

Energy of the Mott insulator

10th order perturbation theory extended
to infinite order using QMC

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Outline

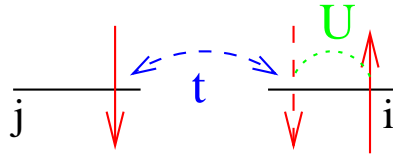
Motivation: Mott-Hubbard transition

Quantum Monte Carlo and strong-coupling PT

extended perturbation theory (ePT)

Introduction

Hubbard model

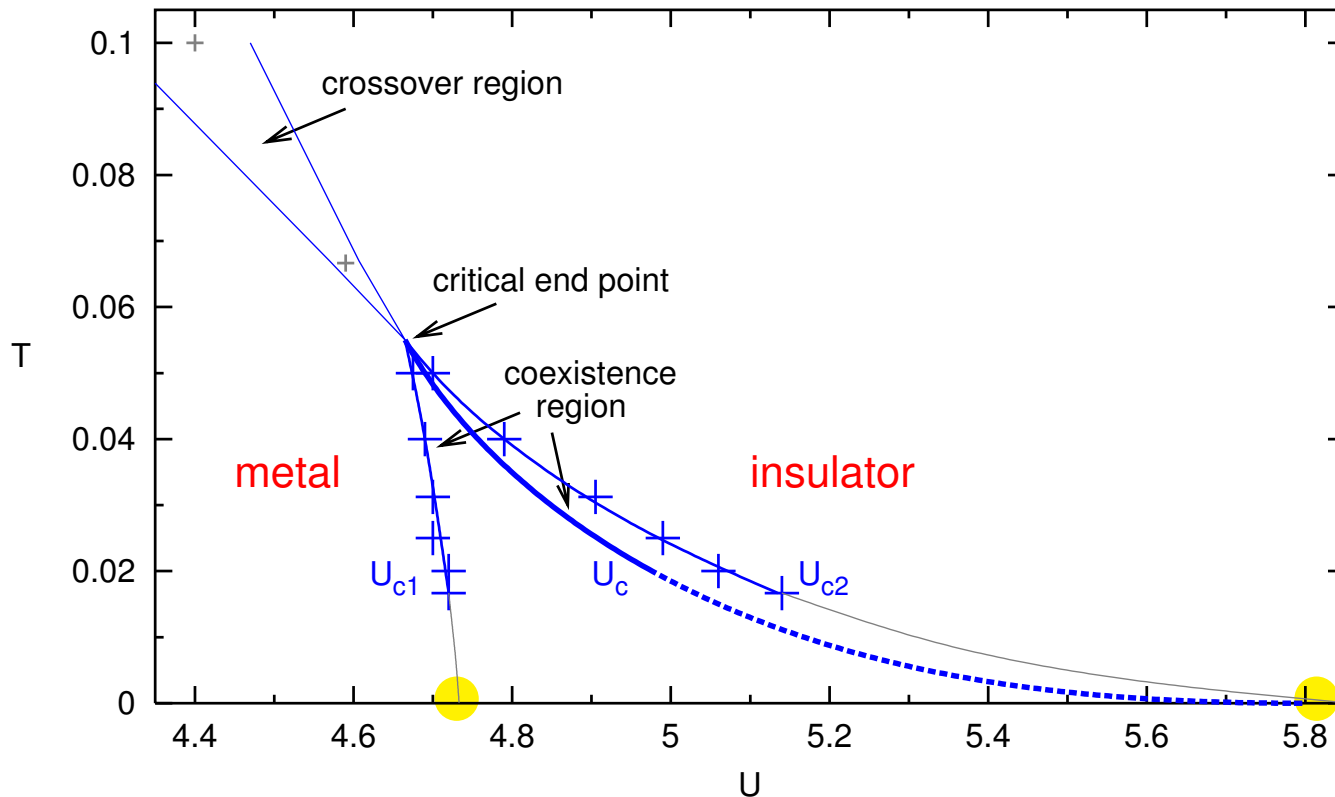
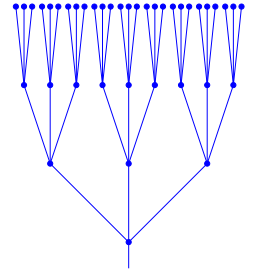


$$\hat{H} = \sum_{(i,j),\sigma} t_{ij} (\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \text{h.c.}) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

dynamical mean-field (DMFT)

semi-elliptic “Bethe” DOS

full frustration (no AF)

