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

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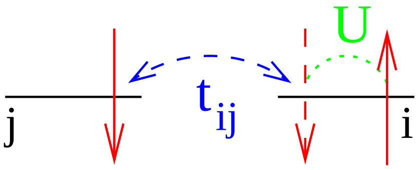
Introduction

1-band Hubbard model, half filling ($n = 1$)



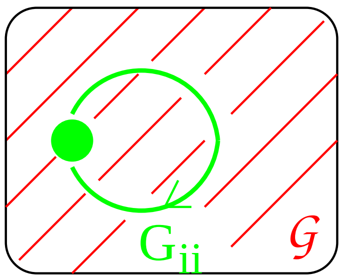
$$\hat{H} = \sum_{\langle ij\rangle\sigma} t_{ij} \left(\hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} + \hat{c}^\dagger_{j\sigma} \hat{c}_{i\sigma} \right) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

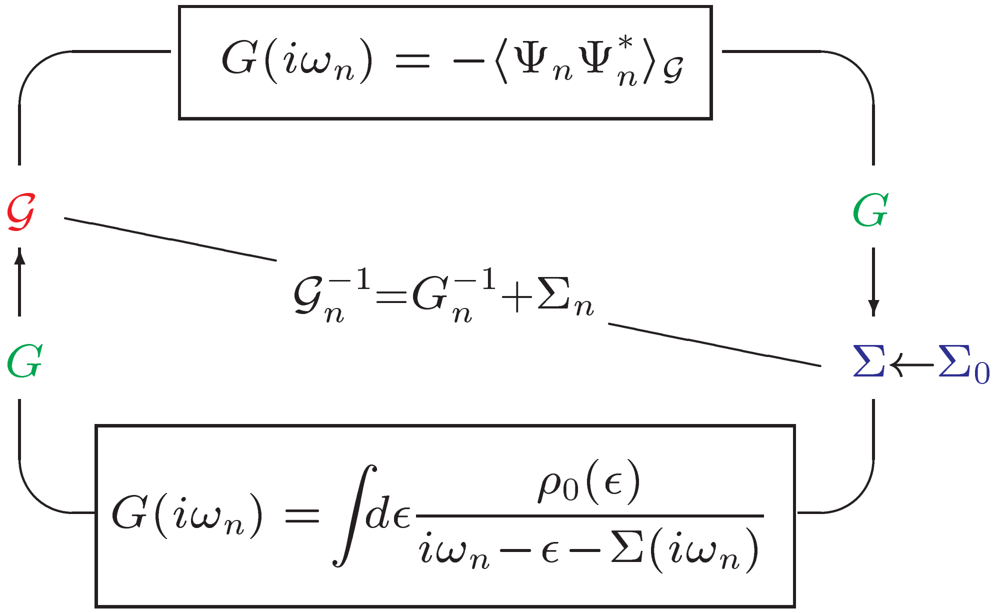
generically:
- metal-insulator transition (MIT) at $U \gtrsim W$
- antiferromagnetism at low T (depending on frustration)

here:
- full frustration $\longrightarrow$ only paramagnetic phase (all T)
- Dynamical Mean-field Theory (DMFT), semielliptic DOS

potential experimental relevance only for $T > T_{\text{order}}$
paramagnetic, bandwidth-controlled 1^{st} order MIT in doped V_2O_3

DMFT: mapping onto impurity model + self consistency condition; exact for $Z \rightarrow \infty$

