Critical exponents in strongly correlated electron systems

Nils Blümer, KOMET Theory

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The trick

(i) mathematical puzzles

1	2	4	8	16	**?**

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1	2	4	8	16	32
4	2	5	2	6	?

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1	2	4	8	16	32
4	2	5	2	6	2
3	1	4	1	5	**?**

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(i) mathematical puzzles

1	2	4	8	16	32
4	2	5	2	6	2
3	1	4	1	5	9

- explicit task: calculate next element(s)

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The trick

(i) mathematical puzzles

1	2	4	8	16	32	?	?	?	. . .
4	2	5	2	6	2				
3	1	4	1	5	9				

- explicit task: calculate next element(s)
- implicit task: derive law (determining all elements)
- hypothesis testable by prediction of selected elements

(ii) Taylor expansions and perturbation series

$$f(x) = \sum_{k=0}^{\infty} a_k \, x^k$$

Function $f(x)$ fully determined by coefficients $\{a_k\}_{k=0}^{\infty}$ within radius of convergence

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a) $\{a_k\} = \boxed{\frac{1}{1}} \; \boxed{\frac{1}{2}} \; \boxed{\frac{1}{6}} \; \boxed{\frac{1}{24}} \; \boxed{\frac{1}{120}} \cdots \boxed{\frac{1}{k!}}$ $\rightsquigarrow$ $f(x) = \sum_{k=0}^{\infty} \frac{x^k}{k!} = e^x$ exponential function

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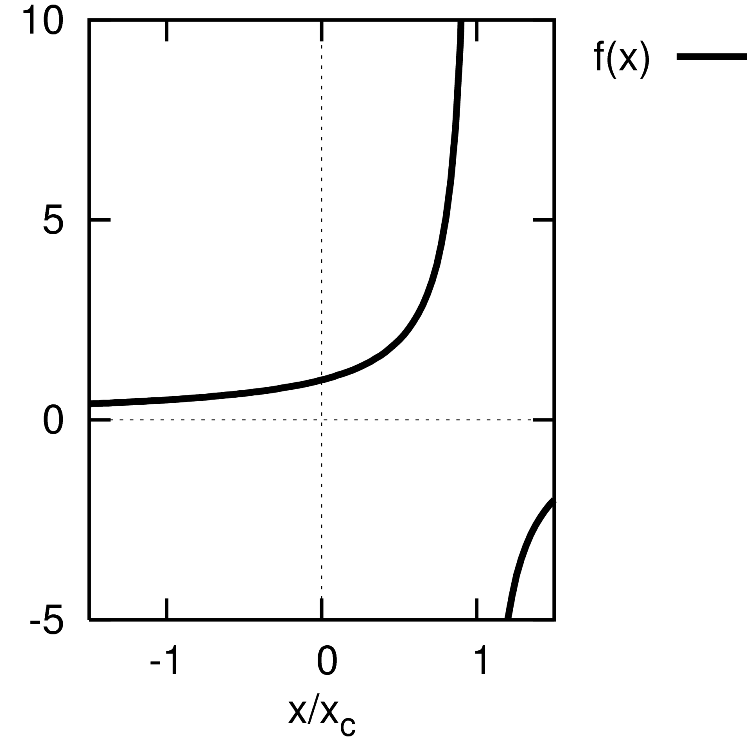
b) $\{a_k\} = \boxed{q^0}\ \boxed{q^1}\ \boxed{q^2}\ \boxed{q^3}\ \boxed{q^4} \cdots \boxed{q^k}$

$$\rightsquigarrow \quad f(x) = \sum_{k=0}^{\infty} (qx)^k = \frac{1}{1-qx} = \frac{1}{q}(x_c - x)^{-1}$$

for $|x| < x_c = q^{-1}$ geometric series



Note: singularity in $f(x)$ at x_c, exponent -1

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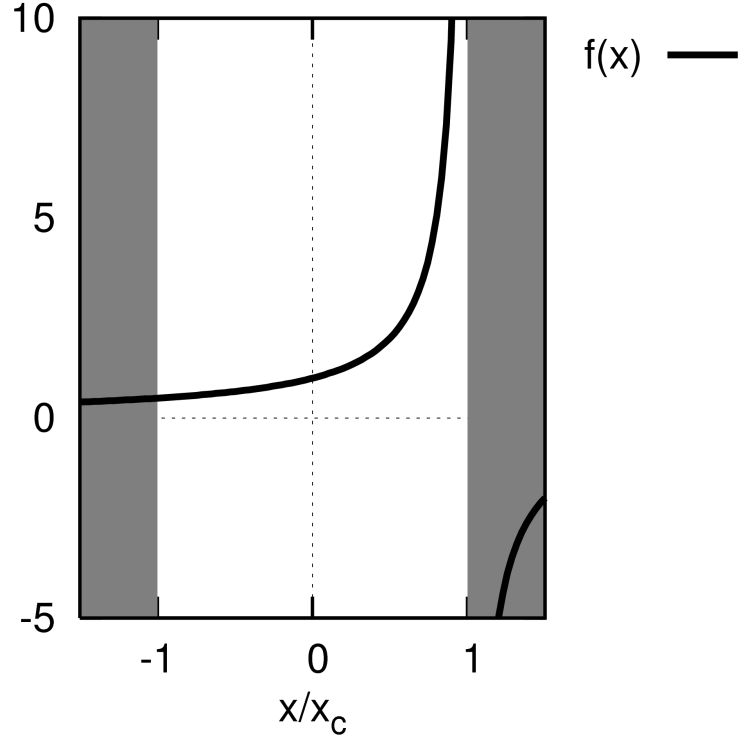

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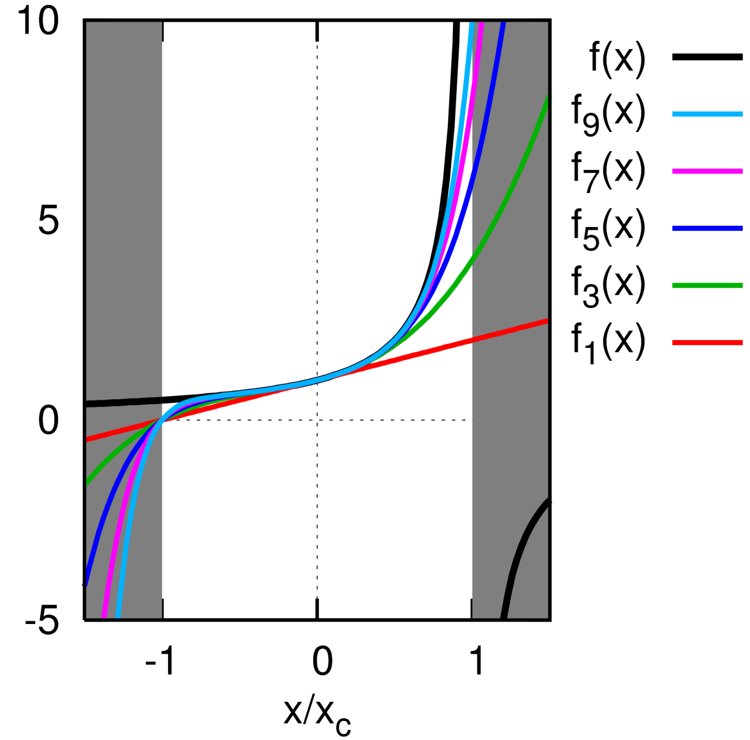
However: finite order approximations

$f_n(x) = \sum_{k=0}^{n} a_k\, x^k$ regular for all x



(iii) Essence of extrapolated perturbation theory (ePT)

1) obtain as many coefficients as possible

2) derive law

3) test law

4) characterize singularity and extract critical exponents

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a_2	a_4	a_6	a_8	a_{10}

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$$f^{\text{irr}}(x) \propto \left| x - q^{-1} \right|^{\tau - 1} \quad \ldots$$

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Outline

Essence of extrapolated perturbation theory (ePT)

Phase transitions and critical exponents

Strongly correlated electron systems

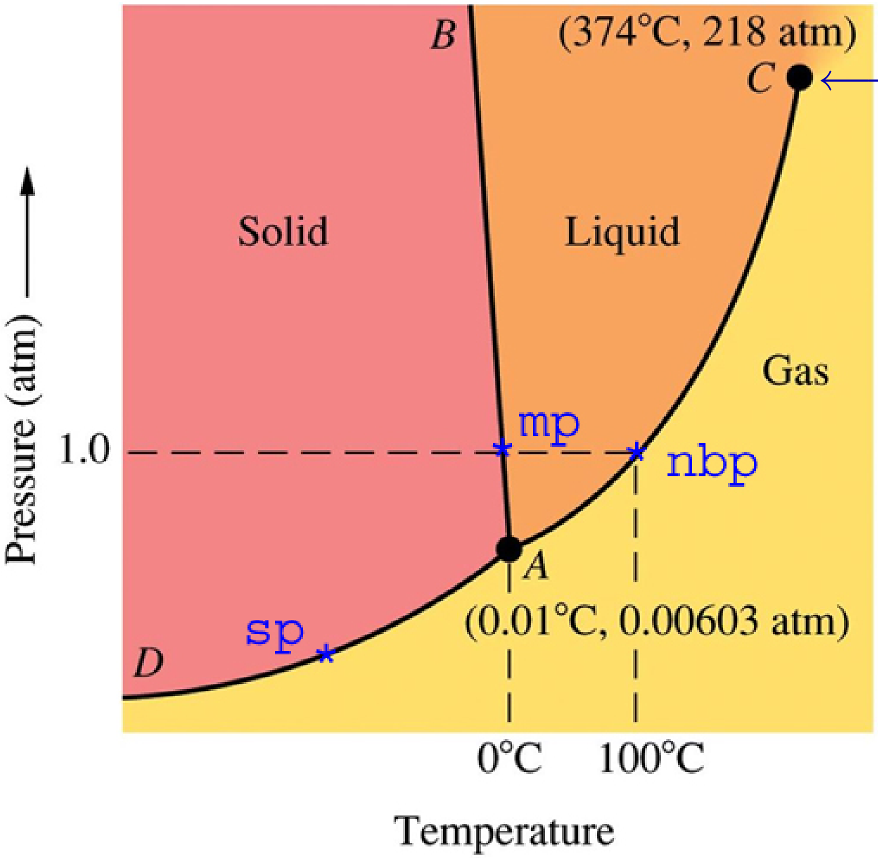
Mott metal insulator transition

Critical exponents

Summary

Phase transitions and critical exponents

Liquid-gas transition of water



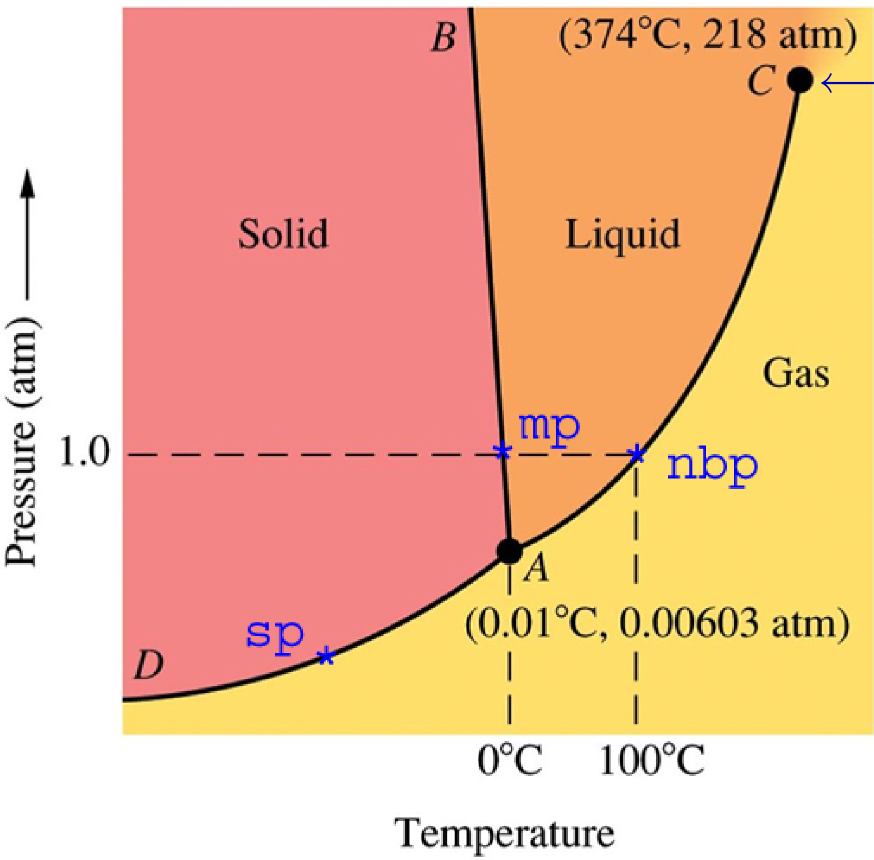
2nd order critical end point

liquid-gas transition: 1st order at $T_t < T < T^*$

2nd order at $T = T^*$

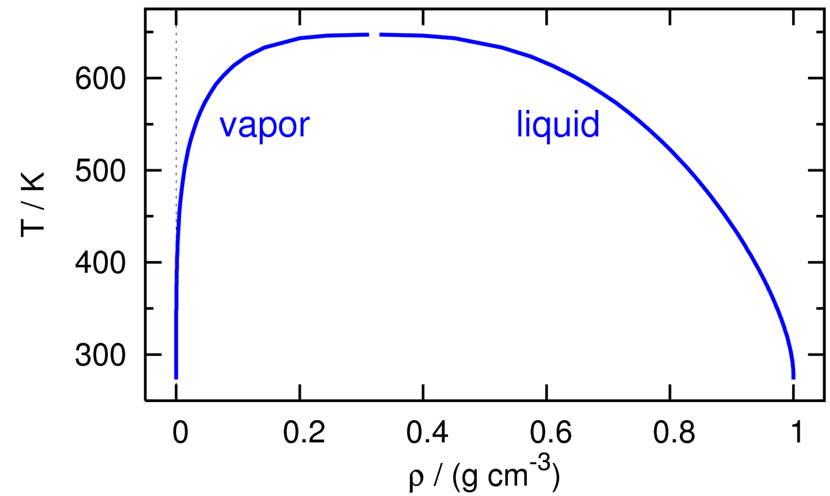
Phase transitions and critical exponents

