# Low-temperature properties of the half-filled frustrated Hubbard model in high dimensions

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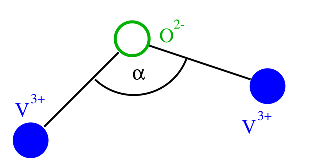
## Introduction

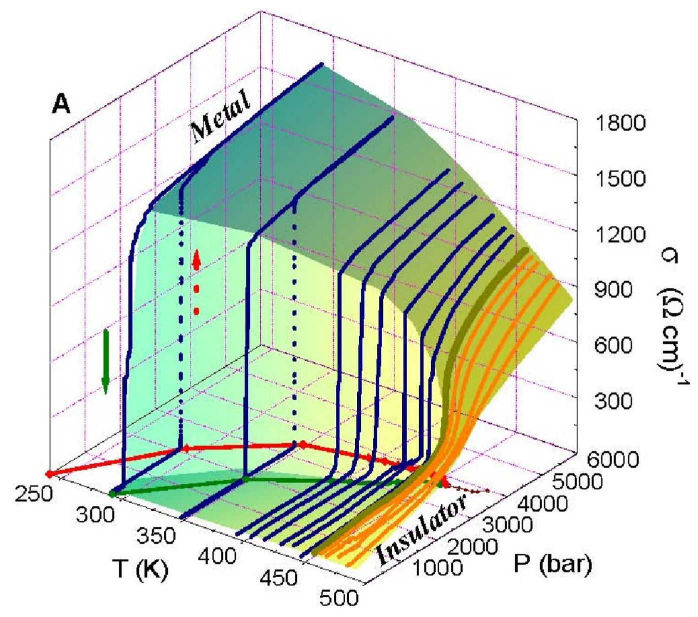
**Motivation:**

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

Hysteresis near MIT!

Bandwidth-control by doping or pressure



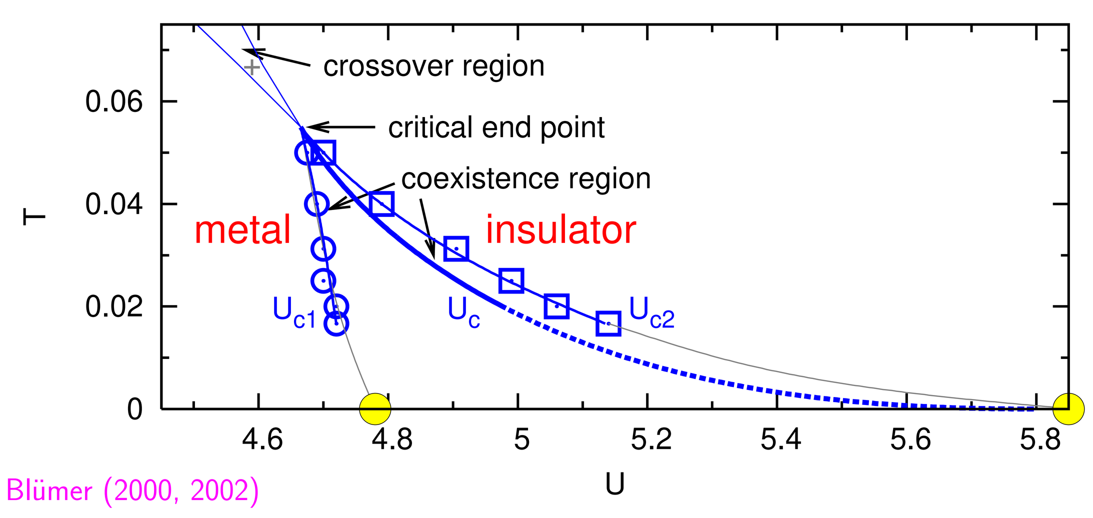




$\alpha_{\rm Cr} < \alpha_{\rm V} < \alpha_{\rm Ti}$   Limelette et al., Science **302**, 89 (2003)