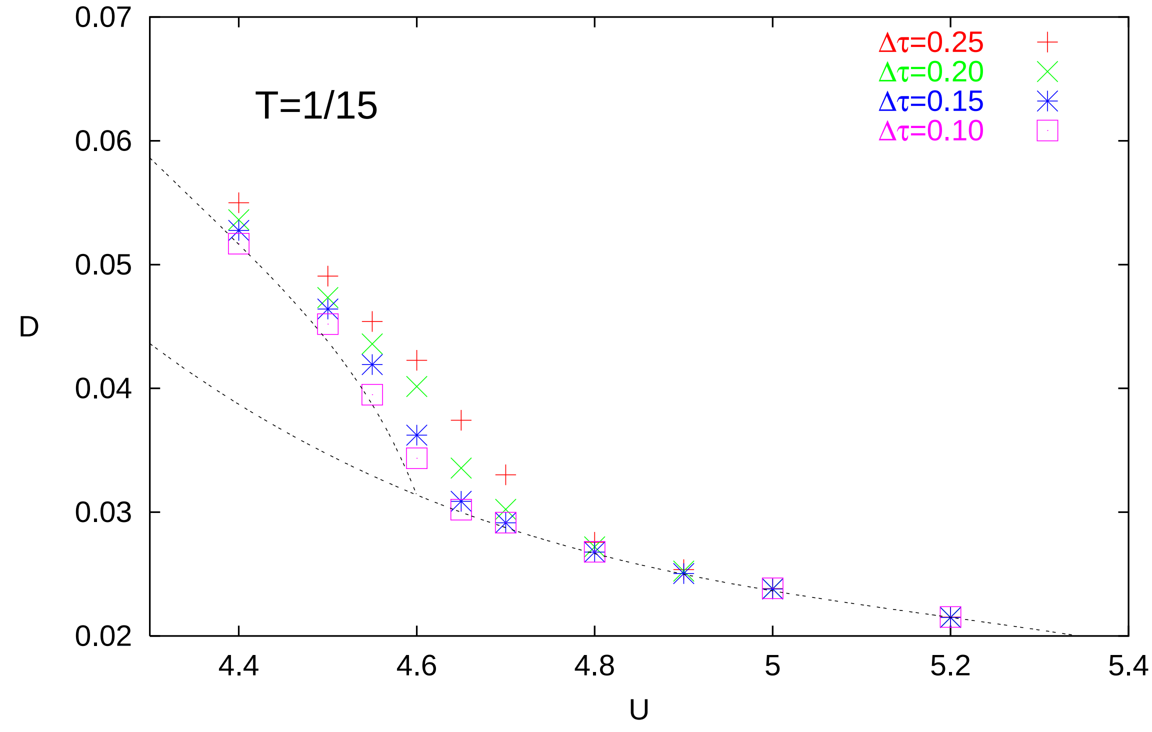




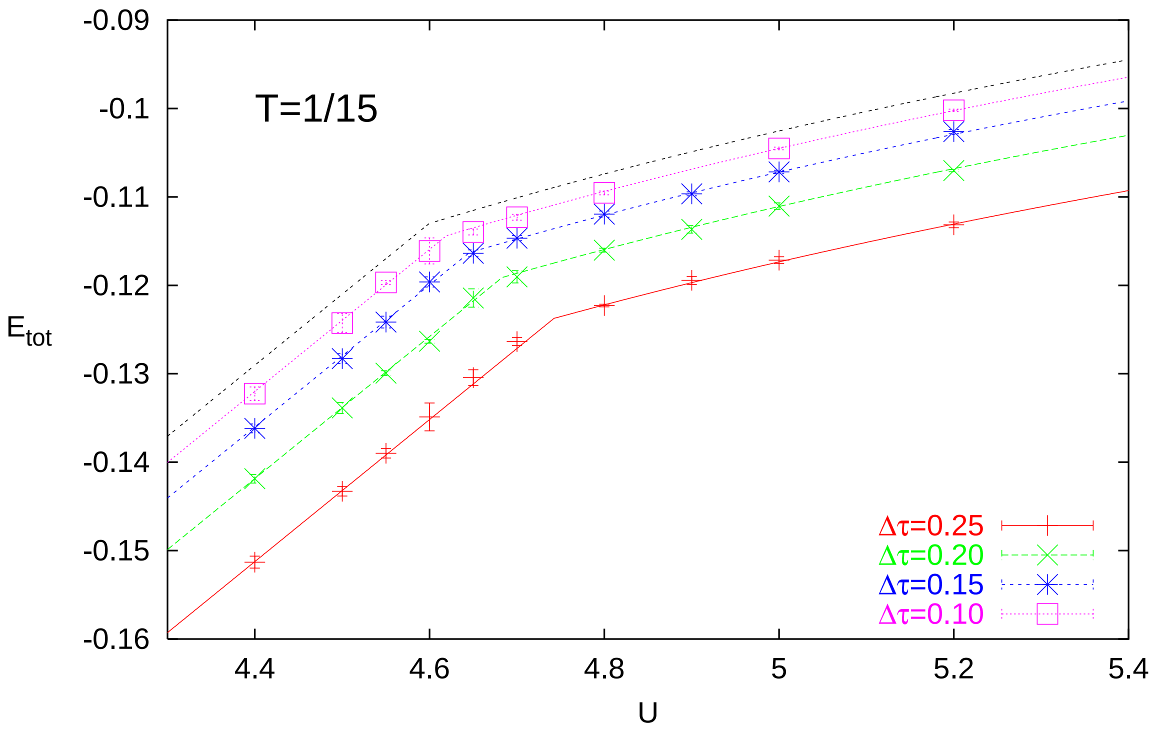
QMC solution of impurity problem:
- discretization of imaginary time $\beta = \Lambda\, \Delta\tau$
- Hubbard-Stratonovich trafo, MC sampling

