Mott transitions at variable spin/orbital degeneracy

Nils Blümer and Elena Gorelik, Univ. Mainz

Outline

Mott transition, 1-band DMFT

SU($2M$) invariant Hubbard model

Multigrid Hirsch-Fye quantum Monte Carlo algorithm

Mott transitions at large degeneracy

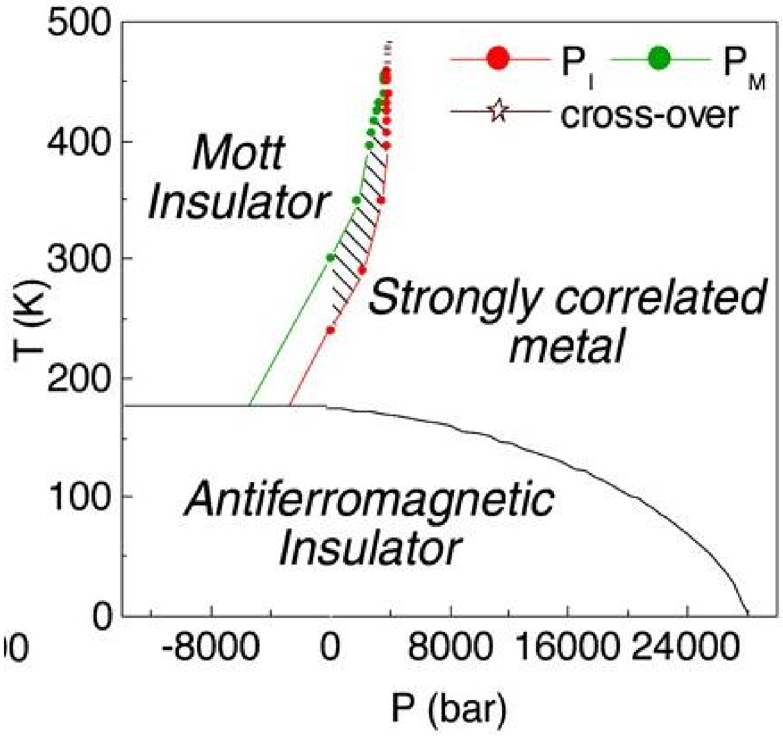
Scaling analysis

Summary

Mott metal-insulator transition (MIT) - experiment

Prototype example: V_2O_3 doped with Cr/Ti and/or under pressure

Phase diagram



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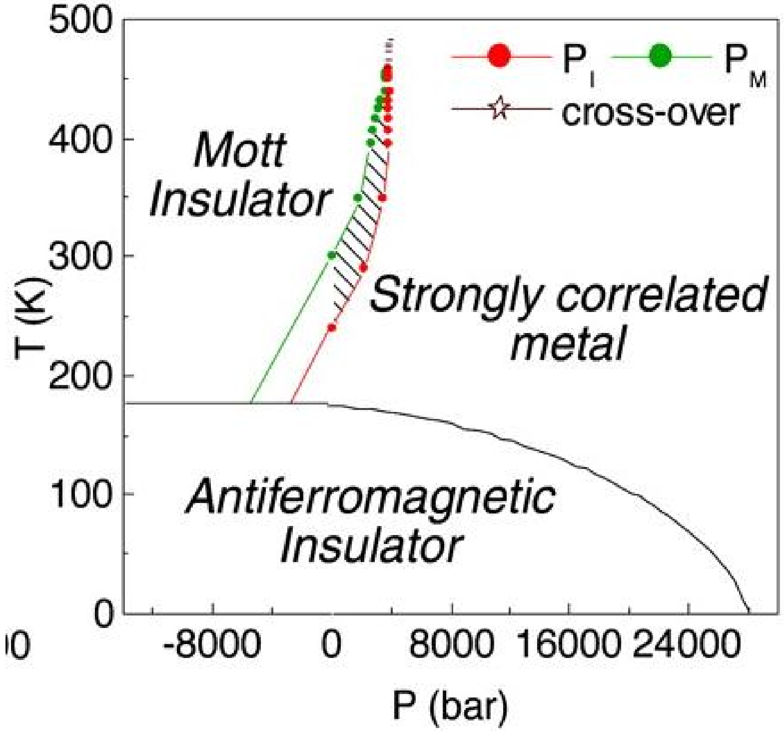