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

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

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 $T \to 0$ from

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

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

**Needed: precise low-T/ground state energetics**

## Mott insulator: $10^{\rm th}$ order PT vs. QMC

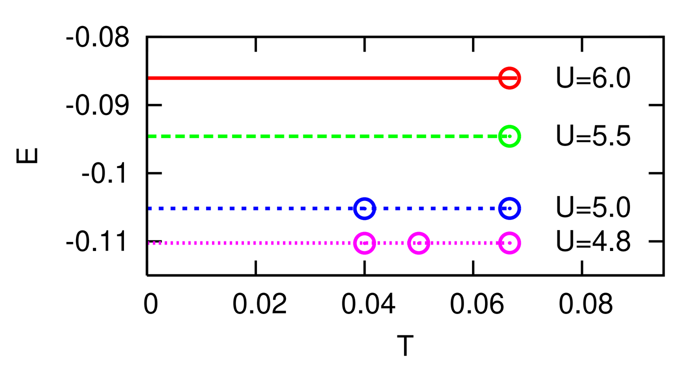
Kato-Takahashi perturbation theory in $d=\infty$ at $T=0$:

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

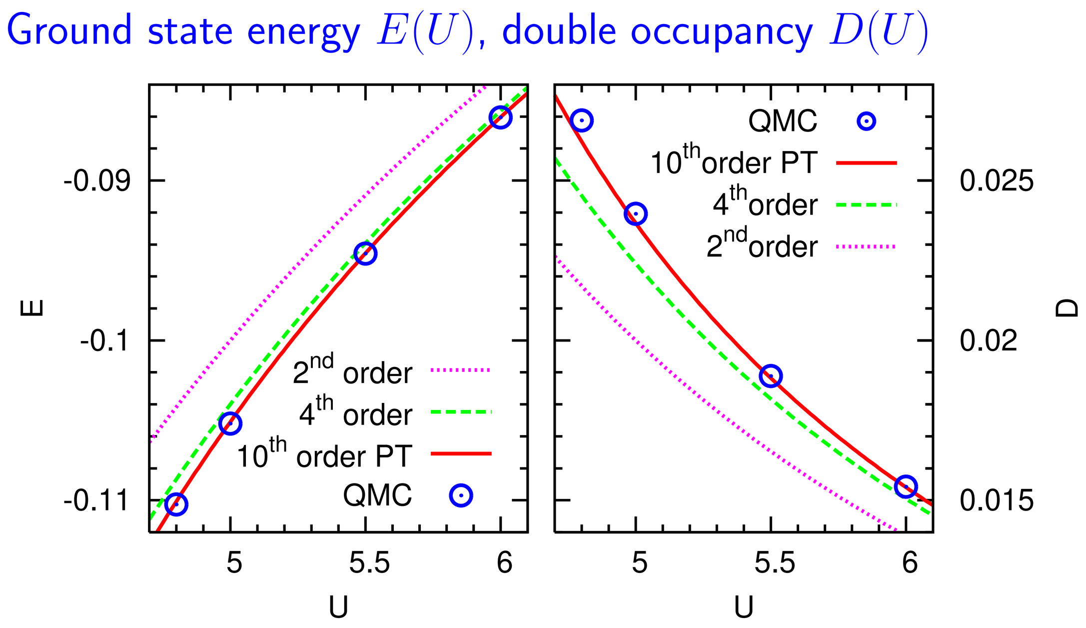
accuracy at $U \gtrsim 6$ [2]: $\Delta E_{\rm PT} \lesssim 10^{-5}$, $\Delta D_{\rm PT} \lesssim 10^{-5}$

Quantum Monte Carlo (QMC) solution of DMFT at finite $T$ using high-frequency corrections (cf. [3]):

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




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

by fitting coefficient ratios $U_{c1}[2i] \equiv (a_{2i+2}/a_{2i})^{1/2}$ to $U_{c1}[n] \approx U_{c1} + u_1\, n^{-1} + u_2\, n^{-2}$

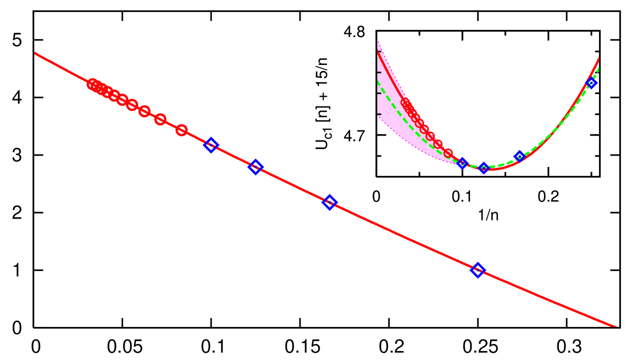
General consequences:

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

$a_n \;\propto\; n^\tau\, U^n_{c1};\ \tau = -\frac{u_1}{U_{c1}}$

$E(U) \;\propto\; (U - U_{c1})^{\tau-1}$

$D(U) \;\propto\; (U - U_{c1})^{\tau-2}$




Specifics / numerical results of extrapolation:

Note: $U_{c1}[n]$ nearly linear in $1/n$.

