How does a Fermi liquid break down – or does it?

Nils Blümer, Univ. Mainz

Outline

Introduction: Specific heat, Fermi liquid theory, DMFT

Kinks in low-T specific heat of correlated electron systems?

Multigrid Hirsch-Fye quantum Monte Carlo algorithm

Summary and outlook

Introduction

Specific heat

Reminder: $$C_V \equiv \left(\frac{\delta Q}{\delta T}\right)_V = \left(\frac{\partial E}{\partial T}\right)_V = T\left(\frac{\partial S}{\partial T}\right)_V$$

absorbed heat Q
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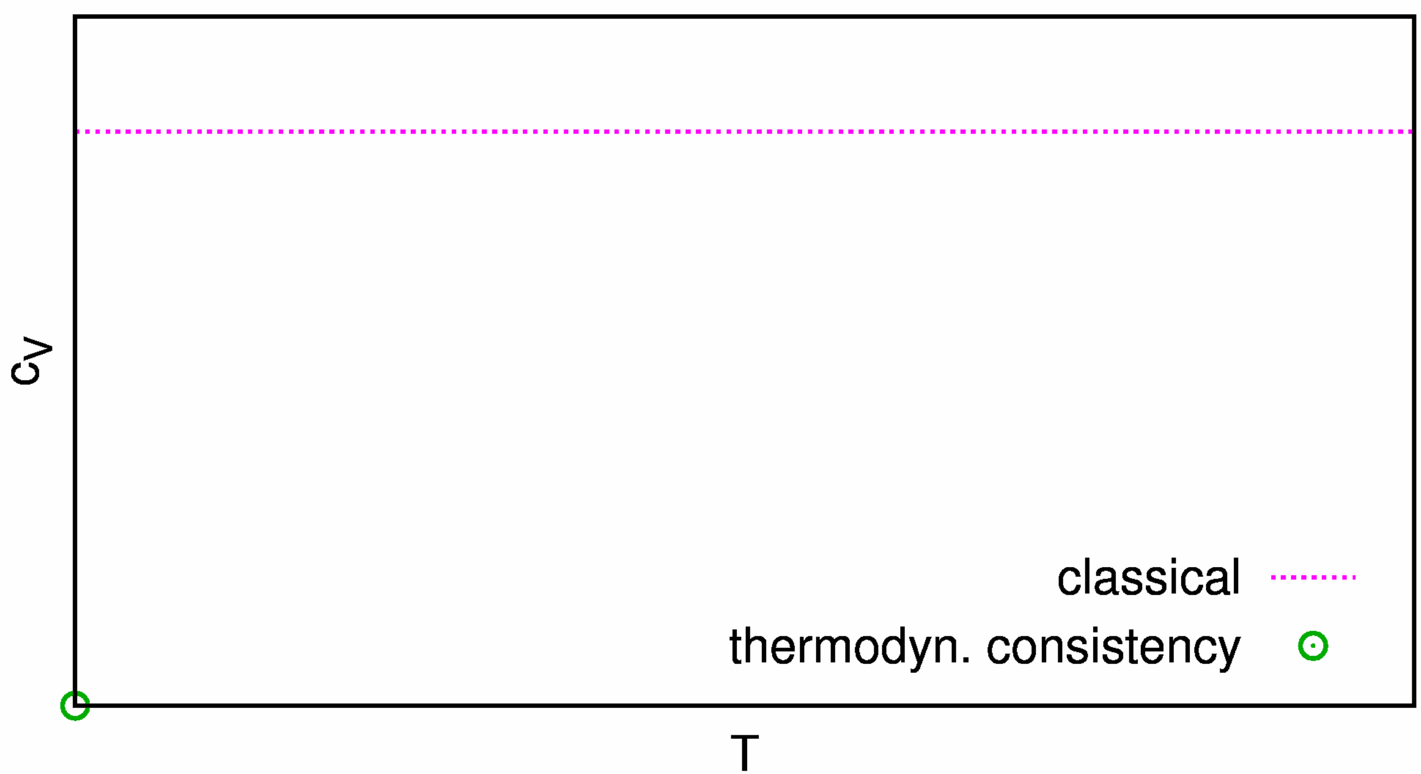

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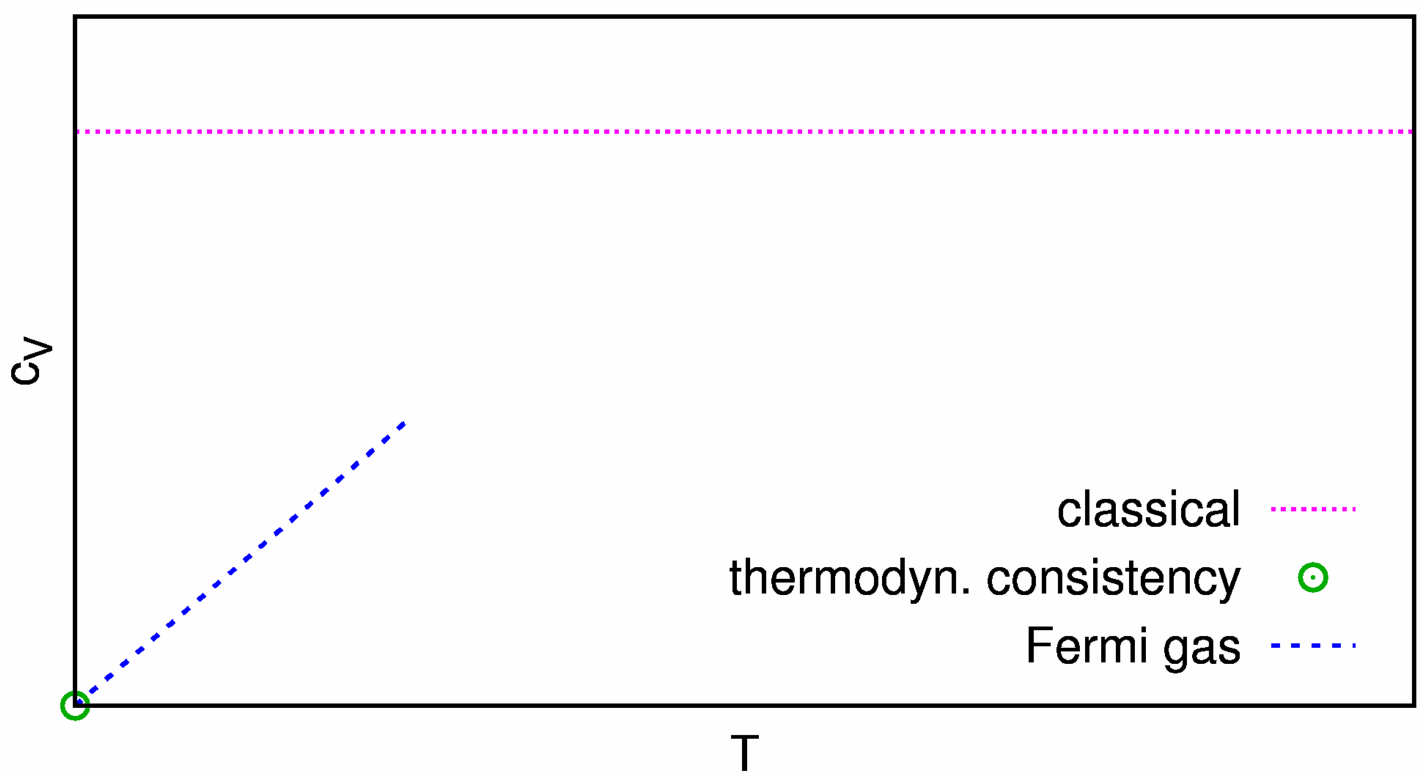

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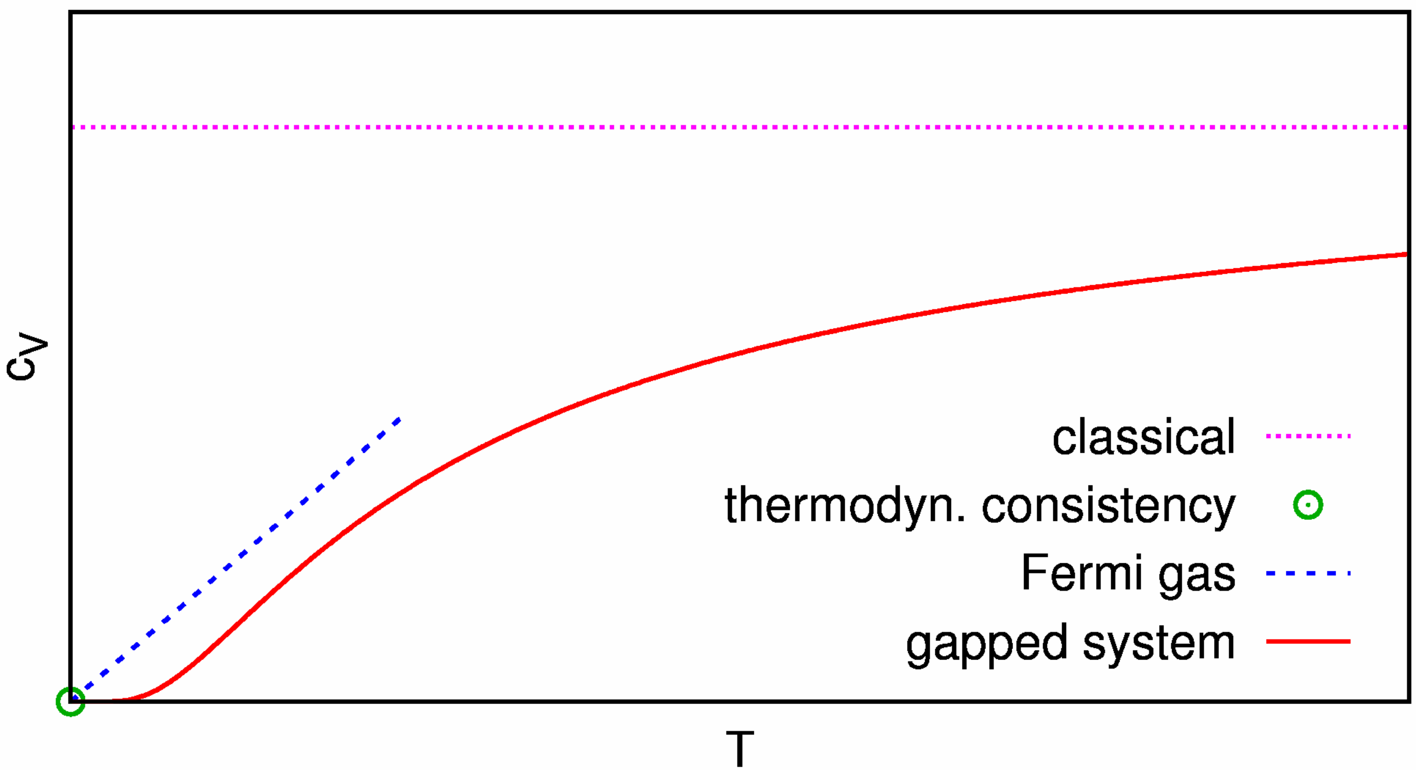

Sommerfeld expansion

For noninteracting Fermions (or effective 1-particle picture):

$$E(T) = \langle \epsilon \rangle_T \equiv \int_{-\infty}^{\infty} d\epsilon \, \epsilon \, \rho(\epsilon) \, f(\epsilon); \quad \text{DOS } \rho(\epsilon); \quad \text{Fermi function } f(\epsilon) = \left[\exp\left(\frac{\epsilon-\mu}{kT}\right) + 1\right]^{-1}$$

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$$I \equiv \int_{-\infty}^{\infty} d\epsilon\, H(\epsilon)\, f(\epsilon) = \int_{-\infty}^{\mu} d\epsilon\, H(\epsilon) + \sum_{n=1}^{\infty} a_n\, (kT)^{2n} \left.\frac{d^{2n-1} H(\epsilon)}{d\epsilon^{2n-1}}\right|_{\epsilon=\mu}$$

$$\text{with } a_1 = \tfrac{\pi^2}{6} \approx 1.64, \quad a_2 = \tfrac{7\pi^4}{360} \approx 1.89, \quad a_3 = \tfrac{31\pi^6}{15120} \approx 1.97, \quad a_n \xrightarrow{n\to\infty} 2$$

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Consequences:

$$E_{\text{electronic}}(T) = E_0 + \frac{\gamma}{2} T^2 + e_4 T^4 + \ldots$$

$$C_{\text{electronic}}(T) = \gamma T + 4 e_4 T^3 + \ldots \qquad \text{with } \gamma = \left.\frac{\pi^2}{3}\rho(\epsilon)\right|_{\epsilon=\mu}$$

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But: lattice contribution $C_{\text{lattice}} \sim T^3$ dominant in most solids for $T \gtrsim 10\text{K}$

Fermi liquid theory

Phenomenological approach [L. D. Landau, Zh. Eksp. Teor. Fiz. **30**, 1058 (1956)]:
mapping between noninteracting and interacting Fermi systems

Predictions:	linear specific heat	$c_V = \gamma T$	
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$$S(T) = \frac{1}{2\pi i T} \int_{-\infty}^{\infty} d\epsilon\, \rho(\epsilon) \int_{-\infty}^{\infty} d\omega\, \omega\, \frac{\partial f(\omega)}{\partial \omega} \left[\log G_R^{-1}(\epsilon,\omega) - \log G_A^{-1}(\epsilon,\omega)\right]$$

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Now assume a T-independent linear (local) self-energy: $\Sigma(\omega) \approx (Z^{-1} - 1)\,\omega$

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Leading Sommerfeld term $\rightsquigarrow$ $S(T) \approx c_V(T) \approx \frac{\pi^2}{3}\frac{\rho(0)}{Z} T = \frac{\gamma_0}{Z} T$

Leading corrections to Fermi liquid theory

$d = 1$: $\Delta c_V(T) \sim T \log(T)$ invalidates FL approach

$d = 2$: $\Delta c_V(T) \sim T^2$

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Fits of experimental data including $T^3 \log(T)$ term for heavy fermion UPt_3
[De Visser, Menovsky, Franse, Physica B+C **147**, 81 (1987)]

Numerical determination of specific heat for correlated systems

Naive approach: (i) compute $E(T)$ on grid $\{T_i\}_{i=1}^{N}$

(ii) use discrete differentiation $$c_V\left(\frac{T_i+T_{i+1}}{2}\right)=\frac{E(T_{i+1})-E(T_i)}{T_{i+1}-T_i}$$

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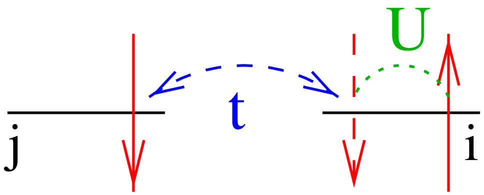
Established alternatives:

- use approximate methods, e.g. IPT (within DMFT) [Georges et al, RMP (1996)]
- fit polynomials to $2d$-QMC data for $E(T)$ [Duffy, Moreo, RPB **55**, 12918 (1997)]
- maximum entropy ansatz for energy levels [Huscroft, Gass, Jarrell, PRB **61**, 9300 (2000)]

Hubbard model

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



Captures important strong-correlation phenomena: Mott metal-insulator transition, (anti-) ferromagnetism, heavy fermions, high-T_c superconductivity (?), . . .

Few parameters: interaction U/W, temperature T/W, filling n, dispersion $\epsilon_{\boldsymbol{k}}$

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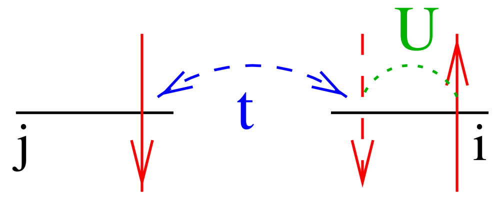

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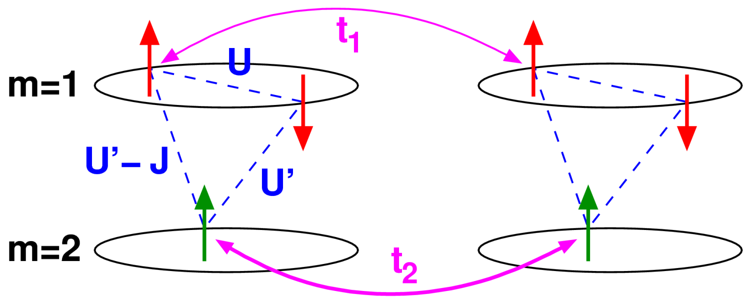

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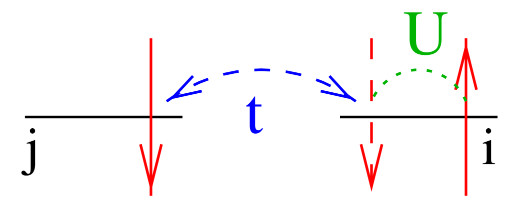

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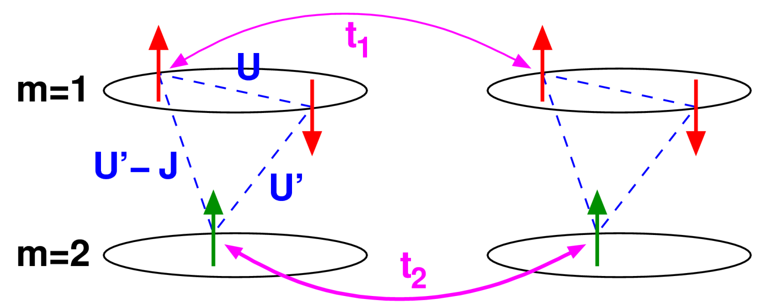

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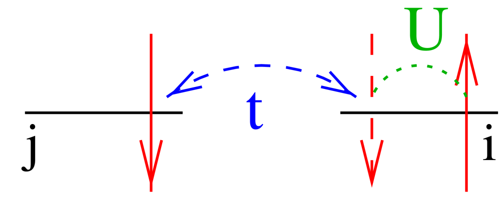

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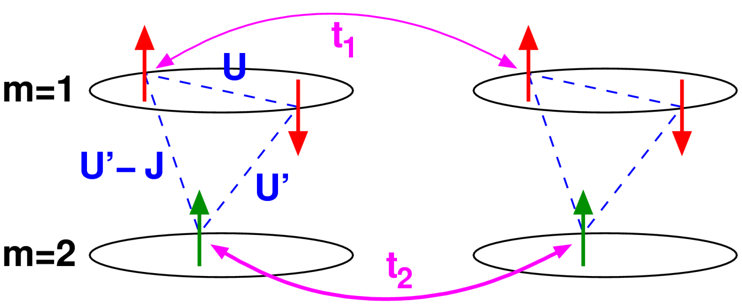
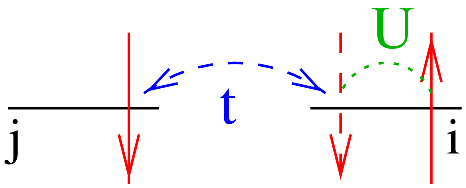


More complexity, more realistic: OSMT, spin+orbital order, LDA+DMFT, . . .