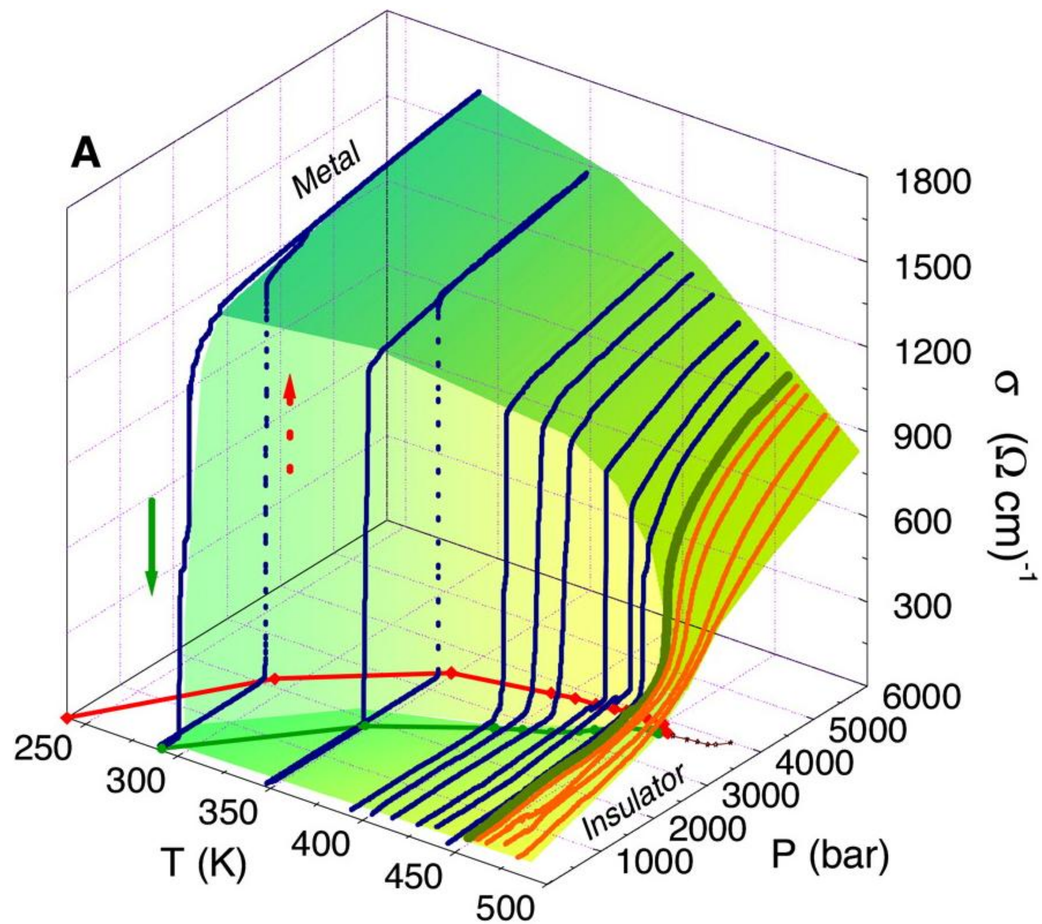


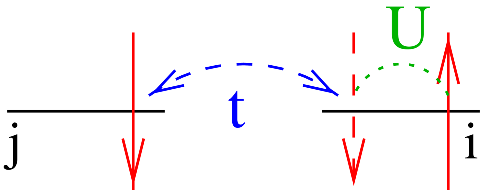
Electrical conductivity



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

Dynamical mean field theory of MIT (1-band case)

Hubbard model: $H = \sum_{(i,j),\sigma} t_{ij} \, (c^\dagger_{i\sigma} c_{j\sigma} + \text{h.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow}$



Semi-elliptic Bethe density of states ($W = 4$), restriction to paramagnetic phase

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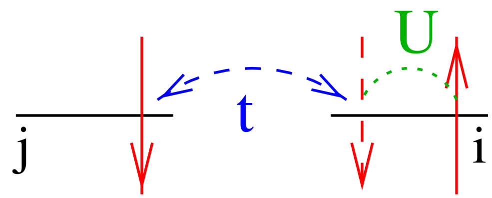

