Center for
Electronic Correlations and Magnetism
University of Augsburg

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

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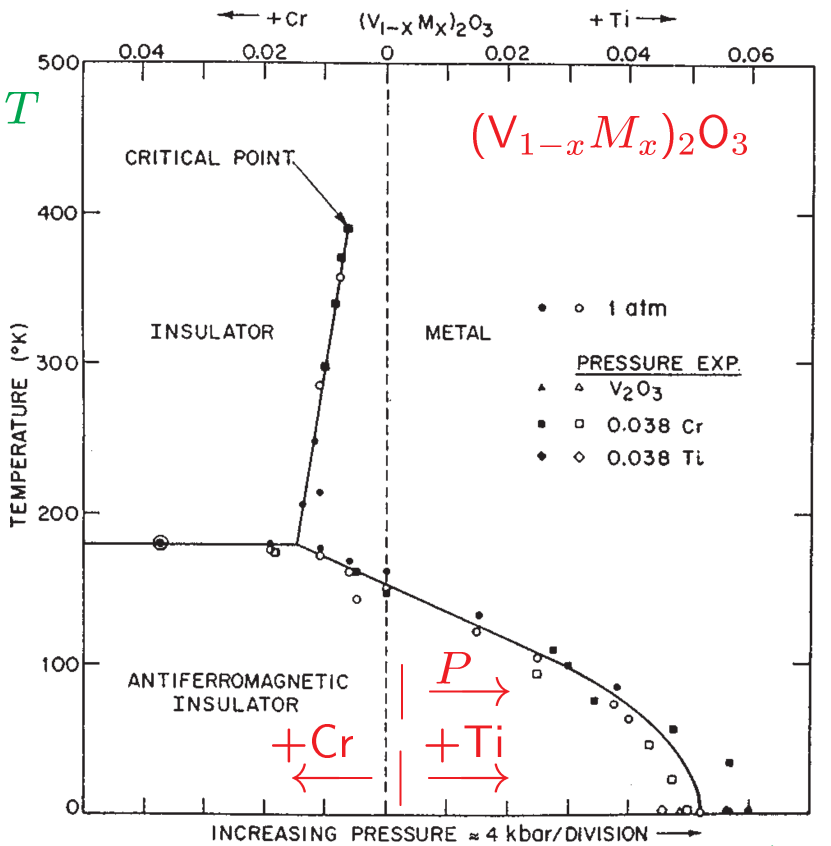
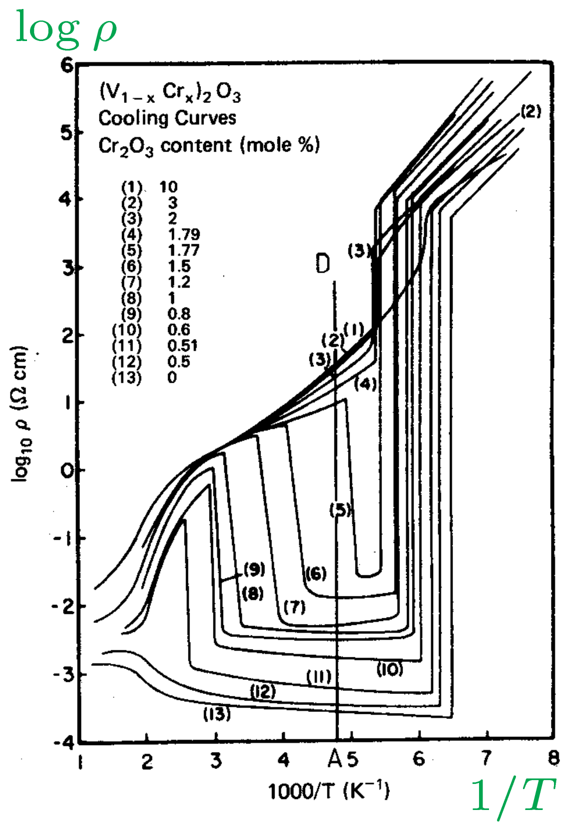
05. 12. 2000

# Introduction



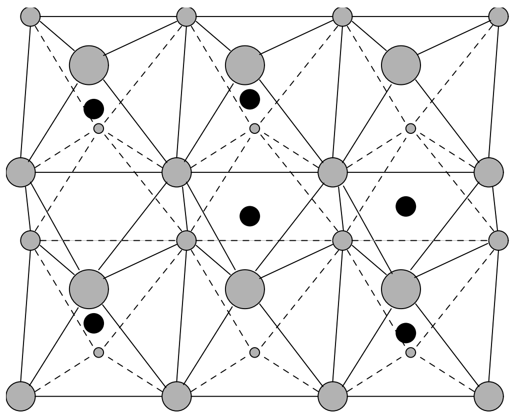

McWhan et al, 1971



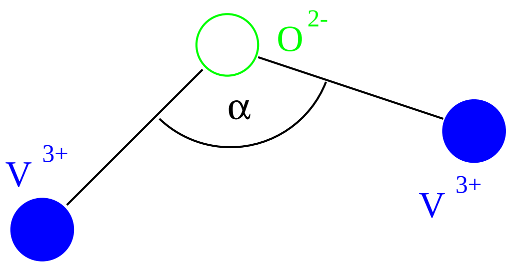

Kawamoto et al, 1980

## Motivation: $V_2O_3$

- MIT without LRO
- drop in resistivity $\rho$ by factor $10^3$
- shift in lattice parameters
- Corundum structure:
  - hcp $O^{2-}$ lattice
  - $V^{3+}$ fill 2/3 of octahedral vacancies
- doping with Ti, Cr:
  - (nearly) isovalent
  - distorts lattice → changes overlap
  - drives MIT (like pressure)
- band degeneracy (Held, cond-mat/0011518)



