Nature and order of orbital-selective Mott transitions

Nils Blümer (Univ. Mainz) and
Krunoslav Požgajčić (Univ. Frankfurt)

Outline

Introduction: orbital/flavor-selective Mott transitions in correlated materials/ultracold atoms on optical lattices

Order of wide-band transition in anisotropic 2-band model

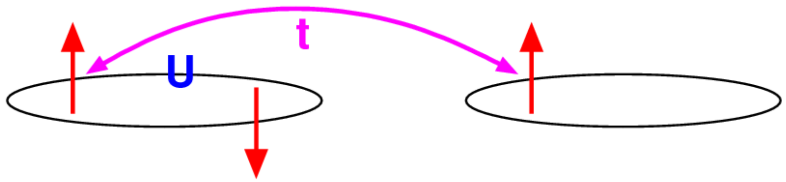
QMC efficiency: Hirsch-Fye vs. continuous time

Summary

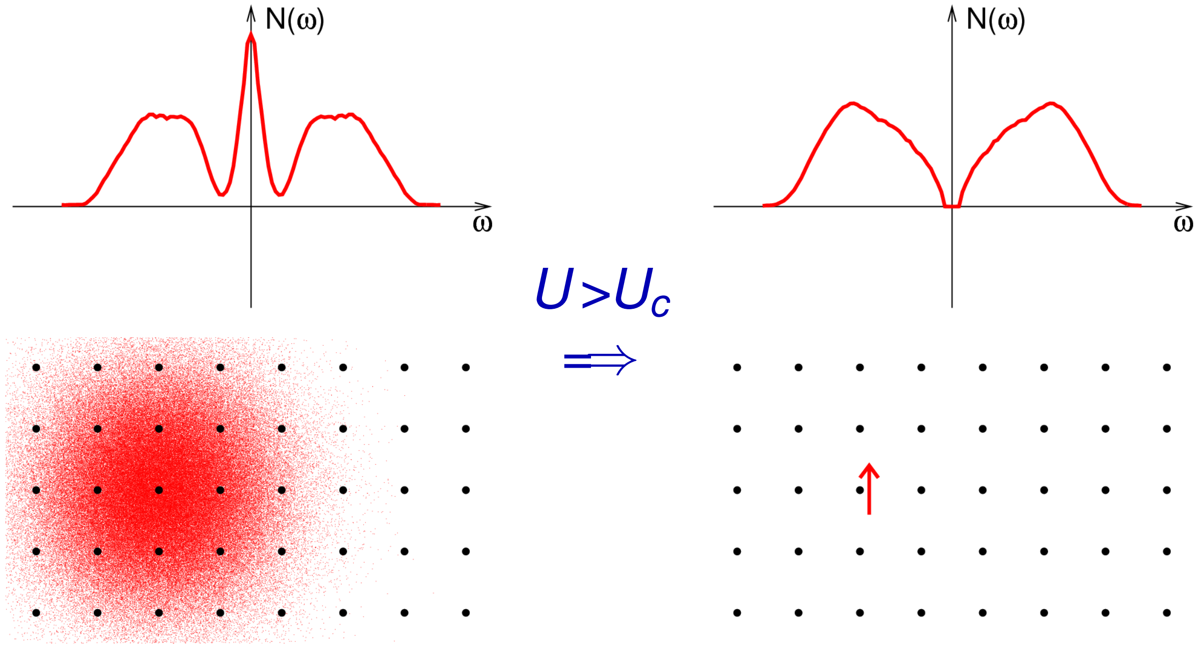
Introduction

Reminder: Mott transition in frustrated 1-band Hubbard model

$$H = -t \sum_{\langle i,j \rangle,\sigma} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$



localization by interactions



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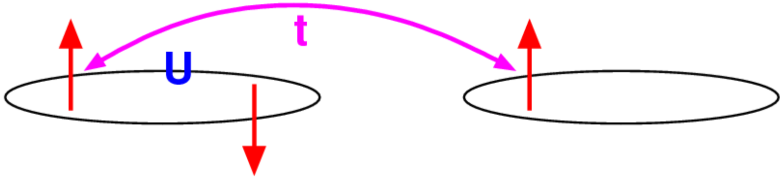

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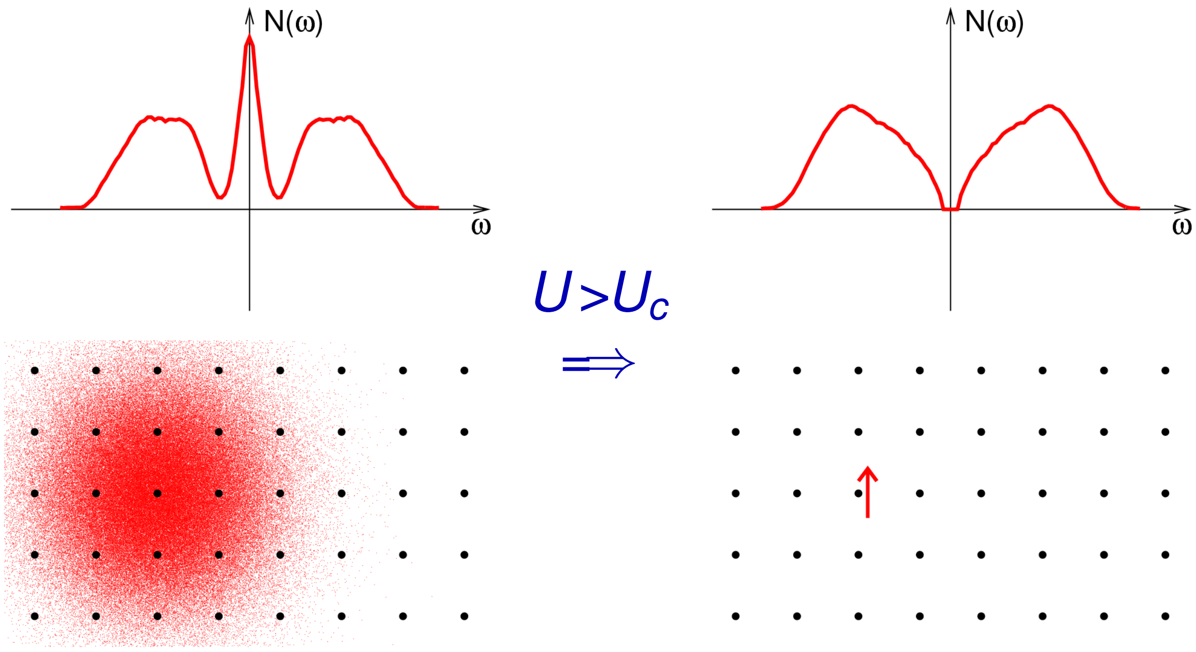

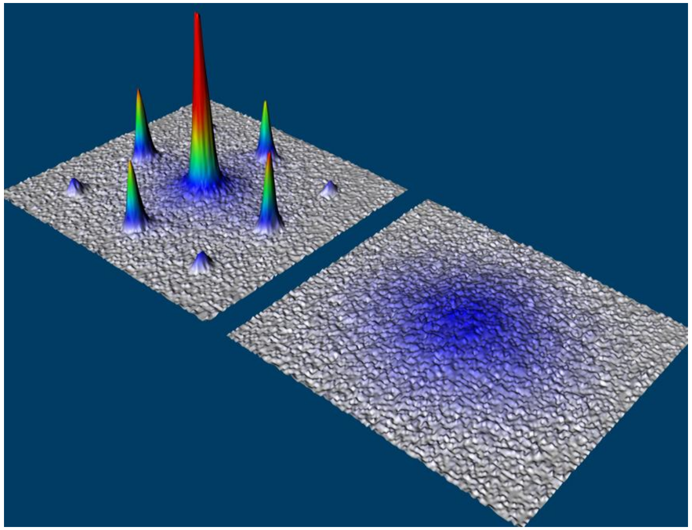

Localization (= decoherence) of ultracold bosons on optical lattice (Bloch group, 2002)

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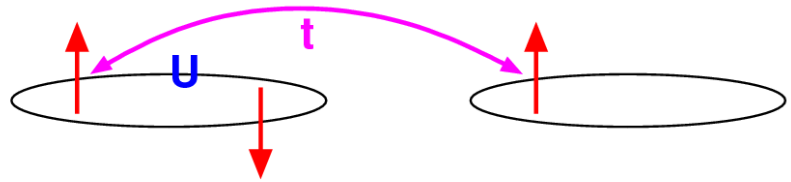

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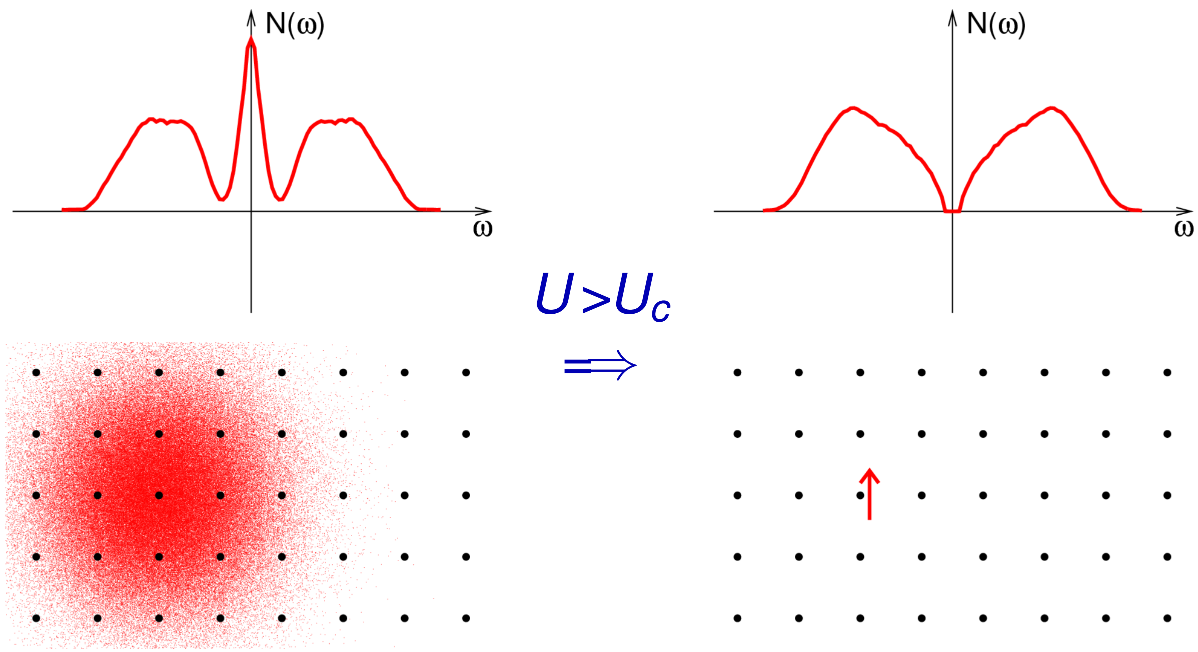
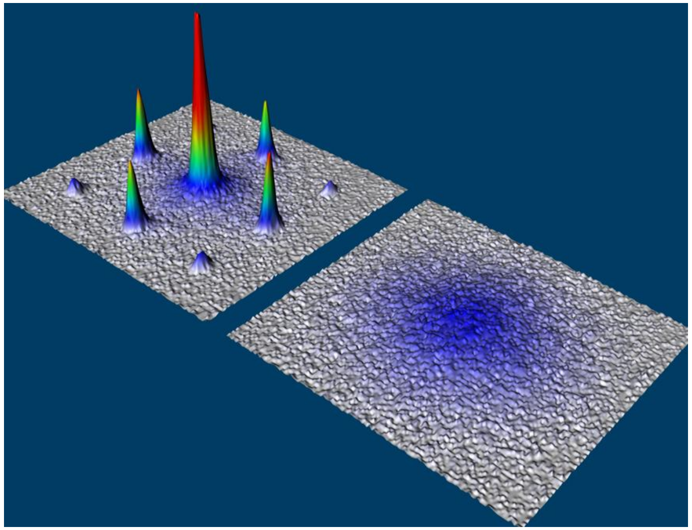




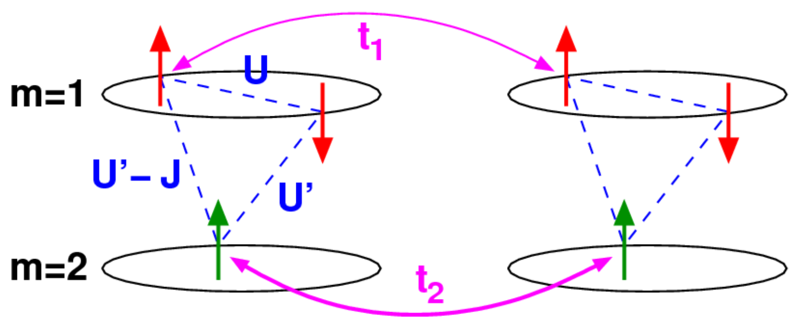
Localization (= decoherence) of ultracold bosons on optical lattice (Bloch group, 2002)

Case of multiple inequivalent orbitals/flavors?