Unrestricted quadratic fit (dashed) $\rightsquigarrow \tau \approx 3.44$, $U_{c1} \approx 4.75$

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 $\tau = 3.5 \rightsquigarrow U_{c1} = 4.782$, $E_{\rm ePT}(U)$, $D_{\rm ePT}(U)$

$U_{c1}$ agrees perfectly with NRG [4], DMRG [5], and SFA [6]; however $U_{c1} \approx 4.45$ and $\tau = 2.5$ in other DMRG study [7].

ePT similar in spirit to Singh's 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

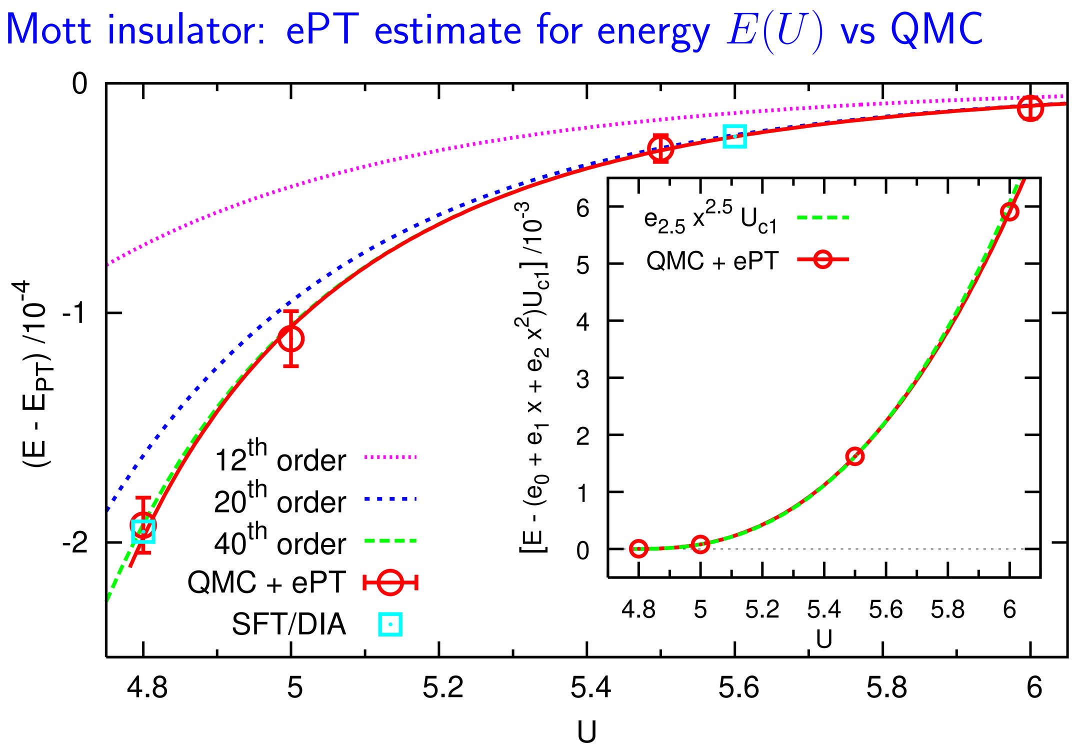



**Fig:** differences between QMC/full ePT/truncated ePT and 10th order PT. Inset: Contributions beyond non-critical terms (solid line) in comparison with leading critical term (dashed).

