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

N. Blümer

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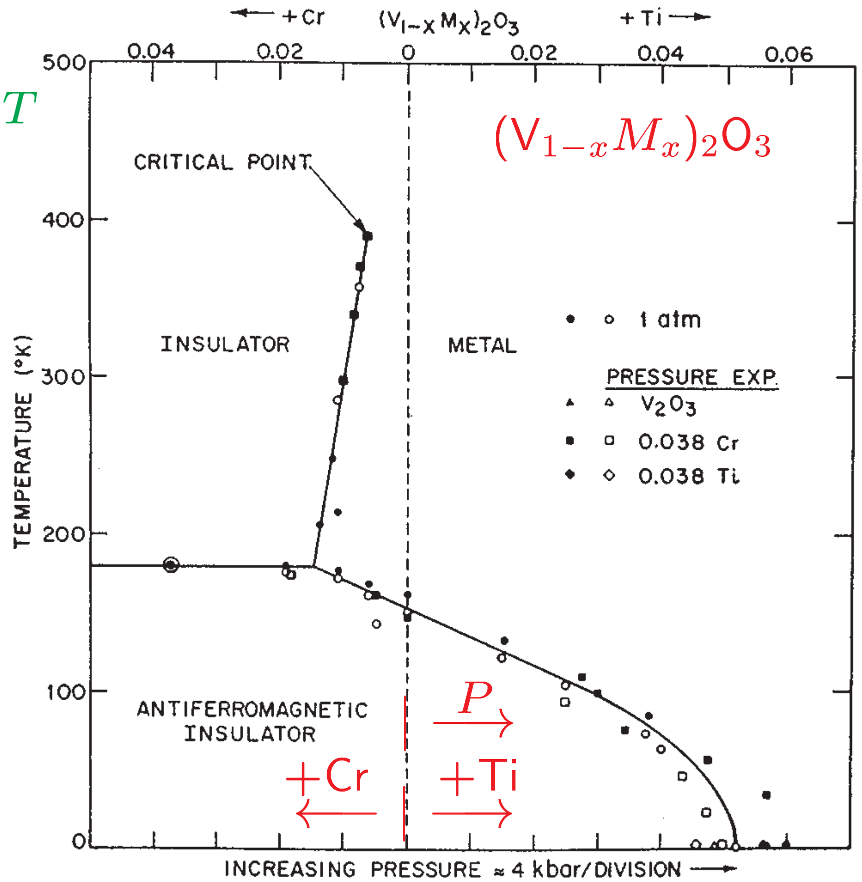
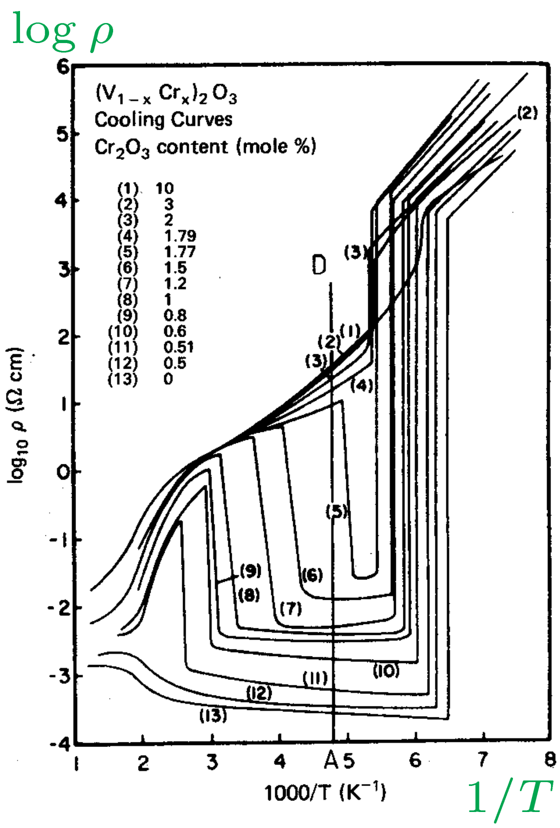
Introduction



McWhan et al, 1971

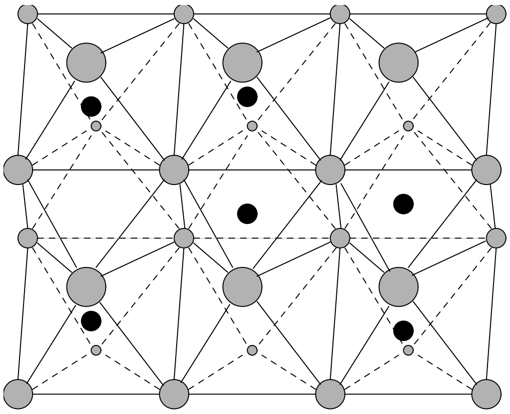
$\longleftarrow U/W$



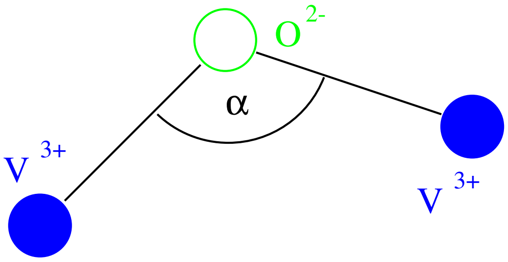
Kawamoto et al, 1980

Motivation: V_2O_3

- MIT without LRO
- drop in resistivity ρ 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 $\rightarrow$ changes overlap
  - drives MIT (like pressure)



Corundum structure

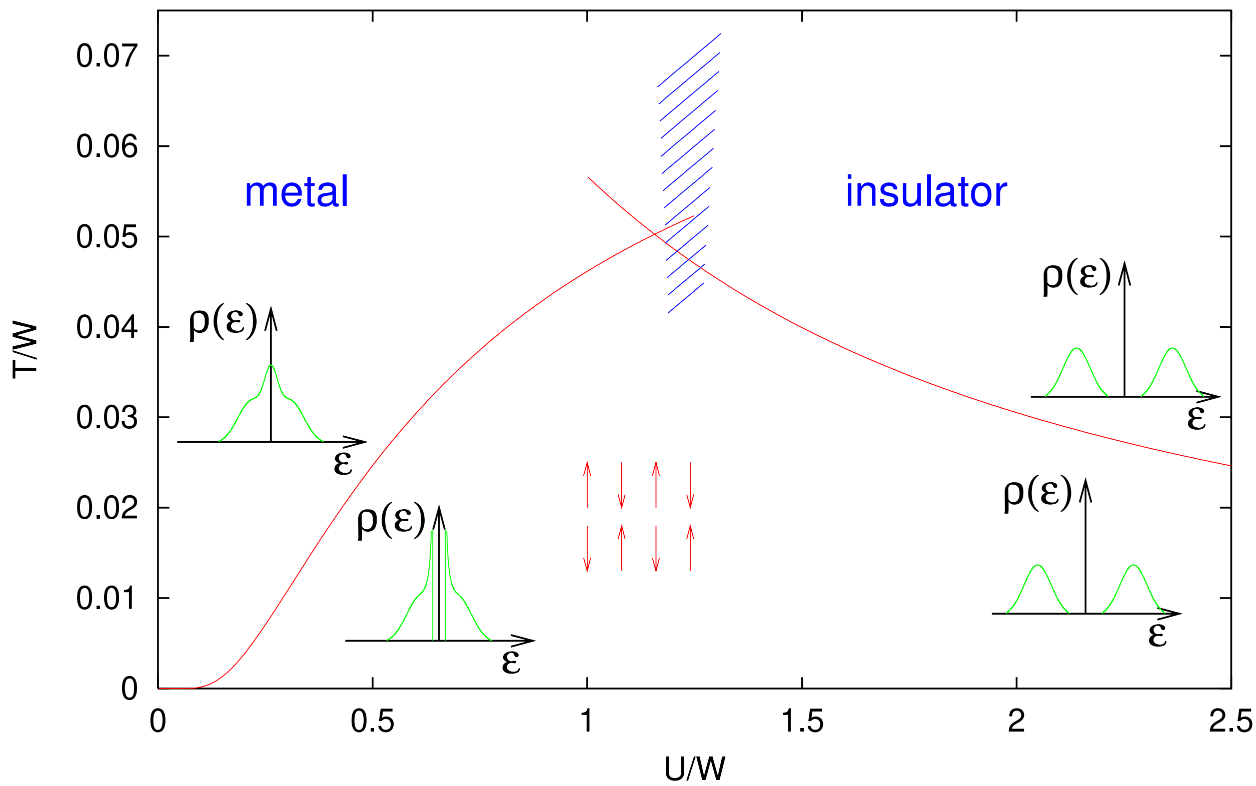


$\alpha_{\mathbf{Cr}} < \alpha_{\mathbf{V}} < \alpha_{\mathbf{Ti}}$

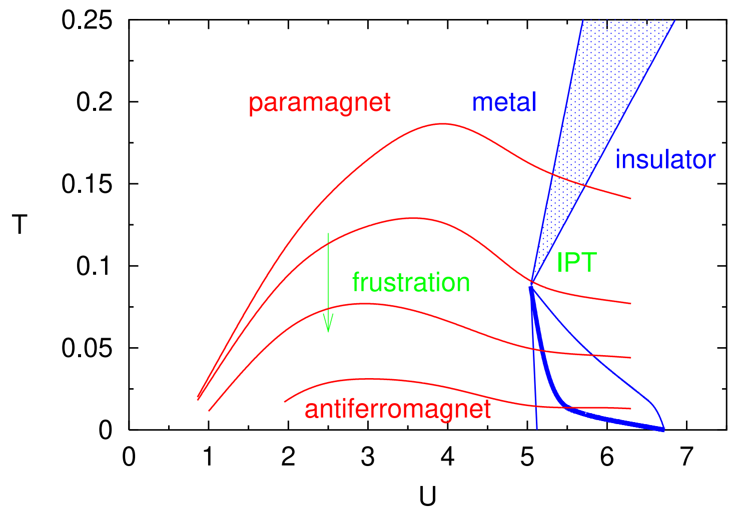
Paramagnetic, bandwidth-controlled metal-insulator transition in V_2O_3

