

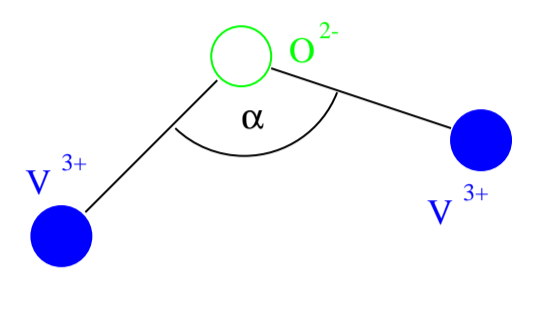
Introduction

Motivation:

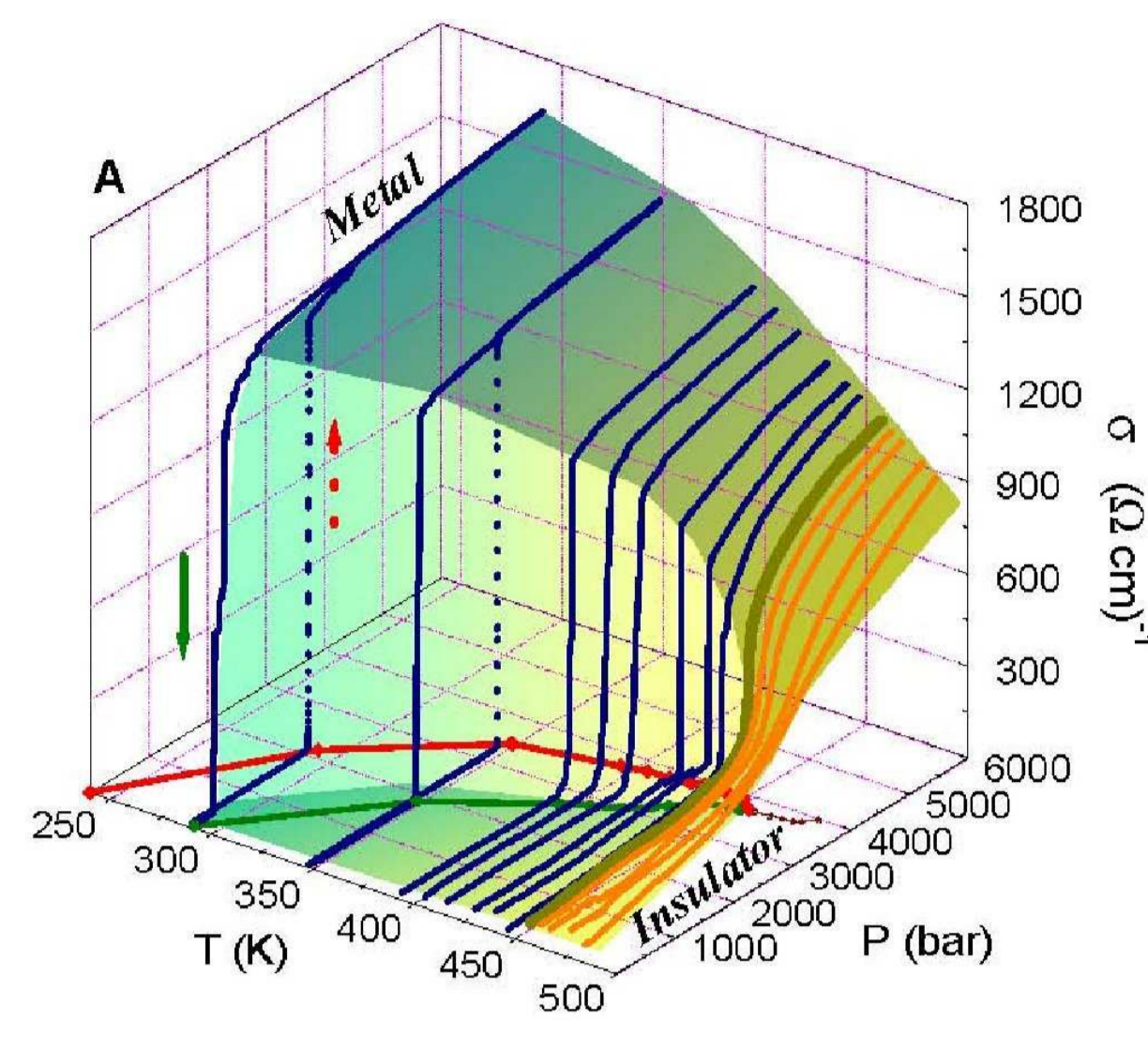
Metal-insulator transition (MIT) in V_2O_3 doped with Cr or Ti

Hysteresis near MIT!