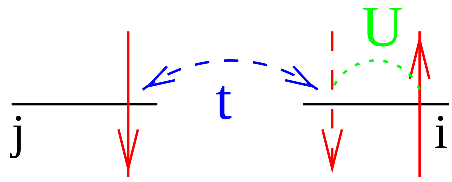
Corundum structure



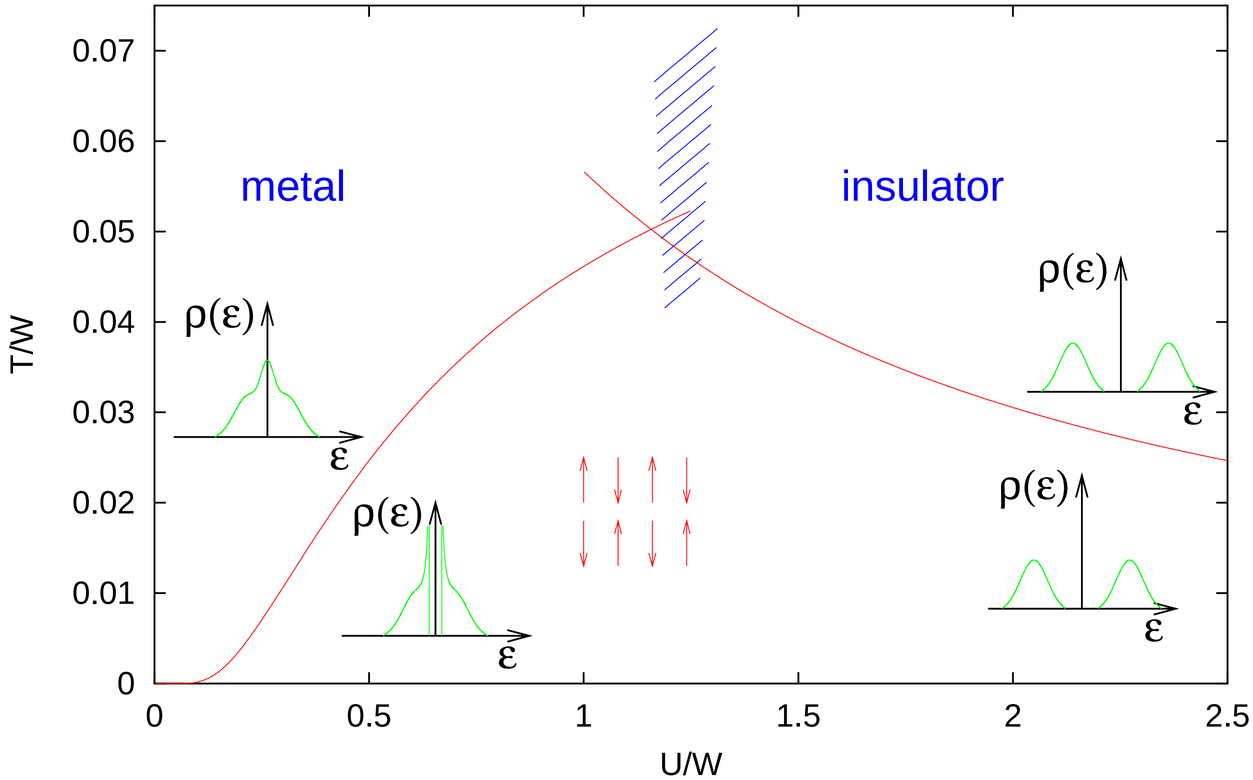

$\alpha_{\mathrm{Cr}} < \alpha_{\mathrm{V}} < \alpha_{\mathrm{Ti}}$

> Paramagnetic, bandwidth-controlled metal-insulator transition in $V_2O_3$

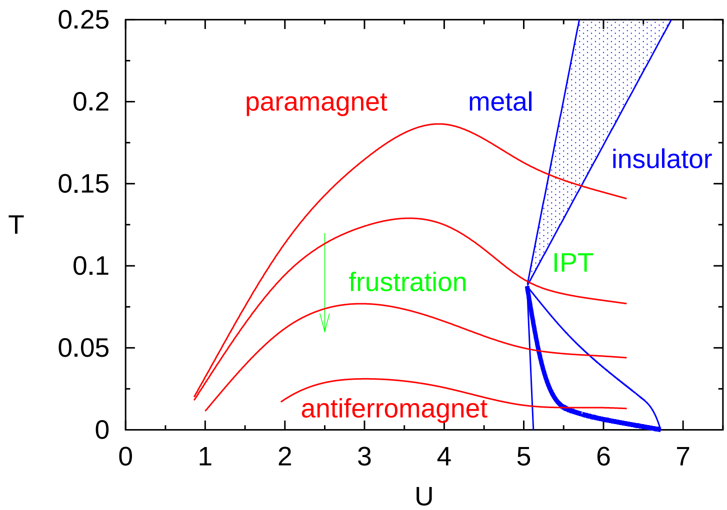
(half-filled) one-band Hubbard model




$$\hat{H} = -t \sum_{\langle ij \rangle \sigma} \left( \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + \hat{c}^{\dagger}_{j\sigma} \hat{c}_{i\sigma} \right) + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$




- here: no MIT, but crossover
- antiferromagnetism is understood at weak and strong coupling
- AF frustrated in many materials
- nonperturbative approach needed
- thermodynamic limit important

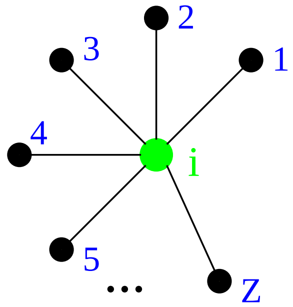



Aim: full phase diagram for

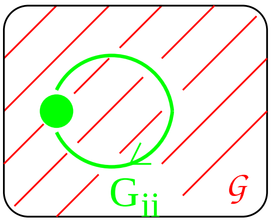
- 1-band Hubbard model at half filling within DMFT
- no AF order (full frustration), semielliptic Bethe DOS ($W = 4$)

# Self-consistent solution of DMFT equations

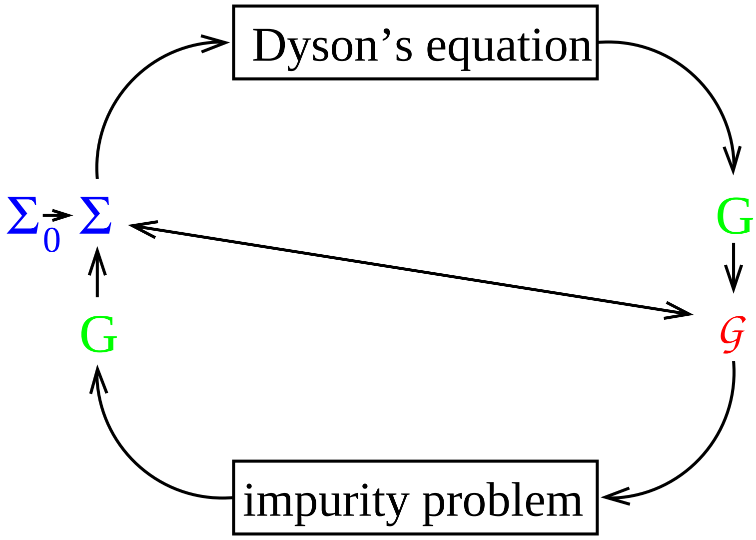
lattice problem




$\Downarrow$ DMFT




impurity problem
+
self consistency




QMC solution of impurity problem:

- discretization $\Delta\tau$ of imaginary time $\beta = 1/T$
- Hubbard-Stratonovich transformation
- MC sampling over auxiliary Ising field
- runs parallel on 4-32 CPUs

$$S_{\rm eff} = -\int_0^\beta d\tau\, d\tau' \sum_\sigma c_\sigma^\dagger(\tau)\mathcal{G}^{-1}(\tau-\tau')c_\sigma(\tau') + U\int_0^\beta d\tau\; c_\uparrow^\dagger(\tau)c_\uparrow(\tau)\; c_\downarrow^\dagger(\tau)c_\downarrow(\tau)$$

# Characterization of phase transitions

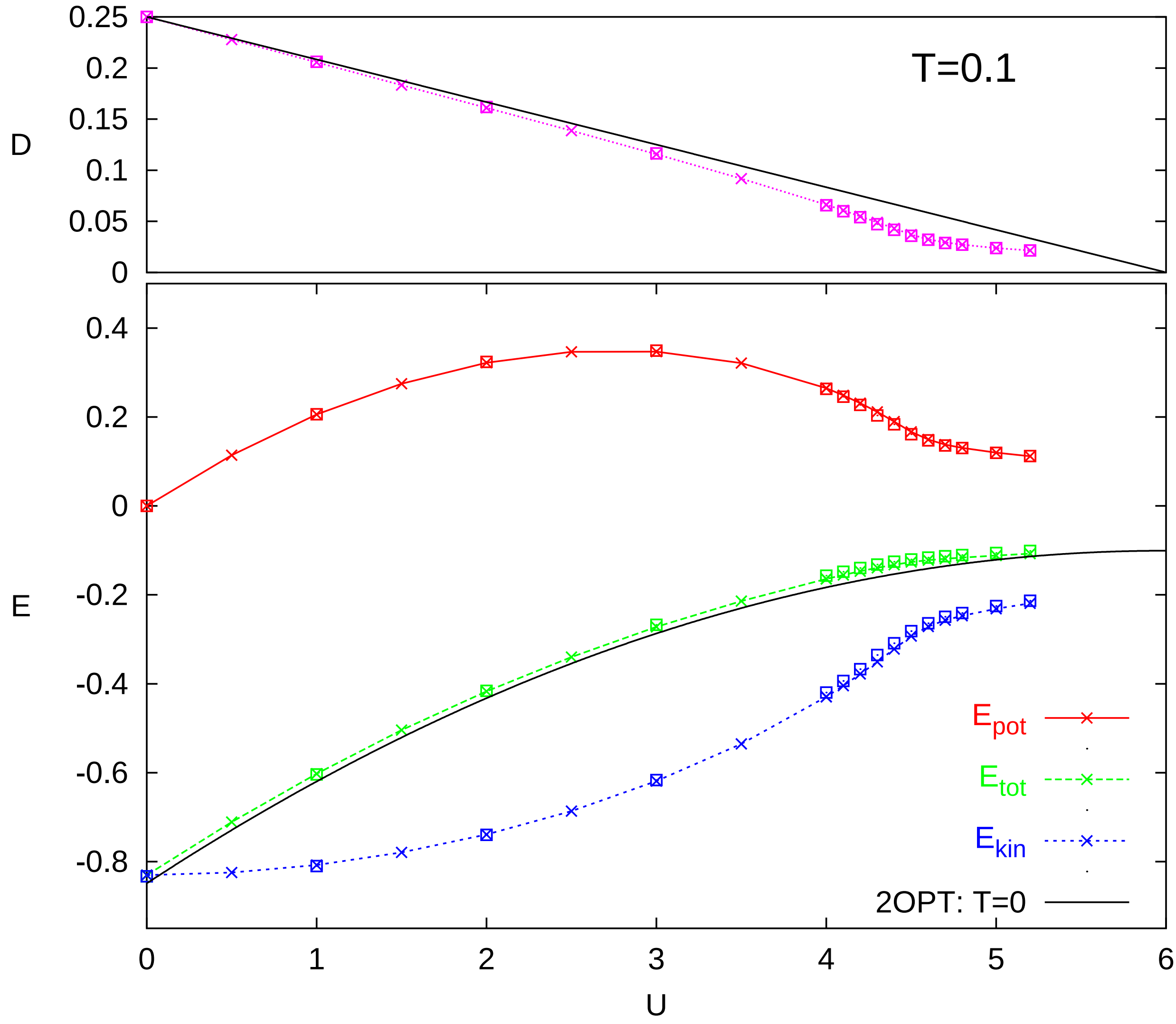
| | |
|---|---|
| continuous phase transition | observables depend continuously and uniquely on U, T |
| first order phase transition | coexistence of 2 different solutions; hysteresis; free energy $\longrightarrow$ transition line |