half-filled one-band Hubbard model

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



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

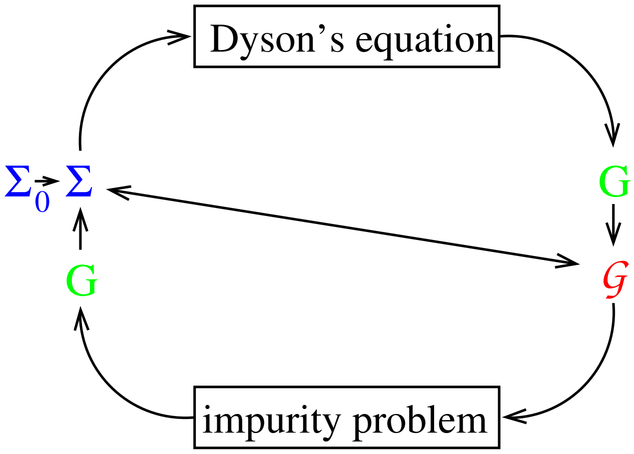


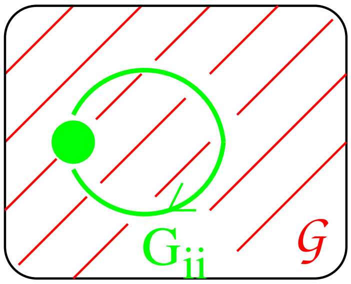
Aim: full phase diagram for

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

Self-consistent solution of DMFT equations

$$
\begin{aligned}
G_n &= \int d\epsilon \frac{\rho(\epsilon)}{i\omega_n - \epsilon - \Sigma_n} \\
G_n &= - < \Psi_n \Psi_n{}^* >_{\mathcal{G}_n} \\
\mathcal{G}_n^{-1} &= G_n^{-1} + \Sigma_n
\end{aligned}
$$





QMC solution of impurity problem:

- discretization $\Delta\tau$ of imaginary time
- Hubbard-Stratonovich trafo
- MC sampling over auxiliary Ising field

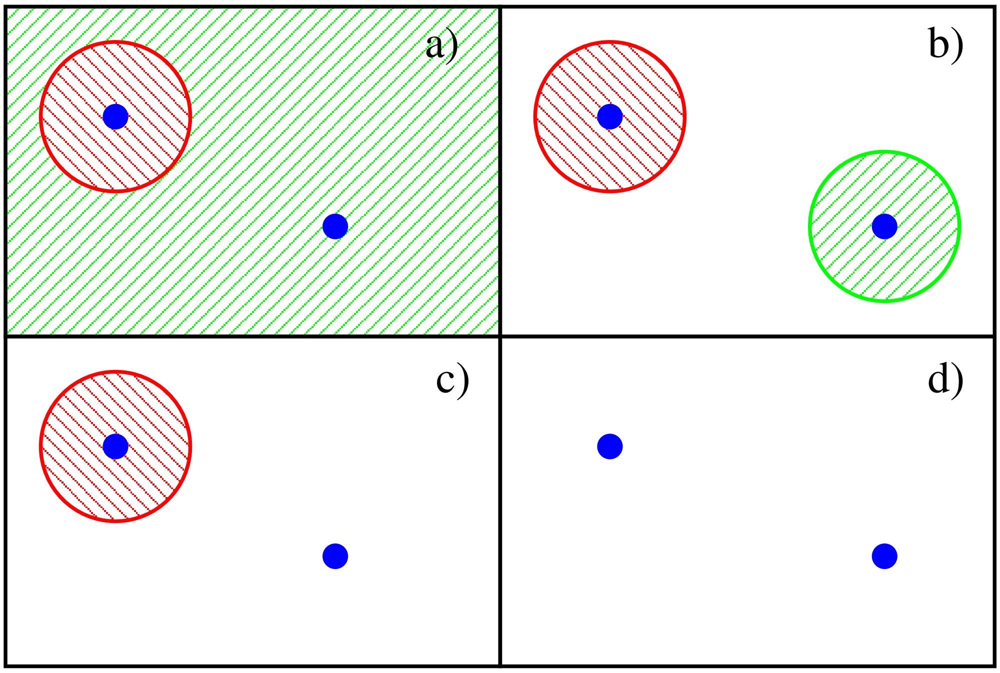
abstract view: solution of fixed point problem by iteration

iteration scheme not determined by lattice problem

instability of fixed point cannot be proven within iteration scheme

but: seems to work in practice!

scheme:
convergence in 2-fixpoint problem (2-dimensional example)



Results: crossover and coexistence regions

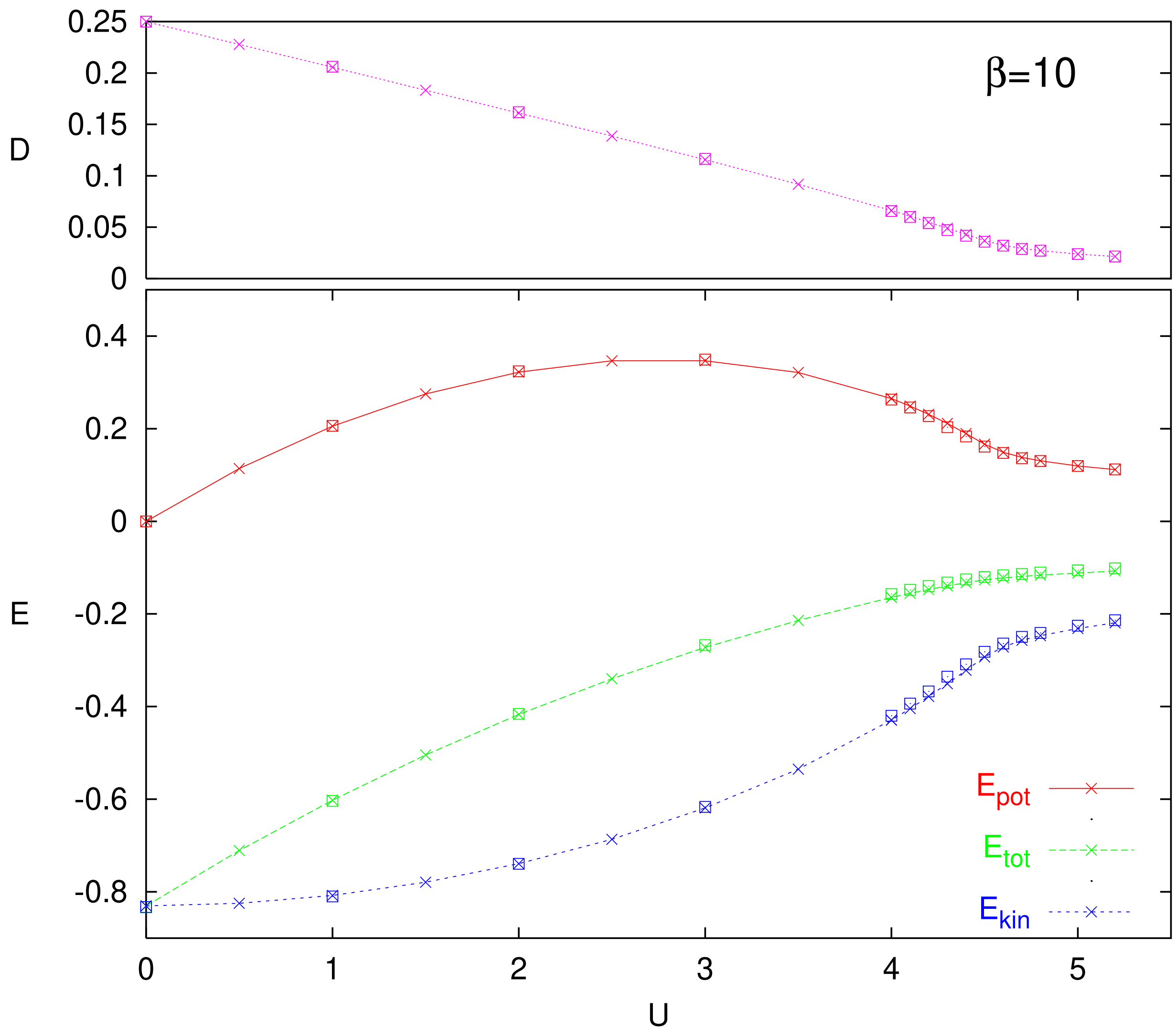
double occupancy D, total energy per lattice site $E = E_{kin} + UD$

