Ferromagnetism in Hubbard model with binary alloy disorder

Krzysztof Byczuk

Institute of Theoretical Physics Warsaw University

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Main results

- New collective effects induced by correlation and disorder
- Enhancement of T_c in binary alloy ferromagnets
- New Mott–Hubbard metal–insulator transition at $n \neq 1$

K. Byczuk, M. Ulmke, D. Vollhardt
Phys. Rev. Lett. **90**, 196403 (2003)
K. Byczuk, W. Hofstetter, D. Vollhardt
Phys. Rev. B **69**, 04512 (2004)
new unpublished results

Collaboration

- Martin Ulmke - FGAN - FKIE, Wachtberg, Germany
- Walter Hofstetter - Aachen, Germany
- Dieter Vollhardt - Augsburg University, Germany

Plan of the talk

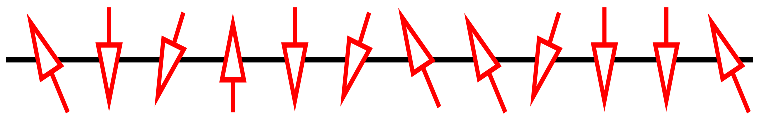
1. Introduction
   - localized vs. itinerant FM
   - itinerant FM in brief history
   - binary alloy
   - alloy FM in Nature
2. Earlier result within DMFT on pure FM
3. Our results on binary alloy FM
   - enhancement of T_c
   - magnetization and Curie–Weiss law
   - Mott–Hubbard MIT at $n \neq 1$
   - non-iso-electronic systems
4. Conclusions

Ferromagnetism of local moments

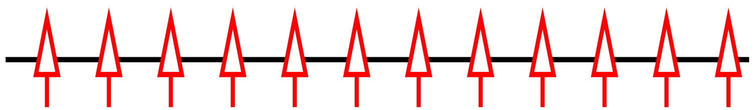
Exchange (Heisenberg) coupling

$$H = \sum_{ij} J_{ij} \, \vec{S}_i \cdot \vec{S}_j$$

$J < 0 \rightarrow$ FM appears at Curie temperature T_c



$T > T_c$



$T < T_c$

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

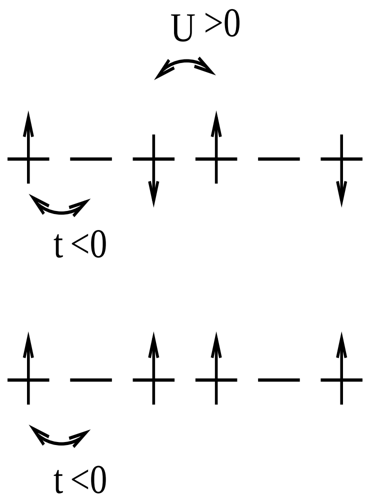
Itinerant Ferromagnetism

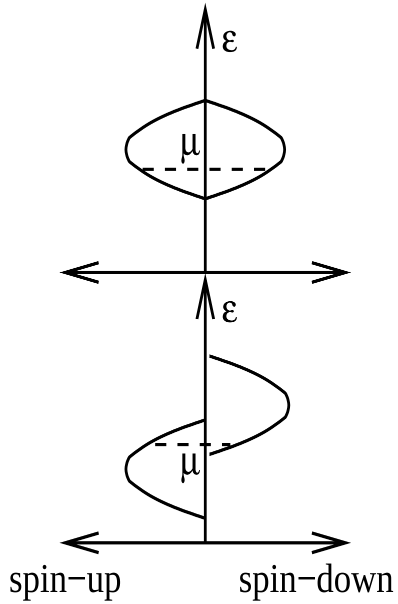
Dynamical way to make FM

To reduce interaction energy electrons prefer FM state

due to Pauli principle $E_{\text{int}}^{\text{FM}} = 0$

However, $|E_{\text{kin}}^{\text{FM}}| < |E_{\text{kin}}^{\text{PM}}|$!





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

FM stable if $U \gtrsim |t|$ - **intermediate coupling problem !!!**

Many itinerant FM are alloys

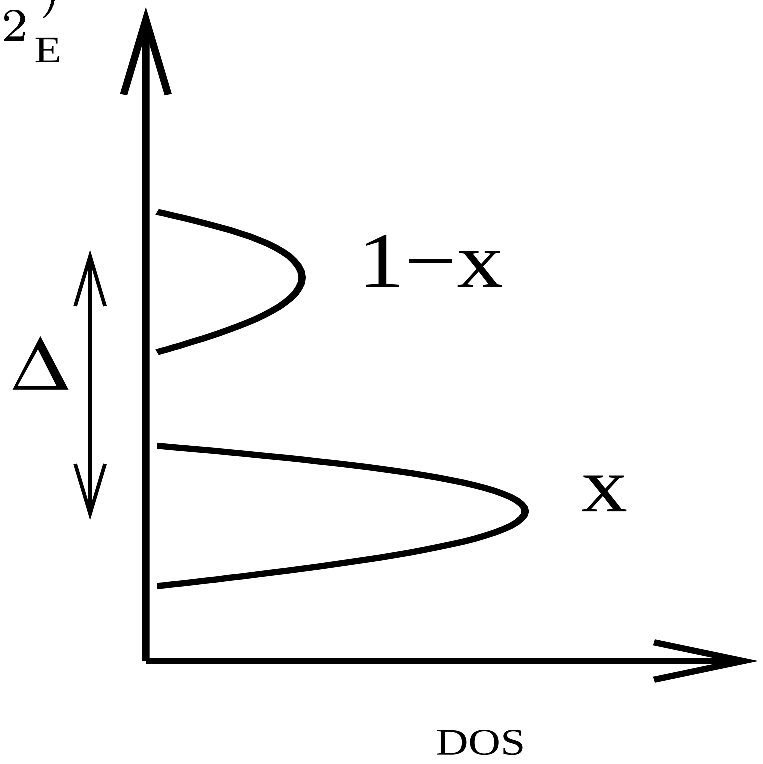
Itinerant Ferromagnetism in brief history