characterize MIT by rapid change / kink in
- double occupancy $D = \langle \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \rangle$
- internal energy $E = E_{\text{kin}} + UD$

$T = 1/15$: sharp transition from metal to insulator, no hysteresis



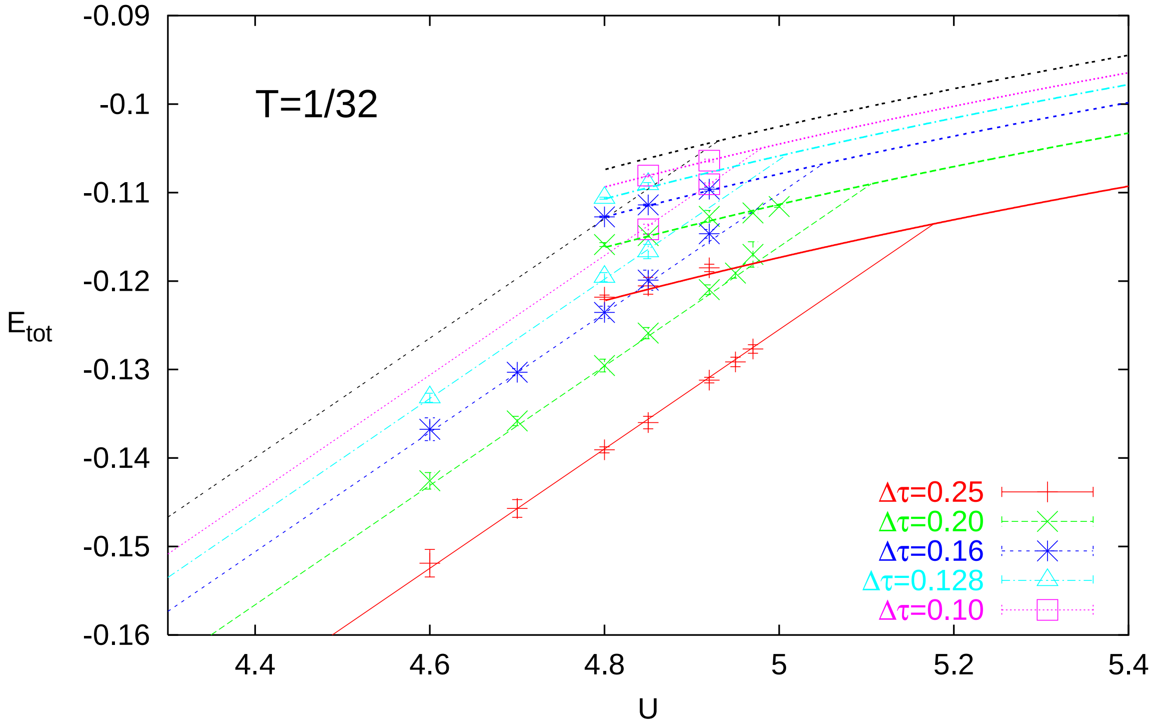
$\Delta\tau$ dependence of D: large at MIT, small below, vanishing above;