$$D = \frac{1}{\beta}\int_0^\beta d\tau \ (1 + G(\tau))^2$$

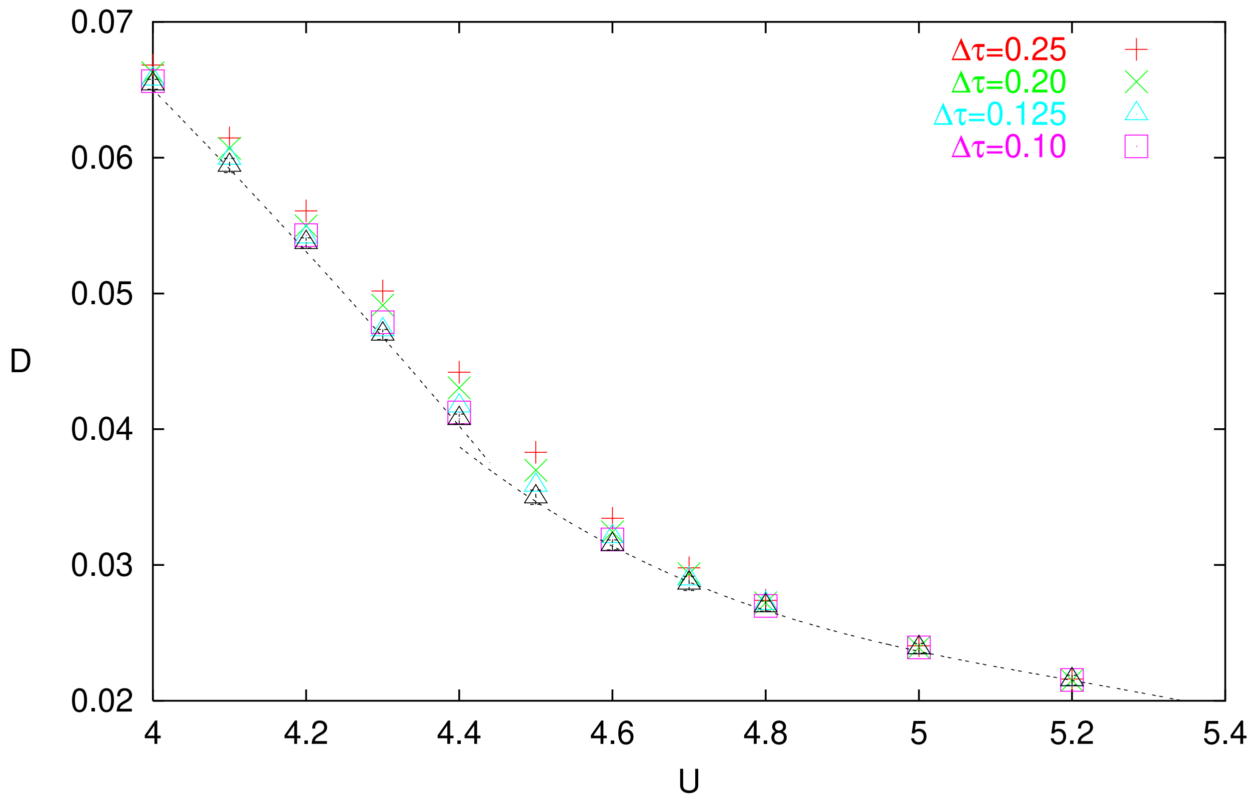
$$E_{kin} = \lim_{\eta\to 0^+} 2T \sum_{n=-\infty}^{\infty} \int_{-\infty}^{\infty} d\epsilon \, \frac{e^{i\omega_n\eta} \ \ \epsilon\rho(\epsilon)\cdot 1}{i\omega_n - \epsilon - \Sigma(i\omega_n)}$$

$$= 2\int_{-\infty}^{\infty} d\epsilon \frac{\epsilon\rho(\epsilon)}{e^{\beta\epsilon}+1}$$

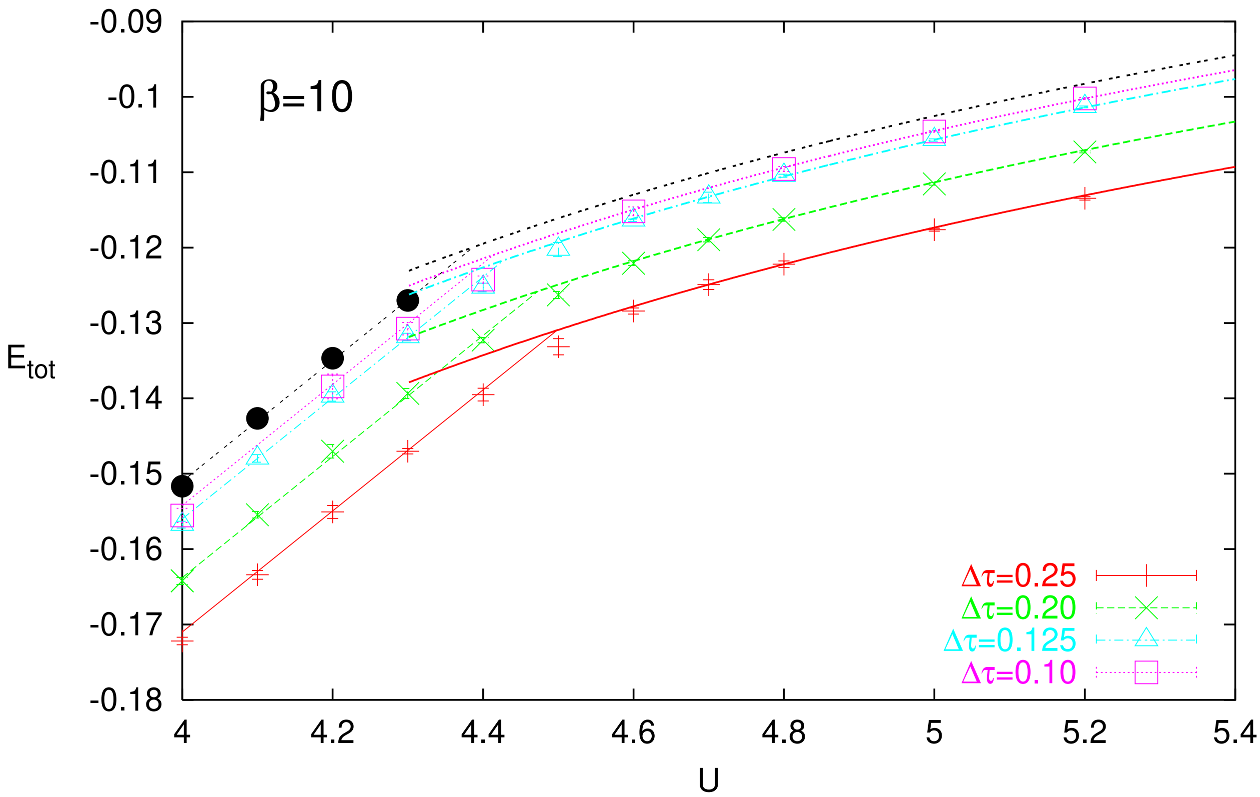
$$+2T \sum_{n=-L/2+1}^{L/2} \int_{-\infty}^{\infty} d\epsilon \ \epsilon\rho(\epsilon) \left(G_\epsilon(i\omega_n) - G^0_\epsilon(i\omega_n) \right)$$