Approaches for Hubbard-type models

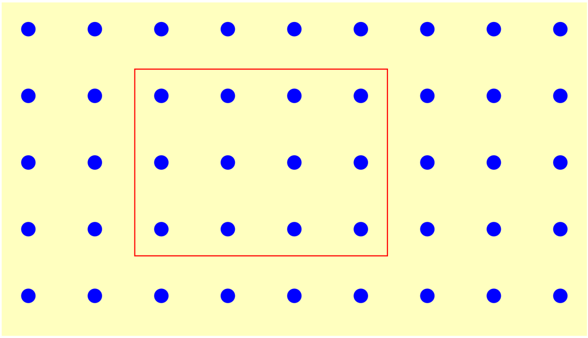
$$\hat{H} = \sum_{(i,j),\sigma} t_{ij} \, (\hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} + \text{h.c.}) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$



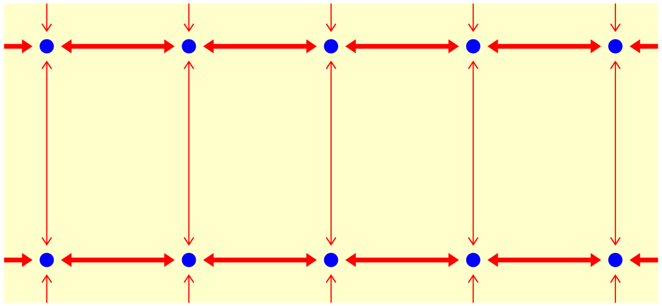
Perturbation theory

- $U \longrightarrow 0$: Hartree-Fock
  2nd order PT, . . .
- $t/U \longrightarrow 0$ (for $n = 1$)
  $\rightsquigarrow$ Heisenberg model

finite clusters: ED, QMC



$d \rightarrow 1$: Bethe ansatz, DMRG



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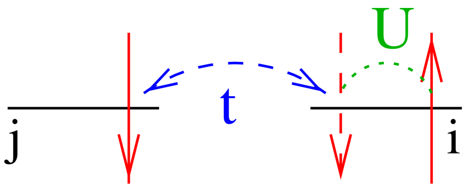

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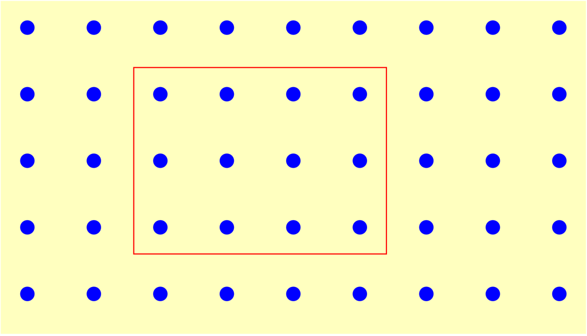

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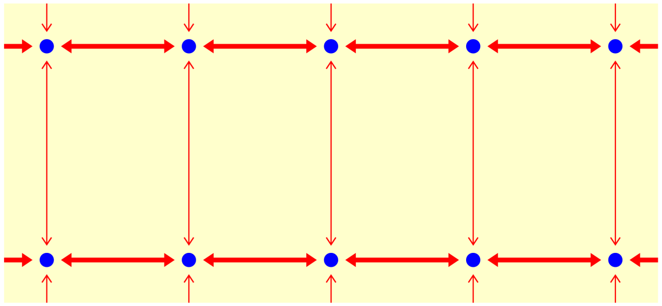
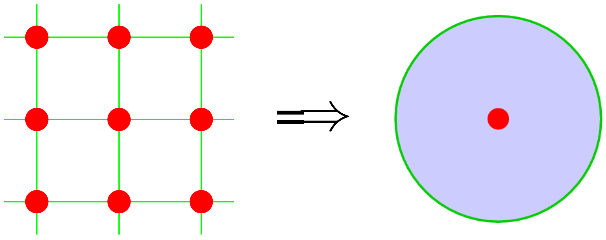


Dynamical mean-field theory (DMFT): local self-energy $\Sigma(\boldsymbol{k}, \omega) \equiv \Sigma(\omega)$

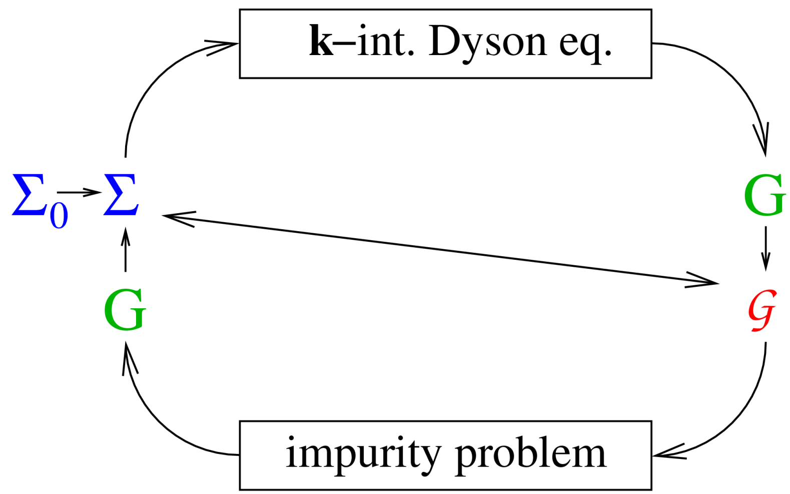
[Metzner, Vollhardt, PRL (1989), Georges, Kotliar, PRL (1992), Jarrell, PRL (1992)]

- \+ non-perturbative $\rightsquigarrow$ valid at MIT
- \+ dynamical on-site correlations preserved
- \+ in thermodynamic limit
- +/− exact for coordination $Z \to \infty$



Iterative solution of DMFT equations

0. Initialize self-energy
1. Solve Dyson equation
2. Solve single impurity Anderson model (SIAM)



$\longleftarrow$ DOS / t_{ij} / $\varepsilon_{\nu\boldsymbol{k}}$

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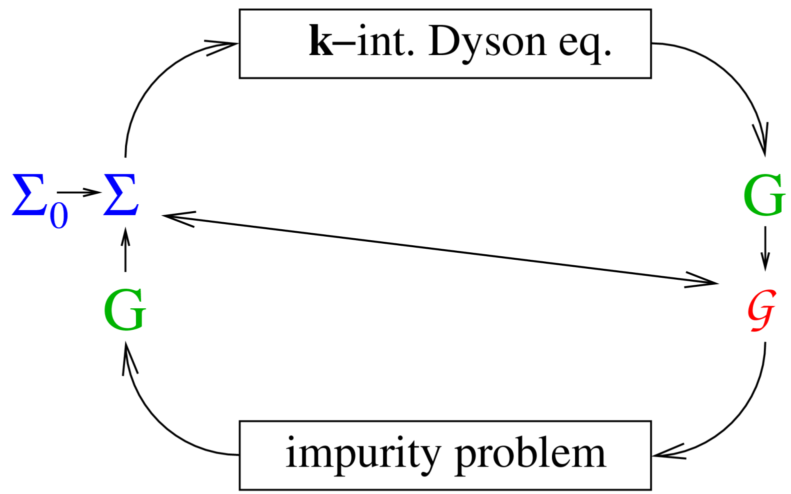

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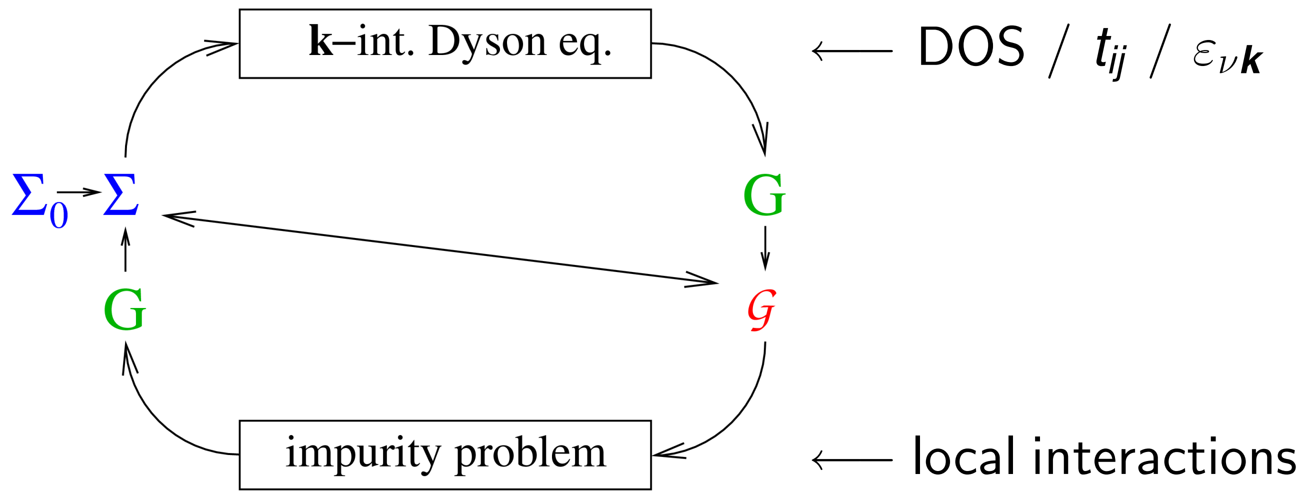
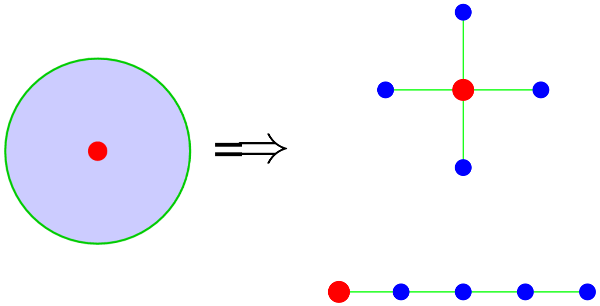


Impurity solver:

- Iterative perturbation theory (IPT; not controlled)
- Quantum Monte Carlo (QMC)
- Exact diagonalization (ED; large finite-size errors)
- Numerical renormalization group (NRG; 1-2 bands)
- Density matrix renormalization group (DMRG)
- Self-energy functional theory (SFT) + ED



Thermal breakdown of a Fermi liquid

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When/how do these laws break down?

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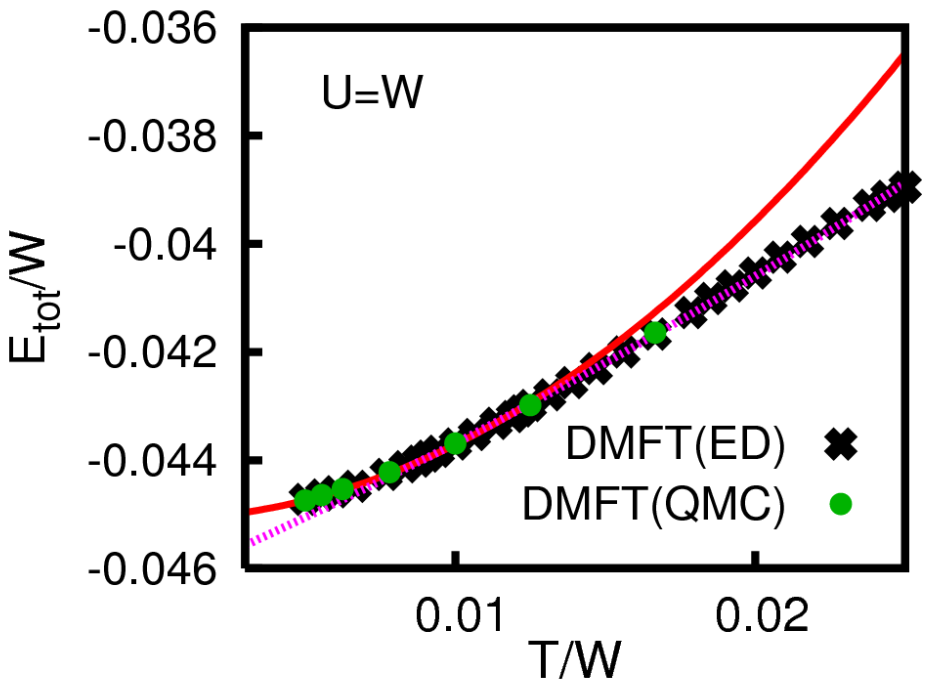
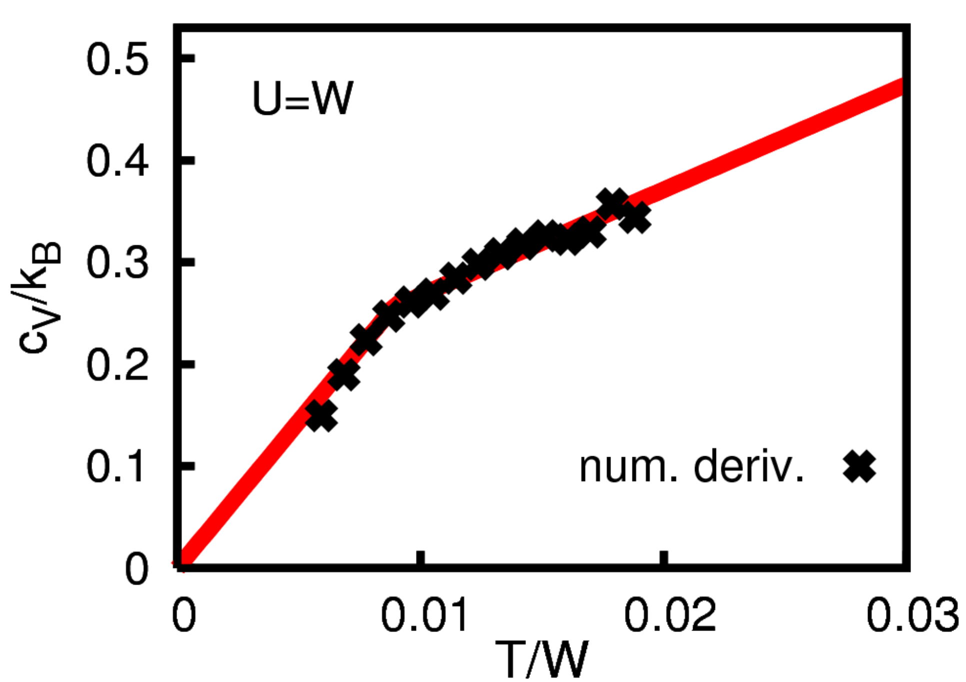
Exact diagonalization study (8 sites) for 1-band Hubbard model

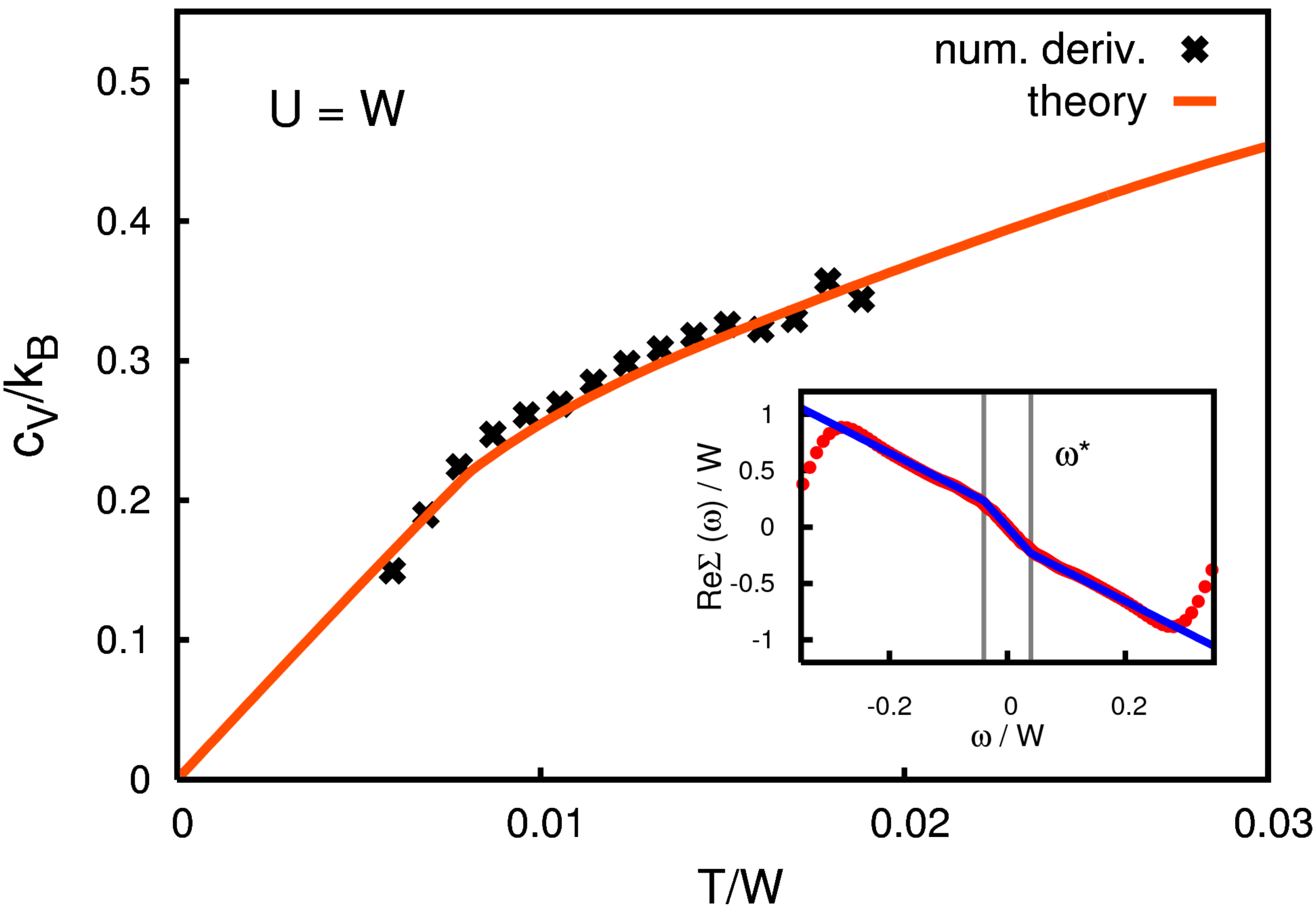




Distinct kink in c_V!

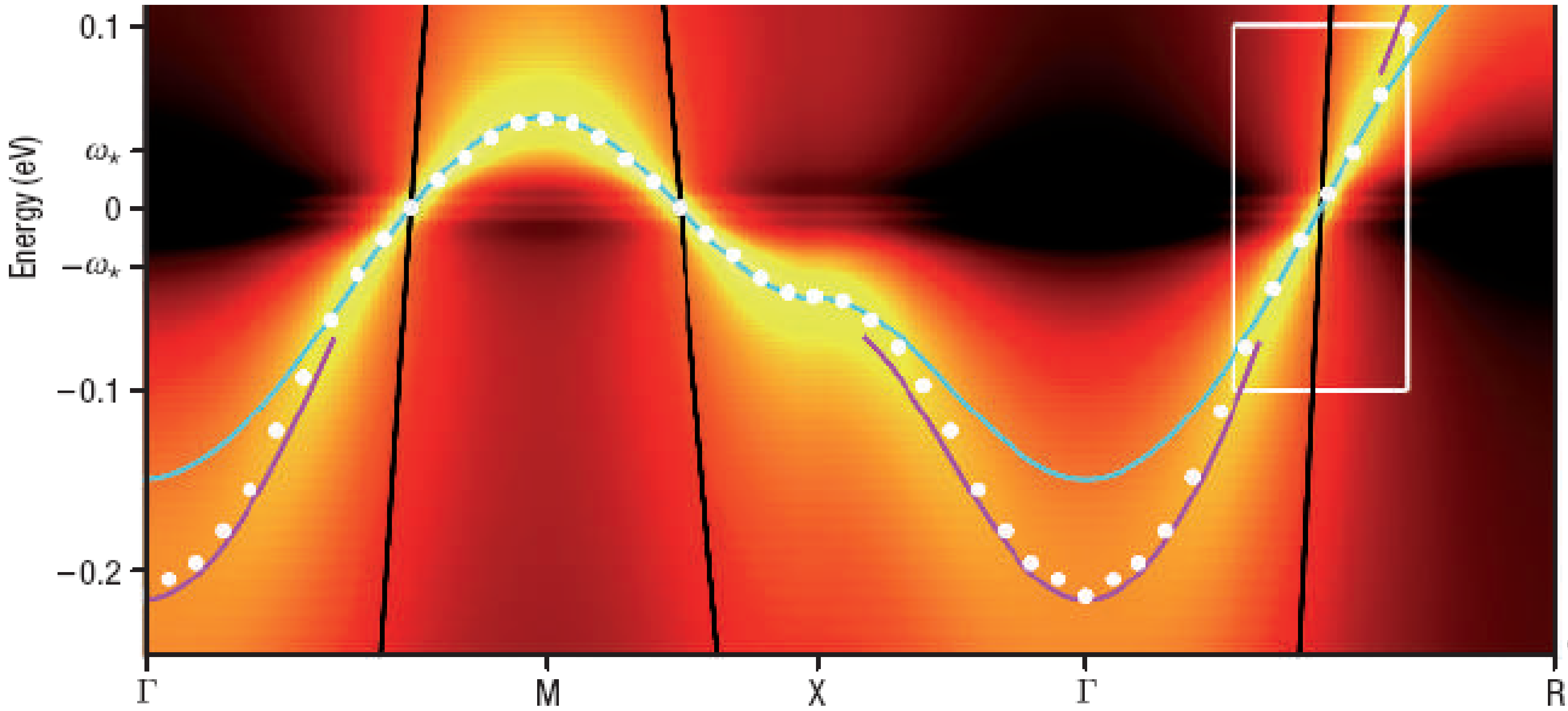
[A. Toschi, M. Capone, C. Castellani, K. Held, arXiv:0712.3723]

Theoretical explanation: kink in self-energy $\rightsquigarrow$ kink in c_V



[A. Toschi, M. Capone, C. Castellani, K. Held, arXiv:0712.3723]

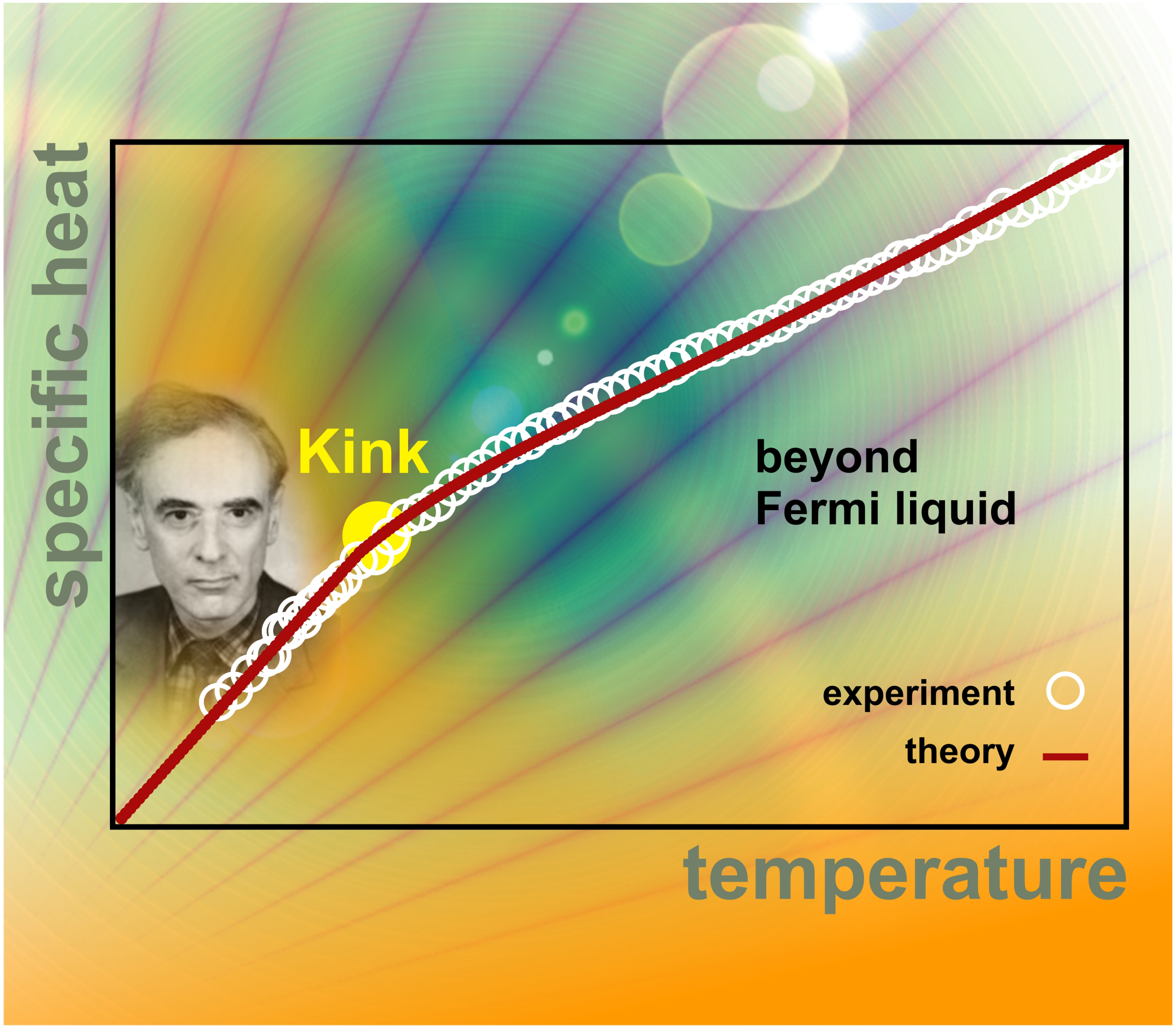
Established: kinks in ARPES spectra



Stronger renormalization of dispersion near Fermi energy

[Byczuk, Kollar, Held, Yang, Nekrasov, Pruschke, Vollhardt, Nature Physics **3**, 168 (2007)]

Kink feature visible in specific heat of heavy fermion LiV_2O_4?



