RUSSIAN ACADEMY OF SCIENCES
URALS DIVISION
Institute of Electrophysics

M. N. Mikheev Institute of Metal Physics
of Ural Branch of Russian Academy of Sciences

Ural Federal University
named after the first President of Russia B.N.Yeltsin

Investigation of Magnetocaloric effect (MCE) in Correlated Metallic Systems

I.A. Nekrasov[1], P.A. Igoshev[2], E.E. Kokorina[1], Lei Xue[3]

[1]Institute of Electrophysics UB RAS, Ekaterinburg, Russia

[2]Institute of Metal physics UB RAS, Ekaterinburg, Russia

[3]Ural Federal University, Ekaterinburg, Russia

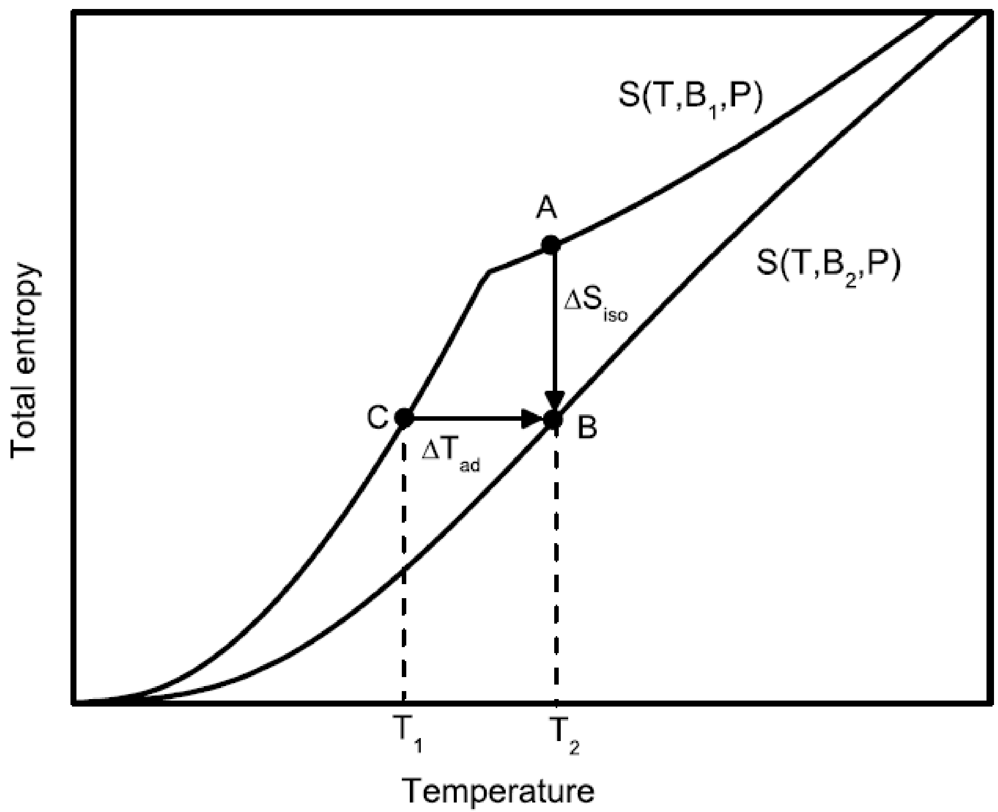
AMM-2016, Ekaterinburg

MCE Thermodynamics

Total entropy

Solid State

$$S(T,B,P) = S_{el}(T,B,P) + S_{mag}(T,B,P) + S_{lat}(T,B,P)$$



Isothermal change of entropy within MCE

$$\Delta S_{iso}(T, B_2 - B_1, P) = S(T, B_2, P) - S(T, B_1, P)$$

Adiabatic change of temperature within MCE

$$\Delta T_{ad}(T, B_2 - B_1, P) = T_2(B_2) - T_1(B_1), S(T_2, B_2, P) = S(T_1, B_1, P)$$

MCE Termodynamics

How to calculate (measure) adiabatic change of entropy within MCE
(the case of second order magnetic phase transition)

$$\Delta S_{iso}(T, \Delta B) = \int_{B_1}^{B_2} \left[\frac{\partial M(T, B)}{\partial T} \right]_B \mathrm{d}B$$

How to calculate (measure) adiabatic change of temperature within MCE
(the case of second order magnetic phase transition)

$$\Delta T_{ad}(T, \Delta B) = -\int_{B_1}^{B_2} \frac{T}{C_B(T, B)} \left[\frac{\partial S(T, B)}{\partial B} \right]_T \mathrm{d}B$$

N.A. de Oliveira*, P.J. von Ranke Physics Reports 489 (2010) 89–159

MCE within the Hubbard model

$$\mathcal{H} = \sum_{ij\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} - h \sum_{i\sigma} \sigma n_{i\sigma}$$

Within the mean-field approximation

$$\mathcal{H}_{\mathrm{MF}} = \sum_{\mathbf{k}\sigma} \tilde{\varepsilon}_{\mathbf{k}\sigma} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} - NU(n^2/4 - m^2)$$