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

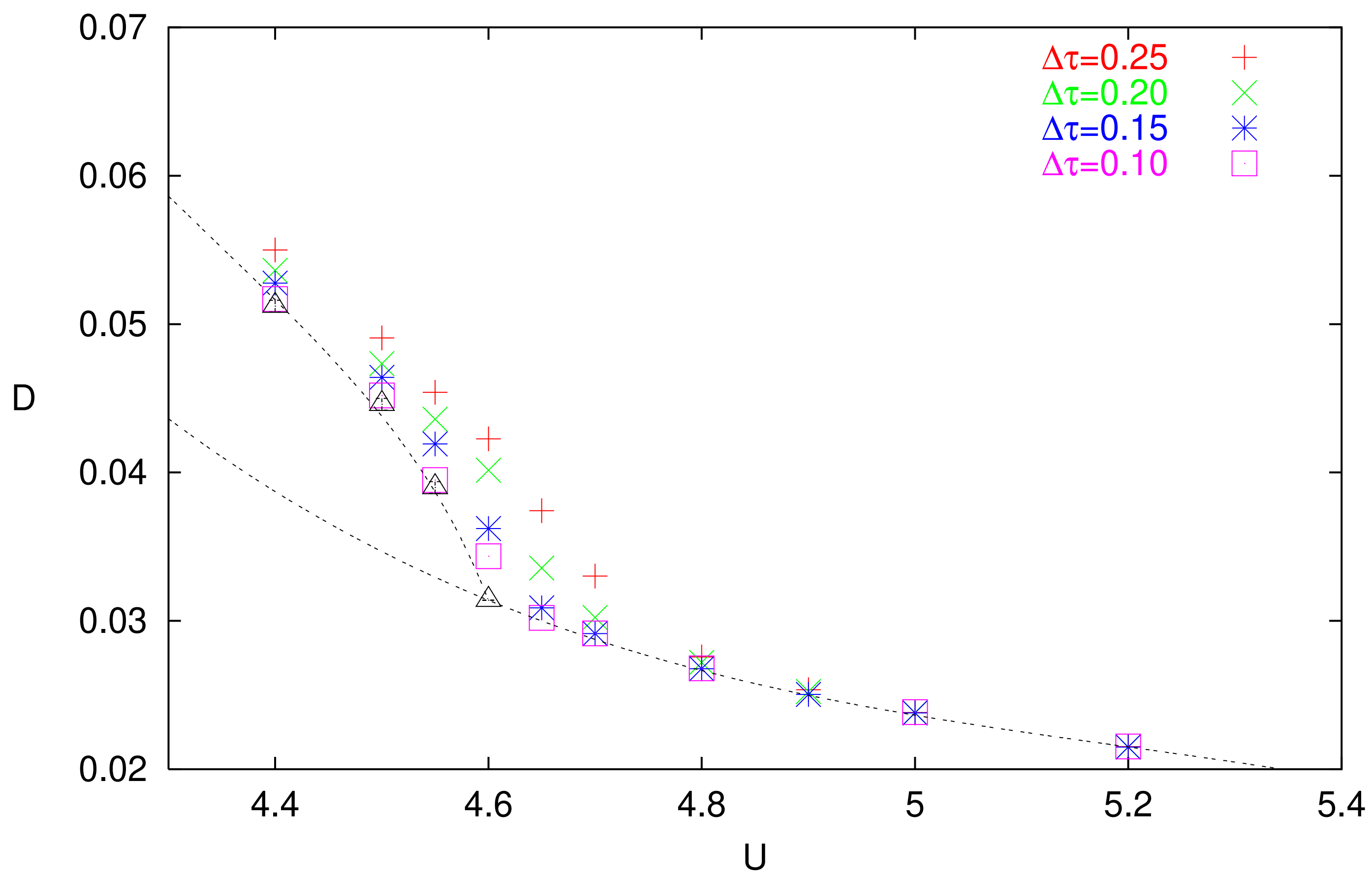


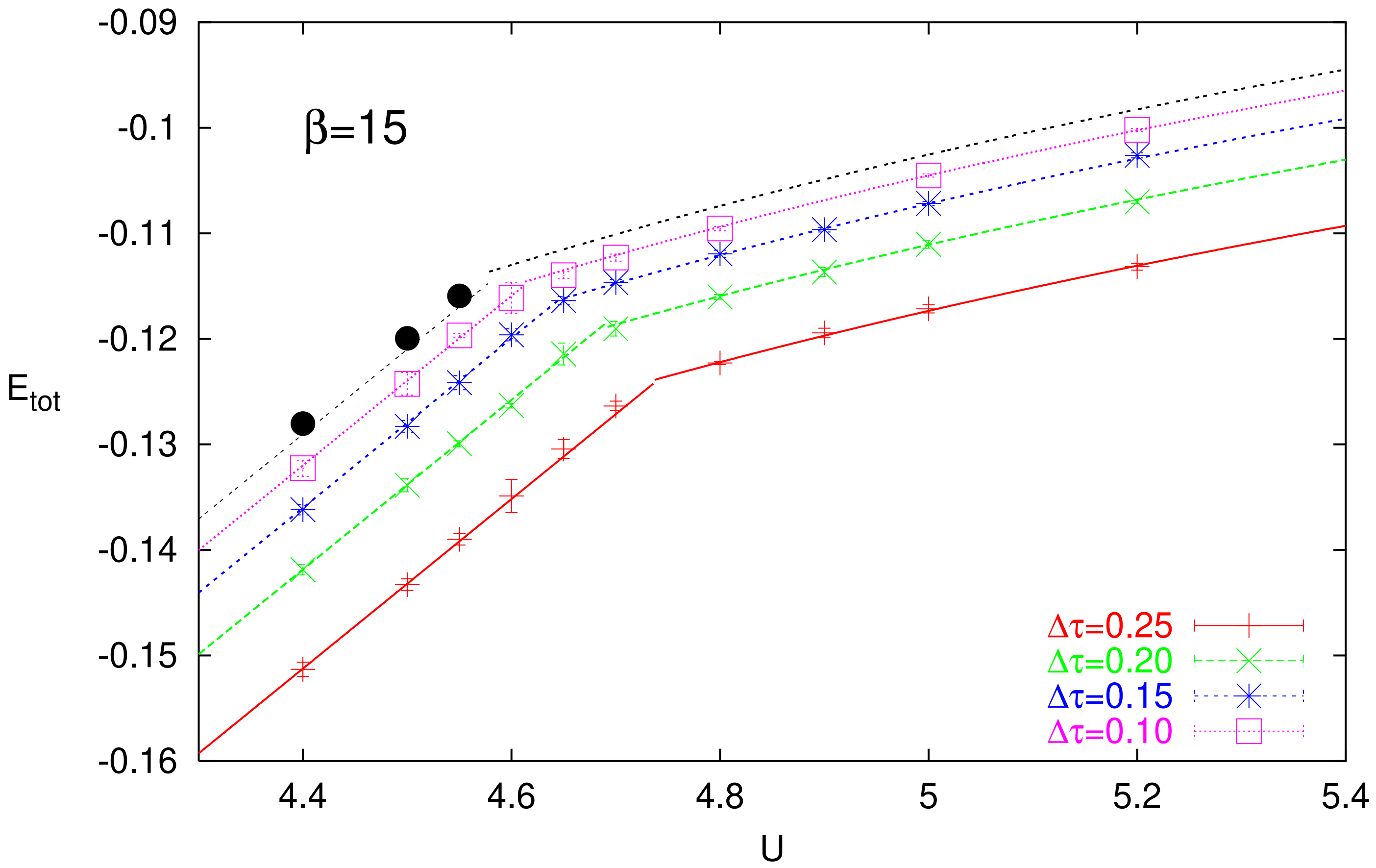
$\Delta\tau$ dependence: large at MIT, small below, vanishing above relatively strong curvature



$\Delta\tau$ dependence: very regular

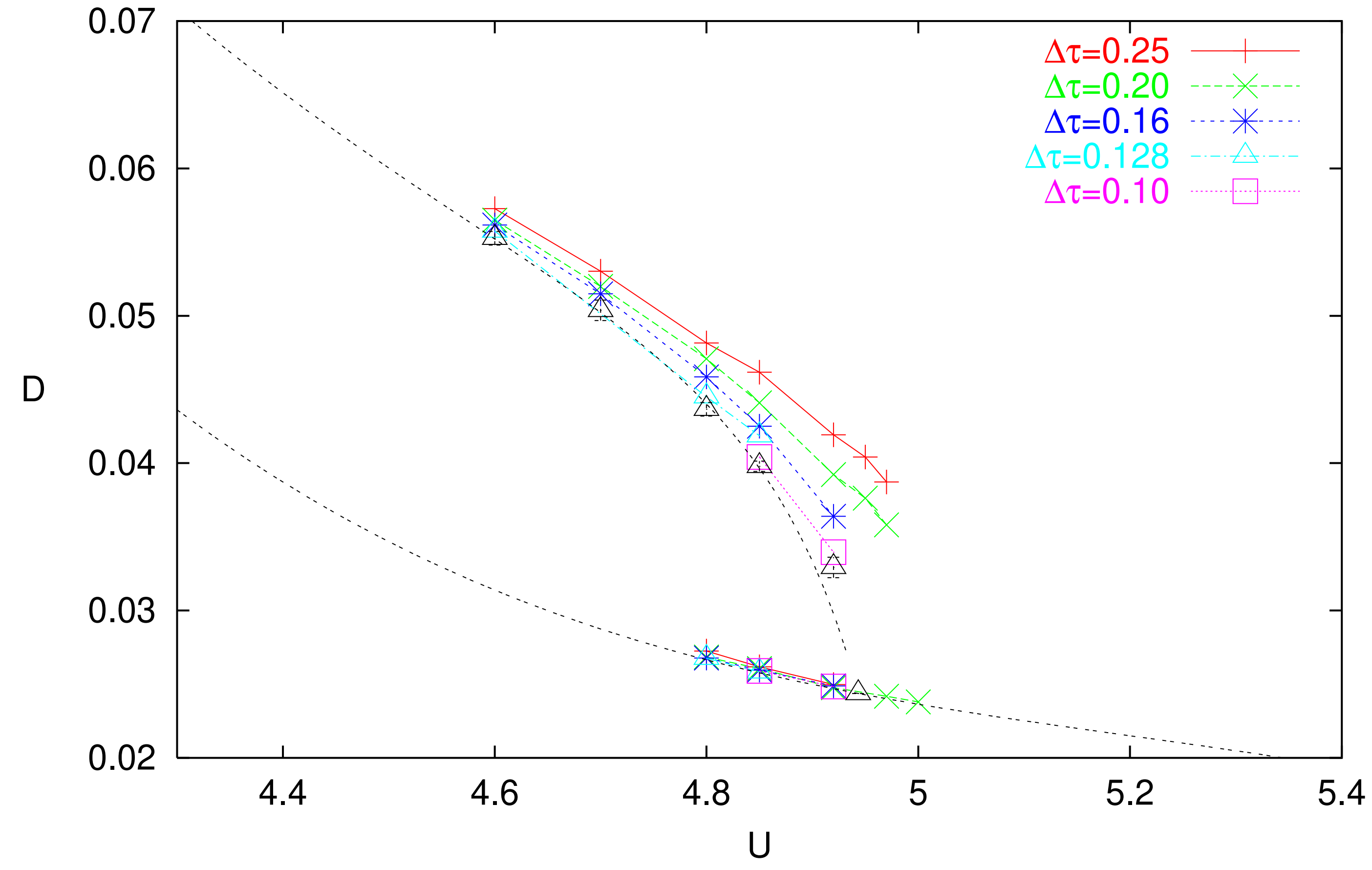
$\beta = 15$: sharp transition from metal to insulator, no hysteresis

