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

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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

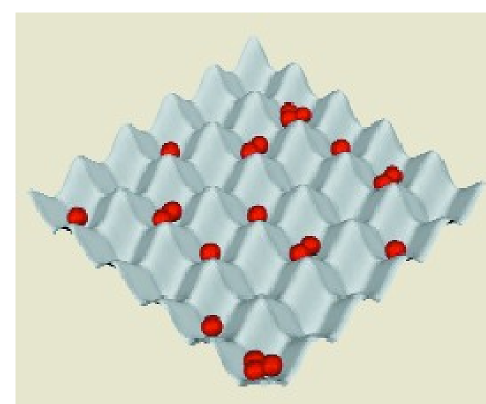
$$H = \sum_{i,j} \sum_{\sigma} T_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + \tfrac{1}{2} I \sum_{i,\sigma} n_{i\sigma} n_{i,-\sigma} - I \sum_{i,\sigma} \nu_{ii} n_{i\sigma}, \qquad (10)$$

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

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

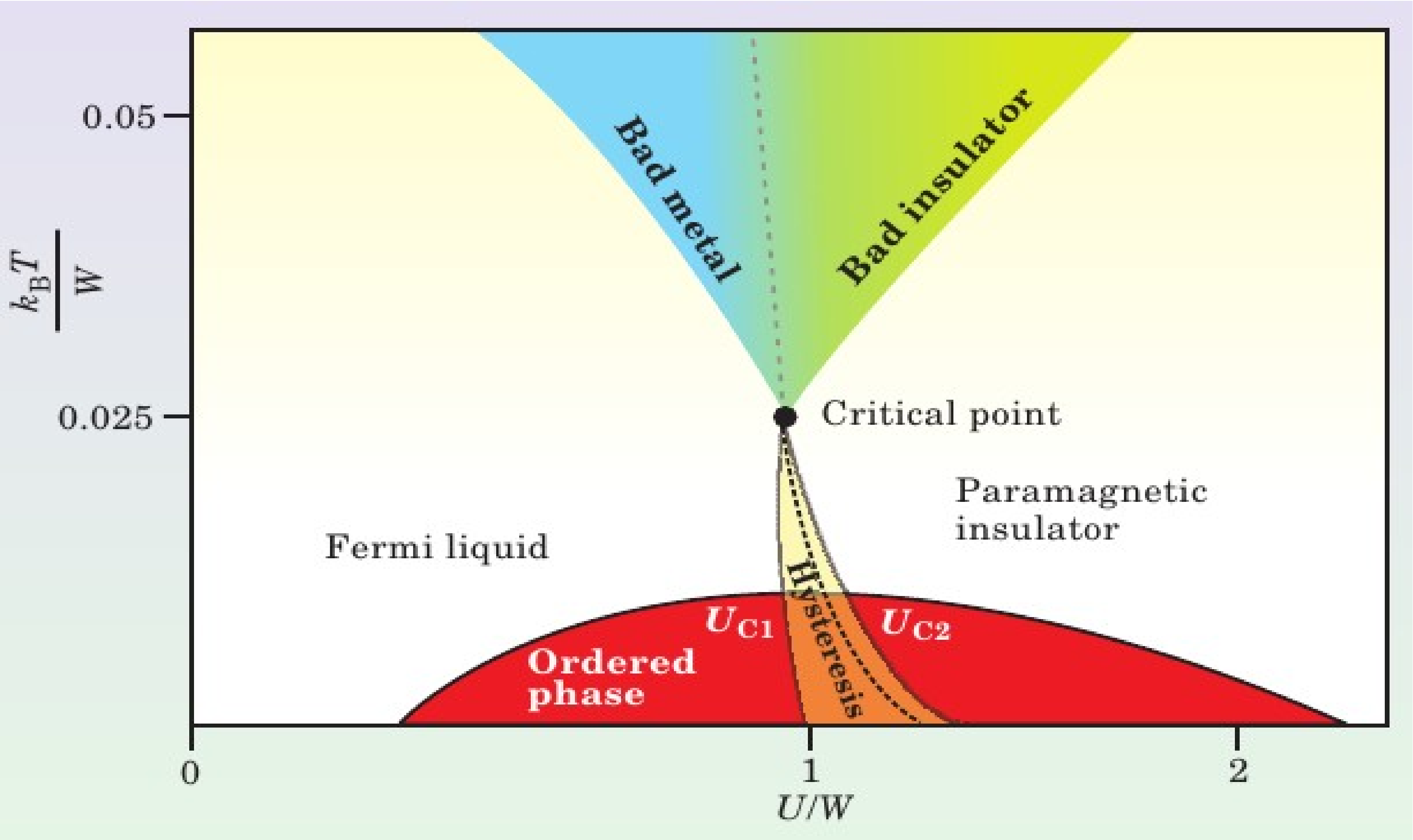
metal – insulator transition
antiferromagnetism