Partition function

$$Z^{d}_{mag}(T, B, P) = \prod_{k\sigma} \left\{ 1 + \exp\left[-\beta \left(\tilde{\varepsilon}^{d}_{k} - \mu \right) \right] \right\}$$

Free energy

$$F^{d}_{mag}(T, B, P) = -\frac{1}{\beta} \sum_{k\sigma} \ln \left\{ 1 + \exp\left[-\beta \left(\tilde{\varepsilon}^{d}_{k} - \mu \right) \right] \right\}$$

Magnetic contribution to the entropy

$$S_{\mathrm{el}}(\mu, \Delta, T) = \frac{1}{N} \sum_{\mathbf{k}\sigma} \left[\ln(1 + \exp\left(-\left(\tilde{\varepsilon}_{\mathbf{k}\sigma} - \mu \right)/T \right)) + \left(\tilde{\varepsilon}_{\mathbf{k}\sigma} - \mu \right) f_{\mathbf{k}\sigma}/T \right]$$

With effective one particle spectrum $\tilde{\varepsilon}_{\mathbf{k}\sigma} = \varepsilon_{\mathbf{k}} + Un/2 - \sigma\Delta$, $\Delta = Um + h$

MCE within the Hubbard model

One can get analytic expression for isothermal change of entropy within MCE

in case of small magnetization or small magnetic field

$$\Delta S = -T_C \rho \frac{\pi^2}{3} \left(2/F_1\right)^{2/3} R \cdot h^{2/3}$$

According to e.g. Moriya T., “Spin fluctuations in itinerant electron magnetism (1985)

$$F_0(M, T) = F_0(0, T) + M^2/2\chi_0(T) + g(T)\, M^4/4 + \ldots, \quad \text{with}$$

$$\chi_0(T) = \tfrac{1}{2}\,\varrho(\varepsilon_0)\,[1 - (\pi^2/6)\, R T^2 + \ldots],$$

$$g(T) = \{F_1/[\varrho(\varepsilon_0)]^3\}\,[1 + (\pi^2/6)\, R_1 T^2 + \ldots], \qquad (2.22)$$

where

$$R = -d^2 \ln \varrho(\varepsilon_0)/d\varepsilon_0^2 = (\varrho'/\varrho)^2 - (\varrho''/\varrho),$$

$$F_1 = (\varrho'/\varrho)^2 - (\varrho''/3\varrho), \qquad (2.23)$$

$$R_1 = 2F_1 + 3R - F_1^{-1}\,[3(\varrho'^2 \varrho''/\varrho^3) - (\varrho''/3\varrho)^2 - 7\varrho' \varrho'''/3\varrho^2 + \varrho^{(4)}/3\varrho],$$

We see that F_1 depends on bare electronic structure and defines sign before M^4 term.

Self-consistent equations for numerical calculations

Total number of particles

$$n = \frac{1}{N} \sum_{\mathbf{k}\sigma} f_{\mathbf{k}\sigma}$$

Magnetic moment per site

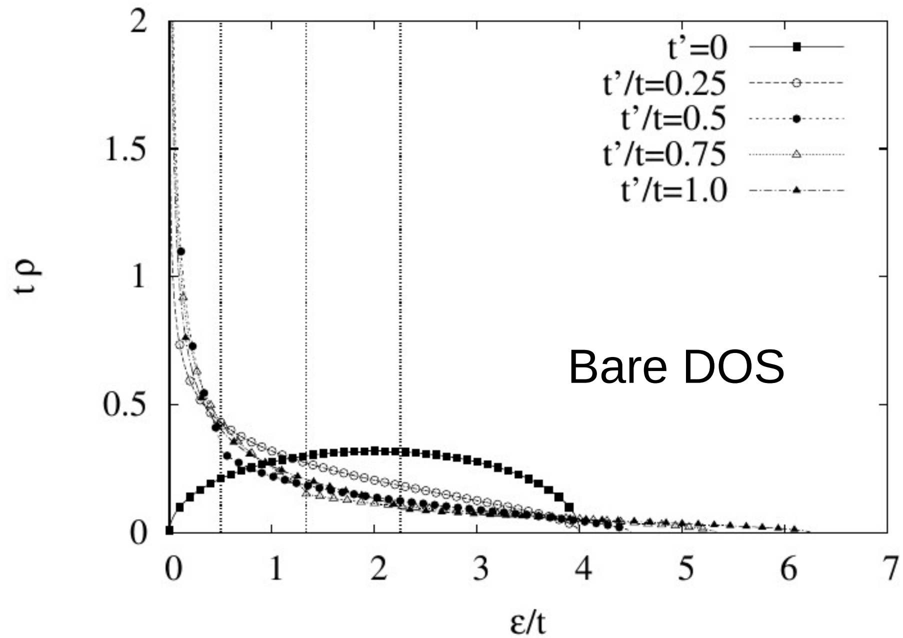
$$m = \frac{1}{2N} \sum_{\mathbf{k}\sigma} \sigma f_{\mathbf{k}\sigma}$$