- Bloch's FM in electron gas $(1/r)$; unstable due to correlations (RPA)
- Stoner model (Hartree-Fock); $U_c \sim N(\mu)$; T_c overestimated
- Kanamori (T-matrix); no FM in Hubbard model
- Gutzwiller, Hubbard I and III - contradictory views
- ...
- LSDA, mode coupling, RG, Hertz, ...
- exact results; $d = \infty$ (Wahle, Kollar, Ulmke, Vollhardt, et al.)
- E.Lieb - *Ground state of Hubbard is singlet on bipartite lattice at half-filling*
- M. Kollar, R. Strack, D. Vollhardt - Exact estimates for extended Hubbard

Alloy Band Splitting

Binary alloy disorder (alloys $A_{1-x}B_x$, e.g $\mathrm{Fe}_{1-x}\mathrm{Co}_x$)

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



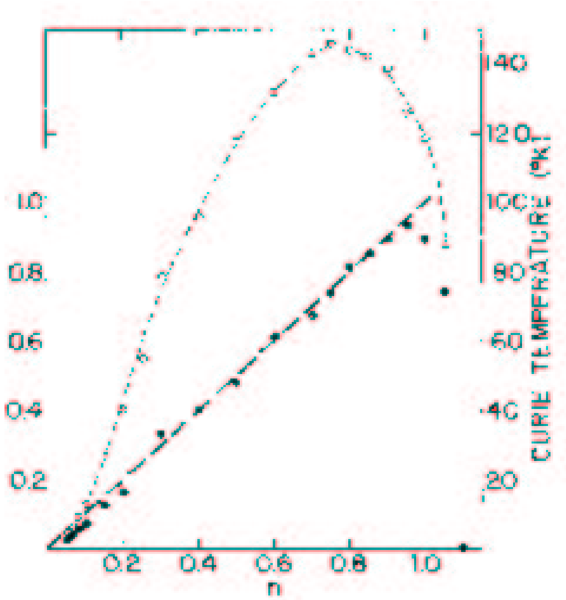
$H = \sum_i \epsilon_i + t\sum_{ij} a_i^\dagger a_j$

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

intermediate "coupling" problem !!!

physical quantity: $O = \int d\epsilon \mathcal{P}(\epsilon) < \hat{O}(\epsilon) >$

Alloy Ferromagnets in Nature I



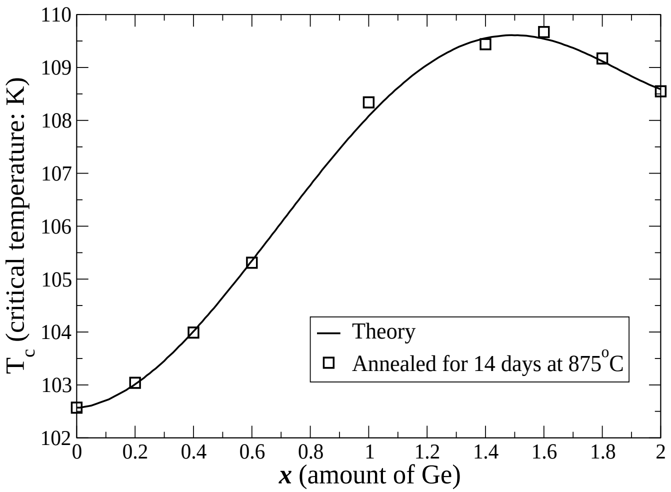
Piryts: $\mathrm{T}_{1-x}(\mathrm{T}+1)_x\mathrm{S}_2$, T=Fe, Co, Ni, Cu, Zn