Liquid-gas transition of water



2^{nd} order critical end point

Coexistence curves of vapor + water



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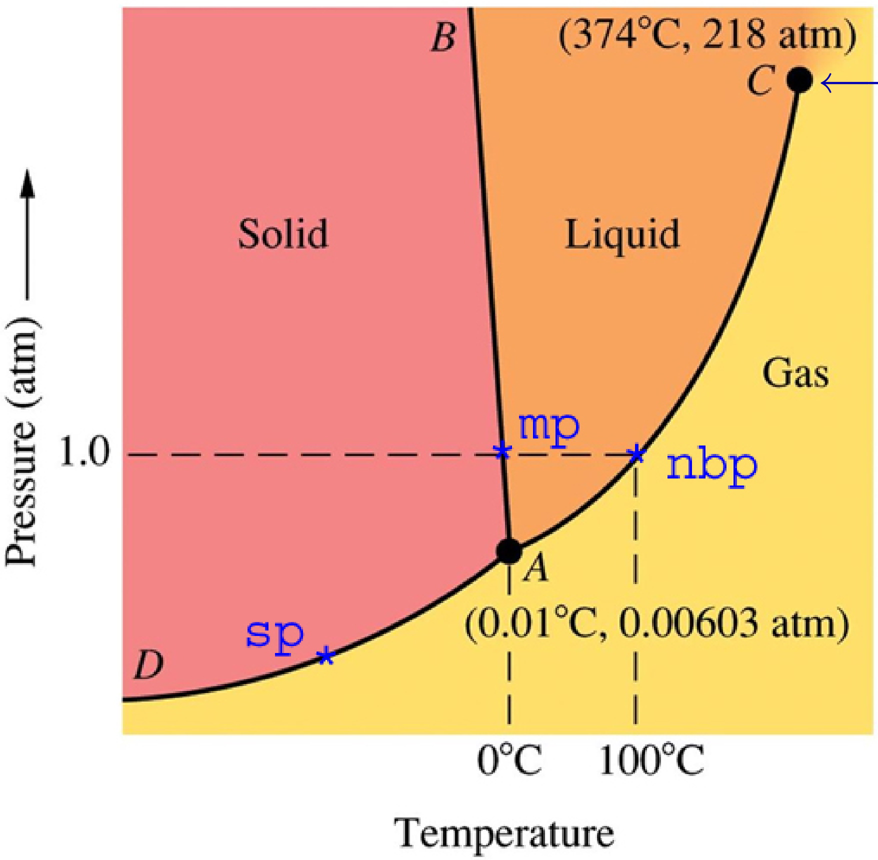

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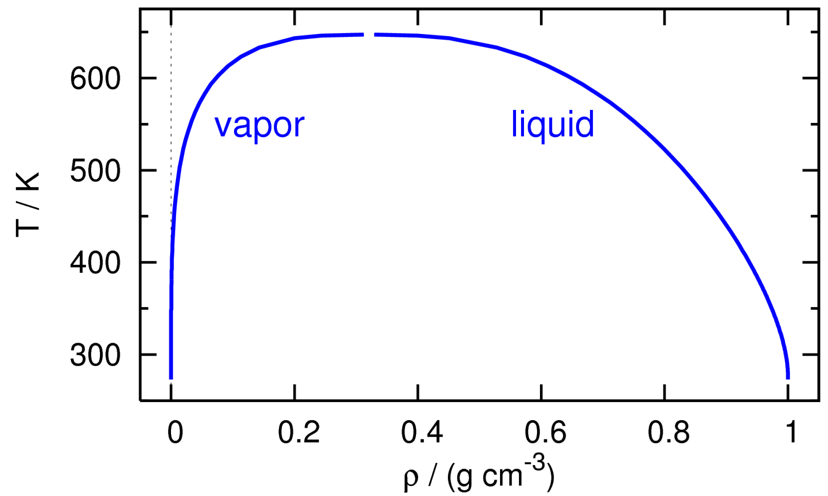
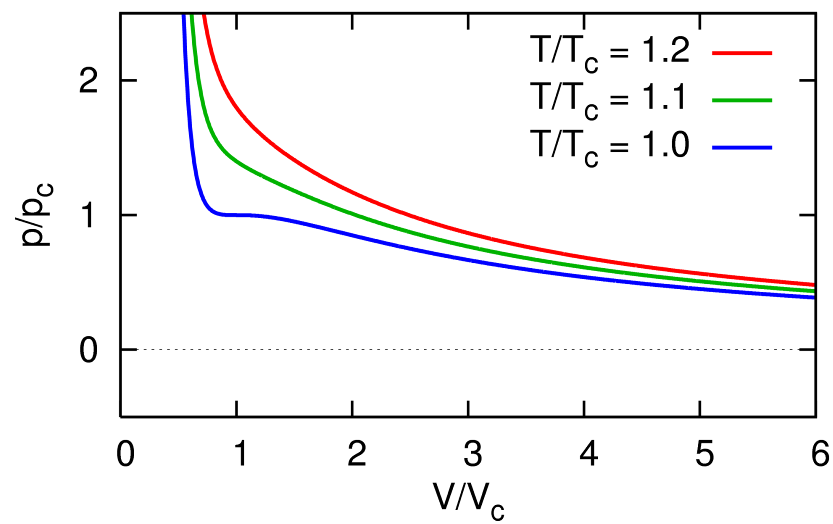


p(V) curves for van der Waals system



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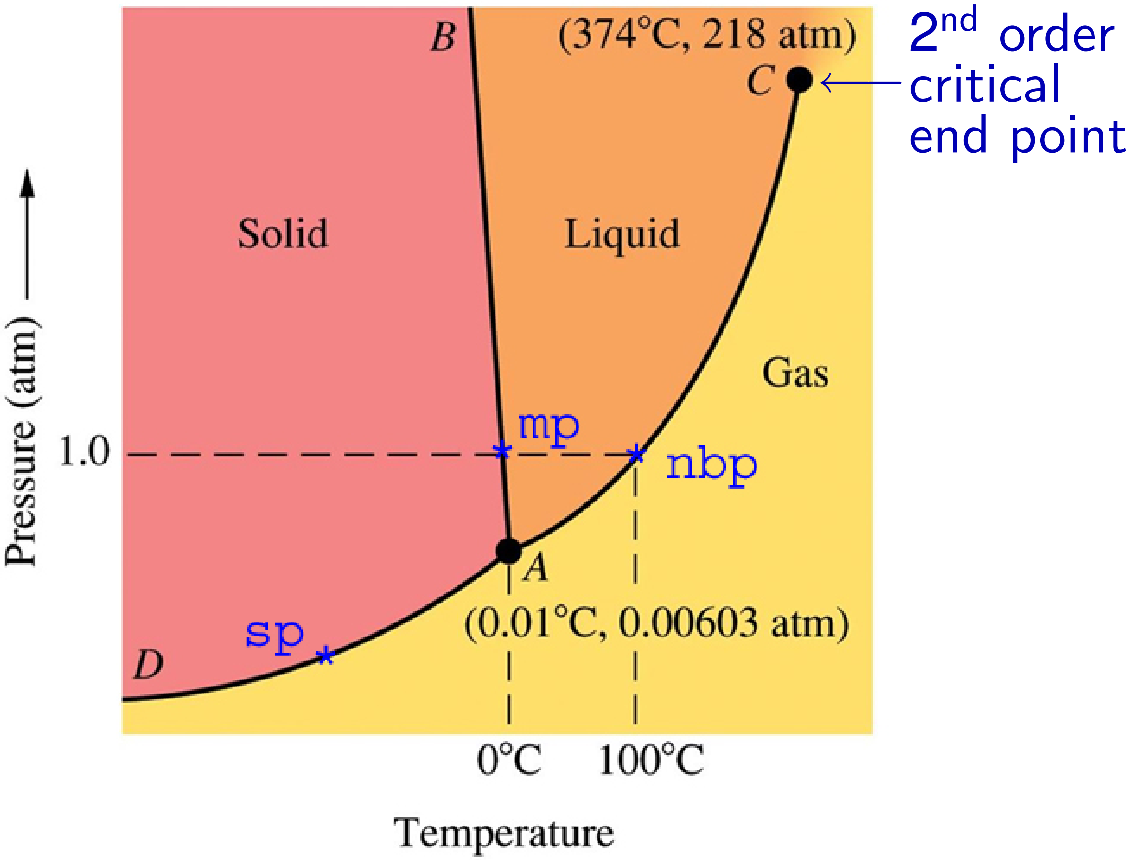

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metastable: superheated/cooled water, ...

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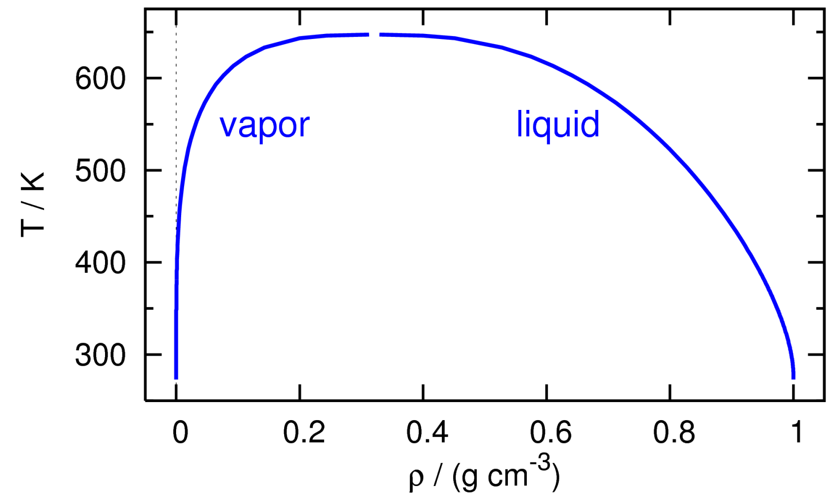

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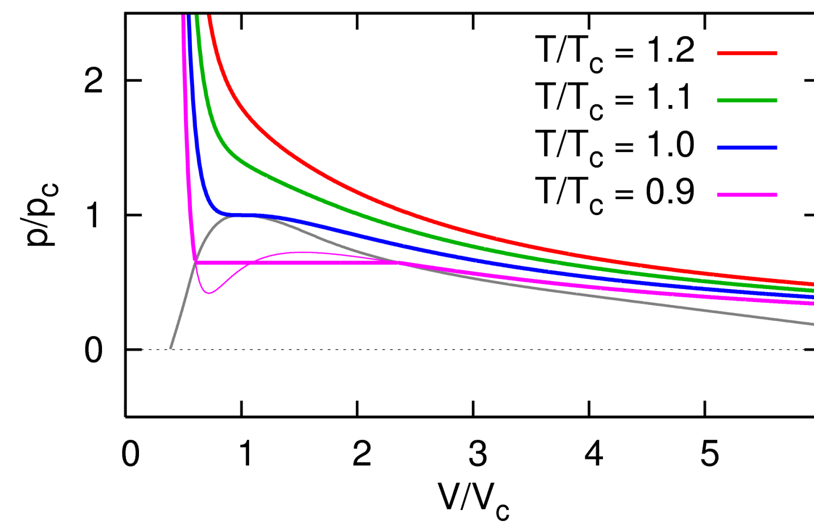

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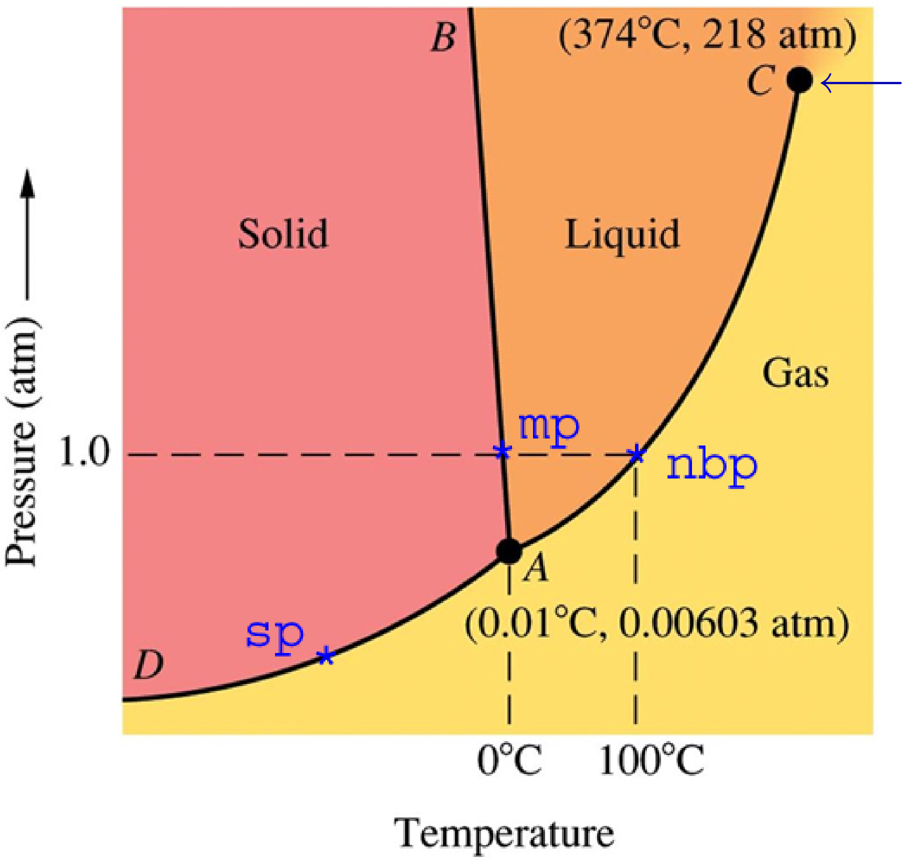

