Thermodynamics of simple cubic Hubbard model – dynamical mean-field study

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Electrons in crystal

Hamiltonian for electrons in crystalline potential

$$H = \sum_{i=1}^{N} \frac{(-i\hbar\nabla_i)^2}{2m} + \sum_{i=1}^{N} V_{ions}(\vec{r}_i) + \sum_{i=1}^{N}\sum_{j<i}^{N} U_{Coulomb}(\vec{r}_i - \vec{r}_j)$$

Kinetic energy

Periodic potential
from ions

Coulomb interactions
between electrons

Electrons in crystal without Coulomb interaction

Hamiltonian for electrons in crystalline potential

$$H = \sum_{i=1}^{N} \frac{(-i\hbar\nabla_i)^2}{2m} + \sum_{i=1}^{N} V_{ions}(\vec{r}_i) + \sum_{i=1}^{N}\sum_{j<i}^{N} U_{Coulomb}(\vec{r}_i - \vec{r}_j)$$

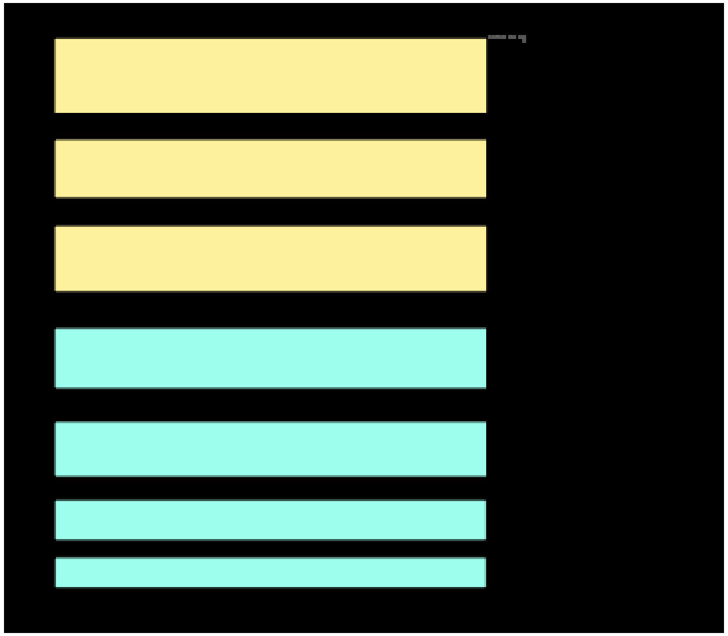
Bloch's wave functions (single particle):

$$\psi_{n\vec{k}}(\vec{r}) = e^{i\vec{k}\vec{r}} u_{n\vec{k}}(\vec{r})$$

$$n = 0, 1, \ldots$$

Possible amount of $\vec{k}$ the same as number of lattice sites

Band structure



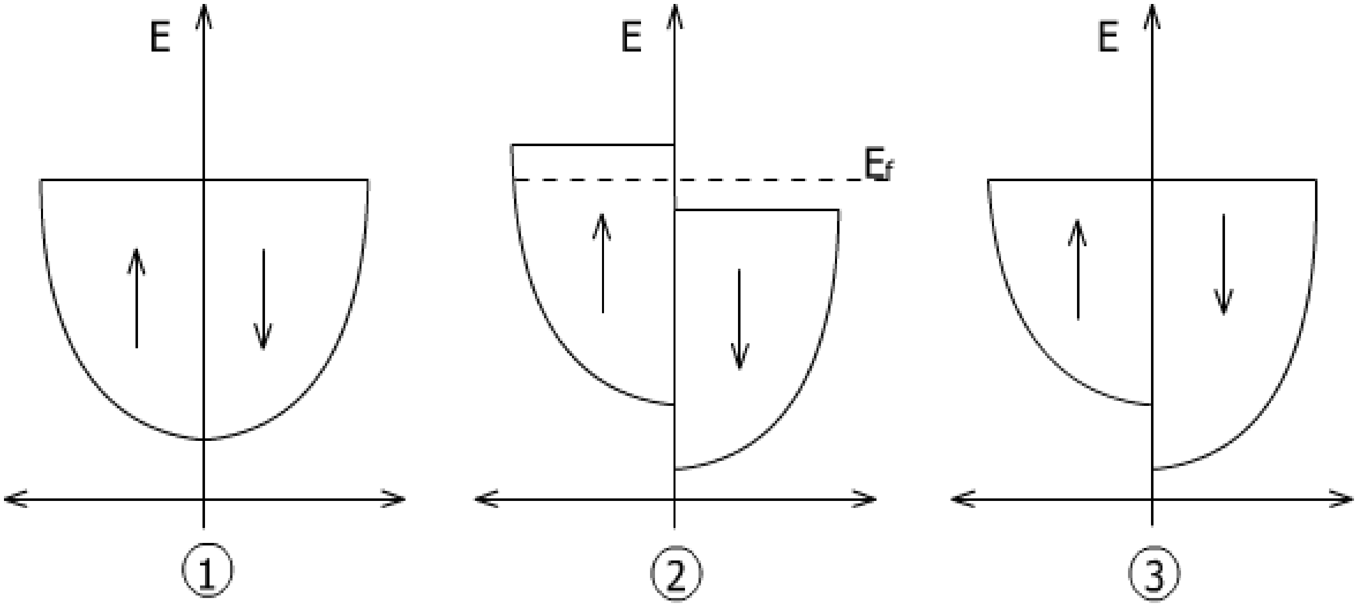
Fermi temperature for Copper: $8.16 \times 10^4 K$

N. W. Ashcroft and N. D. Mermin,

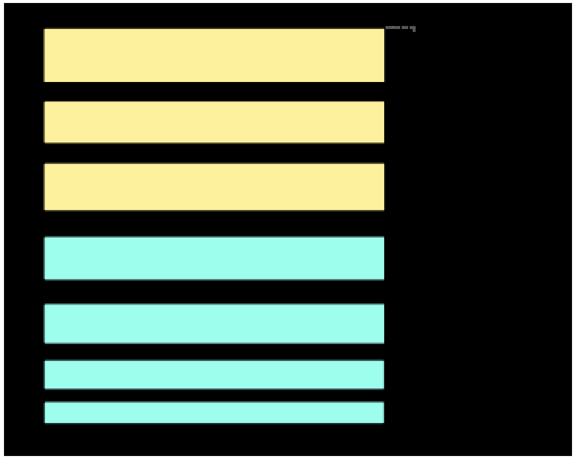
Electrons in crystal without Coulomb interaction – possible magnetic properties