Bandwidth-control by doping or pressure



$$\alpha_{Cr} < \alpha_V < \alpha_{Ti}$$

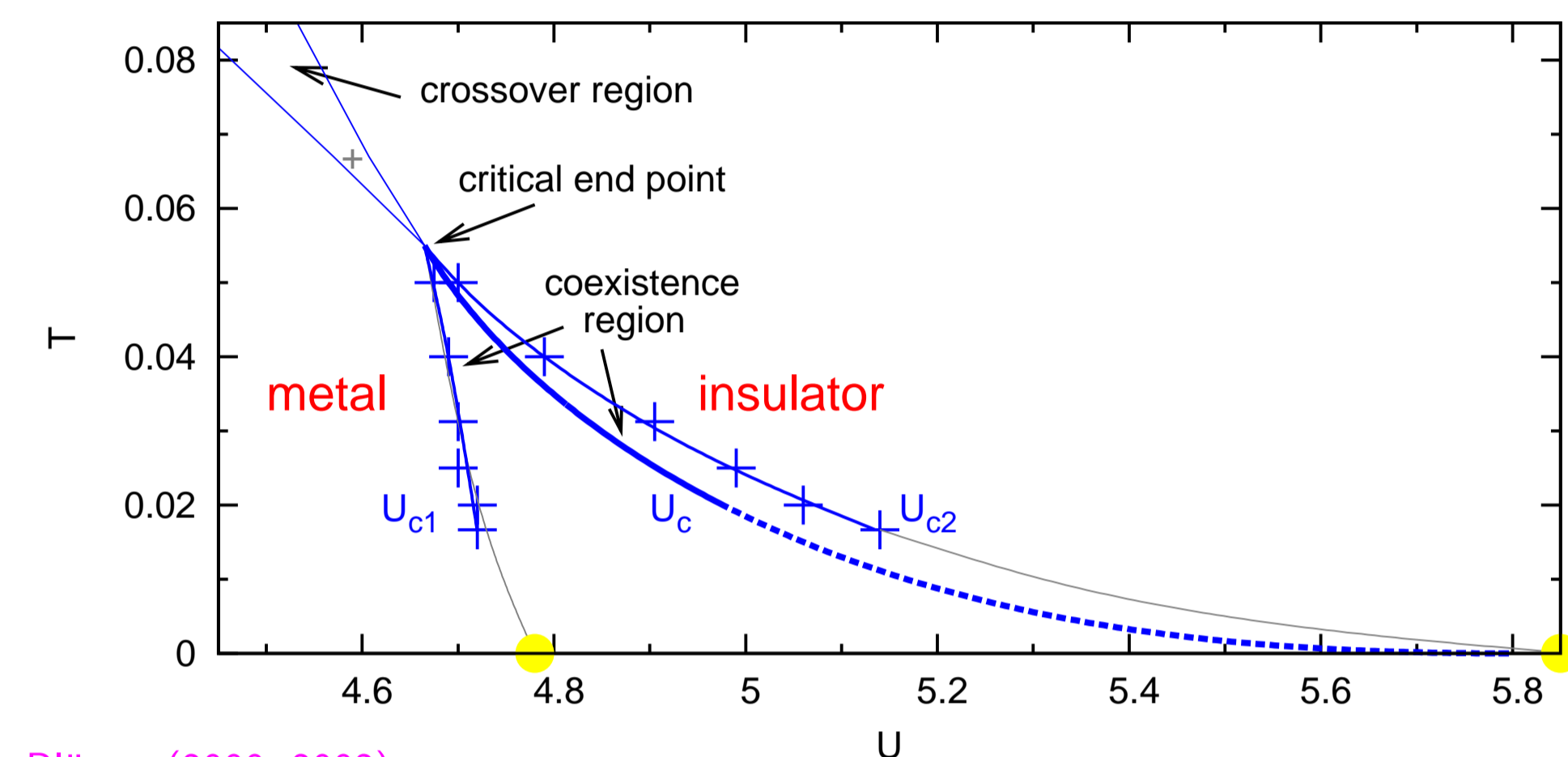


Limelette et al., Science 302, 89 (2003)

Drastically simplified model (no band degeneracy, no lattice degrees of freedom): **half-filled one-band Hubbard model**

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

DMFT, full frustration, semi-elliptic "Bethe" DOS, $n = 1$:
1st order metal-insulator transition for $T < T^* \approx 0.058$:



Blümer (2000, 2002)

1st order line $U_c(T)$ obtained by implicit comparison of free energies using a Clausius-Clapeyron like equation [1] in terms of energy $E = \langle \hat{H} \rangle / L$ and double occupancy $D = \langle \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \rangle$.
Asymptotic curve for $T \rightarrow 0$ from

$$U_c(T) = U_c(0) - \sqrt{2 \log(2) T / a} + \mathcal{O}(T)$$

for $a = d^2 [E_{ins} - E_{met}] / dU^2 |_{T=0, U=U_c(0)}$.

Needed: precise low-T/ground state energetics

Mott insulator: 10th order PT vs. QMC

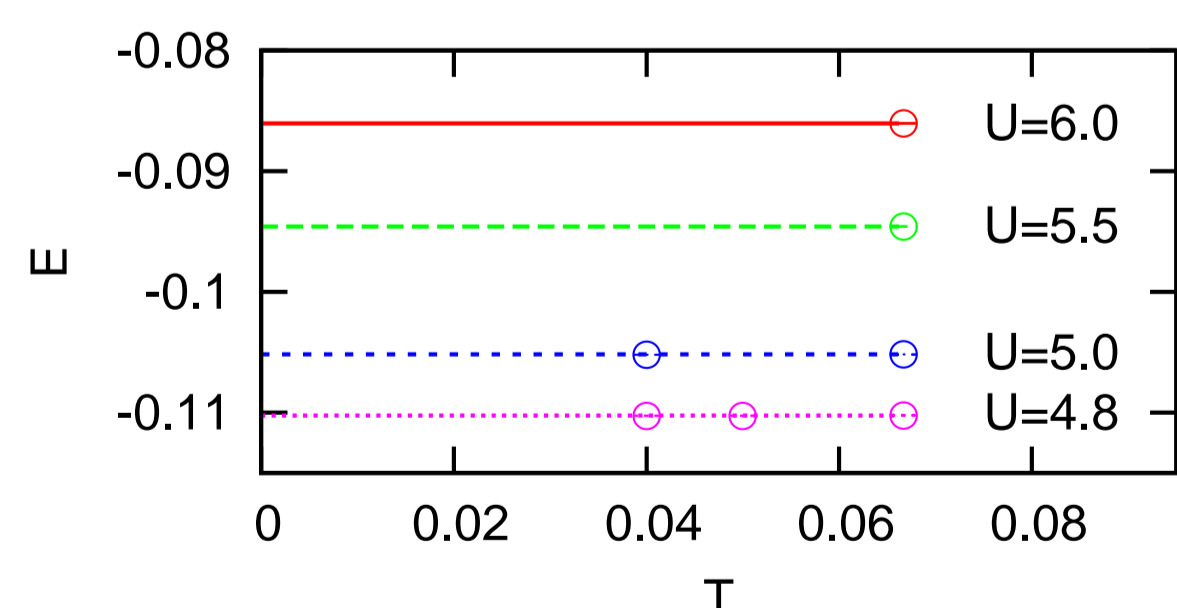
Kato-Takahashi perturbation theory in $d = \infty$ at $T = 0$:

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

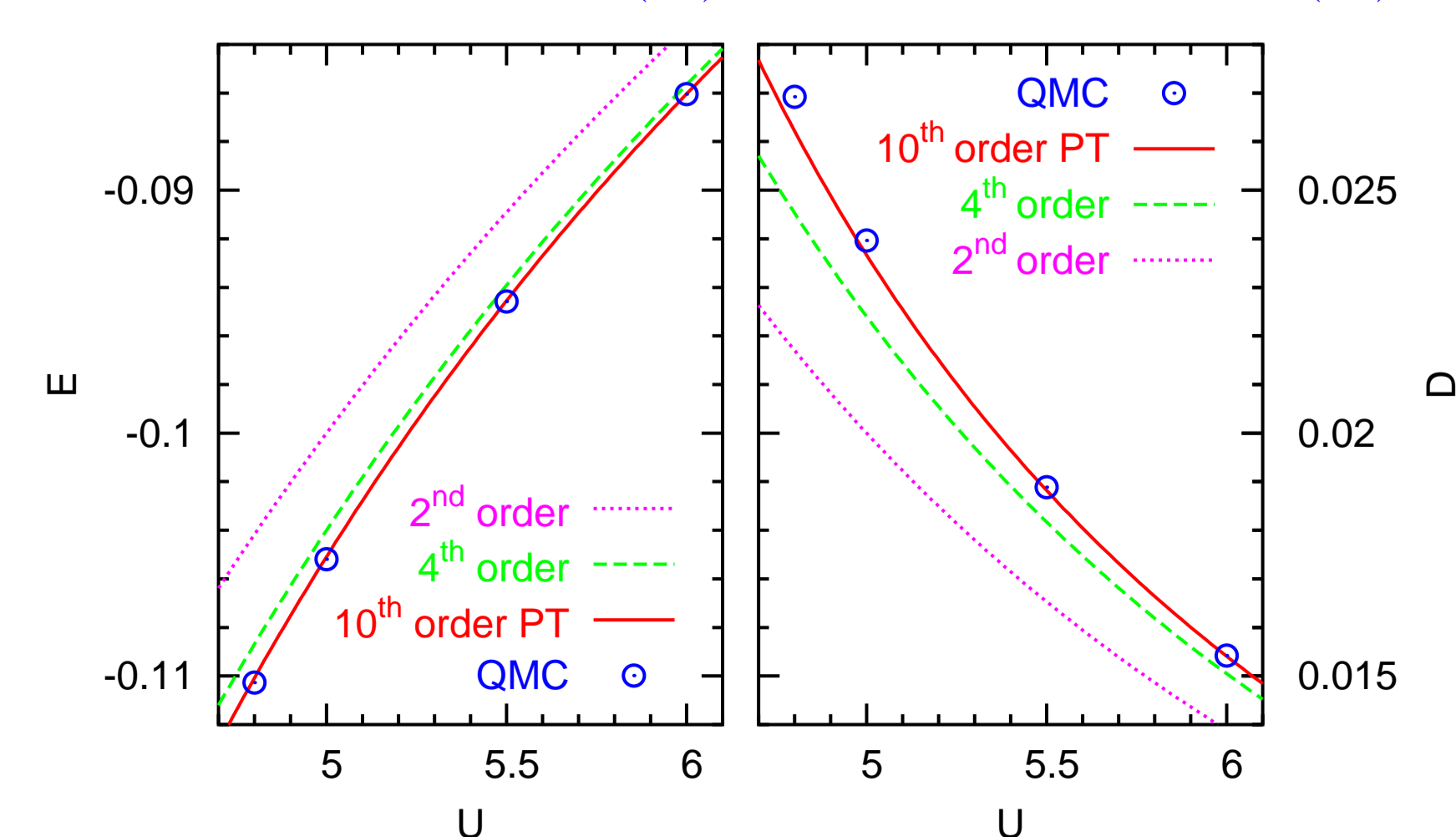
accuracy at $U \gtrsim 6$: $\Delta E_{PT} \leq 10^{-5}$, $\Delta D_{PT} \leq 10^{-5}$

Quantum Monte Carlo (QMC) solution of DMFT at finite T using high-frequency corrections (see poster by C. Knecht)

T -dependence of E , D almost negligible in insulating phase ($U > 4.8$) \rightsquigarrow reliable extrapolation $T \rightarrow 0$



Ground state energy $E(U)$, double occupancy $D(U)$



Excellent agreement at moderately strong coupling ($U = 6.0$).