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

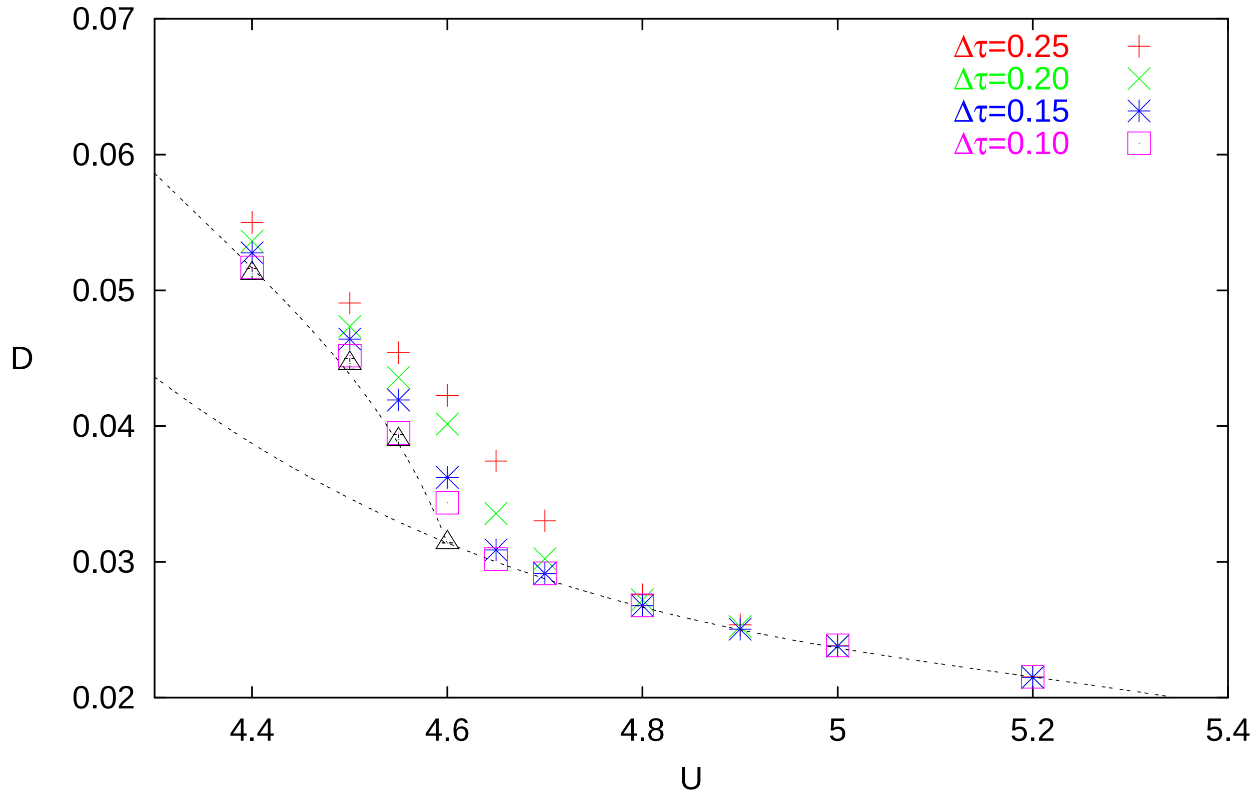
# Results: crossover and coexistence regions

double occupancy $D = \langle \hat{n}_i^{\uparrow} \hat{n}_i^{\downarrow} \rangle$

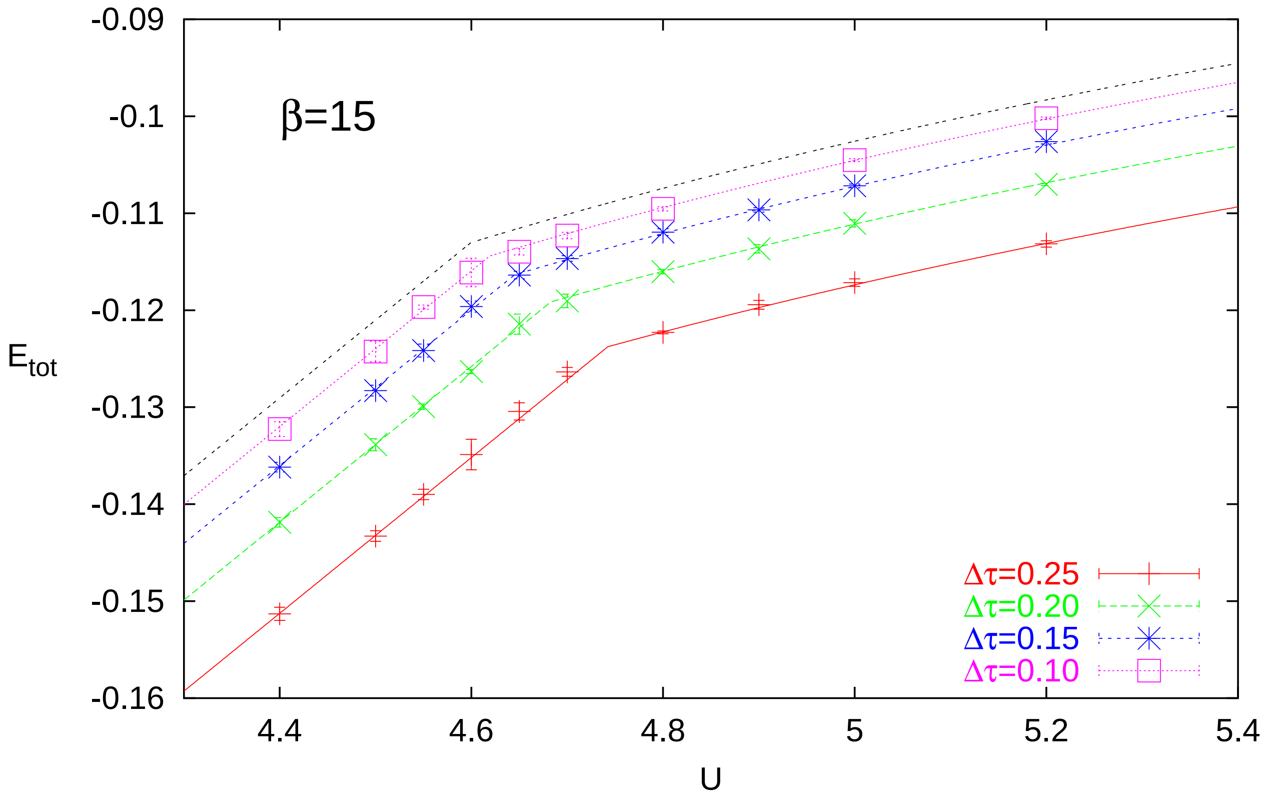
total energy per lattice site $E = E_{kin} + UD$