$t_{2g}^6 e_g^n$ with $n = 0, 1, 2, 3, 4$

$\mathrm{Fe}_{1-x}\mathrm{Co}_x\mathrm{S}_2$, max $T_c(x)$ @ $x \approx 0.76$

Jarrett et al., PRL 1968, Leighton 2004

Alloy Ferromagnets in Nature II



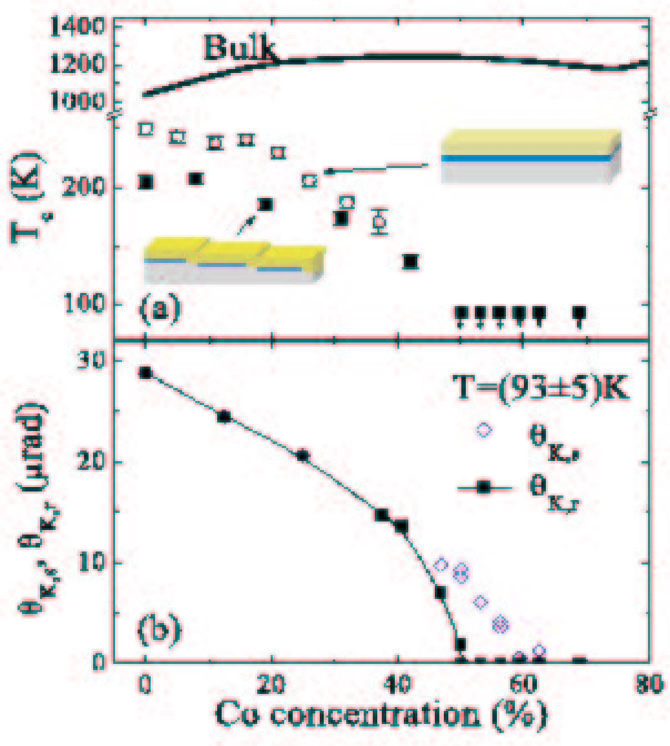
MT_2X_2 ternary intermetallic alloys

$UCu_2Si_{2-x}Ge_x$, max $T_c(x)$ @ $x \approx 1.6$

Silva Neto et al., PRL 2003

Si and Ge isovalent, only structural disorder

Alloy Ferromagnets in Nature III

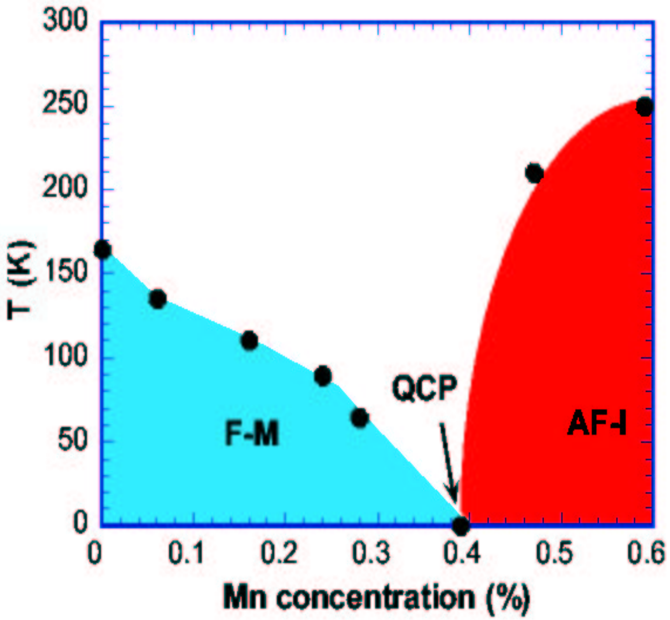


Fe weak FM, Co strong FM, bcc alloy

$Fe_{1-x}Co_x$, max $T_c(x)$ @ $x \approx 0.5$

Pratzer et al., PRL 2003

Alloy Ferromagnets in Nature IV



Alloy ruthenates

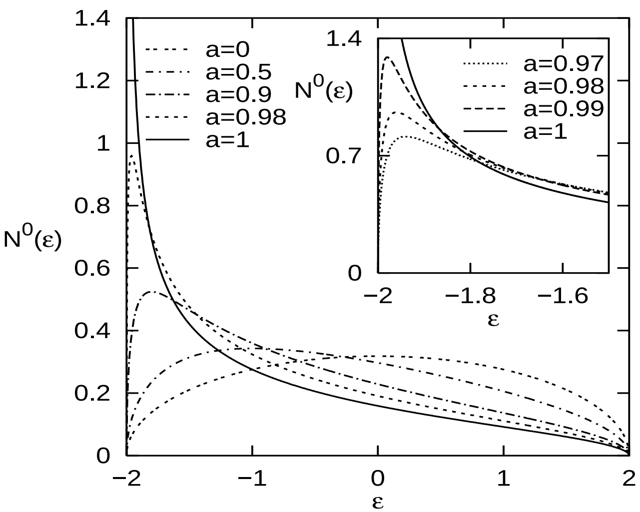
$SrRu_{1-x}Mn_xO_3$, FM Met–AF Ins

Cao et al., cond-mat/0409157

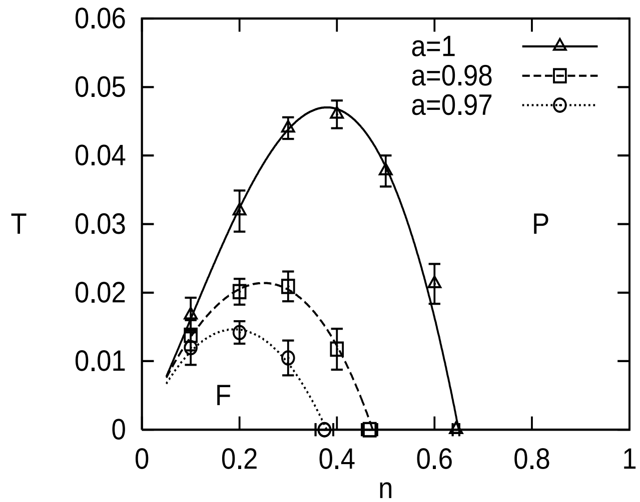
Route to FM in one-band Hubbard (DMFT)