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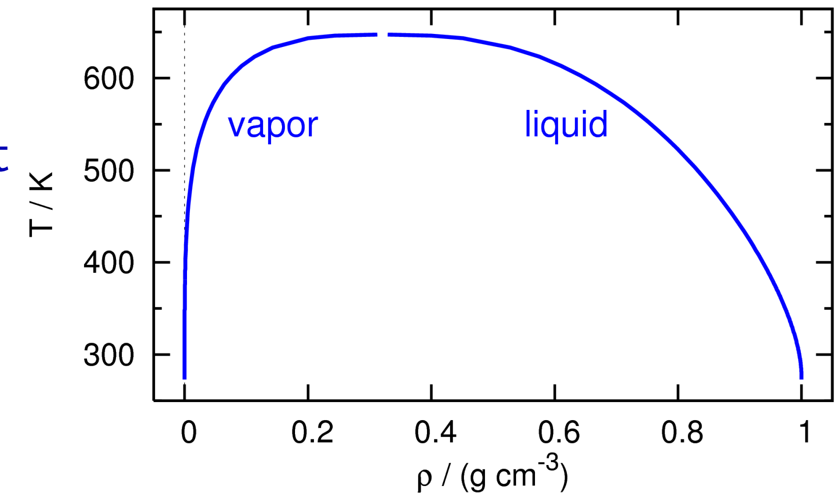

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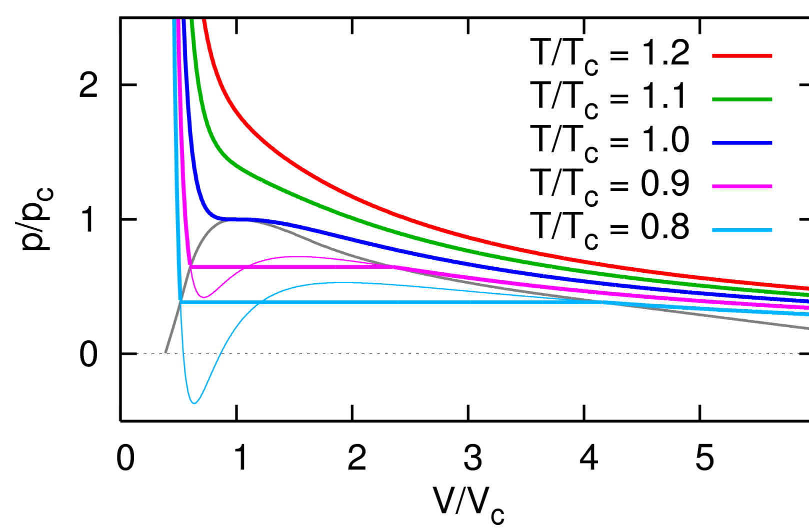

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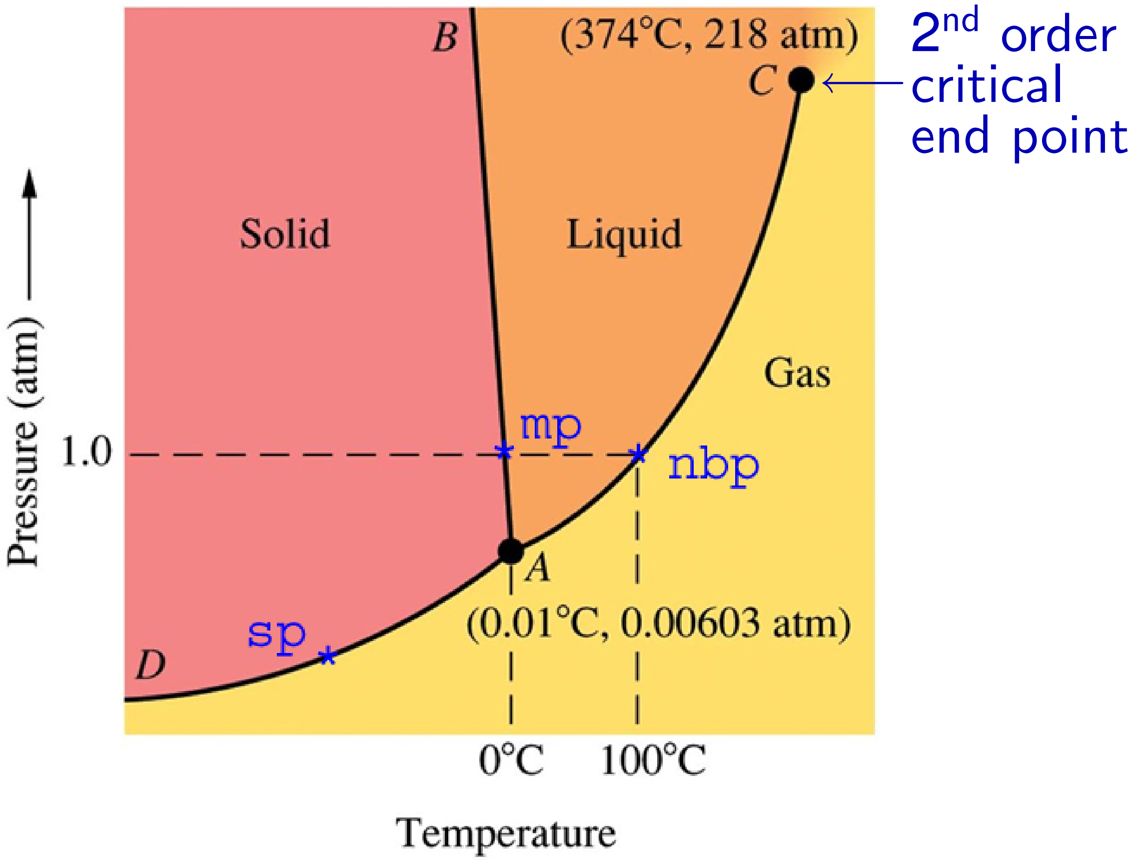

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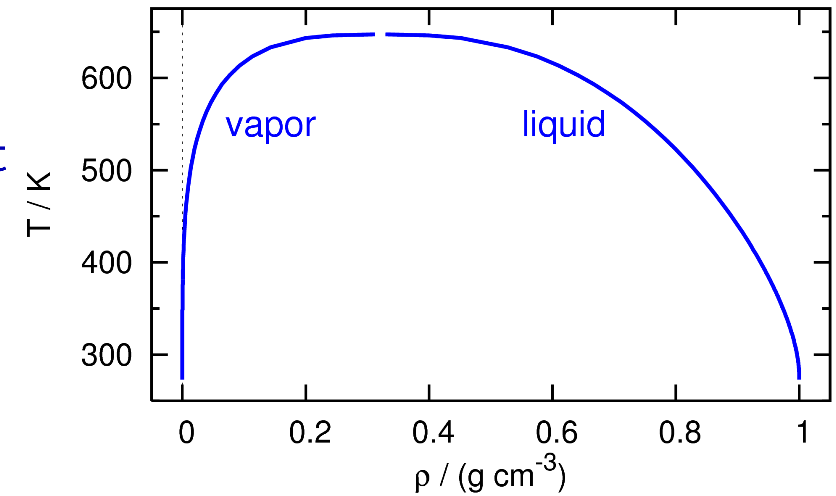

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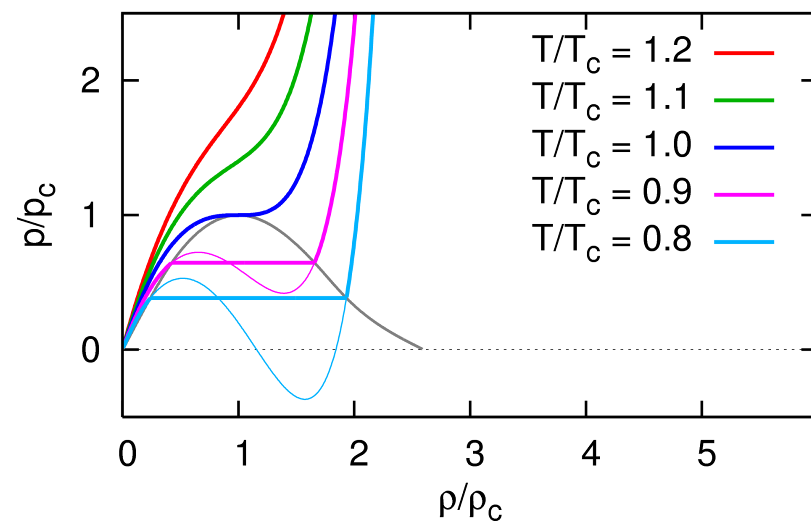
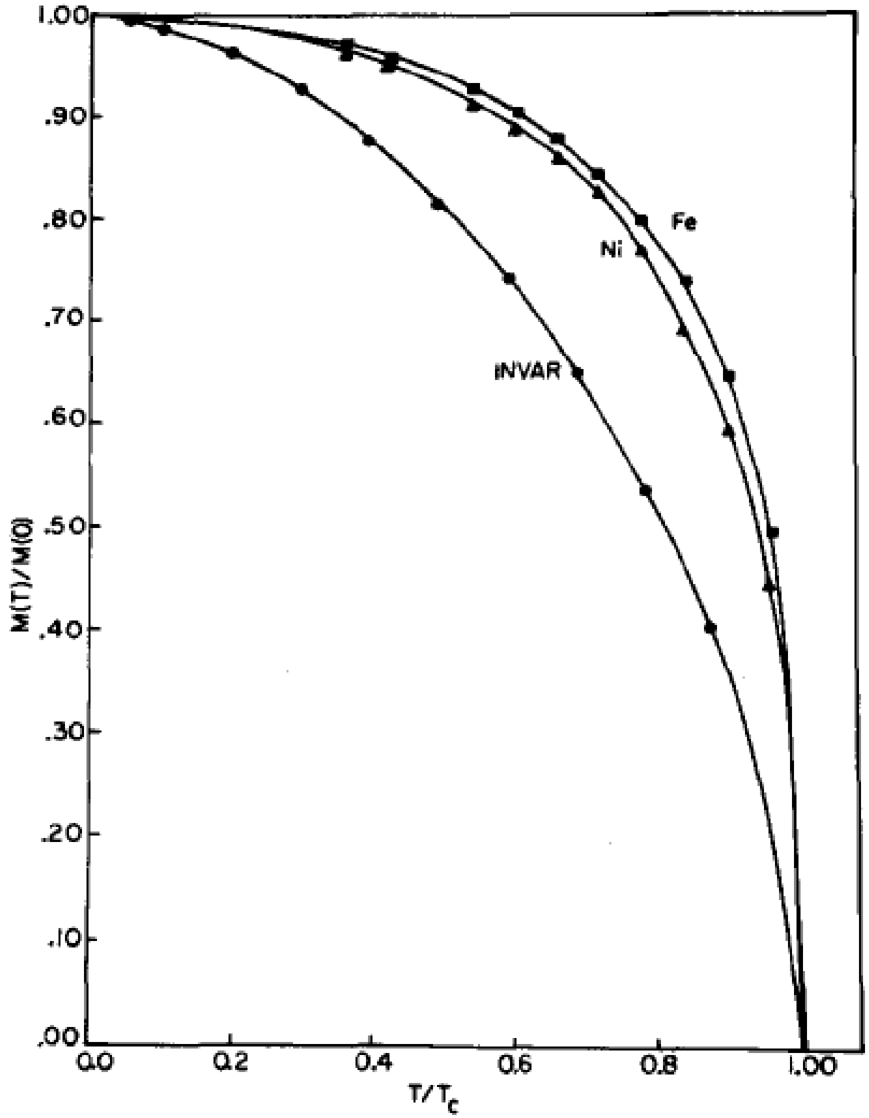


Ferromagnetism

Magnetization of Fe, Ni, INVAR



[Schlosser, Phys. Lett. 40, 195 (1972)]

Critical behavior at 2nd order transition:

$$M(T) \sim |T - T_c|^{\beta} \quad \text{magnetization}$$

$$\chi(T) \sim |T - T_c|^{-\gamma} \quad \text{susceptibility}$$

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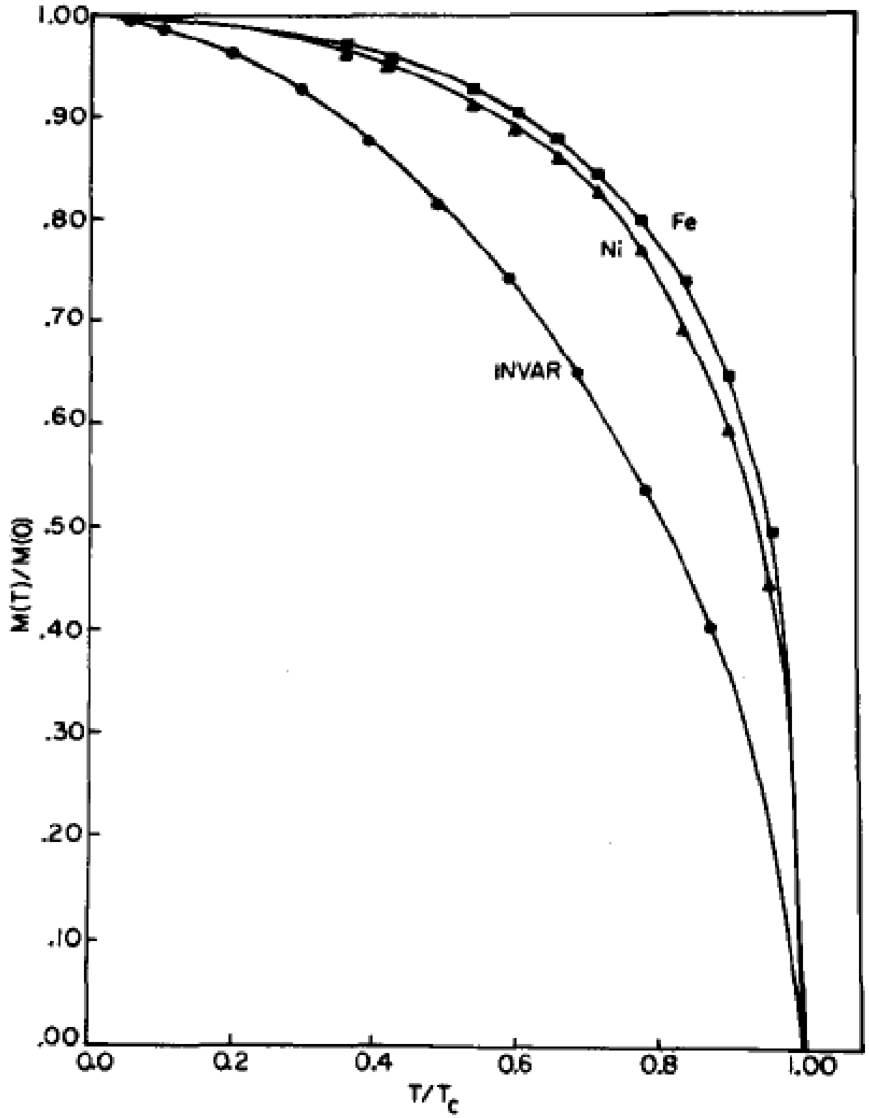