$\Delta\tau$ dependence of E: regular (quadratic); $\sim$ piecewise linear U dependence

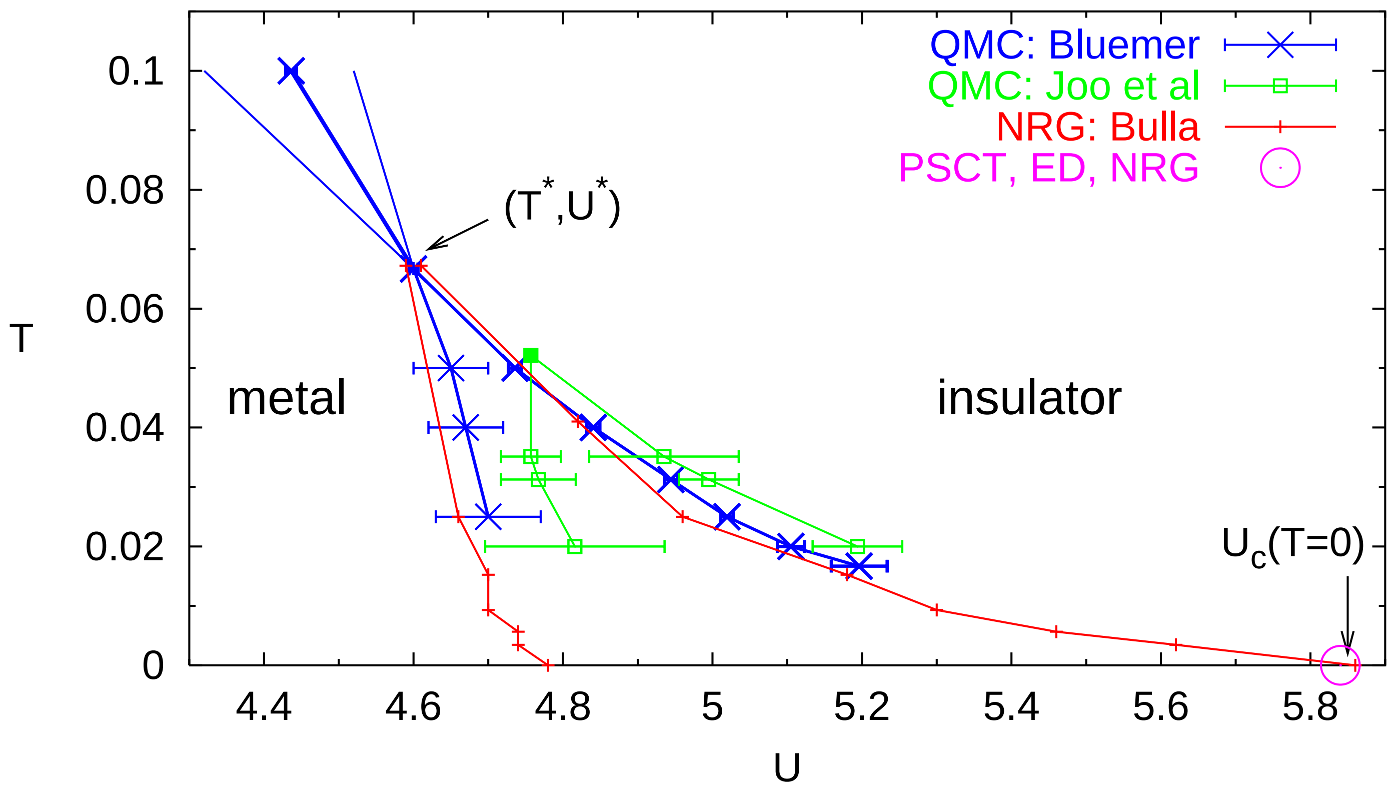
U_c shifts substantially for $\Delta\tau \to 0$

$T = 1/32$: coexistence of metallic and insulating solutions



T dependence of E, D exp. small in insulator

Crossover and coexistence regions



pinpoint 1^{st} order phase transition line $U_c(T)$ for $0 < T < T^*$

Comparing free energies

full absolute computation of $F(T,U)$ far too inaccurate!