$\beta = 15$: sharp transition from metal to insulator, no hysteresis

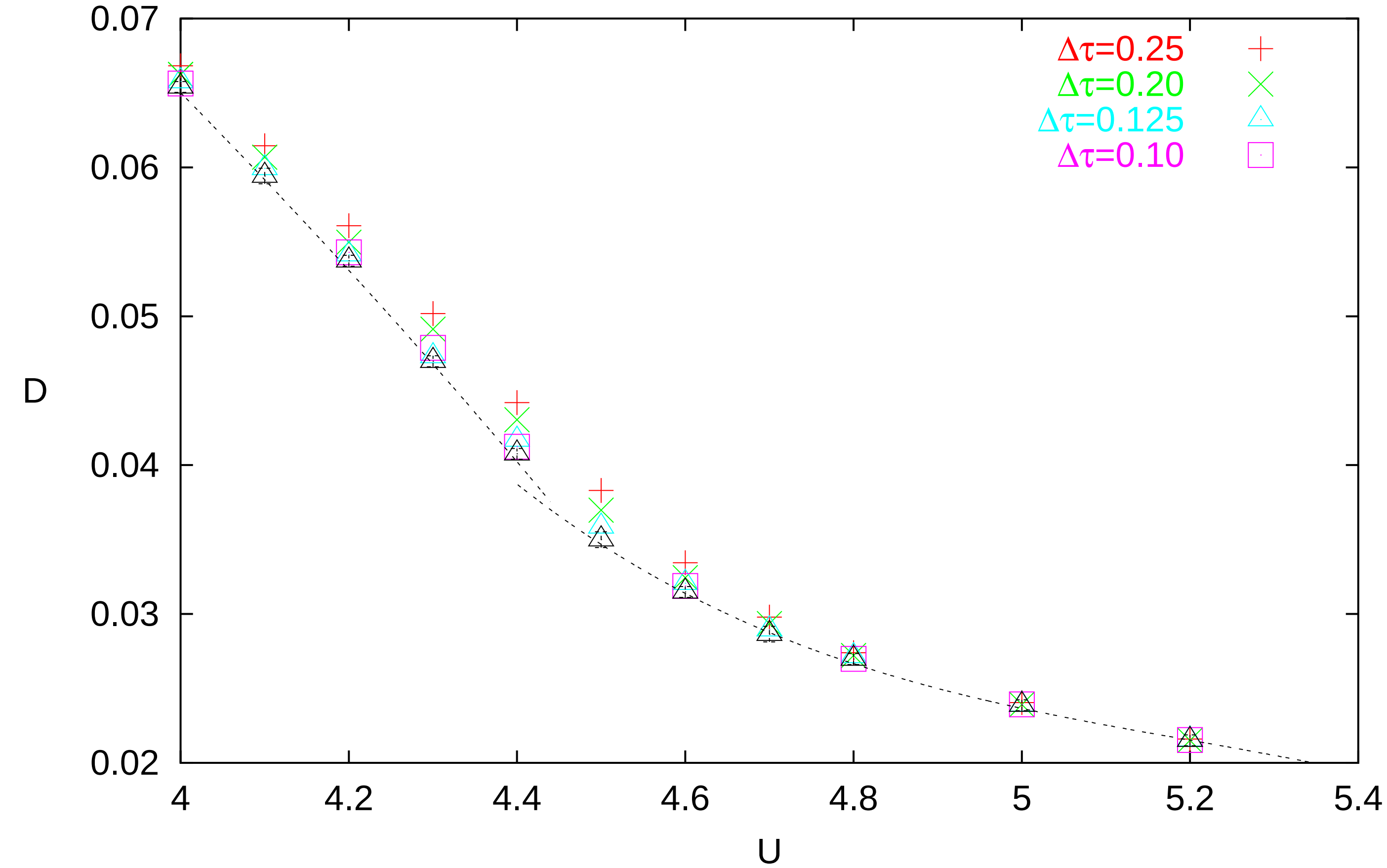


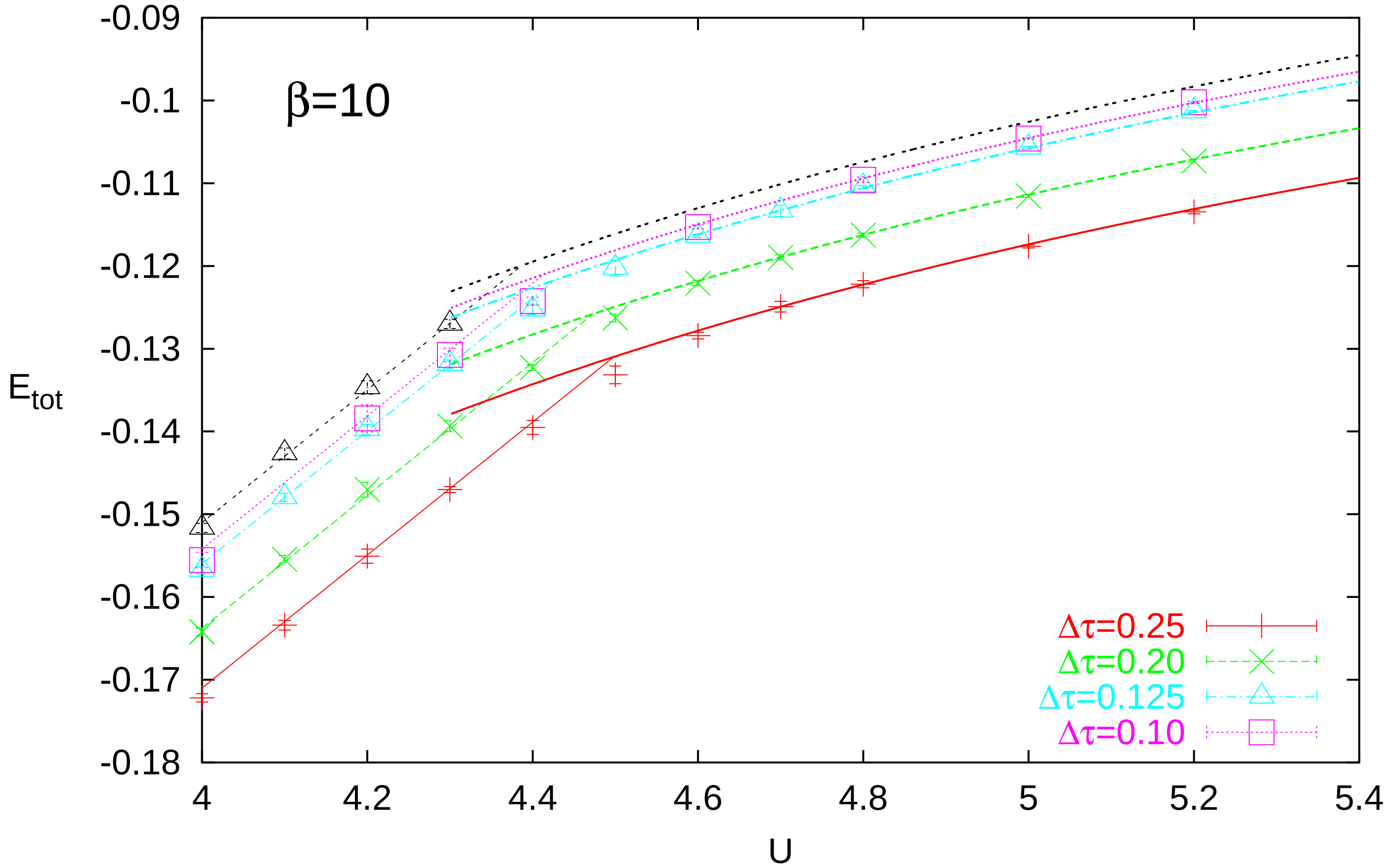

$\Delta\tau$ dependence: large at $MIT$, small below, vanishing above; relatively strong curvature




$\Delta\tau$ dependence: very regular; $U_c$ substantially shifts for $\Delta\tau \to 0$

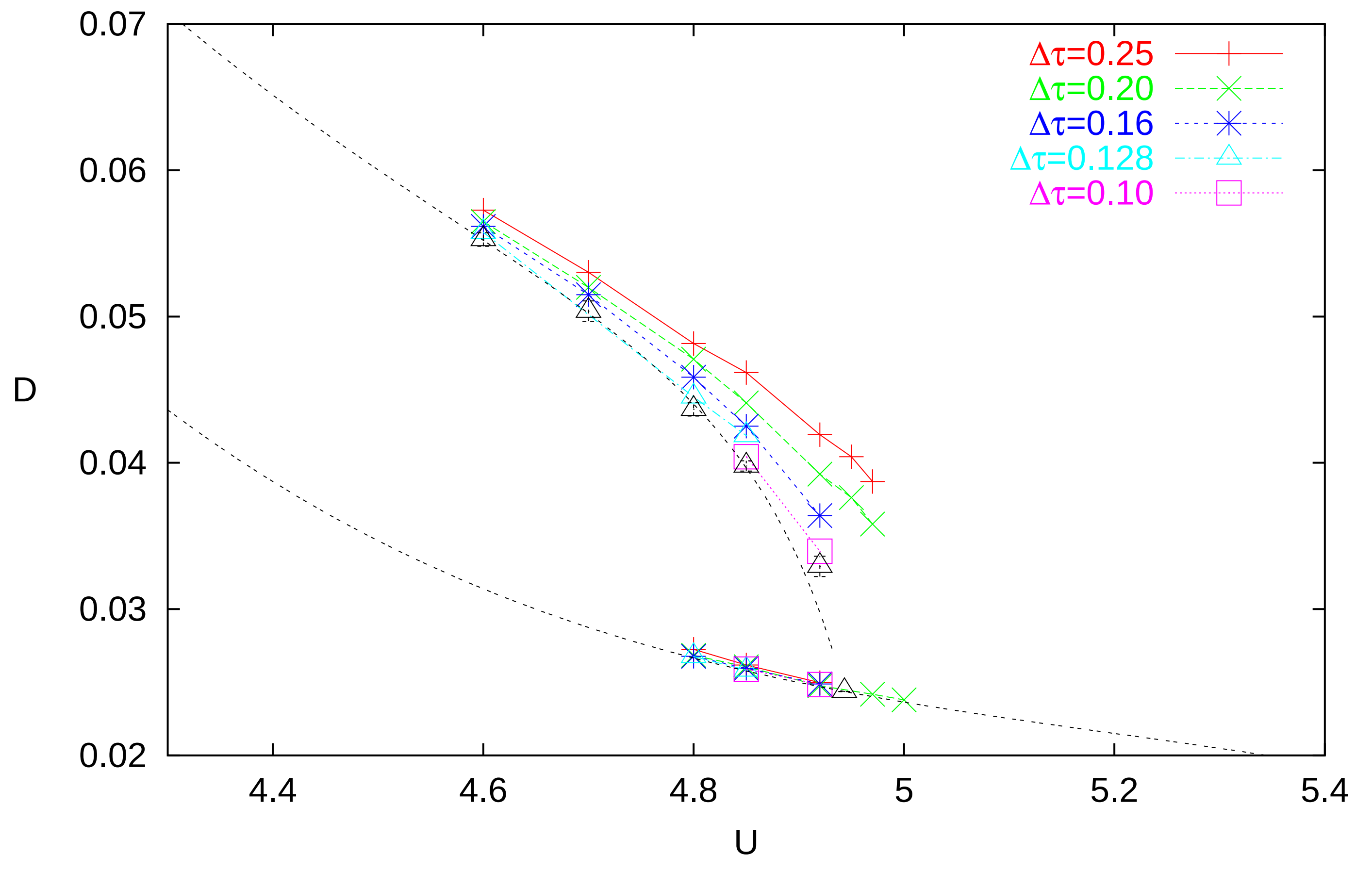
## $\beta = 10$: smooth crossover from metal to insulator