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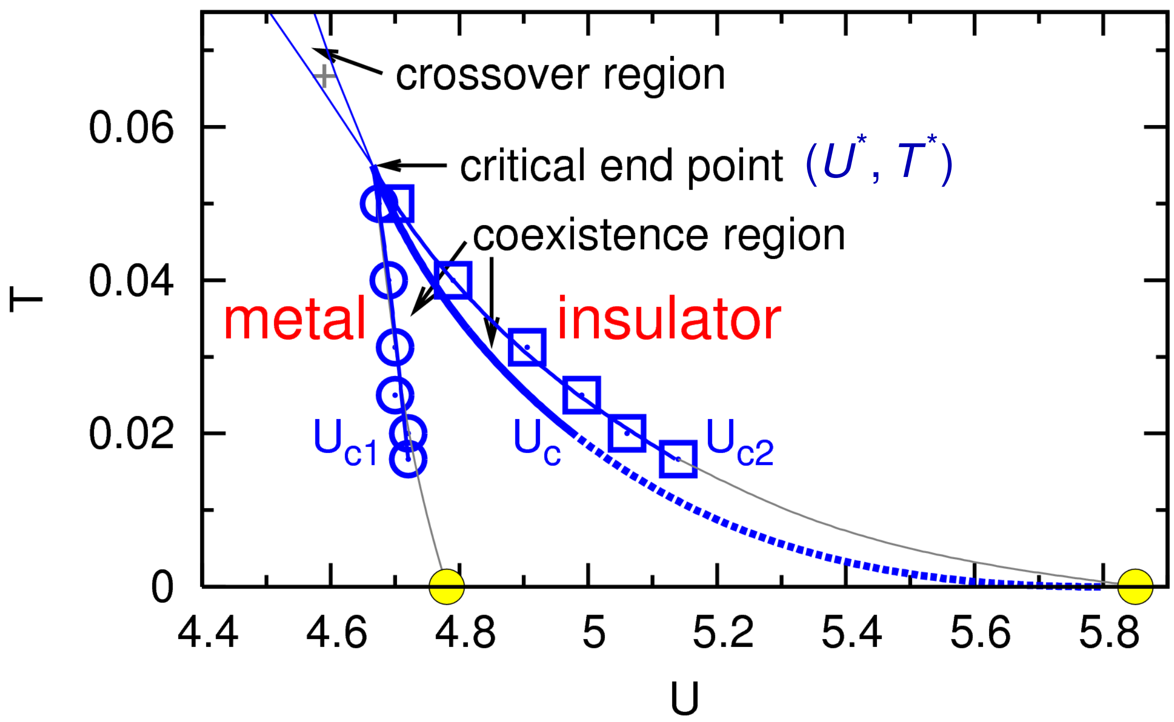

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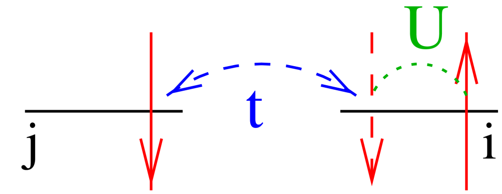

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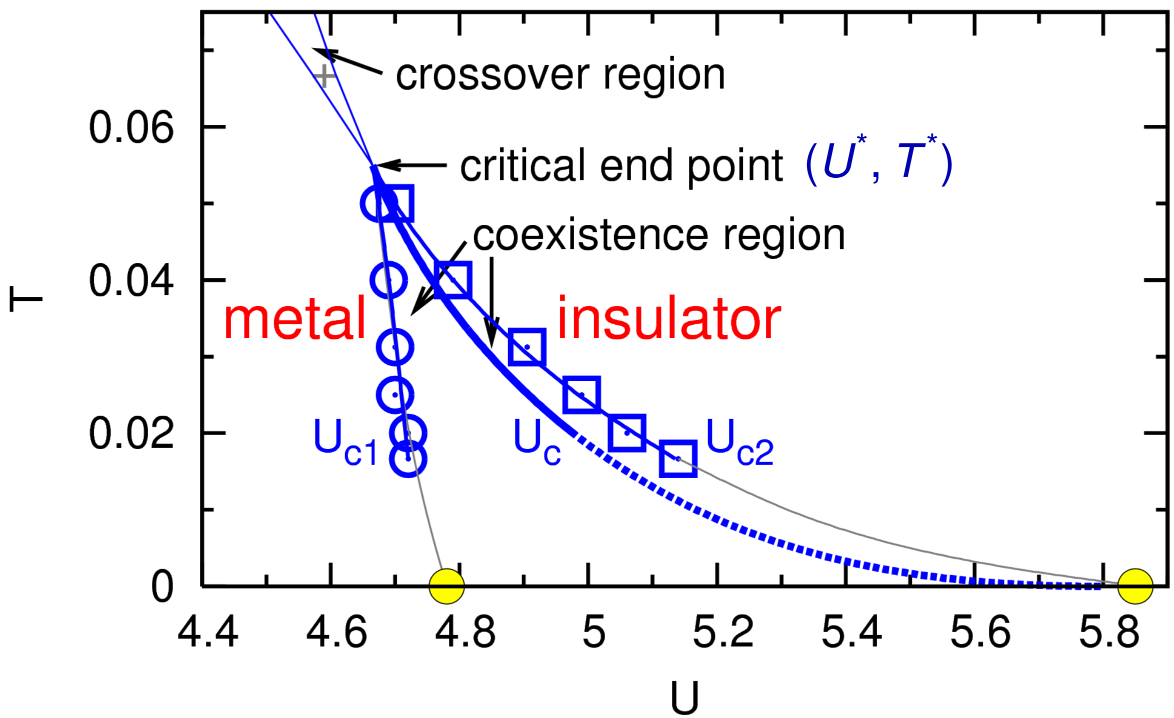

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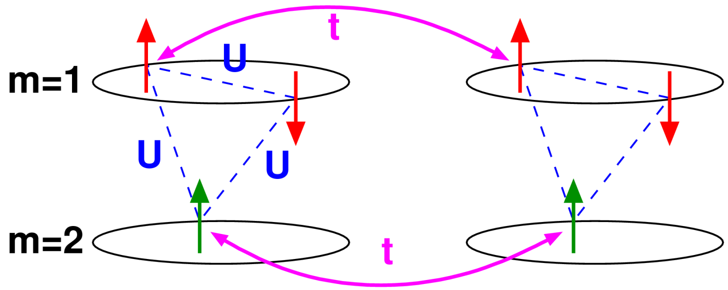
Fundamental differences in multi-band case?