2-band model with orbital-dependent hopping

$$H = \sum_{m=1}^{2} \Big[-\sum_{\langle ij \rangle \sigma} t_m c^\dagger_{im\sigma} c_{jm\sigma} + U \sum_i n_{im\uparrow} n_{im\downarrow} \Big]$$

$$+ \sum_{i\sigma\sigma'} (U' - \delta_{\sigma\sigma'} J_z)\, n_{i1\sigma}\, n_{i2\sigma'}$$



Ising-type Hund couplings [Liebsch, PRL (2003)]

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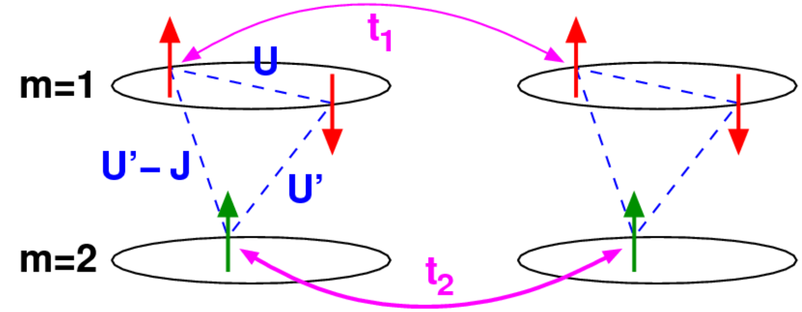

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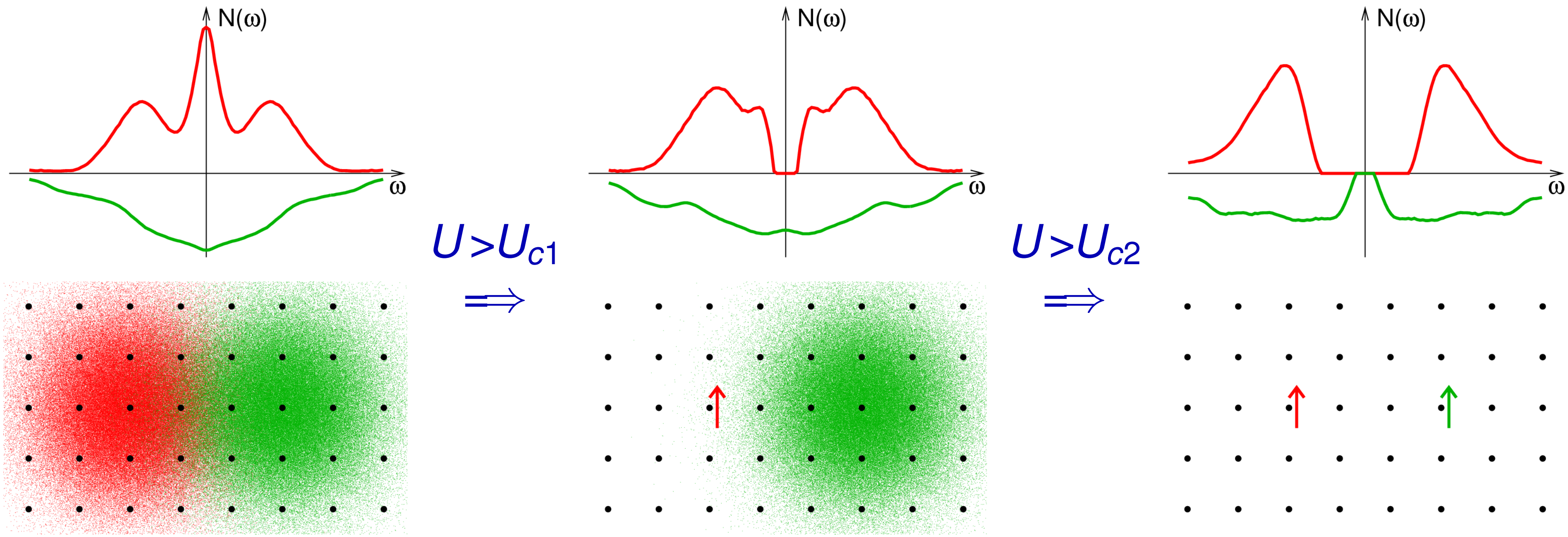

2 phase transitions [Knecht et al. (PRB 2005), de' Medici et al. (PRB 2005), Rüegg et al. (EPJB 2005)]

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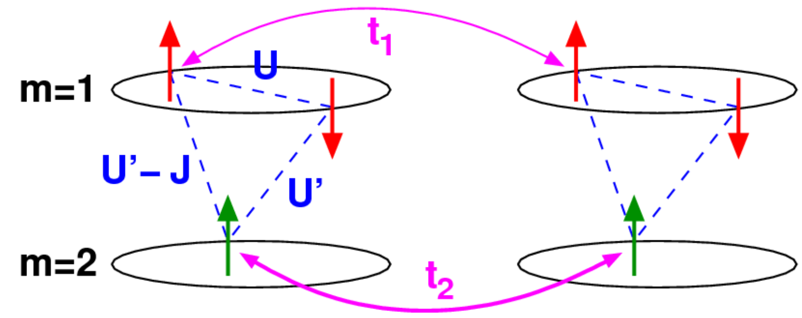

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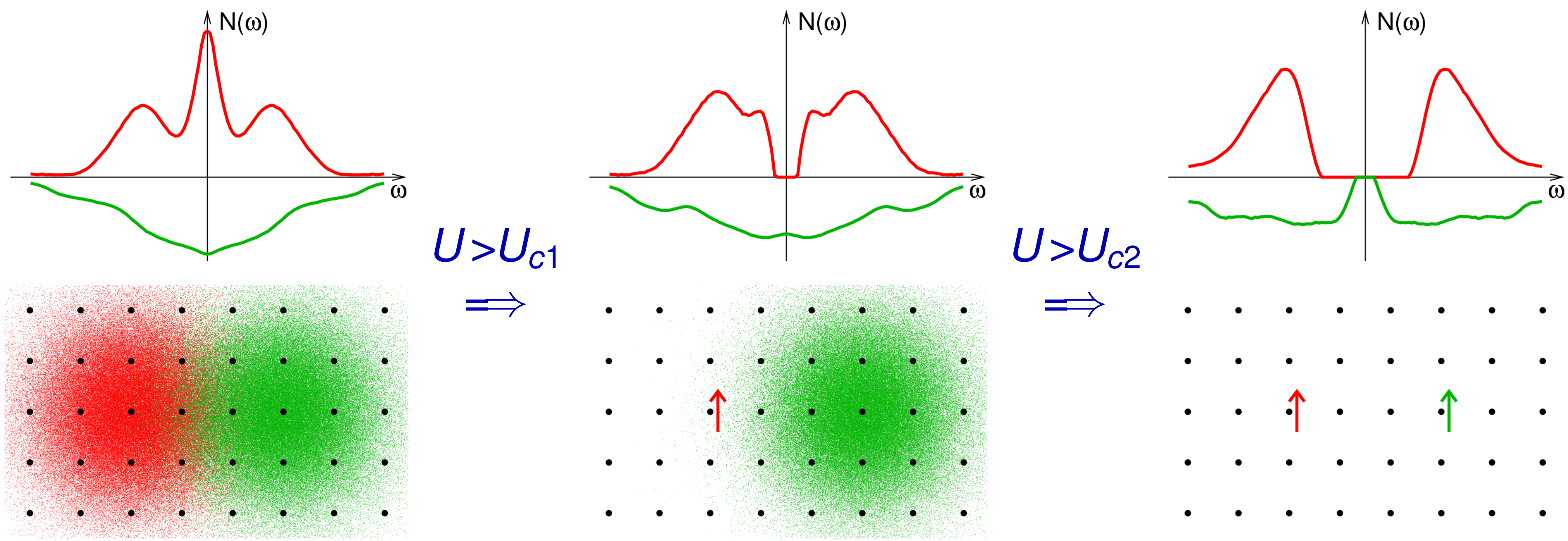

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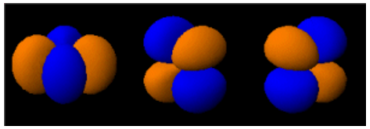
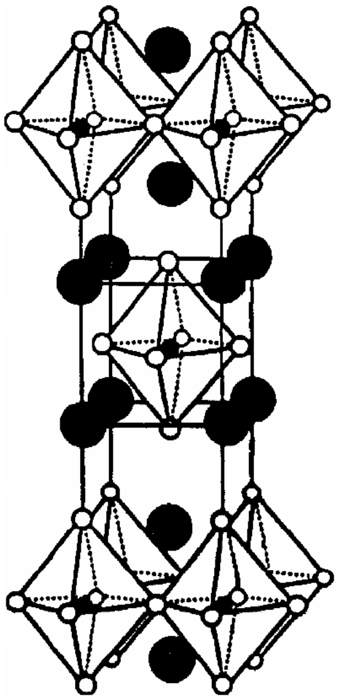
Character of wide-band transition?

Experimental realizations of orbital/flavor-selective physics?

1) t_{2g} electrons
in perovskites





[Nakatsuji, Maeno,
PRL (2000)]

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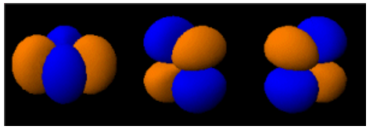
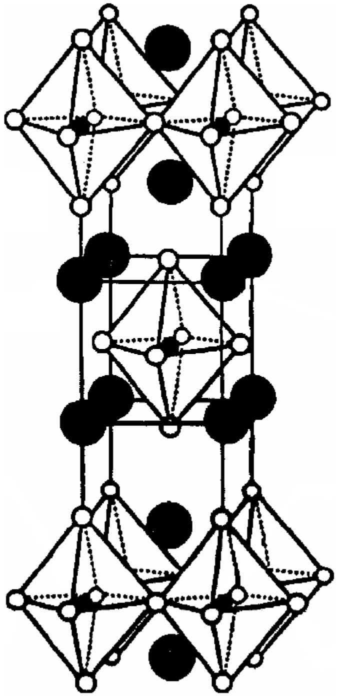
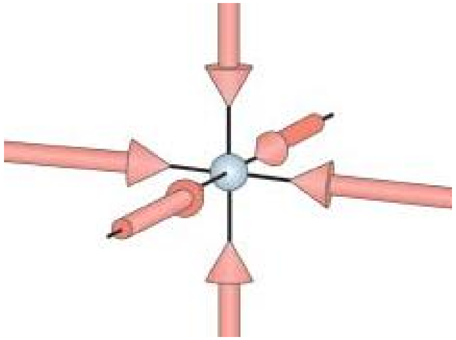
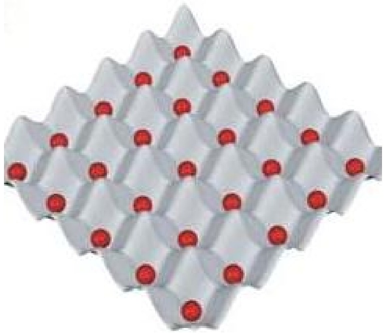




[Nakatsuji, Maeno, PRL (2000)]