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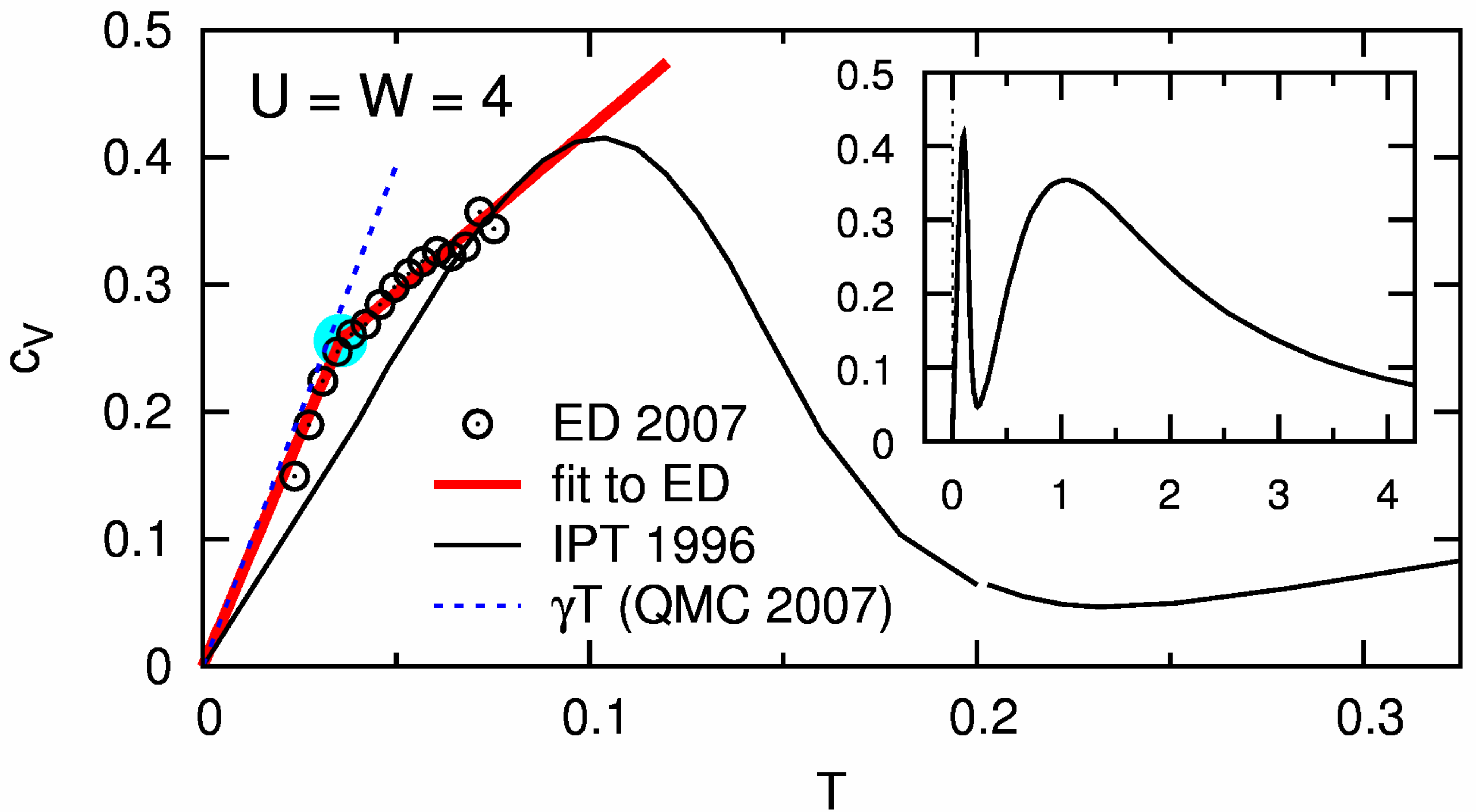
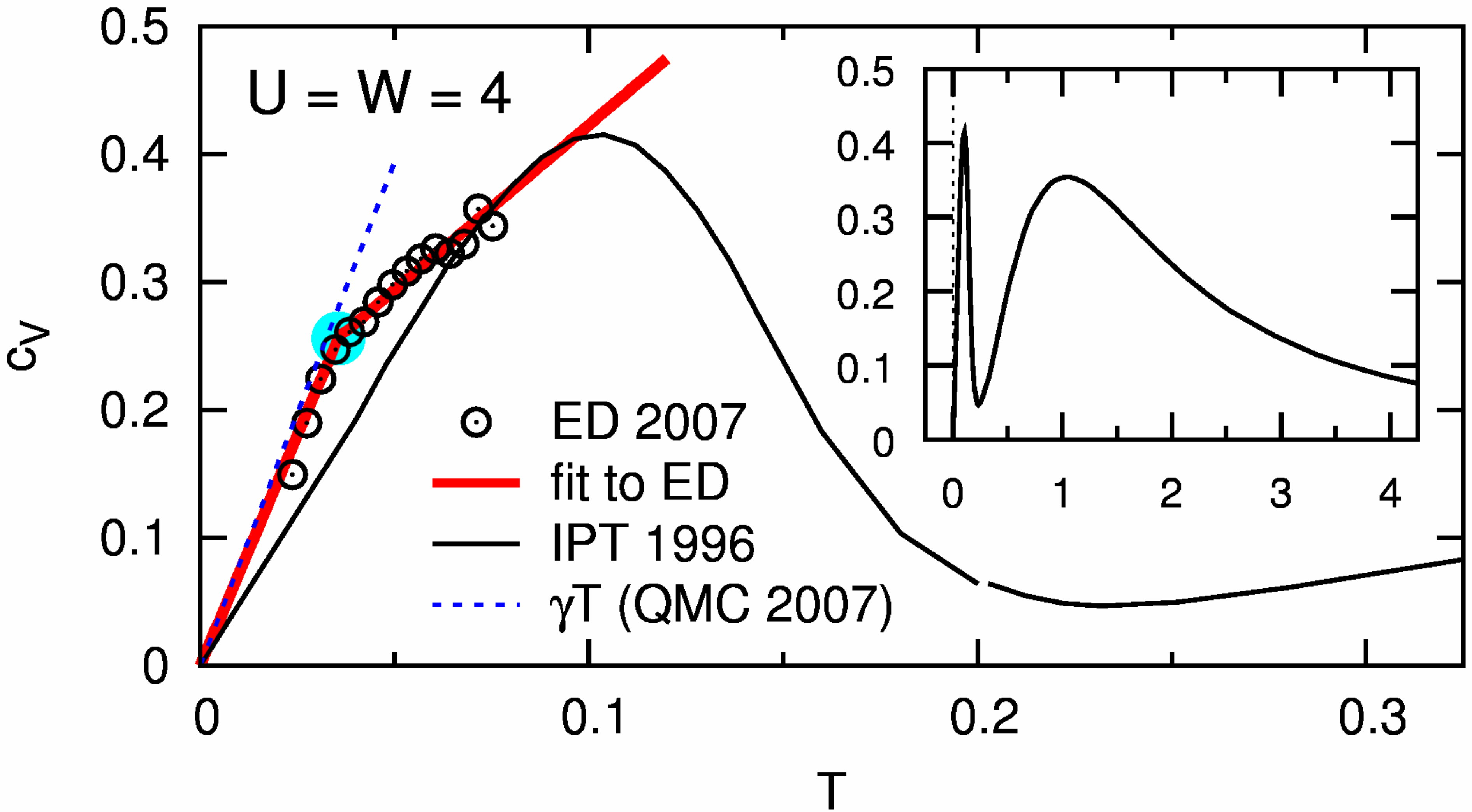
back to the model . . .



IPT: [Georges et al., RMP (1996)]

QMC: [NB, PRB **76**, 205120 (2007)]

ED: [A. Toschi *et al.* (2007)]



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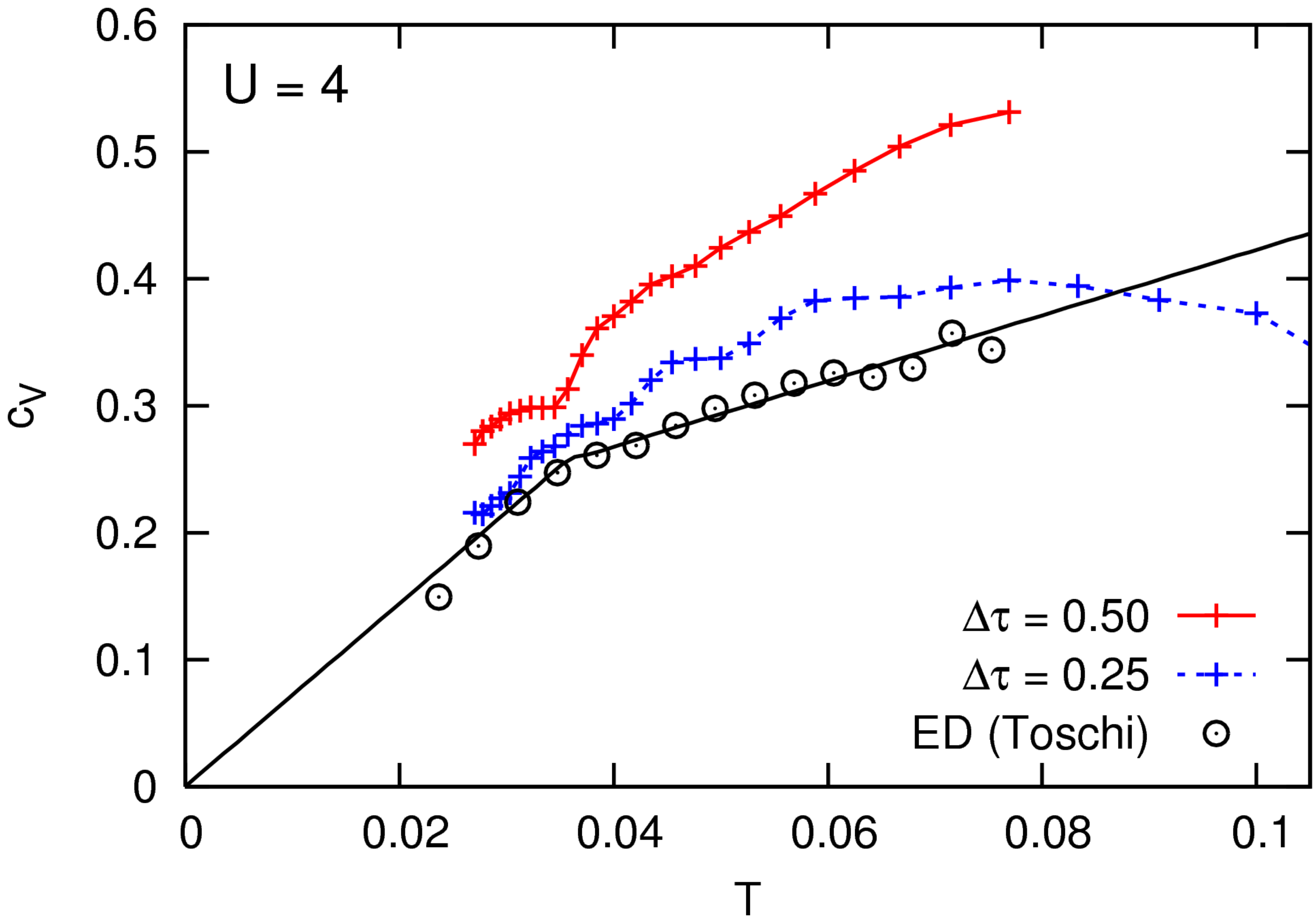
Significant discrepancies

Check using QMC. . .

First shot: conventional HF-QMC at constant discretization $\Delta\tau$,

numerical derivatives from parabolic interpolation of tripels



Roughly consistent with ED, but: no significant kinks, maximum at $T \approx 0.08$?

Best (only?) way to exclude kink: rescale data to straight line!

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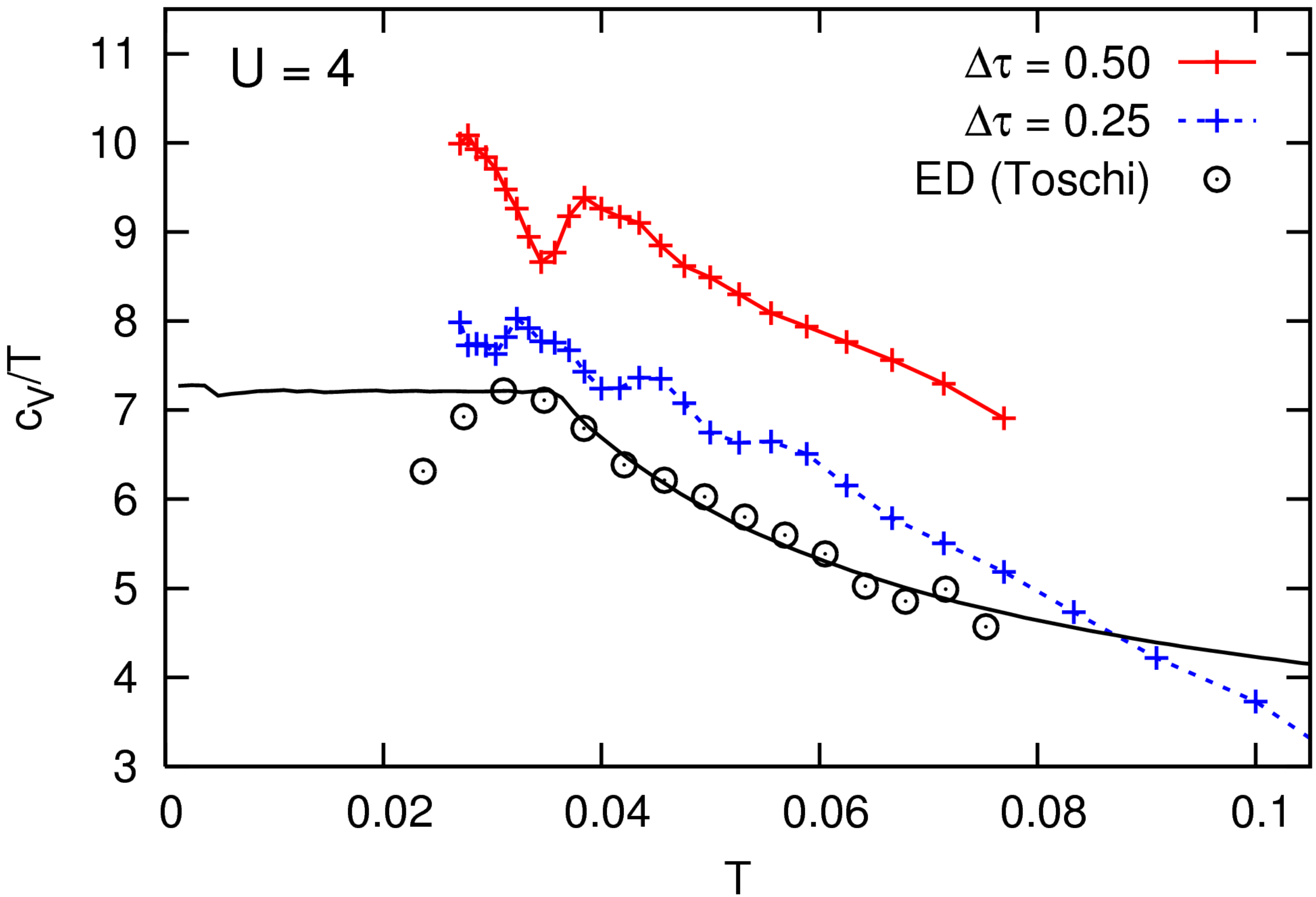
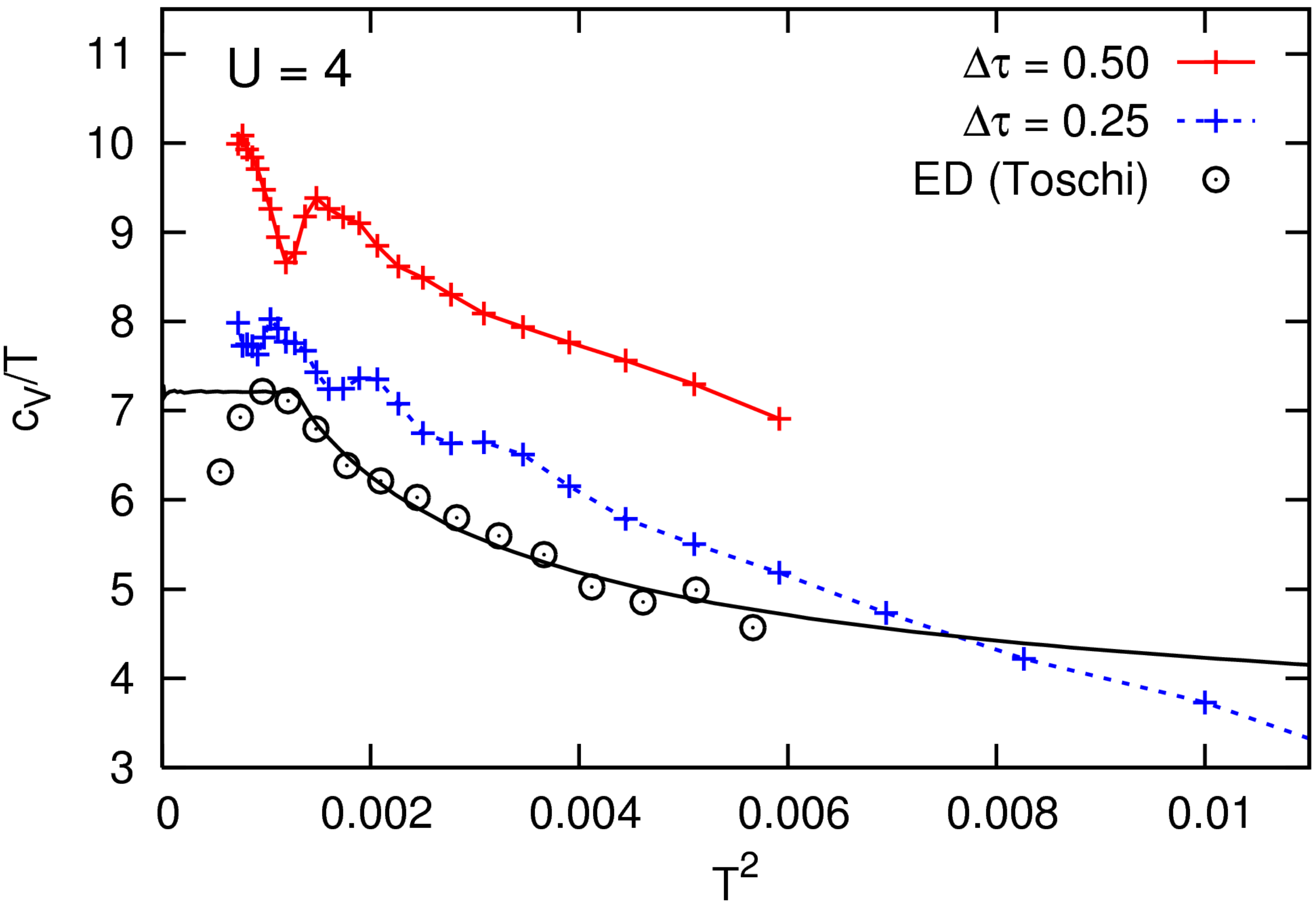
(i) consider c_V/T



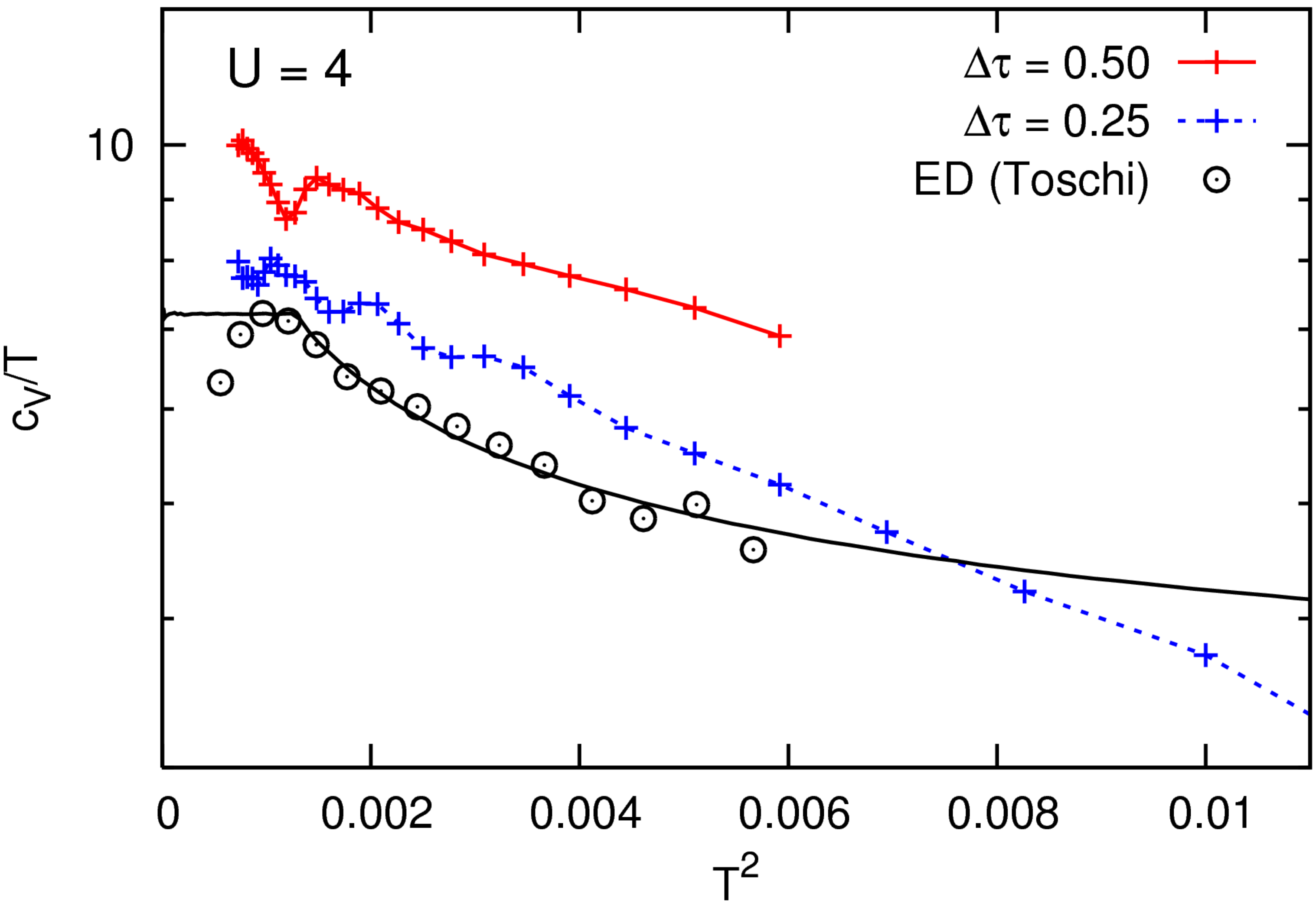
Best (only?) way to exclude kink: rescale data to straight line!