Minimal multiband extension: SU(2M) invariant Hubbard model

$$H = -t \sum_{\langle ij \rangle} \sum_{\alpha} c^{\dagger}_{i\alpha} c_{j\alpha} + \frac{U}{2} \sum_{i} \sum_{\alpha \neq \alpha'} n_{i\alpha} n_{i\alpha'}$$

$\alpha = (m, \sigma), \qquad m = 1, \dots, M, \qquad \sigma = \uparrow, \downarrow$



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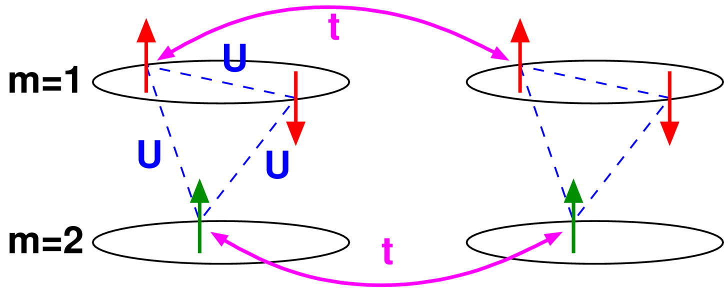

Status quo:

- Mott transition at half filling ($n = M$) for any $M = 1, 2, ...$
- Analytic solutions for $M \to \infty$ (at $T = 0$) [Florens et al., PRB (2002)]

  $U_{c1}, T^* \propto \sqrt{M}$, (unknown prefactors) $\quad U_{c2} \longrightarrow 4|E^0_{\text{kin}}| \propto M$

Verify + complement analytics?

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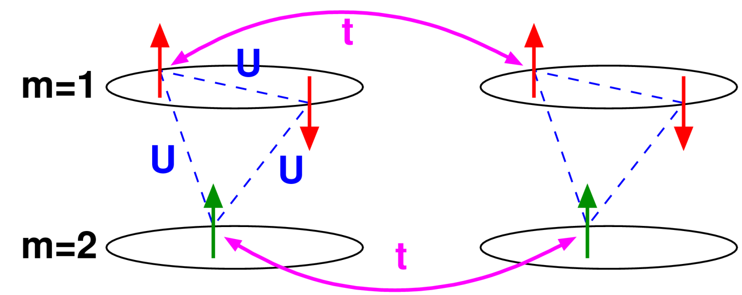

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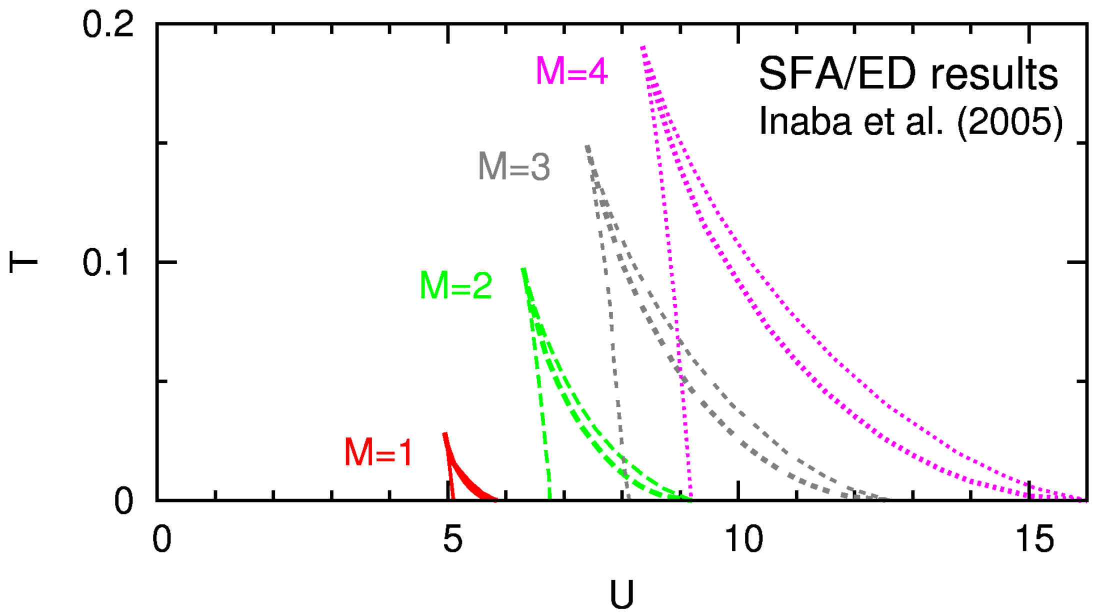