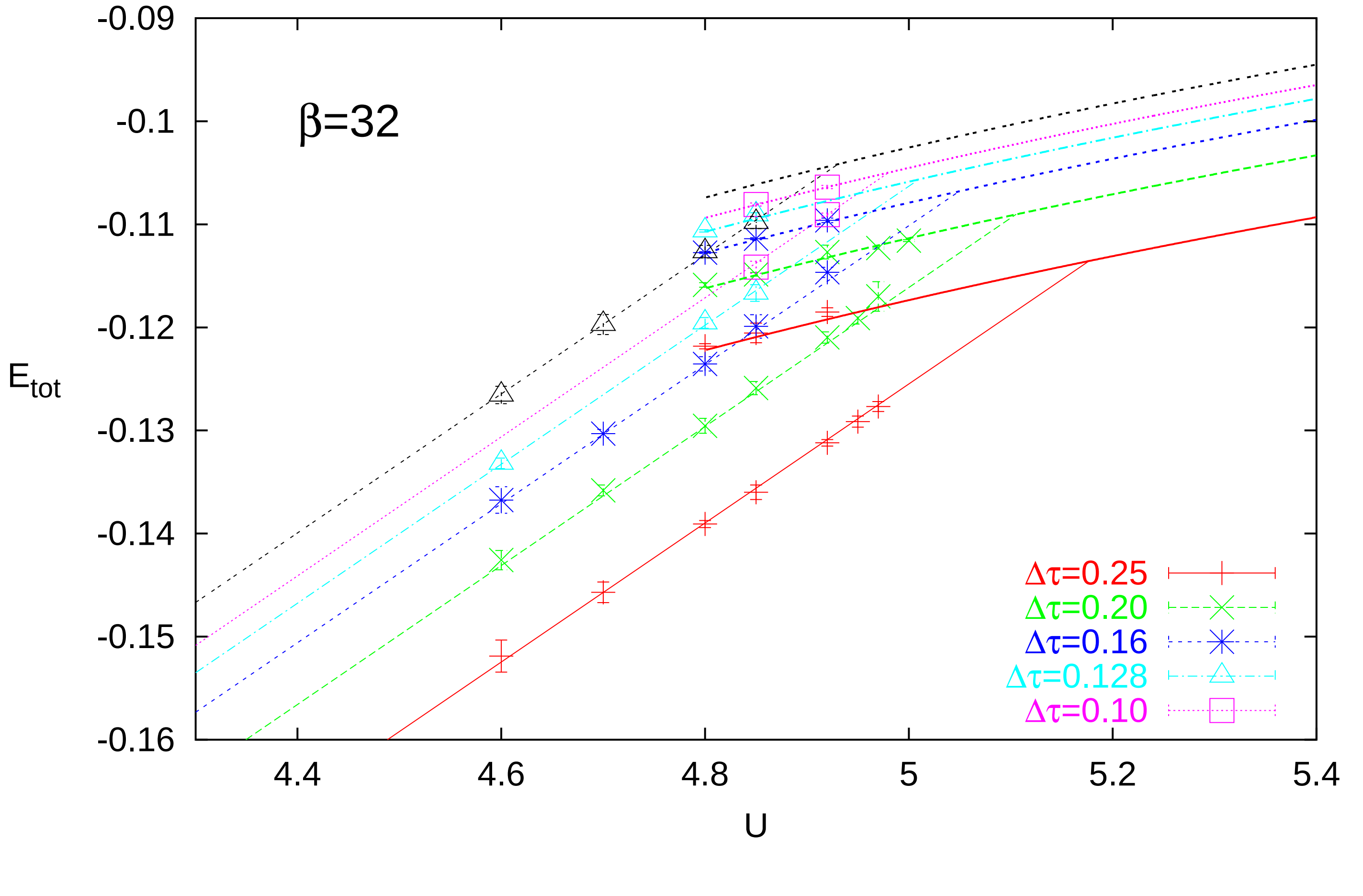


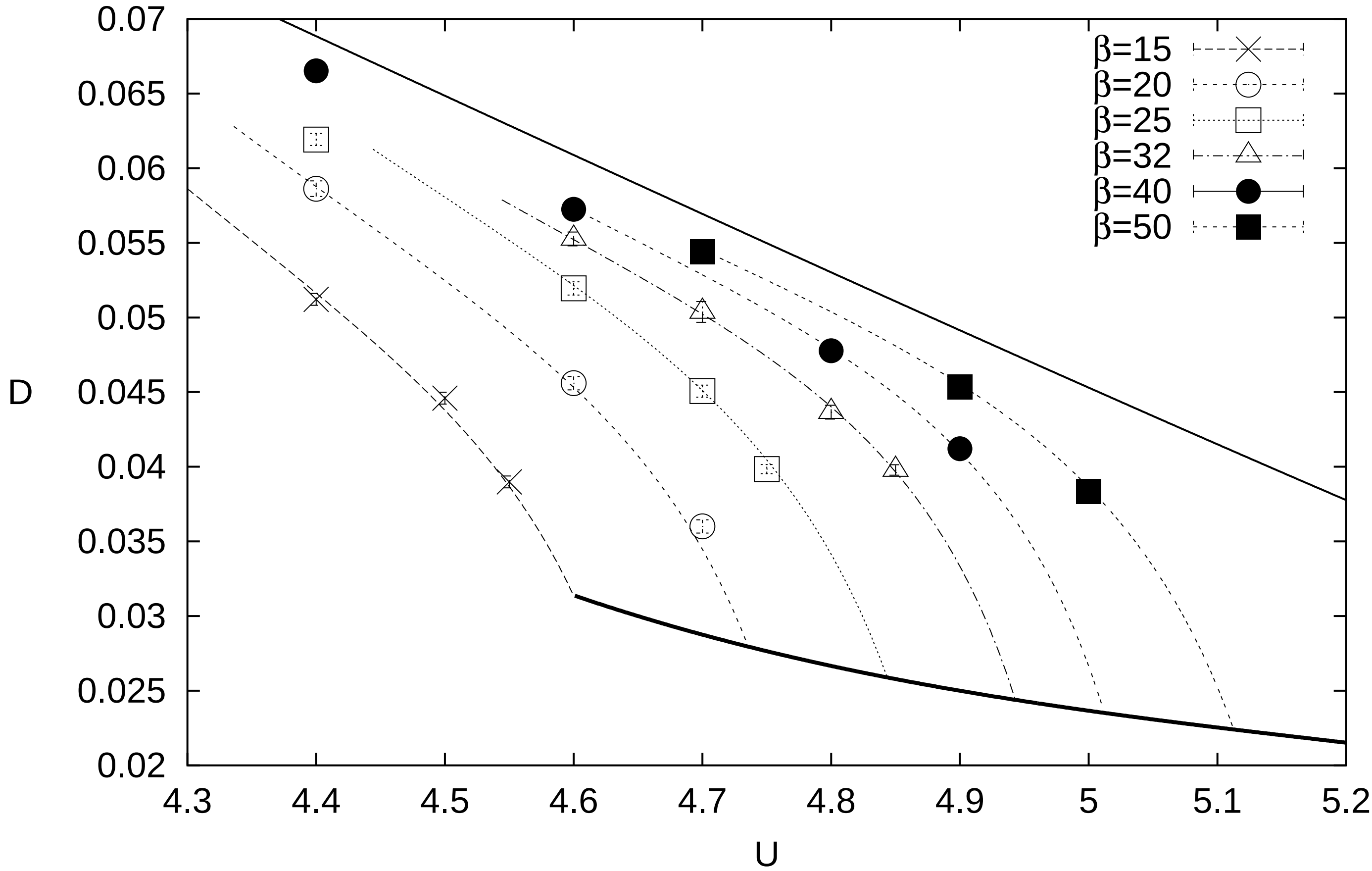

no significant $T$-dependence in insulator (same fitting curves)

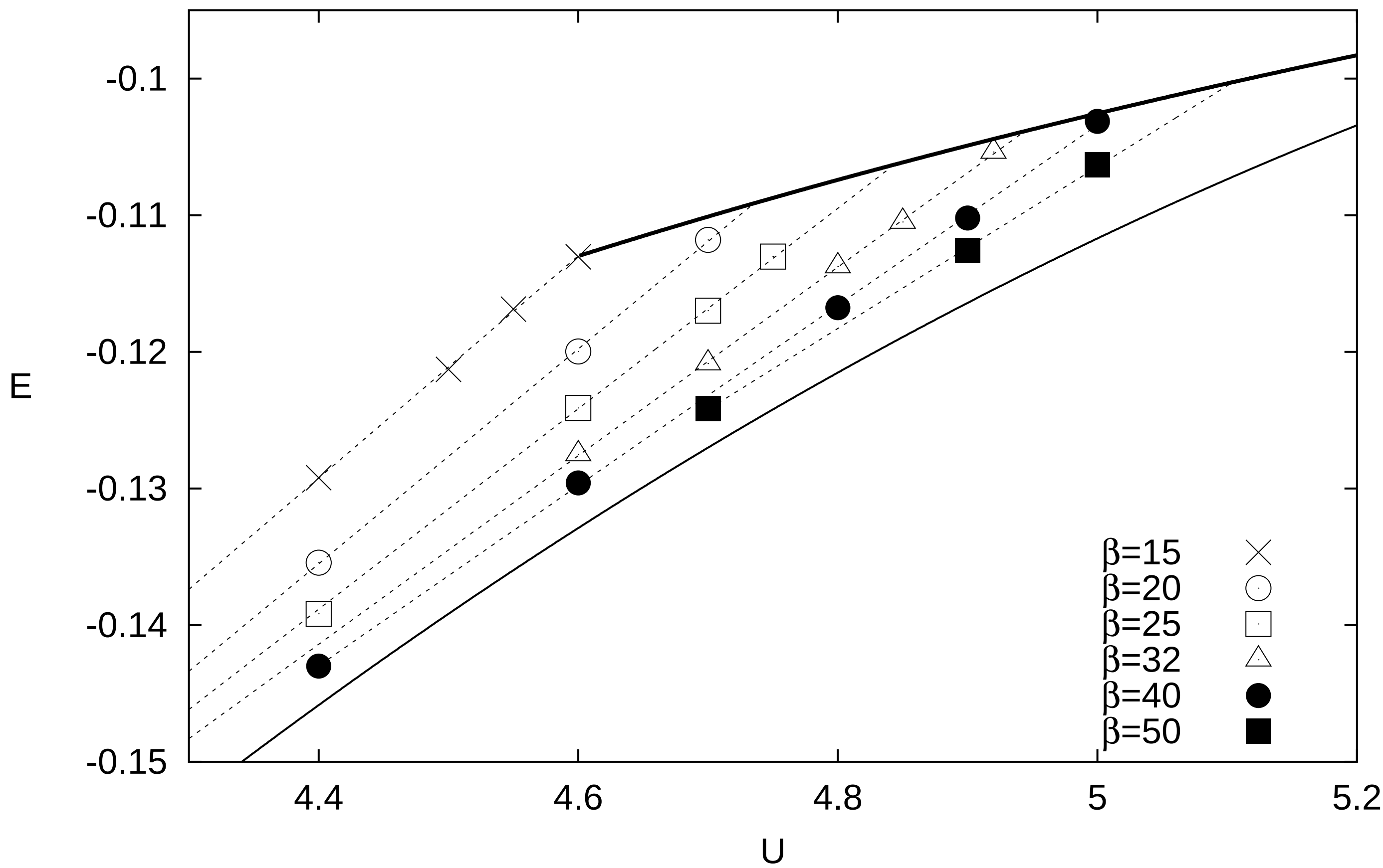
## $\beta = 32$: coexistence of metallic and insulating solutions