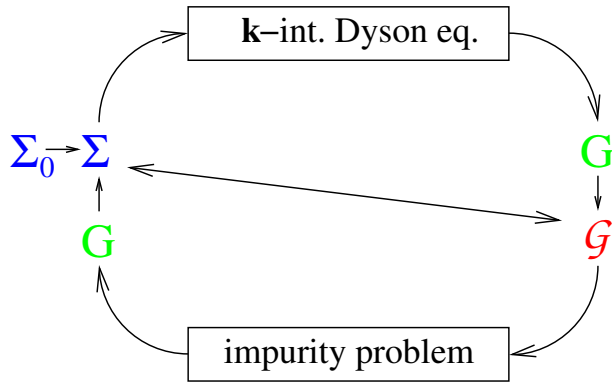


- Georges and Krauth (1993)
- Rozenberg, Kotliar, Zhang (1994)
- Georges et al. (RMP, 1996)
- Schlipf et al. (1999)
- Rozenberg, Chitra, Kotliar (1999)
- Krauth (2000)
- Bulla (1999, 2001)
- Joo, Oudovenko (2001)
- Tong (2001)
- Blümer (2000, 2002)

low-T energetics?

Methods I

DMFT cycle



Quantum Monte Carlo

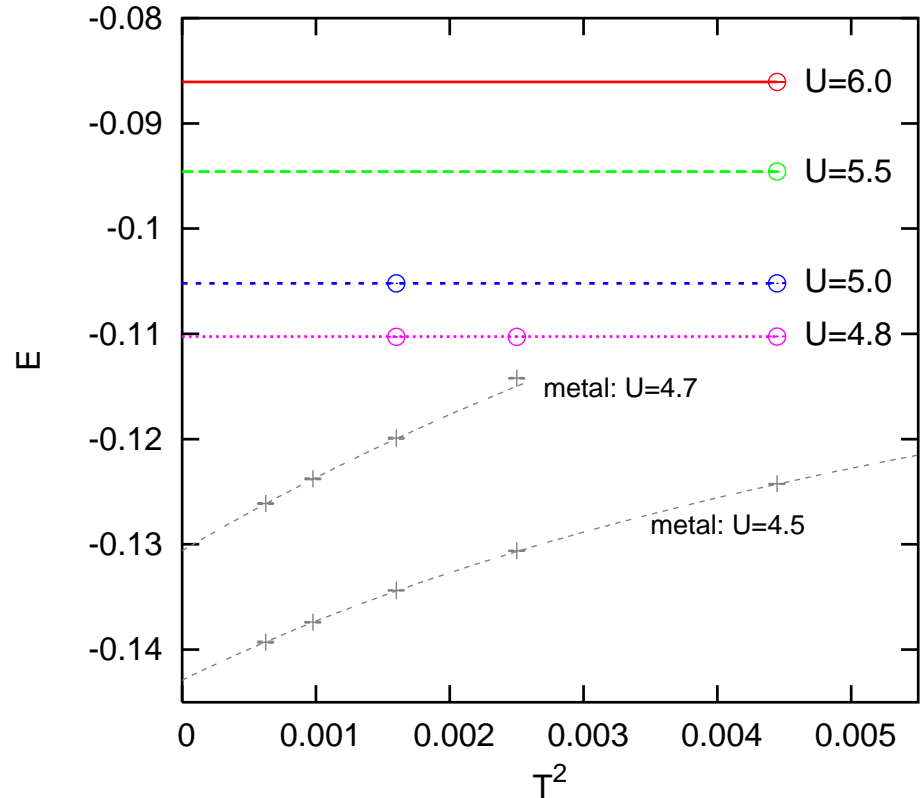