Pauli paramagnetism:

$$\chi = 2\mu_B^2 \rho(E_F)$$



Band insulator - nonparamagnetic

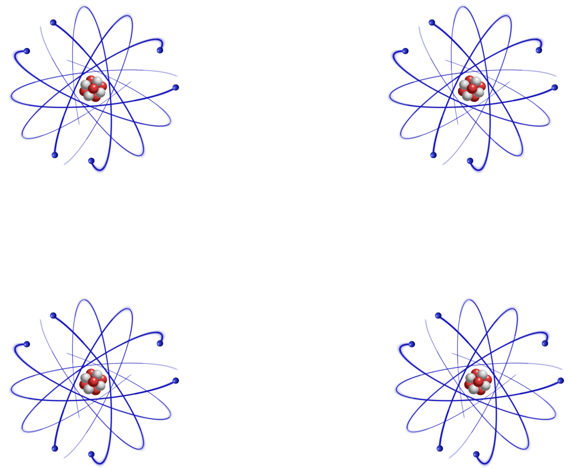


Electrons in crystal – atomic limit

$$H = \sum_{i=1}^{N} \frac{(-i\hbar\nabla_i)^2}{2m} + \sum_{i=1}^{N} V_{ions}(\vec{r}_i) + \sum_{i=1}^{N}\sum_{j<i}^{N} U_{Coulomb}(\vec{r}_i - \vec{r}_j)$$

Simplified, effective Hamiltonian:

$$H = -\mu_B B \sum_{i=1}^{N} (n_{i\uparrow} - n_{i\downarrow})$$



Curie's law:

$$\chi \sim \frac{1}{k_B T}$$

Hubbard Model

Electron correlations in narrow energy bands

By J. Hubbard

that a possible approximation is to neglect all the integrals (8) apart from I. If this approximation, the validity of which is discussed in greater detail below, is made, then the Hamiltonian of (6) becomes

$$H = \sum_{i,j} \sum_{\sigma} T_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + \tfrac{1}{2} I \sum_{i,\sigma} n_{i\sigma} n_{i,-\sigma} - I \sum_{i,\sigma} \nu_{ii} n_{i\sigma}, \qquad (10)$$

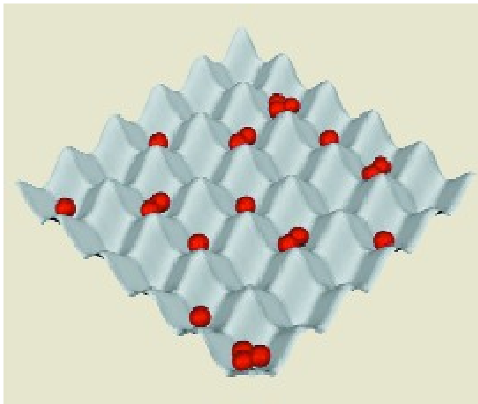
$$H = t \sum_{(i,j)} \sum_{\sigma=\uparrow,\downarrow} \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + \sum_{i} U \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

$$\hat{n}_{i\sigma} \equiv \hat{c}^{\dagger}_{i\sigma} \hat{c}_{i\sigma}$$

Motivation:
d-electrons in transition metals exhibit both kinds of behavior:
-atomic limit
-noninteracting system

Optical lattices

Neutral particles in optical lattice



I. Bloch, Phys. World 17, 25 (2004)

Interacting electrons in materials

Strongly correlated materials

Electron correlations in narrow energy bands

By J. Hubbard

that a possible approximation is to neglect all the integrals (8) apart from I. If this approximation, the validity of which is discussed in greater detail below, is made, then the Hamiltonian of (6) becomes

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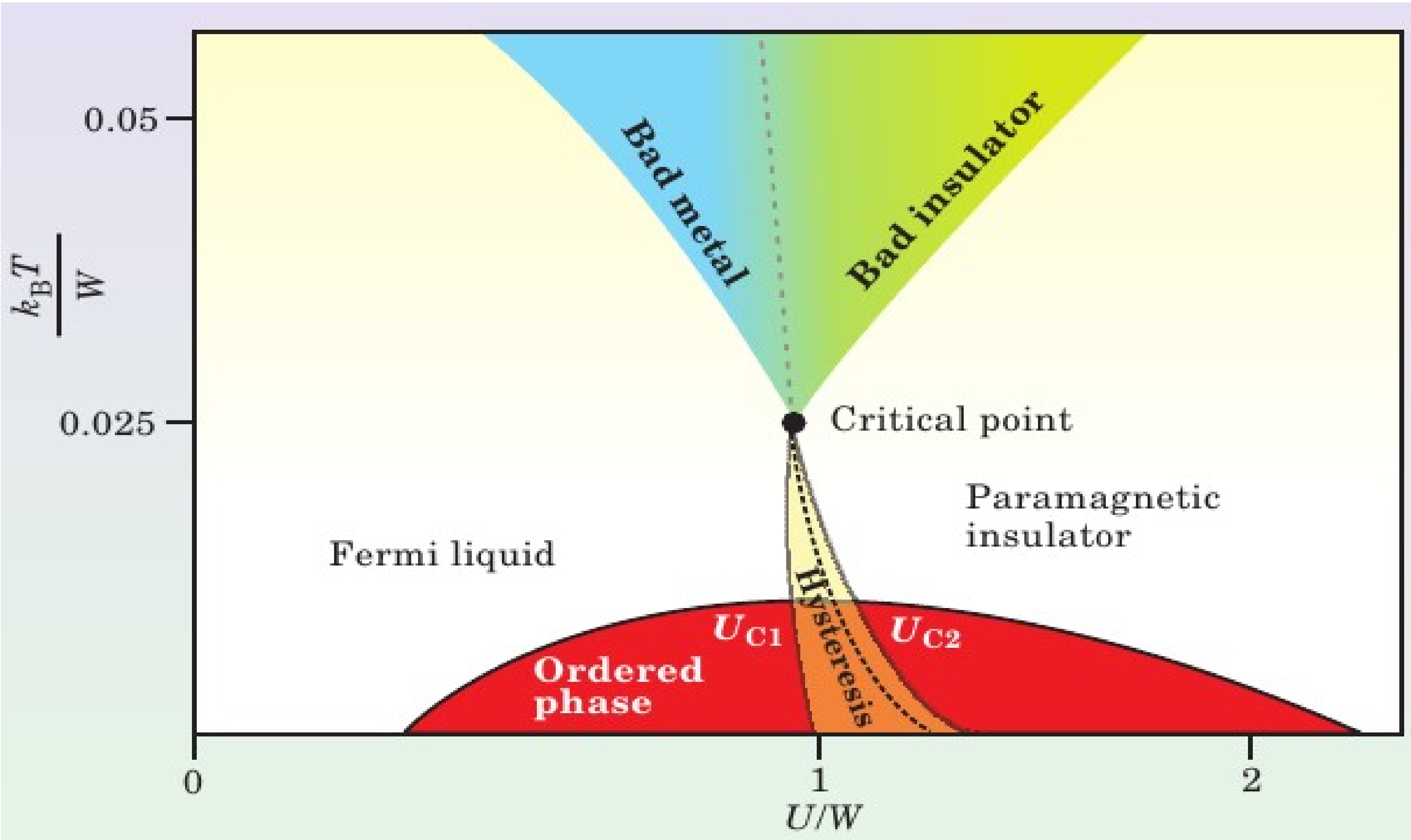
Hubbard model – schematic phase diagram at half-filling (dmft)