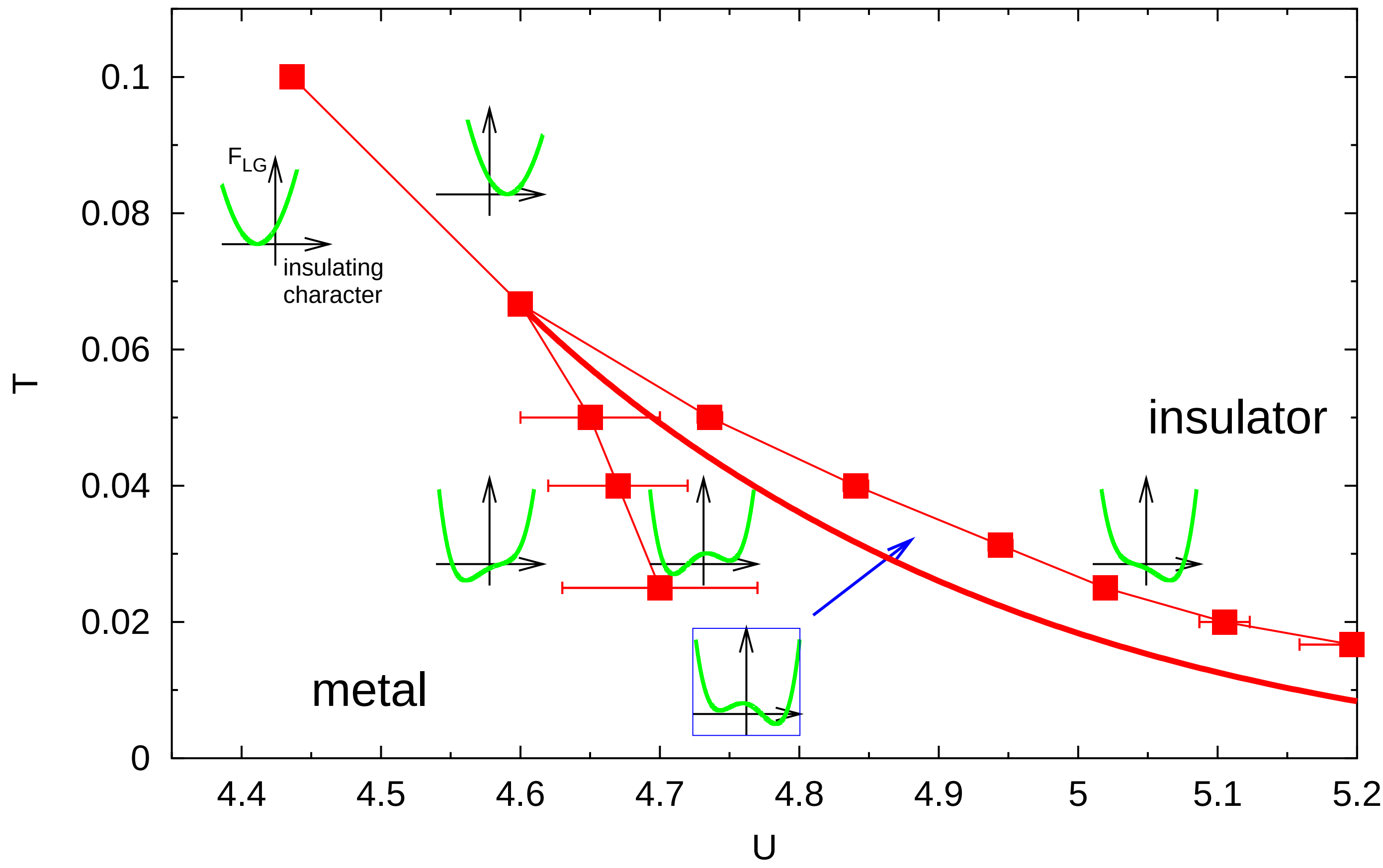
## $D$ and $E$ versus temperature (plus extrapolation $T \to 0$)




no (significant) $T$-dependence of $D$, $E$ in insulating phase

## Phase diagram: coexistence region




## Comparing free energies

$F(U,T)$ cannot be directly computed from QMC, NRG
but differential known:

$$d\left(\beta F_{m/i}(\beta,U)\right) = E_{m/i}(\beta,U)d\beta + \beta D_{m/i}(\beta,U)dU$$

Naive solution: $$F(\beta,U) = F(\beta_0,U_0) + \int_{\beta_0,U_0}^{\beta,U} d\left(\beta' F(\beta',U')\right)$$

Problem: $F_{m/i}(\beta_0,U_0)$ must be known

$1^{st}$ improvement: compute $\Delta F(\beta,U) := F_m(\beta,U) - F_i(\beta,U)$

$$\Delta F(\beta,U) = \int_{\beta_0,U_0}^{\beta,U} d\left(\beta' F_m(\beta',U')\right) - \int_{\beta_0,U_0}^{\beta,U} d\left(\beta' F_i(\beta',U')\right)$$

Problem: different paths of integration introduce different systematic errors for metal and insulator; stability region shifts with $\Delta\tau$

local criterion:

$$d(\beta\Delta F(\beta,U)) = \Delta E(\beta,U)d\beta + \beta\Delta D(\beta,U)dU$$

at (smooth) transition line:

$$\Delta F(\beta,U)|_{U=U_c(\beta)} = 0; \quad d(\beta\Delta F(\beta,U))|_{U=U_c(\beta)} = 0$$

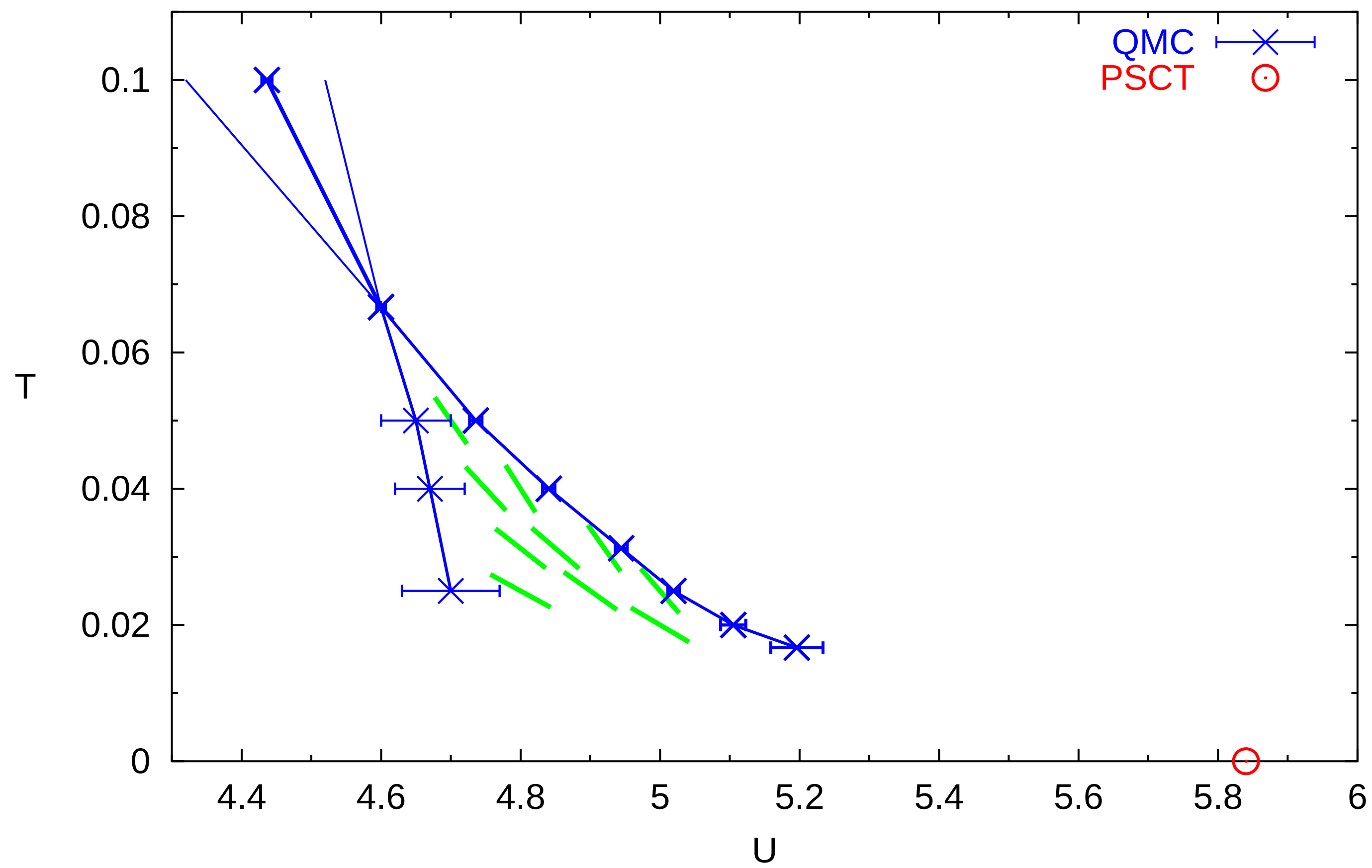
$\longrightarrow$ Clausius-Clapeyron equation:

$$\frac{dU_c(T)}{dT} = f(T,U_c(T))$$

$$f(T,U) := \left.\frac{\Delta E(T,U)}{T\Delta D(T,U)}\right|_{U=U_c(T)}$$

Since $U_c(T^*) = U^*$, we can integrate for the solution,

$$U_c(T) = U^* + \int_{T^*}^{T} dT' f(T', U_c(T')); \quad T < T^*.$$



note: $f(T,U)$ can be linearized in $U$

$$f(T,U) \approx \tilde{f}\,(T)(A+BU); \quad \text{fit parameters } A, B$$

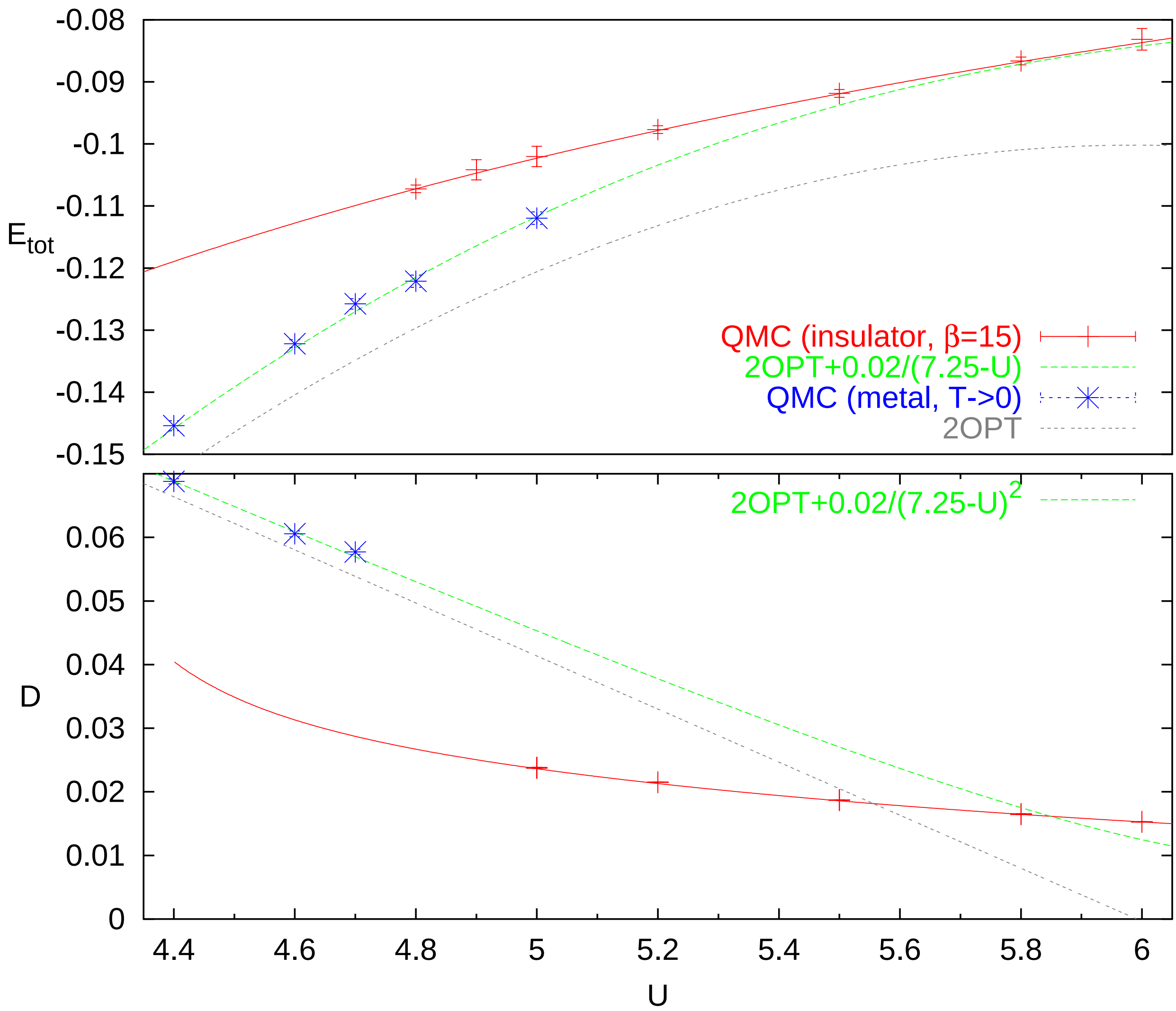
supplement QMC results with low-$T$ information:

Fermi liquid properties in metal, entropy of insulator $S_i(U,T) = S_0$

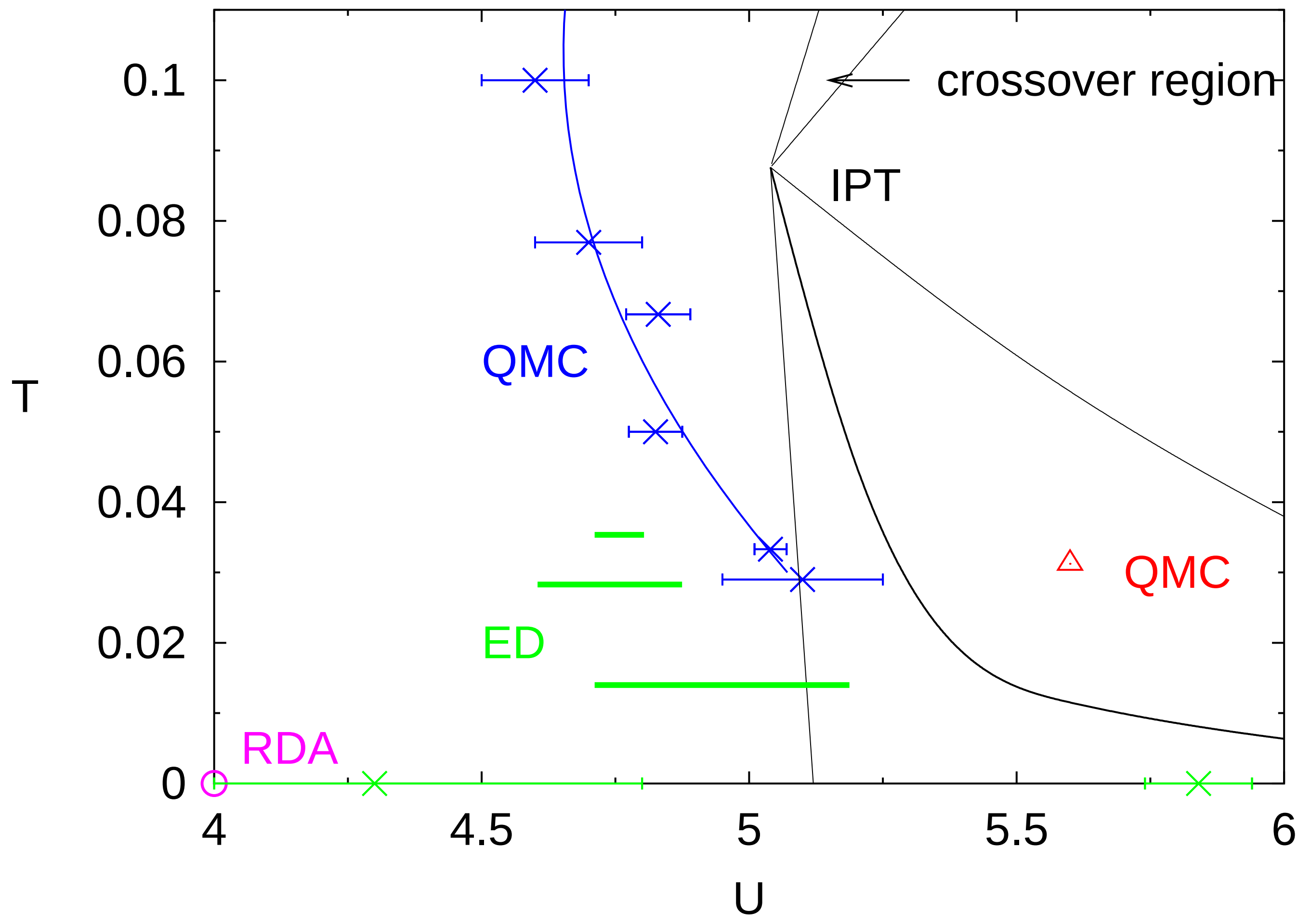
$$\longrightarrow U_c(T) = U_c^0 - \sqrt{\frac{2S_oT}{a}} + \mathcal{O}(T)$$

$$\tilde{f}(T) = CT^{-1/2} + D + ET^{1/2}; \quad C \approx -\sqrt{\frac{S_o}{2a}}$$