Neutral particles in optical lattice



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

Hubbard Model – schematic phase diagram



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 simulators (optical lattices)

Approximated method:

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

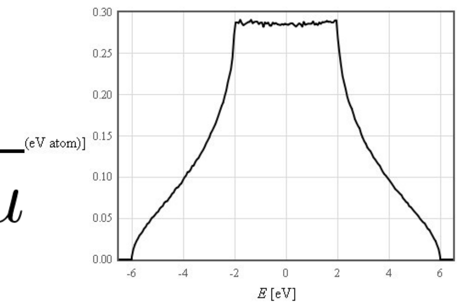
Internal energy: $\langle H \rangle$ → specific heat

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

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):

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

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

CT-QMC

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

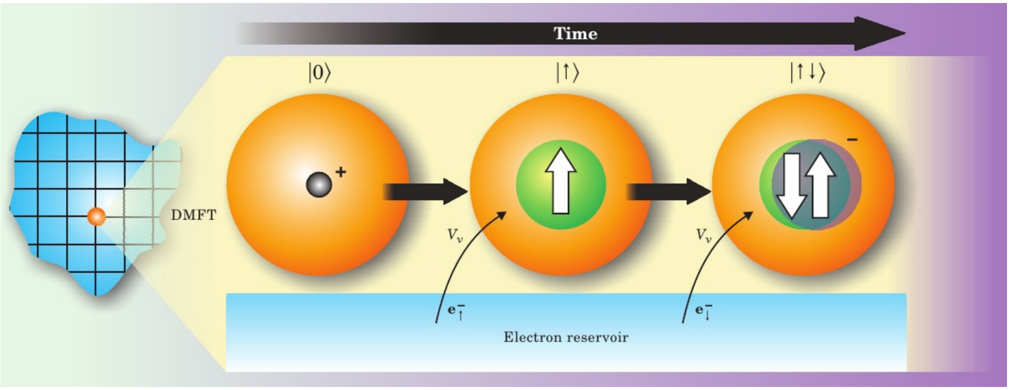
$$+ \sum_{\sigma=\uparrow,\downarrow} \int_0^\beta d\tau \int_0^\beta d\tau' c^*_{0\sigma}(\tau) \Delta(\tau, \tau') c_{0\sigma}(\tau')$$

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

$$\Xi = \Xi_0 \sum_{k=0}^{\infty} \frac{1}{k!} \int_0^\beta d\tau_1 \int_0^\beta d\tau_1' \ldots \int_0^\beta d\tau_k \int_0^\beta d\tau_k' \sum_{\sigma_1,\sigma_1',\ldots,\sigma_k\sigma_k'}$$

$$\times \langle T_\tau c'_{\sigma_1}(\tau_1') c^\dagger_{\sigma_1}(\tau_1) \ldots c'_{\sigma_k}(\tau_k') c^\dagger_{\sigma_k}(\tau_k) \rangle_{\text{local}}$$