Extended perturbation theory: ePT

Extrapolate coefficients in PT series $E_{PT} = \sum_{i=1}^{\infty} a_{2i} U^{1-2i}$

by fitting coefficient ratios $U_{cl}[2i] \equiv (a_{2i+2}/a_{2i})^{1/2}$ to $U_{cl}[n] \approx U_{cl} + u_1 n^{-1} + u_2 n^{-2}$

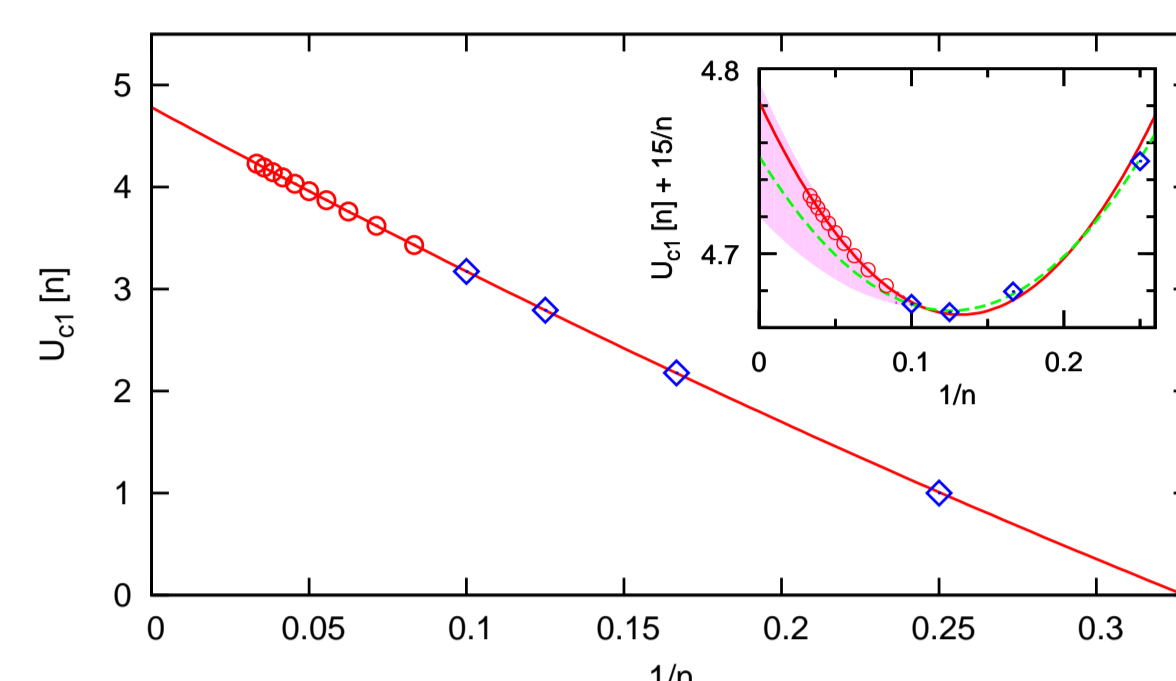
General consequences:

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

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

$$E(U) \propto (U - U_{cl})^{\tau-1}$$

$$D(U) \propto (U - U_{cl})^{\tau-2}$$



Specifics / numerical results of extrapolation:

Note: $U_{cl}[n]$ nearly linear in $1/n$.

Unrestricted quadratic fit (dashed) $\rightsquigarrow \tau \approx 3.44$, $U_{cl} \approx 4.75$

Comparison of $E(U)$, $D(U)$ with QMC $\rightsquigarrow 3.36 \leq \tau \leq 3.53$

Half-integer exponents likely for (dynamical) mean-field theory

Assume $\tau = 3.5 \rightsquigarrow U_{cl} = 4.782$, $E_{ePT}(U)$, $D_{ePT}(U)$

Infinite-order extrapolation method ePT similar in spirit to Singh's vastly successful extrapolation of 10th order PT in J_{\perp}/J_{\parallel} for the 2d Heisenberg AF to the isotropic limit.