2) Flavour mixtures of ultracold (fermionic) atoms on optical lattice





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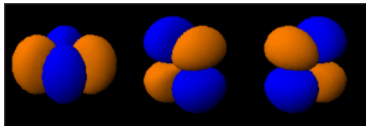

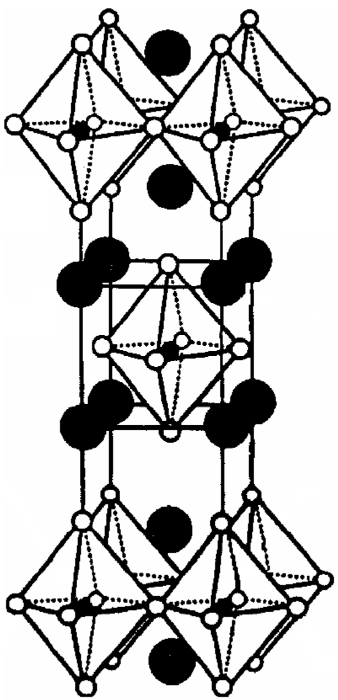

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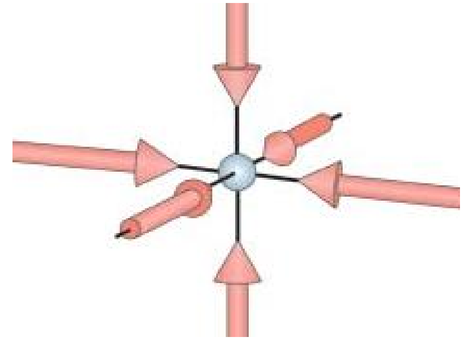
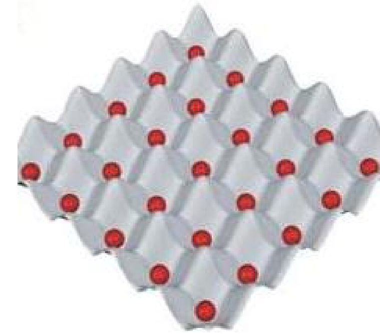
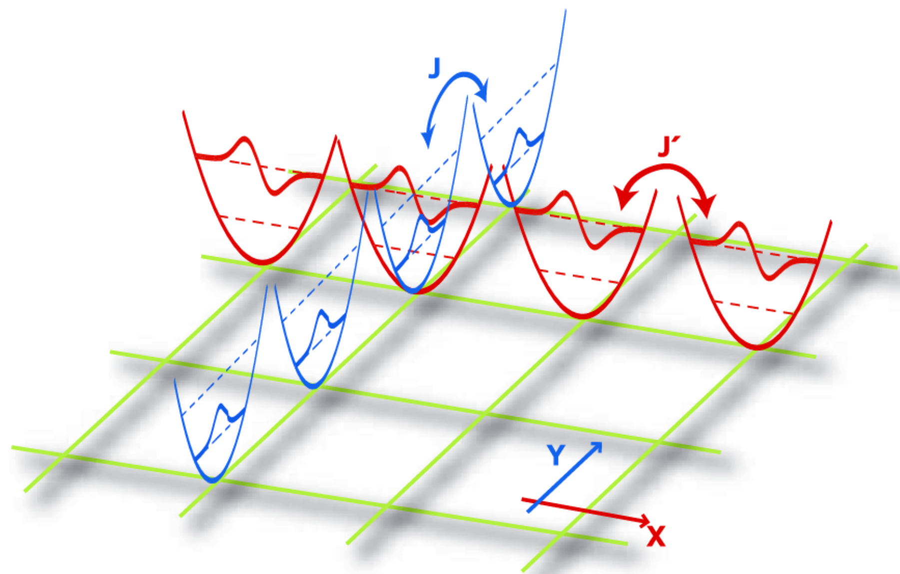




Flavors:

- atomic species, e.g., ^{6}Li and ^{40}K
- hyperfine states
- vibrational levels

Hopping amplitudes are generically flavor dependent!



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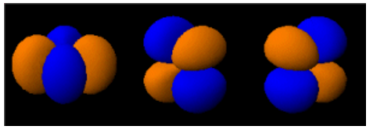

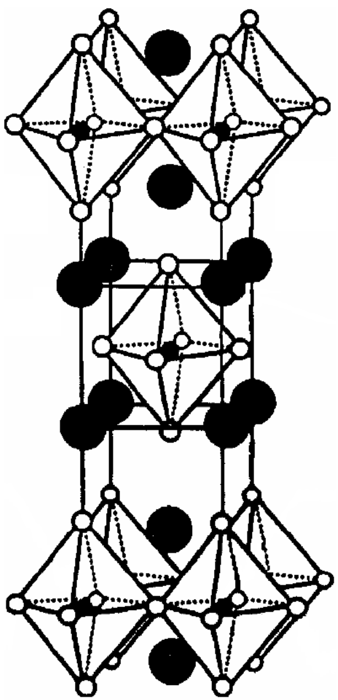

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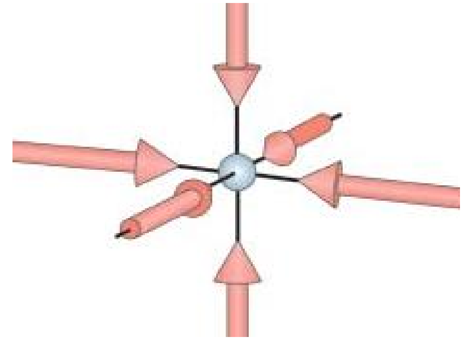

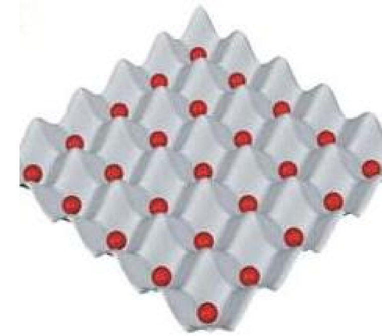

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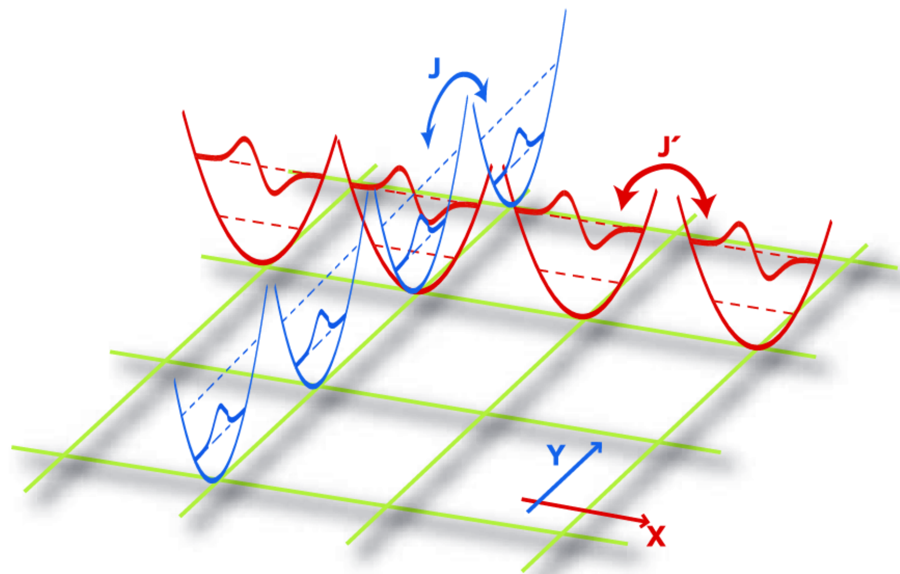
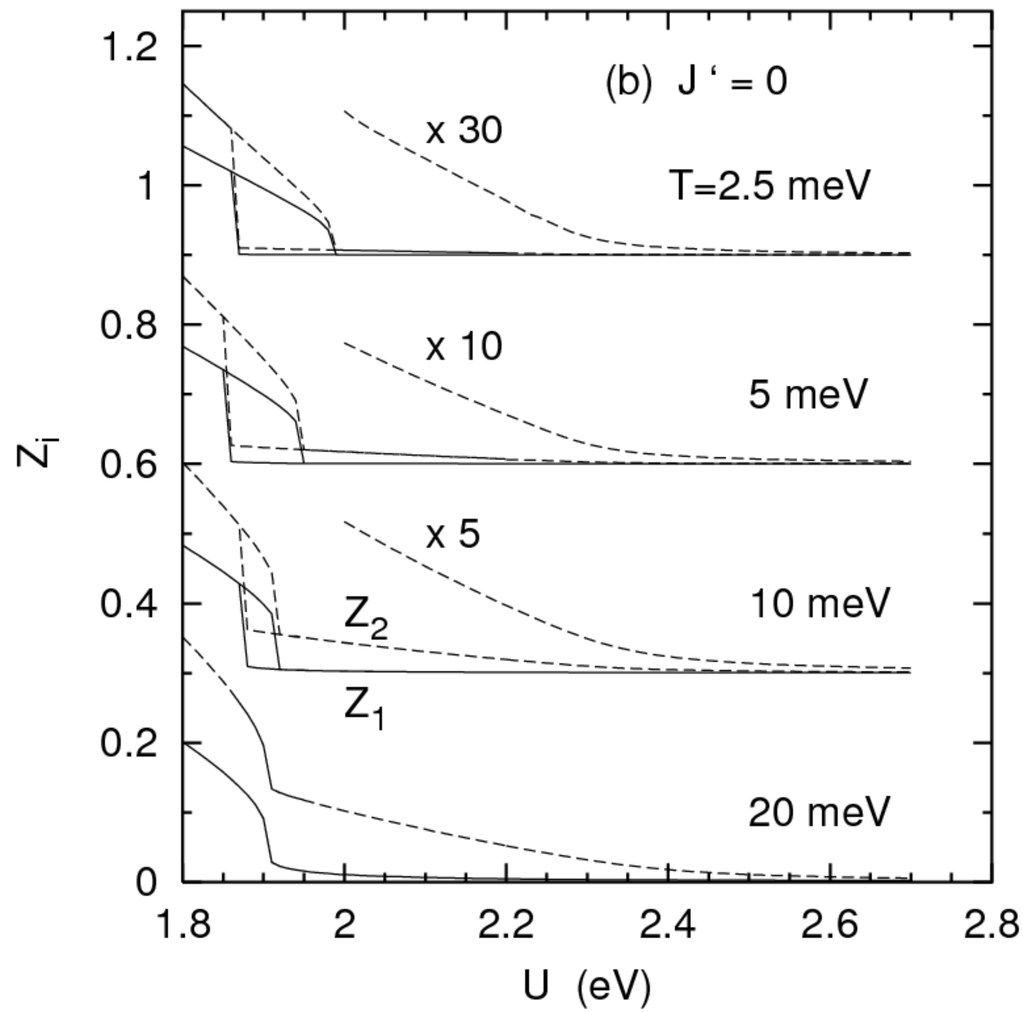
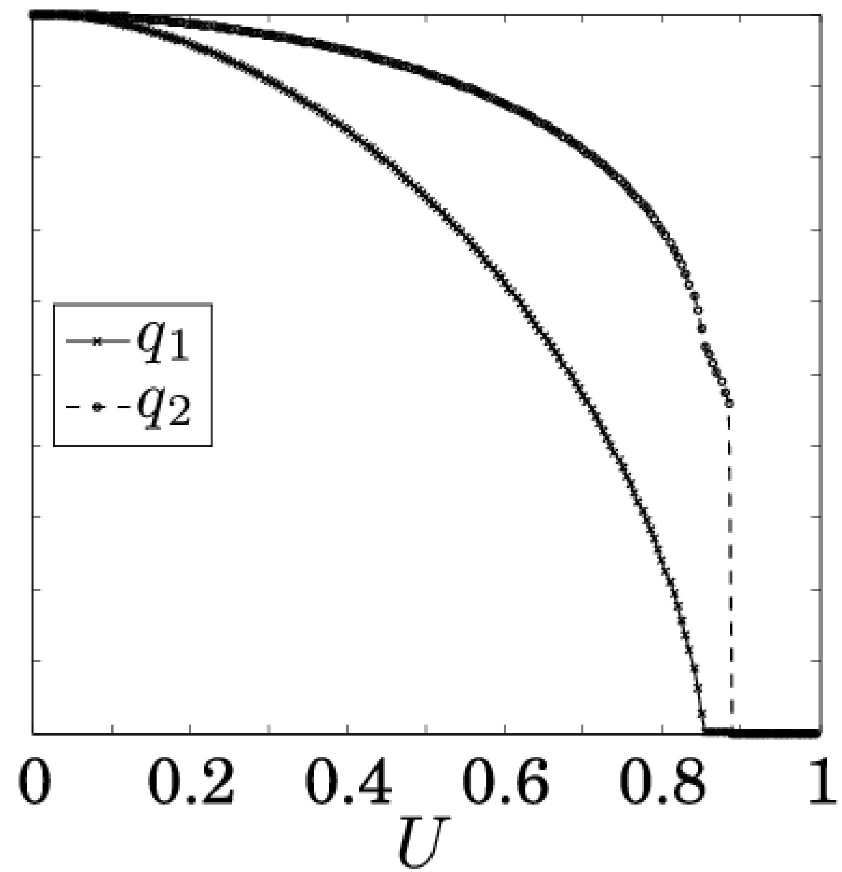


