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

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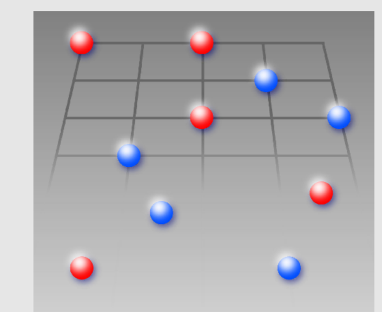


Introduction

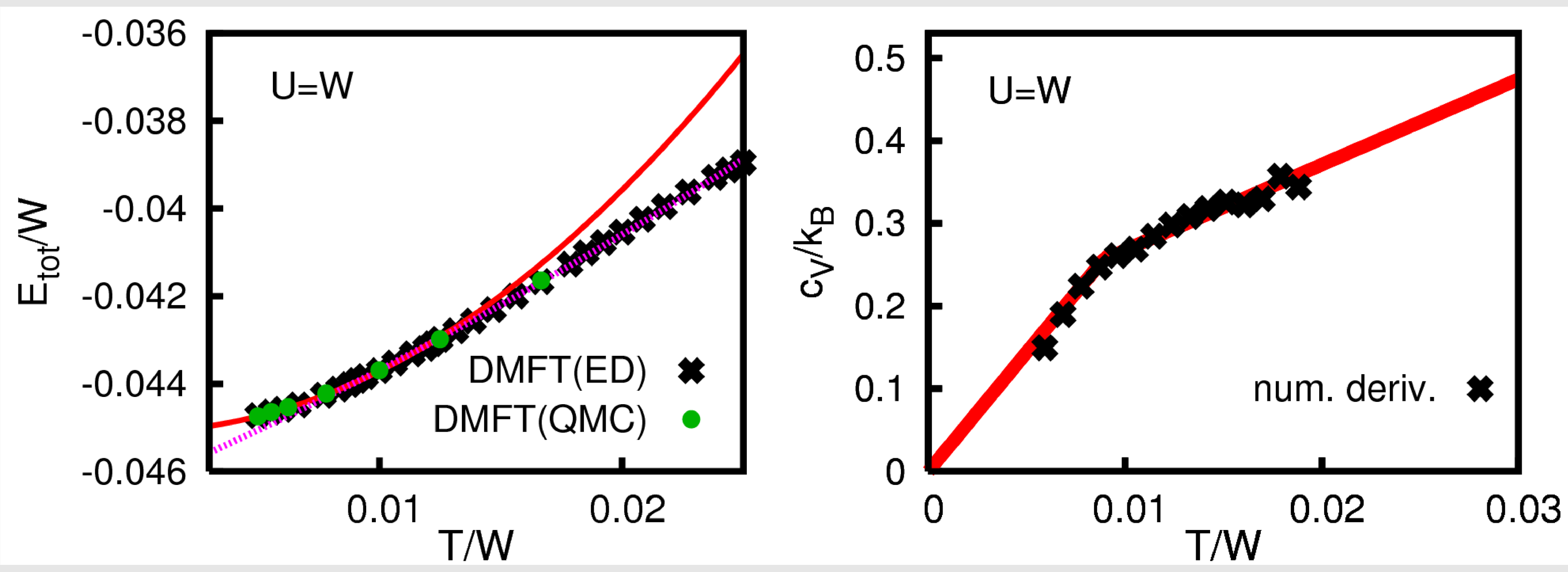
Fermi liquid theory: linear specific heat $c_V = \gamma T$