Kotliar and Vollhardt, Phys. Today 57, 53-60 (2004)

A Mott insulator of fermionic atoms in an optical lattice

NATURE | Vol 455 | 11 September 2008

Robert Jördens[1]*, Niels Strohmaier[1]*, Kenneth Günter[1,2], Henning Moritz[1] & Tilman Esslinger[1]

Hubbard model - challenge

Without rigorous (analytical) solution approximate methods indispensable!

Numerical simulations

Quantum emulators (optical lattices)

Approximated method:

- -Hartree-Fock theory
- -Green function decoupling method
- -slave Boson approach
- -dynamical mean field theory
- -....

Motivation and aim of our work

$$H = t \sum_{(i,j)} \sum_{\sigma=\uparrow,\downarrow} \hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma} + \sum_{i} U \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$$

cubic lattice, equilibrium state (grand canonical ensemble)
half-filling $\mu = U/2$
paramagnetic state (one of motivations: comprehensive thermodynamic within one method, in one place as a reference to other methods)

Comprehensive thermodynamics within dynamical mean-field theory?

Phase diagram (metal-insulator transition)

Charge susceptibility: $$\kappa_c = \left(\frac{\partial n}{\partial \mu}\right)_T$$

Internal energy: $\langle H \rangle$ → specific heat

Double occupation: $$d \equiv \lim_{\infty} \frac{1}{N} \langle \sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} \rangle$$

Green function

Grand canonical potential (thermodynamics):

$$\Xi = \sum_{N,\gamma_N} \langle \gamma_N | e^{-\beta(H-\mu\hat{N})} | \gamma_N \rangle$$

One-particle Green function:

α: $\vec{R}_i$ lattice site, spin

$$G_{\alpha\beta}(\tau,\tau') = -\langle T_\tau \hat{c}_\alpha(\tau) \hat{c}^\dagger_\beta(\tau') \rangle$$

$$\langle \ldots \rangle = \frac{1}{\Xi} \sum_{N,\gamma_N} \langle \gamma_N | e^{-\beta(H-\mu\hat{N})} \ldots | \gamma_N \rangle$$

"time" ordering

$$T_\tau \hat{c}_\alpha(\tau)\hat{c}^\dagger_\alpha(\tau') = \begin{cases} \hat{c}_\alpha(\tau)\hat{c}^\dagger_\alpha(\tau') & \text{dla} \quad \tau > \tau' \\ -\hat{c}^\dagger_\alpha(\tau')\hat{c}_\alpha(\tau) & \text{dla} \quad \tau < \tau' \end{cases}$$

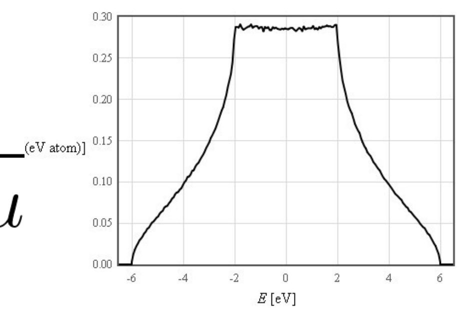
Operator in modified Heisenberg picture

$$\hat{c}_\alpha(\tau) = e^{\tau(H-\mu N)} \hat{c}_\alpha e^{-\tau(H-\mu N)}$$

Method: dynamical mean field theory

- *W. Metzner, D. Vollhardt, Phys. Rev. Lett. 59, 121 (1987)*
- *A. Georges, G. Kotliar, W. Krauth, M. J. Rozenberg, Rev. Mod. Phys. 68, 13 (1996)*

Cubic DOS



Dyson equation:

$$G_{00}(i\omega_n) = \int_{-\infty}^{\infty} d\epsilon \frac{D(\epsilon)}{i\omega_n - \epsilon - \Sigma(i\omega_n) + \mu}$$

Consequences of high dimension limit (local problem):

$$G_{00}(\tau,\tau') = -\langle c_{0\sigma}(\tau) c^*_{0\sigma}(\tau')\rangle_{S_{\mathrm{eff}}[\mathcal{G}_0]}$$

$$G_{00} = \mathcal{G}_0 + \mathcal{G}_0 \Sigma G_{00}$$

CT-QMC

$$S_{\mathrm{eff}} = \sum_{\sigma=\uparrow,\downarrow} \int_0^\beta d\tau \int_0^\beta d\tau' c^*_{0\sigma}(\tau)(\partial_\tau - \mu) c_{0\sigma}(\tau') + \int_0^\beta d\tau U n_{0\downarrow}(\tau) n_{0\uparrow}(\tau)$$

