Mott-Hubbard metal-insulator transition in $d = \infty$

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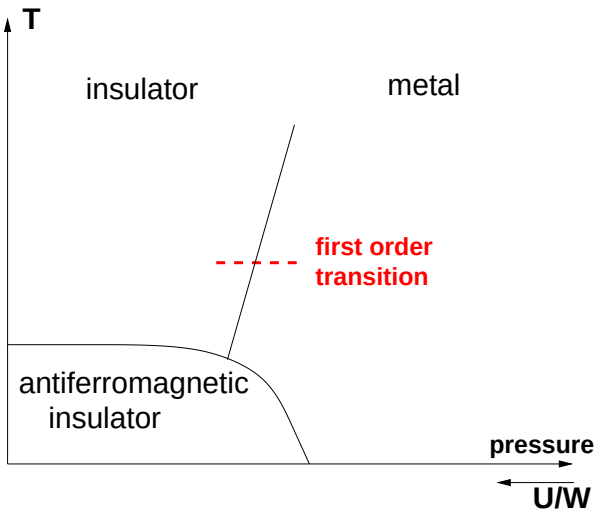
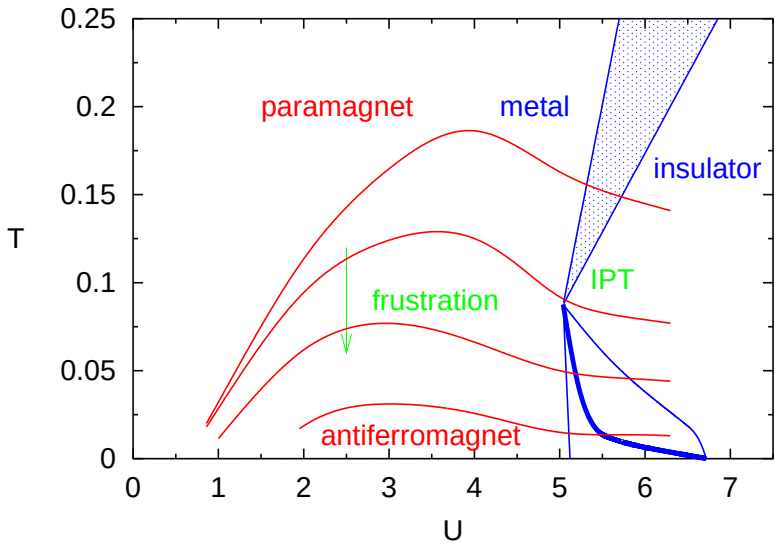
Motivation: V_2O_3



1-band Hubbard model

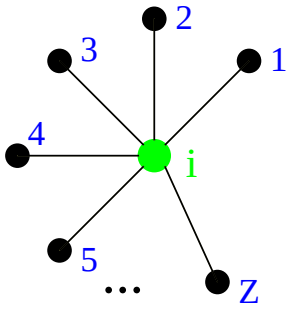


Aim: Phase diagram / order of phase transition for

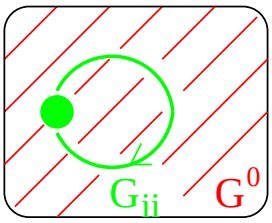
- 1-band Hubbard model at half filling
- no antiferromagnetic order (full frustration)
- Dynamical Mean-Field Theory (DMFT)
- semielliptic Bethe density of states ($W = 4$)