Mott insulator: ePT estimate for energy $E(U)$ vs QMC

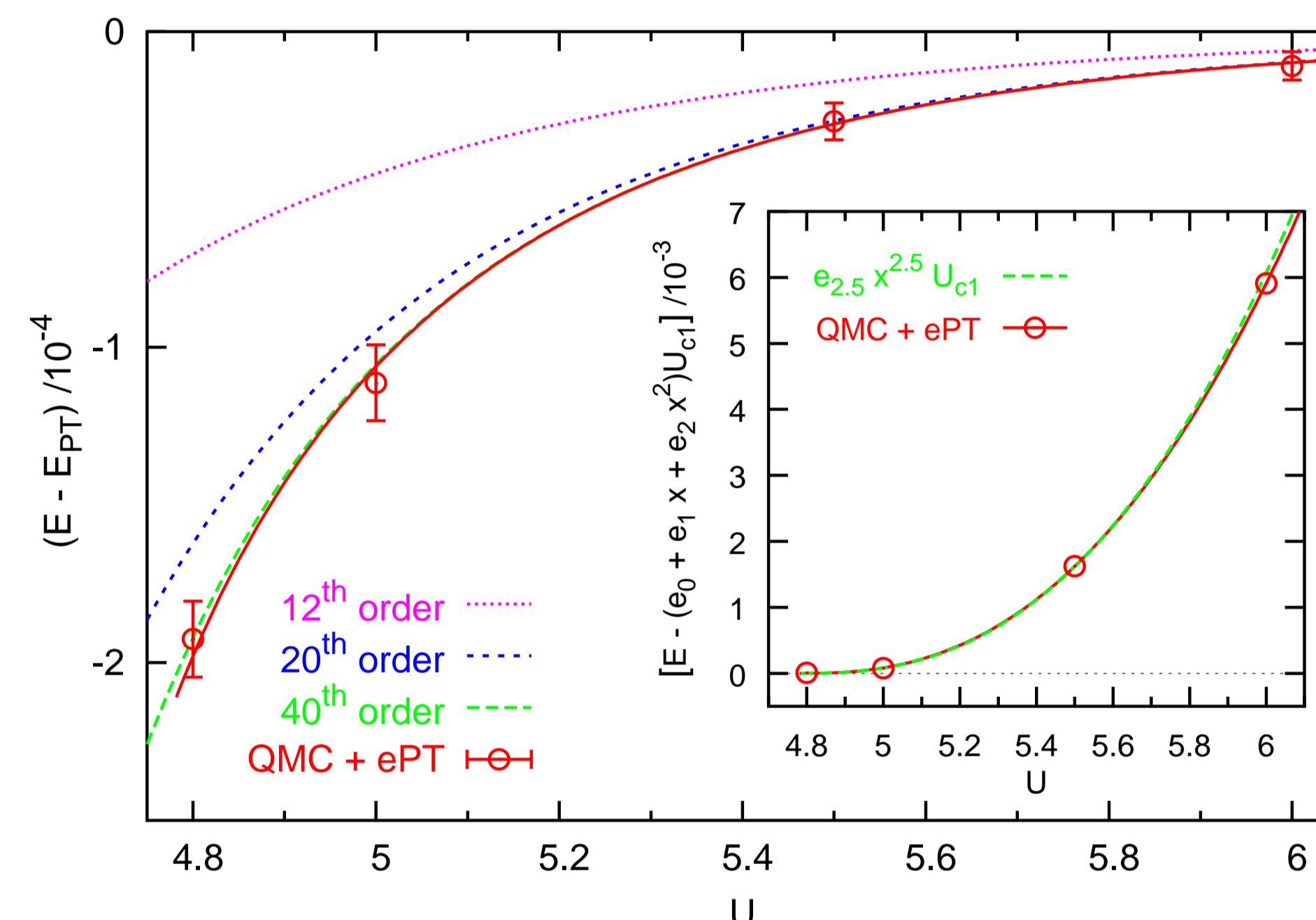


Fig: differences between QMC/full ePT/truncated ePT and 10th order PT. Inset: Contributions beyond non-critical terms (solid line) in comparison with leading critical term (dashed).

Mott insulator: ePT estimate for double occupancy $D(U)$

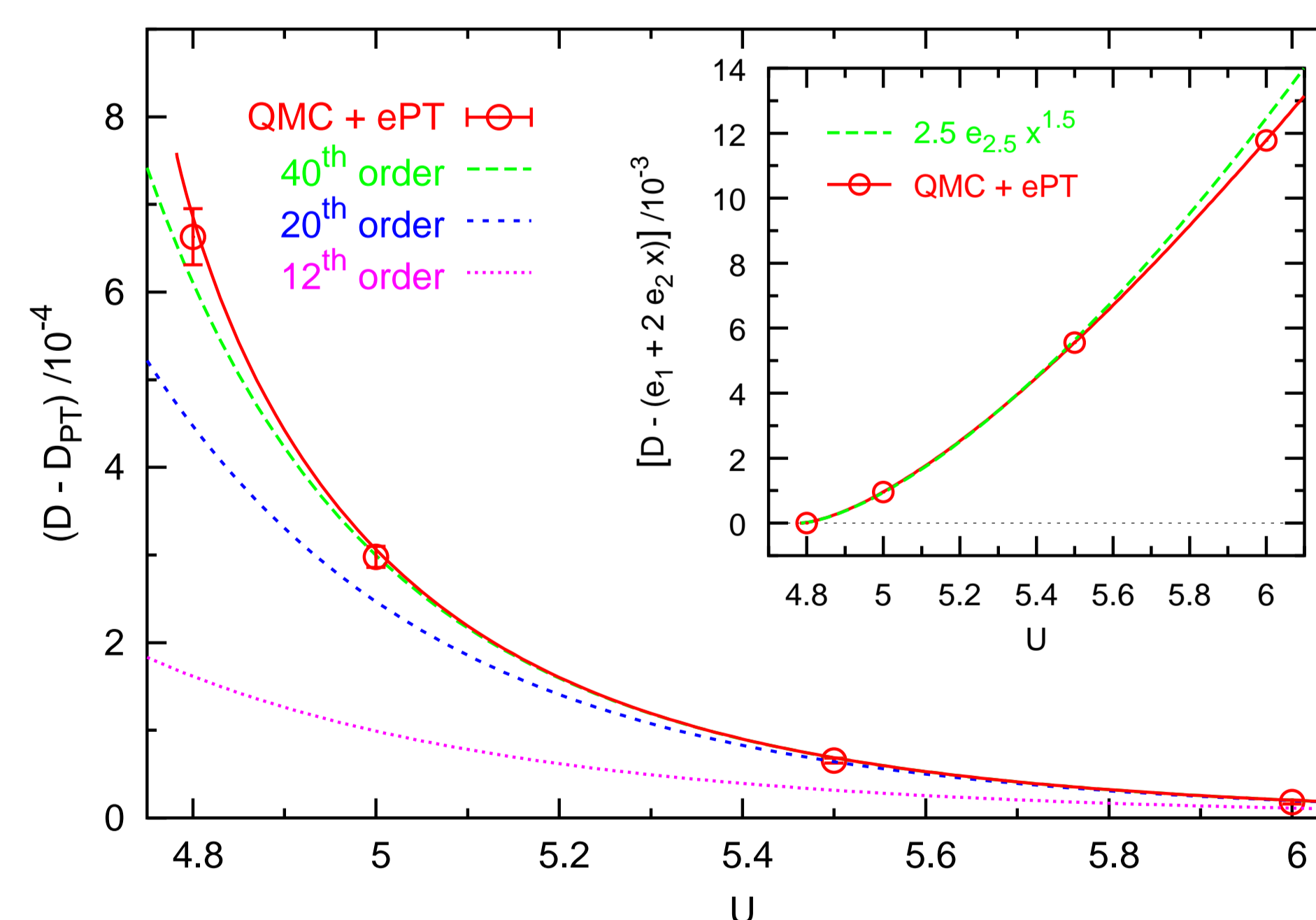


Fig: Double occupancy from QMC (circles) and ePT (solid lines) in complete analogy with previous figure [2].