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

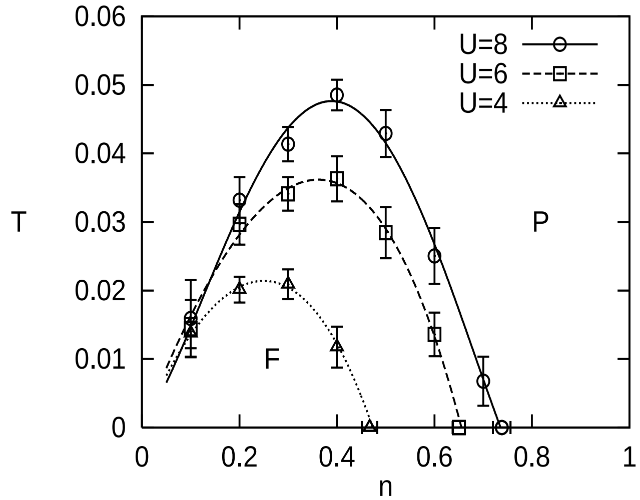
DOS asymmetry - a



Interaction - U



$U = 4$

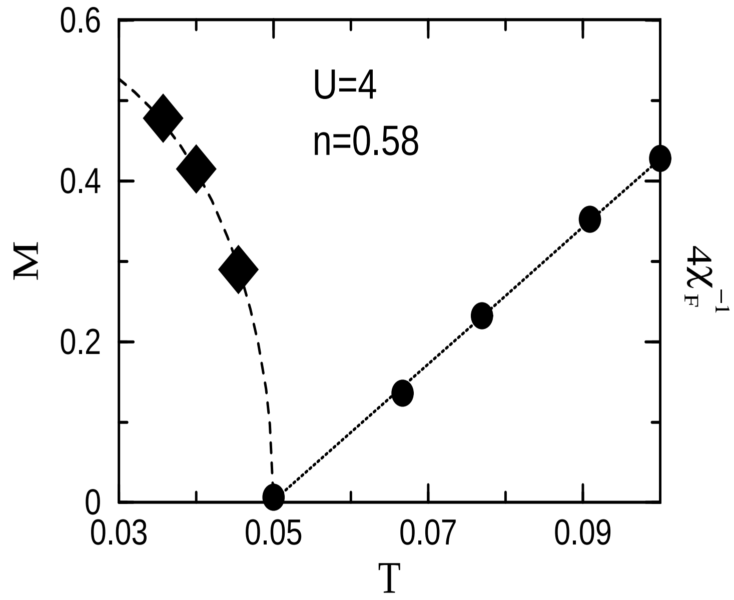


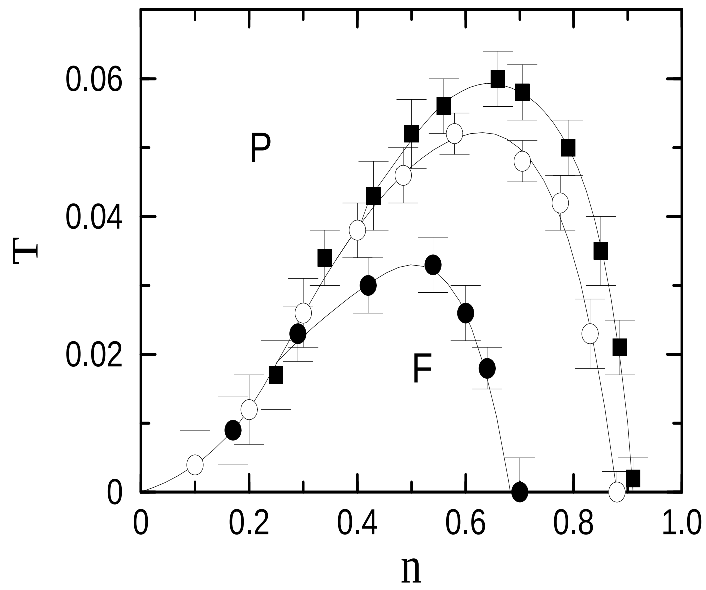
$a = 0.98$

Wahle et al. 1998

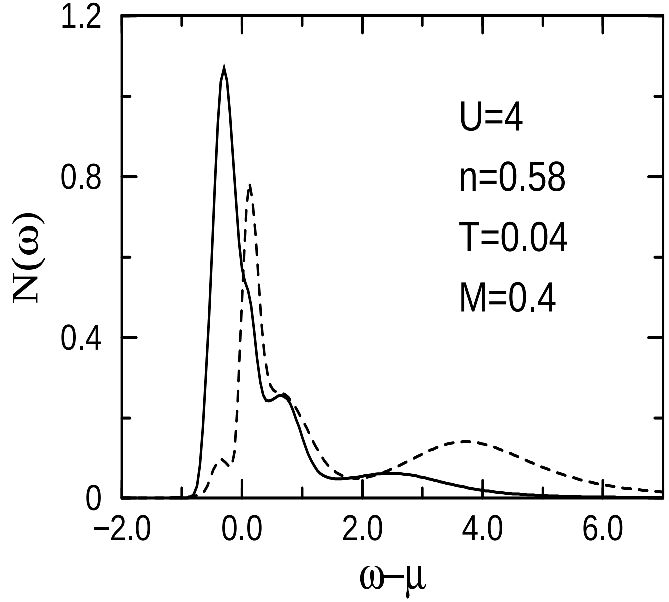
FCC $d = \infty$ FM in one-band Hubbard

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





$U = 2, 4, 5$



Ulmke et al. 1998

FM in binary alloy itinerant electrons

Anderson–Hubbard Hamiltonian

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

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 observable averaged arithmetically

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

$d = \infty$ FCC DOS stabilizes FM

$$N^0(\omega) = \frac{\exp[-\frac{1+\sqrt{2}\omega}{2}]}{\sqrt{\pi(1+\sqrt{2}\omega)}}$$

Dynamical Mean–Field Theory

Local Green function - Hilbert transform of DOS with self–energy