Self-consistent solution of DMFT equations

lattice problem



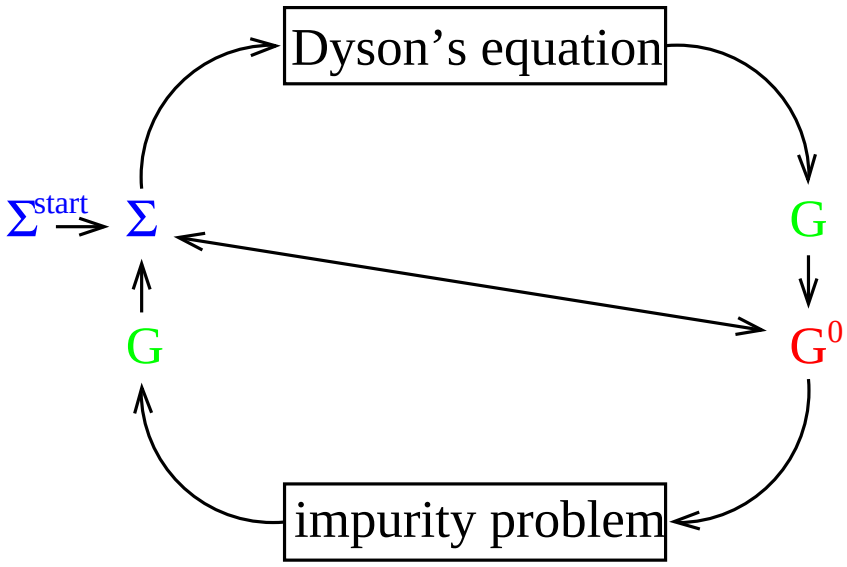
$\Downarrow$ DMFT



impurity problem

+

self consistency



QMC solution of impurity problem:

- discretization $\Delta\tau$ of imaginary time
- Hubbard-Stratonovich transformation
- MC sampling over auxiliary Ising field
- runs parallel on 4-32 CPUs

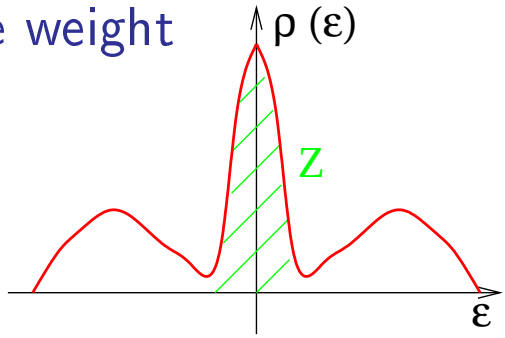
Characterization of phase transitions

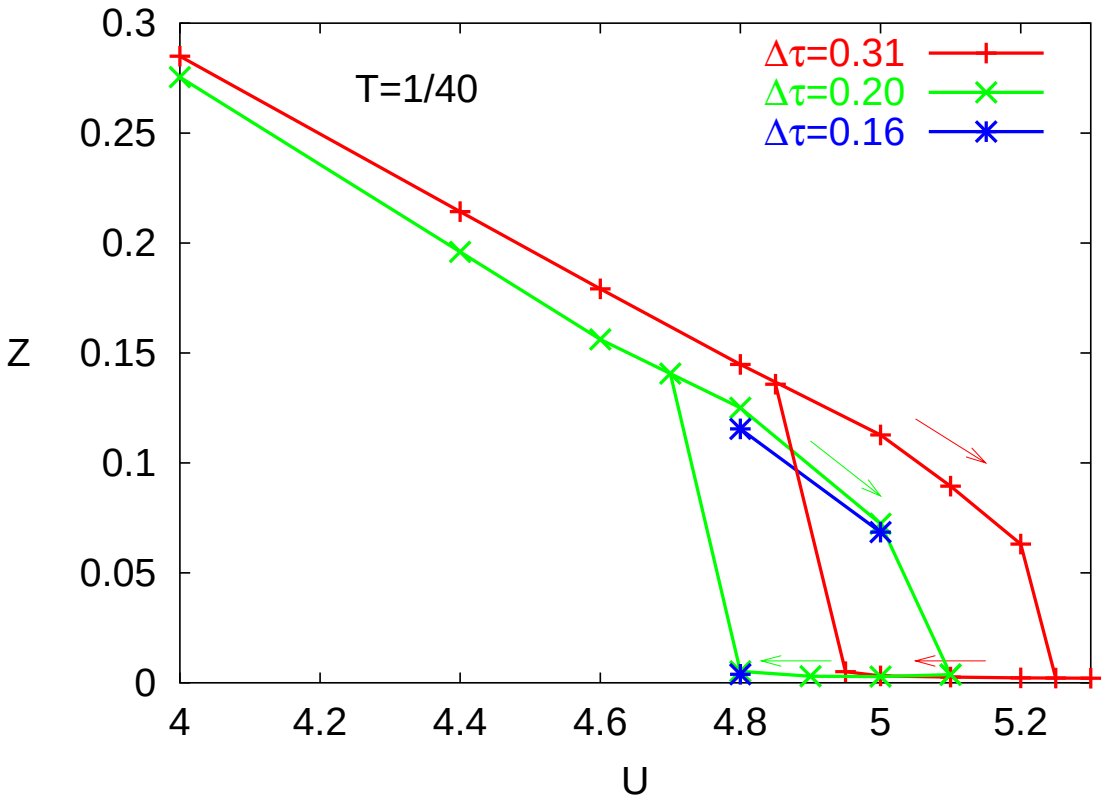
continuous phase transition	observables depend continuously and uniquely on U, T
first order phase transition	coexistence of 2 different solutions; hysteresis; free energy $\longrightarrow$ transition line