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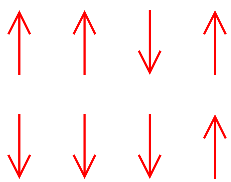
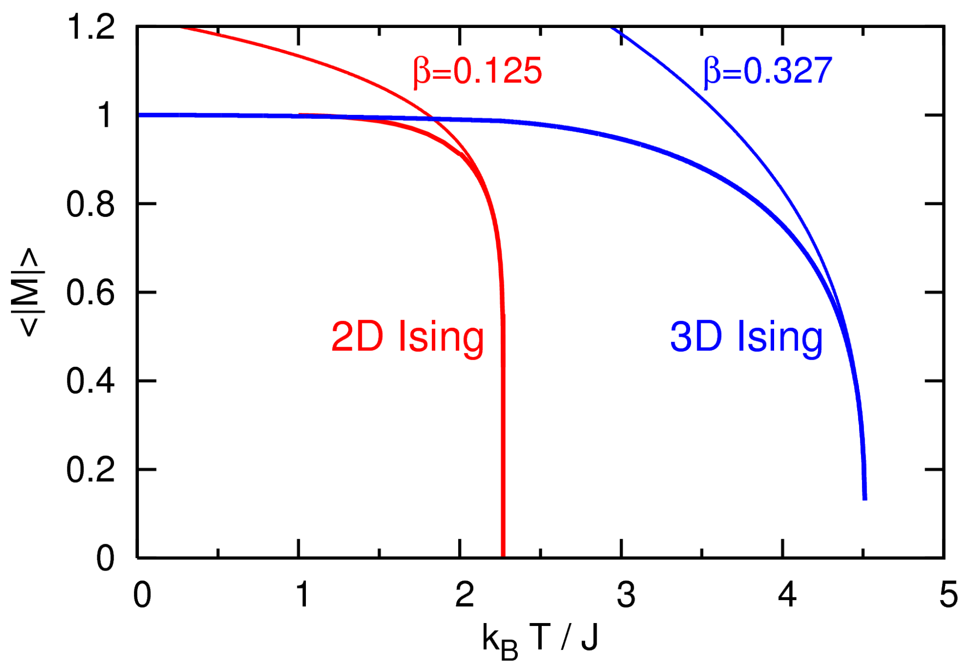
Ising model $H = J \sum_{\langle ij \rangle} s_i^z s_j^z$





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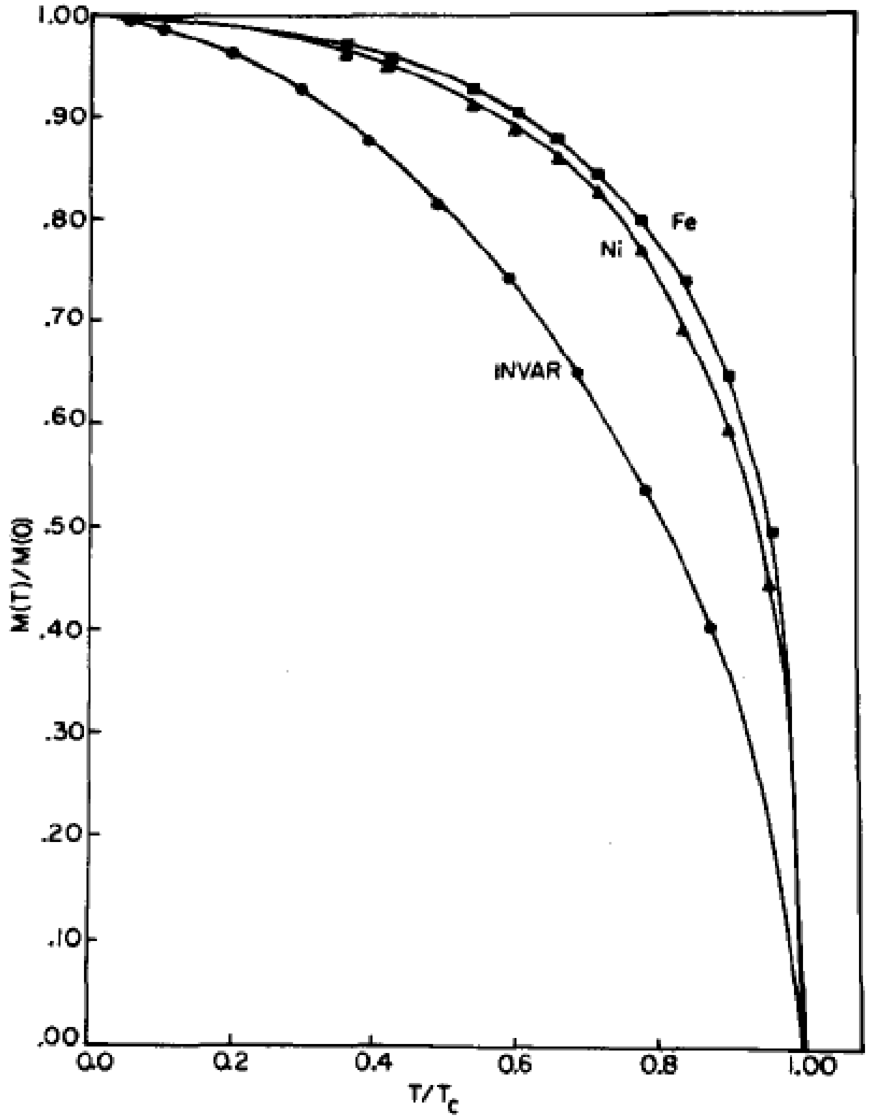

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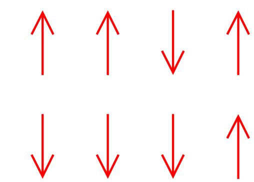

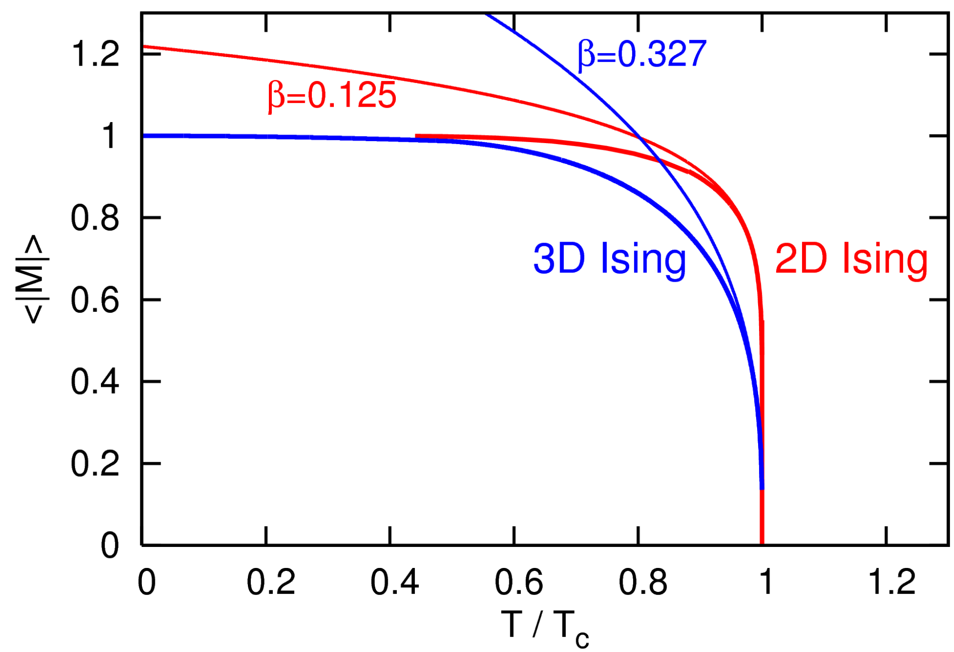

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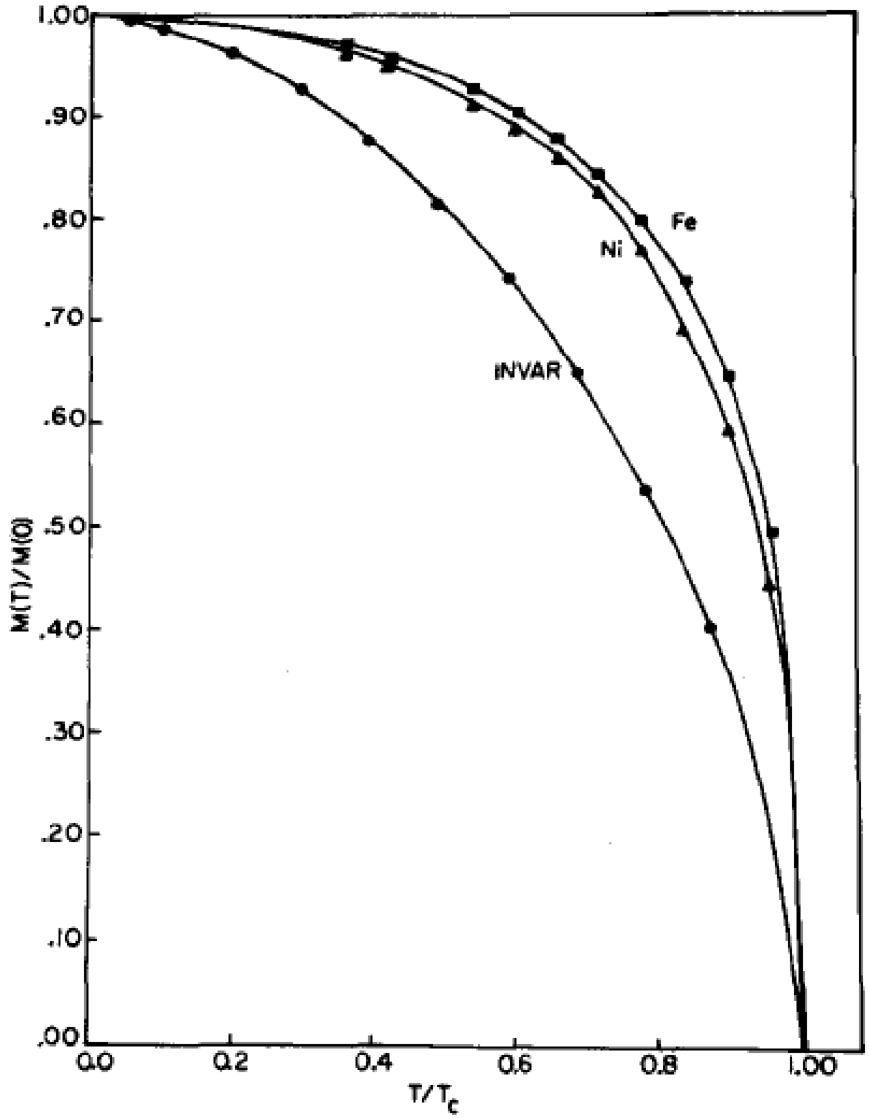

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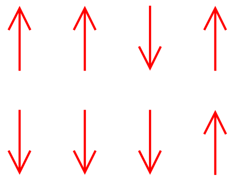
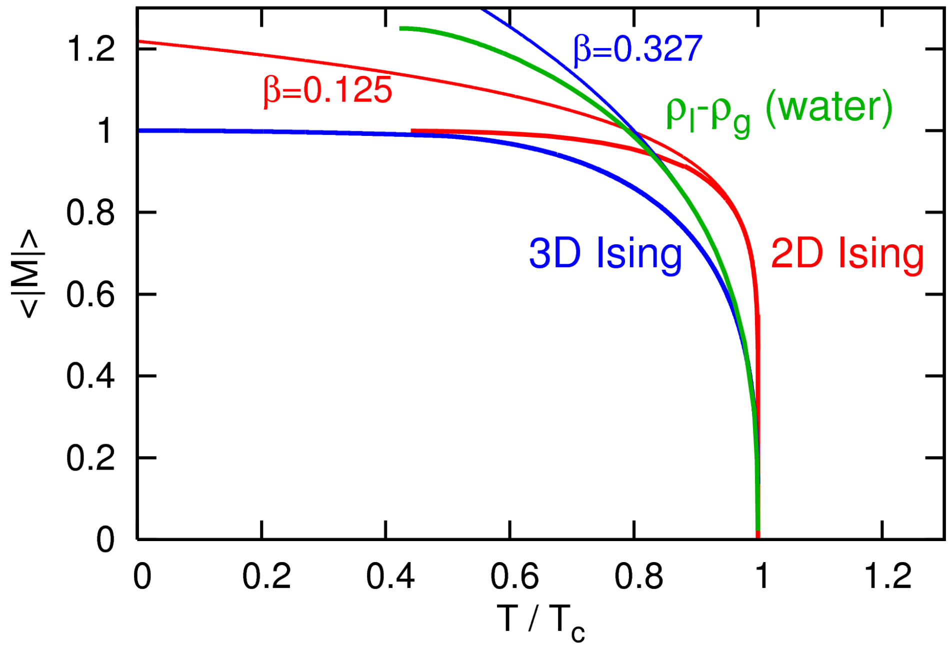