Summary

New method ePT: 10th order PT extended to infinite order. \rightsquigarrow extreme precision for insulator and critical exponents:

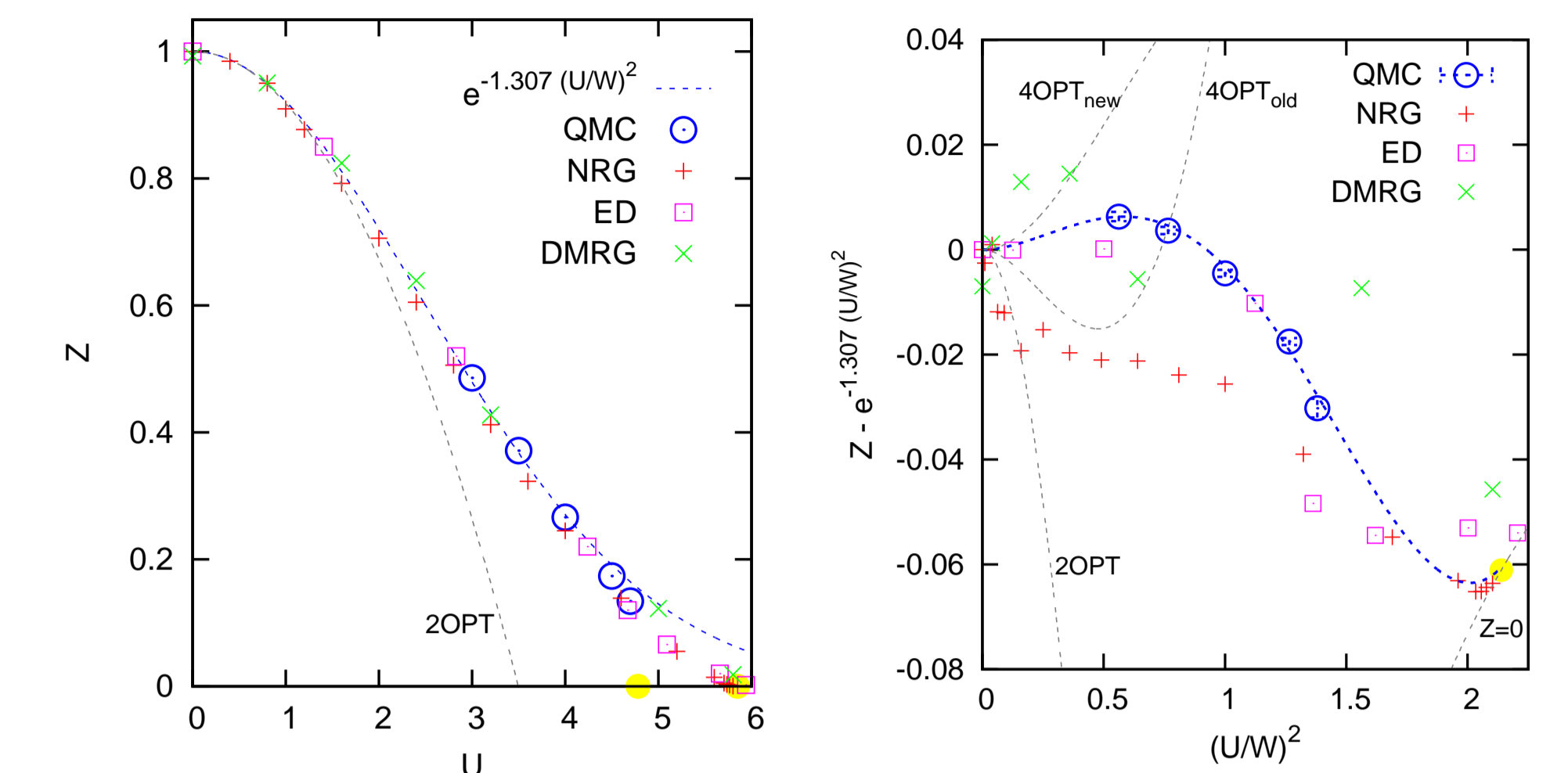
$$E_{crit} \propto (U - U_{cl})^{2.5}, D_{crit} \propto (U - U_{cl})^{1.5}$$

Extreme precision at finite T from improved QMC scheme.

High-precision extrapolations to $T = 0$ for metal at all U possible by using (i) $\gamma^{-1} \propto Z$, (ii) weak-coupling PT/ thermodynamic consistency, and (iii) matching condition at U_{c2} .

QMC estimates for metal ($T \rightarrow 0$)