$$G_{\sigma n} = \int d\epsilon \frac{N^0(\epsilon)}{i\omega_n + \mu - \Sigma_{\sigma n} - \epsilon}$$

expressed by path integral, which is calculated with
Hubbard–Stratonovich and QMC over auxiliary Ising spins

$$G_{\sigma n} = -\left\langle \frac{\int D\left[c_\sigma, c_\sigma^\star\right] c_{\sigma n} c_{\sigma n}^\star e^{\mathcal{A}_i\{c_\sigma, c_\sigma^\star, \mathcal{G}_\sigma^{-1}\}}}{\int D\left[c_\sigma, c_\sigma^\star\right] e^{\mathcal{A}_i\{c_\sigma, c_\sigma^\star, \mathcal{G}_\sigma^{-1}\}}} \right\rangle_{\mathrm{dis}}$$

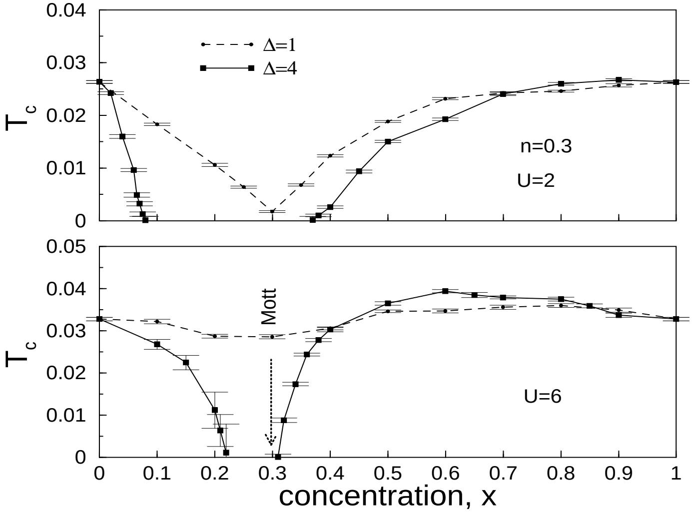
single impurity action for each $\epsilon_i = \pm\Delta/2$

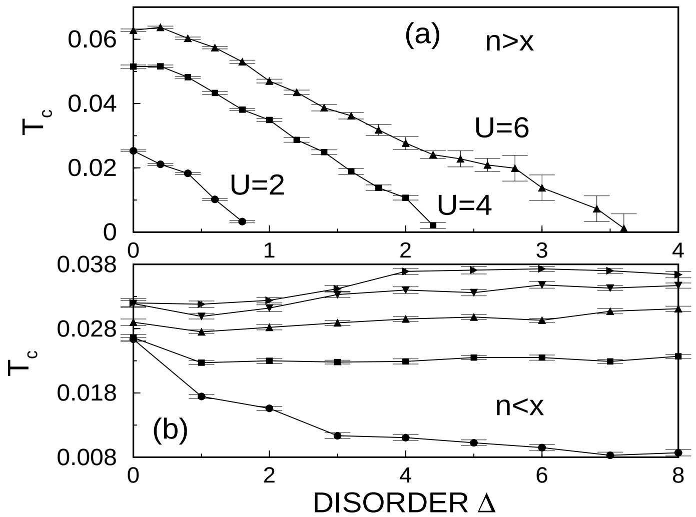
$$\mathcal{A}_{\mathrm{i}}\{c_\sigma, c_\sigma^\star, \mathcal{G}_\sigma^{-1}\} = \sum_{n,\sigma} c_{\sigma n}^\star \mathcal{G}_{\sigma n}^{-1} c_{\sigma n} - \epsilon_i \sum_\sigma \int_0^\beta d\tau\, n_\sigma(\tau) - \frac{U}{2} \sum_\sigma \int_0^\beta d\tau\, c_\sigma^*(\tau) c_\sigma(\tau) c_{-\sigma}^*(\tau) c_{-\sigma}(\tau)$$

