Delta^y$

Periodic Anderson model with alloy disorder at $U = 0$

Different splitting scheme, e.g. c-electron disorder

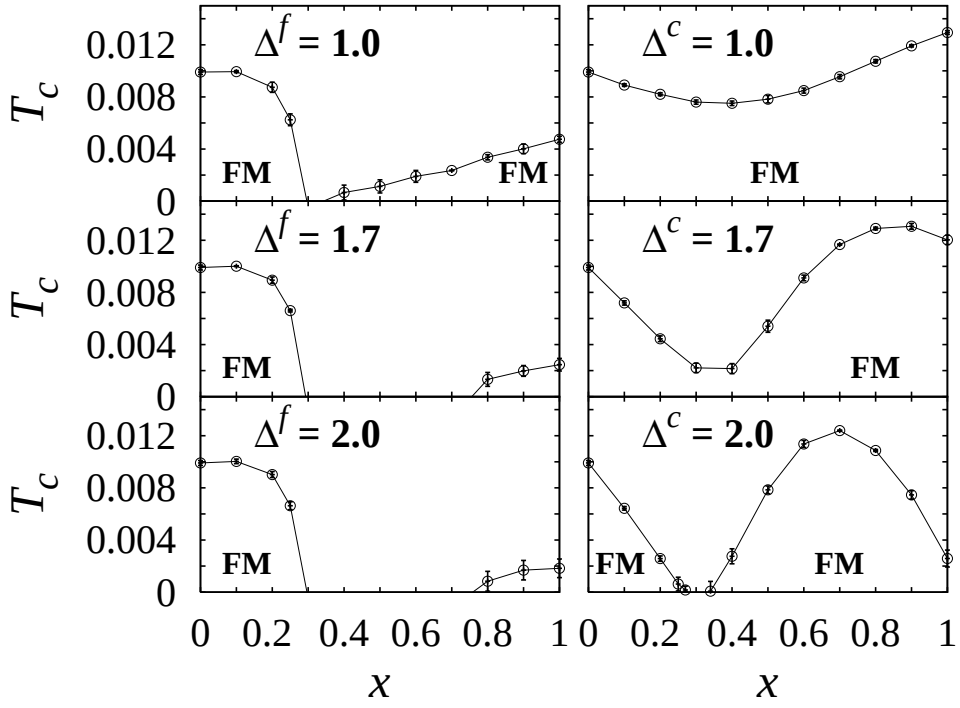
$$G^{cc}_{\sigma n} = \frac{x}{(\mathcal{G}^{cc}_{\sigma n})^{-1} - |V_0|^2 \mathcal{G}^{ff}_{\sigma n}} + \frac{1-x}{(\mathcal{G}^{cc}_{\sigma n})^{-1} - |V_0|^2 \mathcal{G}^{ff}_{\sigma n} - \Delta^c}$$

$$G^{ff}_{\sigma n} = \frac{x}{(\mathcal{G}^{ff}_{\sigma n})^{-1} - |V_0|^2 \mathcal{G}^{cc}_{\sigma n}} + \frac{1-x}{(\mathcal{G}^{ff}_{\sigma n})^{-1} - \frac{|V_0|^2}{(\mathcal{G}^{cc}_{\sigma n})^{-1} - \Delta^c}}$$