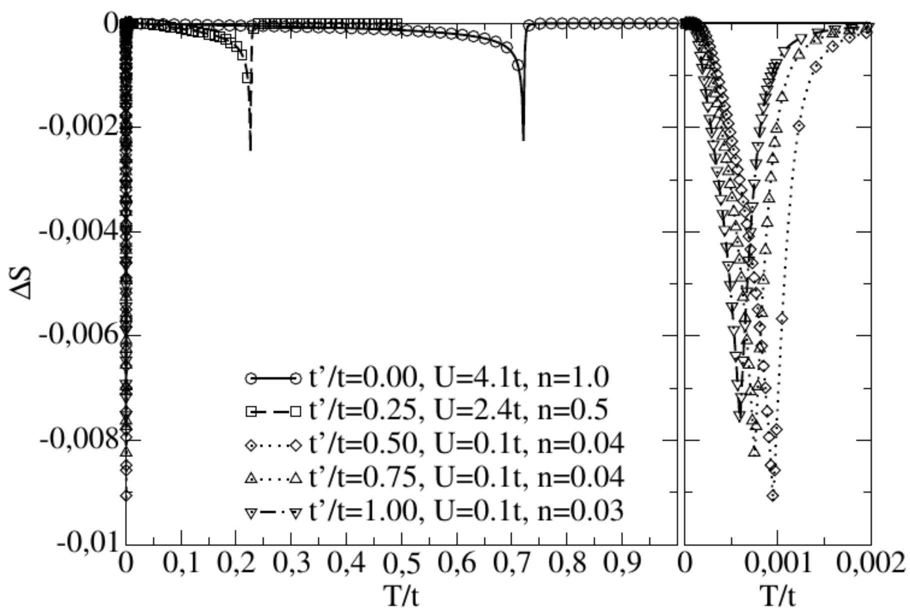
$$S_{\mathrm{el}}(\mu, \Delta, T) = \frac{1}{N} \sum_{\mathbf{k}\sigma} [\ln(1 + \exp\left(-\left(\tilde{\varepsilon}_{\mathbf{k}\sigma} - \mu\right)/T\right)) + \left(\tilde{\varepsilon}_{\mathbf{k}\sigma} - \mu\right) f_{\mathbf{k}\sigma}/T]$$

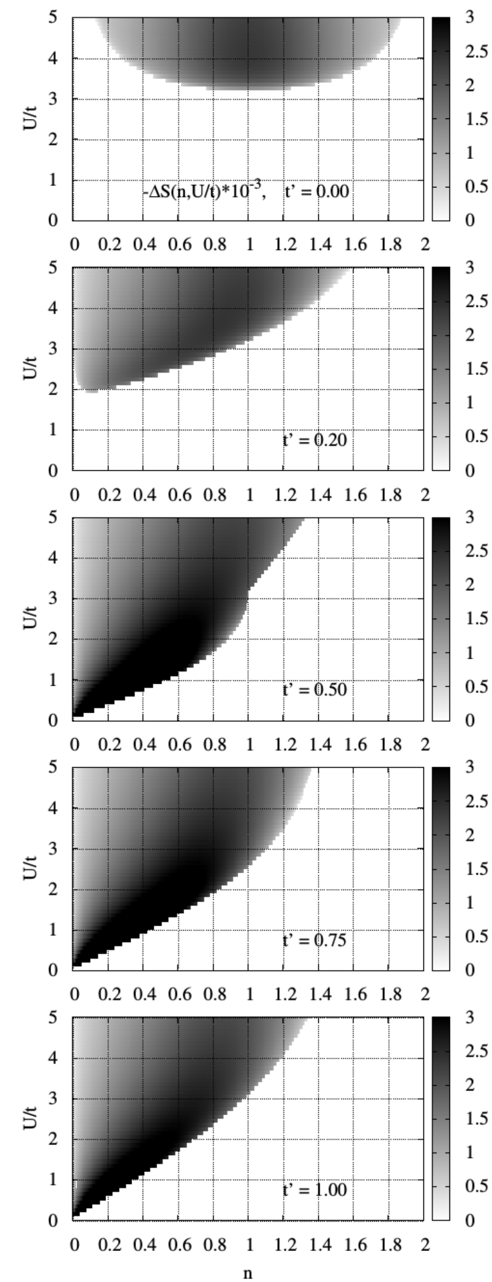
With effective one particle spectrum $\tilde{\varepsilon}_{\mathbf{k}\sigma} = \varepsilon_{\mathbf{k}} + Un/2 - \sigma\Delta$