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Approximate solutions ($M \leq 4$) based on self-energy functional theory (1 bath site per orbital) [Inaba et al., PRB (2005)]

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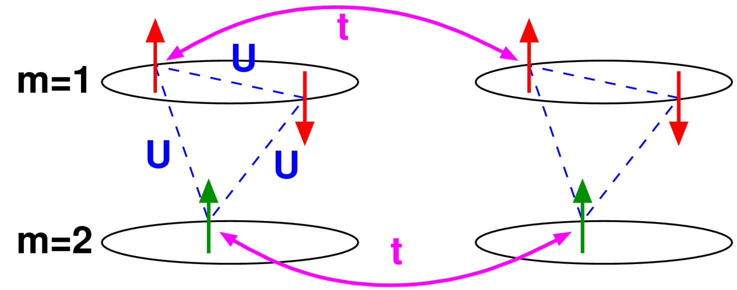

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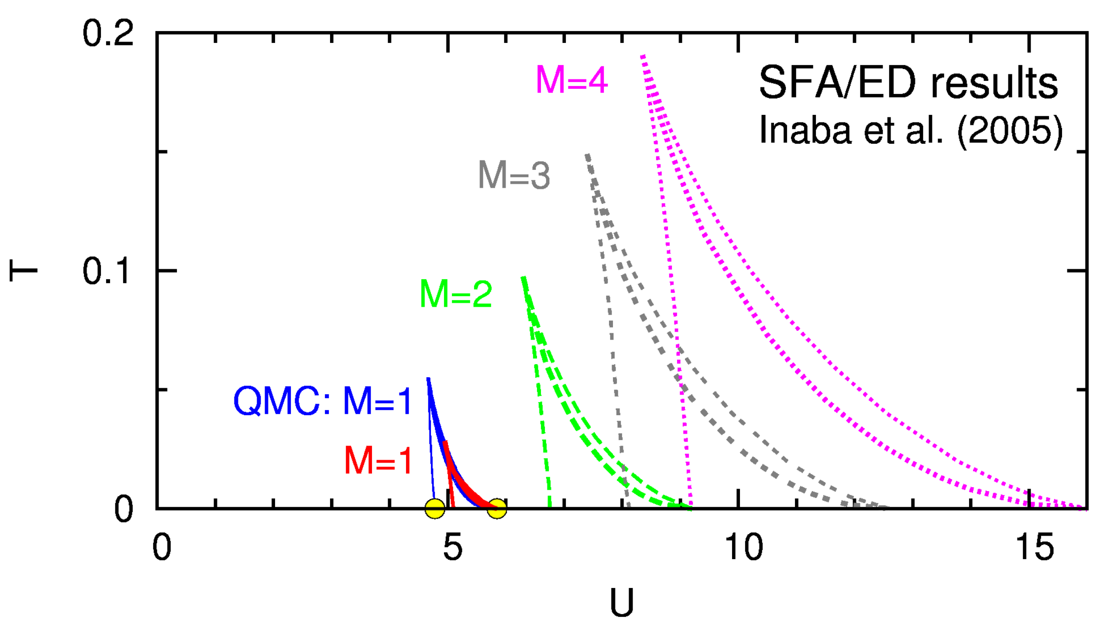