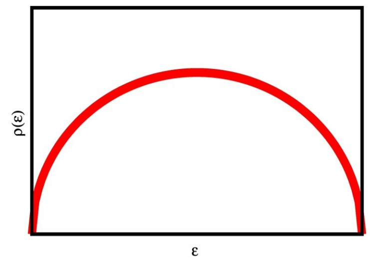
$$\times \frac{1}{k!} Det \begin{bmatrix} \Delta(\tau_{\sigma_1}, \tau'_{\sigma_1}) & \Delta(\tau_{\sigma_1}, \tau'_{\sigma_2}) & \ldots & \Delta(\tau_{\sigma_1}, \tau'_{\sigma_k}) \\ \ldots & \ldots & \ldots & \ldots \\ \ldots & \ldots & \ldots & \ldots \\ \Delta(\tau_{\sigma_k}, \tau'_{\sigma_1}) & \ldots & \ldots & \Delta(\tau_{\sigma_k}, \tau'_{\sigma_1}) \end{bmatrix}$$

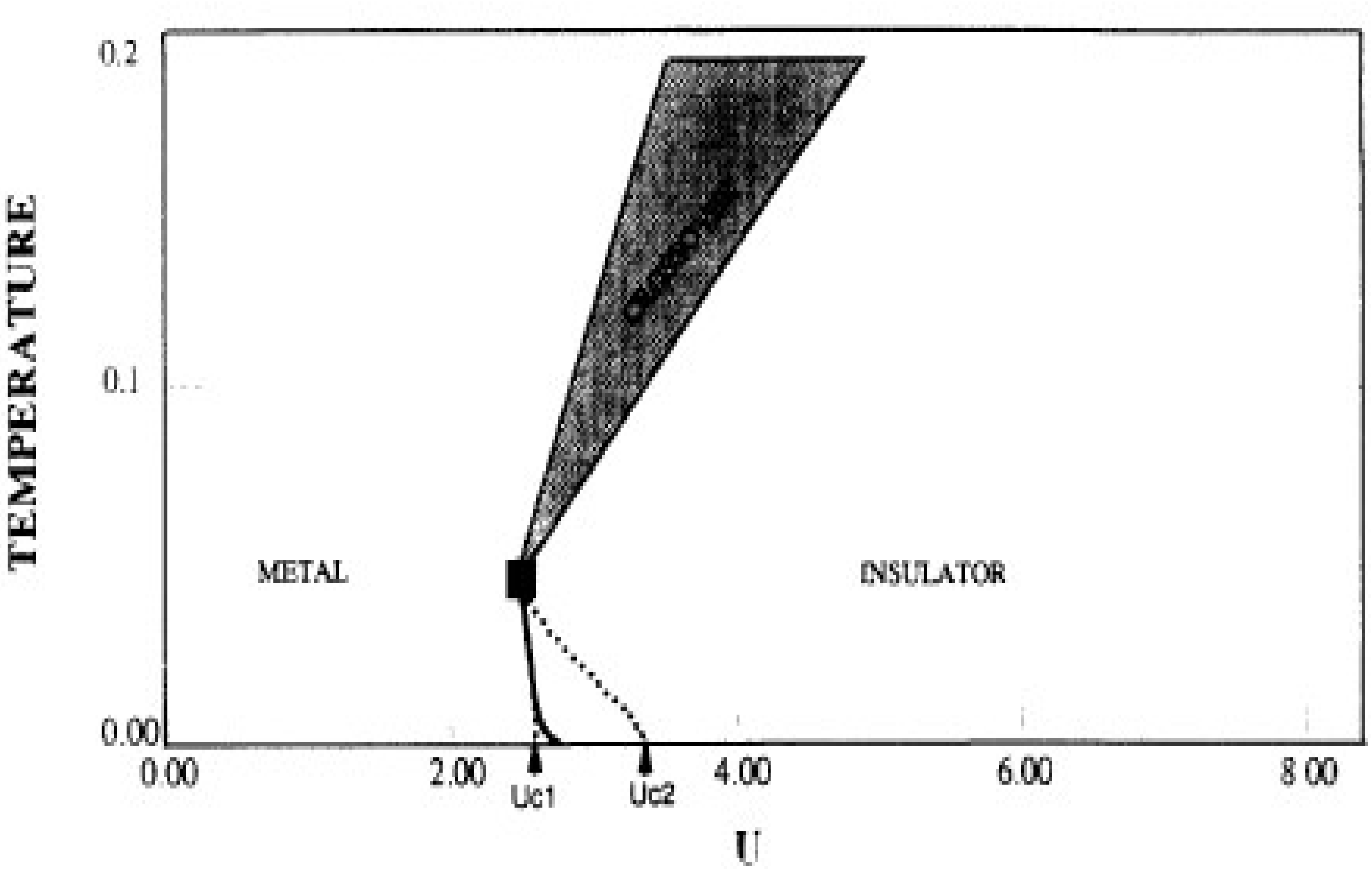
$$X \equiv k, \tau_1, \sigma_1, \tau_1', \sigma_1' \ldots \tau_k, \sigma_k \tau_k', \sigma_k',$$