$\mathbf{k}$–integrated Dyson equation for Weiss function

$$\mathcal{G}_{\sigma n}^{-1} = G_{\sigma n}^{-1} + \Sigma_{\sigma n}$$

Curie temperature

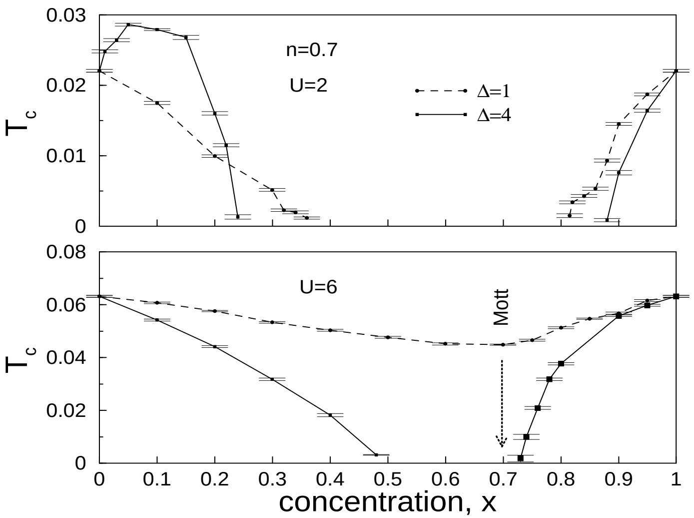


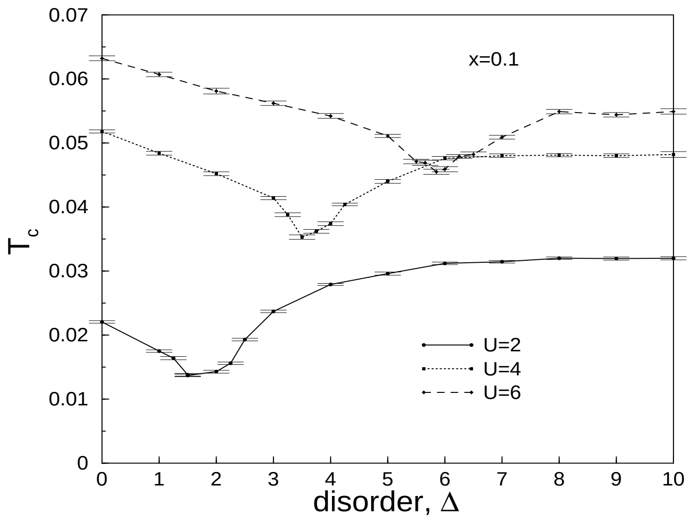


$n = 0.7 \; x = 0.5$

$n = 0.3 \; x = 0.5$

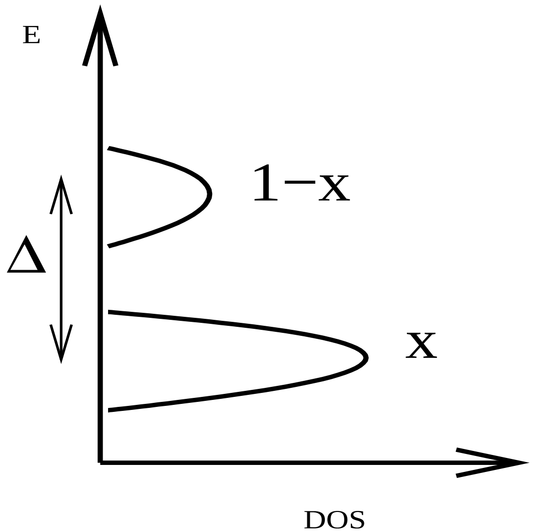
$T_c(x)$ increases !!! at some cases



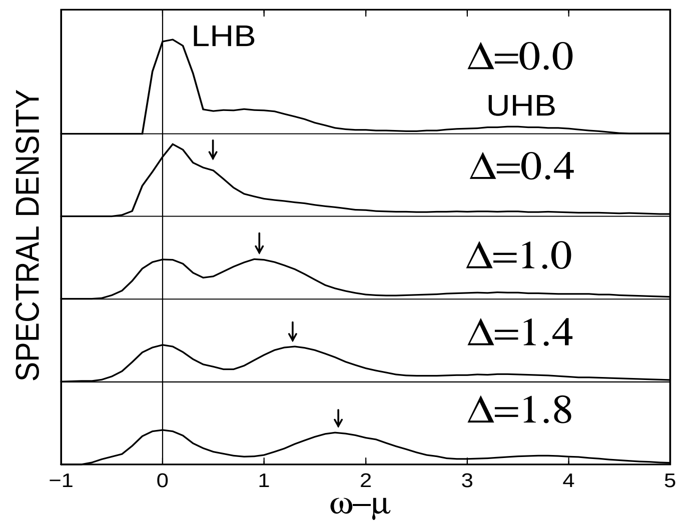


$n = 0.7$

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

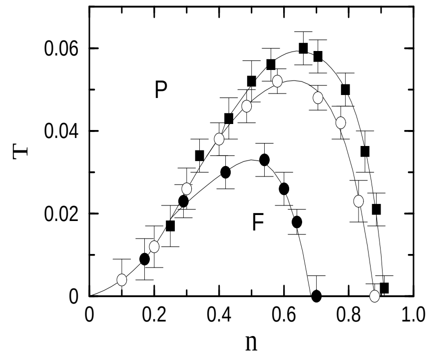


$U = 4,\ n = 0.3,\ n = 0.5,\ T = 0.071,$ MEM

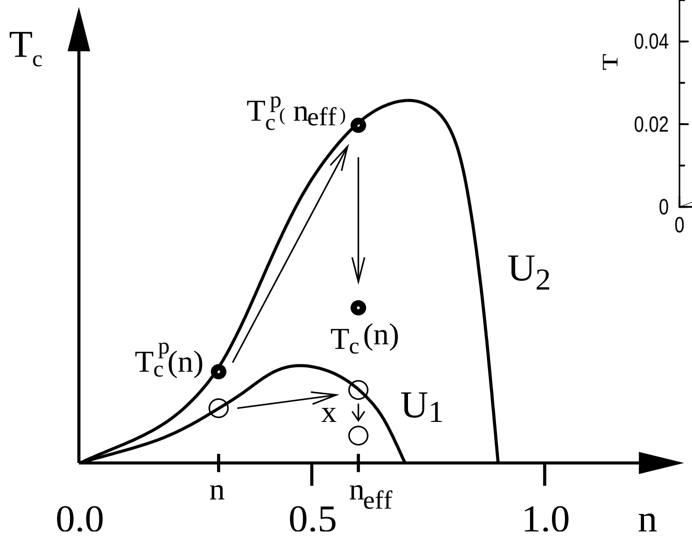


Subtle interplay between Δ and U increases T_c!

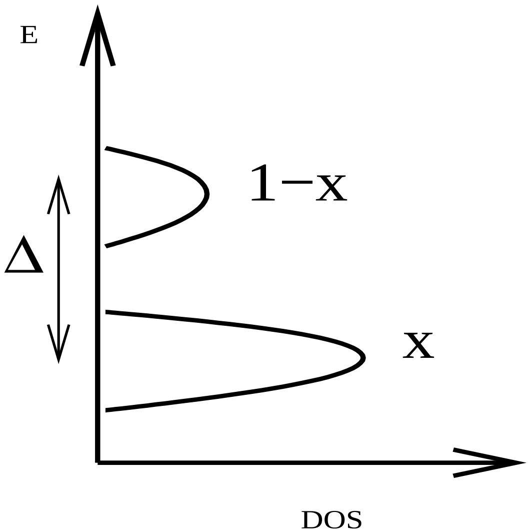
Why is Curie temperature enhanced?



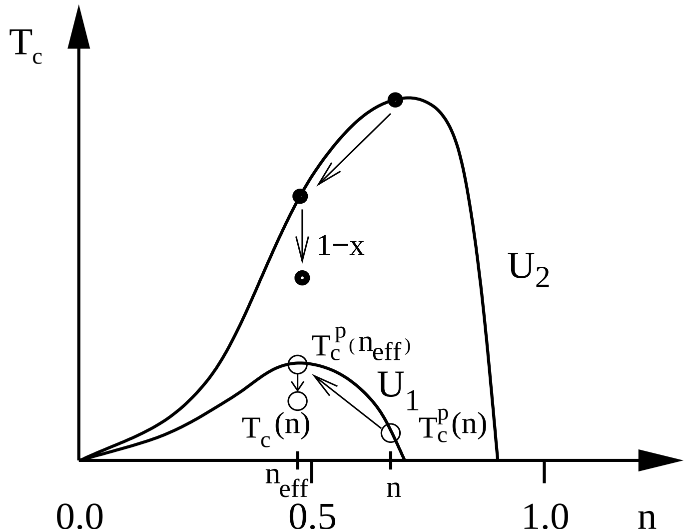
$$n < 2x \rightarrow n_{\text{eff}} = \frac{n}{x}$$
$$T_c = xT_c^p$$