Related: Dual nature of 5f electrons in UPt_3 [Zwicknagl, Yaresko, Fulde, PRB (2002)]

Order of wide-band transition in anisotropic model



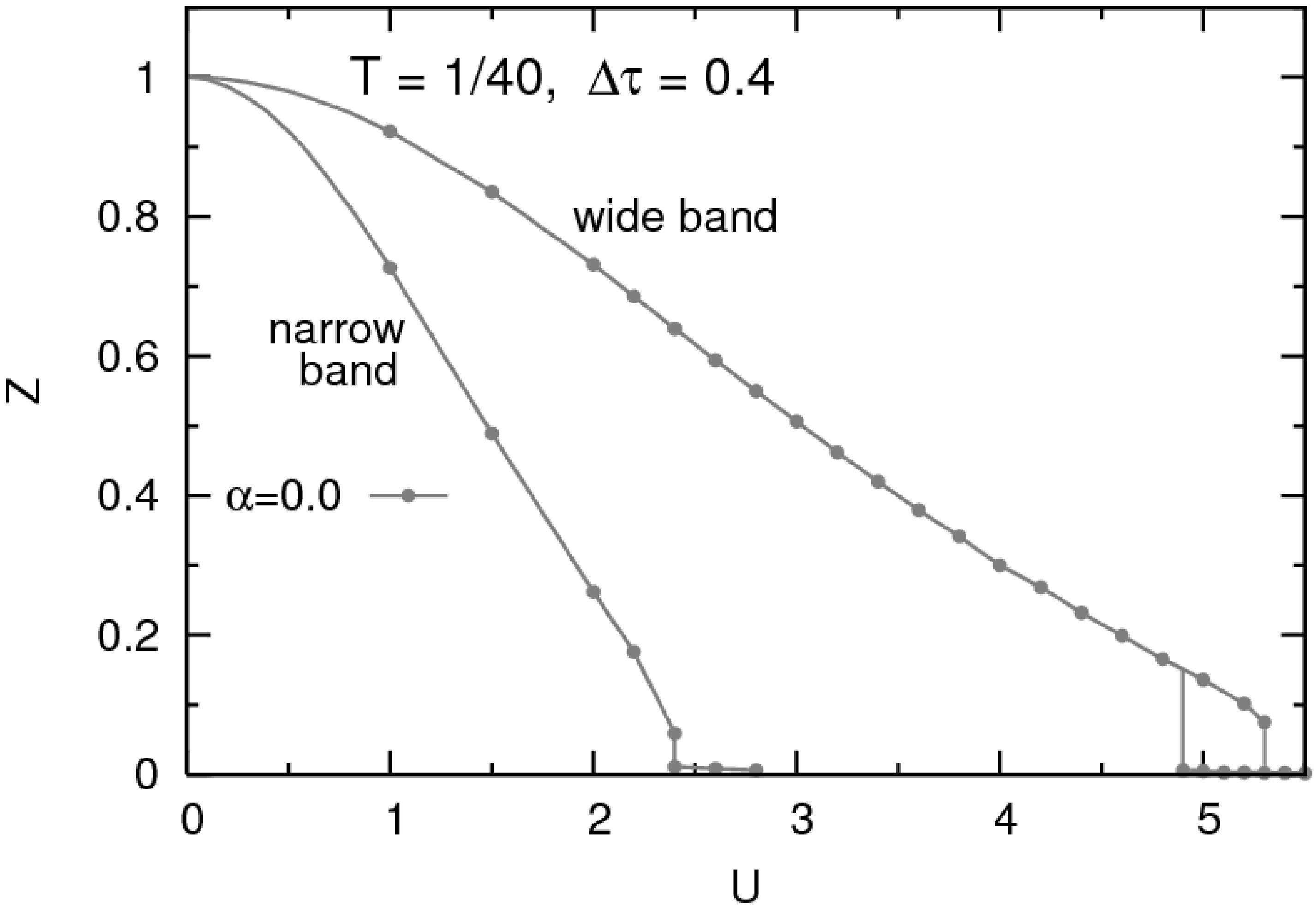
ED ⇝ no hysteresis at low T for wide-band transition [Liebsch, PRL (2005)]



Slave-boson MF ⇝ 1st order wide-band transition (at $T = 0$) [Rüegg, Indergand, Pilgram, Sigrist, EPJB (2005)]

Systematic study: effect of inter-orbital coupling

$$H = \sum_{m=1}^{2} \Big[-\sum_{\langle ij\rangle\sigma} t_m c^{\dagger}_{im\sigma} c_{jm\sigma} + U \sum_i n_{im\uparrow} n_{im\downarrow} \Big] + \alpha \sum_{i\sigma\sigma'} (U/2 - \delta_{\sigma\sigma'} U/4)\, n_{i1\sigma}\, n_{i2\sigma'}$$



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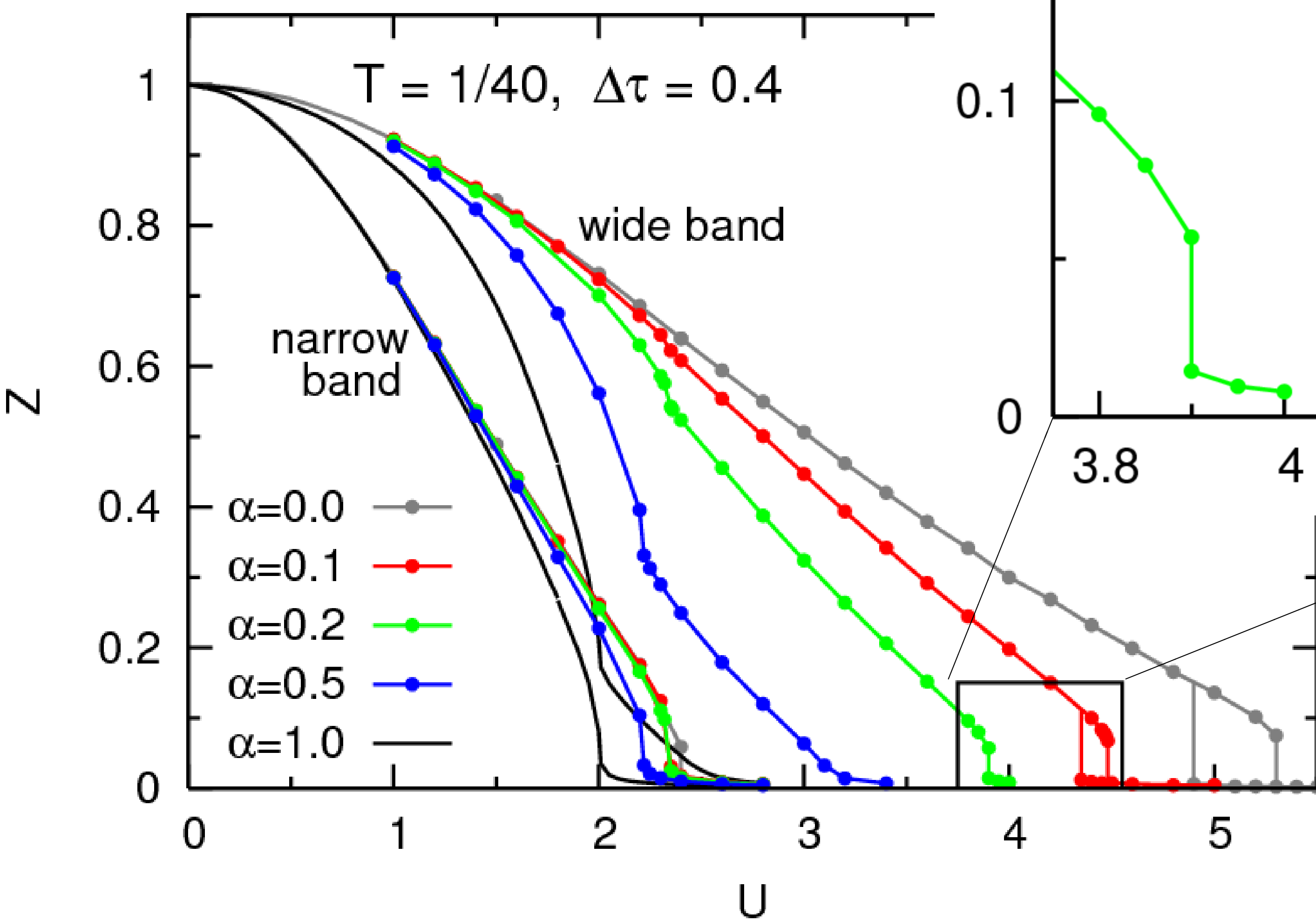
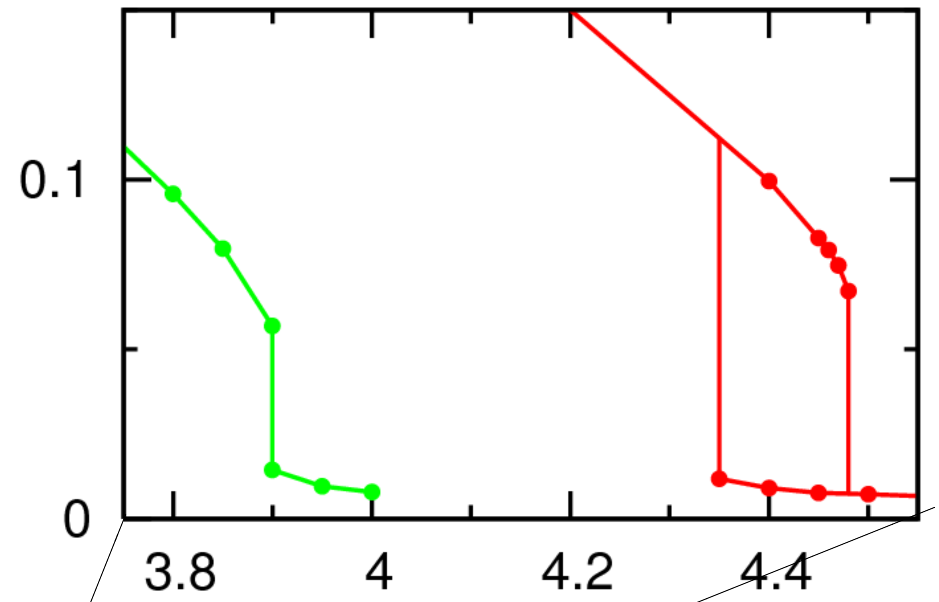