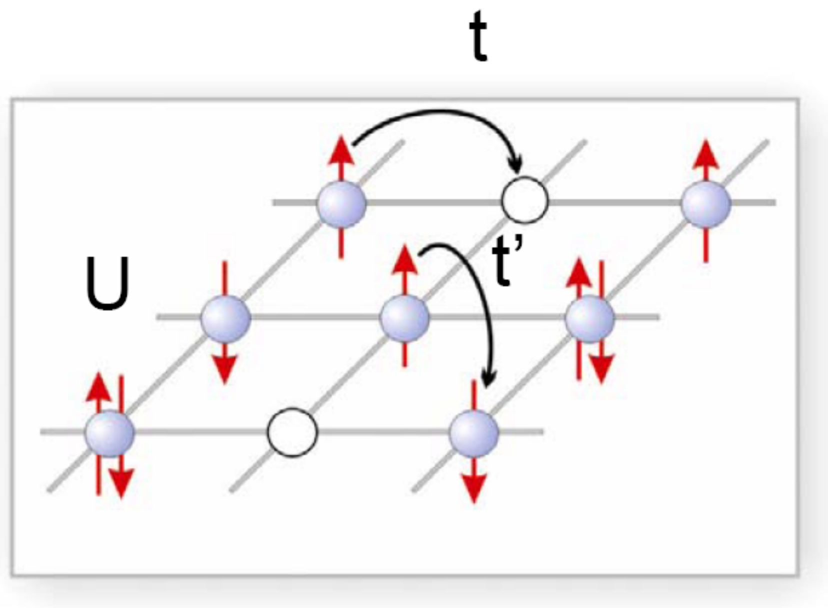


Liquid-gas: 3D Ising universality class

Strongly correlated electron systems

Valence electrons in solids:

correlated by Coulomb repulsion and Pauli principle $\rightsquigarrow$ Hubbard type models



Charge and spin degrees of freedom

Competition between kinetic energy ($W(t, t')$) and potential energy (U)

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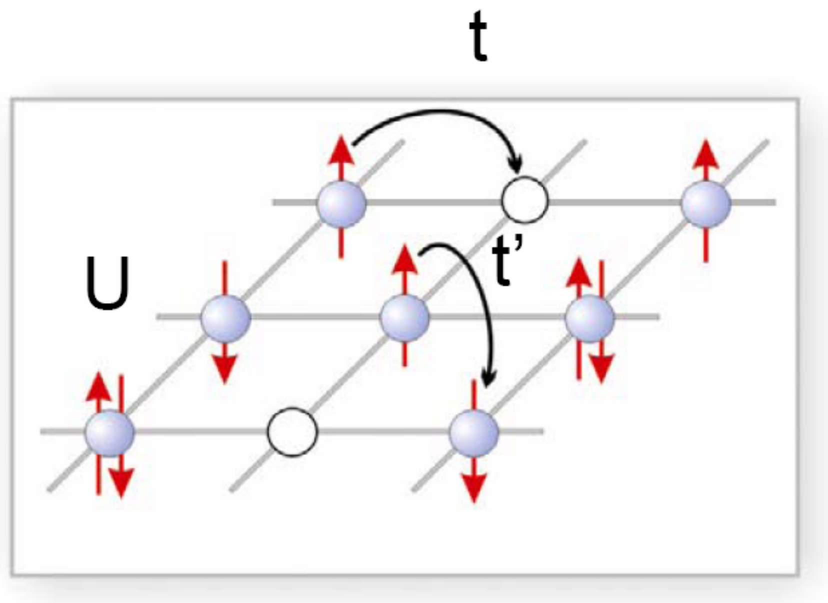

Charge and spin degrees of freedom

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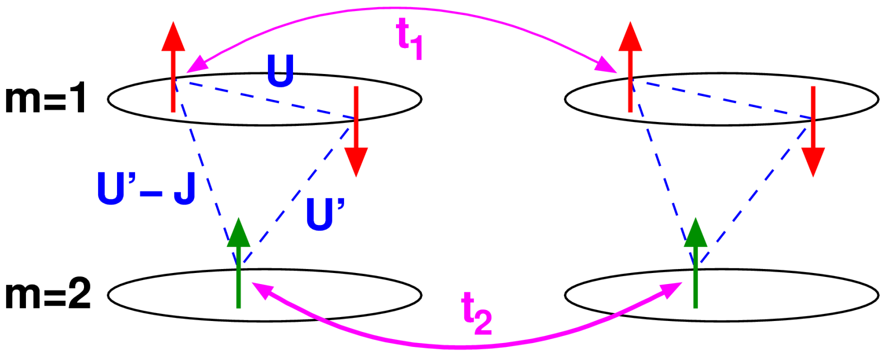
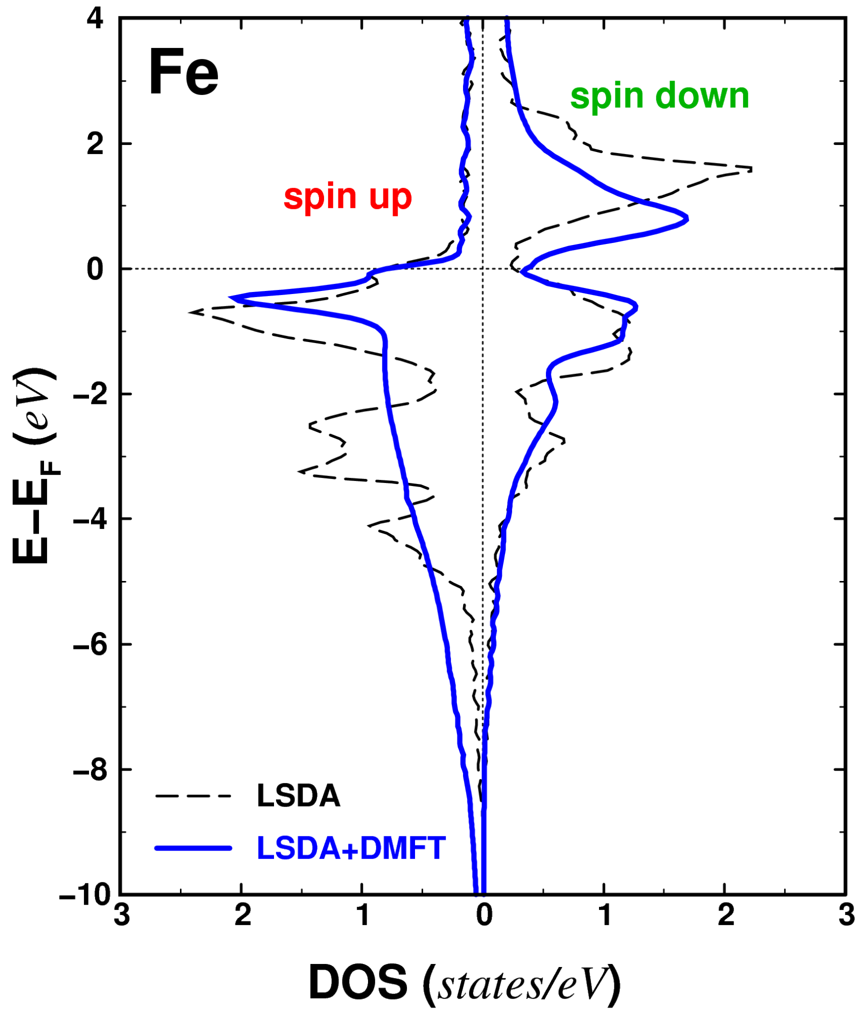
Multi-band case: Hund rule couplings



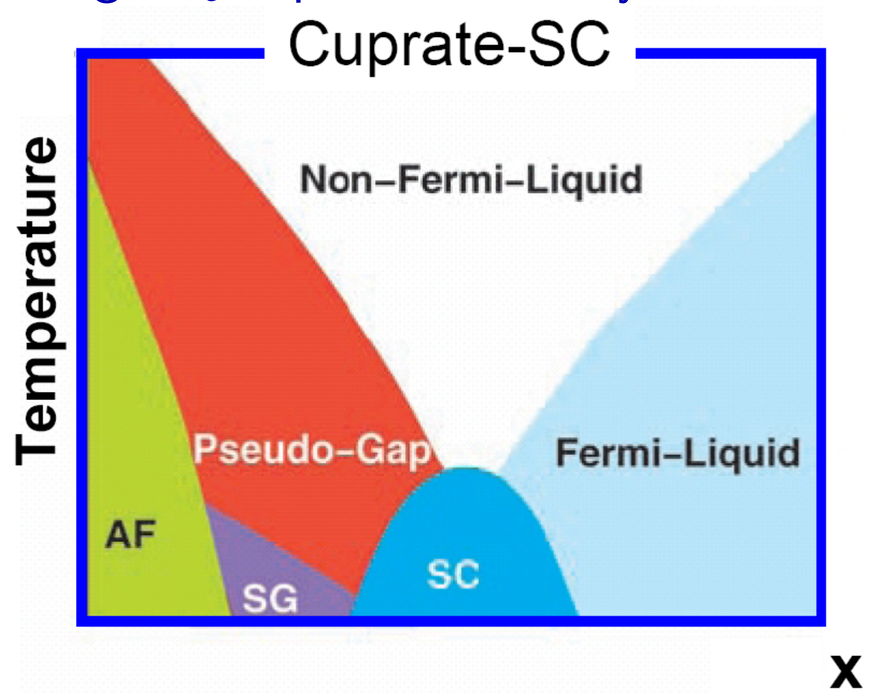
Systems and phenomena

- Itinerant (ferro)magnetism



[Chioncel et. al, PRB (2003)]

- High-T_c superconductivity



- **Metal-insulator transitions**

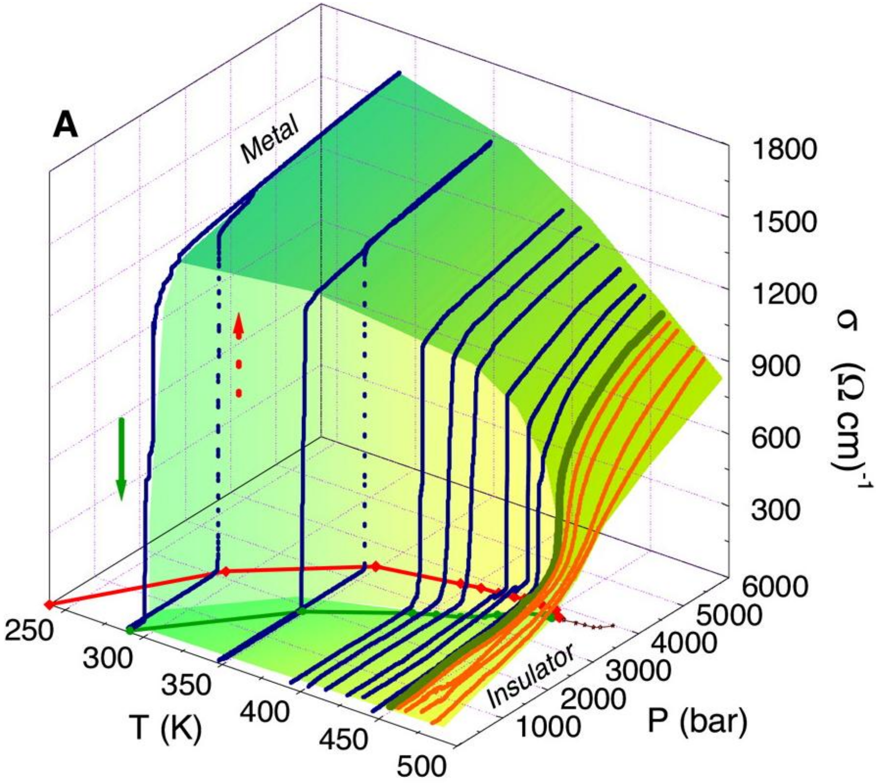
- Ultracold atoms on optical lattices

. . .

The Mott metal-insulator transition

Mott transition in $(V_{1-x}Cr_x)_2O_3$:

Hysteresis in conductivity



[Limelette et al., Science 302, 89 (2003)]

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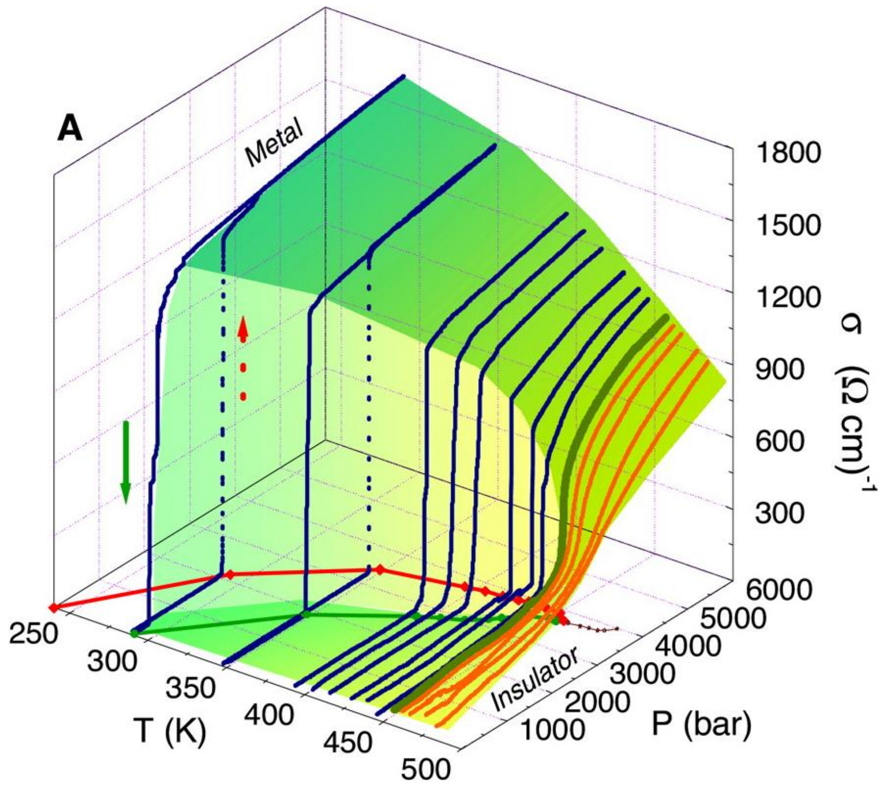