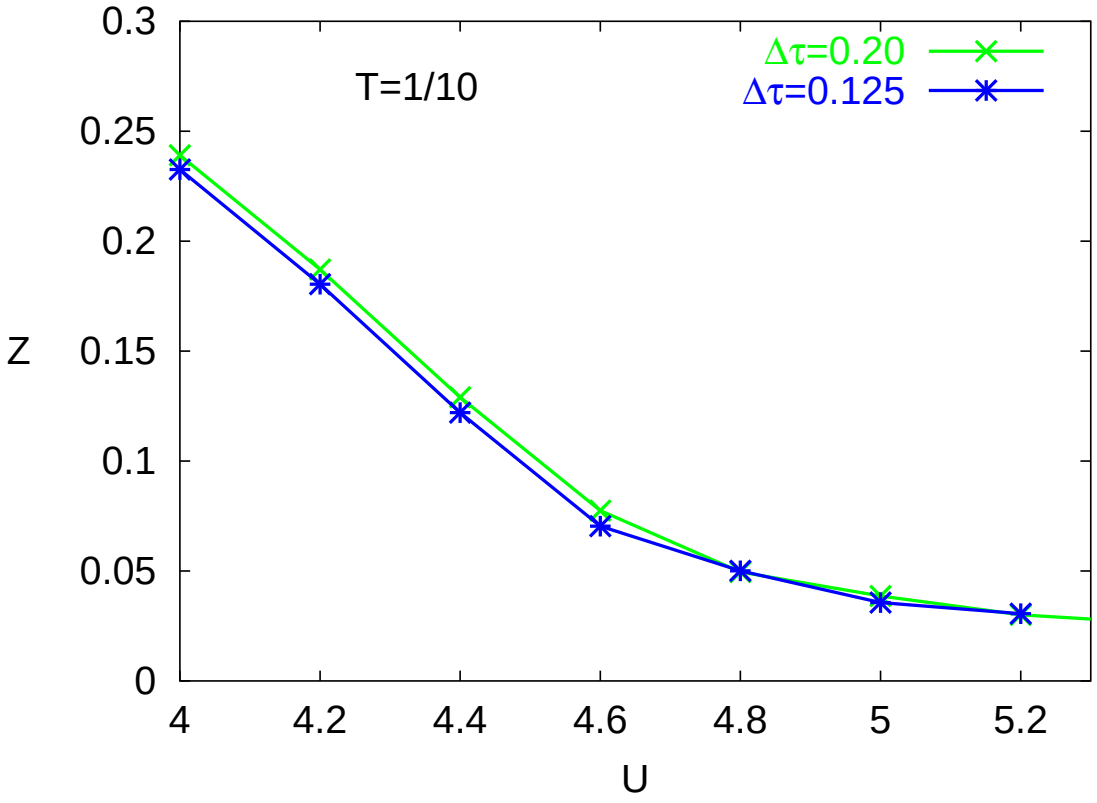
in the physical limit ($\Delta\tau \to 0$ for QMC, $\Lambda \to 1$ for NRG etc.)