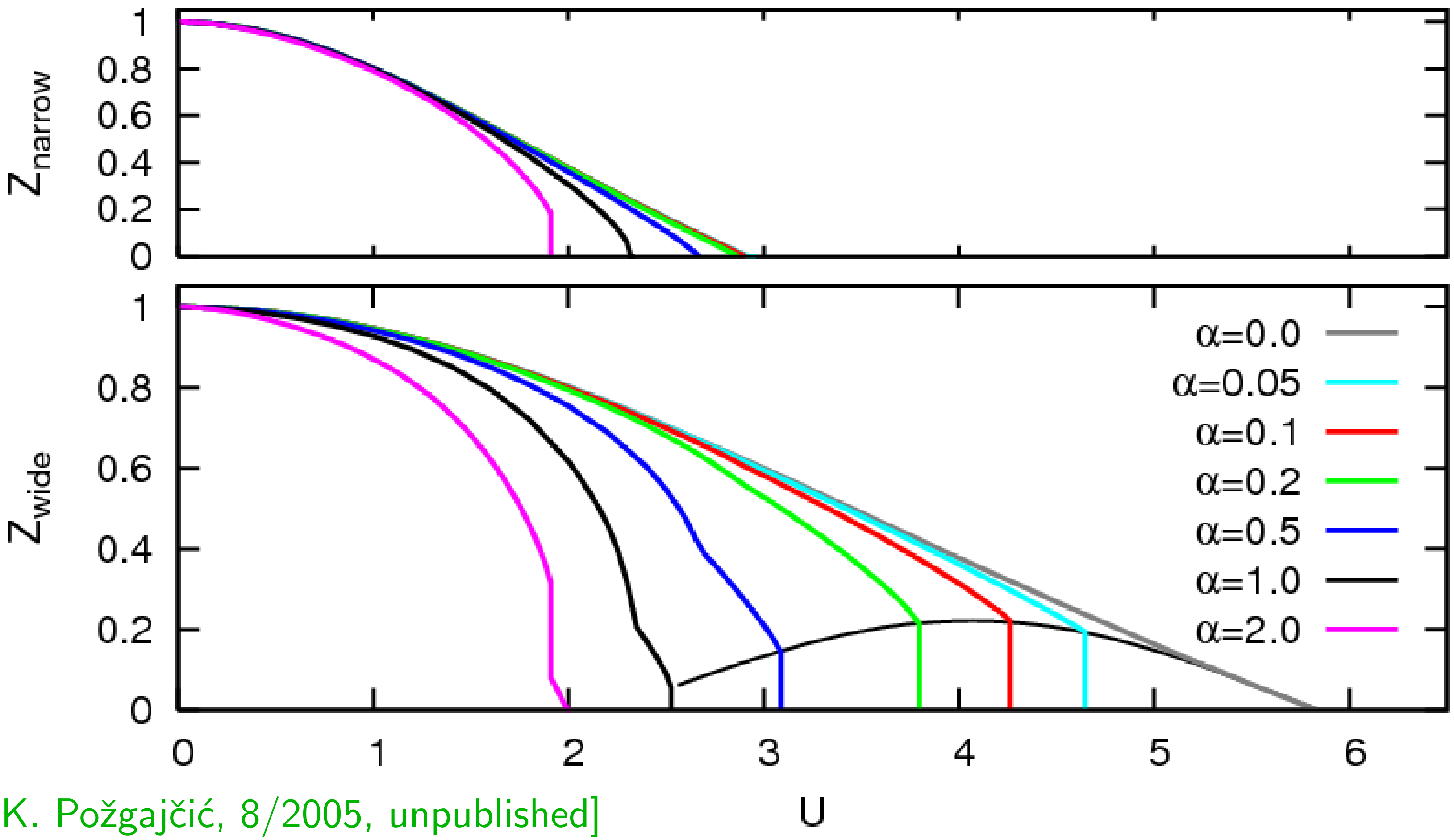


QMC at $T = 1/40$:

wide-band OSMT remains 1st order for small α

1st order at T=0?

Self-energy functional theory (SFT+ED) with 1 bath site per orbital



[K. Požgajčić, 8/2005, unpublished]

◦ 1st order wide-band transition for $0 < \alpha \lesssim 1.5$ ◦ larger α: 2nd order ↔ 1st order

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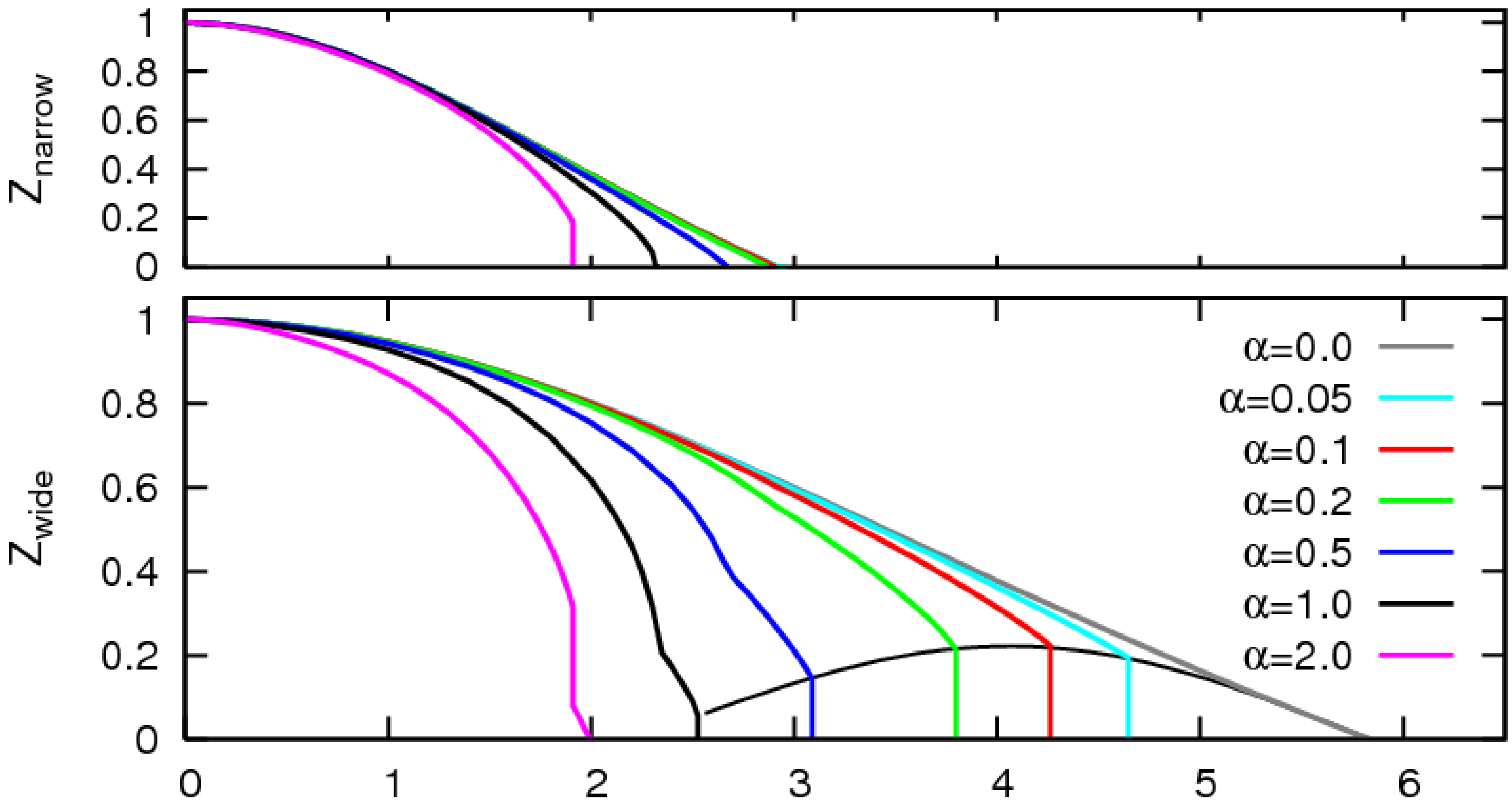

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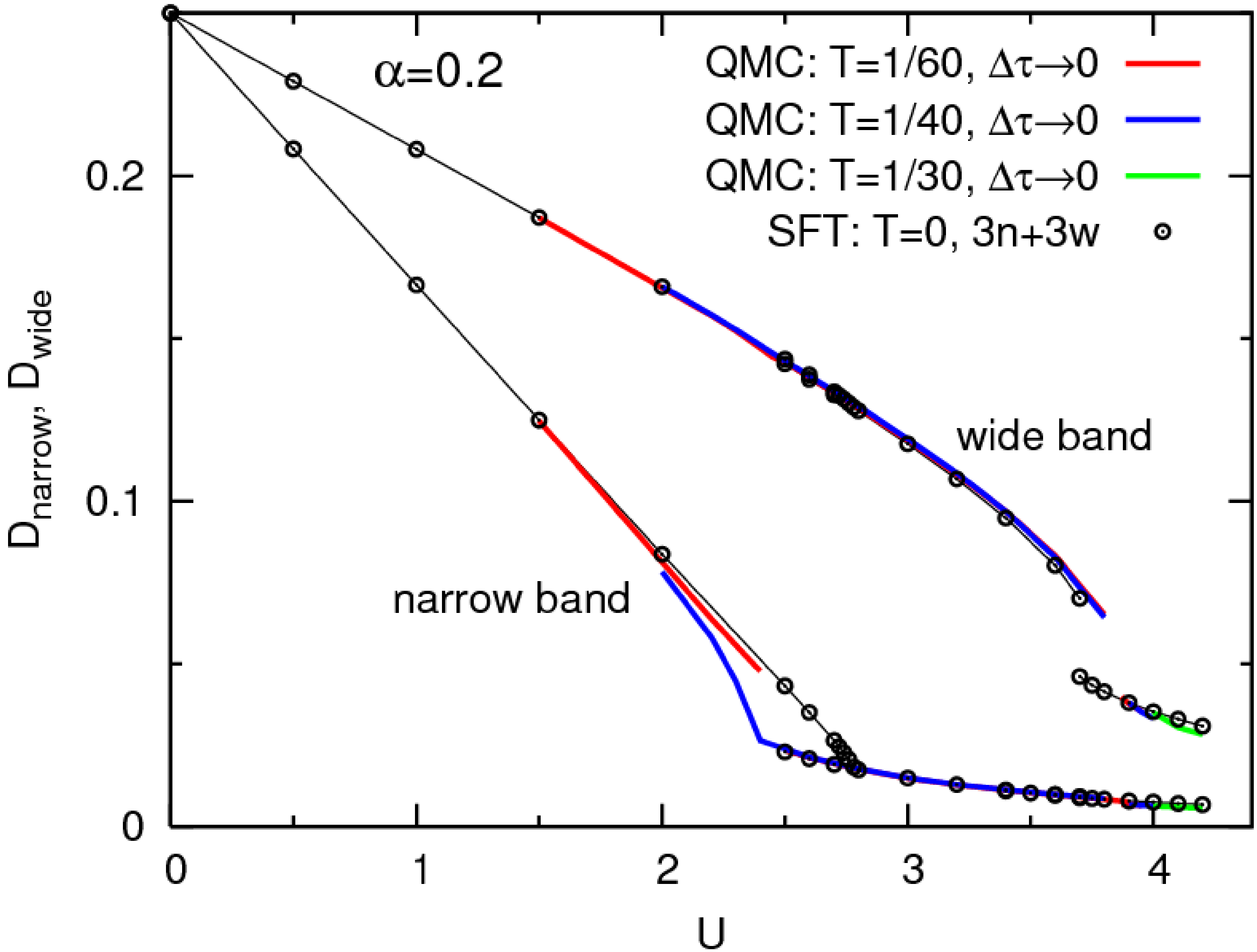
◦ 1st order wide-band transition for $0 < \alpha \lesssim 1.5$ ◦ larger α: 2nd order ↔ 1st order

Problems: ◦ Low-frequency part of $\Sigma(\omega)$ inconsistent with QMC

◦ Z ill-defined in OSM phase ◦ strong finite-size effects

Double occupancy (1st order derivative of Ω)



Excellent agreement between SFT and QMC

1st order at $T = 0$ (at least) for $0 < \alpha \leq 0.2$

QMC efficiency: Hirsch-Fye vs. continuous time

Performance analysis of continuous-time solvers for quantum impurity models

Emanuel Gull,[1] Philipp Werner,[2] Andrew Millis,[2] and Matthias Troyer[1]

[1] *Institut für theoretische Physik, ETH Zürich, CH-8093 Zürich, Switzerland*
[2] *Columbia University, 538 West, 120th Street, New York, NY 10027, USA*

Impurity solvers play an essential role in the numerical investigation of strongly correlated electrons systems within the "dynamical mean field" approximation. Recently, a new class of continuous-time solvers has been developed, based on a diagrammatic expansion of the partition function in either the interactions or the impurity-bath hybridization. We investigate the performance of these two complimentary approaches and compare them to the well-established Hirsch-Fye method. The results show that the continuous-time methods, and in particular the version which expands in the hybridization, provide substantial gains in computational efficiency.