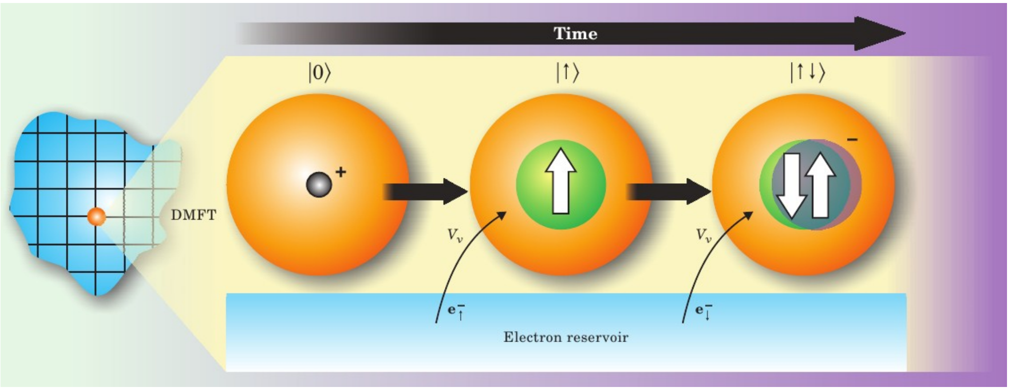
$$+ \sum_{\sigma=\uparrow,\downarrow} \int_0^\beta d\tau \int_0^\beta d\tau' c^*_{0\sigma}(\tau) \Delta(\tau,\tau') c_{0\sigma}(\tau')$$

Single impurity problem

Anderson, P. W. (1961). Phys. Rev., 124, 41

$$H = t\sum_{(i,j)}\sum_{\sigma=\uparrow,\downarrow}\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma} + U\hat{n}_{0\uparrow}\hat{n}_{0\downarrow}$$

$$\Xi = \sum_{N,\gamma_N}\langle\gamma_N|e^{-\beta(H-\mu\hat{N})}|\gamma_N\rangle$$



Kotliar and Vollhardt, Phys. Today 57, 53-60 (2004)

Resummation over noninteracting sites

$$\Xi = \int D\phi^* D\phi e^{-S_{eff}}$$

$$\begin{aligned} S_{\text{eff}} &= \sum_{\sigma=\uparrow,\downarrow}\int_0^\beta d\tau\int_0^\beta d\tau' c^*_{0\sigma}(\tau)(\partial_\tau-\mu)c_{0\sigma}(\tau') \\ &+ \int_0^\beta d\tau U n_{0\downarrow}(\tau)n_{0\uparrow}(\tau) \\ &+ \sum_{\sigma=\uparrow,\downarrow}\int_0^\beta d\tau\int_0^\beta d\tau' c^*_{0\sigma}(\tau)\Delta(\tau,\tau')c_{0\sigma}(\tau') \end{aligned}$$

Gull et al. Rev Mod Phys 83, 349 (2011)

Hirsch, J. E., and R. M. Fye, Phys. Rev. Lett. 56, 2521 (1986,)

Continuous time – hybridization expansion quantum Monte Carlo

Continuous time: Prokof'ev, N. V., and B. V. Svistunov, 1998, Phys. Rev. Lett. 81, 2514

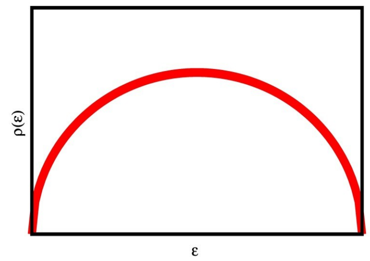
$$
\begin{aligned}
\Xi \;=\; & \Xi_0 \sum_{k=0}^{\infty} \frac{1}{k!} \int_0^{\beta} d\tau_1 \int_0^{\beta} d\tau_1' \ldots \int_0^{\beta} d\tau_k \int_0^{\beta} d\tau_k' \sum_{\sigma_1, \sigma_1', \ldots, \sigma_k \sigma_k'} \\
& \times \langle T_\tau c'_{\sigma_1}(\tau_1') c^\dagger_{\sigma_1}(\tau_1) \ldots c'_{\sigma_k}(\tau_k') c^\dagger_{\sigma_k}(\tau_k) \rangle_{\text{local}} \\
& \times \frac{1}{k!} Det \begin{bmatrix} \Delta(\tau_{\sigma_1}, \tau'_{\sigma_1}) & \Delta(\tau_{\sigma_1}, \tau'_{\sigma_2}) & \ldots & \Delta(\tau_{\sigma_1}, \tau'_{\sigma_k}) \\ \ldots & \ldots & \ldots & \ldots \\ \ldots & \ldots & \ldots & \ldots \\ \Delta(\tau_{\sigma_k}, \tau'_{\sigma_1}) & \ldots & \ldots & \Delta(\tau_{\sigma_k}, \tau'_{\sigma_1}) \end{bmatrix}
\end{aligned}
$$