(i) consider c_V/T (ii) $T \longrightarrow T^2$



Best (only?) way to exclude kink: rescale data to straight line!

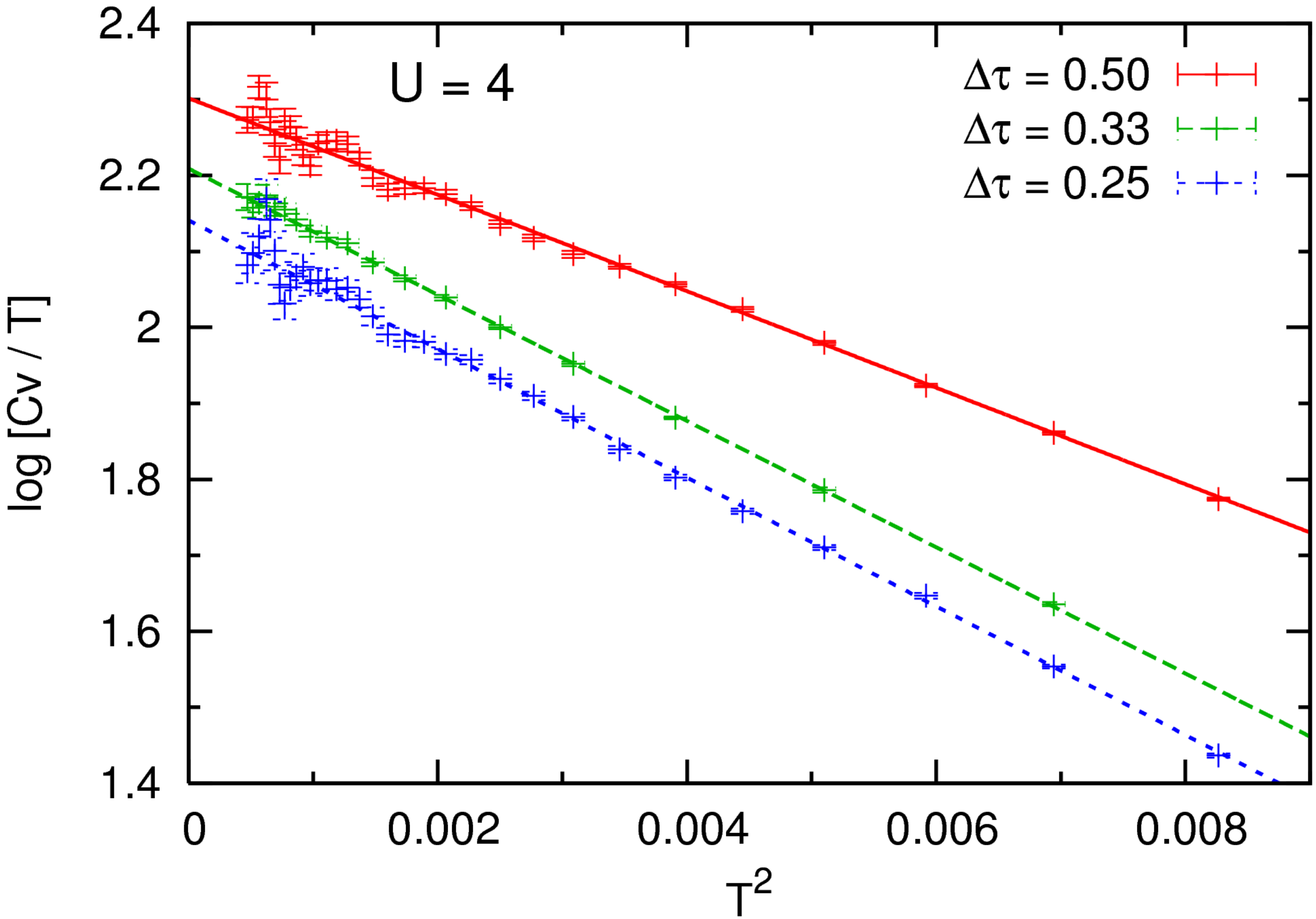
(i) consider c_V/T (ii) $T \longrightarrow T^2$ (iii) logarithmic scale



New hypothesis (for quasiparticle contribution): $c_V(T) \approx \gamma T\, e^{-aT^2}$

Now: more QMC sweeps + iterations, extended T range, smaller $\Delta\tau$

derivatives with error bars (via parabolic least-squares fits to 5-tupels)



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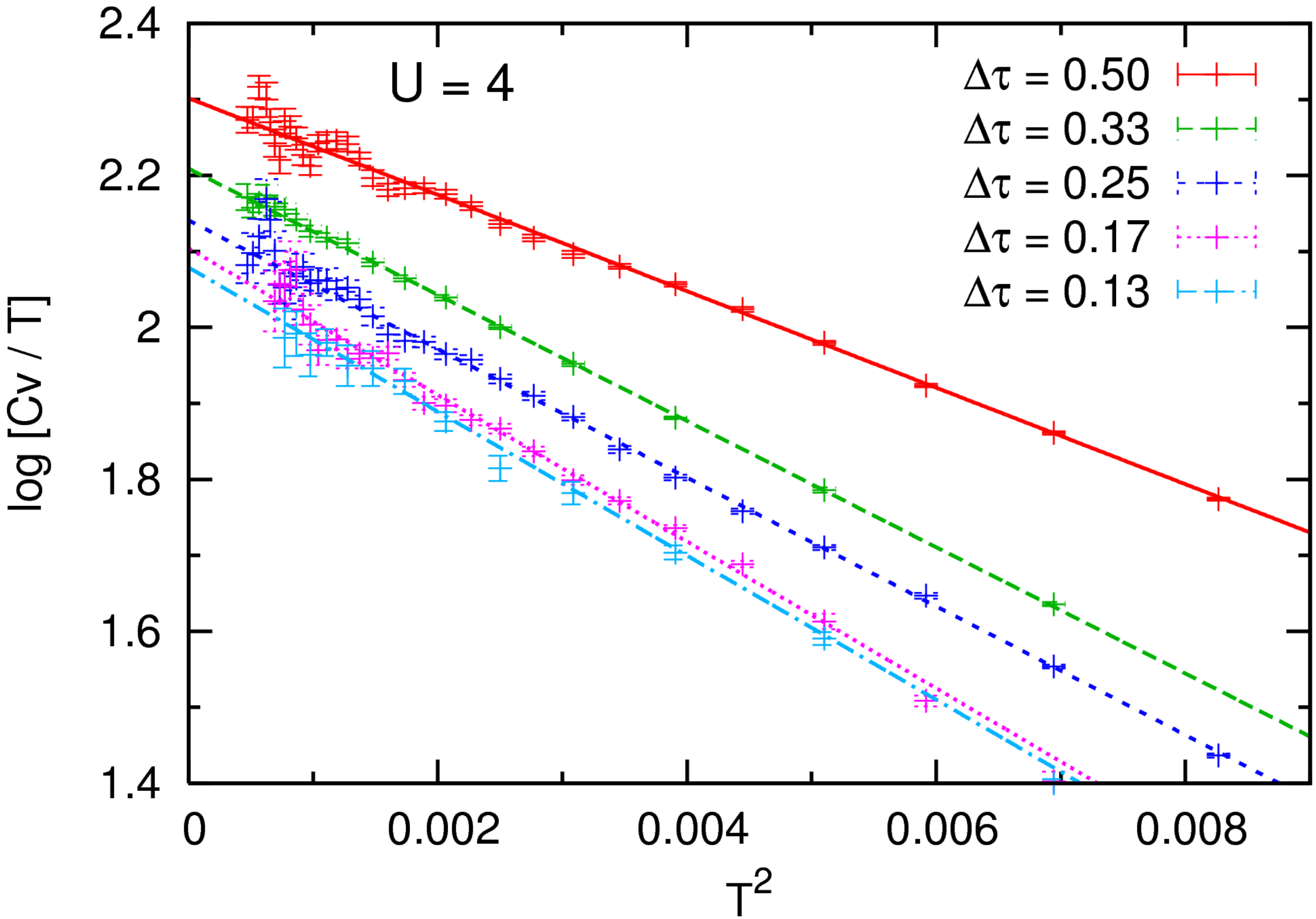

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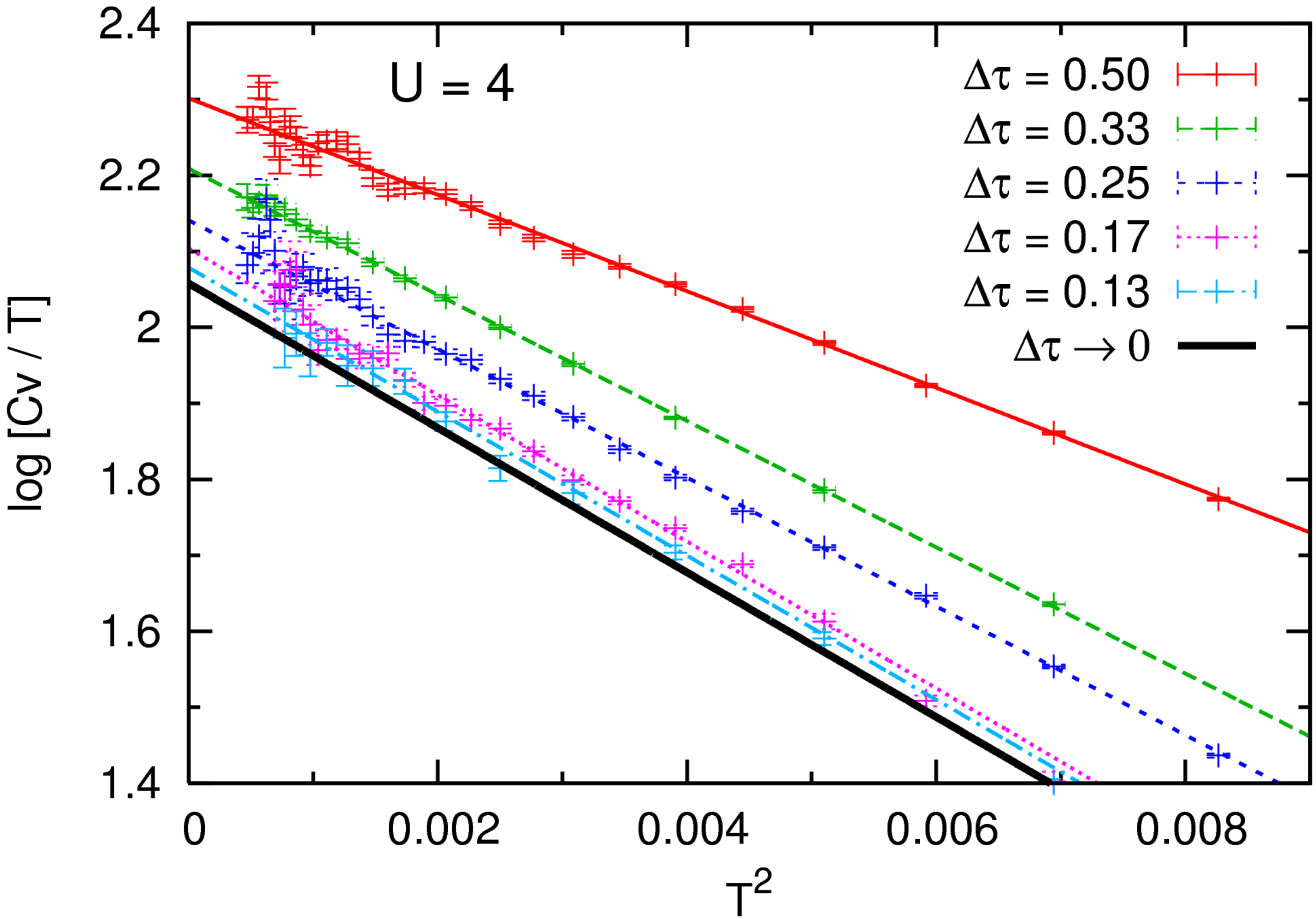
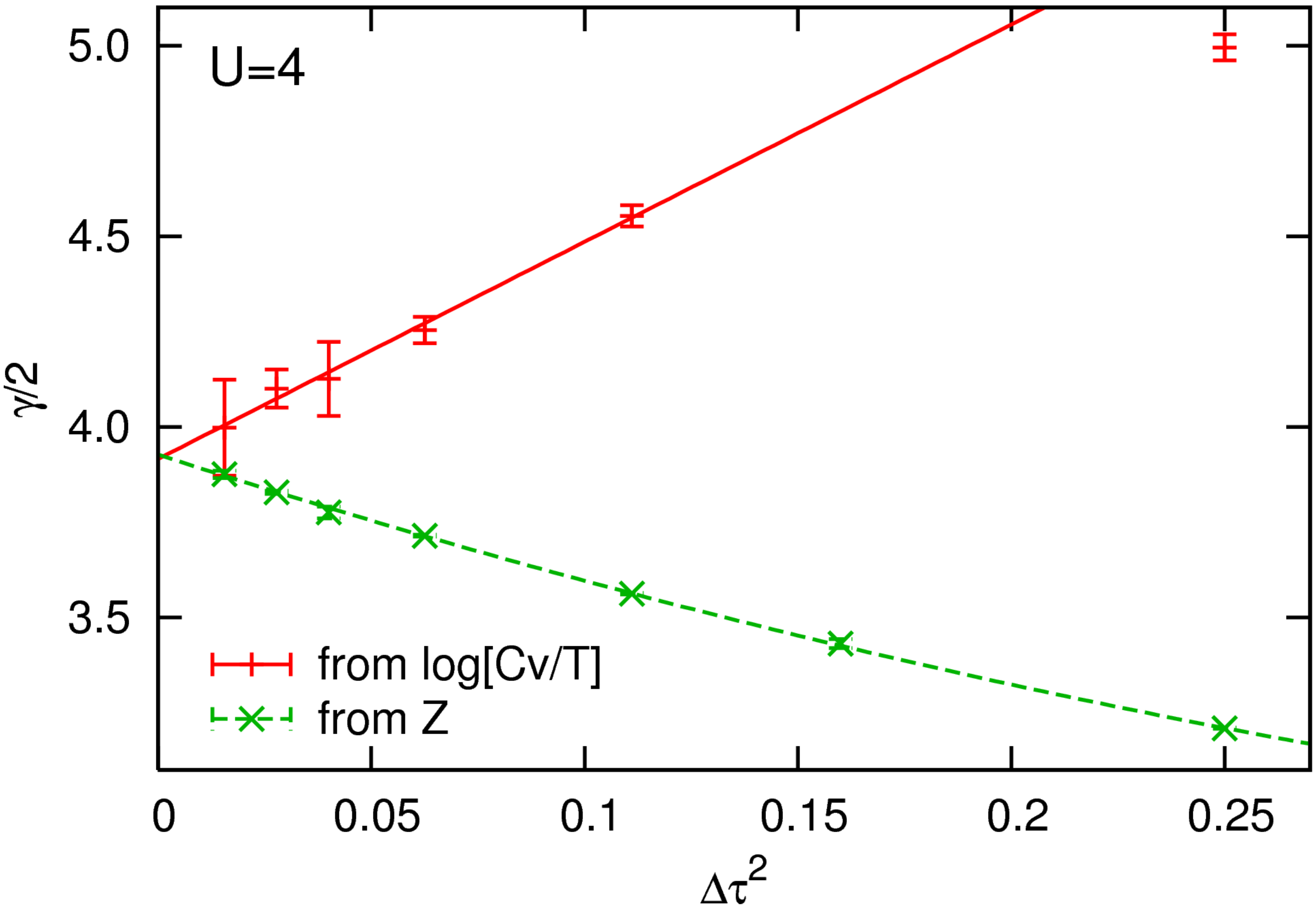


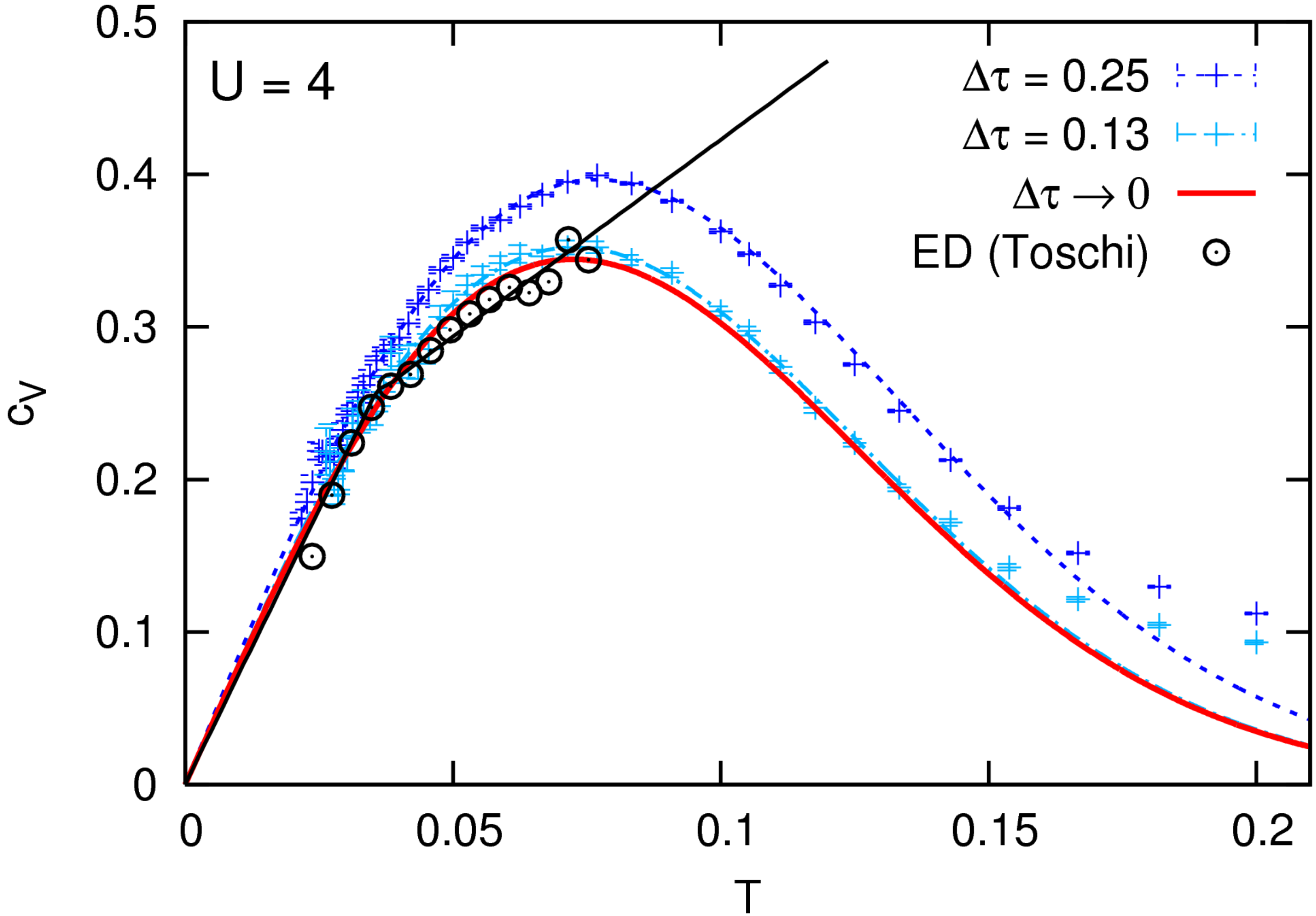
Parametric extrapolation $\Delta\tau \to 0$ is reliable