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

Paramagnetic phase diagram – (semi-circular dos)

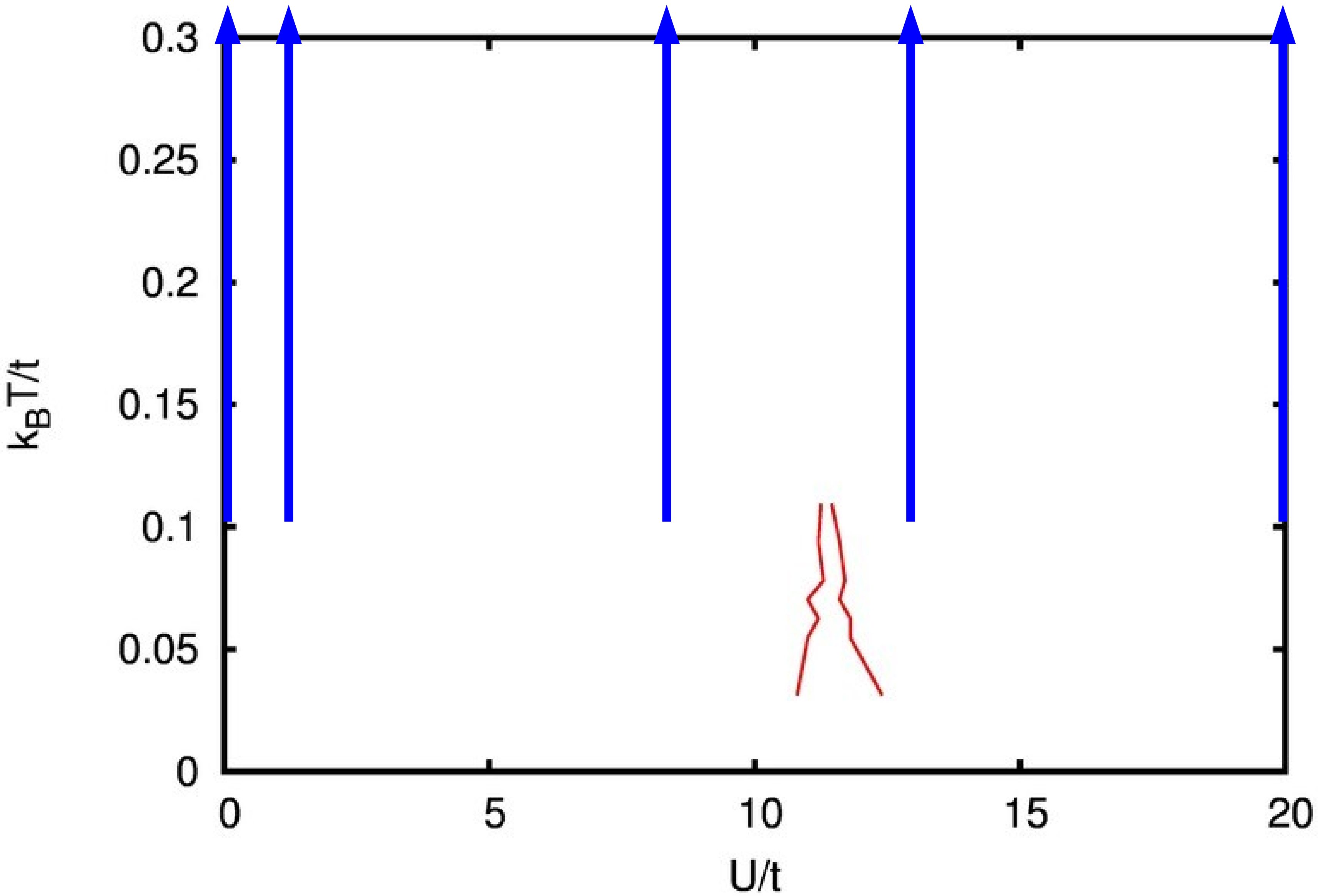
DOS:





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

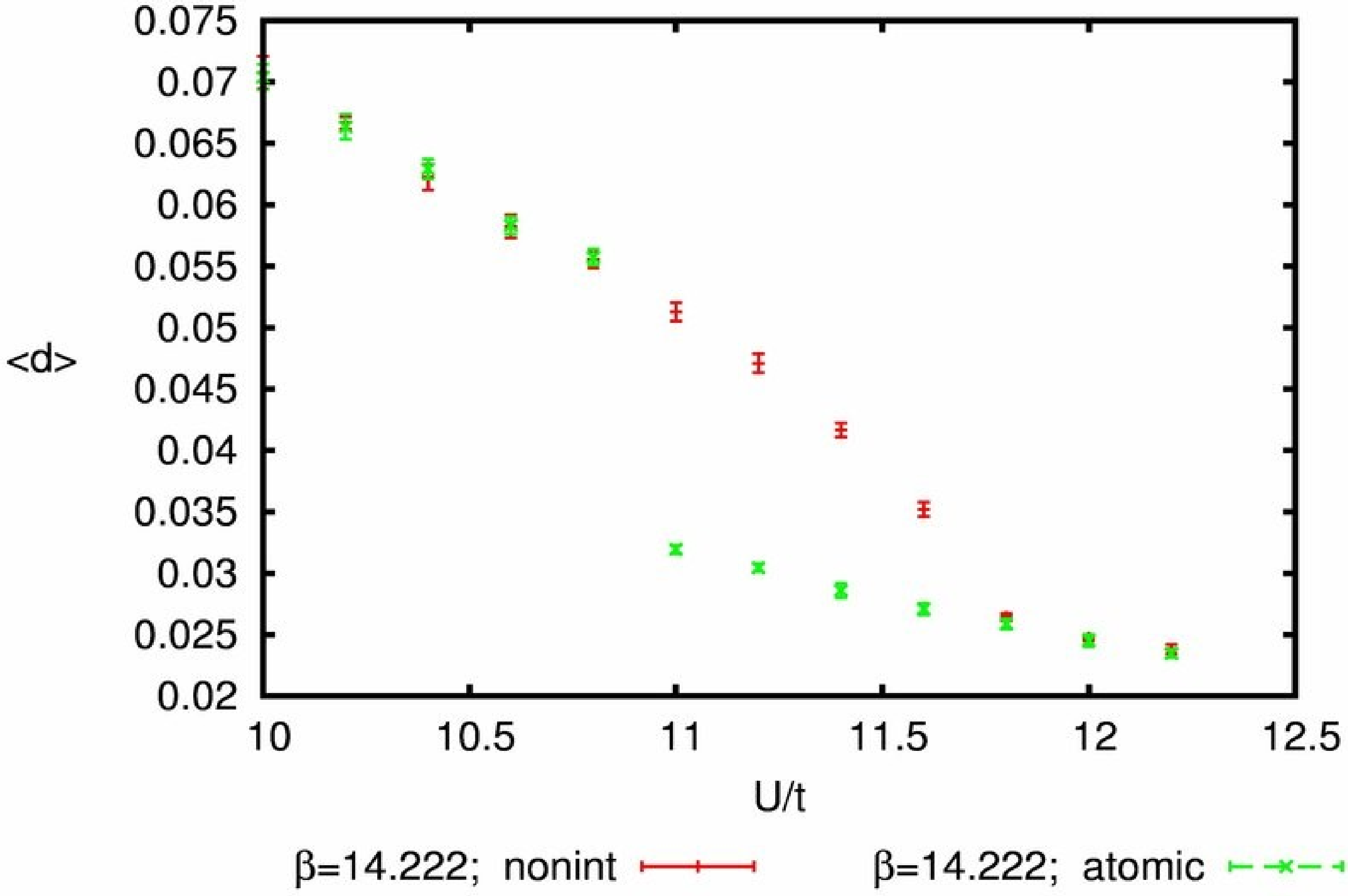
Results – phase diagram



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

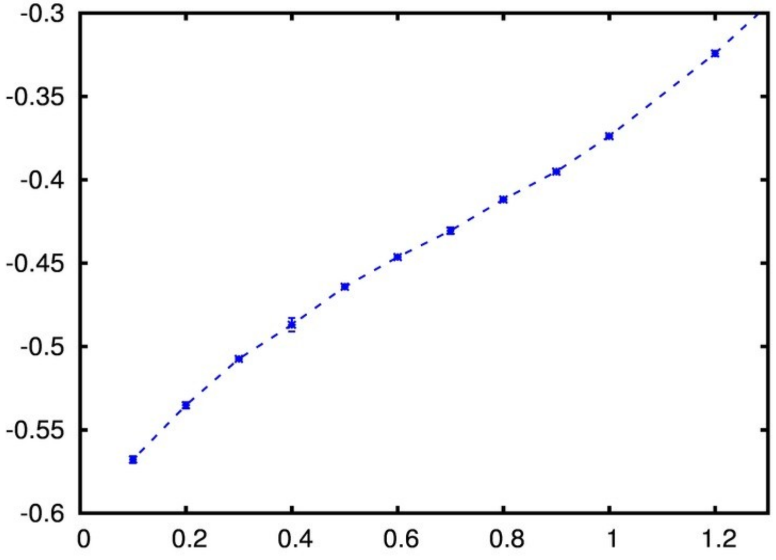
Results Example of determination of coexistence region