linear entropy $S = \gamma T$

quadratic resistivity $\rho \propto T^2$ for "low enough" T

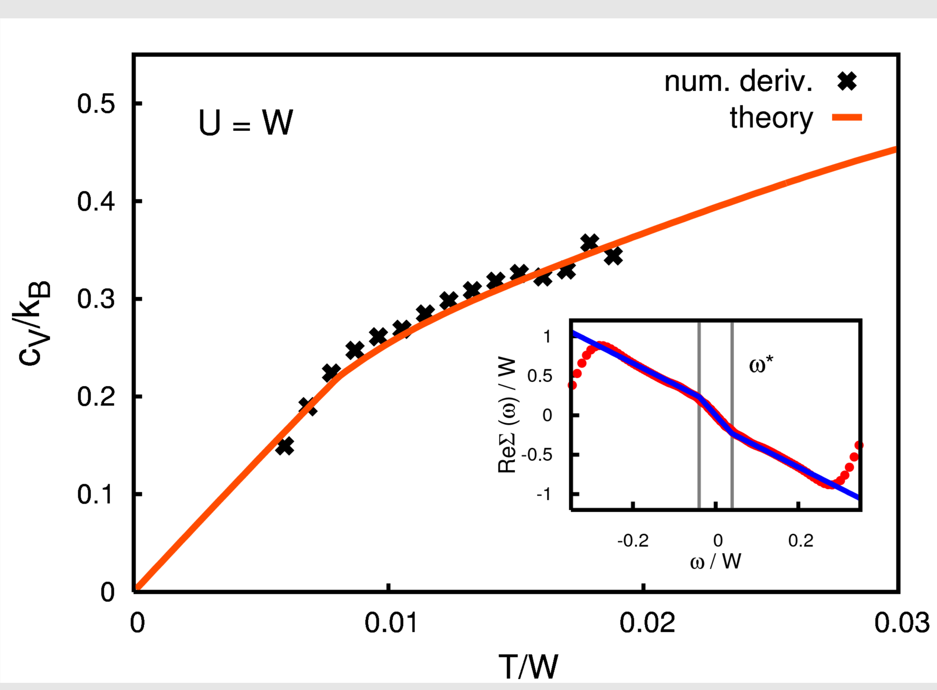
When/how do these laws break down?

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



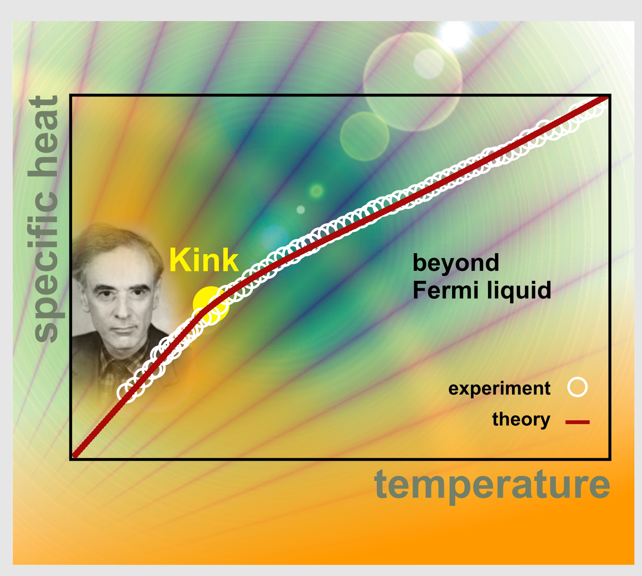
Distinct kink in c_V! [A. Toschi, M. Capone, C. Castellani, K. Held, arXiv:0712.3723]

Theoretical explanation: kink in self-energy ⇝ kink in c_V



[A. Toschi *et al.*, arXiv:0712.3723]

Kink feature visible in specific heat of heavy fermion LiV_2O_4?



[A. Toschi *et al.*, arXiv:0712.3723]

Comparison with literature:

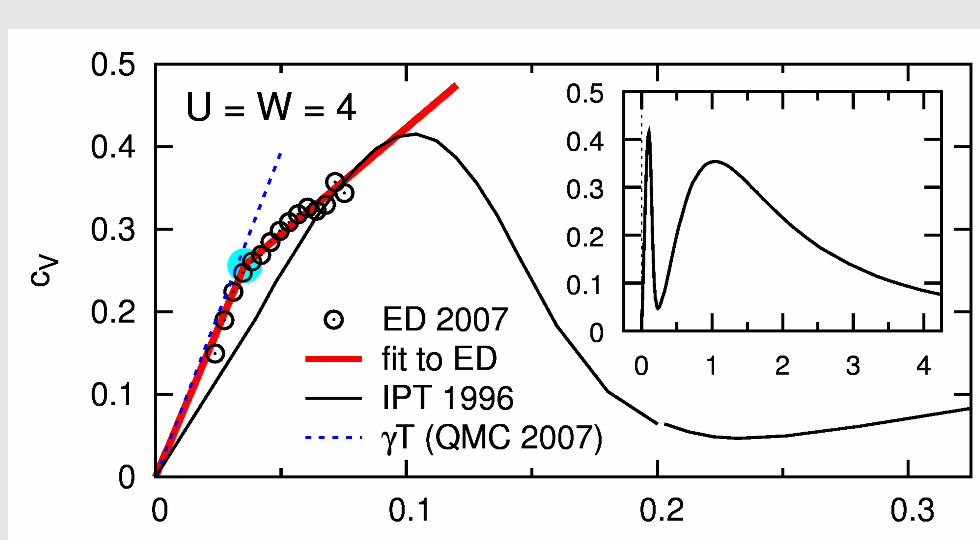
IPT: [Georges et al., RMP (1996)]

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

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

Significant discrepancies

Check using QMC ...



Results for moderately strong coupling ($U = W$)

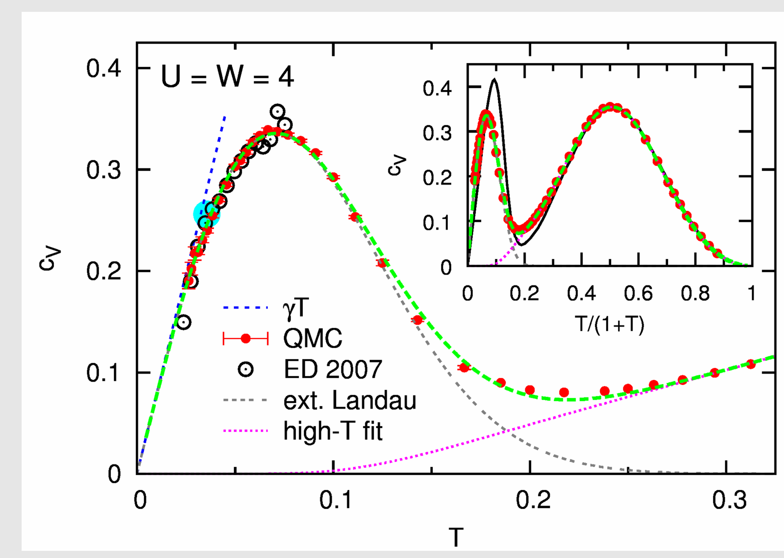
Model: Frustrated 1-band Hubbard model within dynamical mean-field theory (DMFT)

Semi-elliptic "Bethe" density of states with bandwidth $W = 4$

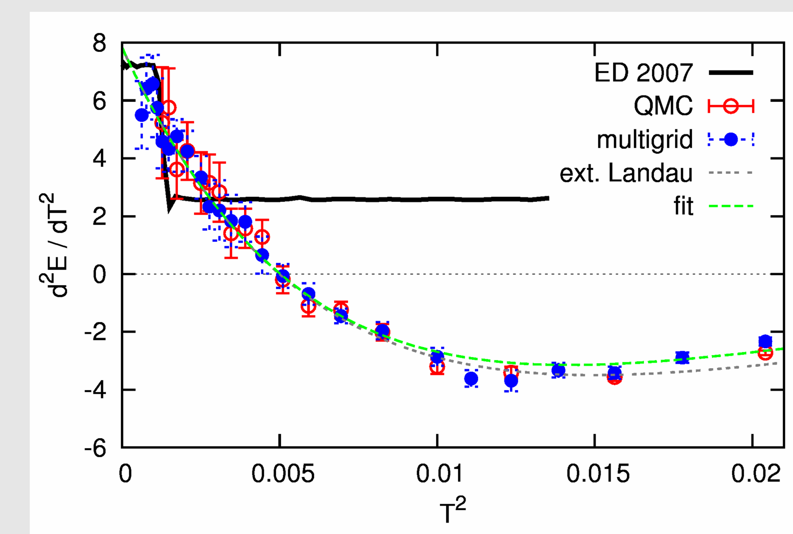
Method: Conventional or multigrid HF-QMC ⇝ $E(T)$