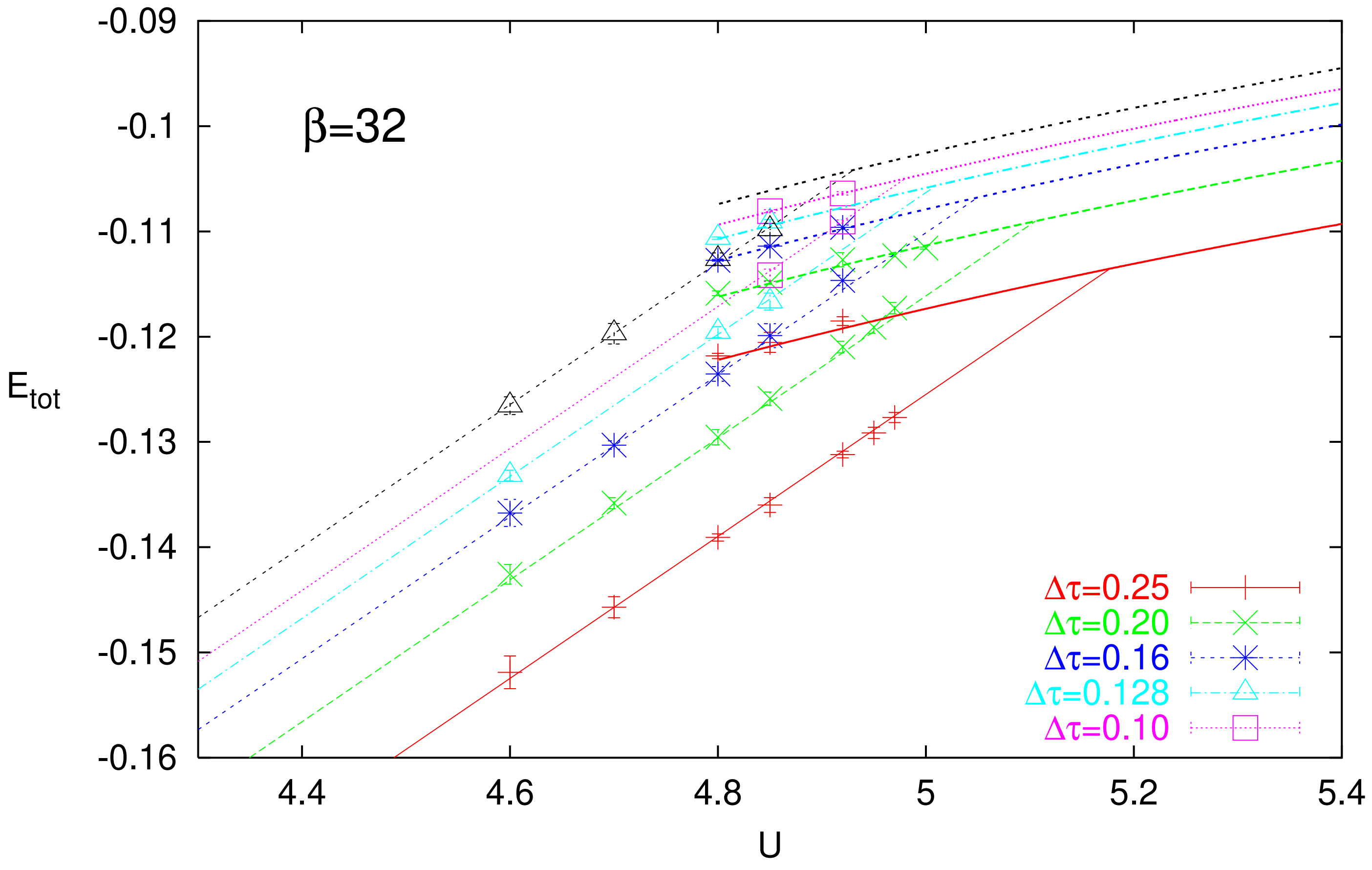




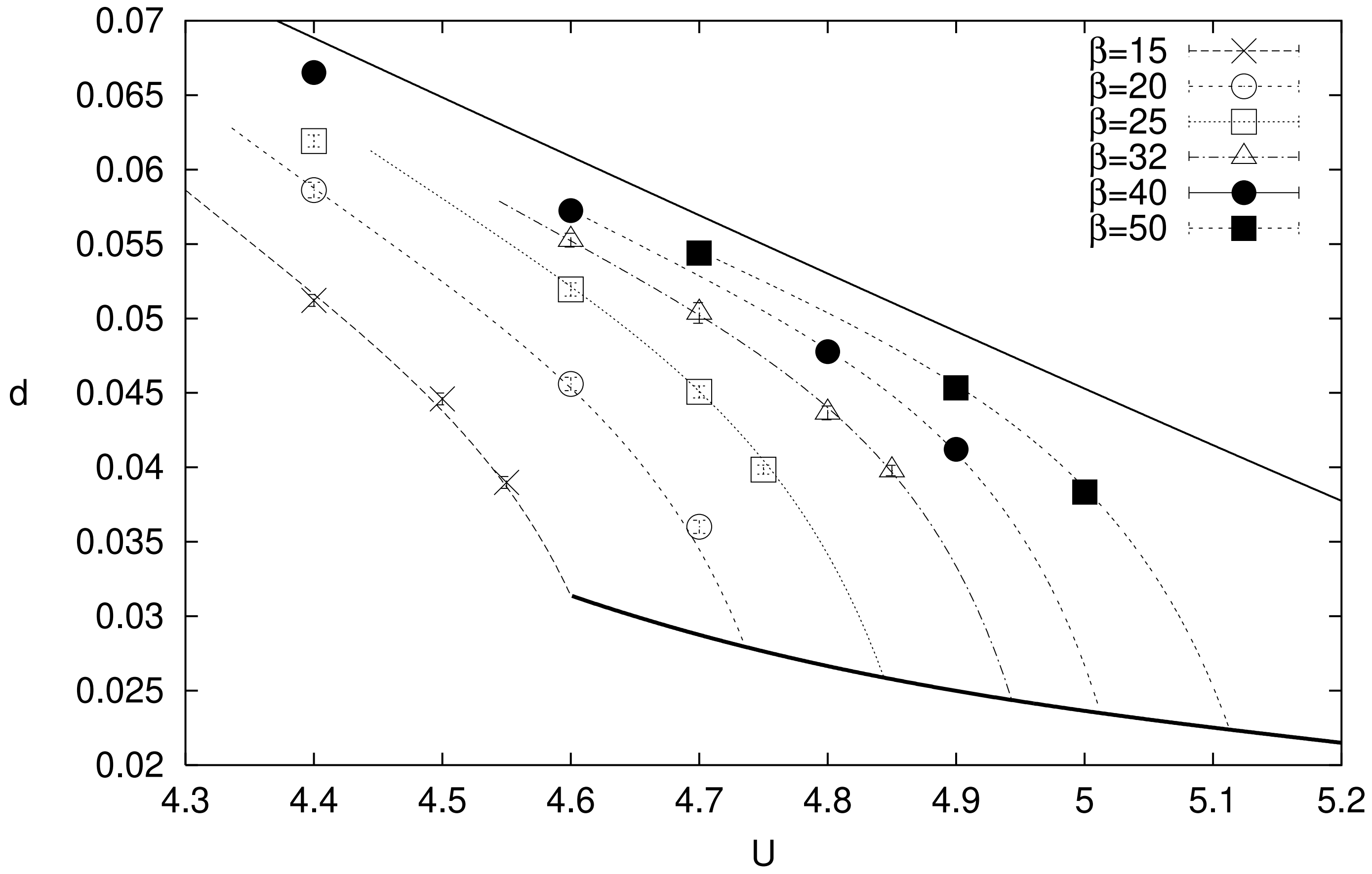
U_c substantially shifts for $\Delta\tau \to 0$