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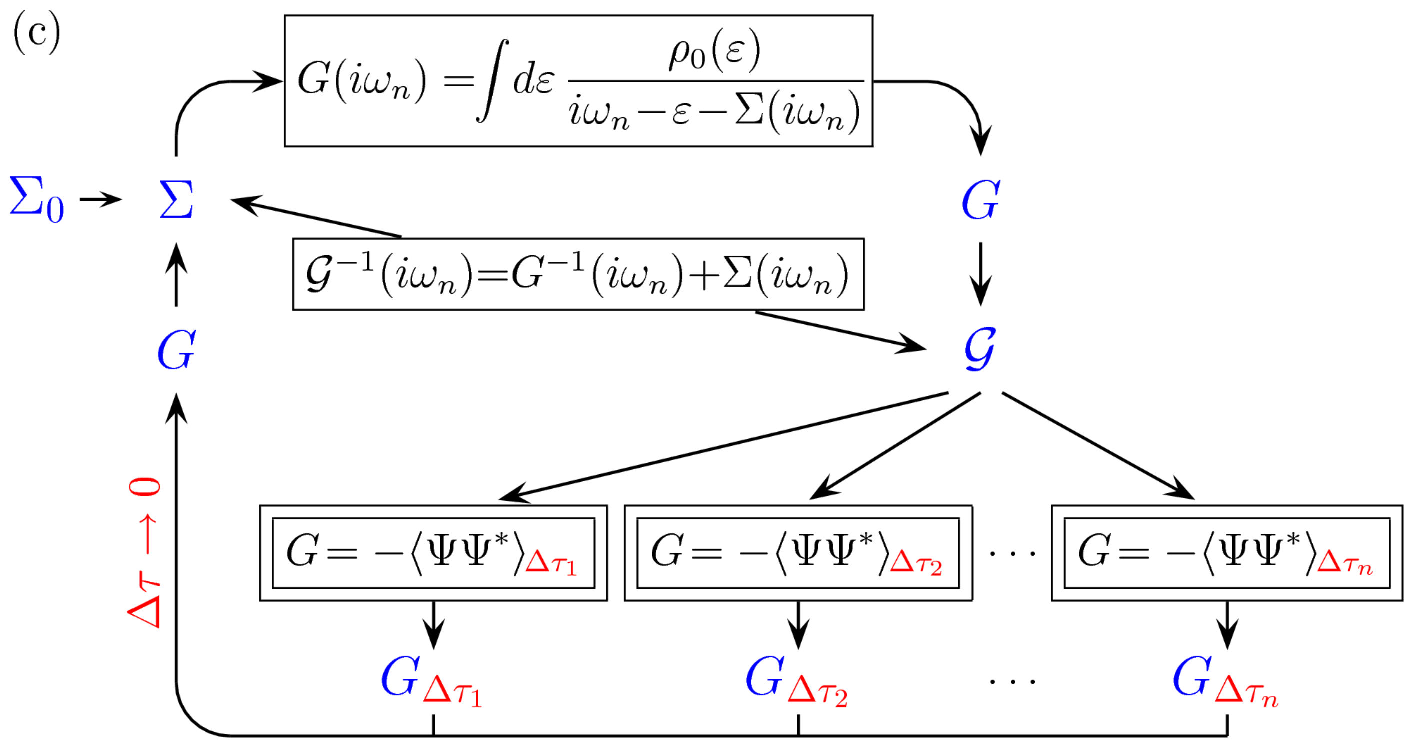
But: SFA biased for $M = 1$

Needed: exact method, larger M

Unbiased method: Multigrid Hirsch-Fye quantum Monte Carlo



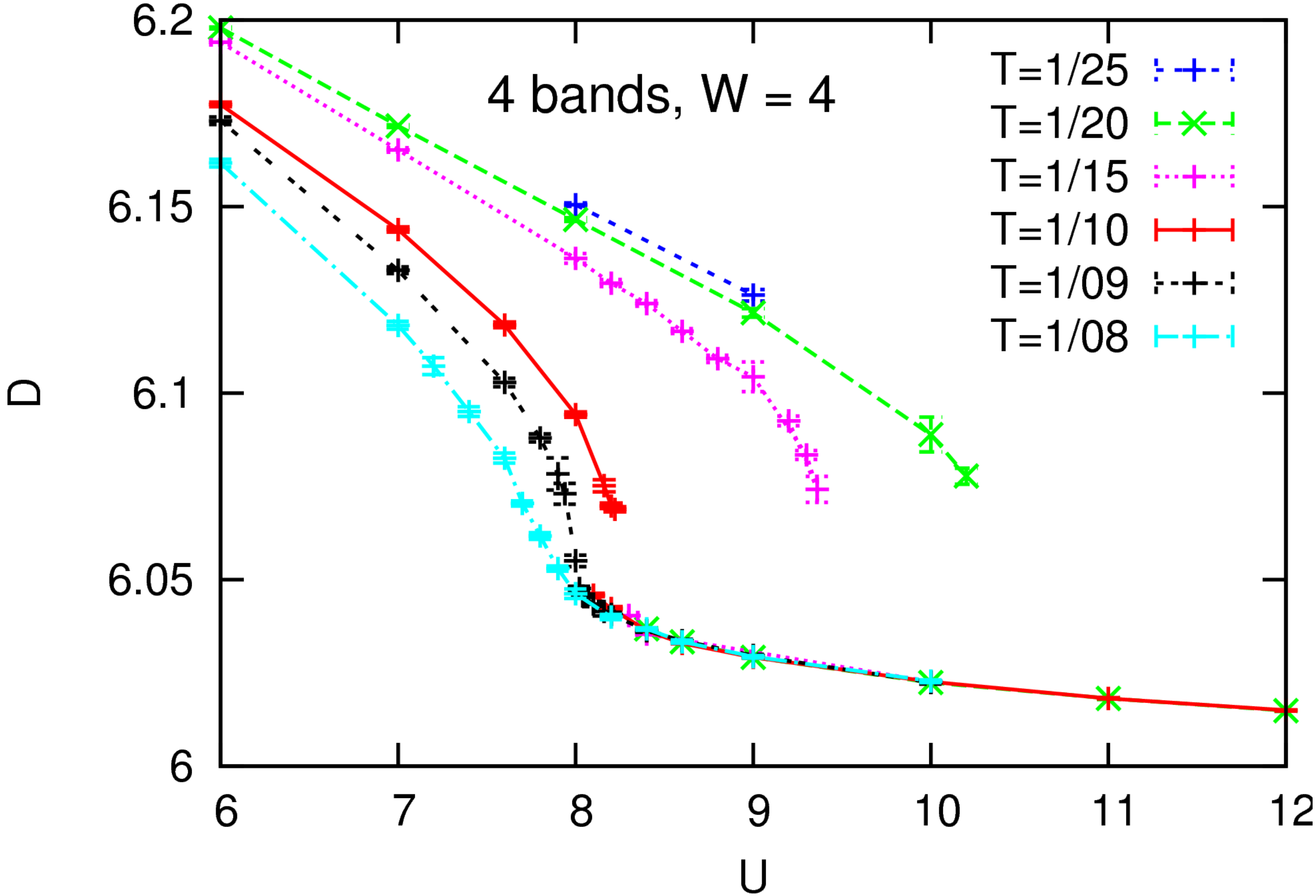
Quasi continuous-time QMC impurity solver, numerically exact