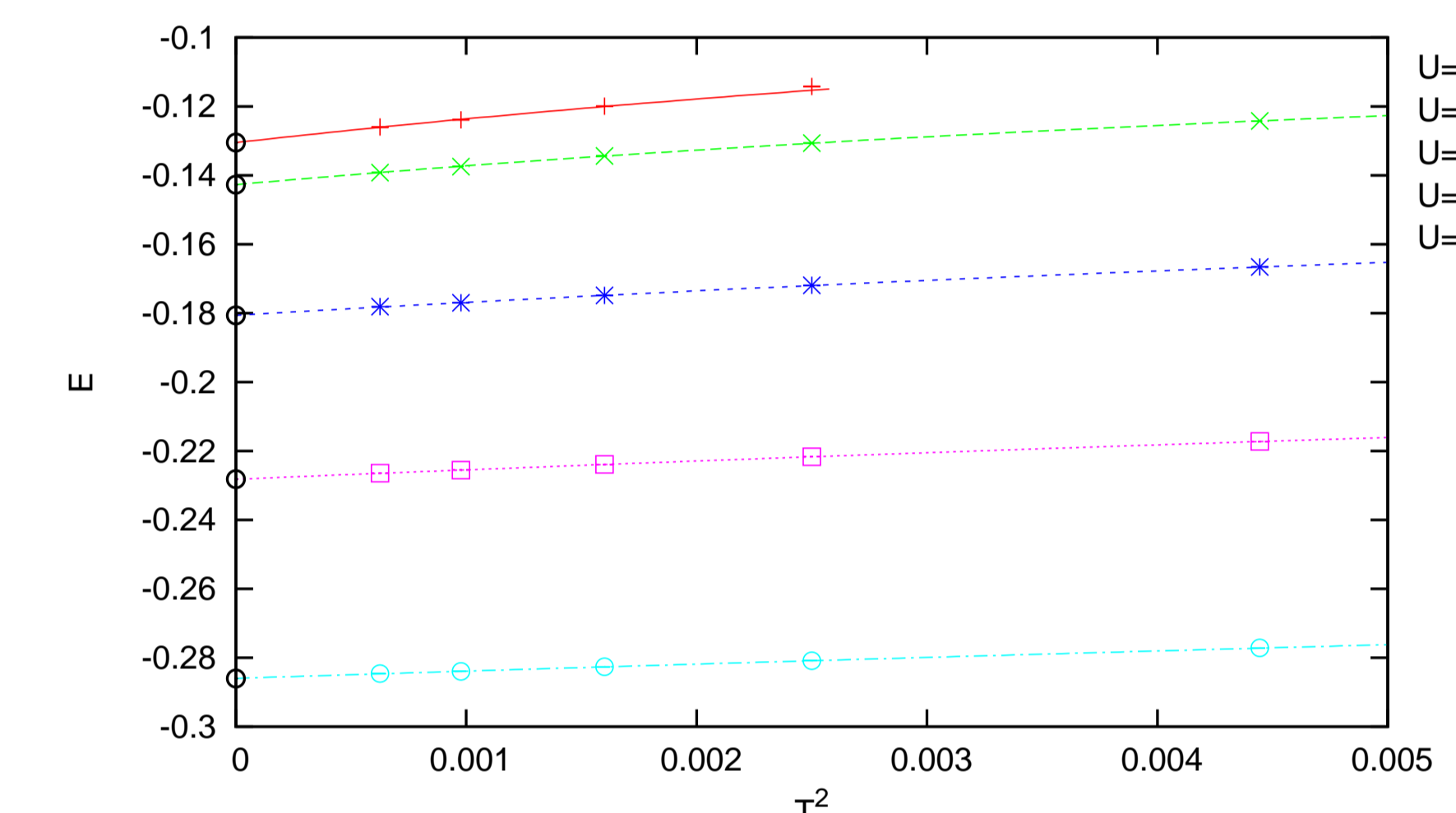
Quasiparticle weight/mass enhancement $Z = m/m^*$ at $T = 0$



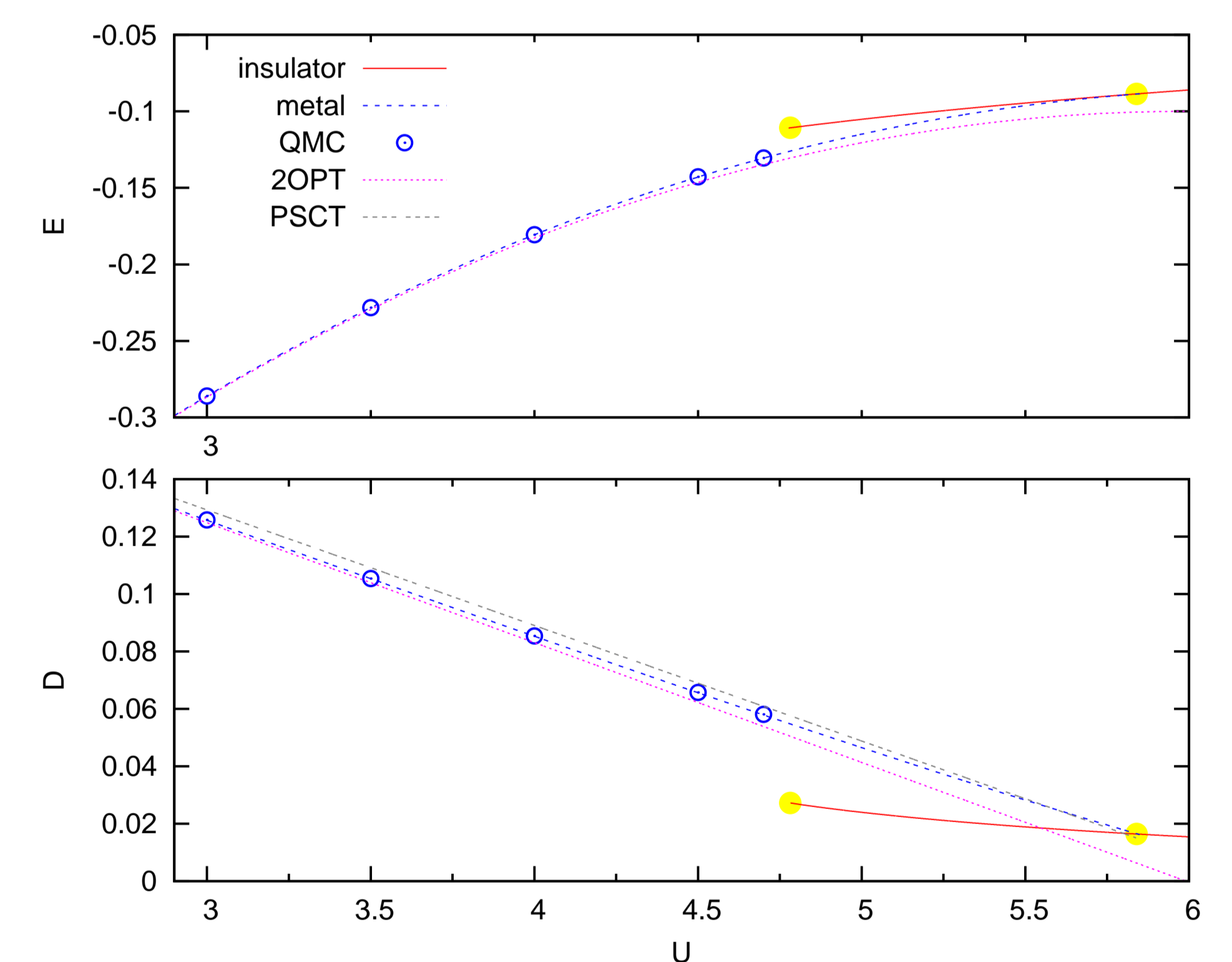
Fits to QMC roughly consistent with new 4OPT results [3].