Good for large U



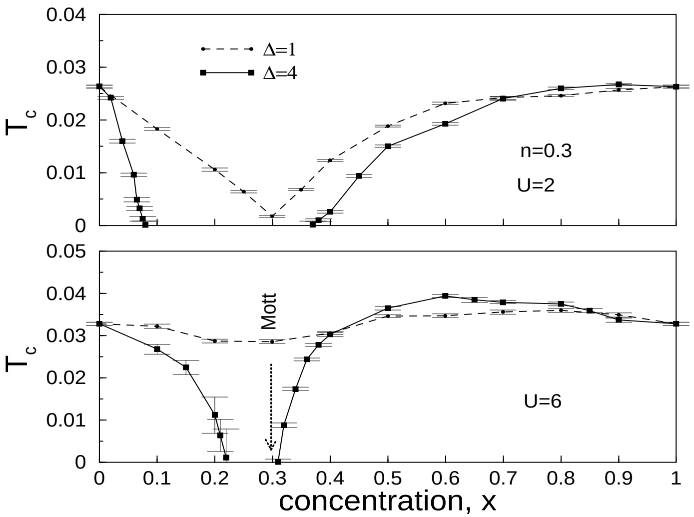
$T_c(x)$ increases !!! at some cases

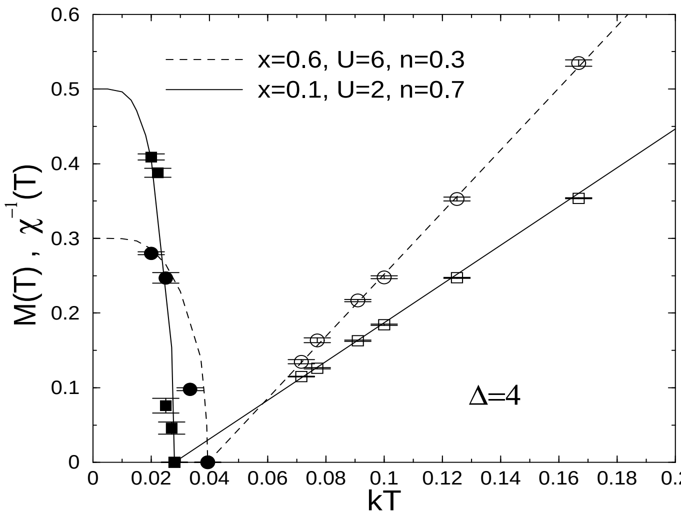


$$n > 2x \rightarrow n_{\text{eff}} = \frac{n-2x}{1-x}$$
$$T_c = (1-x)T_c^p$$

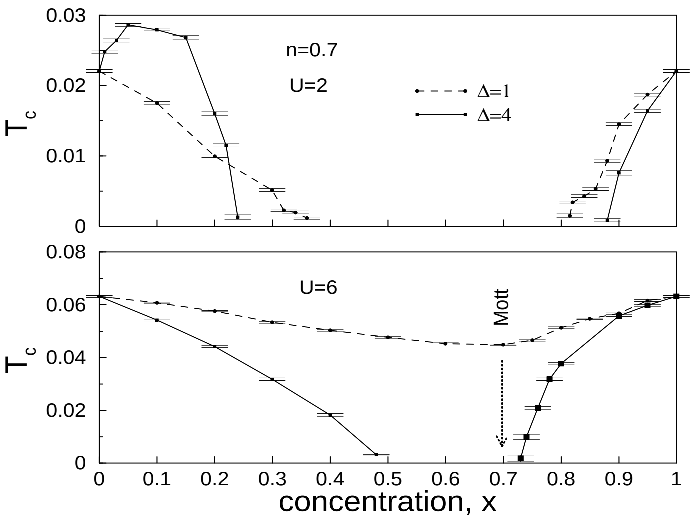
Good for small U

Magnetization and Curie-Weiss law





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

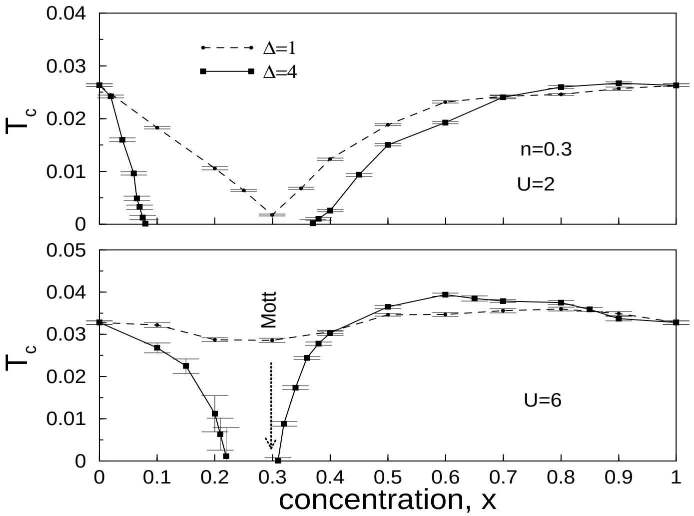


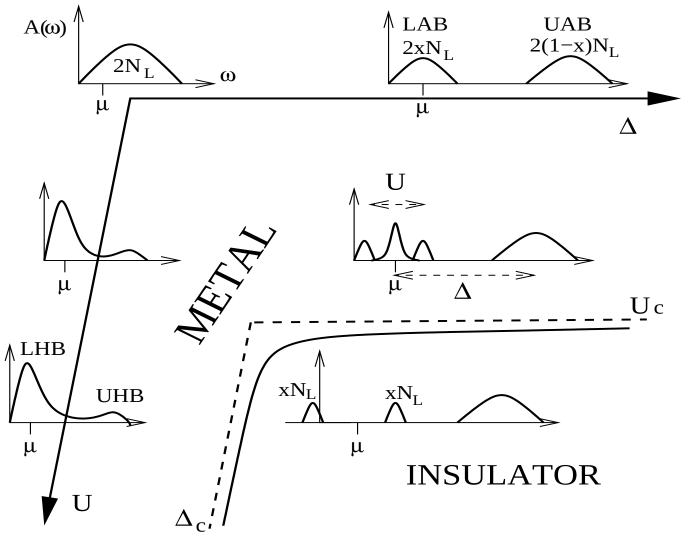
$$\frac{M(T)}{M_s} = \tanh\left[\frac{T_C M(T)}{T M_s}\right]$$

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

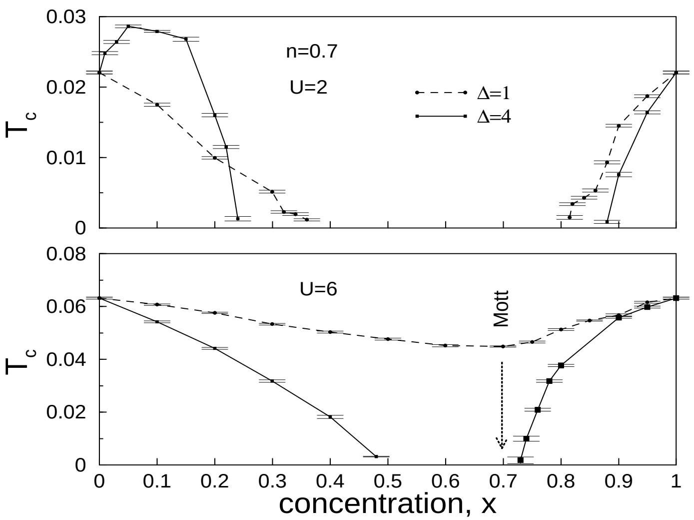
$\frac{C_1}{C_2} = 0.623$ close to $\frac{3}{5}$

Mott–Hubbard metal–insulator transition

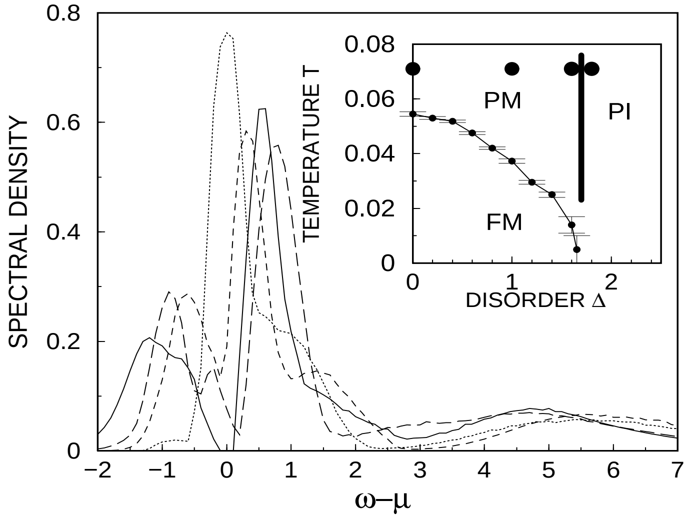




If $n = x$ (or $1 + x$) Mott-Hubbard MIT occures for $\Delta > \sqrt{x}$ and $U > 6\sqrt{x}$ (or $\sqrt{1-x}$ and $6\sqrt{1-x}$)