employs internal $\Delta\tau \to 0$ extrapolation for Green function (within DMFT cycle)

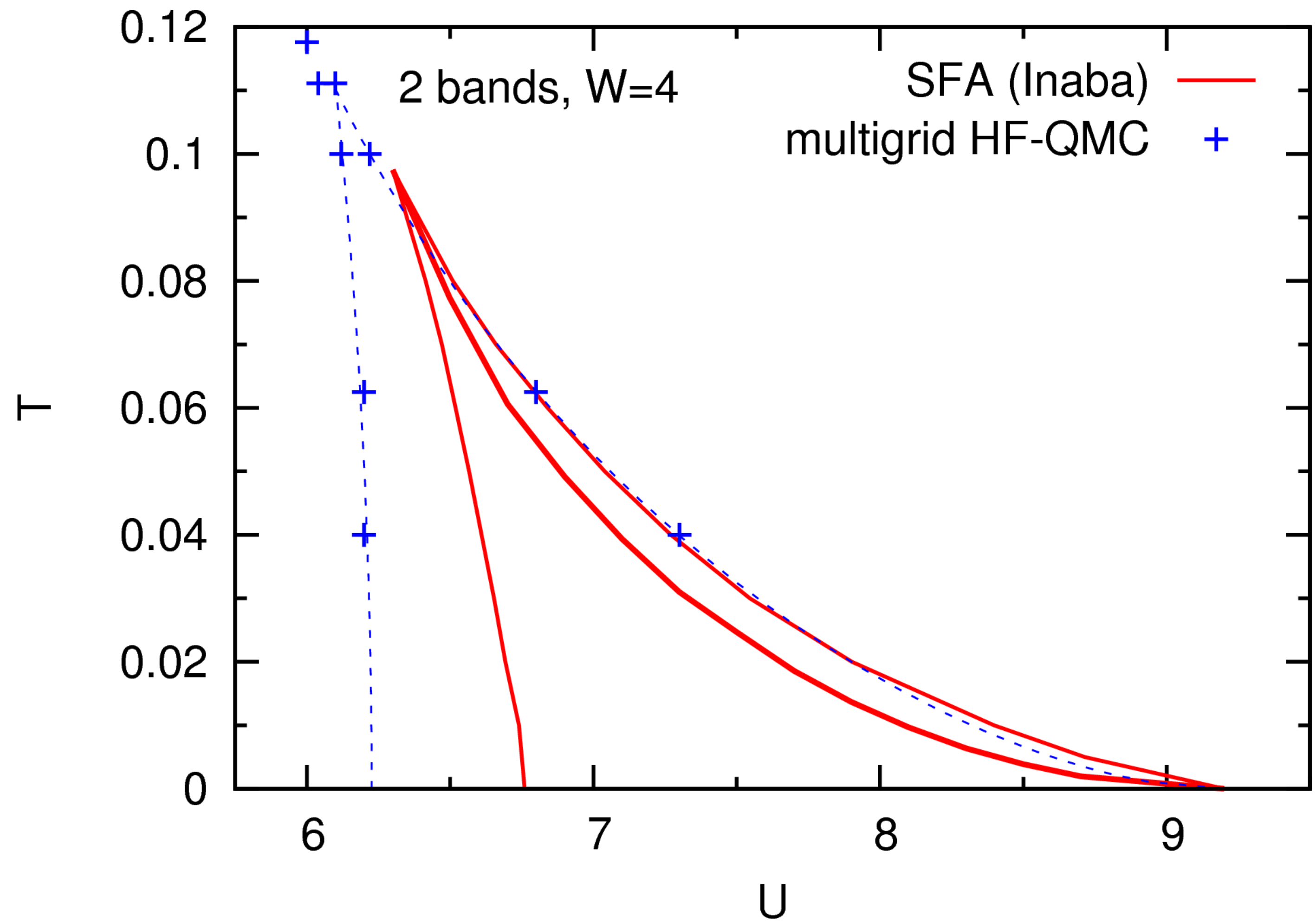
High precision and efficiency established in 1-band case [N.Blümer, arXiv:0801.1222]