Independent check of γ via quasiparticle weight (from self-energy)



Perfect agreement (also with PRB **56**, 205120 (2007))

Now back to unscaled specific heat



Exponential law valid far beyond fit range ($T \leq 0.084$)

ED raw data has reasonable accuracy, but fit lines are incorrect

Is entropy consistent? Yes!

$$S(T) = \int_0^T dT' \, \frac{c_V(T')}{T'} = \int_0^T dT' \, 7.83\, T' e^{-95.14\, T'^2} \stackrel{T\to\infty}{\longrightarrow} 0.711 \approx 0.693 \approx \log(2)$$

Interpretation: free spins at $T \gtrsim 0.2$ (in subspace without double occupancies)

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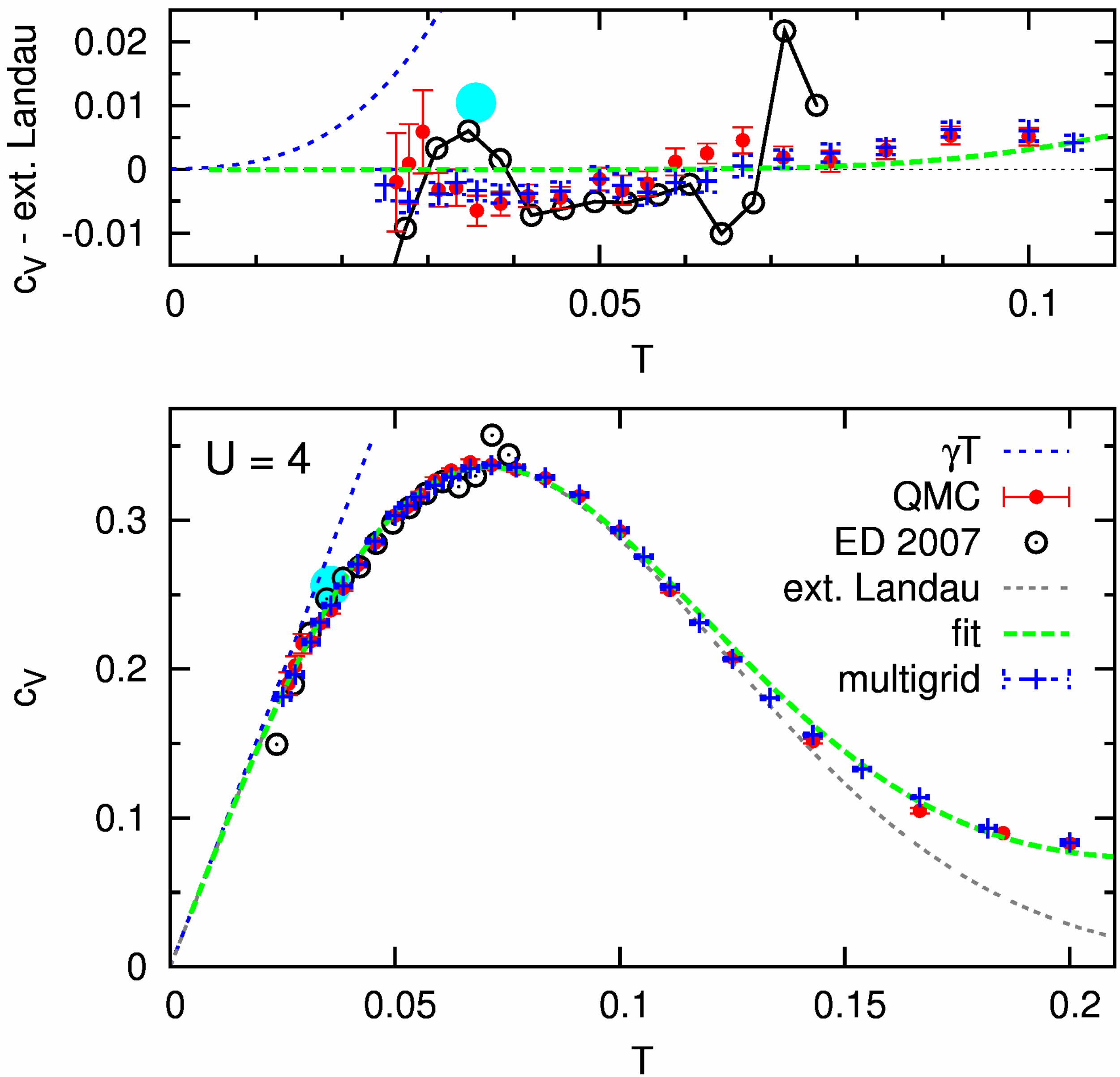
Generalized Fermi liquid law for quasiparticle contribution to specific heat

$$c_V(T) = \frac{2\pi}{3Z} T \exp\left[-(T/T_0)^2\right]; \quad T_0 = \frac{3\log(2)}{\pi^{3/2}} Z \qquad \text{(Bethe DOS)}$$

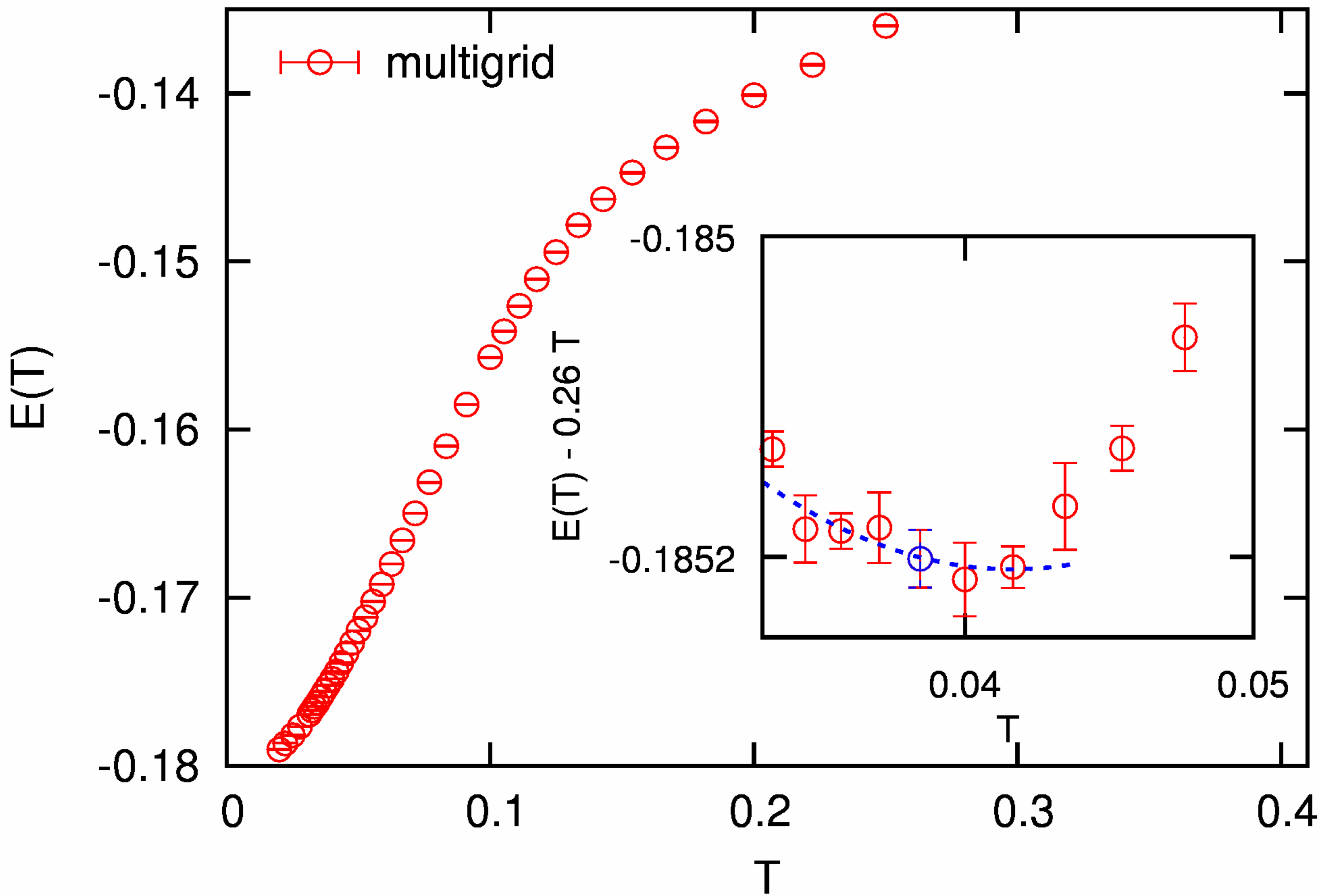
Single (low-frequency) qp weight $Z = \left.\frac{d\Sigma(\omega)}{d\omega}\right|_{\omega=0}$ governs c_V!

Prediction with no free parameters, to be tested at smaller/larger U.

Unbiased high-precision results from multigrid HF-QMC



In detail: numerical differentiation procedure



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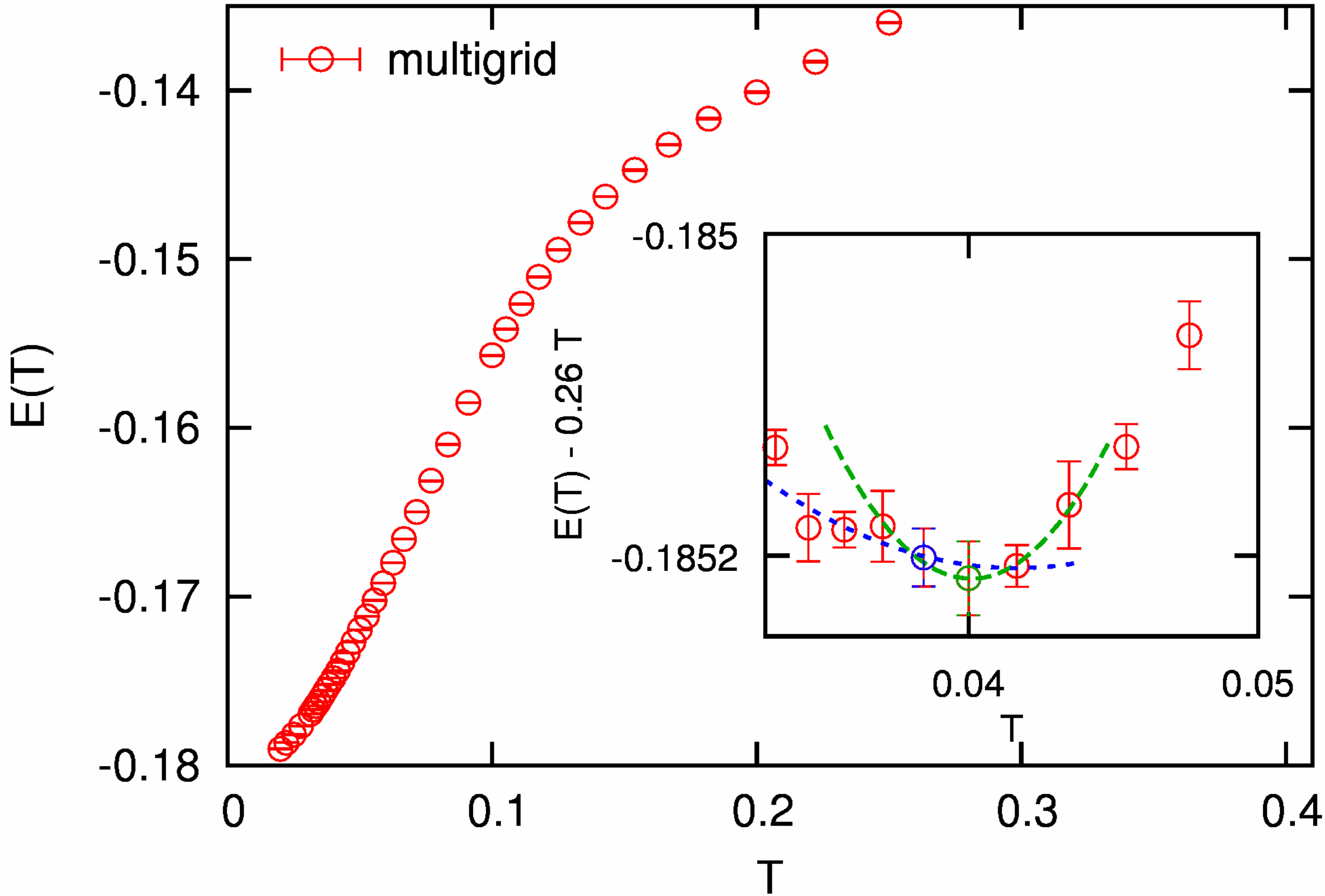

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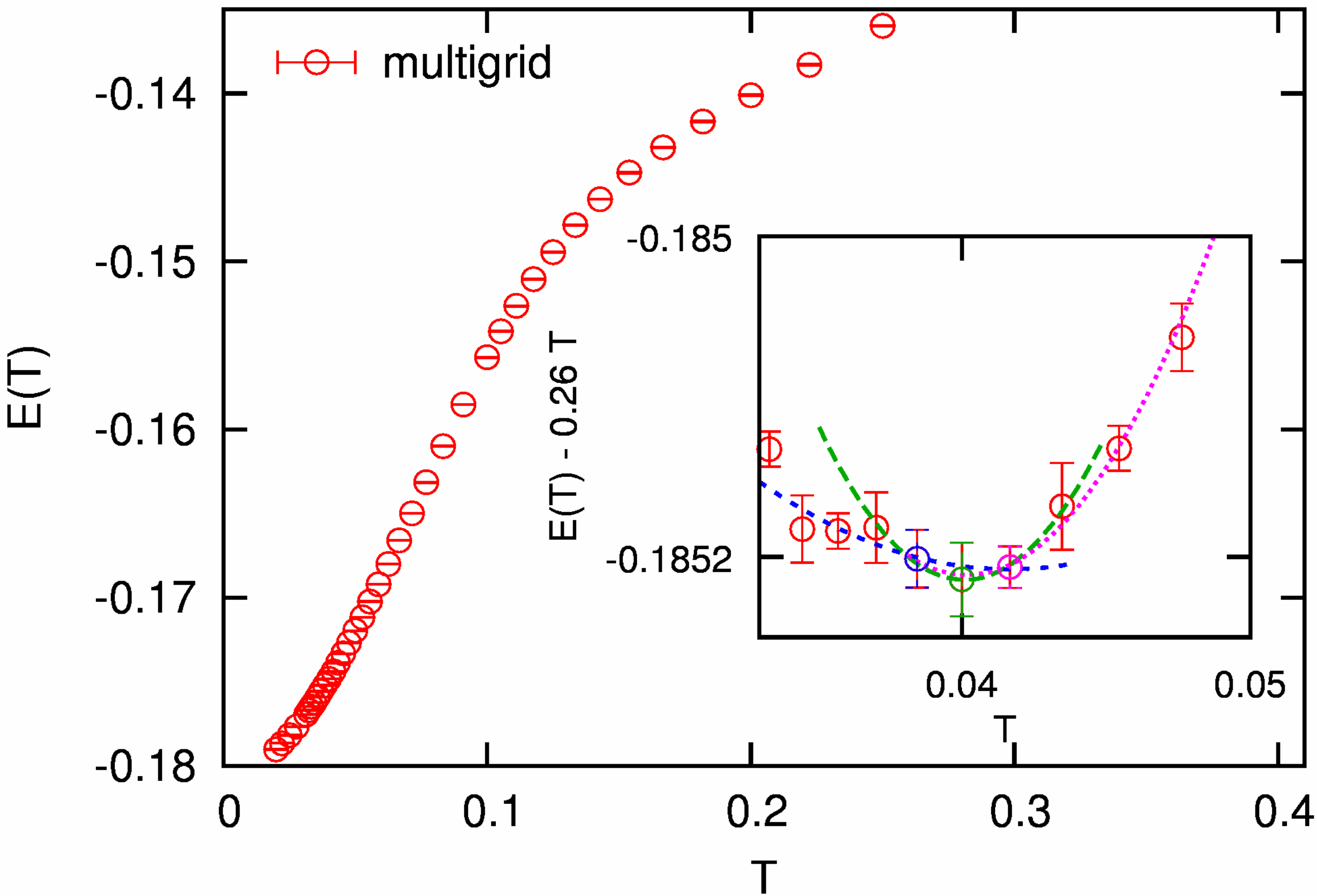

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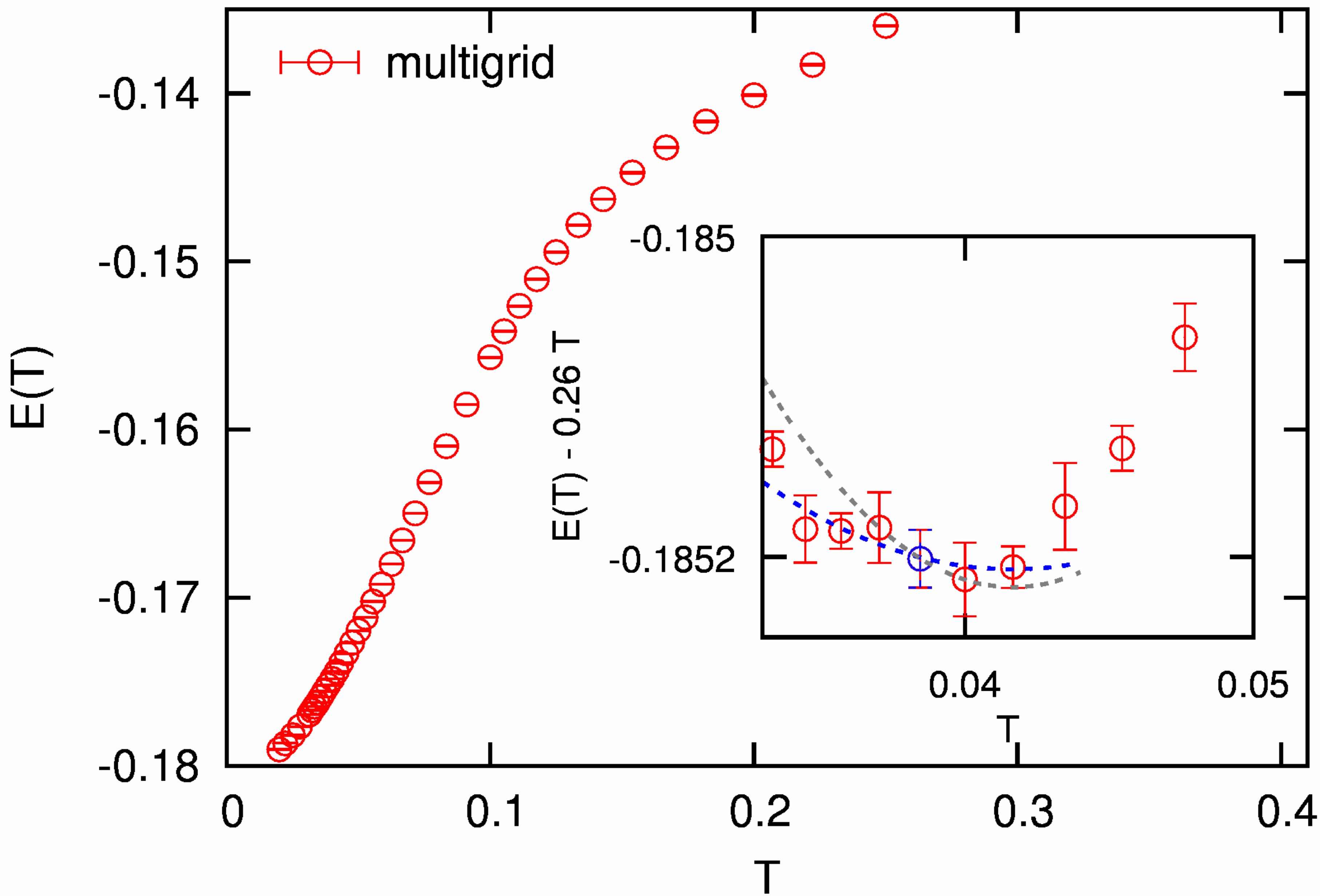
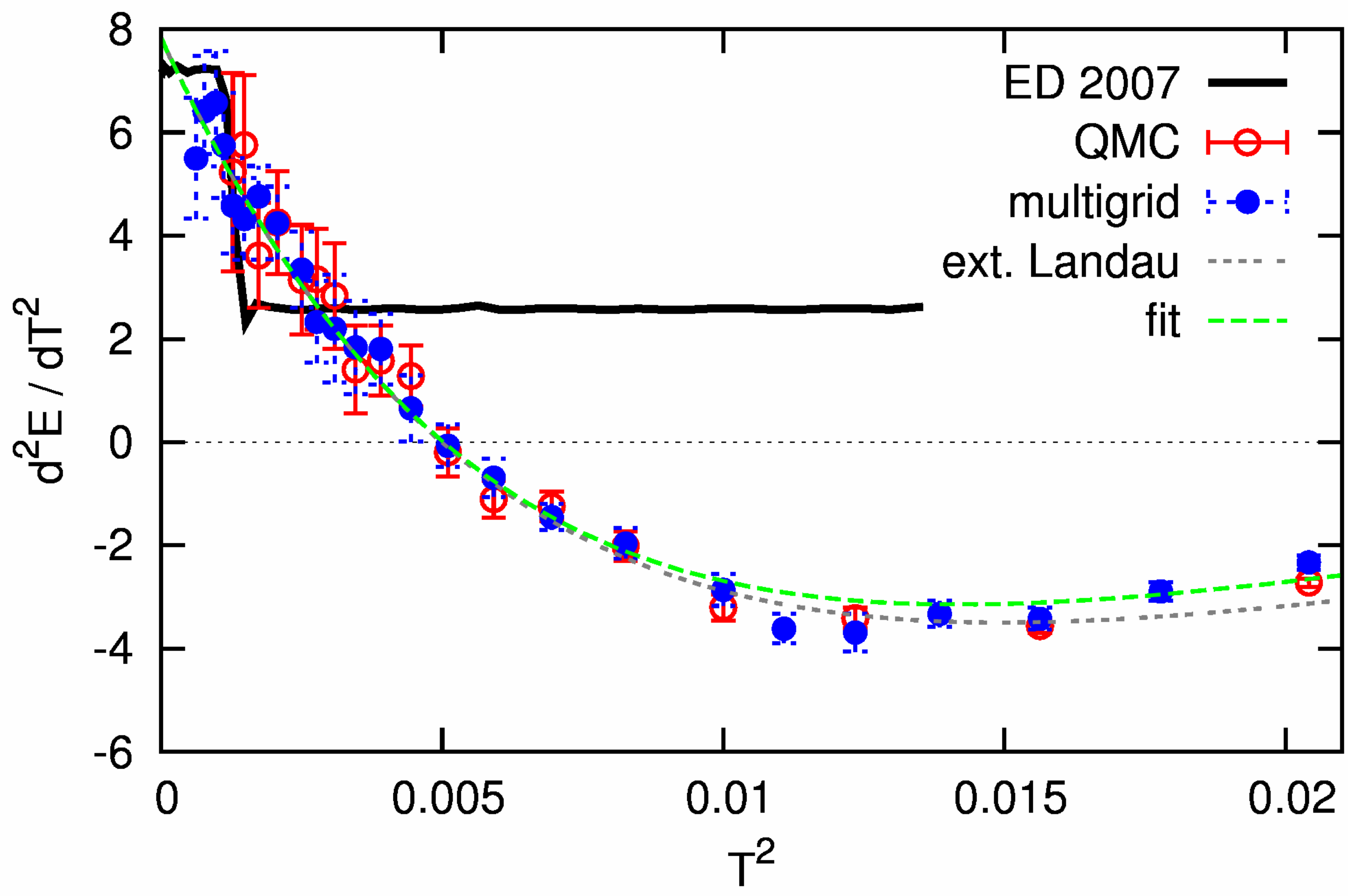