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

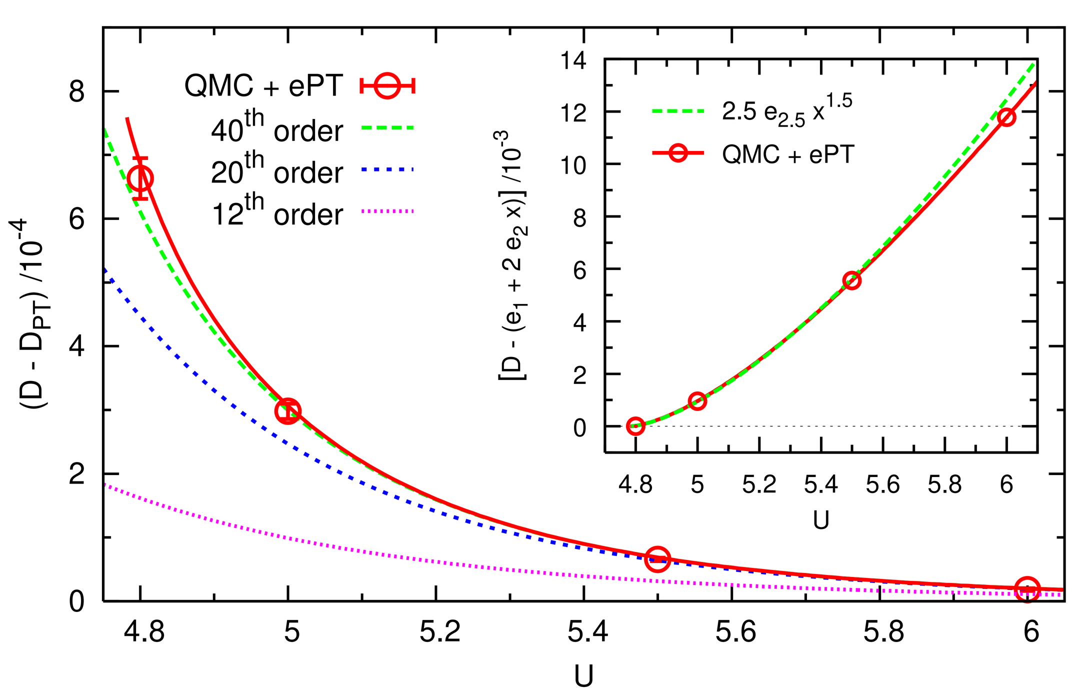



**Fig:** Double occupancy from QMC (circles) and ePT (solid lines) in complete analogy with previous figure [2].

## Summary

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

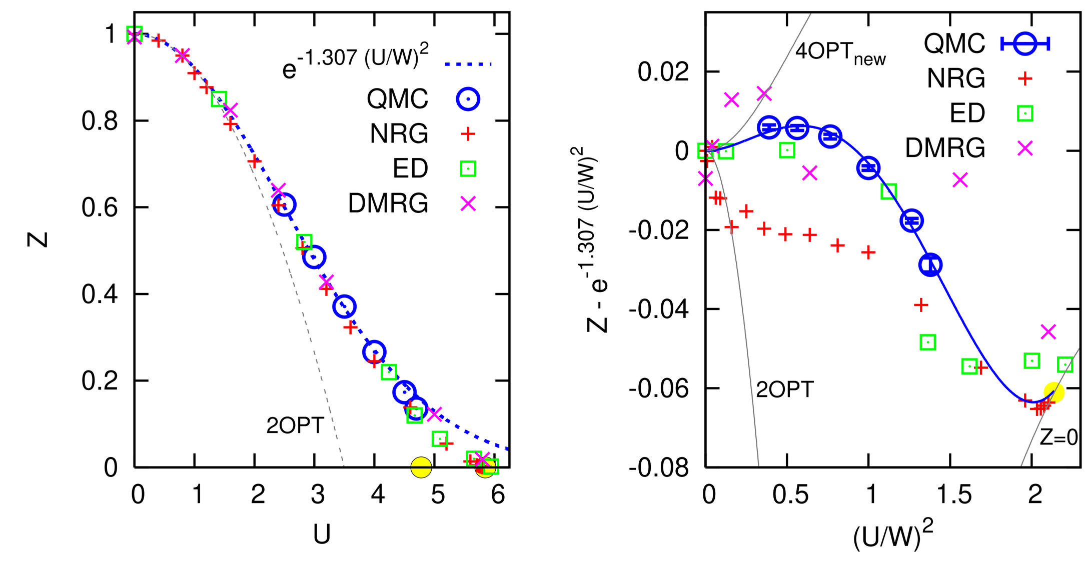
$E_{\rm crit} \propto (U - U_{c1})^{2.5}$, $D_{\rm crit} \propto (U - U_{c1})^{1.5}$.