Z determines linear coefficient of specific heat $c = \gamma T + \mathcal{O}(T^3)$ as $\gamma = \pi/(3Z)$ (for Bethe DOS) \rightsquigarrow reliable E extrapolation

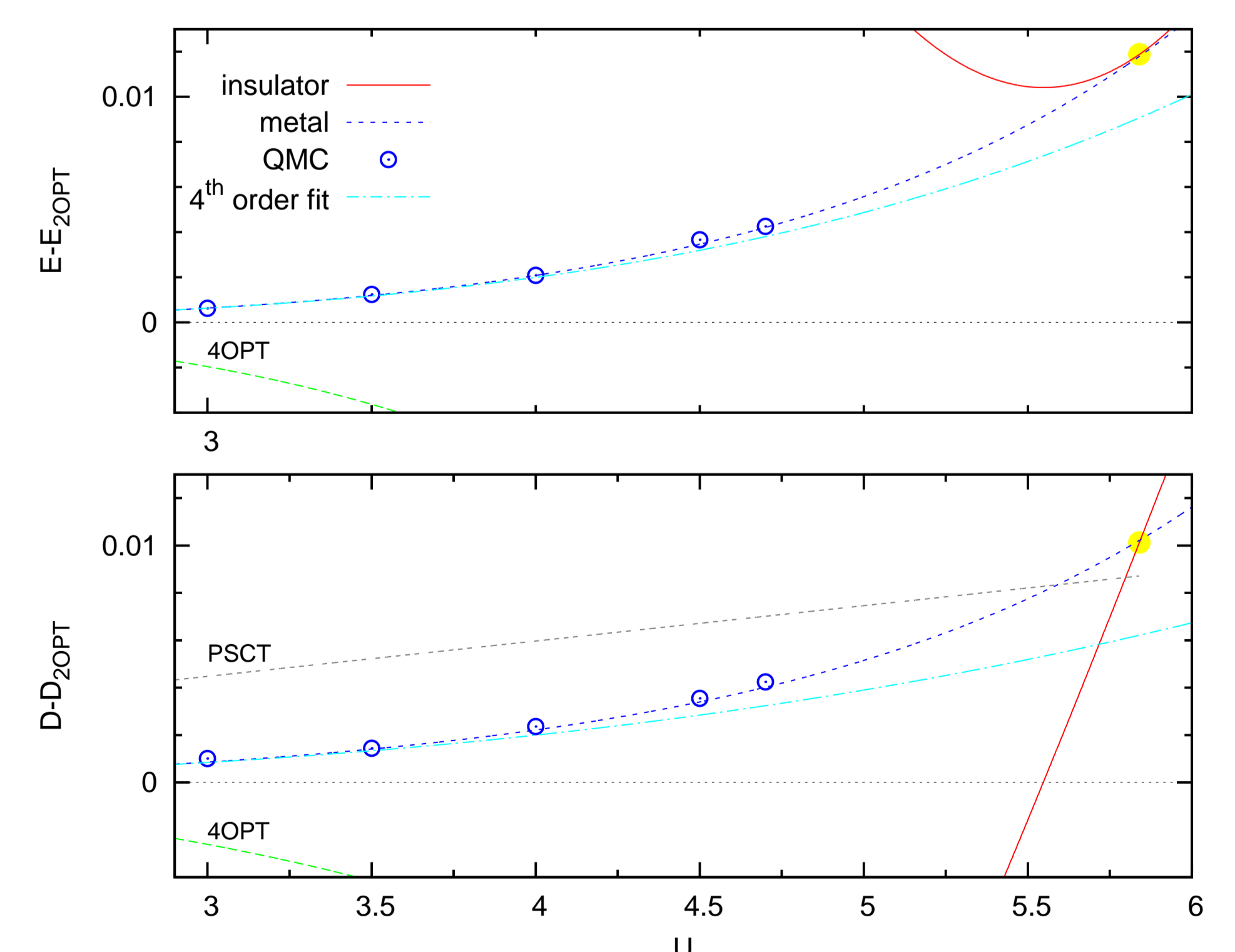
Energy $E(T, U)$ from QMC and extrapolation $T \rightarrow 0$



Continuous precise estimates for E , D at all U from QMC, weak-coupling PT, ePT, and matching conditions at U_{c2}



2nd order weak-coupling PT (2OPT) surprisingly good \rightsquigarrow plot differences w.r.t. 2OPT results for E and D :



Analytic 4OPT results for E and D [3] evidently incorrect.

References

- [1] N. Blümer, Thesis, Univ. Augsburg (2002) and Shaker, Aachen, (2003).
- [2] N. Blümer and E. Kalinowski, Phys. Rev. B, in press [cond-mat/0404568].
- [3] F. Gebhard et al., Eur. Phys. J. B 36, 491 (2003).
- [4] N. Blümer and E. Kalinowski, Physica B, in press [cond-mat/0407442].