40×10^7 sweeps

$$\Sigma(\omega) = \frac{U^2}{4\omega} + \mathcal{O}(\omega^2)$$

$$0.1 \leq \Delta\tau \leq 0.25$$

$$\Delta E \approx 10^{-5}$$

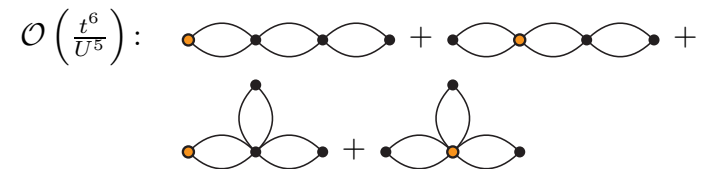
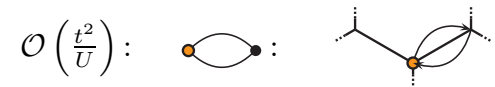
$$\Delta D \approx 10^{-5}$$



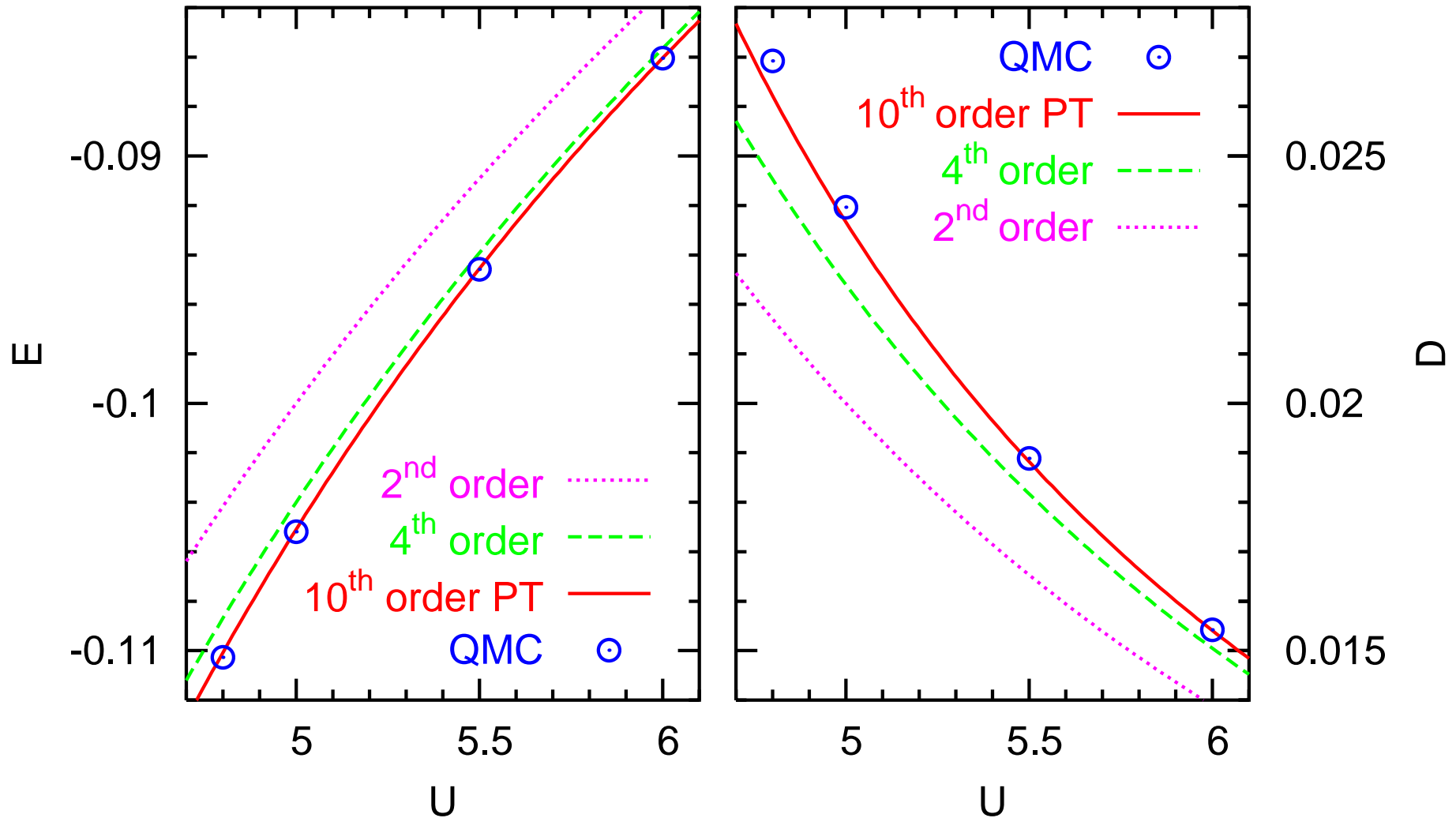
Kato-Takahashi perturbation theory at $T = 0$ ($t^* = 1$):