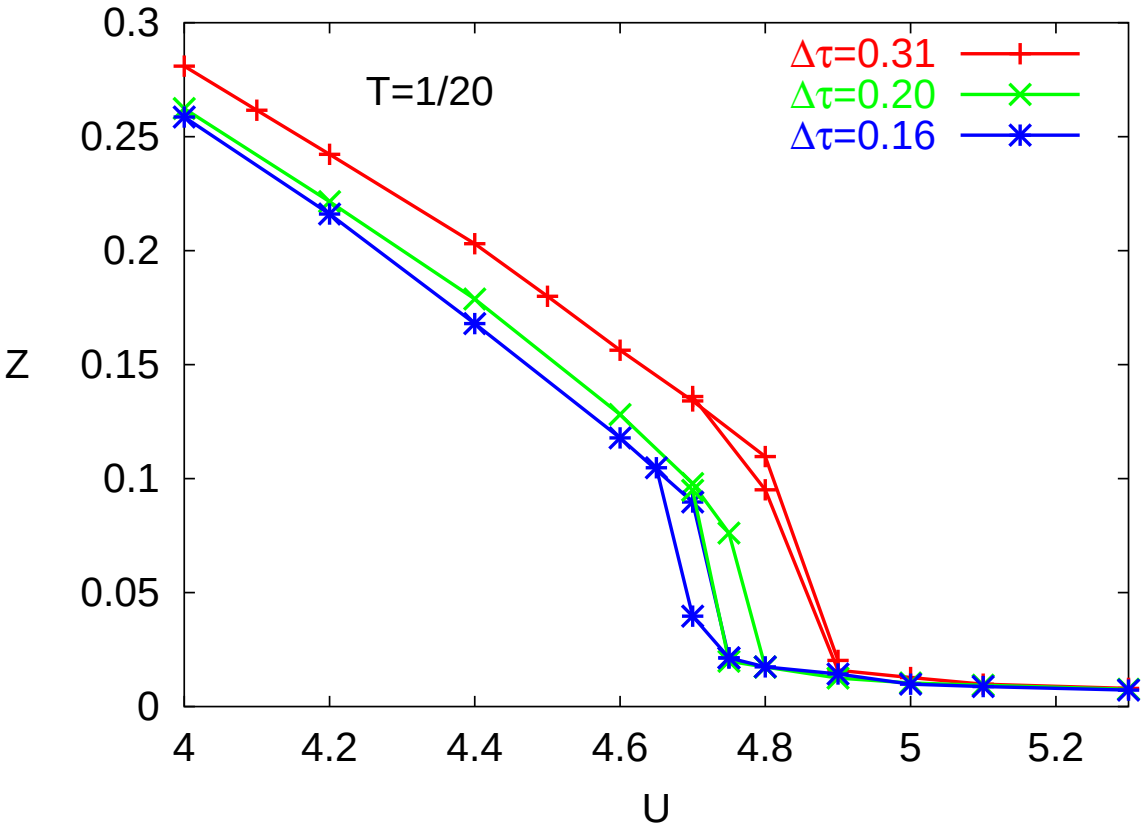
Results: quasiparticle weight

$$Z = \frac{m}{m^*} = \left(1 - \frac{\partial Re\Sigma(\omega)}{\partial \omega}\right)^{-1}$$