and spin splitting $\Delta = Um + h$

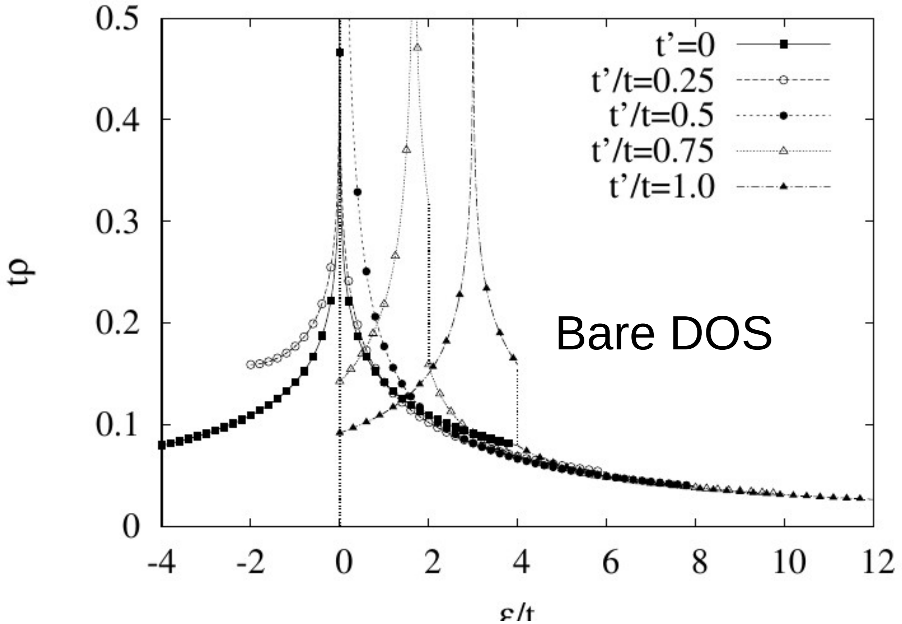
ΔS: Bethe lattice results

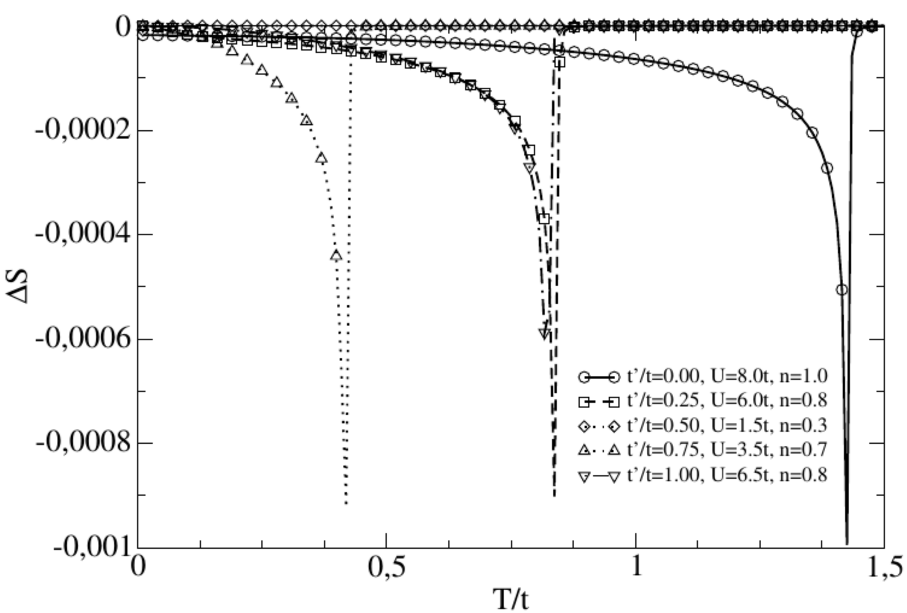


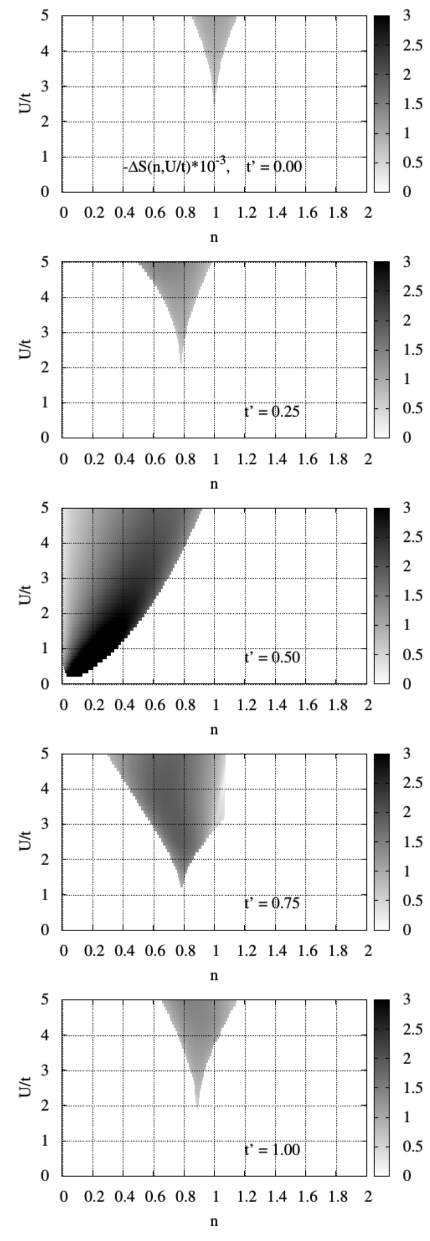




ΔS: Square lattice results

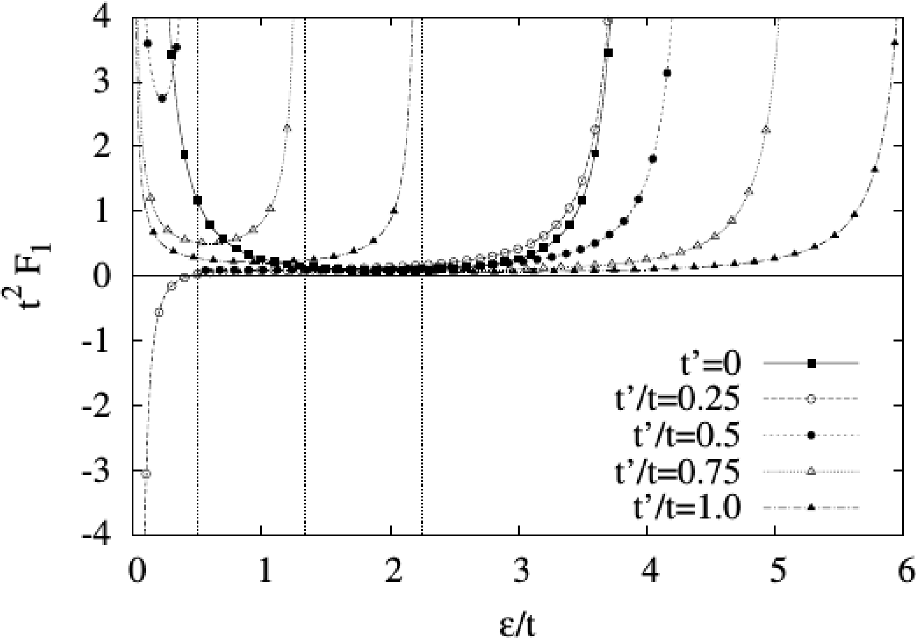


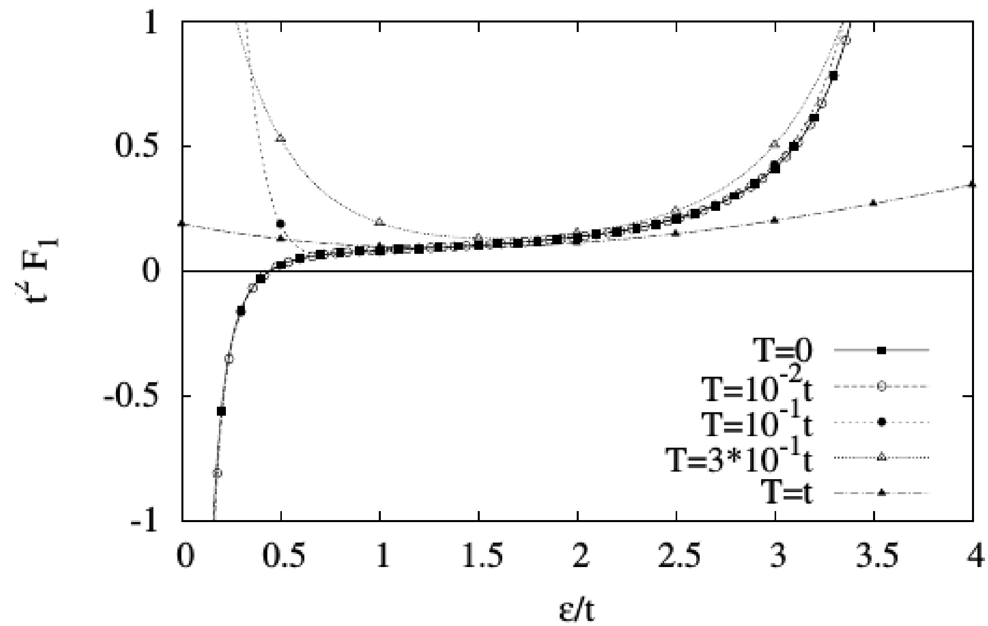




First order magnetic phase transition in the present model

Since F_1 depends on bare electronic structure and defines sign before M^4 term for $F_1<0$ one should consider possibility of first order phase transition as a function of nnn hopping or temperature.