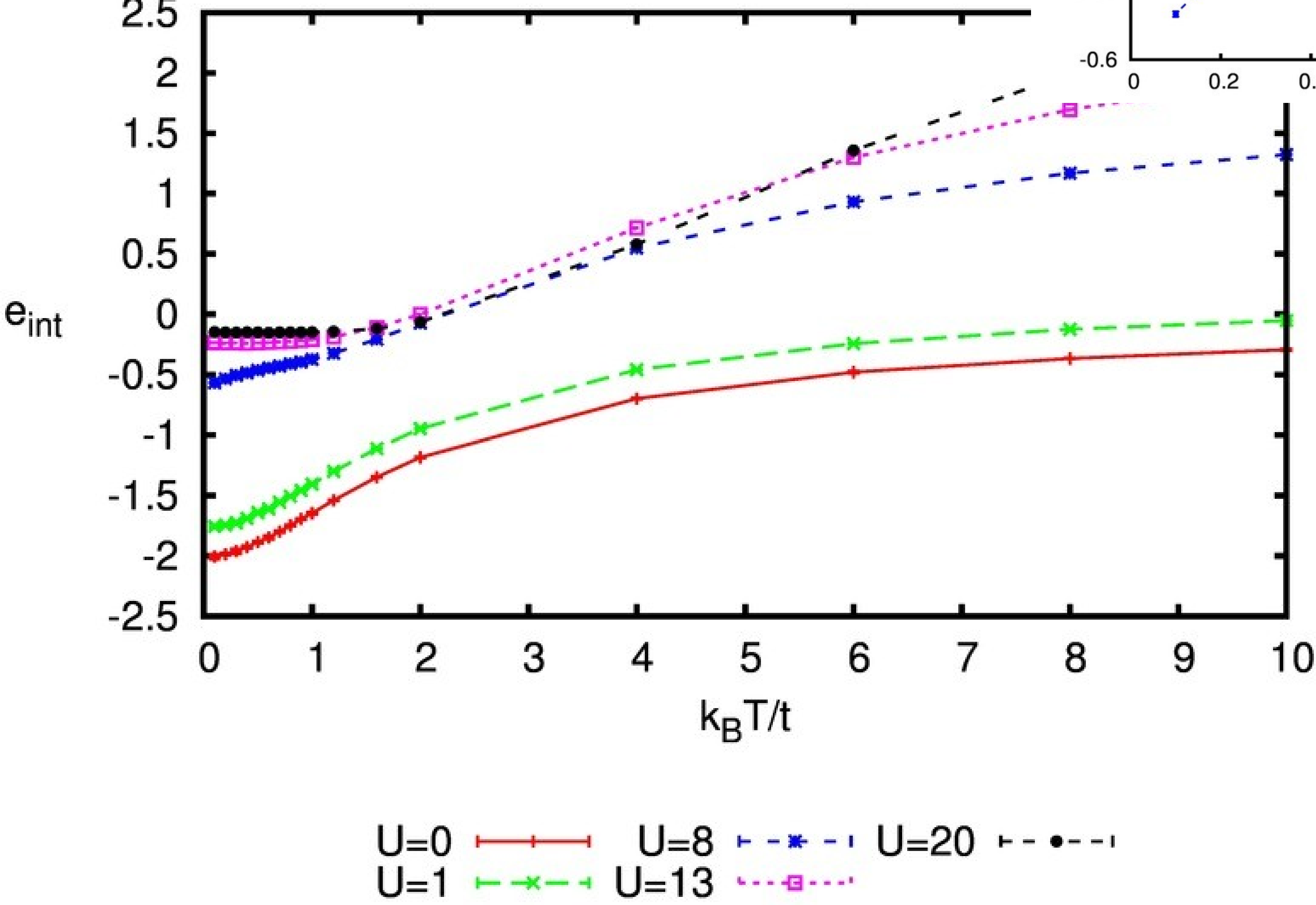
$$d \equiv \lim_{\infty} \frac{1}{N} \langle \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \rangle$$