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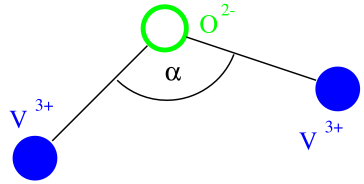
Pressure changes W/U



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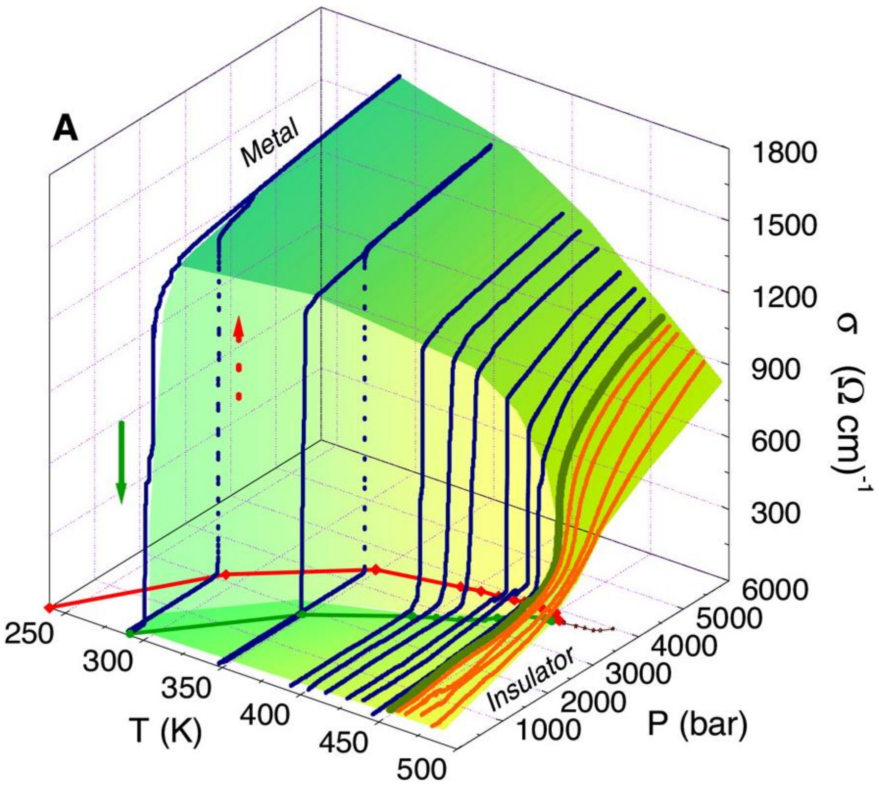

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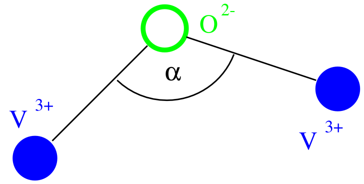
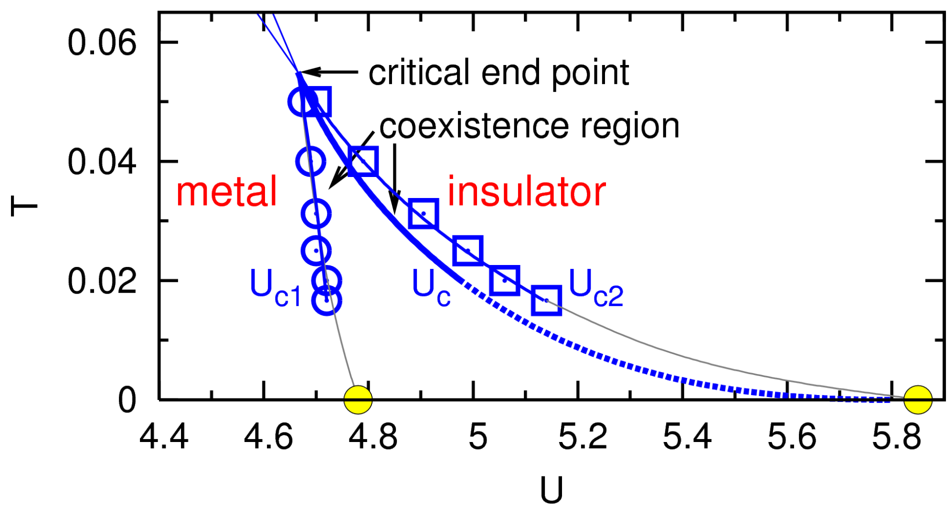


Theoretical phase diagram:

Dynamical mean-field theory (DMFT)

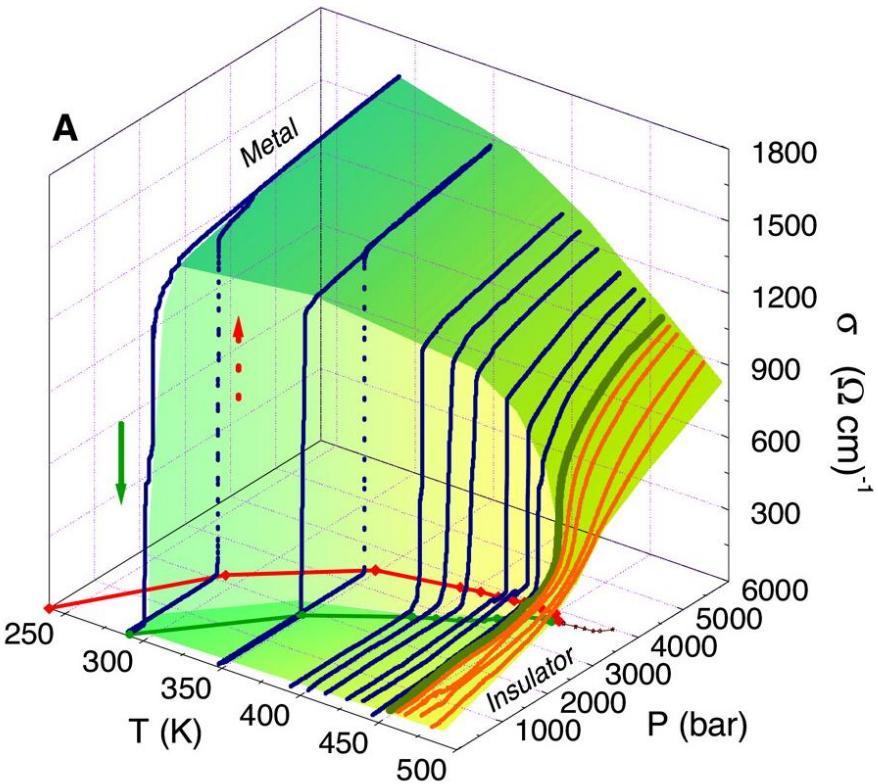
Quantum Monte Carlo (QMC)



The Mott metal-insulator transition

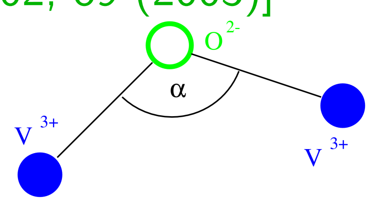
Mott transition in $(V_{1-x}Cr_x)_2O_3$:

Hysteresis in conductivity



[Limelette et al., Science 302, 89 (2003)]

Pressure changes W/U



Theoretical phase diagram:

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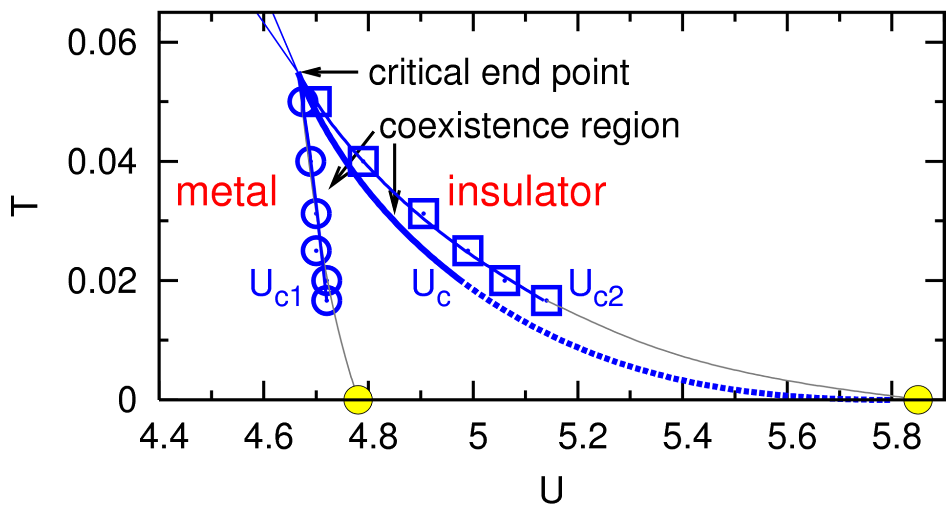

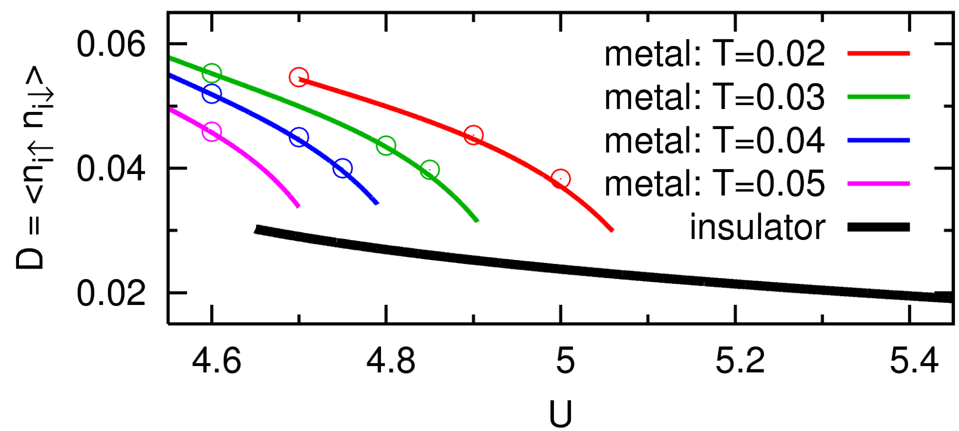

Critical exponents from ePT (using PT + QMC)

Kato-Takahashi strong-coupling perturbation theory ($T=0$)

$$E_{\mathrm{PT}}(U) = -\frac{1}{2}\frac{t^2}{U} - \frac{1}{2}\frac{t^4}{U^3} - \frac{19}{8}\frac{t^6}{U^5} - \frac{593}{32}\frac{t^8}{U^7} - \frac{23877}{128}\frac{t^{10}}{U^9} + \mathcal{O}\left(\frac{t^{12}}{U^{11}}\right)$$

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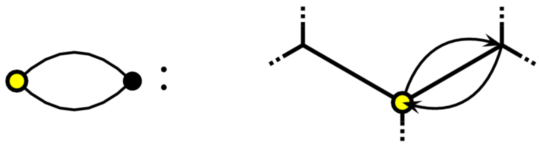

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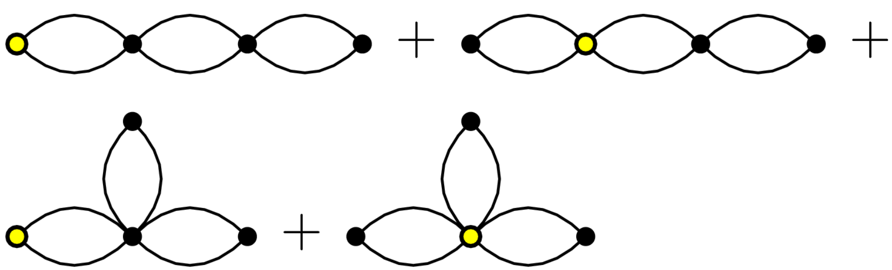

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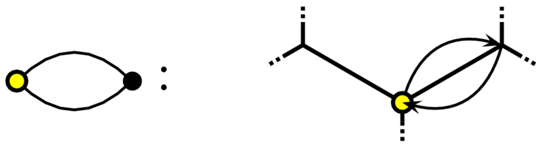

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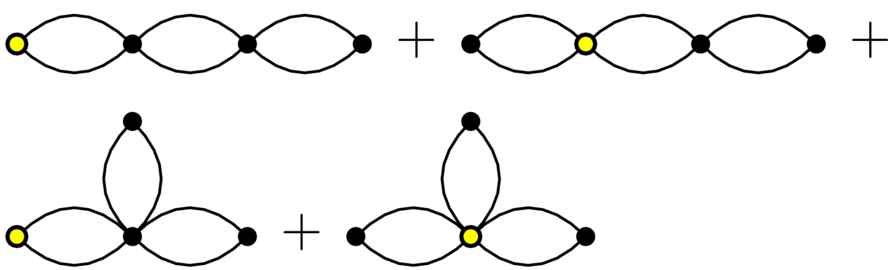

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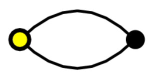
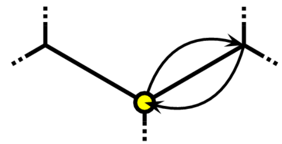
coefficient ratios: 1 4.8 7.8 10.1

$\mathcal{O}\left(\frac{t^2}{U}\right)$:  : 

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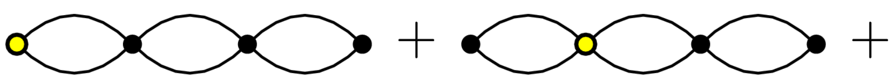
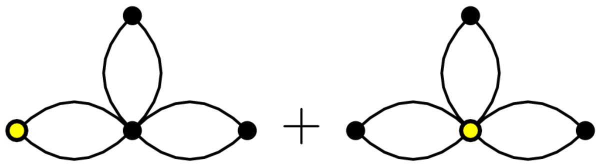
$\mathcal{O}\left(\frac{t^6}{U^5}\right)$: 