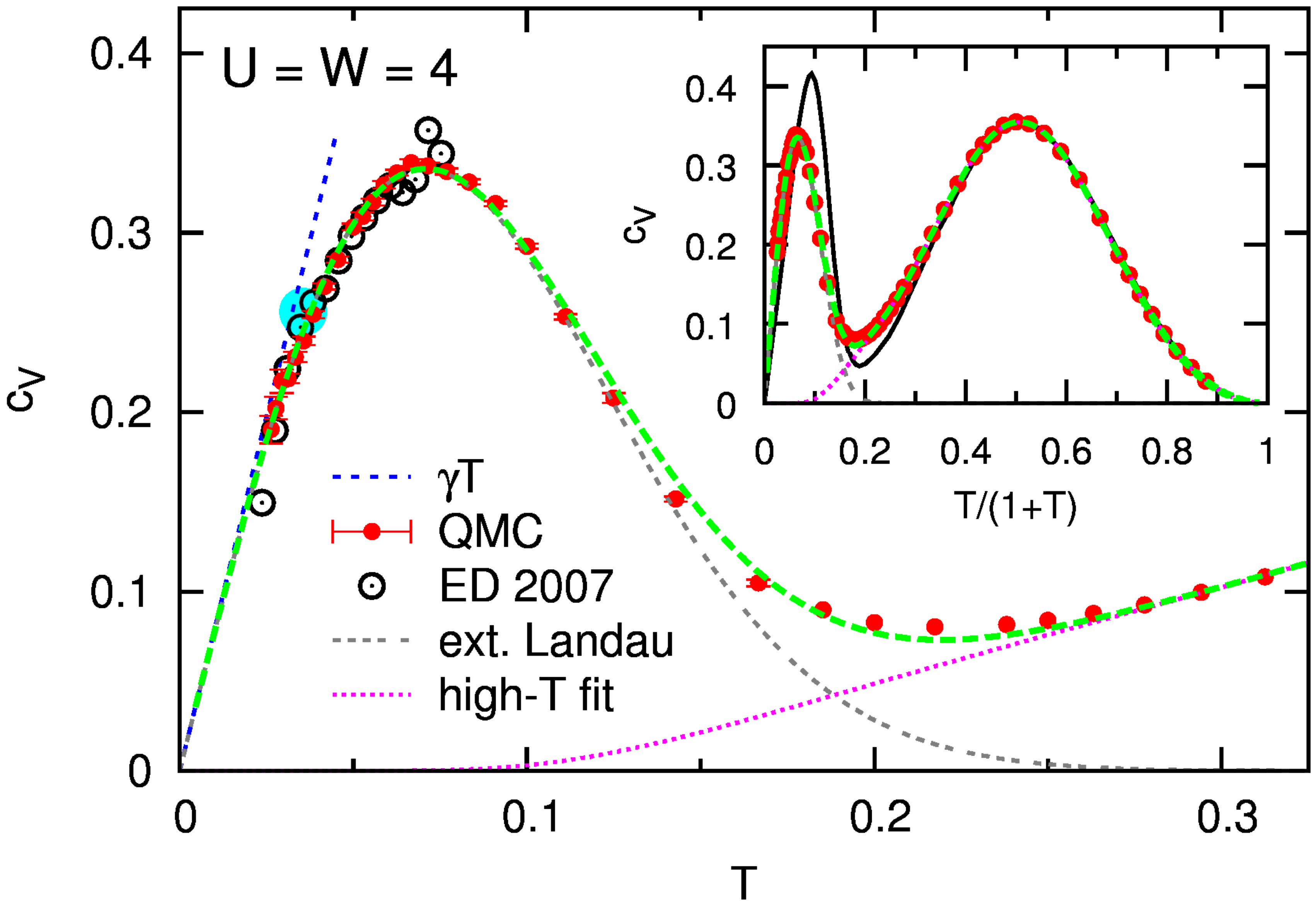
Direct measure of "kinkiness": energy curvature



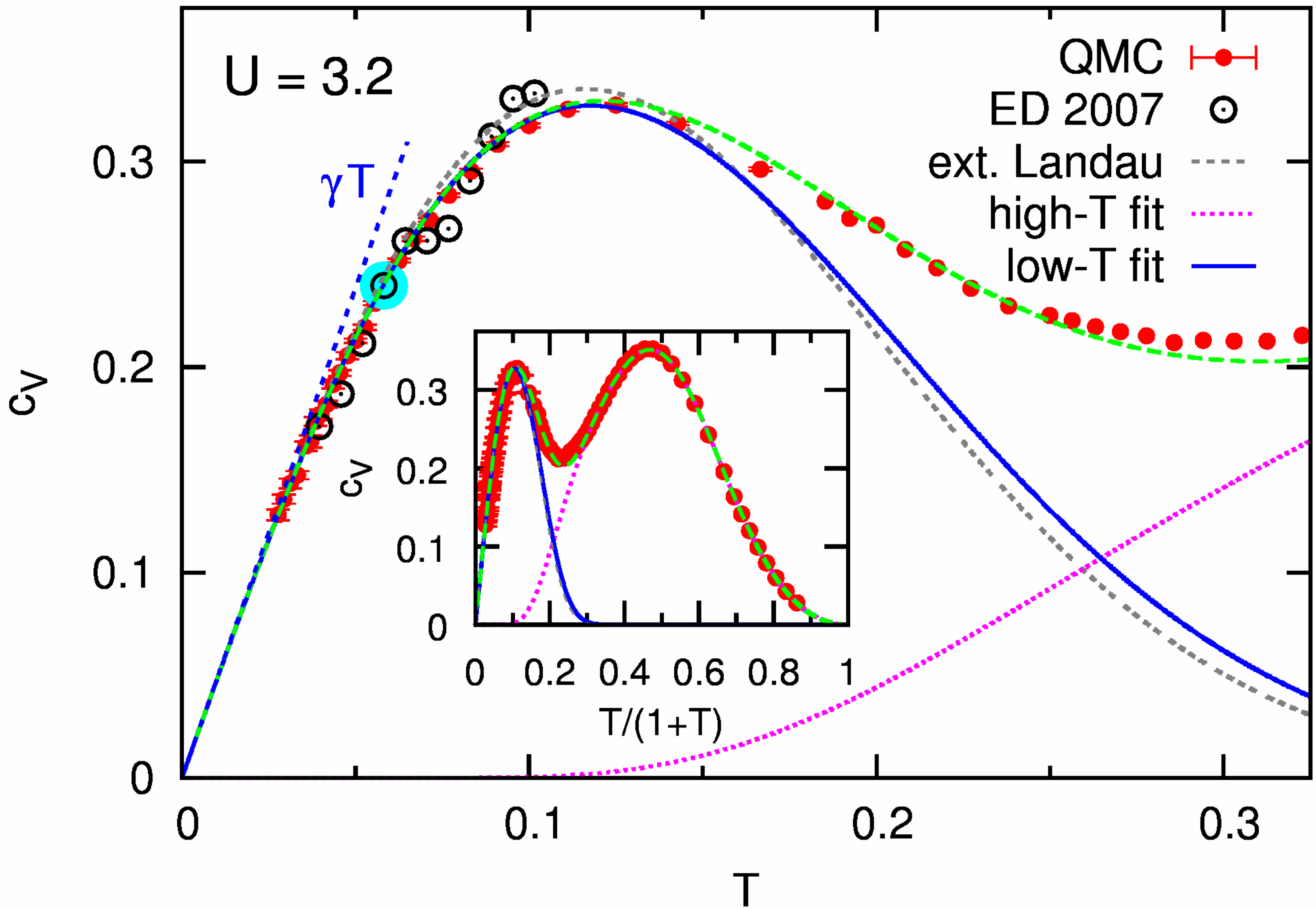
Full agreement of (multigrid) HF-QMC with extended Landau theory (parameter: Z)

Initial slope: contributions from Sommerfeld expansion + T-dependence of $\Sigma(\omega)$

Specific heat over full temperature range

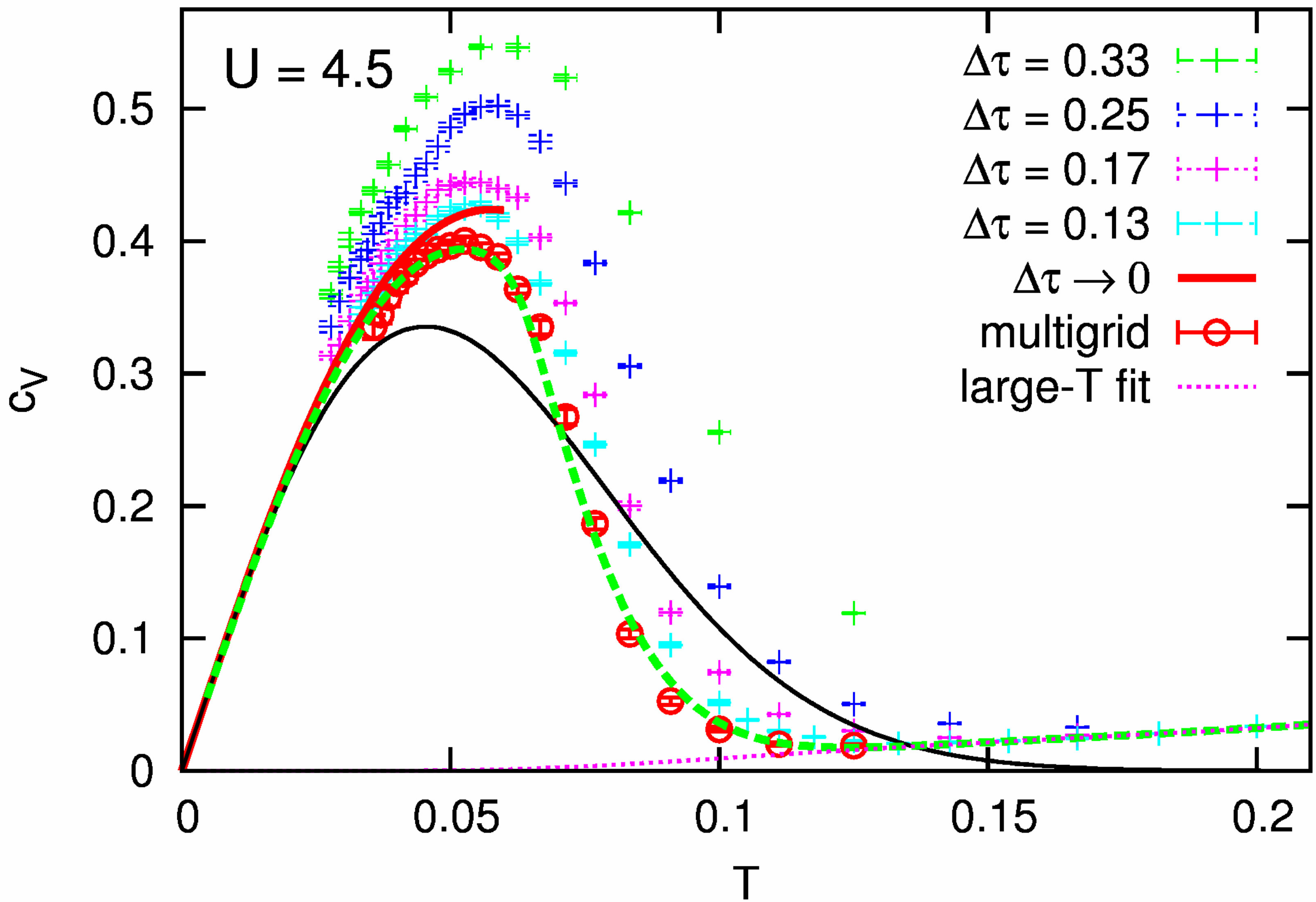


Weaker coupling



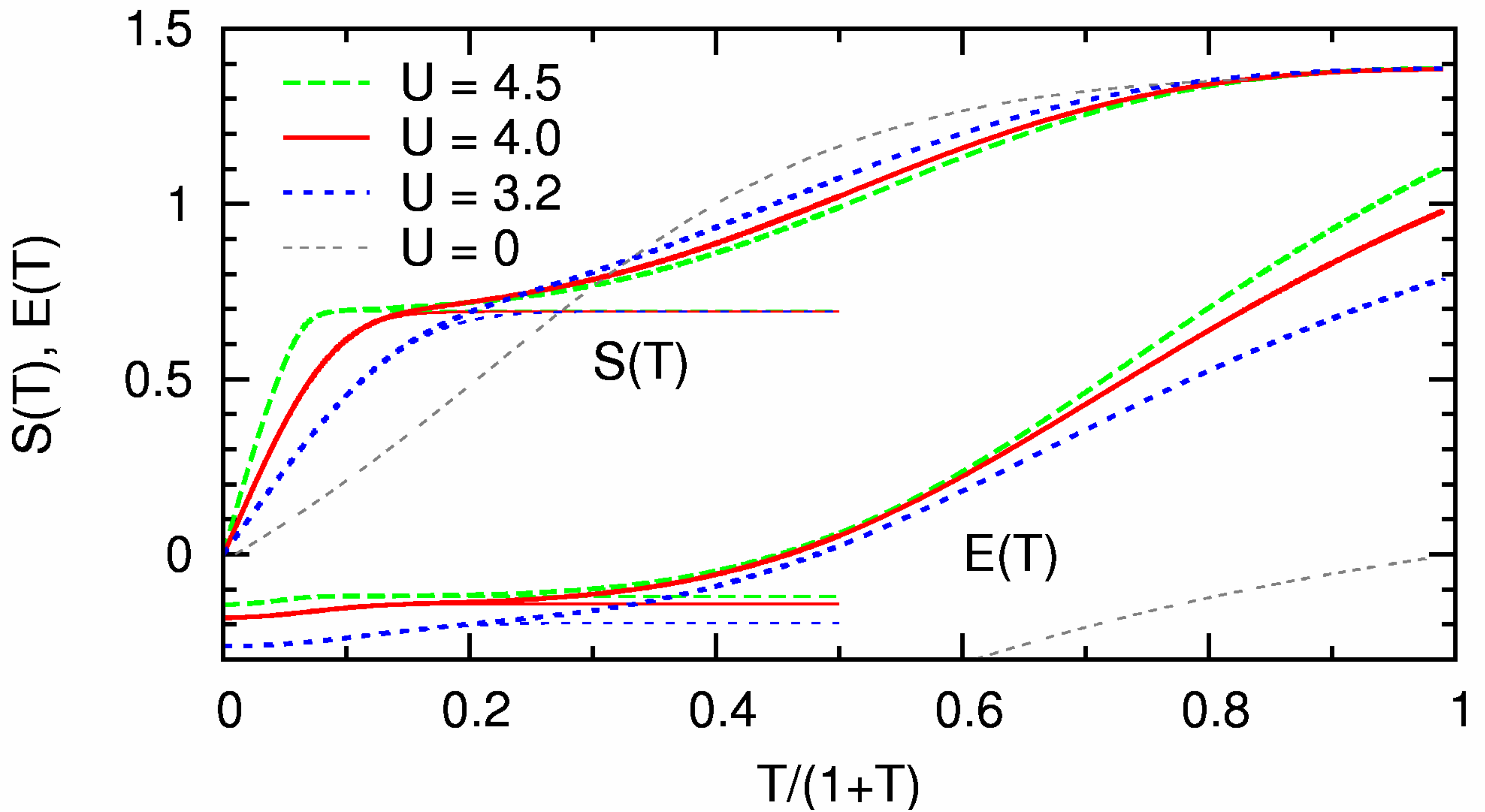
Empirical "extended Landau" fit remains accurate for lower U