Quadratic least-squares-fits to 5-tupels ⇝ derivatives

Specific heat over full temperature range



Measure of "kinkiness": energy curvature



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

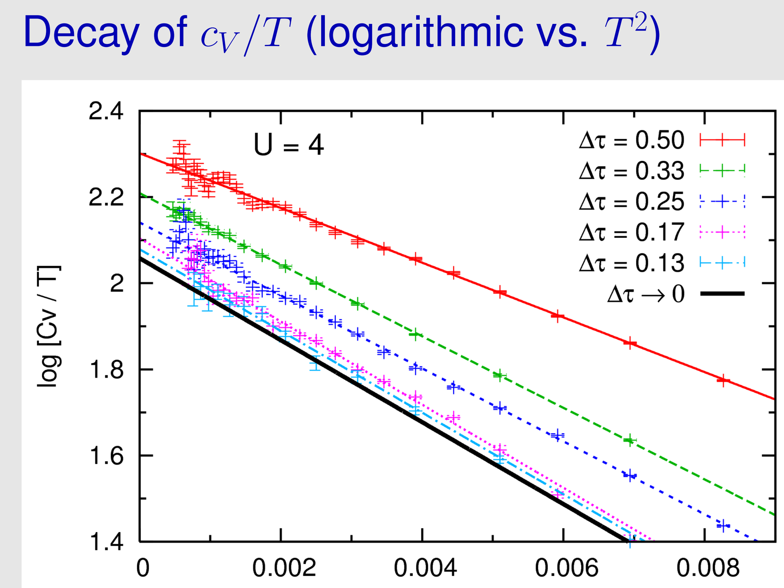
Generalized Fermi liquid law for quasiparticle contribution to specific heat

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

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

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

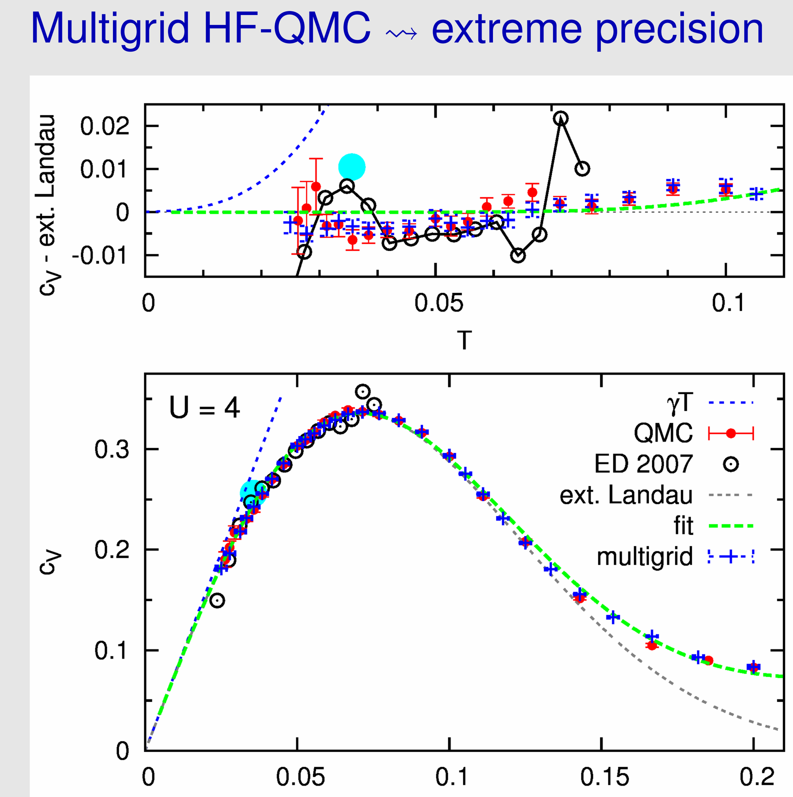
Decay of c_V/T (logarithmic vs. T^2)



Conventional HF-QMC (at finite $\Delta\tau$) and extrapolated result:

Regular decay of c_V/T without any kinks or significant curvature (up to $T \approx 0.12$)

Multigrid HF-QMC ⇝ extreme precision



Conclusions so far: (i) no kinks seen at very high accuracy (one order of magnitude better than previous ED), (ii) surprisingly good fit of qp contribution to c_V by empirical fit.