Extreme precision at finite $T$ from improved QMC scheme. Current application: orbital-selective Mott transitions [3].

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 ($T \to 0$)

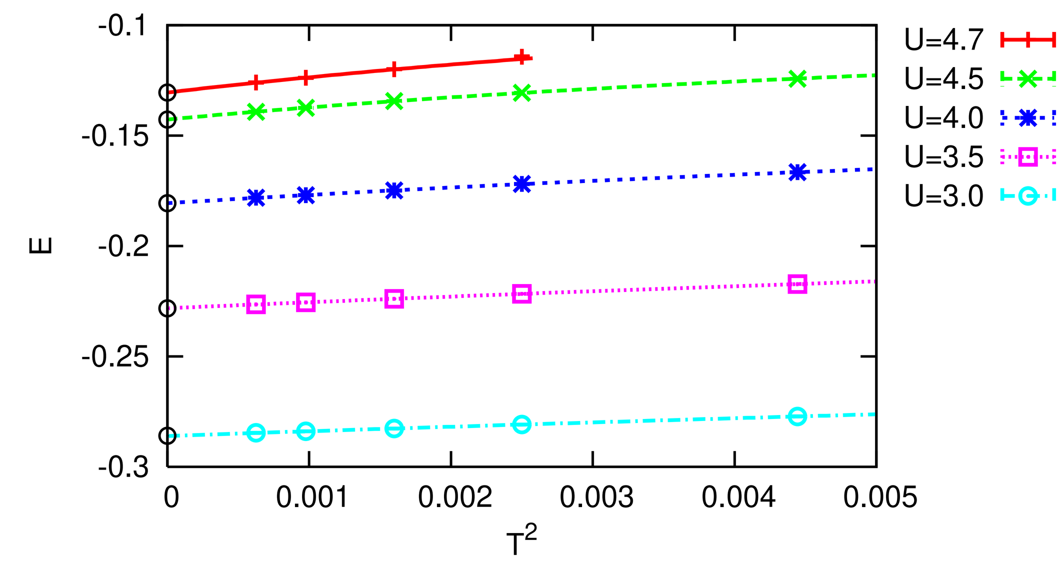
Quasiparticle weight/mass enhancement $Z = m/m^*$ at $T=0$