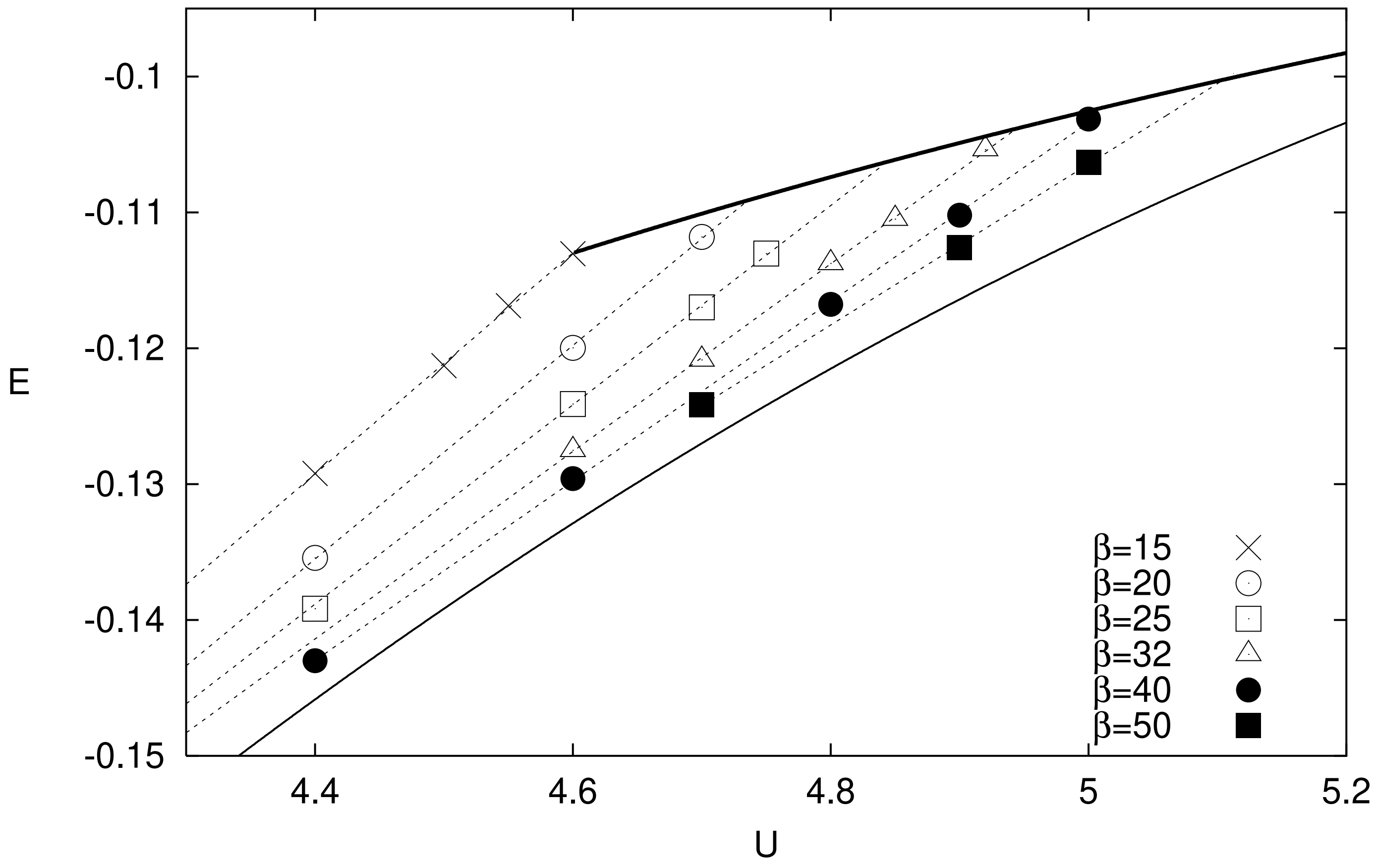
$\beta = 32$: coexistence of metallic and insulating solutions





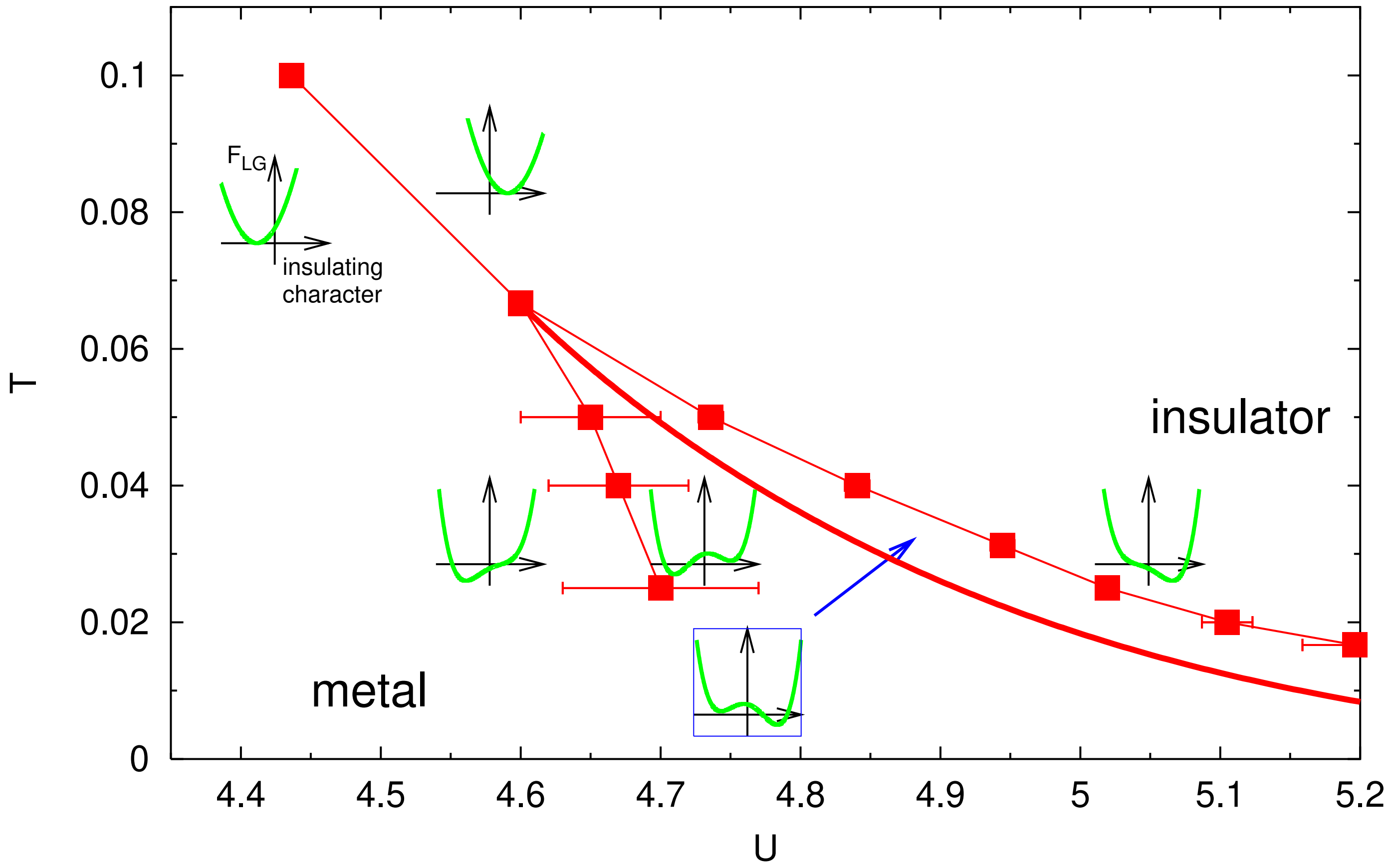
D and E versus temperature (plus extrapolation $T \to 0$)





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:

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

Naive solution: $F(\beta,U) = F(\beta_0,U_0) + \int_{\beta_0,U_0}^{\beta,U} d(\beta' F_{m/i}(\beta',U'))$

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

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

$$\Delta F(\beta,U) = \int_{\beta_0,U_0}^{\beta,U} d(\beta' F_{m/i}(\beta',U'))$$

Problem: different paths of integration introduce different systematic errors for metal and insulator local criterion:

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

at (smooth) transition line:

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

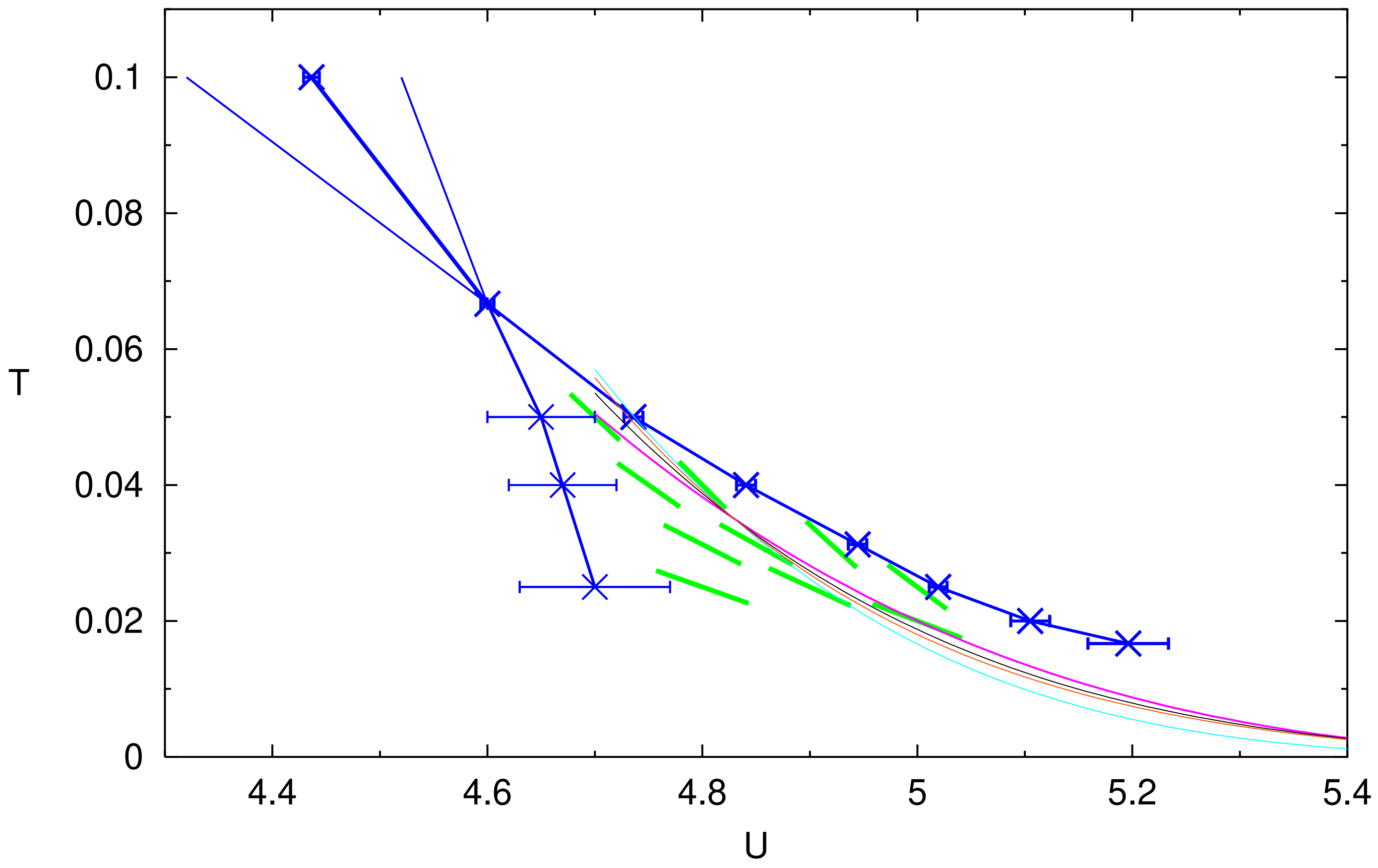
$\longrightarrow$ Clausius-Clapeyron equation:

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

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

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

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

supplement QMC results with low-T information:

entropy of insulator (almost) independent of U

$$E_i(U,T) = E_i^0(U); \quad S_i(U,T) = S_0\ . \tag{1}$$

Fermi liquid properties in metal

$$E_m(U,T) = E_m^0(U) + \frac{1}{2}\gamma(U)T^2; \quad S_i(U,T) = \gamma(U)T \tag{2}$$

zero-temperature information $(U_c^0 := U_c(T=0) = U_{c2}(T=0))$

$$E_i^0(U) - E_m^0(U) = \frac{a}{2}(U-U_c^0)^2; \quad \gamma(U) = \frac{\gamma_0}{U_c^0 - U}. \tag{3}$$

Equate free energies,

$$0 = \Delta F(U_c,T) = \frac{a}{2}(U-U_c^0)^2 + \frac{1}{2}\gamma(U)T^2 - TS_0, \tag{4}$$

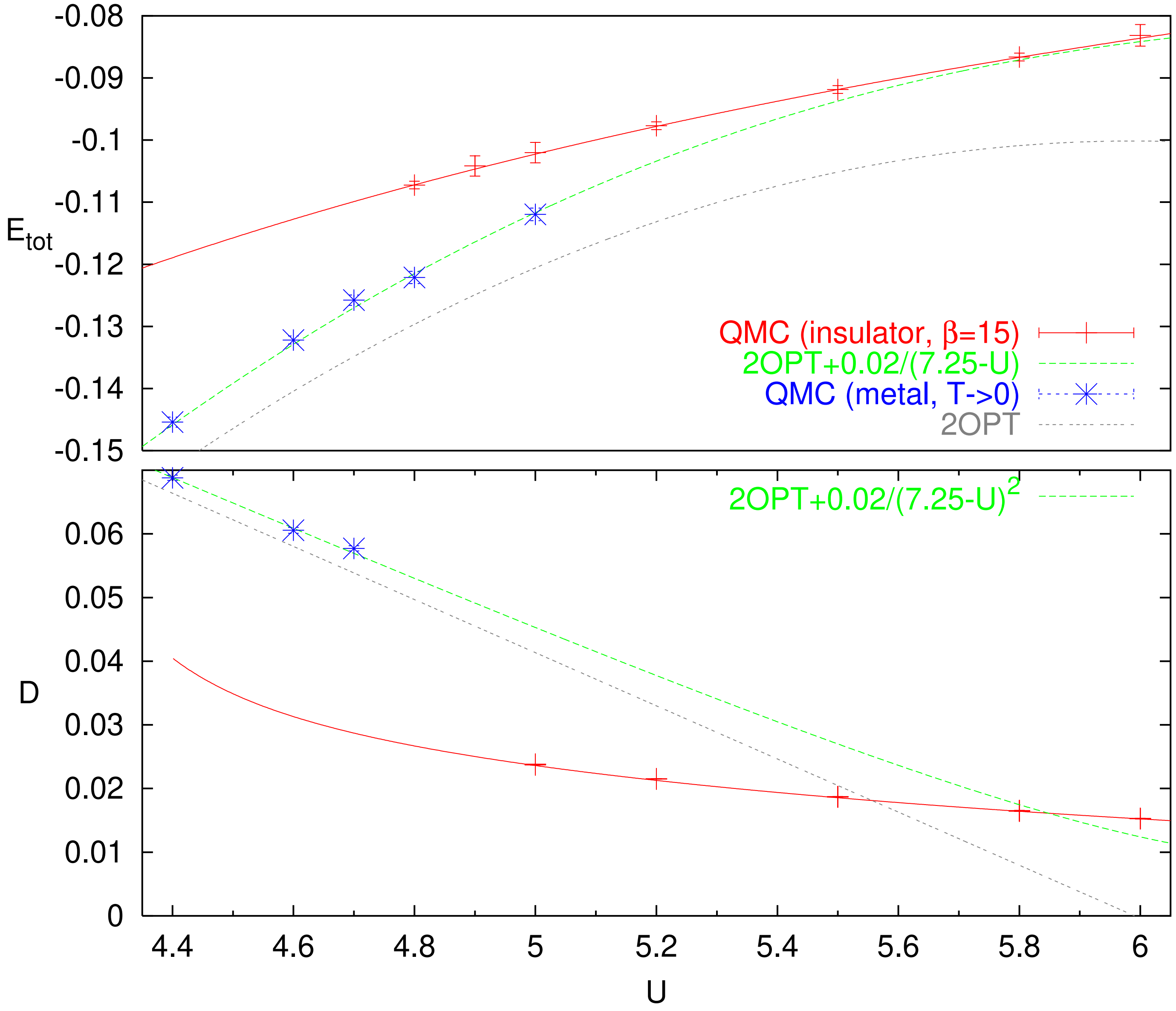
to obtain the low-temperature solution,

$$U_c(T) = U_c^0 - \sqrt{\frac{2S_oT}{a}} + \mathcal{O}(T) \tag{5}$$

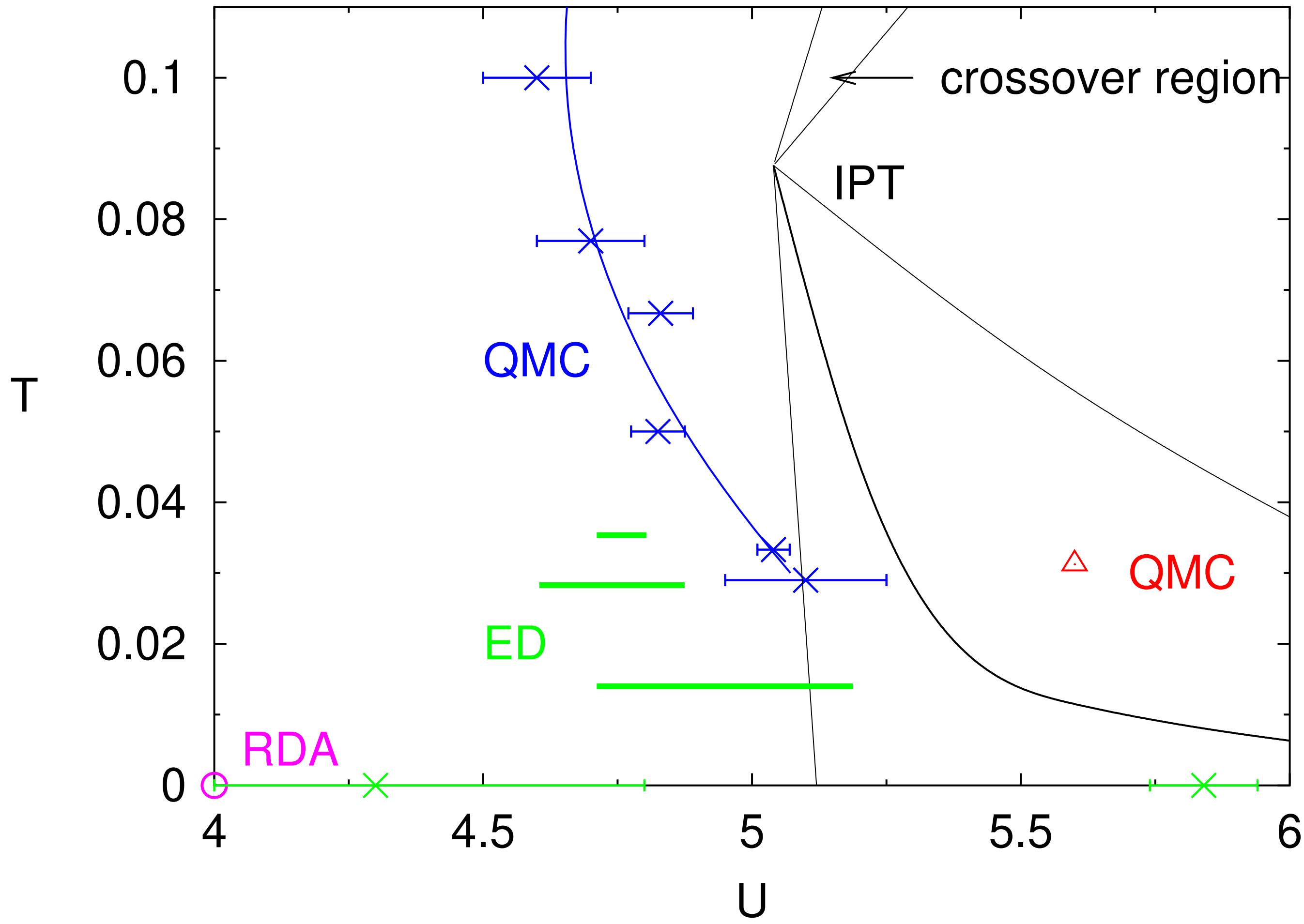
$\longrightarrow$ fitting Ansatz

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

determination of $T = 0$ parameters from second order PT + QMC

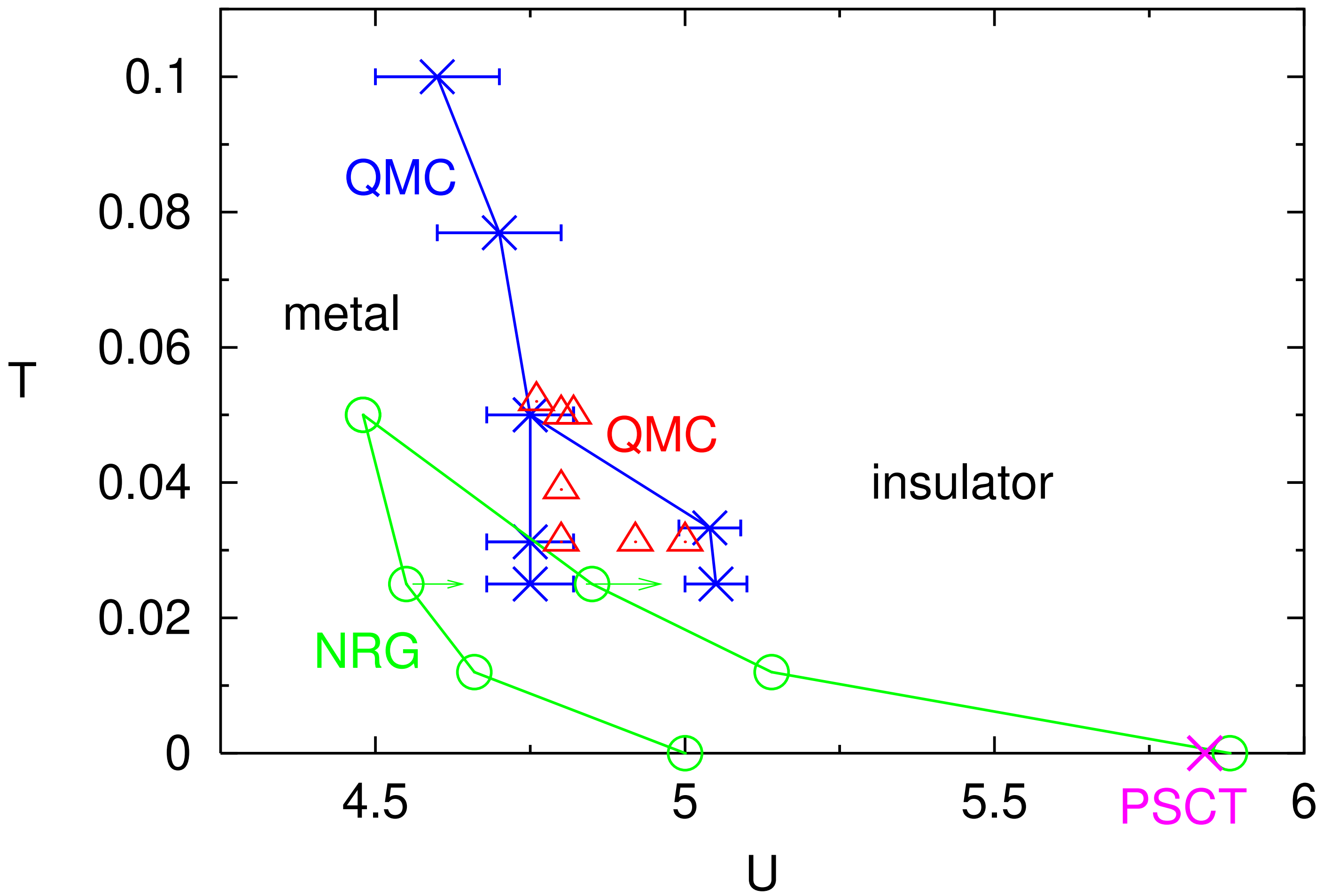


Status of phase diagram in spring 1999



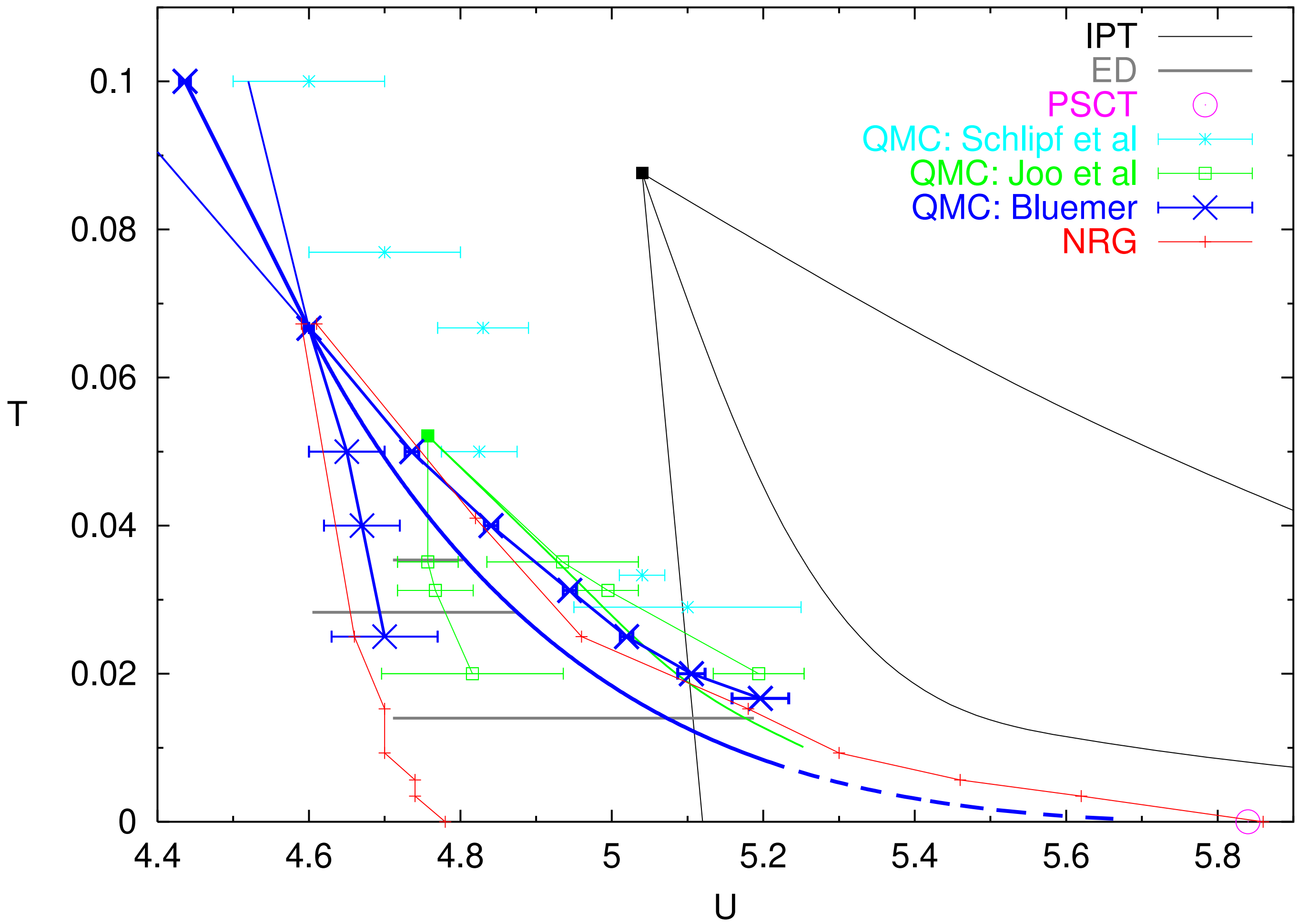
Georges et al. (1996)
Rozenberg, Kotliar, and Zhang (1994)
Noack and Gebhard (1999)
Georges et al (1996); Hofstetter
Schlipf et al (1999)

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