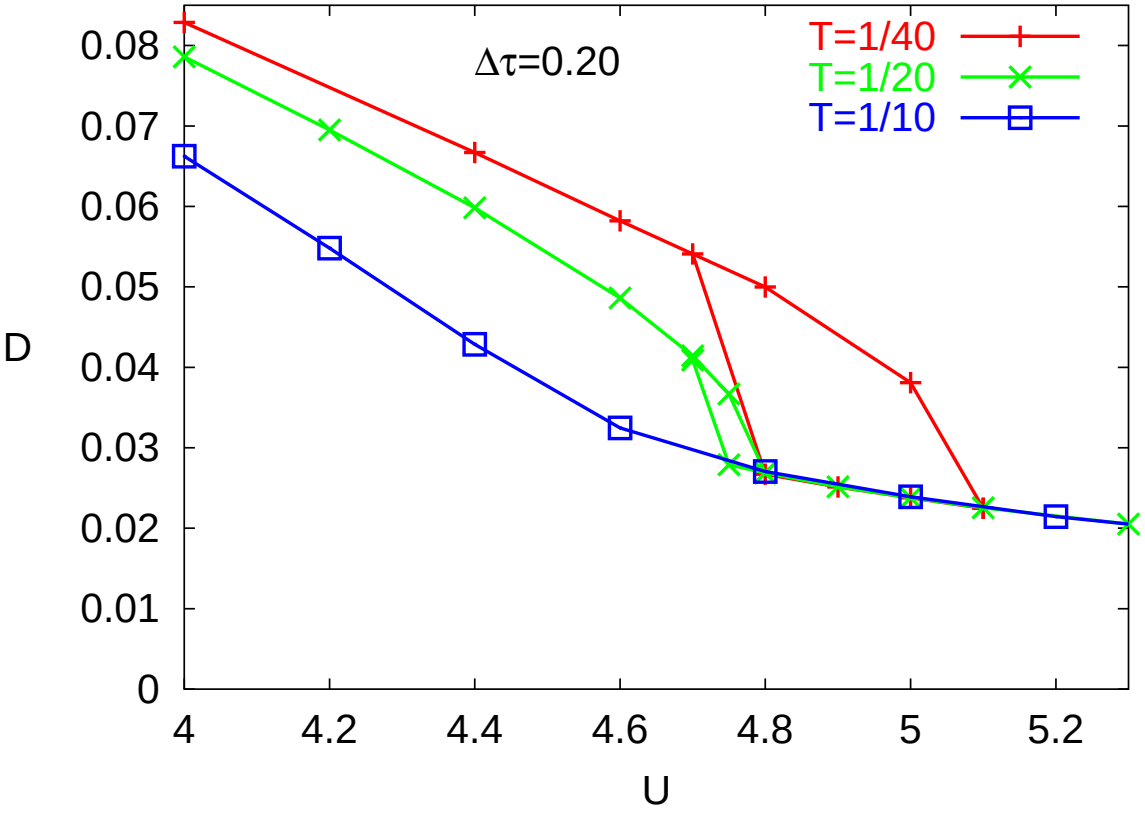




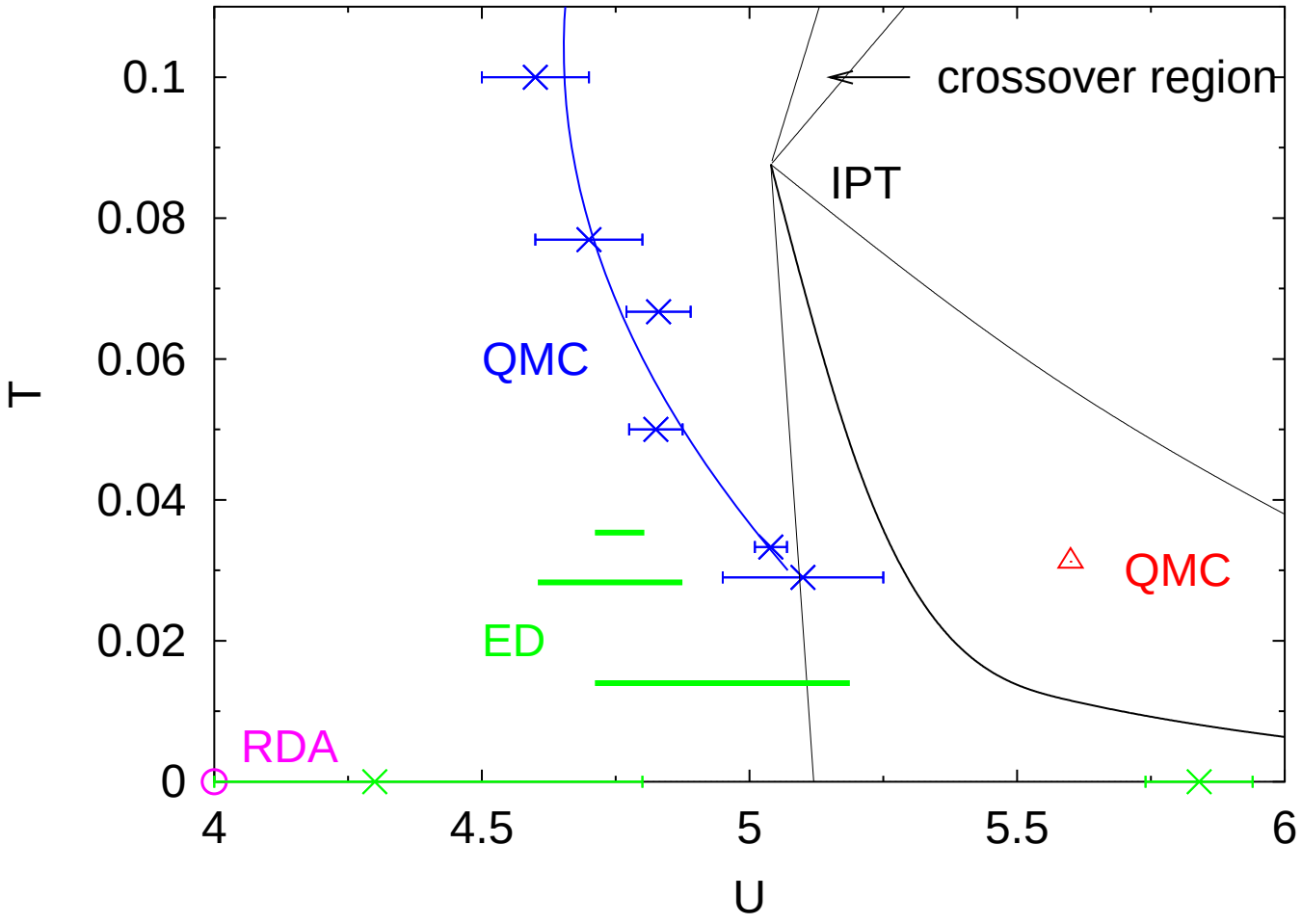




Double occupancy $D = \langle n_i^{\uparrow} n_i^{\downarrow} \rangle$

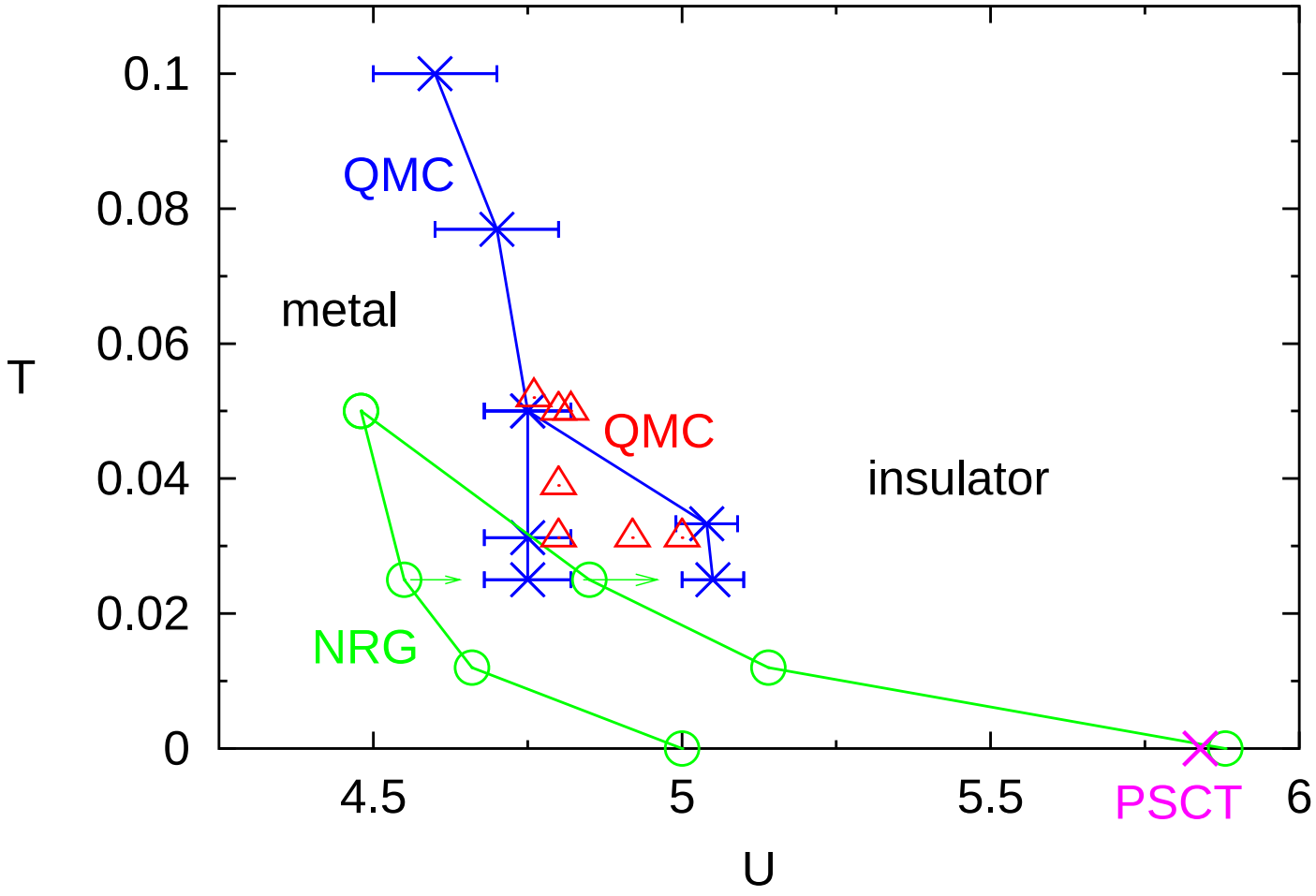


Status of phase diagram in spring 1999



Georges et al. (1996)
Rozenberg, Kotliar, and Zhang (1994)
Noack and Gebhard (1999)
Georges et al (1996); Hofstetter
Schlipf et al (1999)

Phase diagram of 1-band Hubbard model ($n = 1$)



Rozenberg, Chitra and Kotliar (1999)
Moeller et al. (1996)

Conclusions

- results from fundamentally different methods now converge towards a reliable phase diagram
- coexistence region at low T $\longrightarrow$ first order transition

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