$T = 0$ parameter $a$ from second order PT + QMC

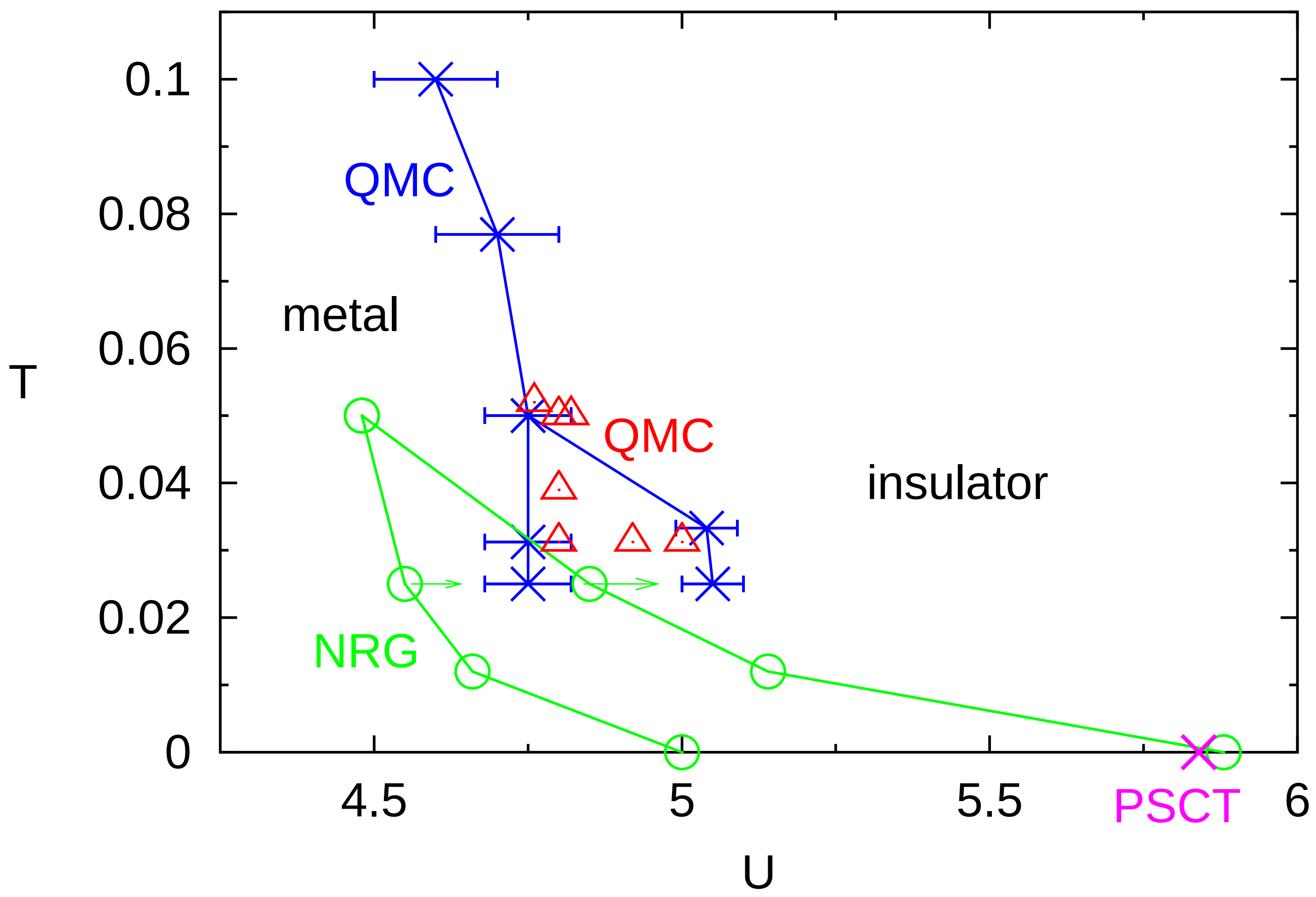


# Status of phase diagram in spring 1999



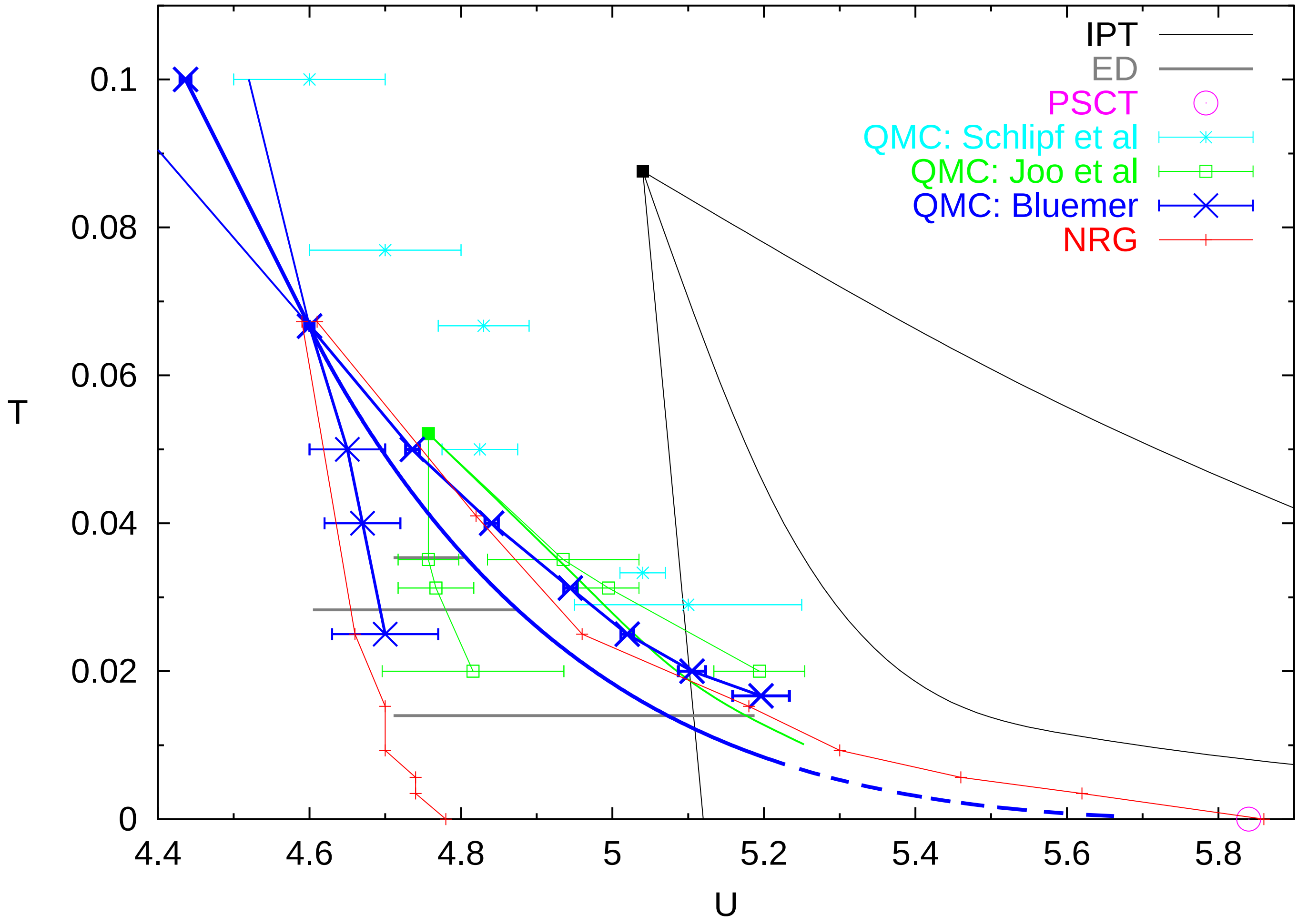

Georges et al. (1996)
Rozenberg, Kotliar, and Zhang (1994)
Noack and Gebhard (1999)
Georges et al (1996); Hofstetter
Schlipf et al (1999)

# Status of phase diagram in spring 2000




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

# Full phase diagram: Comparison




# Conclusions

- results from fundamentally different methods now converged towards a reliable phase diagram
- coexistence region at low T $\rightarrow$ first order transition
- first controlled computation of $U_c(T)$

Work supported by DFG through SFB484