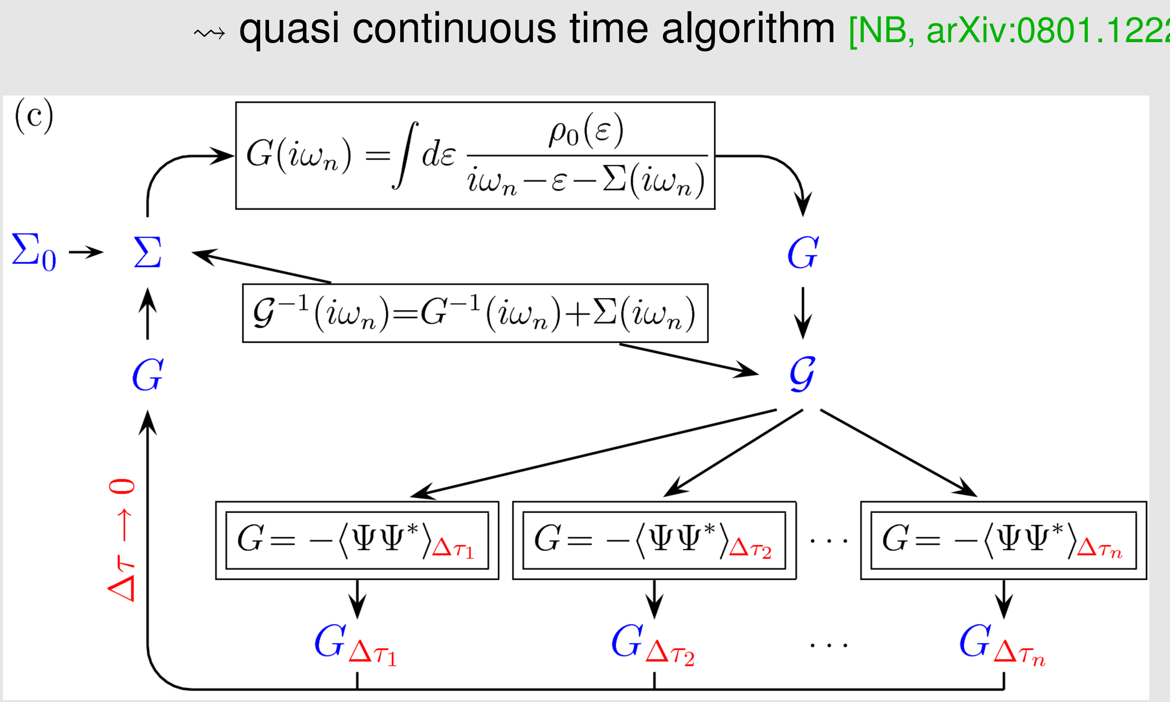
Multigrid Hirsch-Fye quantum Monte Carlo

State of the art: (a) conventional HF-QMC – systematic errors from discretization $\Delta\tau$

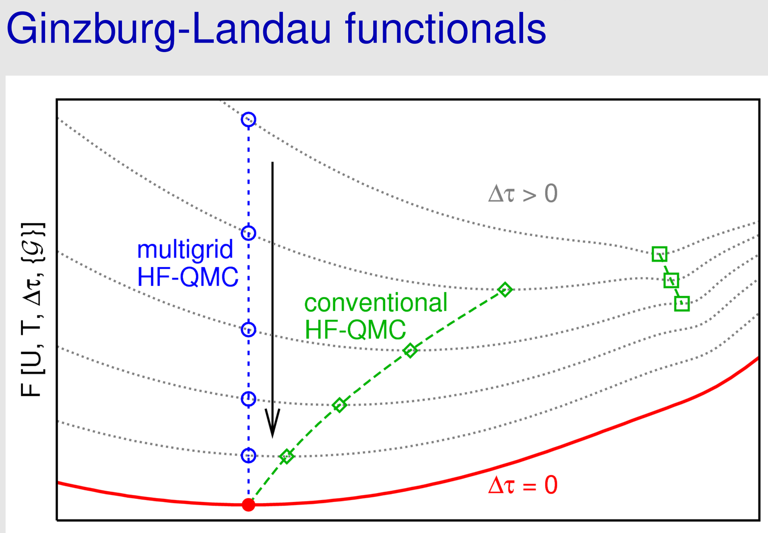
(b) *a posteriori* extrapolation of selected observables