PACS numbers: 71.10.-w, 71.10.Fd, 71.28.+d, 71.30.+h

[cond-mat/0609438]

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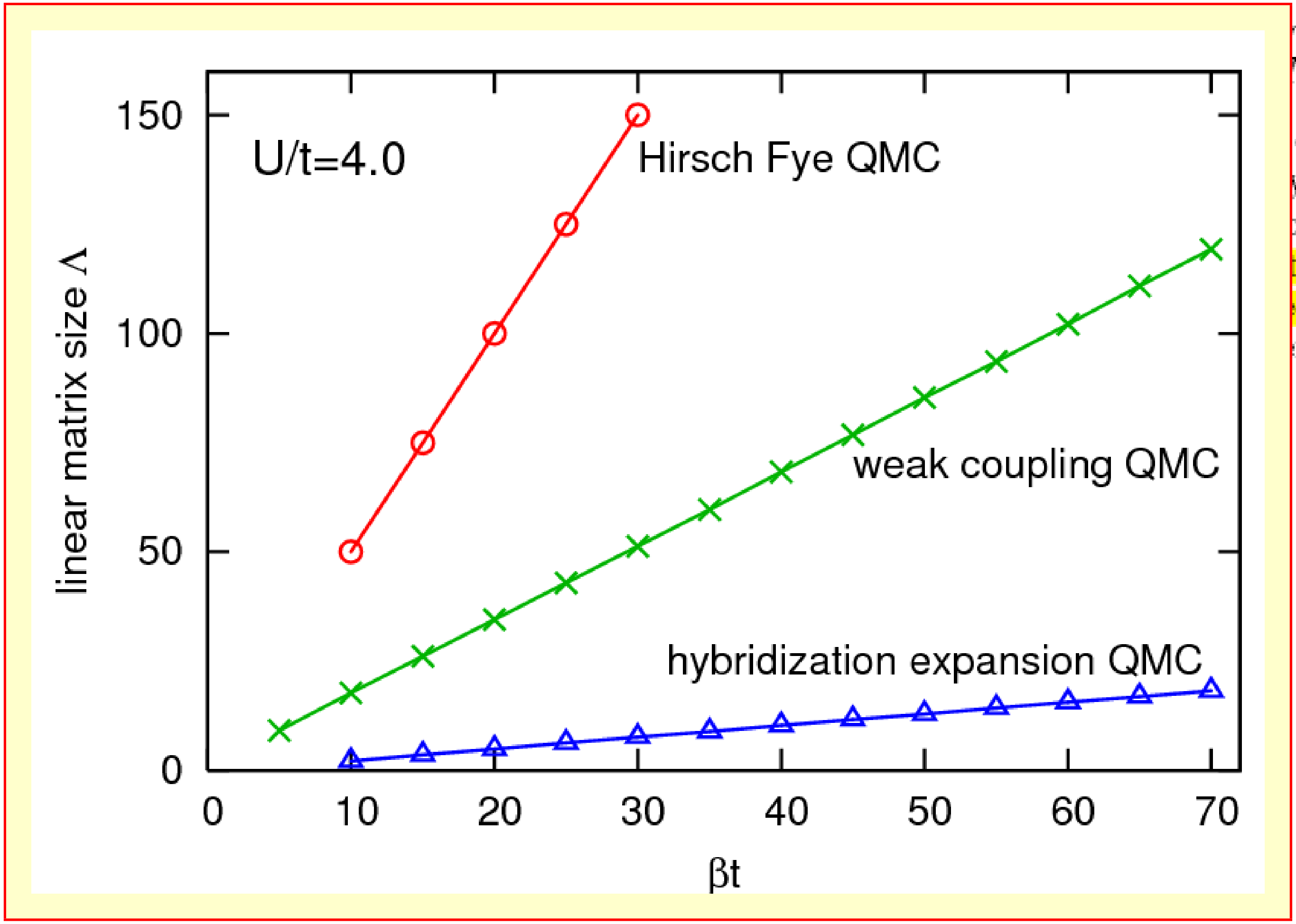

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NY 10027, USA

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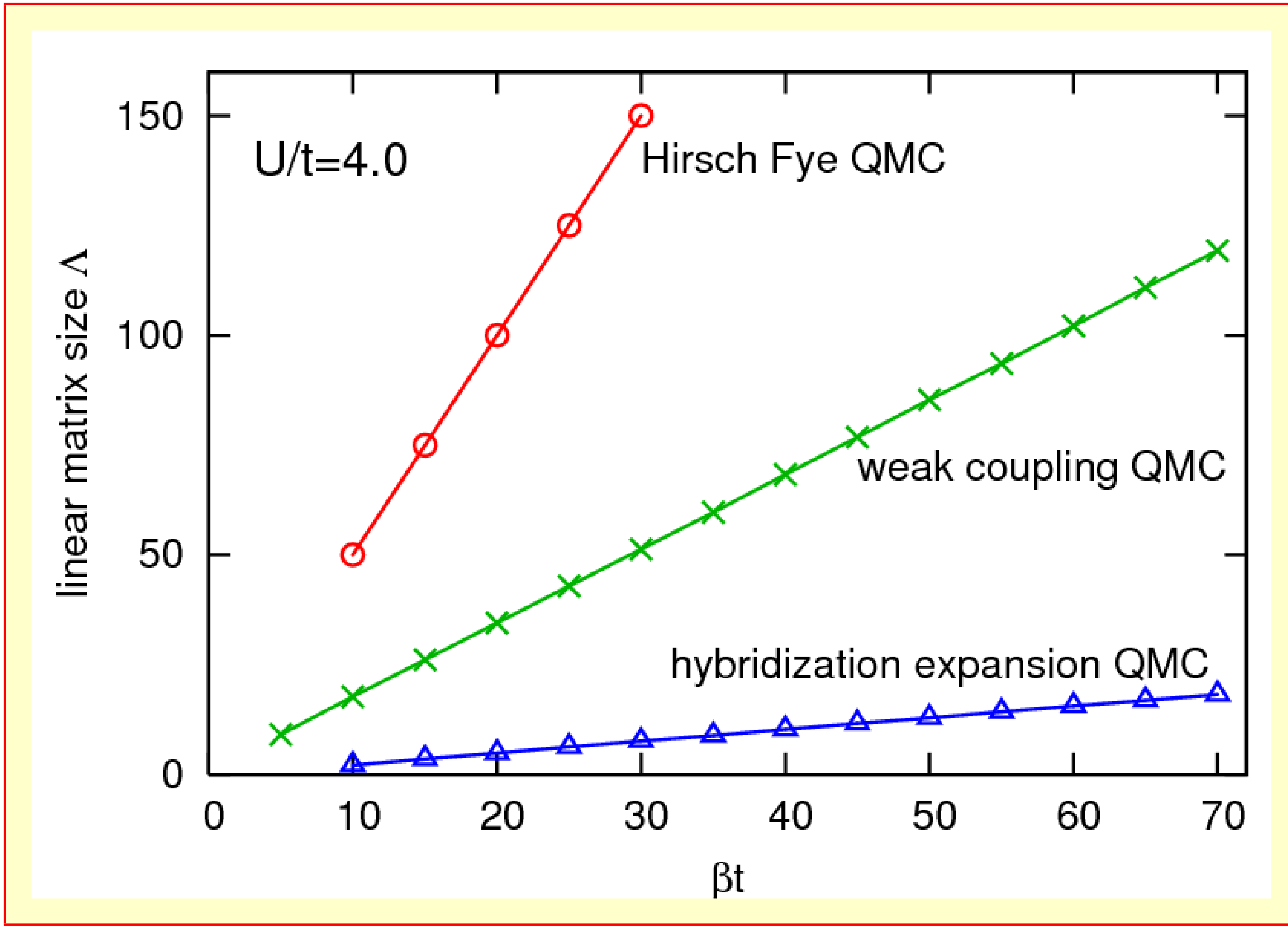

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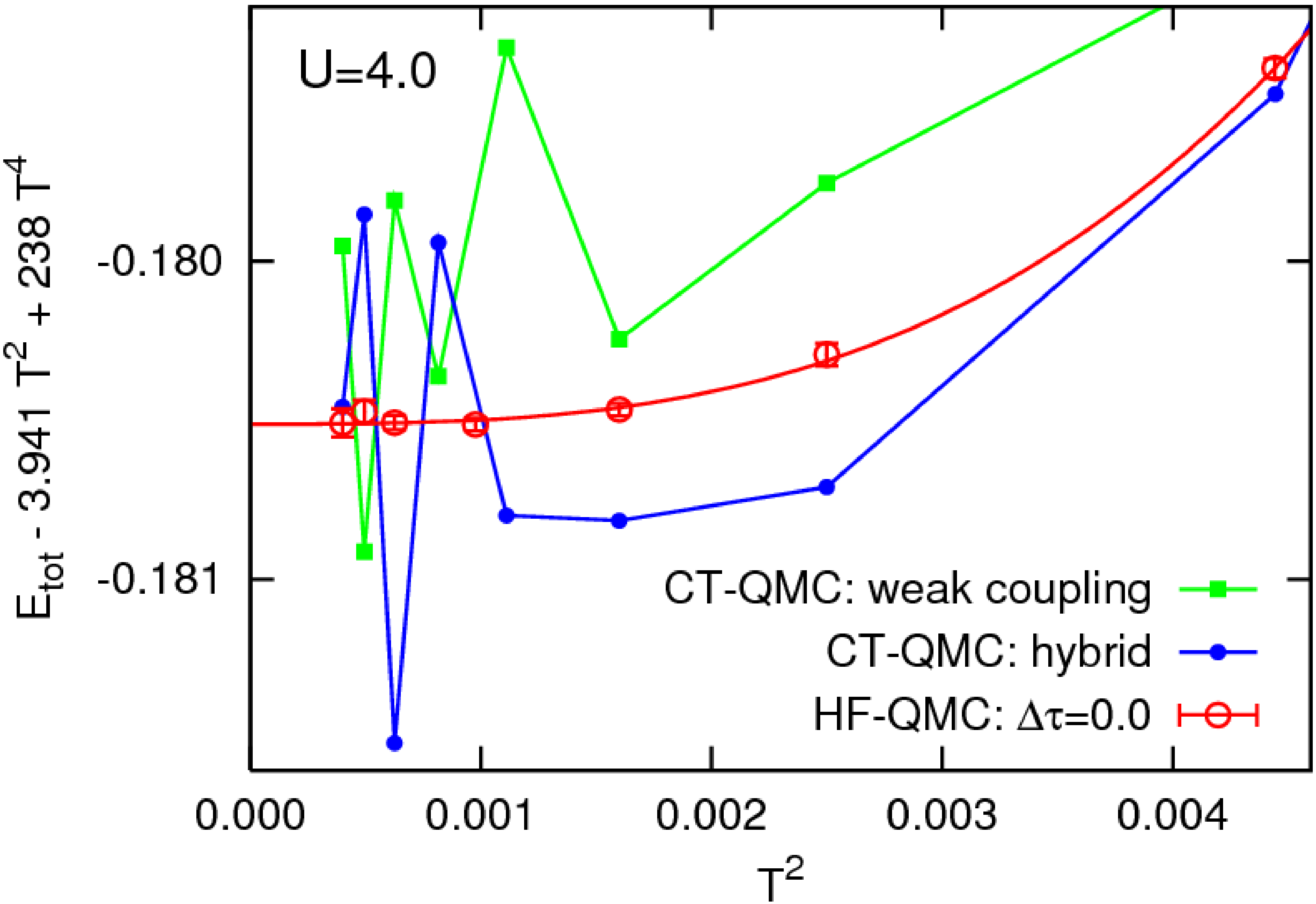
problem: numerical cost scales as Λ^3 $\rightsquigarrow$ **HF-QMC dead!**