$$E_{\text{PT}}(U) = -\frac{1}{2U} - \frac{1}{2U^3} - \frac{19}{8U^5} - \frac{593}{32U^7} - \frac{23877}{128U^9}$$

$$D_{\text{PT}}(U) = dE_{\text{PT}}(U)/dU$$



Results I



Excellent agreement at $U = 6.0$.

continuous fit + critical behavior?

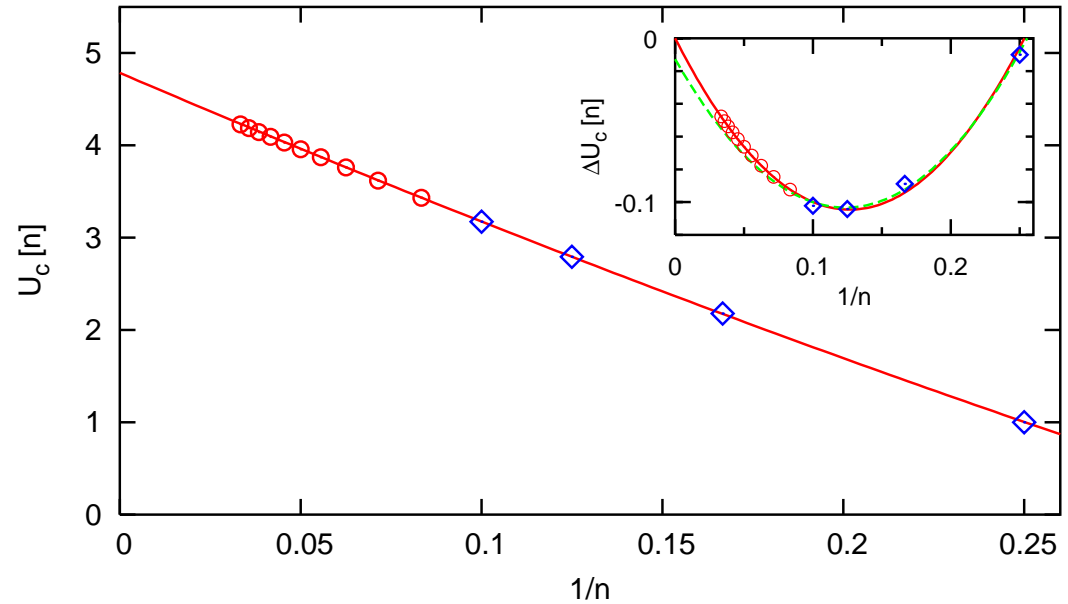
Methods II

Idea: extrapolate PT coefficients in

$$E_{\text{PT}} = \sum_{i=1}^{\infty} a_{2i} U^{1-2i}$$

using $U_{c1}[2i] \equiv \sqrt{a_{2i+2}/a_{2i}}$.