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

⇝ quasi continuous time algorithm [NB, arXiv:0801.1222]



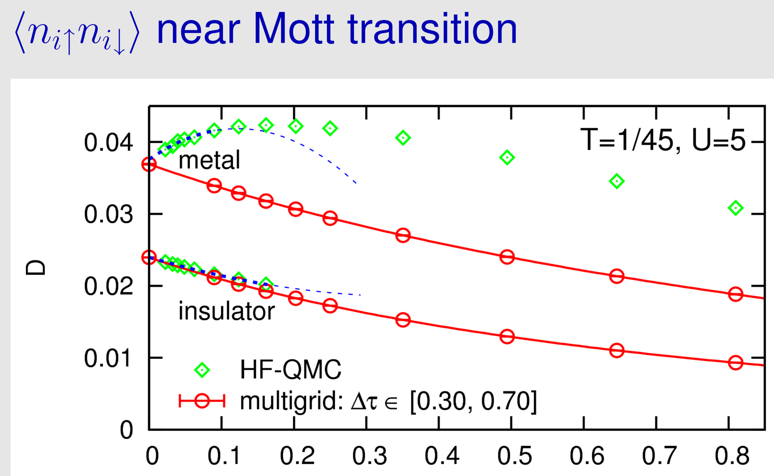
Schematic comparison via generalized Ginzburg-Landau functionals



HF-QMC: DMFT fixed point shifts with $\Delta\tau$

Multigrid: convergency to exact fixed point

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

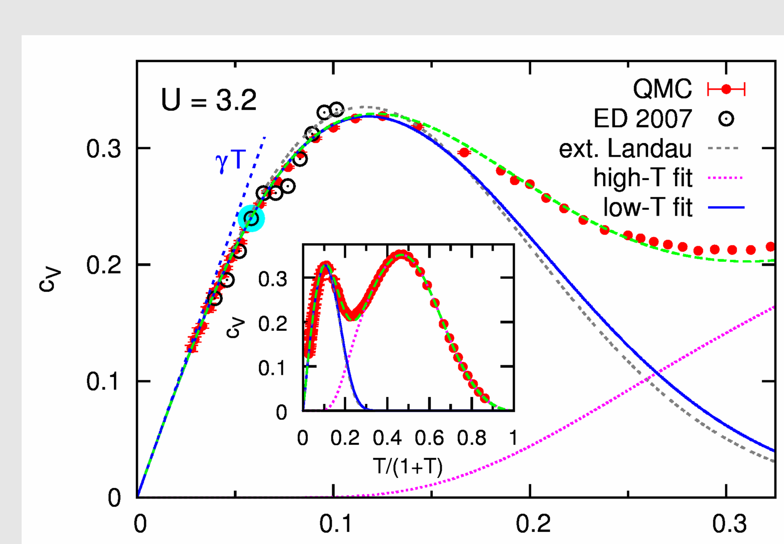


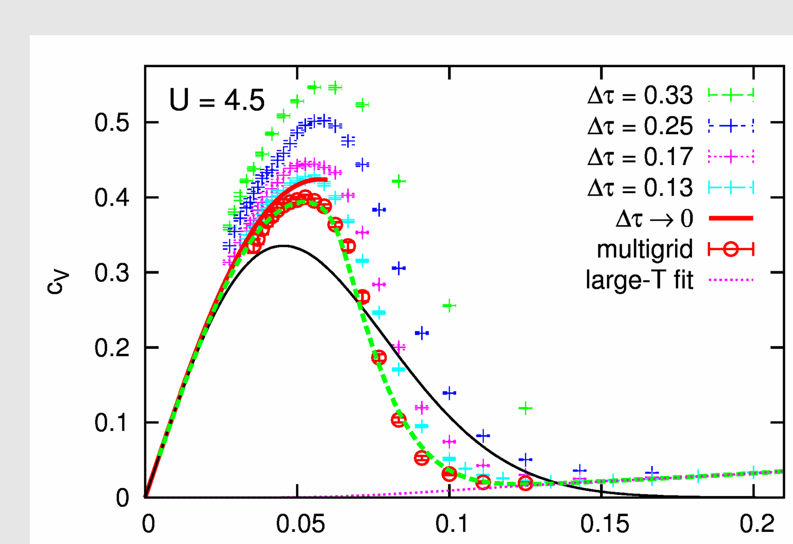
HF-QMC: no insulating phase for $\Delta\tau \gtrsim 0.4$