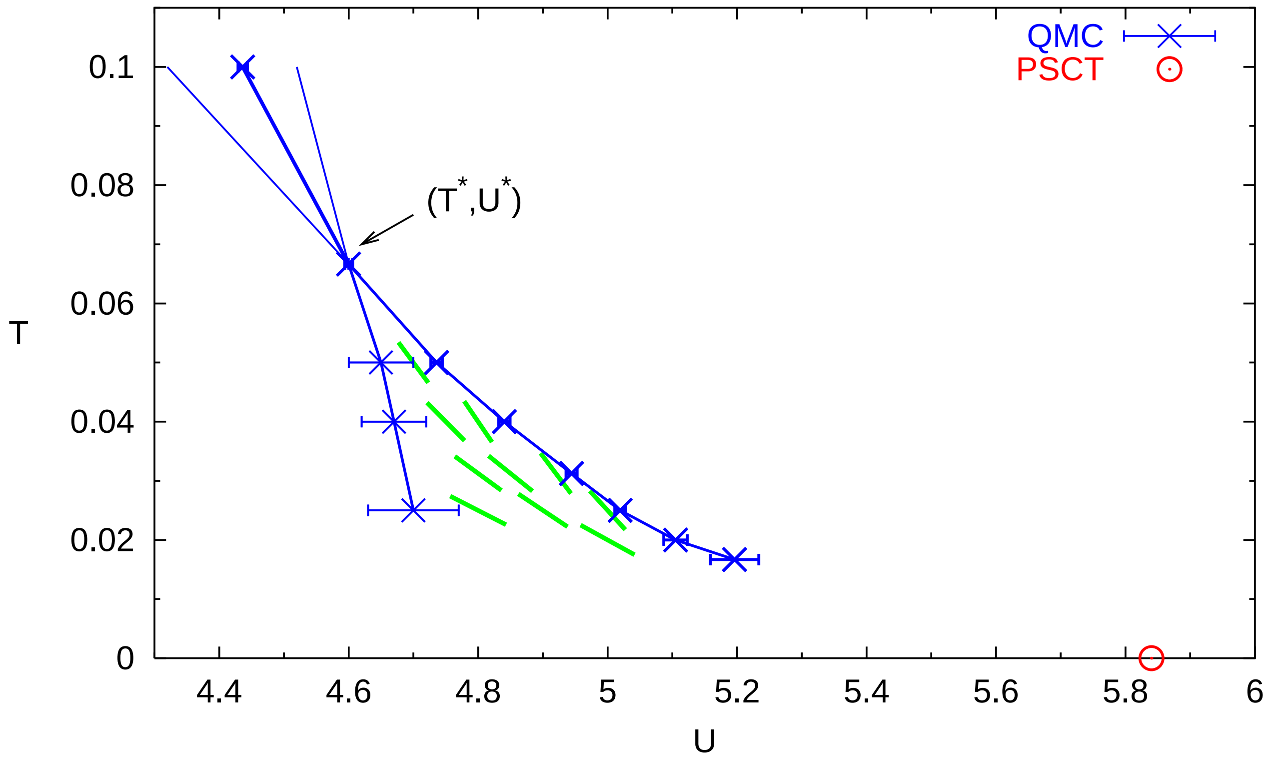
- consider $\Delta F(T,U) = F_{\text{metal}}(T,U) - F_{\text{insulator}}(T,U)$
- local criterion $d(\beta\Delta F(\beta,U)) = \Delta E(\beta,U)d\beta + \beta\Delta D(\beta,U)dU$

Clausius-Clapeyron equation:

$$\frac{dU_c(T)}{dT} = f(T,U_c(T)); \quad f(T,U) := \frac{\Delta E(T,U)}{T\Delta D(T,U)}$$