Energy of 1-band Hubbard model (semi-elliptic DOS, $W = 4$)



HF-QMC is 2 orders of magnitude more precise (after extrapolation $\Delta\tau \rightarrow 0$)

Summary

Orbital-selective Mott transitions (OSMTs)

- new concept, motivated by experiments on $Ca_{2-x}Sr_xRuO_4$
- flavor-selective phases expected in ultracold quantum gases
- there: many fascinating possibilities

Nature and order of OSMTs in 2-band Hubbard model ($J_z > J_\perp$)

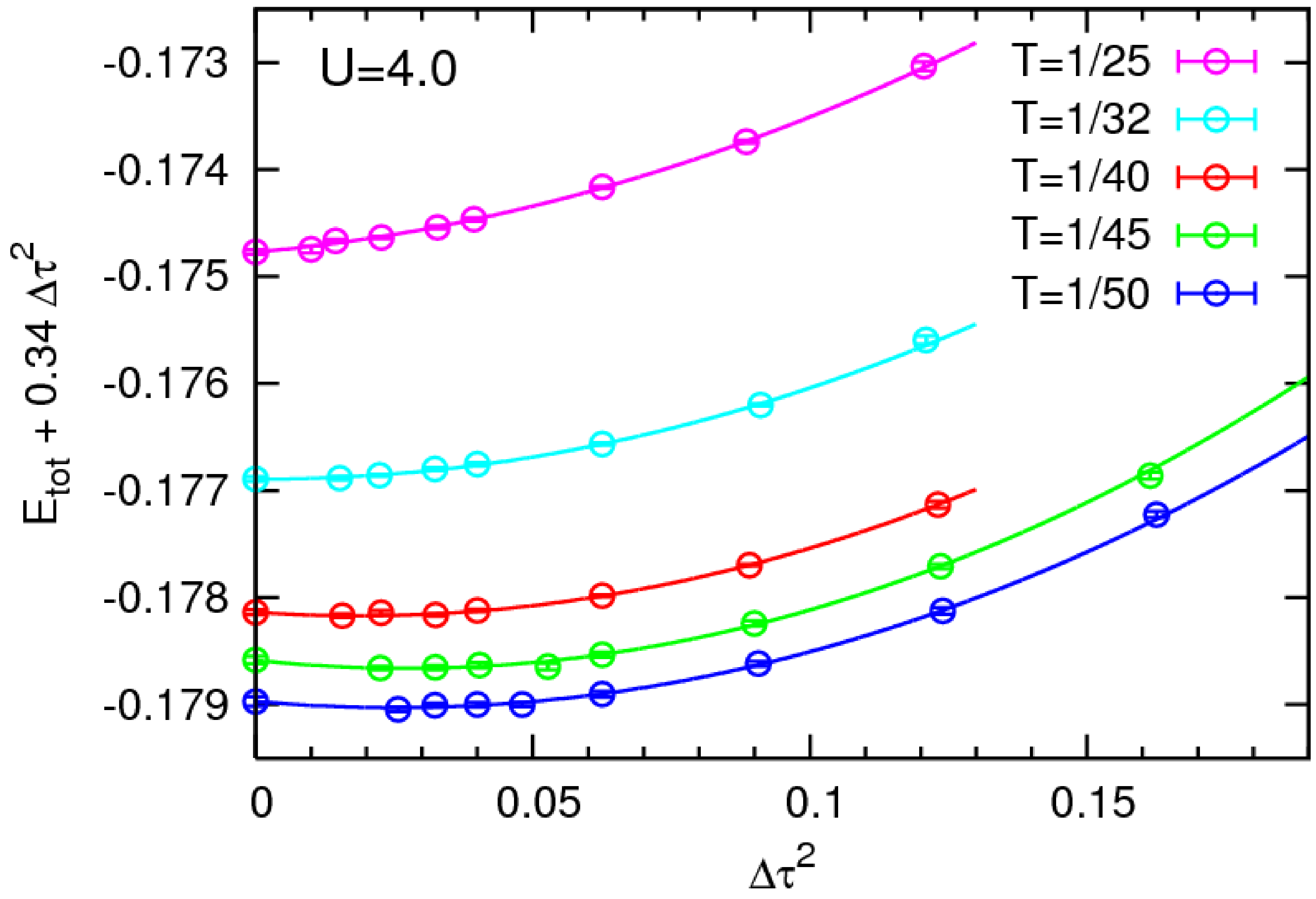
- narrow-band transition unchanged from single-band case
- non-FL phase for $U_{c1} < U < U_{c2}$
- wide-band OSMT 1st order (for small α) at $T > 0$ and $T = 0$

  [NB, C. Knecht, K. Požgajčić, P.G.J. van Dongen, JMMM **310**, 922 (2007)]

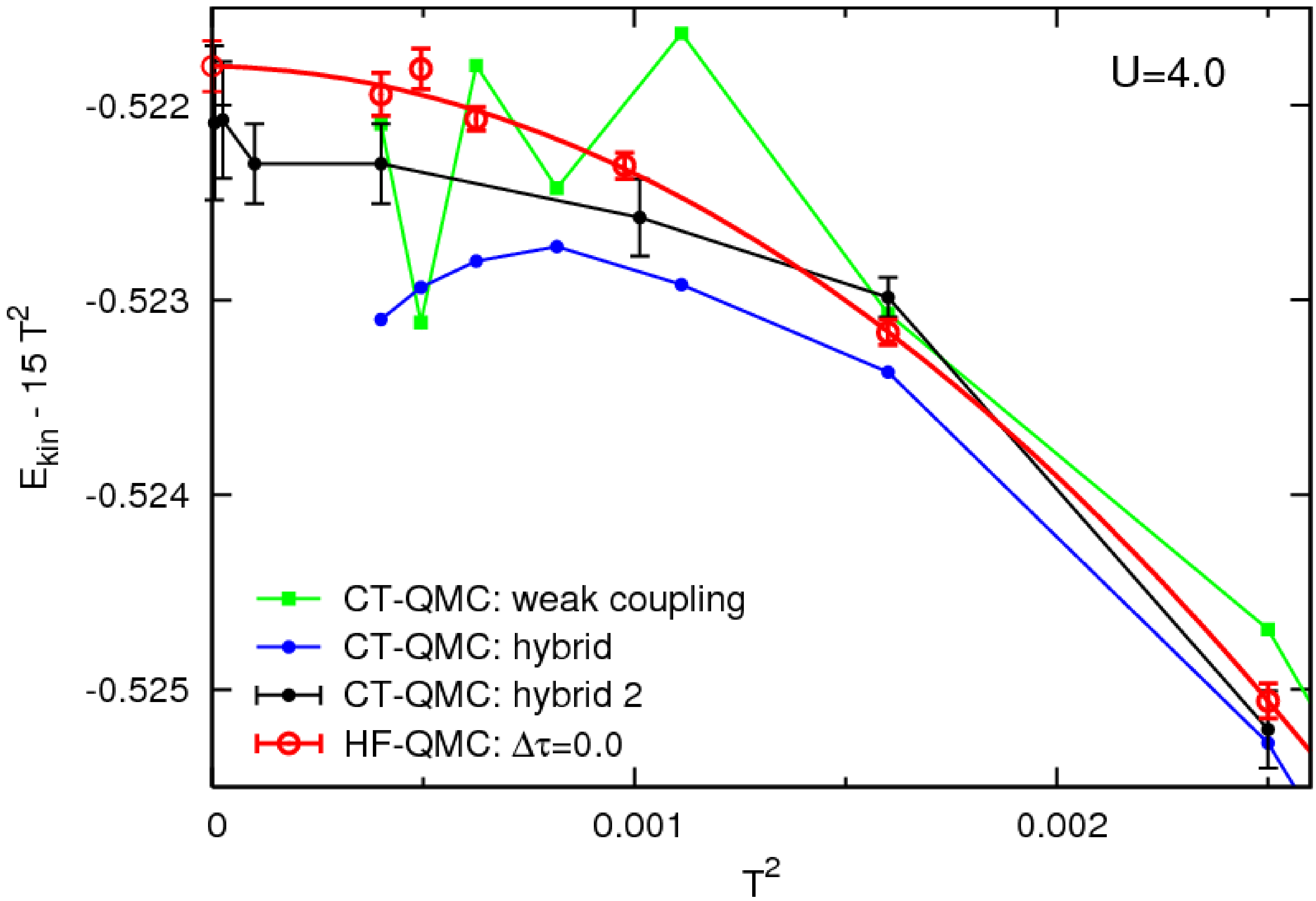
Continuous-time quantum Monte Carlo methods (CT-QMC)

- promising, direct access to low-temperature phases
- less severe sign problem in case of spin-flip terms
- but: HF-QMC competitive at moderate T (for $\Delta\tau \to 0$)

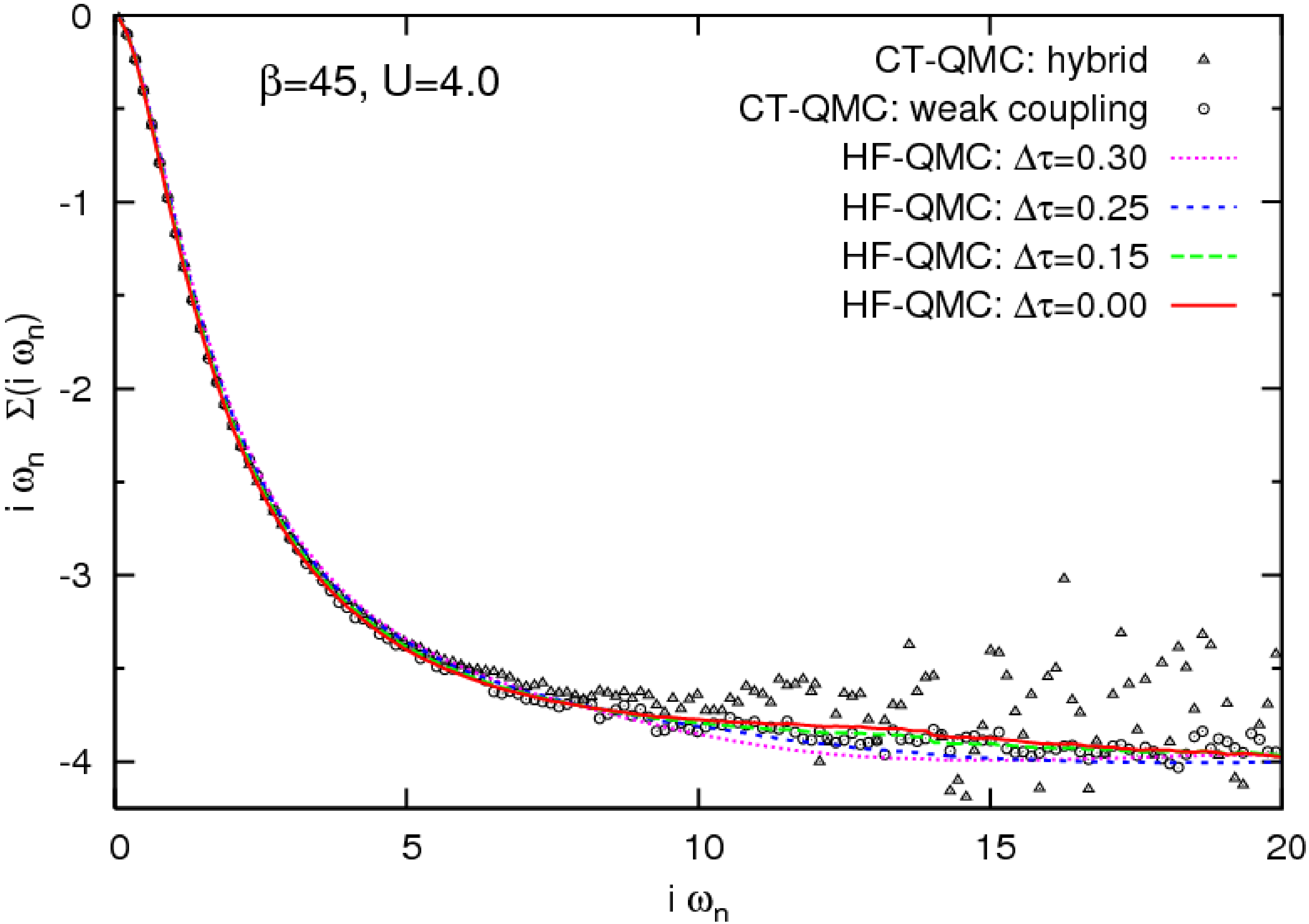
Extrapolation of energy of 1-band Hubbard model $\Delta\tau \to 0$