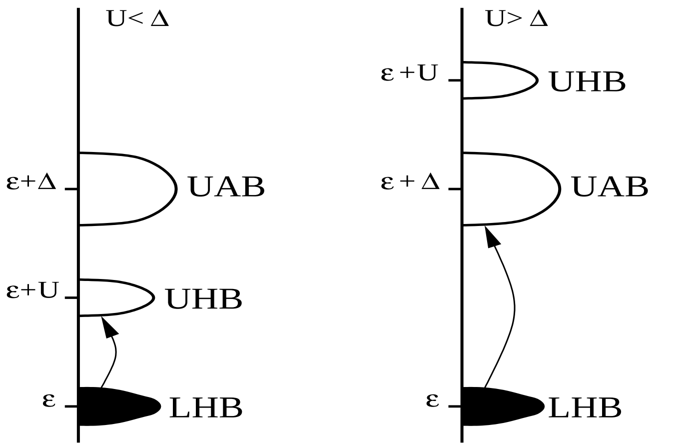


$U = 6,\ x = 0.5,\ n = 0.5,\ T = 0.071$, MEM



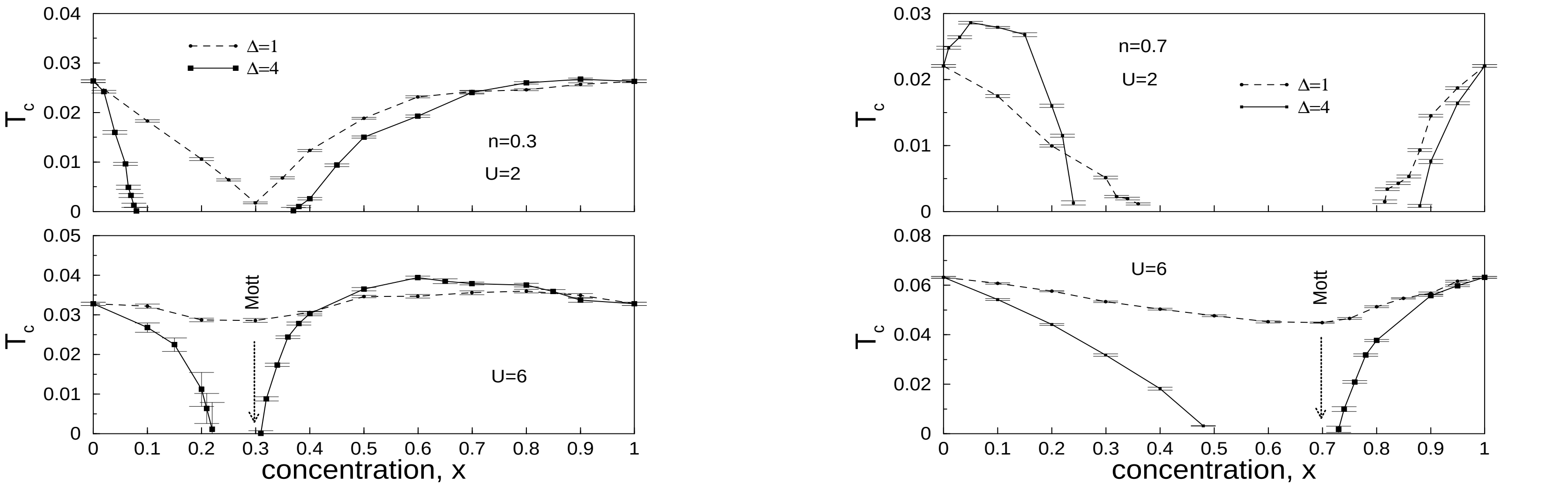
Correlated insulators

- alloy Mott insulator
- alloy charge transfer insulator



alloy Mott insulator | alloy charge transfer insulator

Quantum critical points



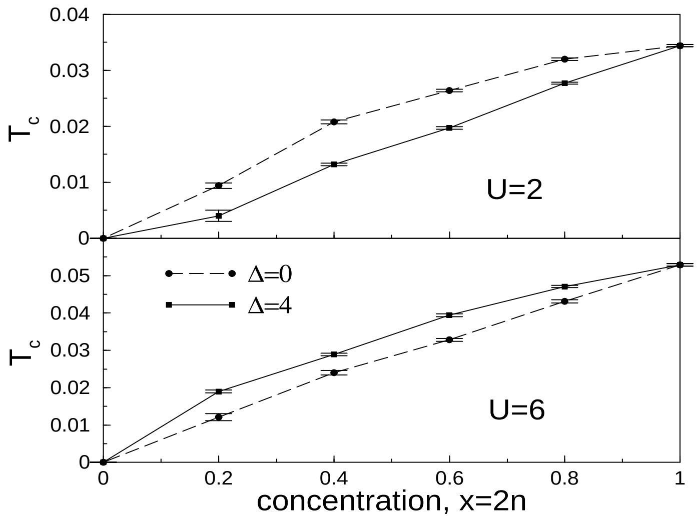
At $T = 0$ quantum phase transitions: FM met $\rightarrow$ PM ins or FM met $\rightarrow$ PM ins (Mott).

Correlation (band-width) controlled, Filling controlled, Alloy concentration controlled Mott MITs.

Is non-Fermi liquid in $d < \infty$? Role of correlations in space.

Non-iso-electronic alloyed Hubbard model

$x = 2n$ as in $\mathrm{Fe}_{1-x}\mathrm{Co}_x$, "empty $e_g^0 \rightarrow e_g^1$ quarter filled"



Summary

- New collective effects induced by correlation and disorder
- Possibilities of T_c increase in binary alloy ferromagnet
- New Mott–Hubbard metal–insulator transition at $n \neq 1$
- Alloy Mott insulator vs. Alloy charge transfer insulator
- Alloy concentration controlled Mott MIT

Outlook

- $T_c(x)$ - QPT ? 2nd vs 1st order PT ?
- Multi-band Hubbard model, role of Hund and exchange coupling, which from our findings are generic for many orbitals ?
- Material specific models ?? LDA+DMFT+disorder ???