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

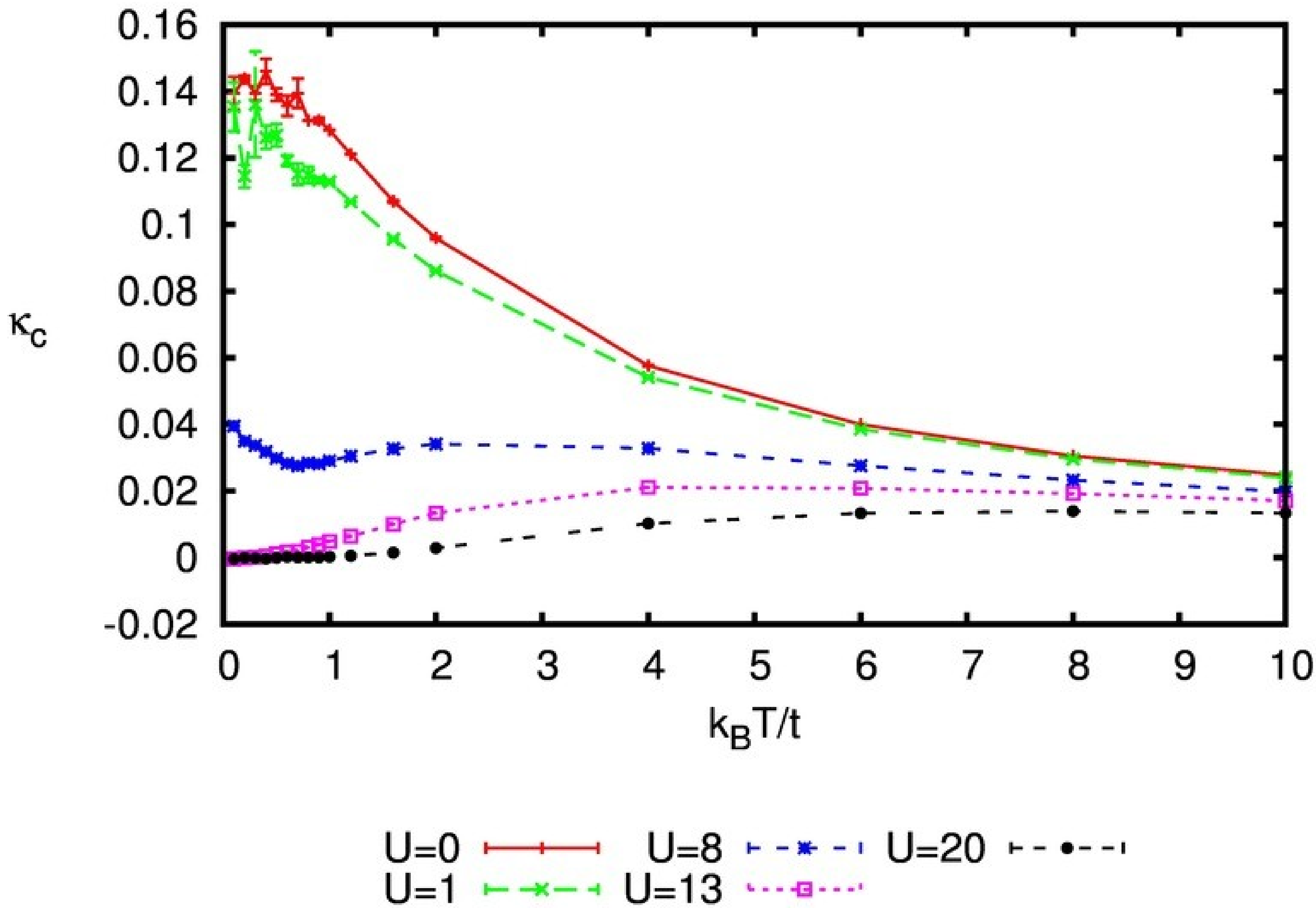
Results – internal energy





Results – charge susceptibility

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



Summary