Results for Bethe lattice

Peculiarities of MCE in metallic correlated systems with first order magnetic phase transition

MCE for the case of first order magnetic phase transition

Now we should consider thermodynamic potential

$$\Omega(T,\mu,h|m) = A_0(T,\mu) + A_2(T,\mu)m^2 + A_4(T,\mu)m^4 + A_6(T,\mu)m^6 - hm, \qquad A_2 > 0, A_4 < 0, A_6 > 0.$$

Condition of phase separation

$$\Omega(T,\mu_c(h),h|m_1) = \Omega(T,\mu_c(h),h|m_2)$$

Total phase derivative

$$\frac{d}{dh} \equiv \frac{\partial}{\partial h} + \eta\frac{\partial}{\partial \mu}. \qquad \eta \equiv \frac{d\mu_c}{dh} = \frac{m_2 - m_1}{n_1 - n_2}$$

Define behavior of different phase fractions

$$\frac{dm_i}{dh} = \frac{\partial m_i}{\partial h} + \eta\frac{\partial m_i}{\partial \mu}$$

Illustration for the case of the Hubbard model within mean-field approximation

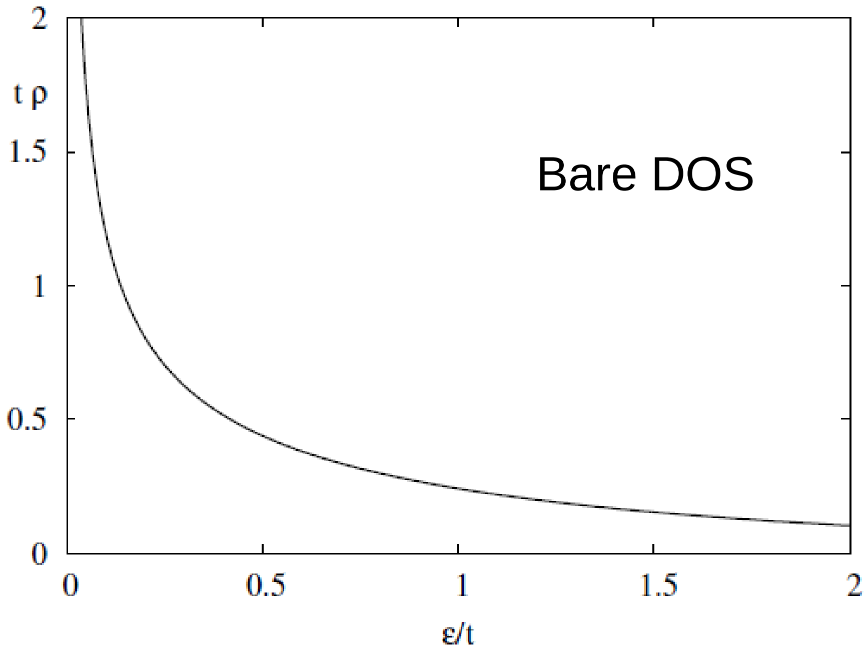
$$\Omega(\mu,T,h|n,m) = Um^2/4 - Un^2/4 + \sum_{\mathbf{k}\sigma} \ln(1+\exp\left(-\beta(\varepsilon_{\mathbf{k}} + Un/2 - \sigma(Um/2+h) - \mu)\right))$$

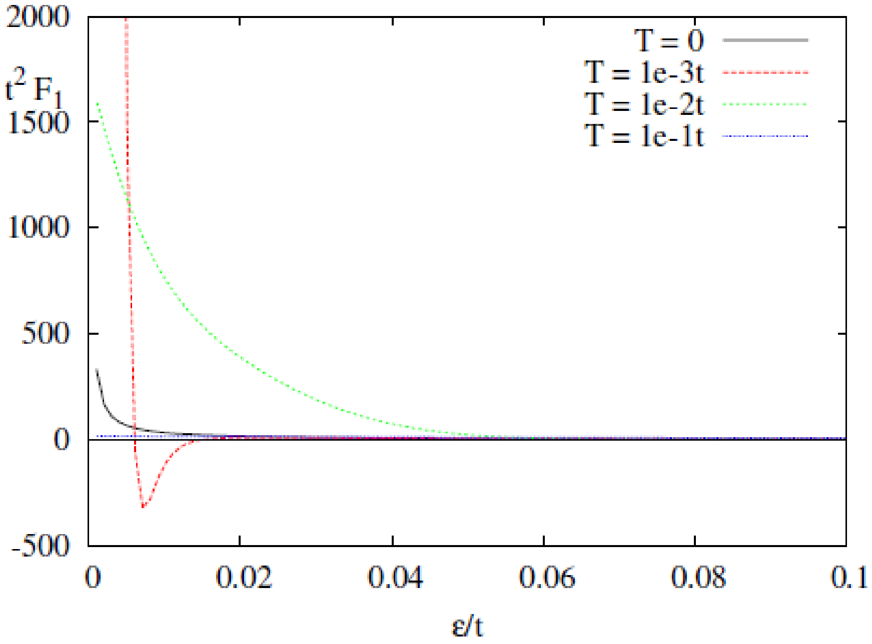
Where *n* and *m* are internal variables or grand canonical ensemble.

Thus for fixed chemical potential, temperature and magnetic field values different sets of *n* and *m* can give two different solutions – phase separation.