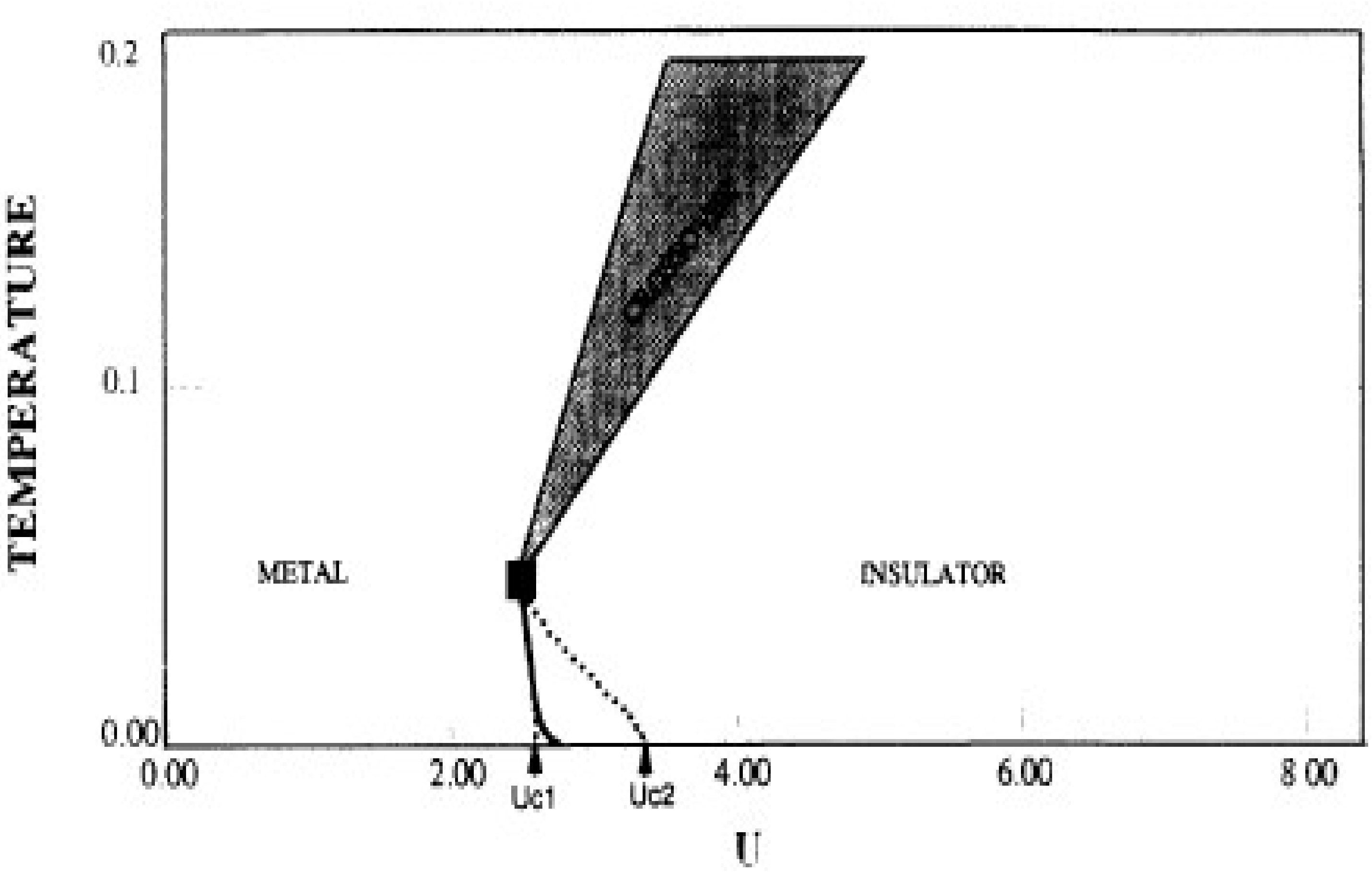
$$X \equiv k, \tau_1, \sigma_1, \tau_1', \sigma_1' \ldots \tau_k, \sigma_k \tau_k', \sigma_k',$$

$$\int_X A(X) p(X) \longrightarrow \frac{1}{N_{MC}} \sum_{i=1}^{N_{MC}} A(X_i)$$

Paramagnetic phase diagram – (semi-circular dos)

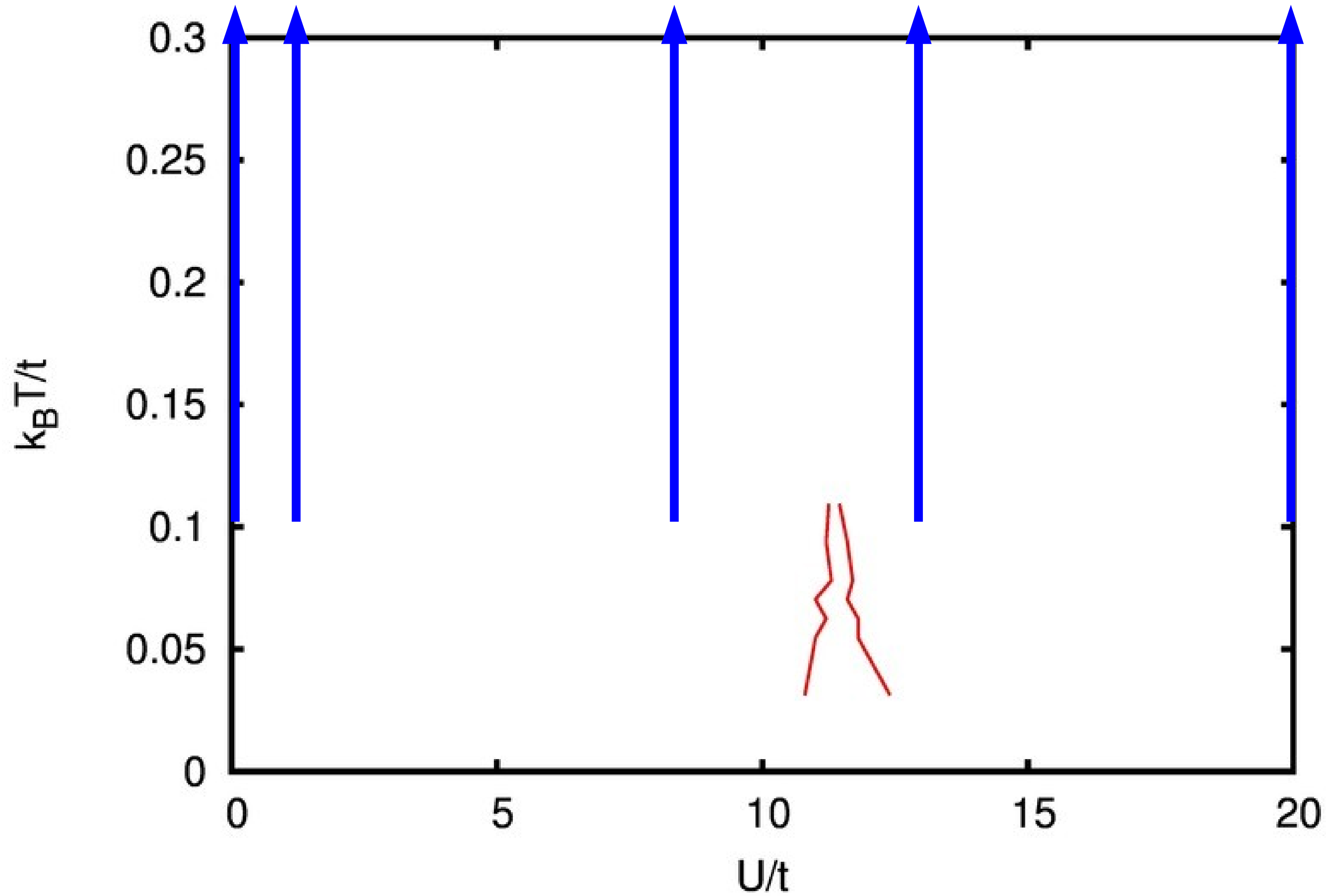
DOS:





M.J. Rozenberg, G. Kotliar, X.Y. Zhang, PRB 49,10181 (1994)

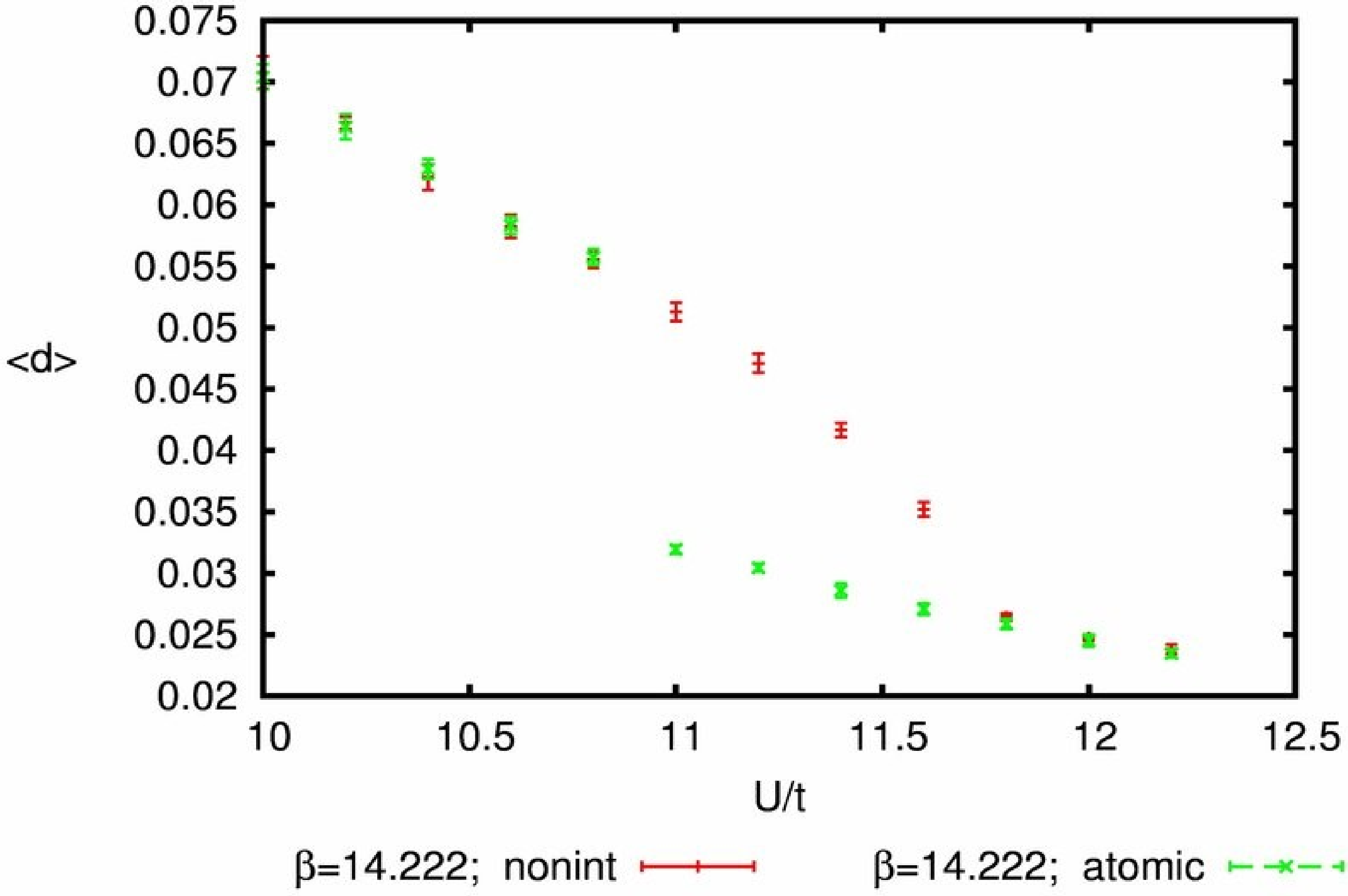
Results – phase diagram



$$k_B T_c \approx 0.1t \approx 0.083W$$
$$U_c \approx 11.3t$$

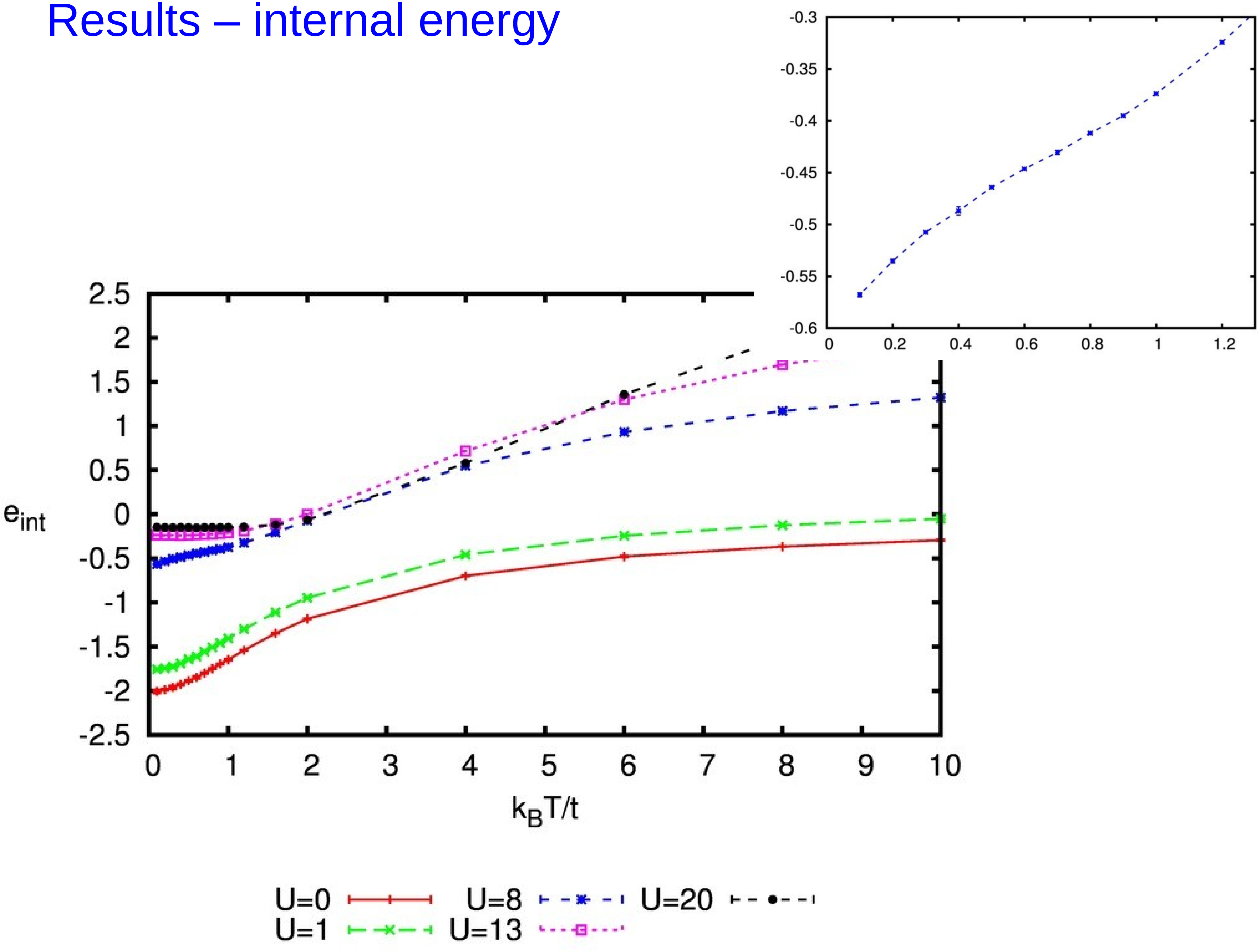
Results Example of determination of coexistence region

$$d \equiv \lim_{\infty} \frac{1}{N} \langle \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \rangle$$