Stronger coupling: $U = 4.5 \lesssim 4.7 \approx U^*$



Corrections to “extended Landau” fit close to phase transitions

Entropy and energy for various couplings couplings

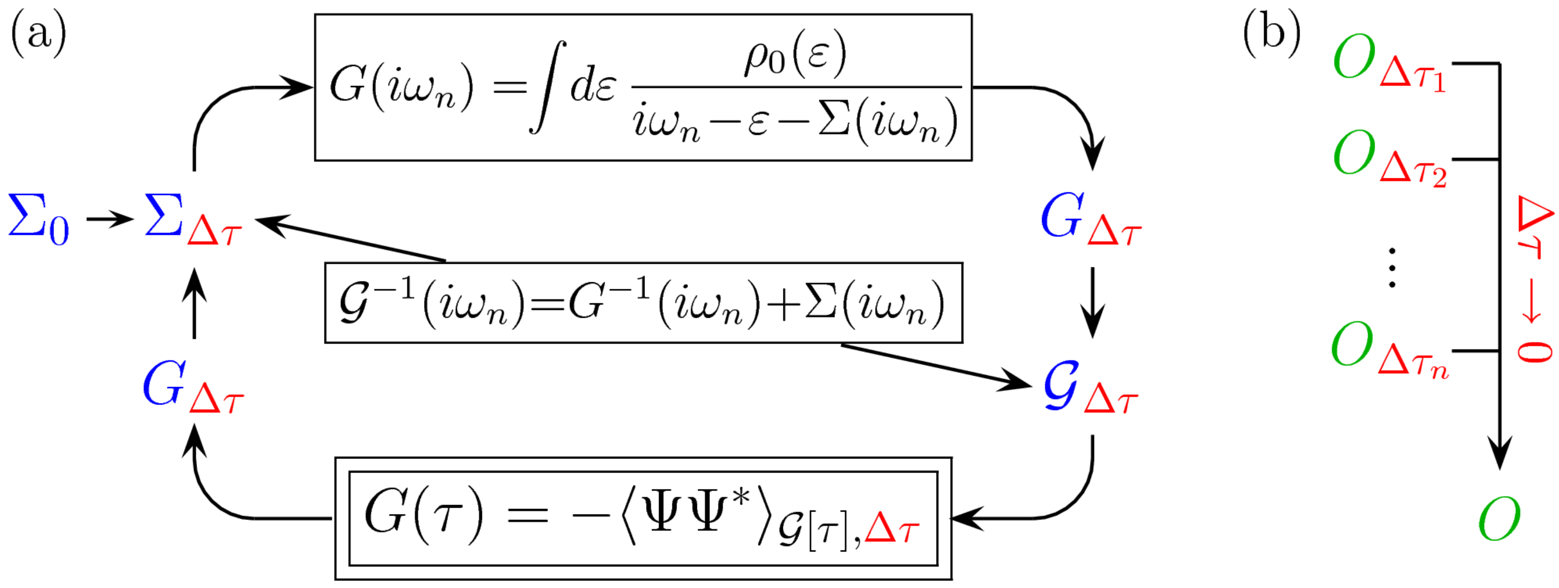


Thick lines: global fits; thin lines: qp contribution only

Multigrid Hirsch-Fye quantum Monte Carlo algorithm

State of the art: (a) conventional HF-QMC

(b) *a posteriori* extrapolation of selected observables



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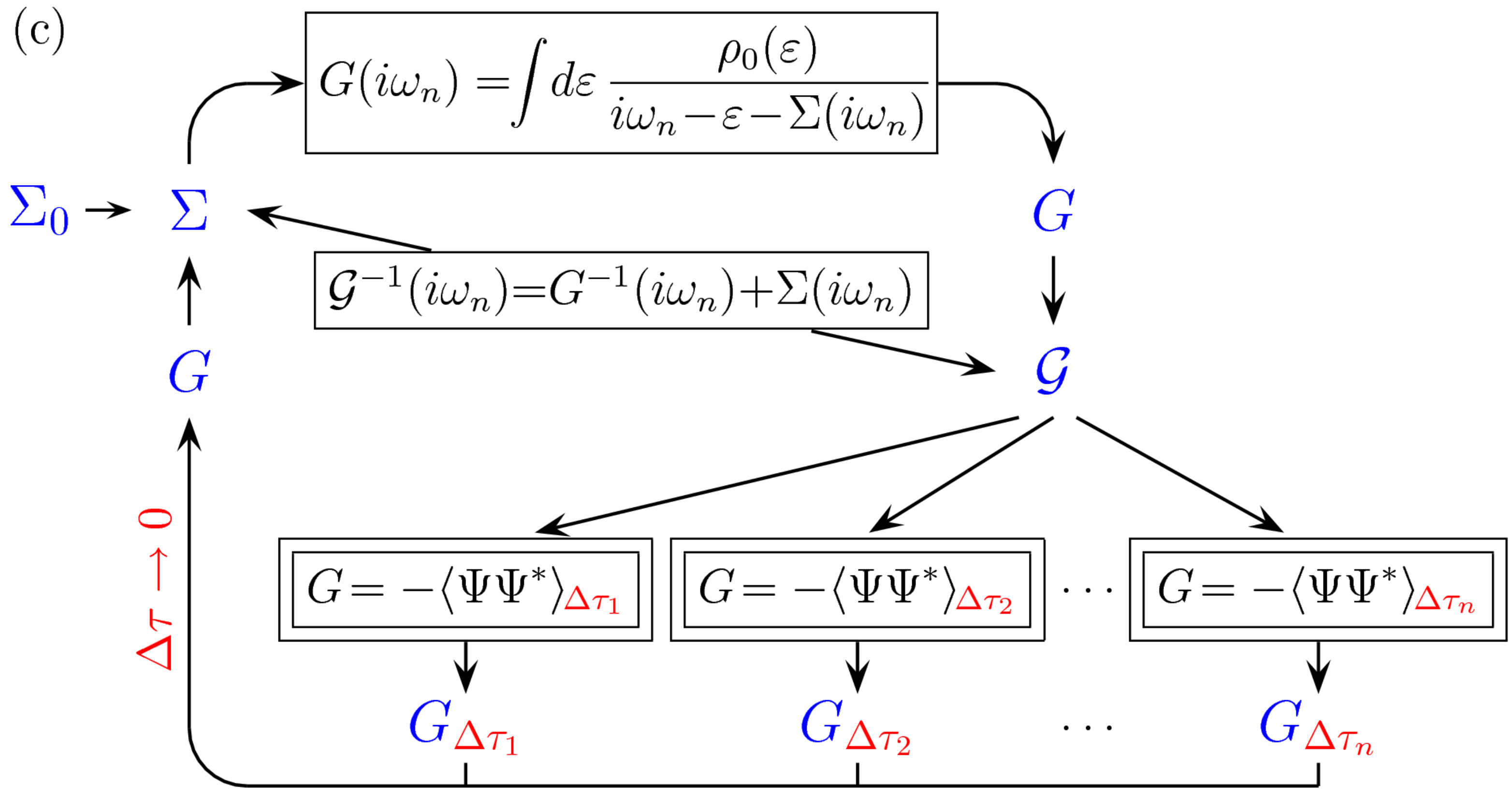
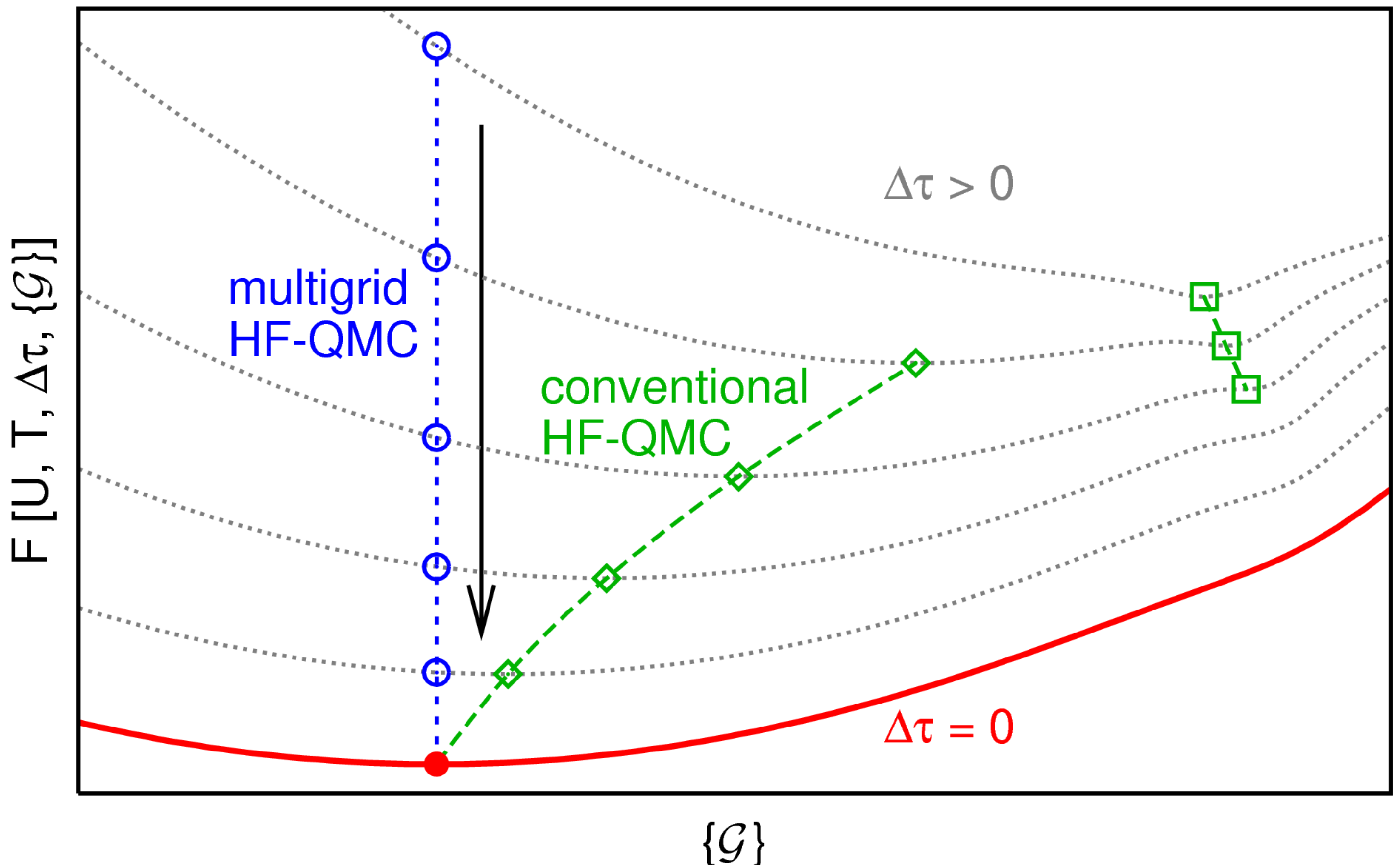
(c)



(c) Multigrid HF-QMC: internal elimination of Trotter error

$\rightsquigarrow$ quasi continuous time algorithm [NB, arXiv:0801.1222]

Schematic comparison via generalized Ginzburg-Landau functionals



Conventional Hirsch-Fye QMC: DMFT fixed point shifts with $\Delta\tau$

Multigrid Hirsch-Fye QMC: DMFT iteration towards exact fixed point

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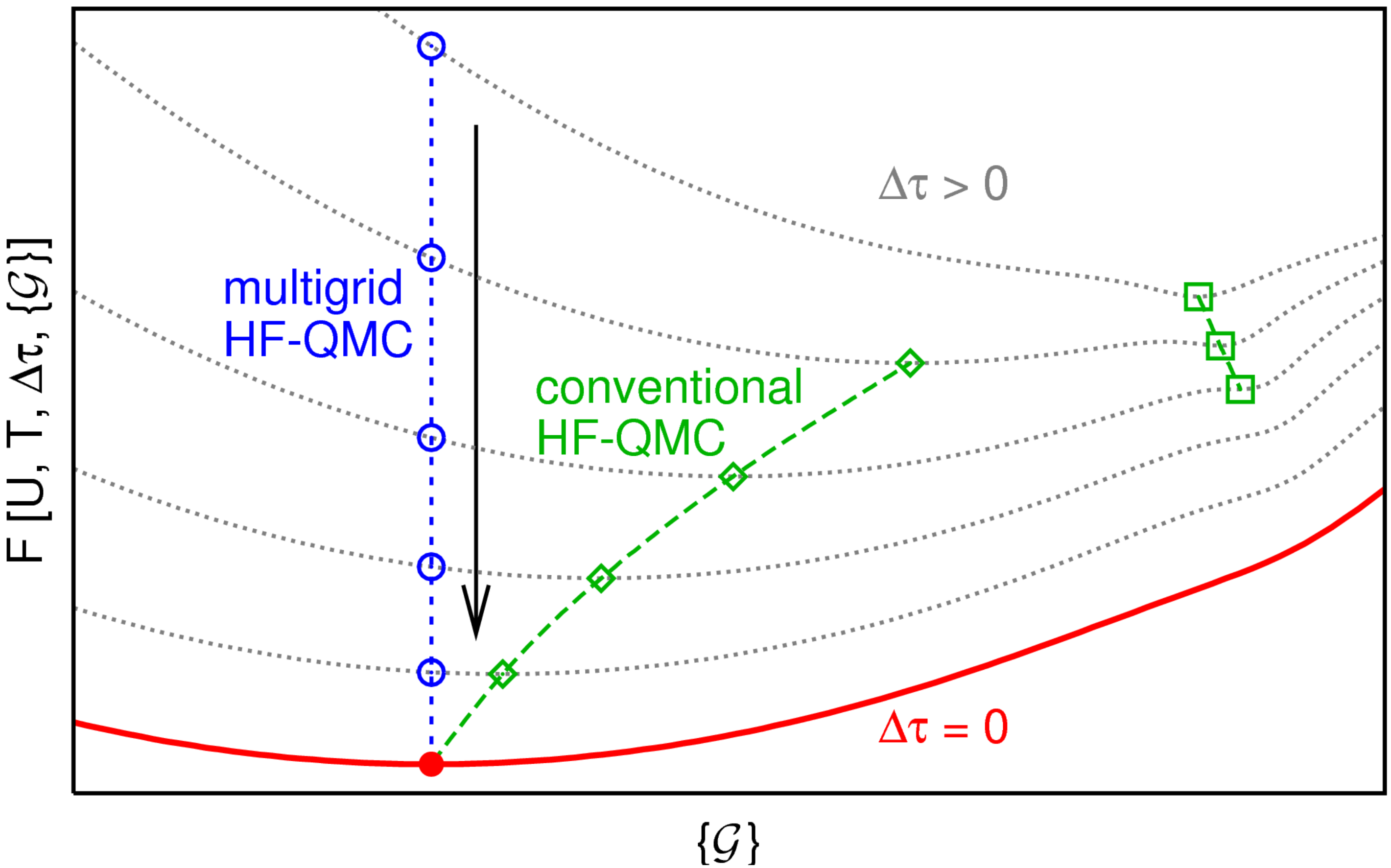

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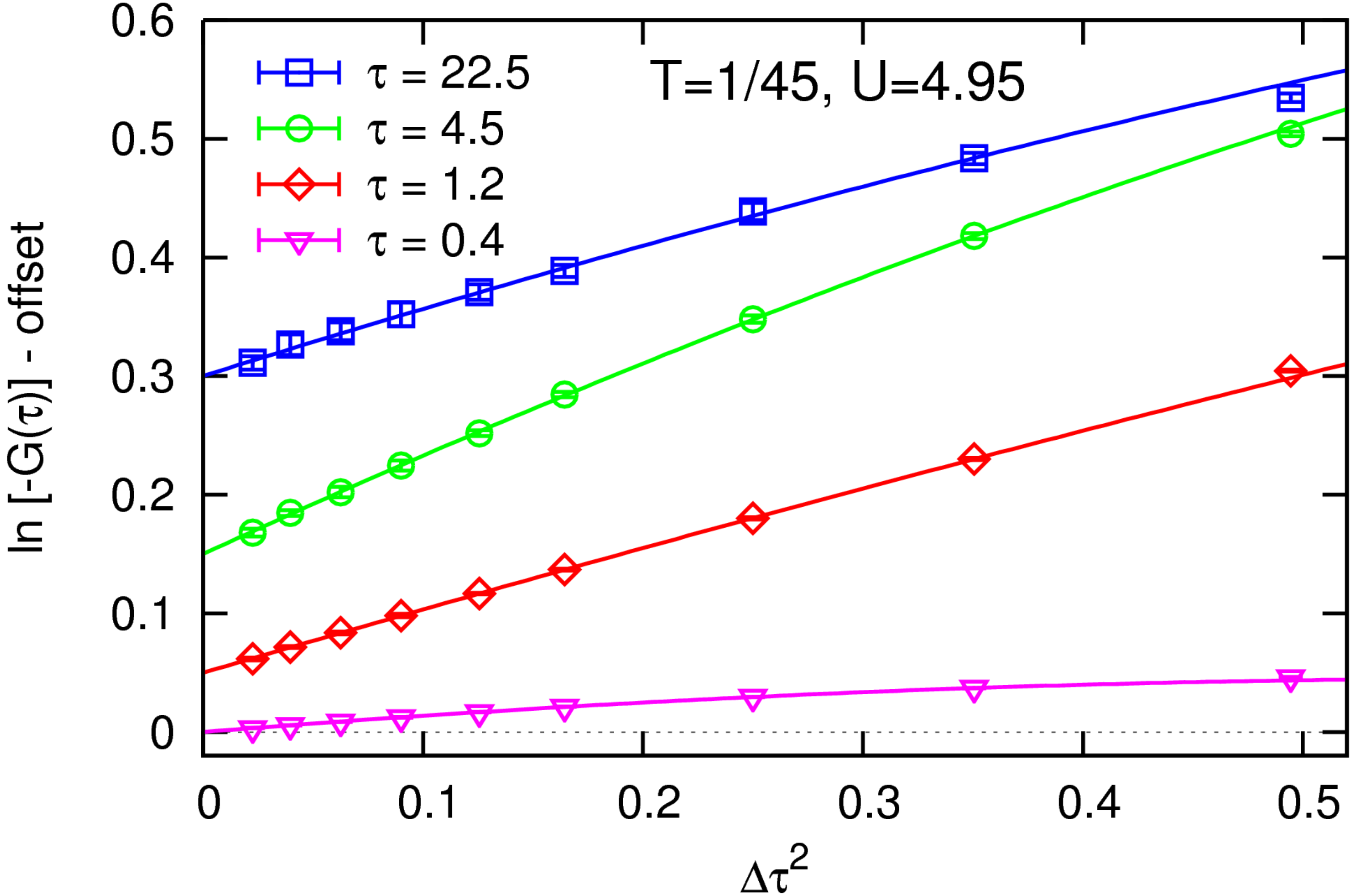
Multigrid Hirsch-Fye QMC: DMFT iteration towards exact fixed point

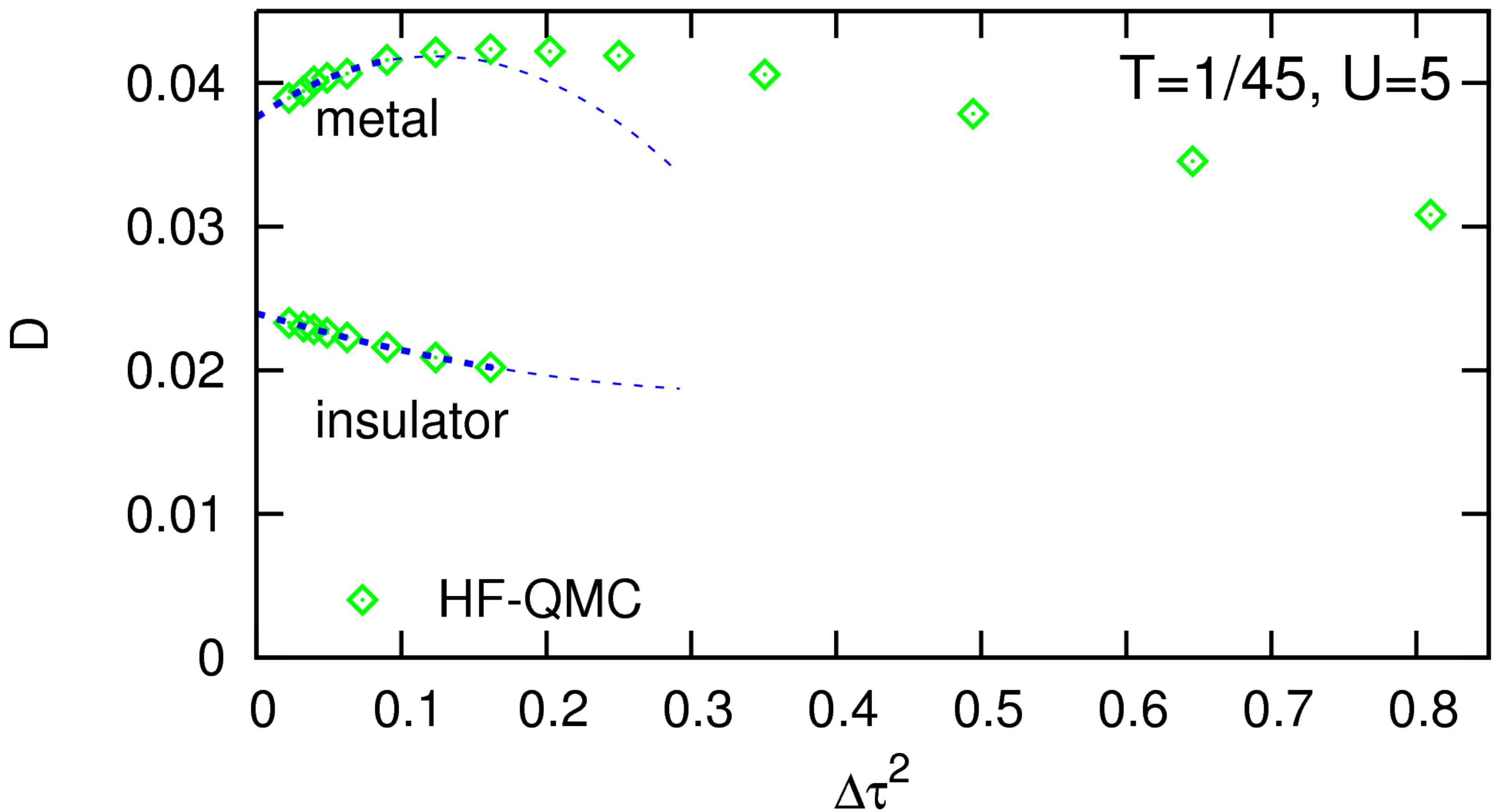
Implementation: Green function extrapolation, hierarchy of frequency scales

Fundamental step: extrapolation $\Delta\tau \to 0$ of Green function $G(\tau)$

First: interpolation to common fine grid (using high-frequency expansion for $\Sigma(\omega)$), then extrapolation using least-squares fits



Comparison: double occupancy $D = \langle n_{i\uparrow} n_{i\downarrow} \rangle$ near Mott transition



Conventional HF-QMC: no insulating solution for $\Delta\tau \gtrsim 0.4$

very irregular $\Delta\tau$ dependence beyond $\Delta\tau \approx 0.3$

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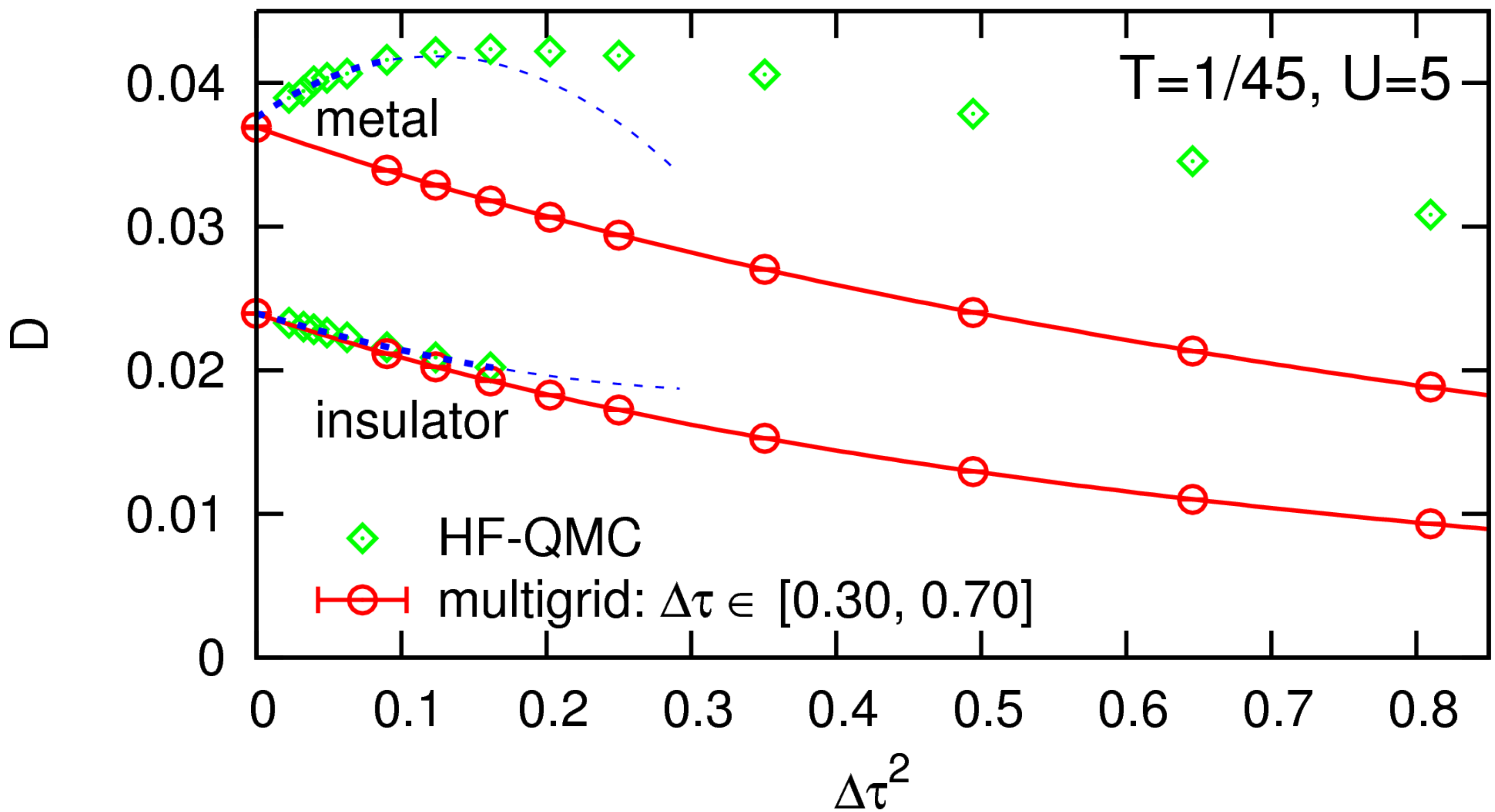