MCE for the case of first order magnetic phase transition in the Hubbard model

Let us consider infinite dimensional fcc lattice with nnn hopping only





So we see that there is F1<0 for some temperature range

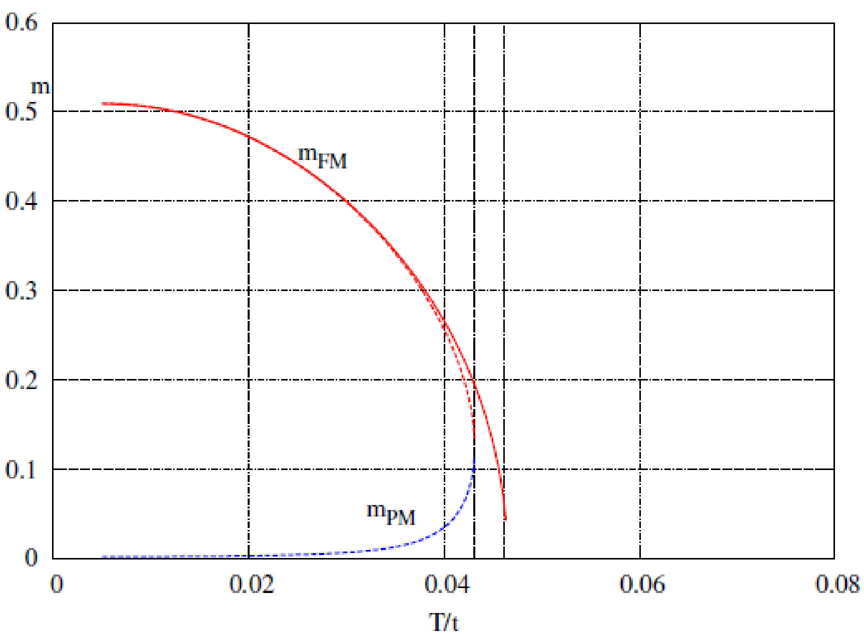
MCE for the case of first order magnetic phase transition in the Hubbard model

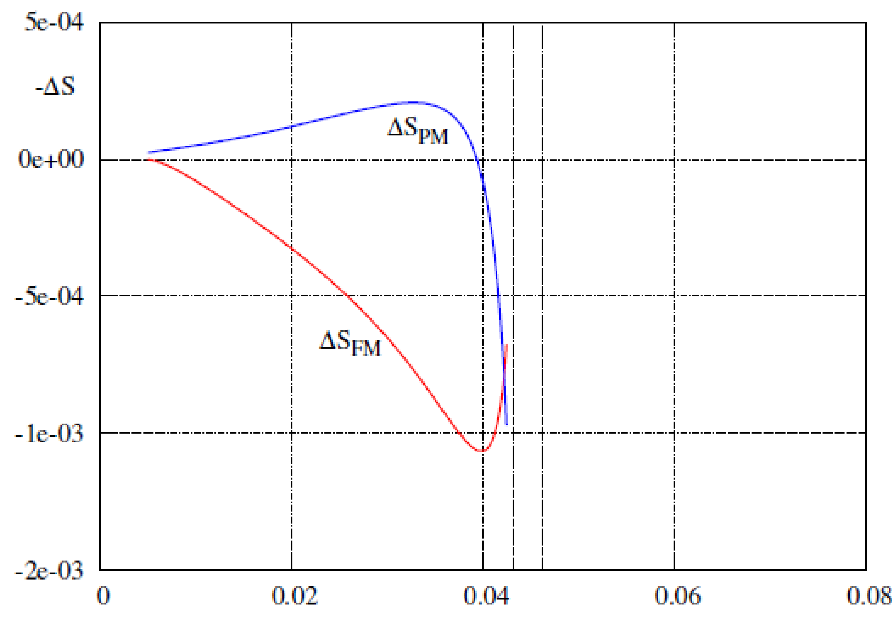
Magnetization and entropy are now depend on phase volume fractions:

1 – paramagnetic; 2 – ferromagnetic.