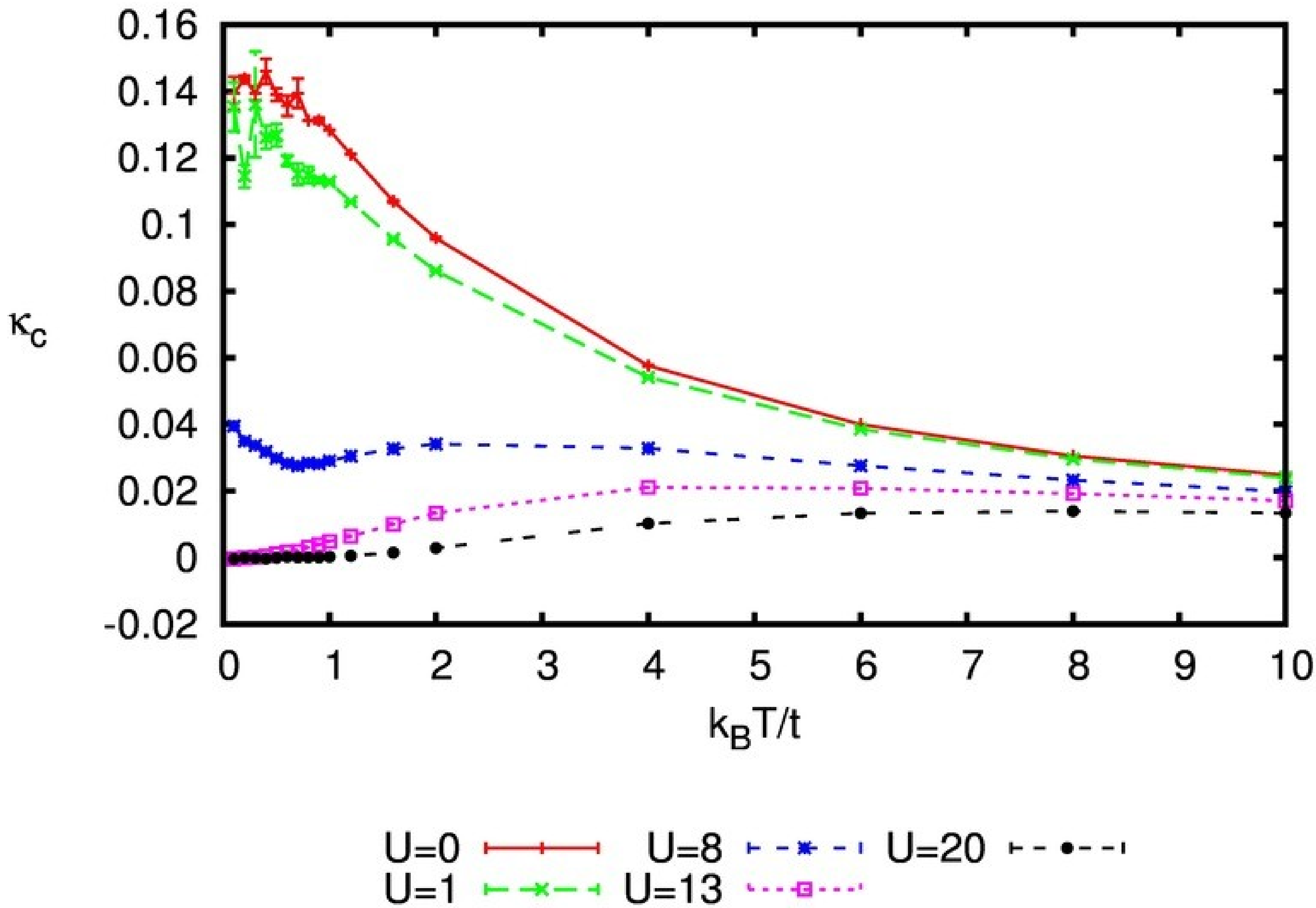
$$\beta = \frac{t}{k_B T}$$

Results – internal energy



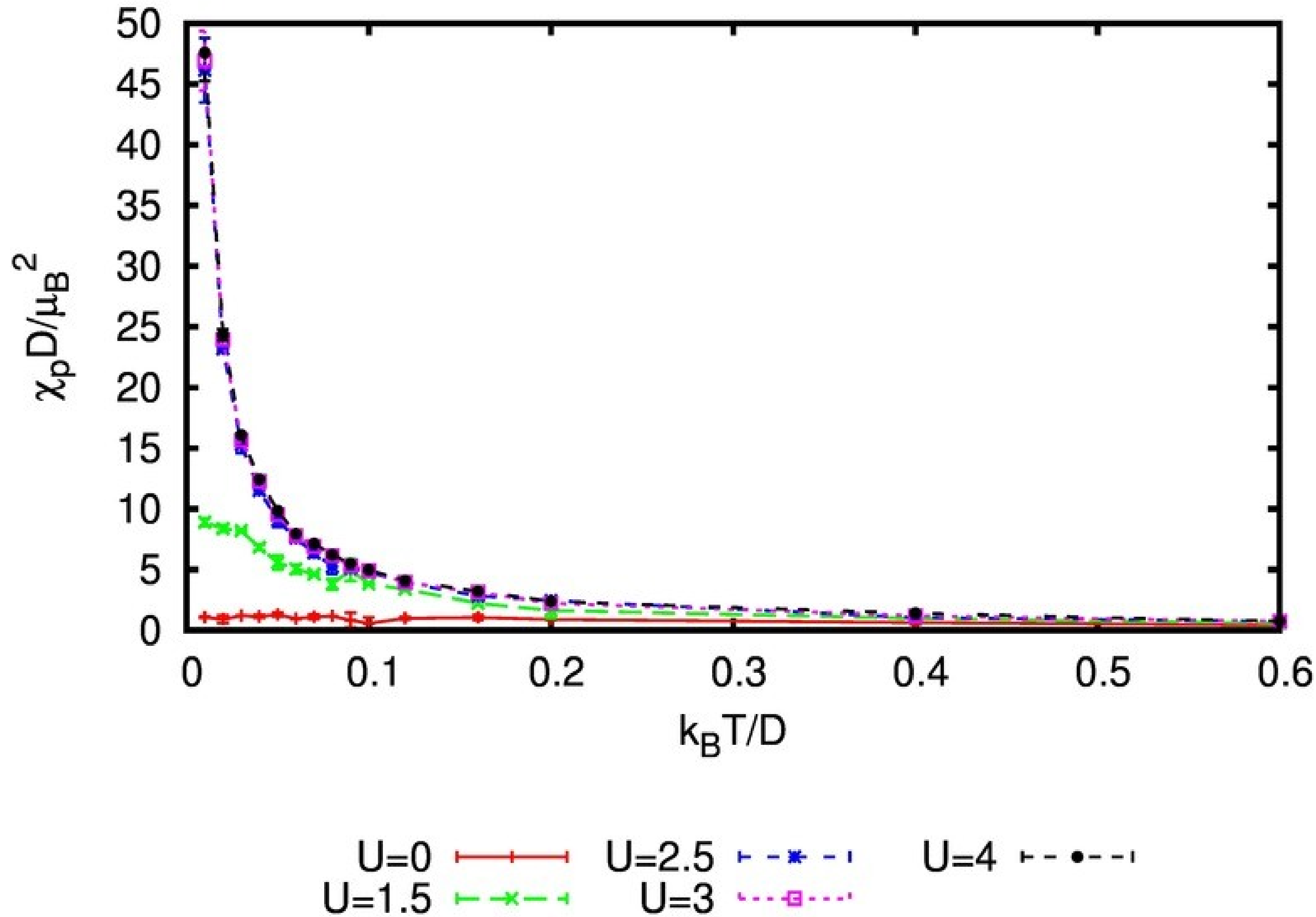
Results – charge susceptibility

$$\kappa_c = \left(\frac{\partial n}{\partial \mu}\right)_T$$



Results – magnetic susceptibility

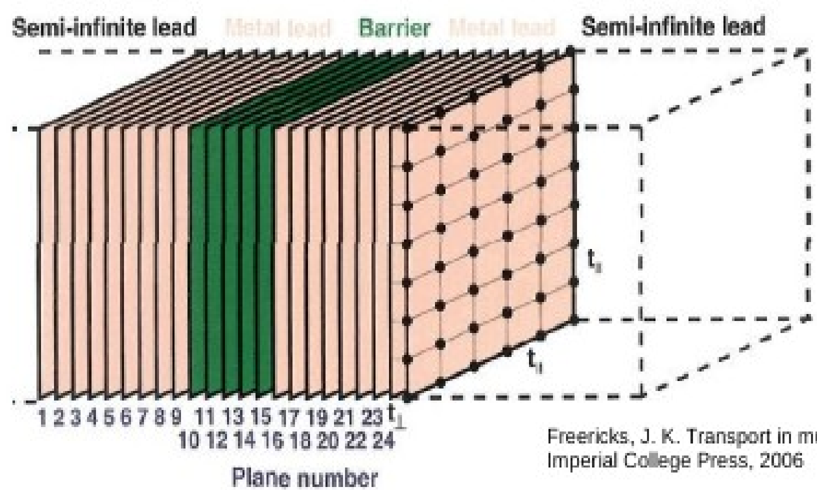
$$\chi_p = \left(\frac{\partial m}{\partial B}\right)_T$$



Summary

Thermodynamic properties in frame of dynamical mean-field aproximation
-single impurity problem by CTQMC – test of solver
-thermodynamics of Hubbard model in one place - within one method – as a reference to other methods/systems

Future perspective:
-calculation of other thermodynamic properties also for antiferromagnetic case
-heterostructures (e.g. band metal – Mott insulator – band metal)



Freericks, J. K. Transport in multilayered nanostructures, Imperial College Press, 2006