Fit to $U_{c1}[n] \approx U_{c1} + u_1 n^{-1} + u_2 n^{-2}$



Consequences:

$$U_{c1} = \lim_{i \rightarrow \infty} U_{c1}[2i]$$

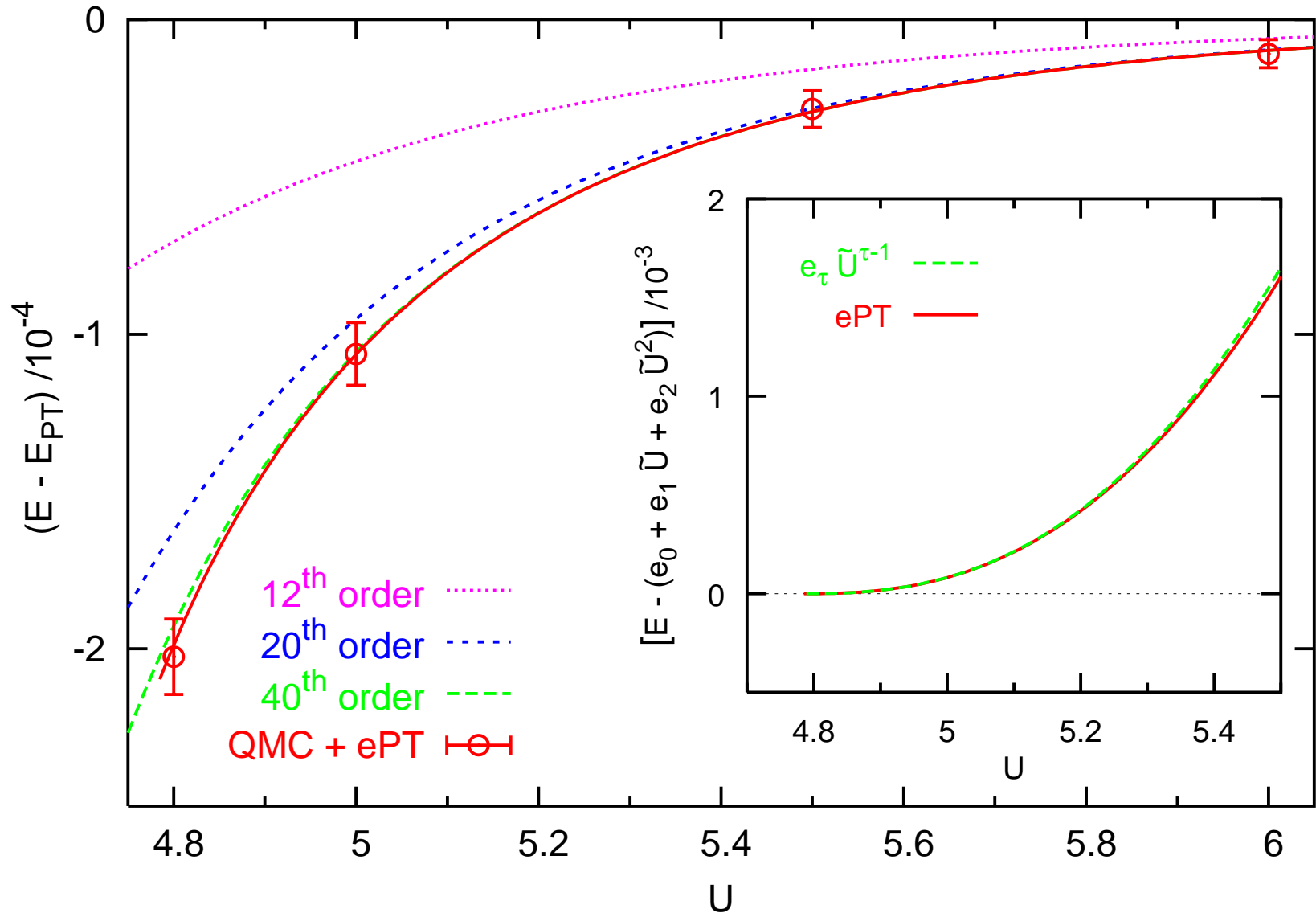
$$a_n \propto n^\tau U_{c1}^n$$

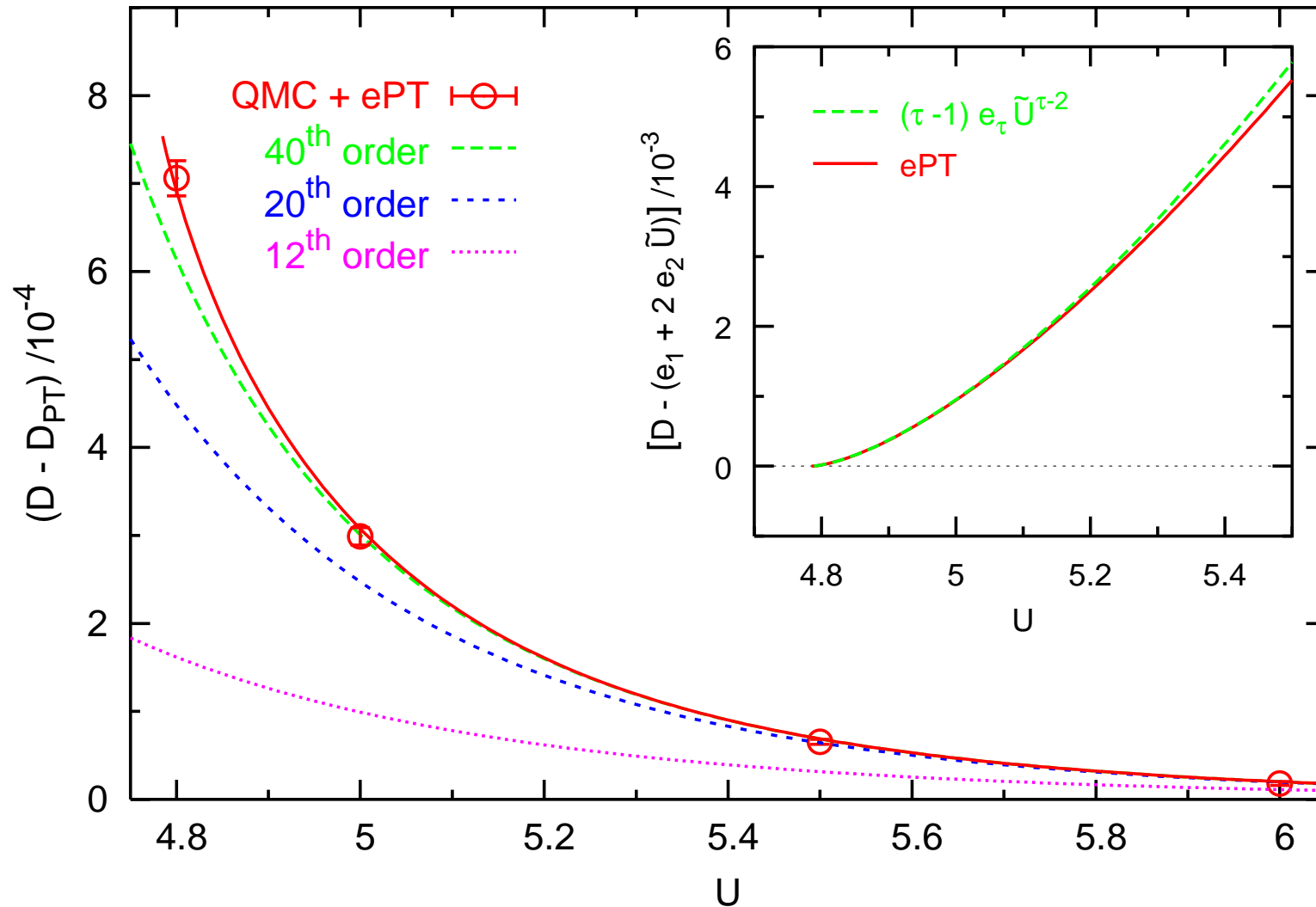
$$E_{\text{critical}}(U) = e_\tau (U - U_{c1})^{\tau-1}$$

$$D_{\text{critical}}(U) = (\tau - 1) e_\tau (U - U_{c1})^{\tau-2}$$

Results II

$$\tau = 3.48 \pm 0.05 \approx 3.5, \quad U_{c1} = 4.785 \quad (\text{unrestricted: } U_{c1} = 4.77)$$





Conclusions:

Mott insulator: new estimate of lower stability edge U_{c1} , critical exponents
 high-precision results for E , D at all U (parametrizations available)
 \rightsquigarrow low- T parameter for $U_c(T)$, benchmark for old and new methods