$$m = x_1 m_1(\mu_c, T, h) + x_2 m_2(\mu_c, T, h),$$

$$S = x_1 S_1(\mu_c, T, h) + x_2 S_2(\mu_c, T, h),$$



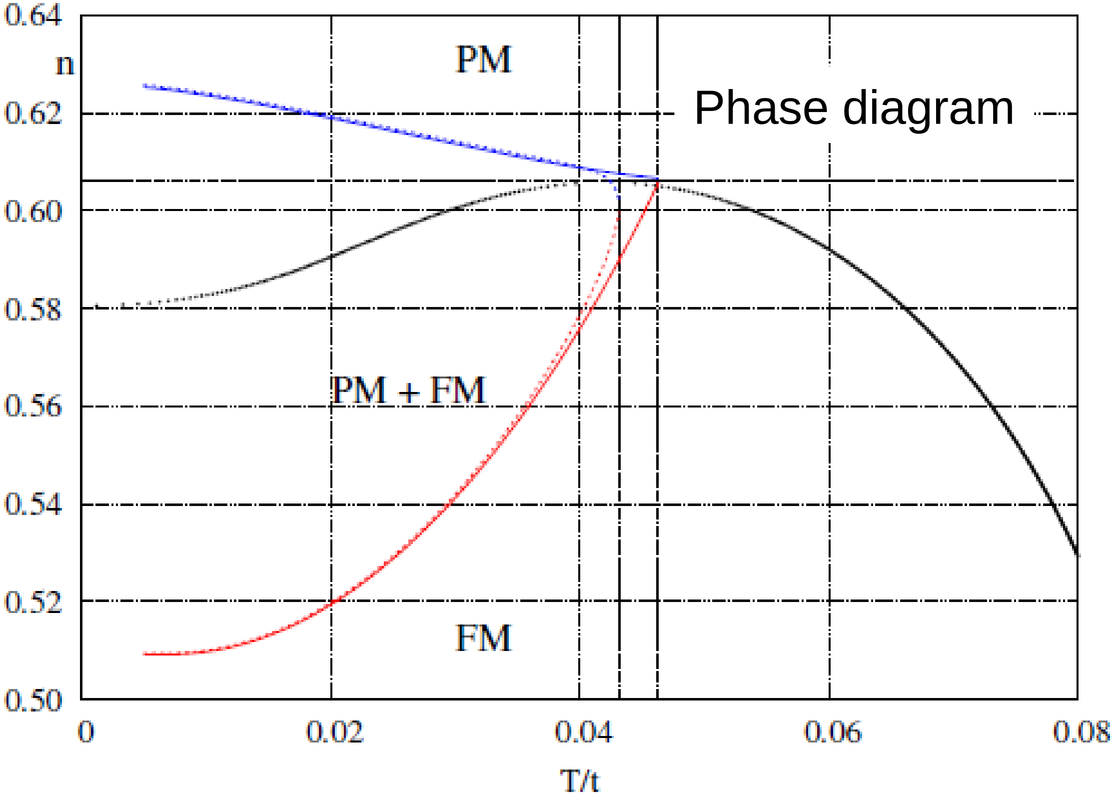


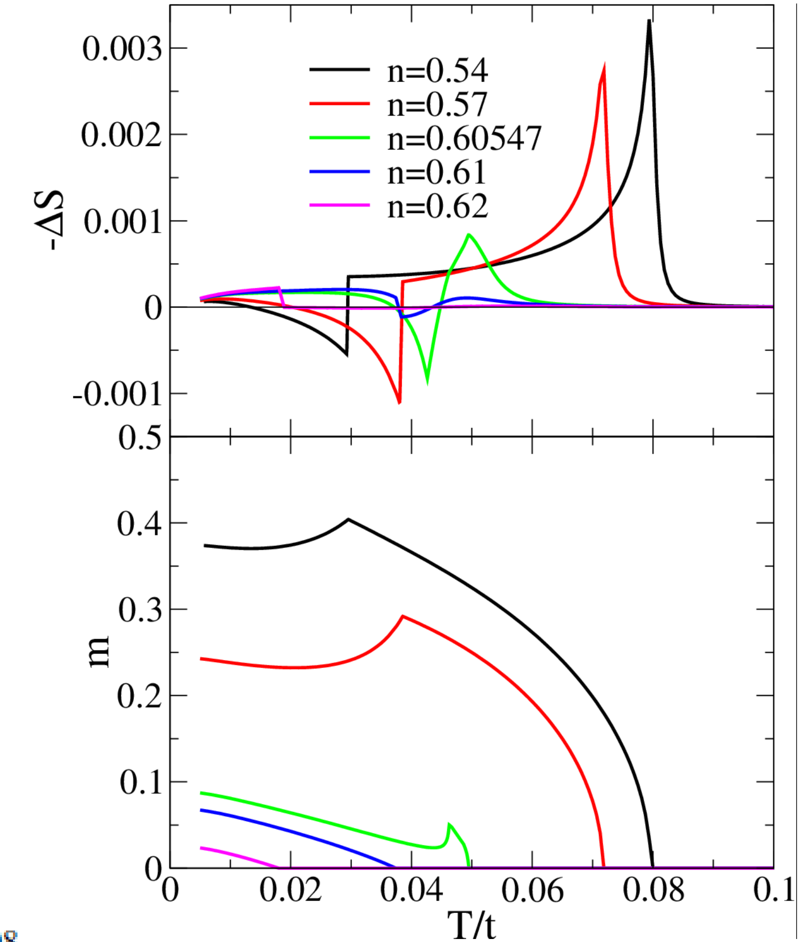
$$U = t, n = n^*(h = 0) = 0.60547, h = 10^{-4} t$$

MCE for the case of first order magnetic phase transition in the Hubbard model

Let us consider infinite dimensional fcc lattice

with nnn hopping only





$$U = t, n = n^*(h = 0) = 0.60547, h = 10^{-4}t$$

Conclusions

1. It is shown that presence of van Hove singularity in bare spectrum near the Fermi level essentially increases ΔS for metallic correlated systems.

2. It is shown that first order phase magnetic transition can be induced just by presence of van Hove singularity near the Fermi level at low enough Temperatures and is general property of metallic system (does not depend on approximations done)

3. It is obtained that ΔS can change sign in the case of first order phase transition as a function of temperature or concentration. That gives theoretical Possibilities to construct new type of devices.