10$^{\mathrm{th}}$order PT accurate (only) at $U \gtrsim 6$: $\Delta E_{\mathrm{PT}} \leq 10^{-5}$ **extrapolation?**

Extrapolated perturbation theory: ePT

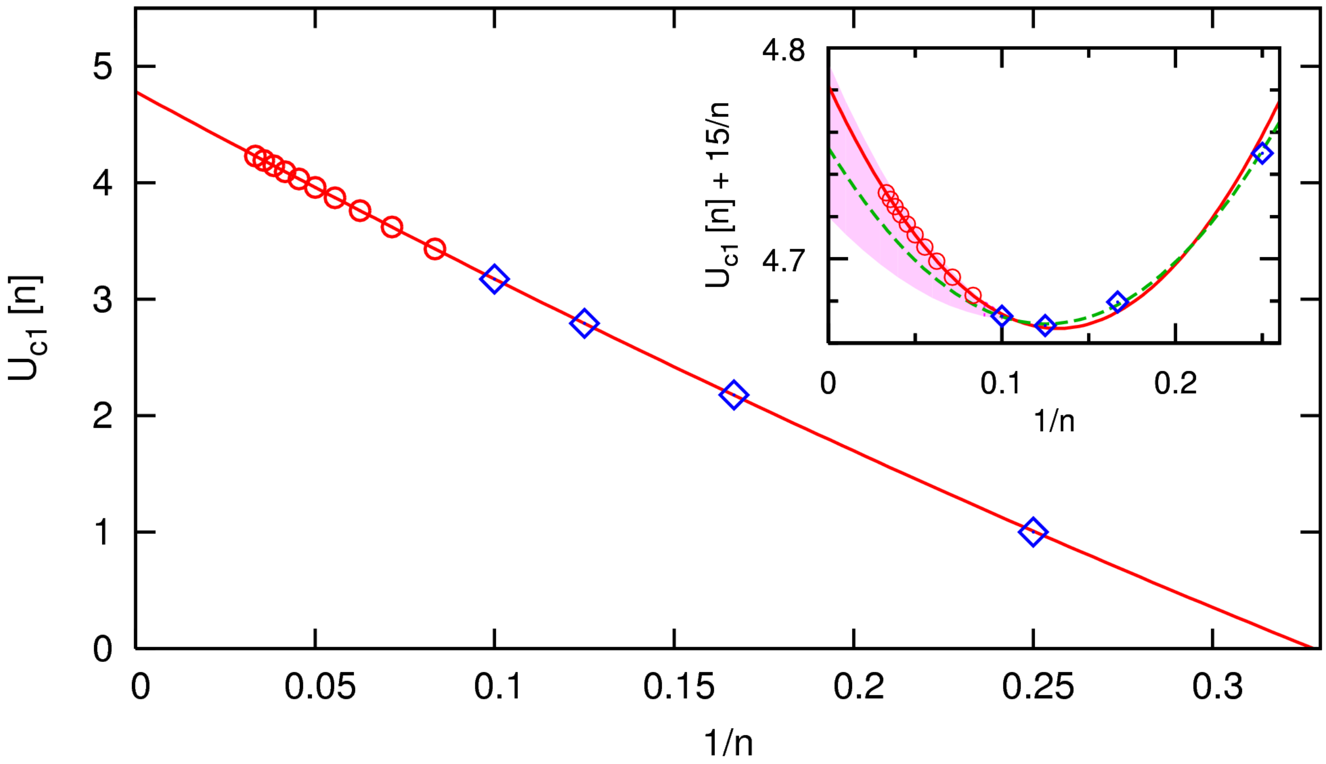
Extrapolate coefficients

$$E_{\mathrm{PT}} = \sum_{i=1}^{\infty} a_{2i}\, U^{1-2i}$$

by fitting ratios

$U_{c1}[2i] \equiv \sqrt{a_{2i+2}/a_{2i}}$ to

$$U_{c1}[n] \approx U_{c1} + u_1 n^{-1} + u_2 n^{-2}$$



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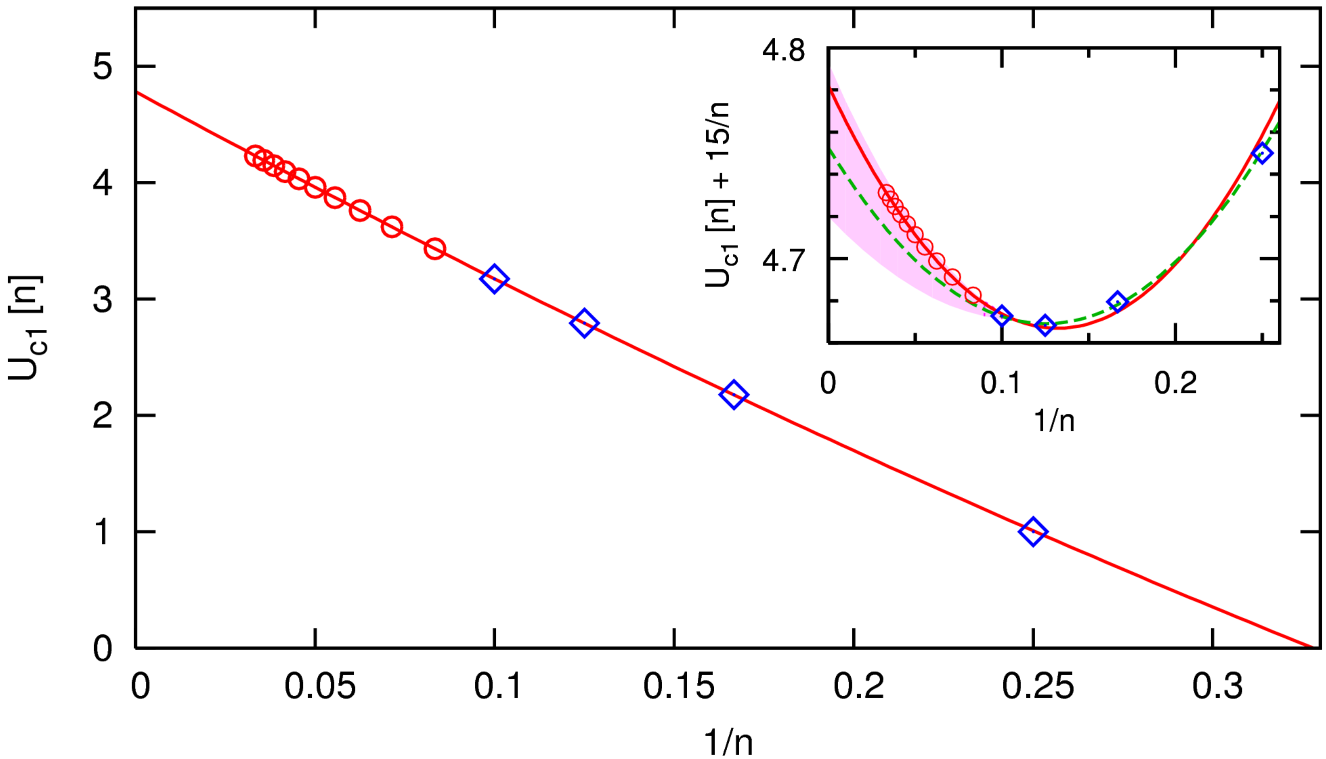

General consequences:

$$U_{c1} = \lim_{i\to\infty} U_{c1}[2i]$$

$$a_n \propto n^{\tau}\, U_{c1}^{n}; \quad \tau = -\frac{u_1}{U_{c1}}$$

$$E^{\mathrm{irr}}(U) \propto (U - U_{c1})^{\tau-1}$$

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Specifics / numerical results of extrapolation:

Unrestricted quadratic fit $\rightsquigarrow \tau \approx 3.44,\ U_{c1} \approx 4.75$

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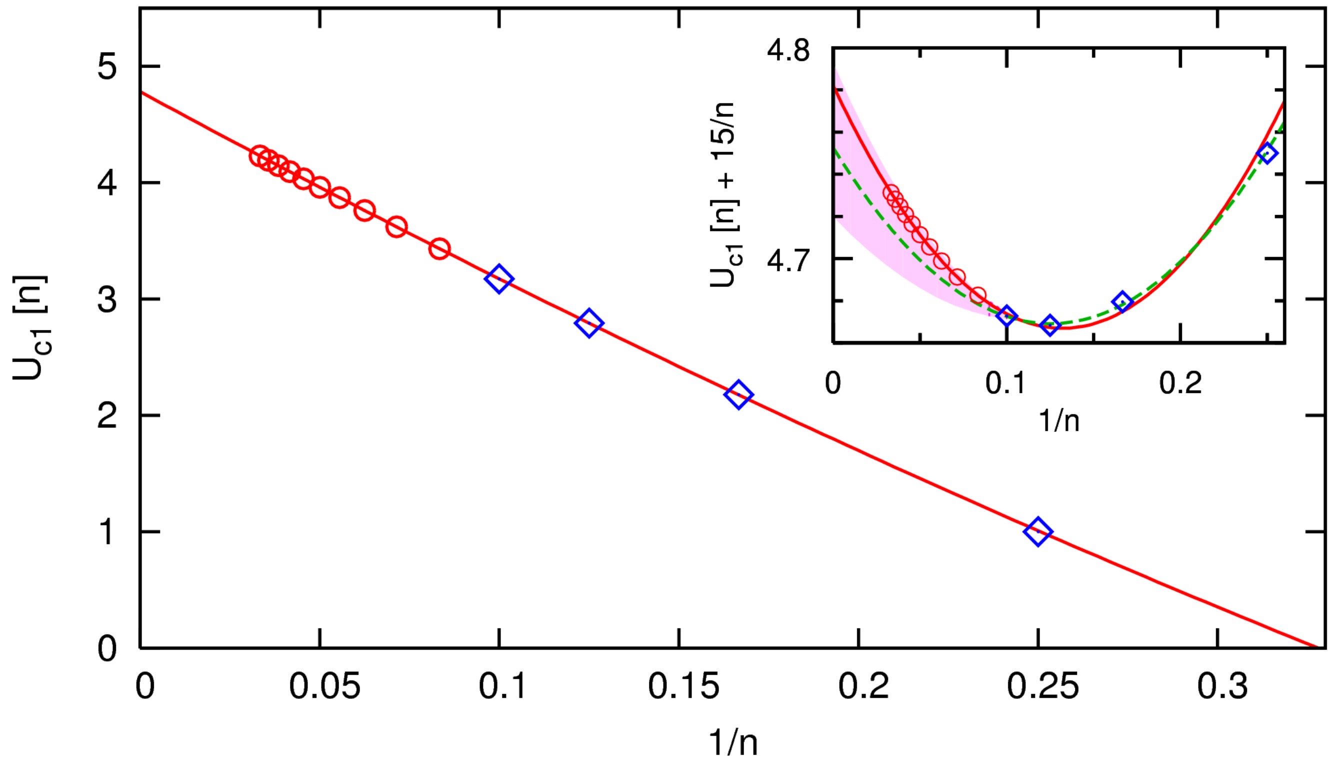

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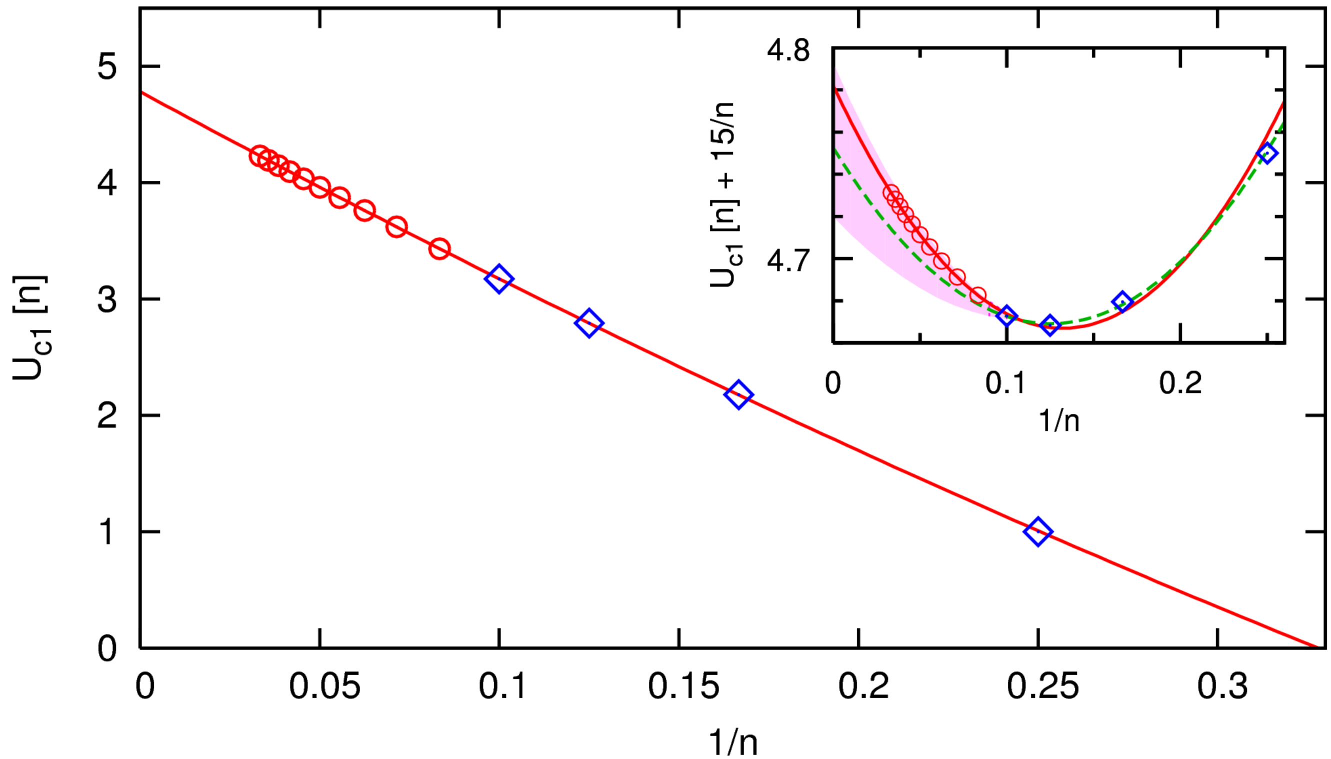