irregular $\Delta\tau$ depend. in metal

Multigrid: vastly larger useful range of $\Delta\tau$

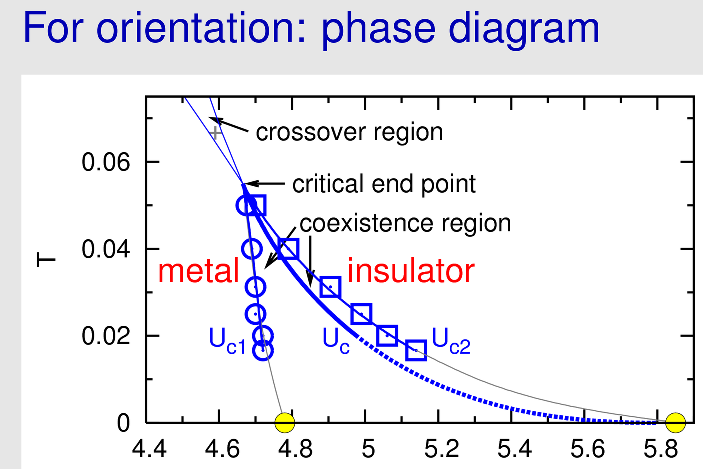
Different couplings





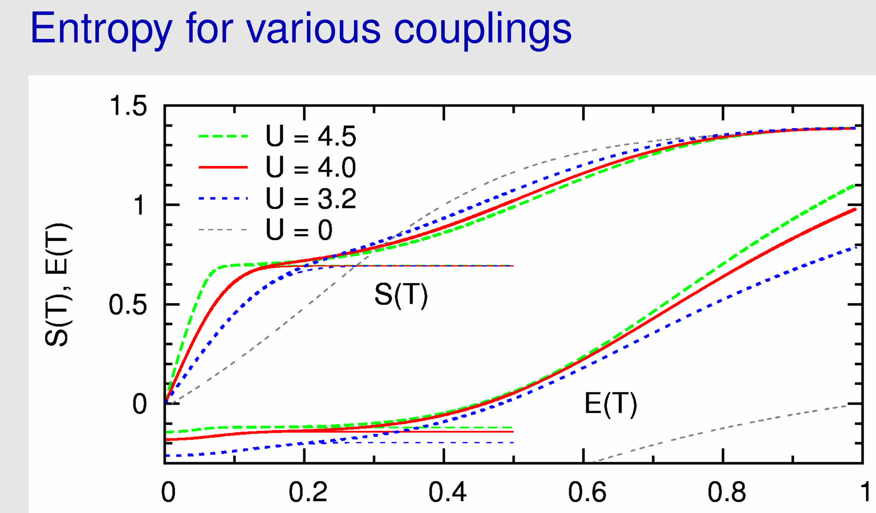
Empirical "extended Landau" fit remains accurate for lower U, significant corrections in vicinity of phase transitions

For orientation: phase diagram



[NB (2002, 2005)]

Entropy for various couplings



Mechanisms for decay of c_V/T

Dominant factors: (i) next-to-leading Sommerfeld terms,

(ii) temperature dependence of $dRe\Sigma/d\omega\big|_{\omega\to 0}$

Analysis similar to derivation of nonanalytic term in $d = 2$ [Gangadharaiah *et al.*, PRL (2005)].

UPPT 2008, International workshop on *Unconventional Phases and Phase Transitions in Strongly Correlated Electron Systems*, June 04 - 07, 2008, Dresden, Germany