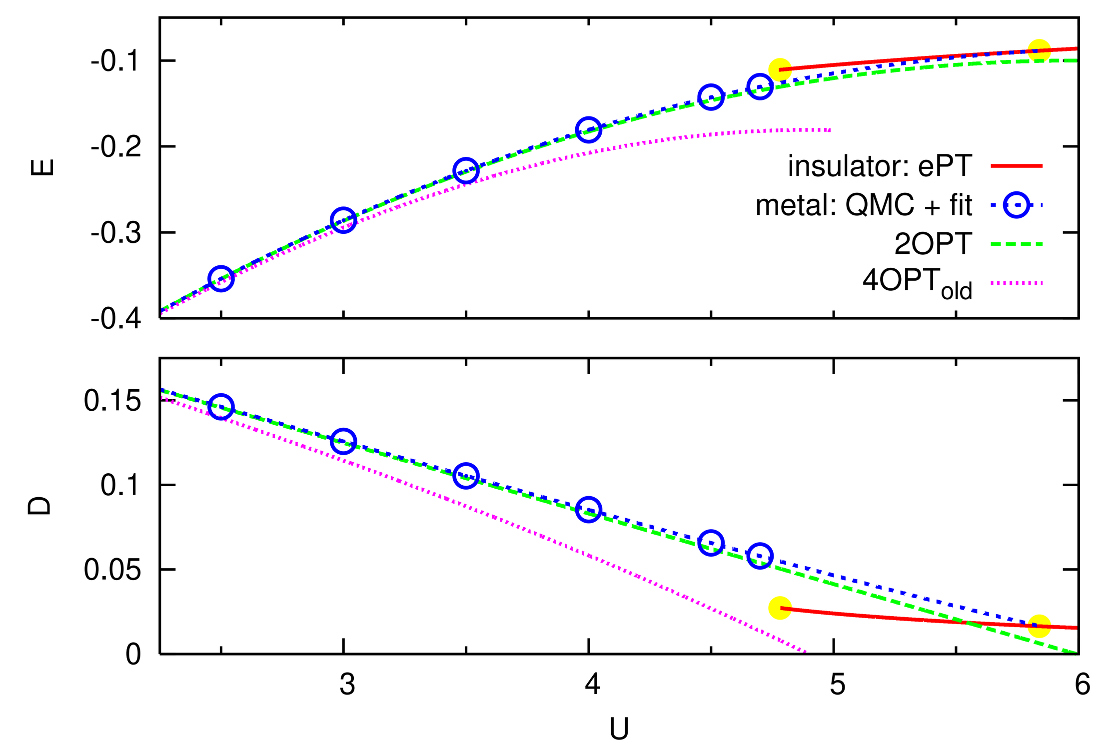

Fits to QMC roughly consistent with new 4OPT results [8].

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

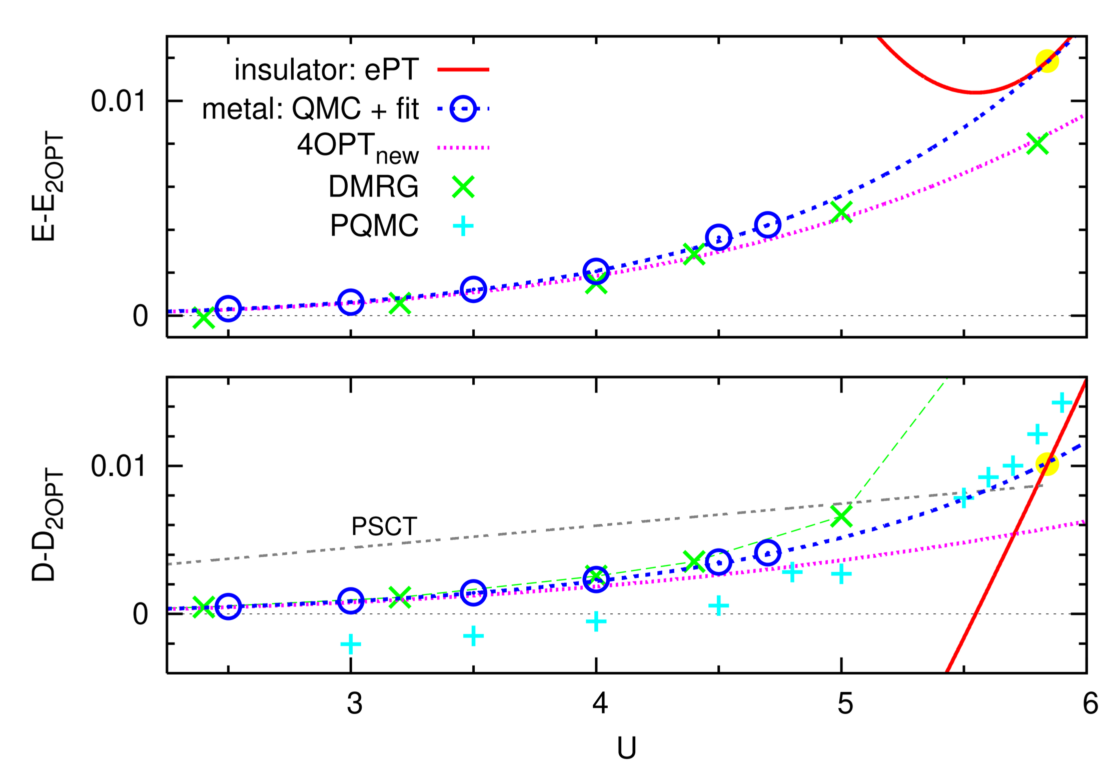
Energy $E(T,U)$ from QMC and extrapolation $T \to 0$




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 results 4OPT$_{\rm old}$ for $E$ and $D$ [8] corrected by QMC.

## References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[7] S. Nishimoto, F. Gebhard, and E. Jeckelmann, J. Phys. C **16**, 7063 (2004).

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