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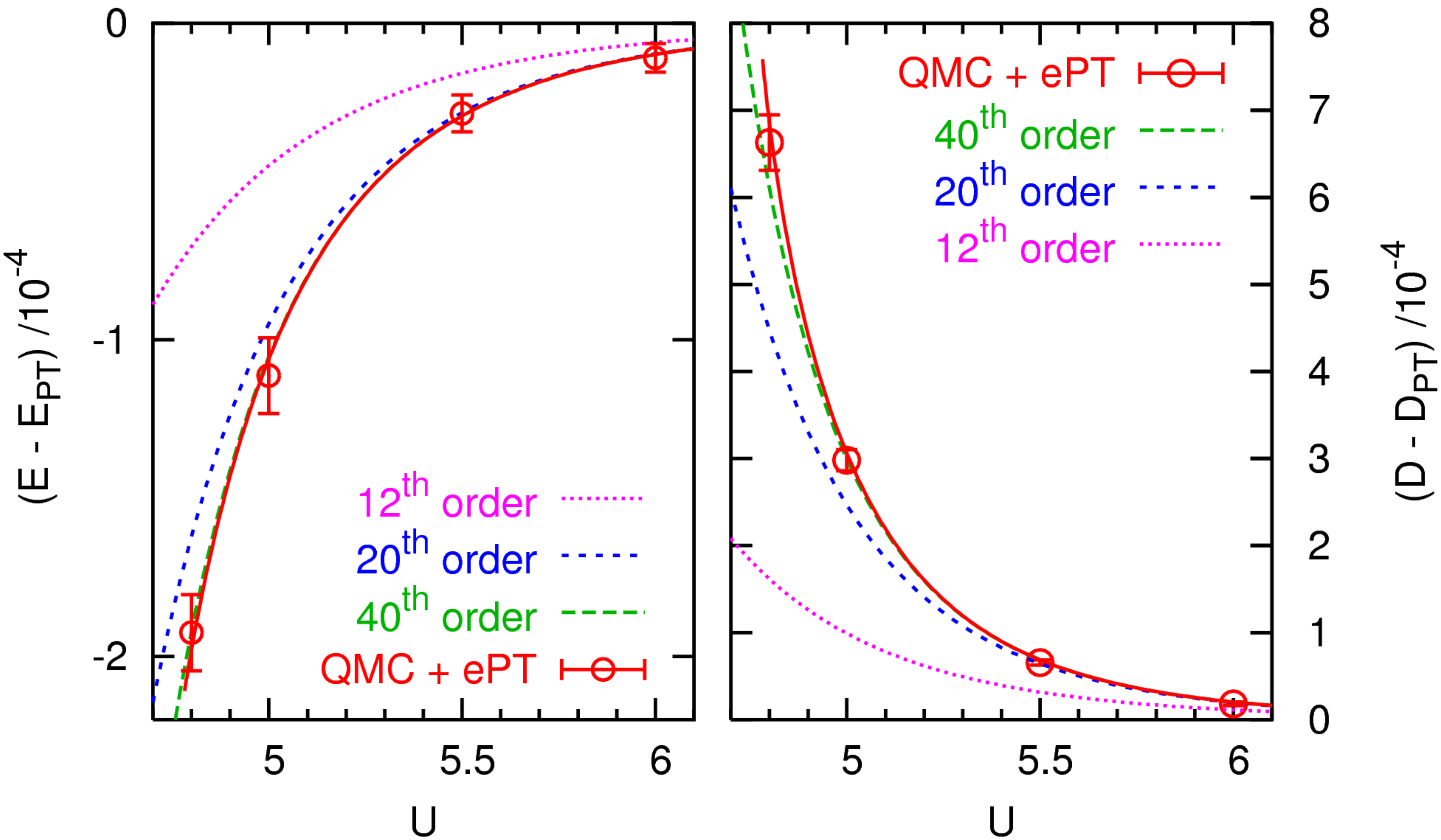
Half-integer exponents likely for mean-field theories

Assume $\tau = 3.5 \rightsquigarrow U_{c1} = 4.782,\ E_{\mathrm{ePT}}(U),\ D_{\mathrm{ePT}}(U)$

Comparisons: energy E and double occupancy $D = dE/dU$

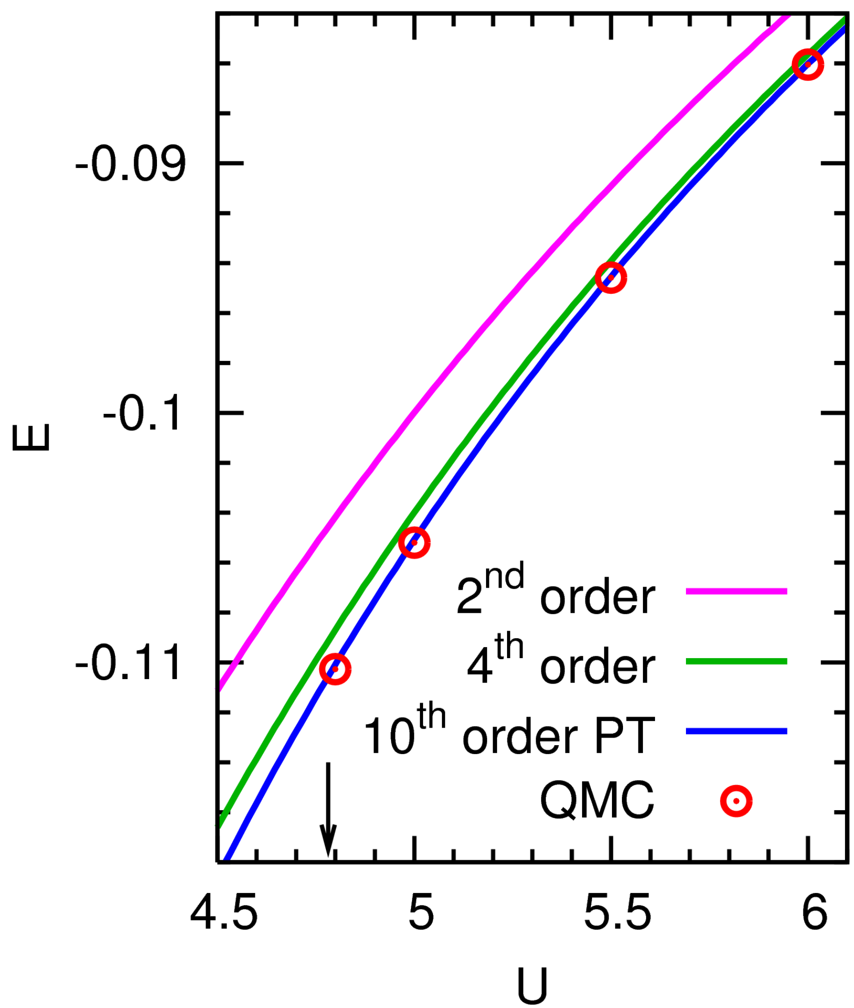


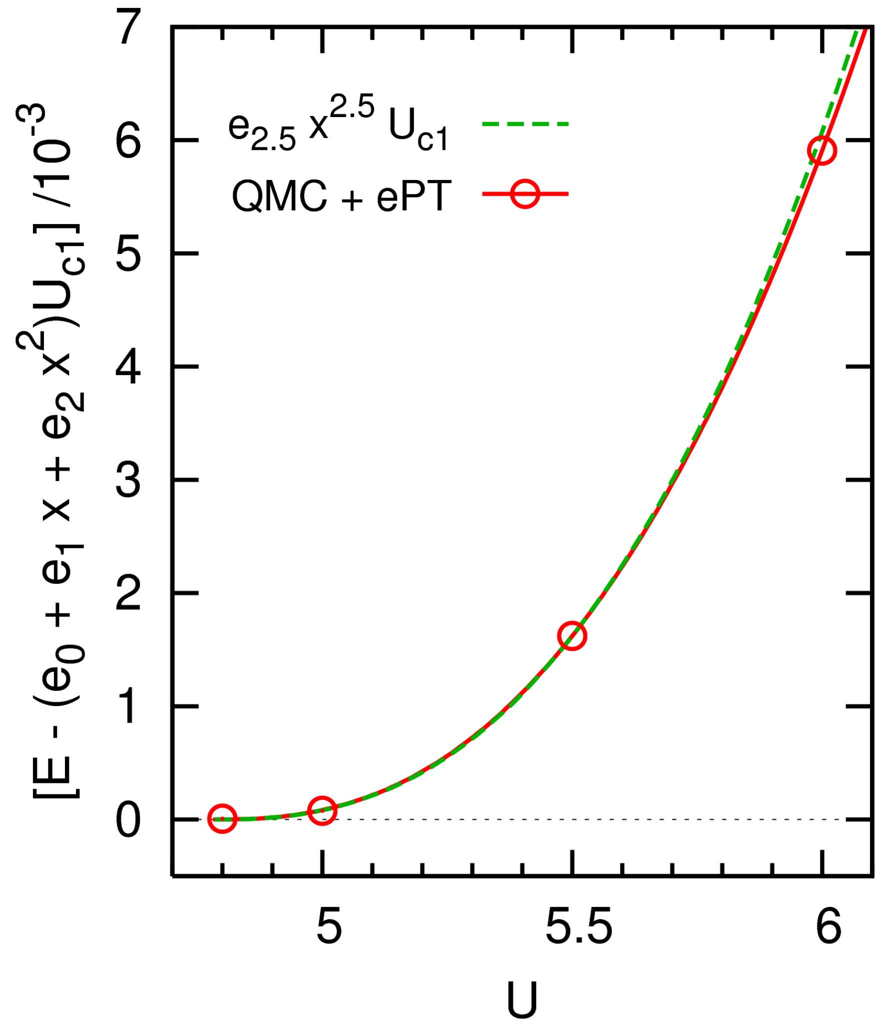
Excellent agreement ⇝ reliable exponents, fully parametrized benchmark results

[Blümer, Kalinowski, Phys. Rev. B **71**, 195102 (2005)]

Prediction of spinodal point U_{c1} confirmed by (most) DMRG, SFA results

A posteriori: coefficients of irregular parts confirmed by QMC





$$E(U) = e_0 + e_1 x + e_2 x^2 + e_{2.5} x^{2.5} + \mathcal{O}(x^3); \qquad x \equiv \frac{U - U_{c1}}{U_{c1}}$$

Summary

Critical exponents in strongly correlated electron systems:

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for insulating ground state at spinodal U_{c1}

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Multi-band: orbital-selective Mott transitions
Theory of half-metallic double perovskites (Eberhard Jakobi)
Realistic material-specific calculations with LDA+DMFT
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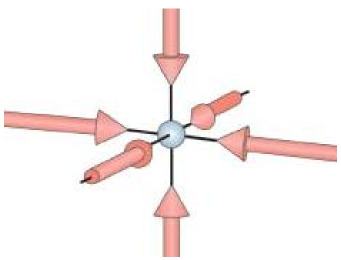
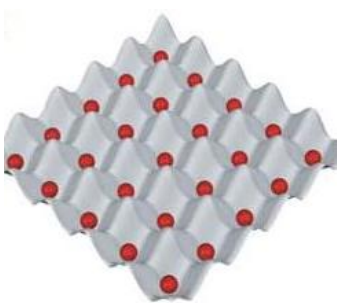
Thanks to: Eva Kalinowski, Carsten Knecht, Peter van Dongen
Florian Gebhard, Wolfgang Paul, Kurt Binder

Starting in 7/2007: SFB/TRR 49 (Frankfurt - Kaiserslautern - Mainz)
Condensed matter systems with variable many-body interactions

A1 [Bloch] – Ultracold Fermi mixtures in optical lattices
A2 [Kuhr/Bloch] – Spatially addressable quantum gases in optical lattices
A3 [Hofstetter] – Inhomogeneous quantum phases in ultracold gases with strong correlations
A5 [Fleischhauer/Eggert] – Advanced numerical methods for correlated quantum gases
A6 [Blümer] – Flavour-selective Mott transitions of ultracold quantum gases on optical lattices
A7 [Hillebrands/Serha] – Collective effects and instabilities of a magnon gas
A8 [Kopietz] – Interacting magnons and critical behaviour of bosons

project area B: real materials



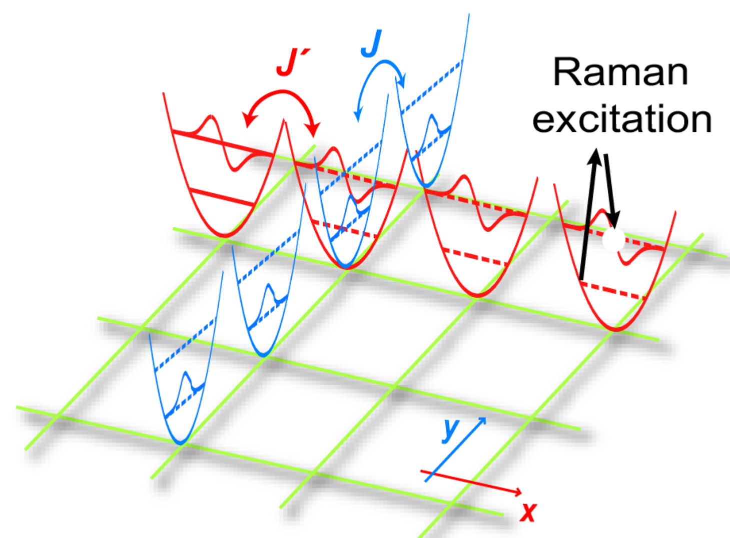


A1 + A6: flavor selectivity in Fermi mixtures of different

- atomic species: ^{6}Li and ^{40}K
- hyperfine states
- vibrational levels

on optical lattices

Hopping amplitudes tunable and flavor-dependent!



[Müller, Fölling, Widera, Bloch (2007)]