$1 - x$ fraction of f-electrons is not mixed with c-electron

FM in Periodic Anderson model with alloy disorder

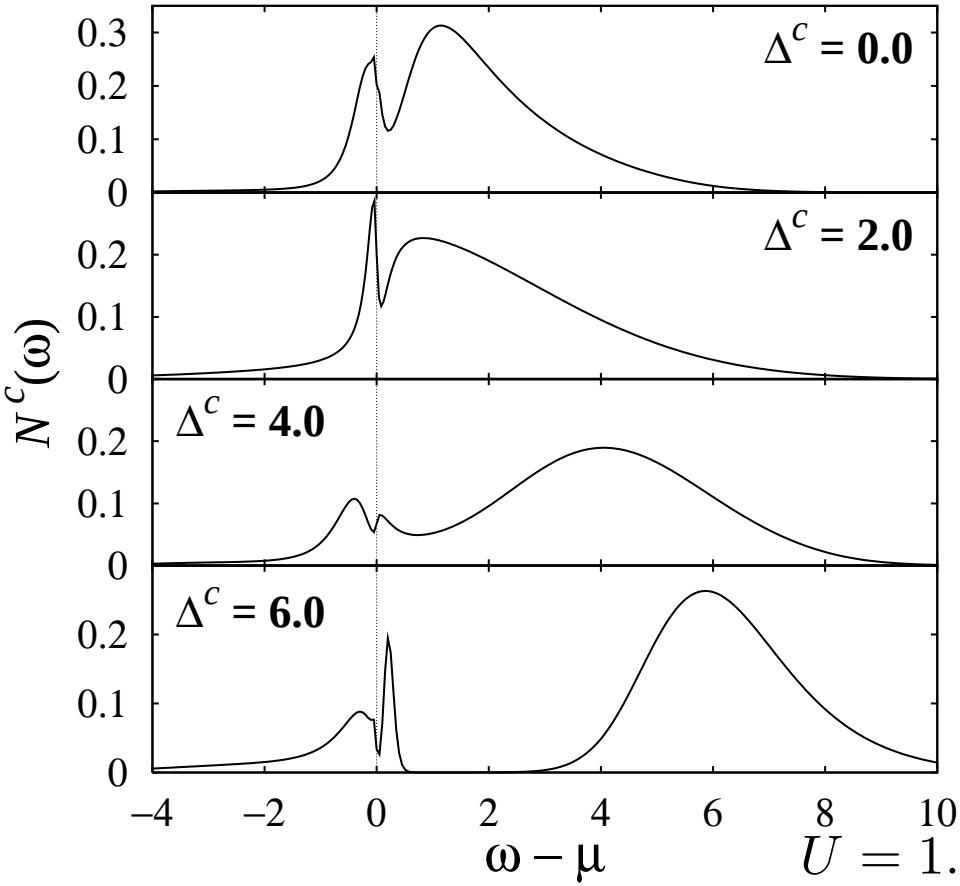


c-electron disorder enhances T_c

$U = 1.5$, $V = 0.6$, $n_{\rm tot} = 1.3$, $\epsilon_c^0 - \epsilon_f^0 = 3.25$

U. Yu, K.B., D. Vollhardt, Phys. Rev. Lett. **100**, *246401 (2008)*

Kondo insulator in PAM with alloy disorder



$$4N_L \to (4 - 2(1-x))N_L$$

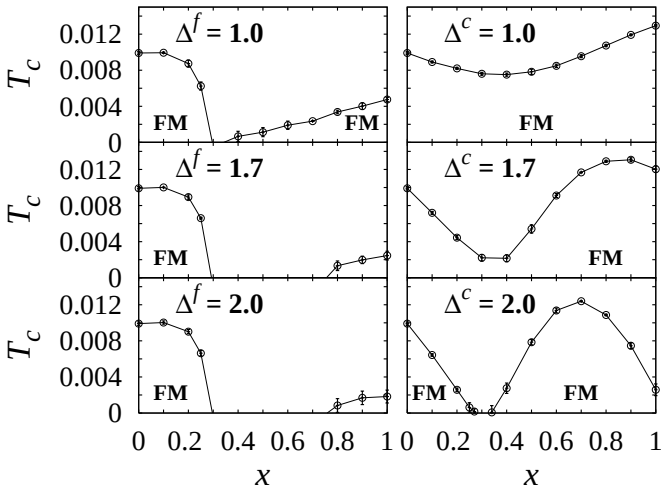
$$n_{\rm tot}^{\rm eff} = n_{\rm tot} \times 4/(2(1+x))$$

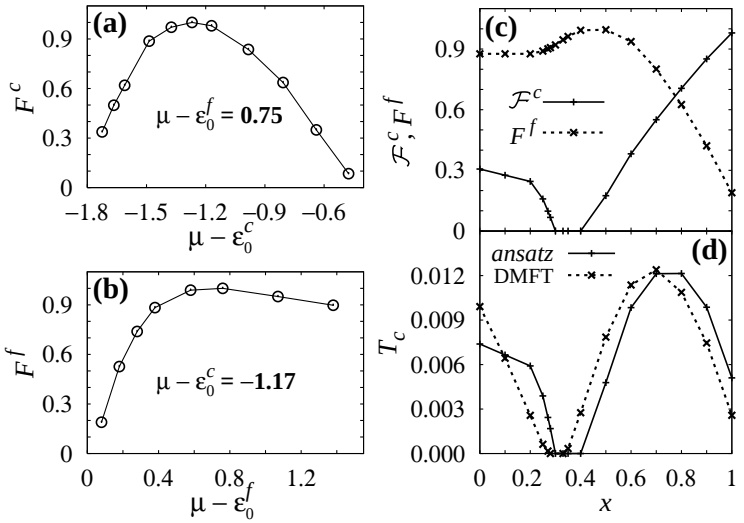
$$n_{\rm tot}^{\rm eff} = 2n_{\rm tot}/(1+x) = 2$$

$U = 1.5,\ V = 0.6,\ n_{\rm tot} = 1.3,\ \epsilon_c^0 - \epsilon_f^0 = 3.25,\ x = 0.3$

U. Yu, K.B., D. Vollhardt, Phys. Rev. Lett. **100**, *246401 (2008)*

FM in PAM with alloy disorder - discussion





ansatz for pure system: $T_c = T_c^0 F^c(\mu - \epsilon_c^0) F^f(\mu - \epsilon_f^0)$

for disorder system: $\mathcal{F}^c(x, \mu - \epsilon_0^c) = [xF^c(\mu - \varepsilon_0^c + \Delta^c) + (1-x)F^c(\mu - \varepsilon_0^c)]$

U. Yu, K.B., D. Vollhardt, Phys. Rev. Lett. **100**, *246401 (2008)*

Conclusions

- Binary alloy disorder leads to interesting effects in correlated electron systems
- Enhancement of T_c
- Correlated insulators at non-integer densities

Collaboration

- Walter Hofstetter - Frankfurt, Germany
- Martin Ulmke - FGAN - FKIE, Wachtberg, Germany
- Dieter Vollhardt - Augsburg University, Germany
- Unjong Yu - Augsburg University, Germany