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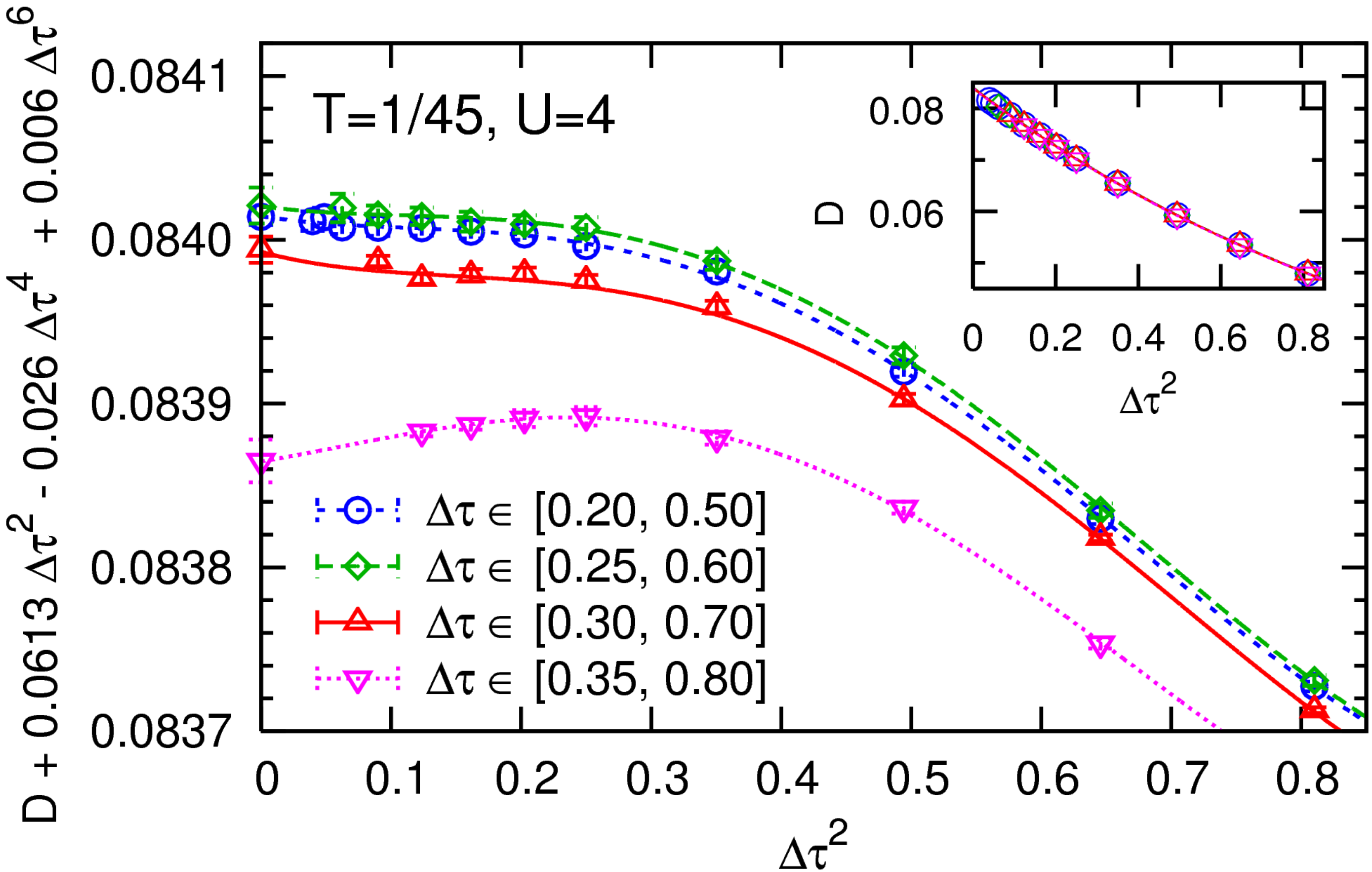
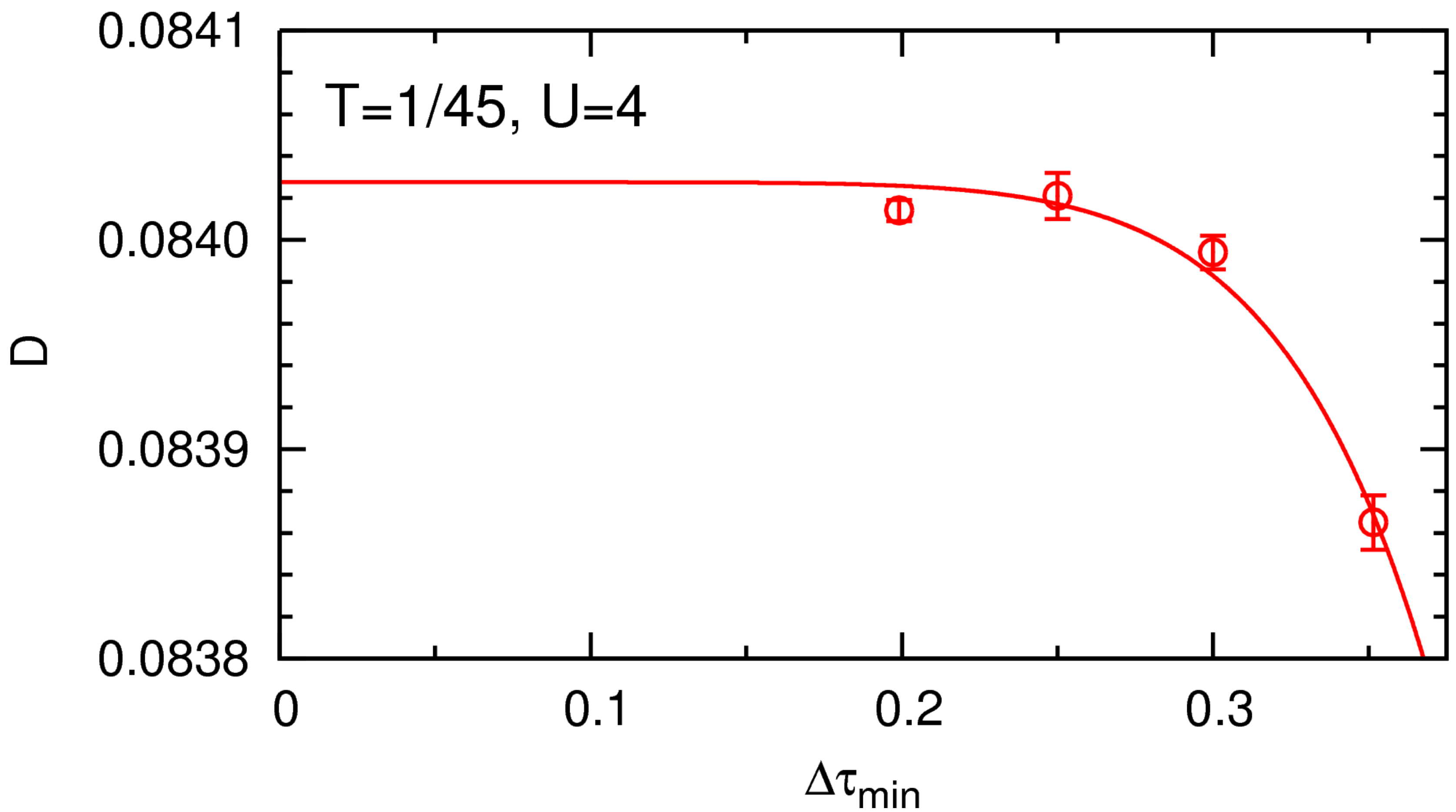
Multigrid HF-QMC: vastly larger useful range of $\Delta\tau$

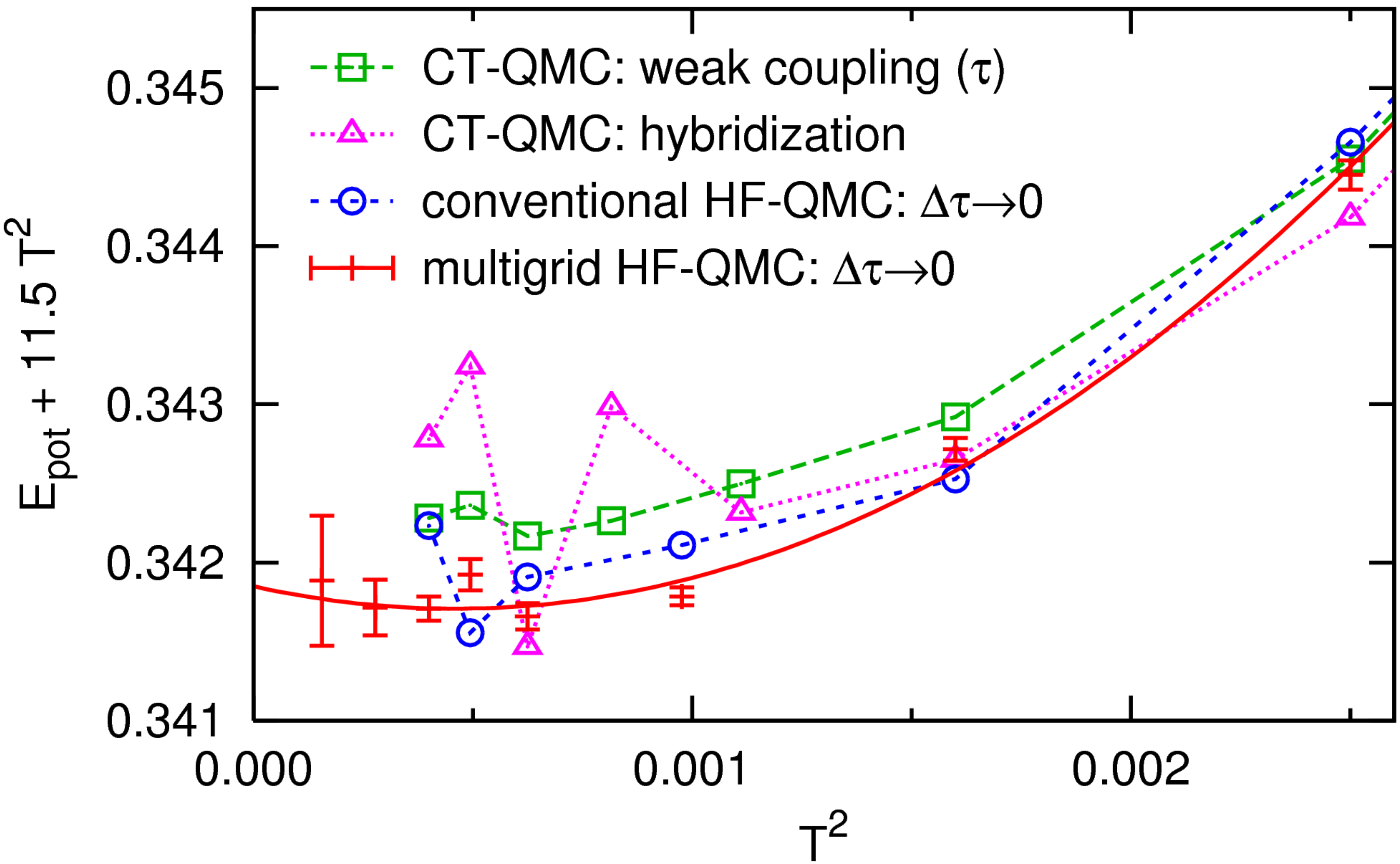
Systematic study: impact of grid range (on double occupancy)





Multigrid HF-QMC usually "numerically exact" for $\tau_{\rm min} \lesssim 0.3$

Efficiency: potential energy $E_{\text{pot}} = UD$ (at $U = W = 4$)



No more "difficult observables" for multigrid HF-QMC

Higher precision than CT-QMC methods at same effort

Summary

Multigrid Hirsch-Fye quantum Monte Carlo algorithm

- Quasi continuous time $\rightsquigarrow$ strictly "numerically exact"
- Stable and precise even at phase boundaries
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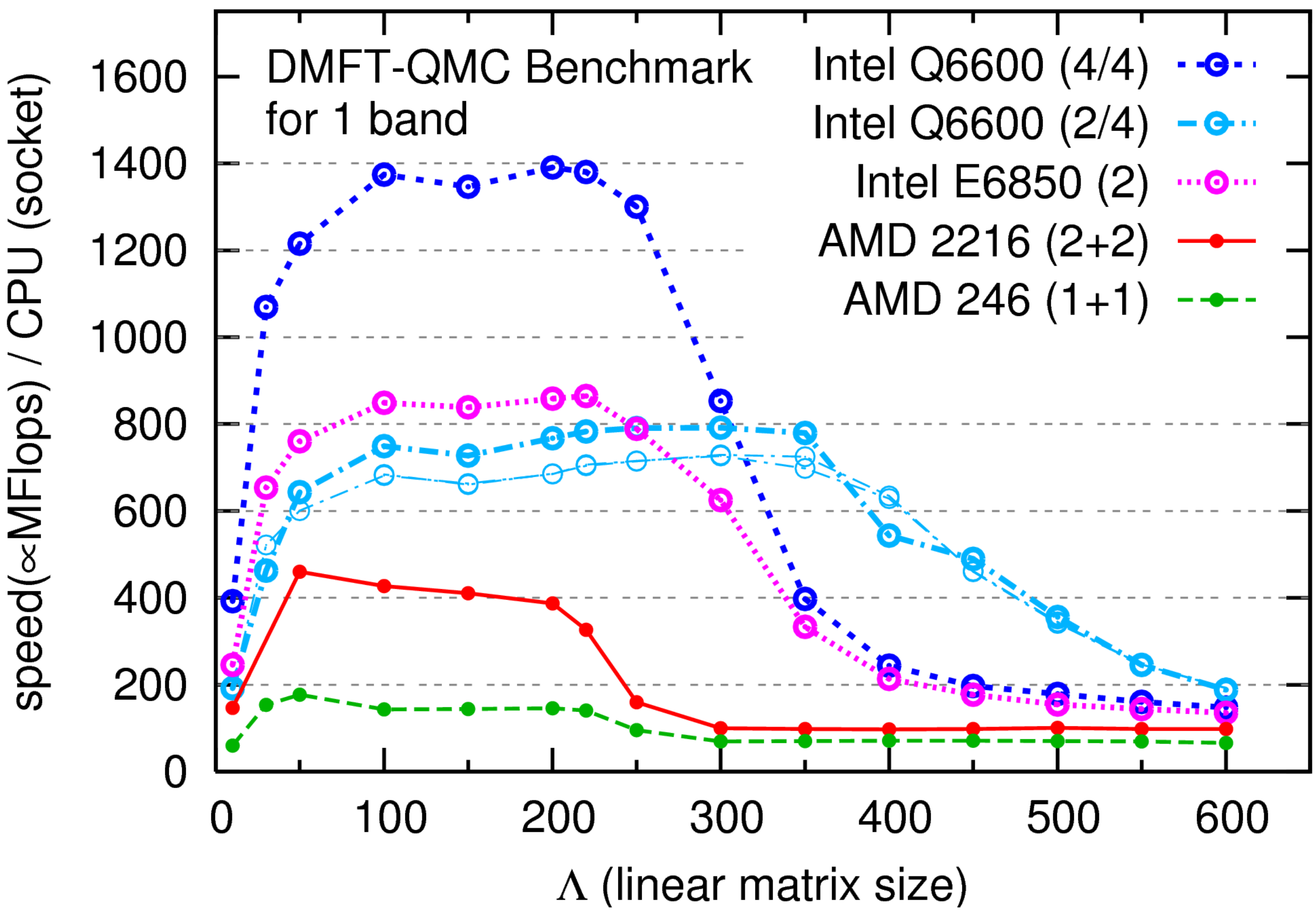
Outlook

Flavor-selective Mott transitions in ultracold quantum gases (SFB/TR 49)

Material-specific multiband calculations in context of LDA+DMFT

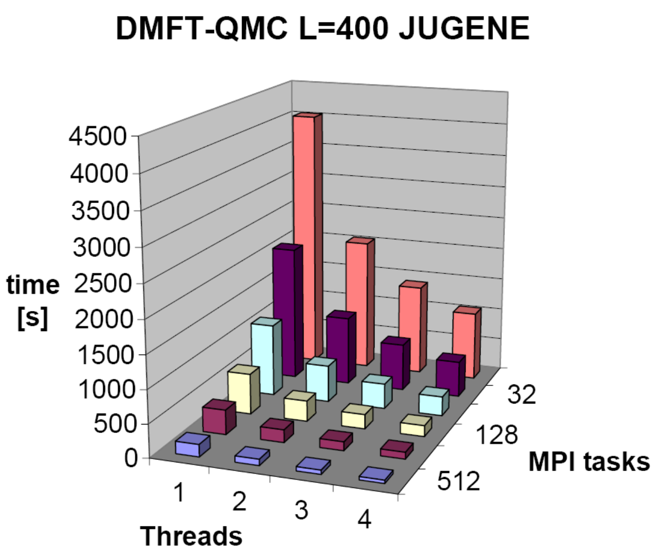
New: hybrid parallelization (MPI and OpenMP) . . .

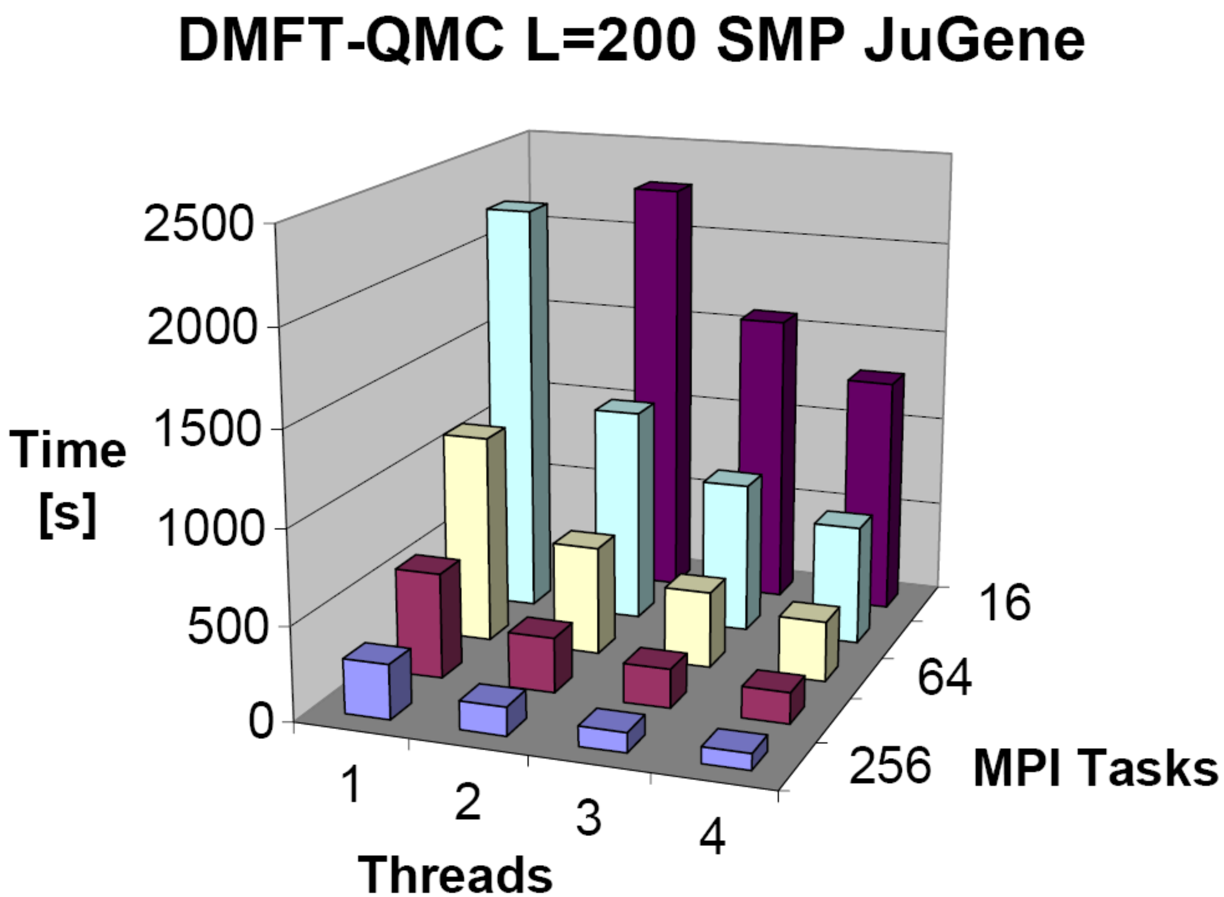
Benchmarks



HF-QMC profits strongly from modern large-cache architectures

New (4/2008): hybrid parallelization (MPI + OpenMP)





Very good scaling: speed roughly linear with number of CPU cores

Superlinear scaling on JUMP