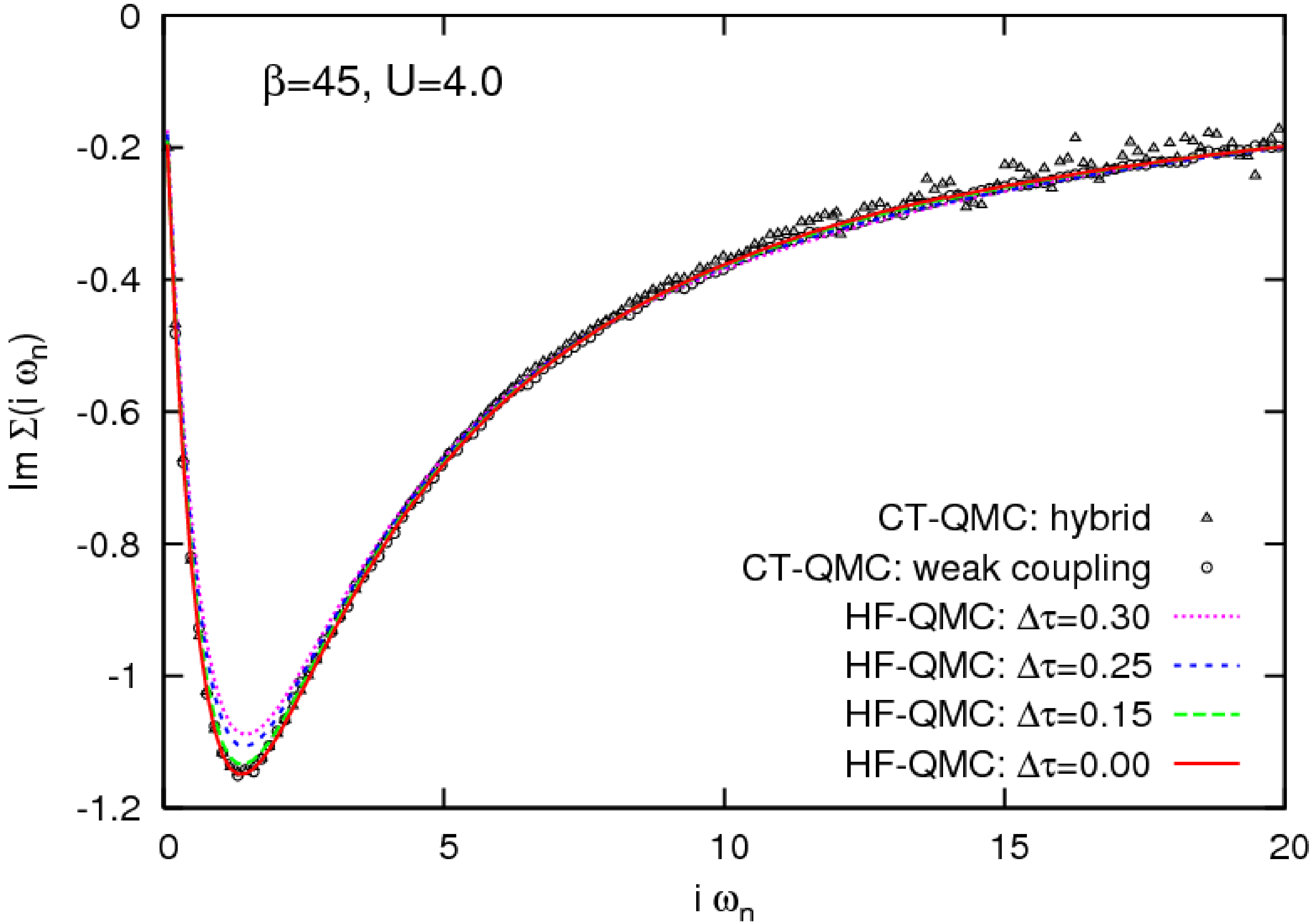
Kinetic energy of 1-band Hubbard model



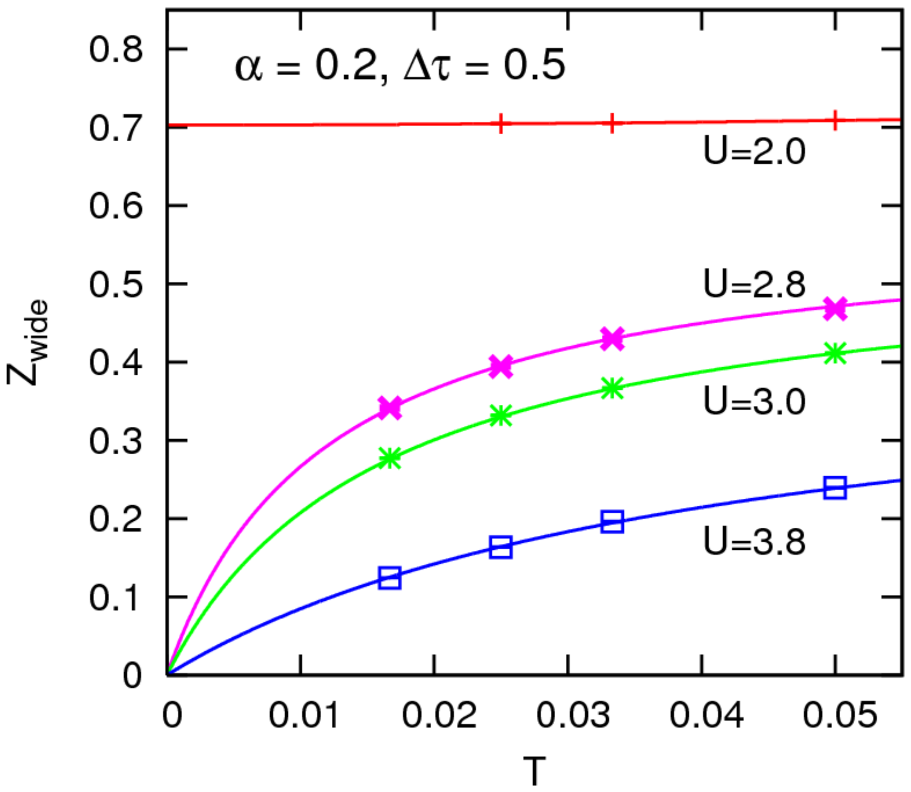
Self-energy of 1-band Hubbard model



Rescaled self-energy of 1-band Hubbard model



Self-energy and quasiparticle weight Z in OSM phase



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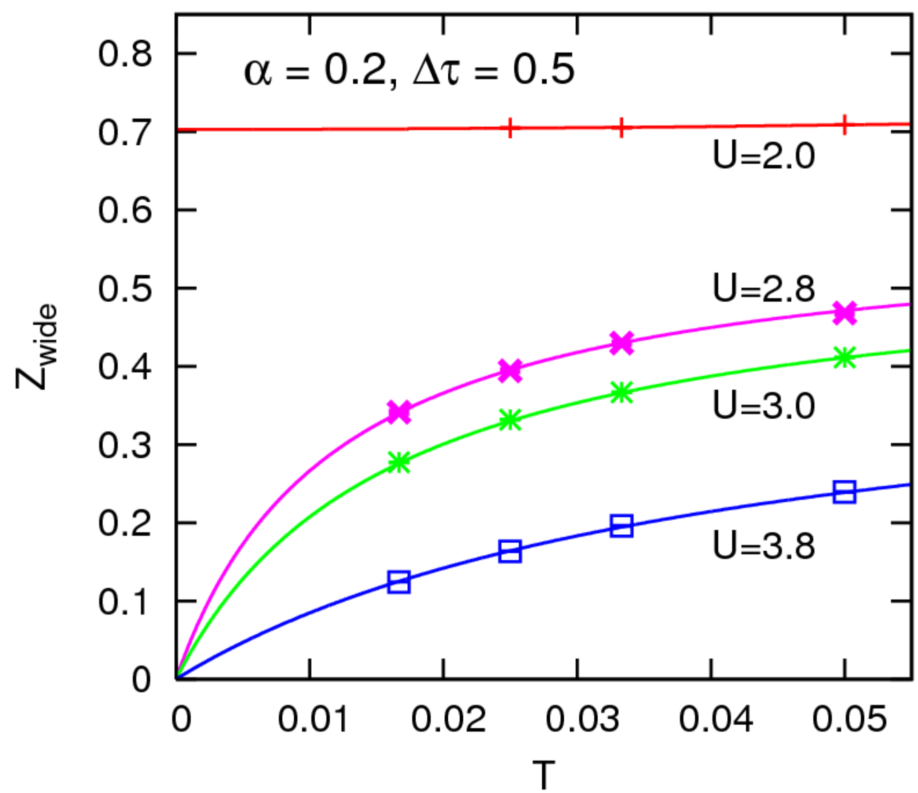

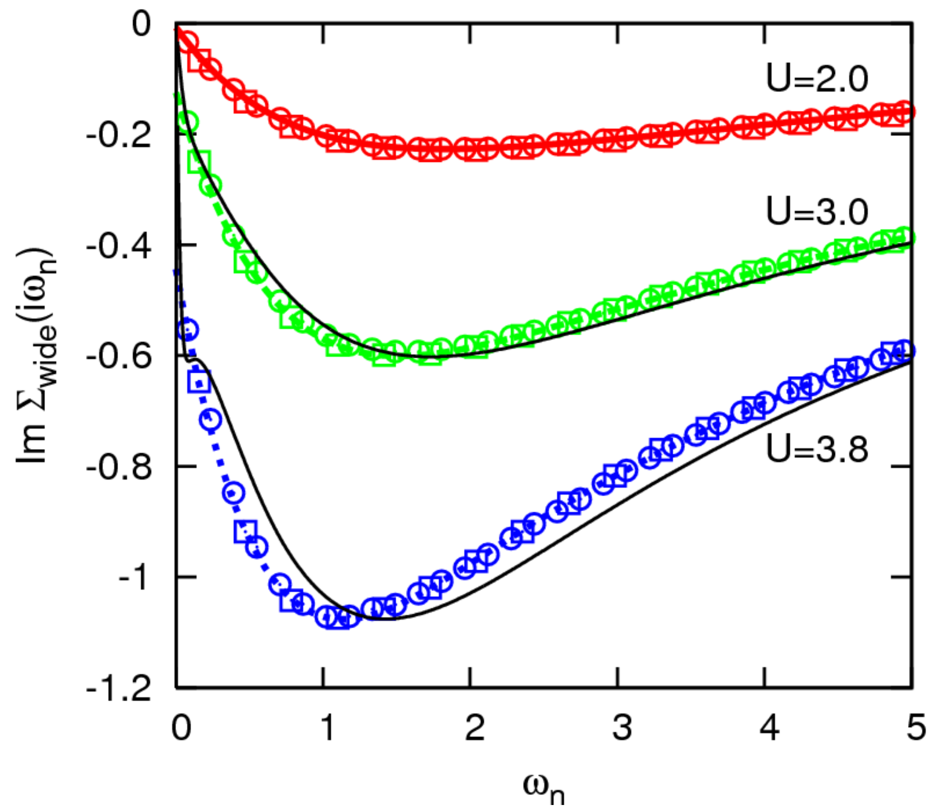

T-dependence of Z_{wide} in non-FL OSM phase:

artifact of QMC estimate $Z = \left[1 - \frac{\text{Im}\Sigma(i\pi T)}{\pi T}\right]^{-1}$

Antiferromagnetic order in bipartite case