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

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



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

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

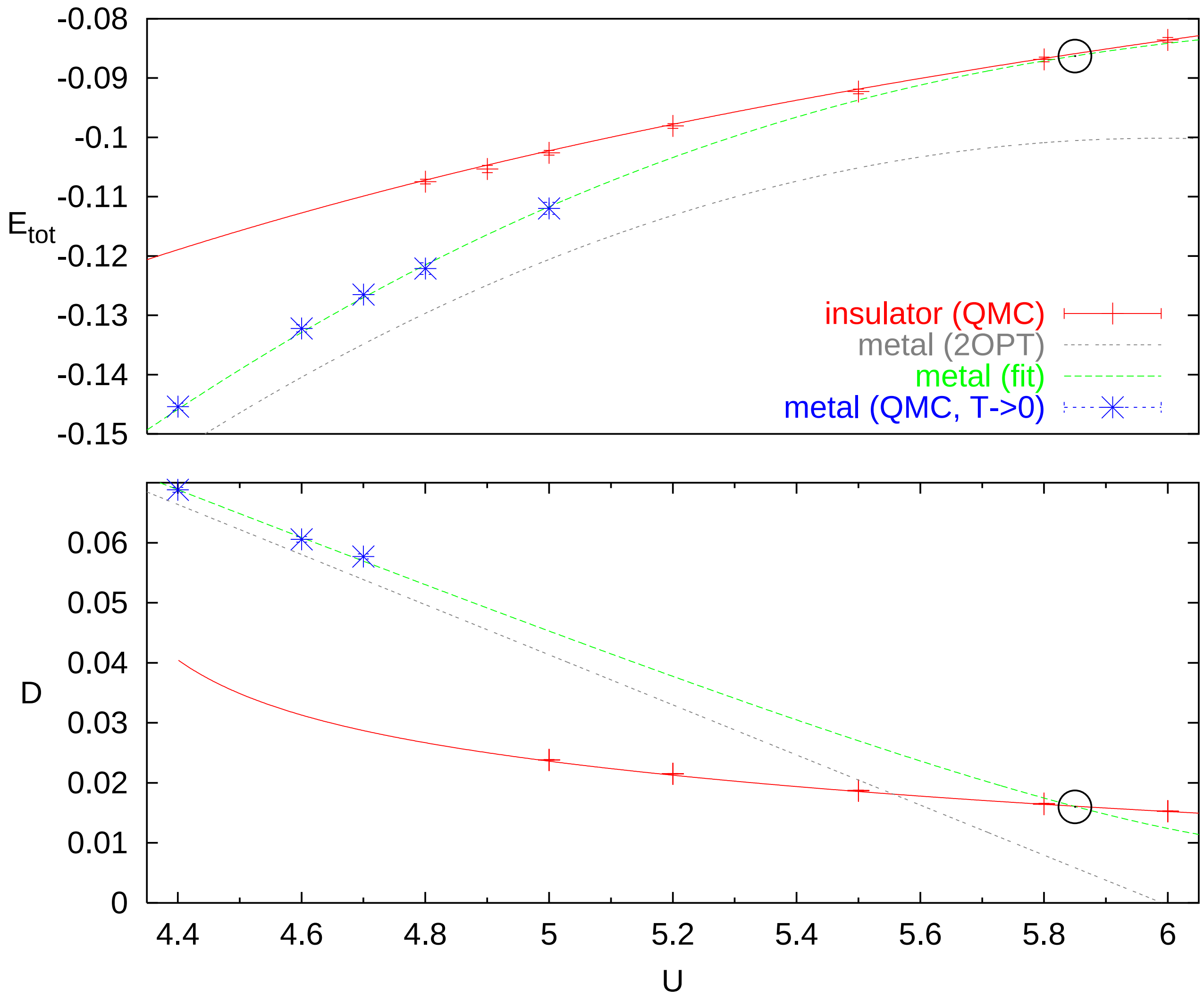
Low temperature information

Fermi liquid properties in metal, entropy $S_{\text{insulator}}(T,U) = S_0$

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

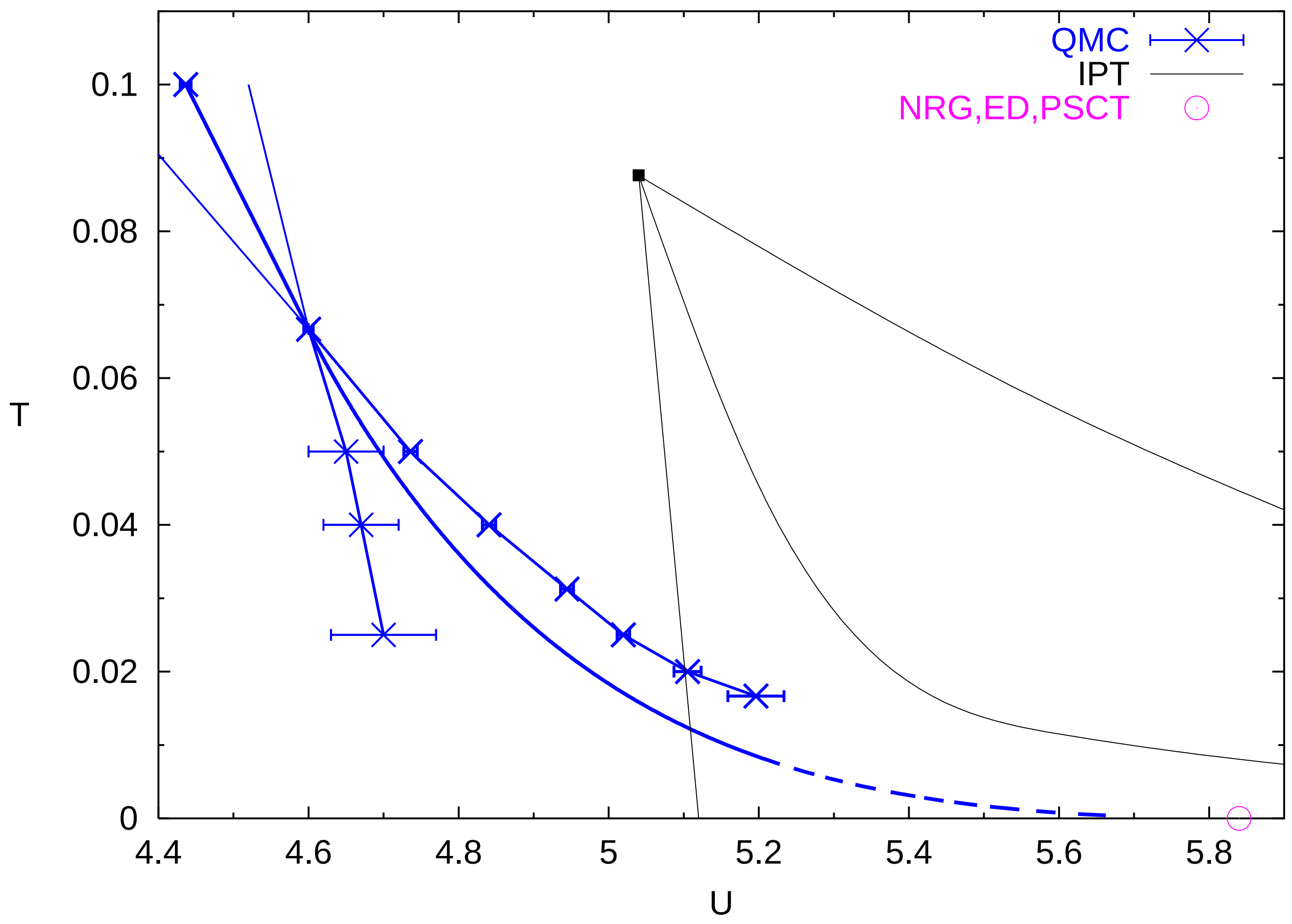
$$\tilde{f}(T) = CT^{-1/2} + D + ET^{1/2}; \quad C \approx -\sqrt{\frac{S_o}{2a}}$$

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



substantial improvement over PSCT estimates for value of a.

Full phase diagram



Conclusions

- results from fundamentally different methods now converged towards a reliable phase diagram
- first controlled computation of $U_c(T)$
- full thermodynamics, e.g., $E(T,U)$, $c_v(T,U)$

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