Thermodynamic properties in frame of dynamical mean-field aproximation

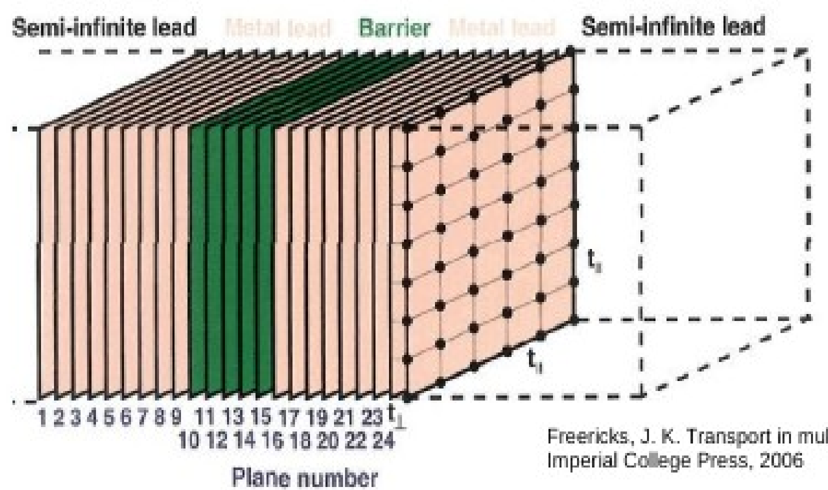
-single impurity problem by CTQMC – test of solver

-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