Mapping the coexistence regions

Pair occupancy $D = \sum_{\alpha \neq \alpha'} \langle n_{i\alpha} n_{i\alpha'} \rangle \quad \left(\frac{M(M-1)}{2} \leq D \leq \frac{2M(2M-1)}{8} \right)$



Phase diagram: $M = 2$



Excellent agreement for $U_{c2}(T)$

SFA underestimates stability of insulating phase and T^* (but better than $M = 1$)

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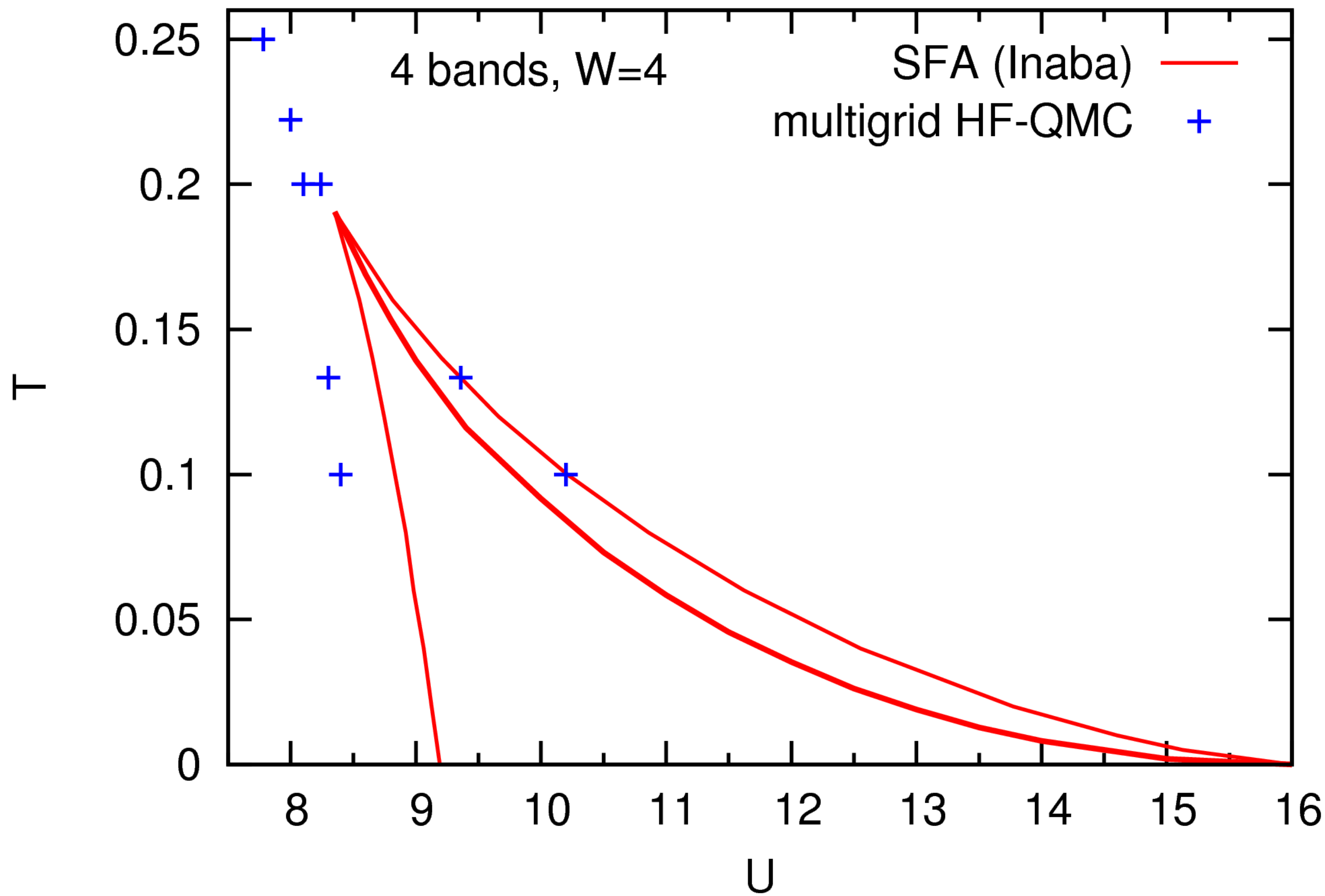
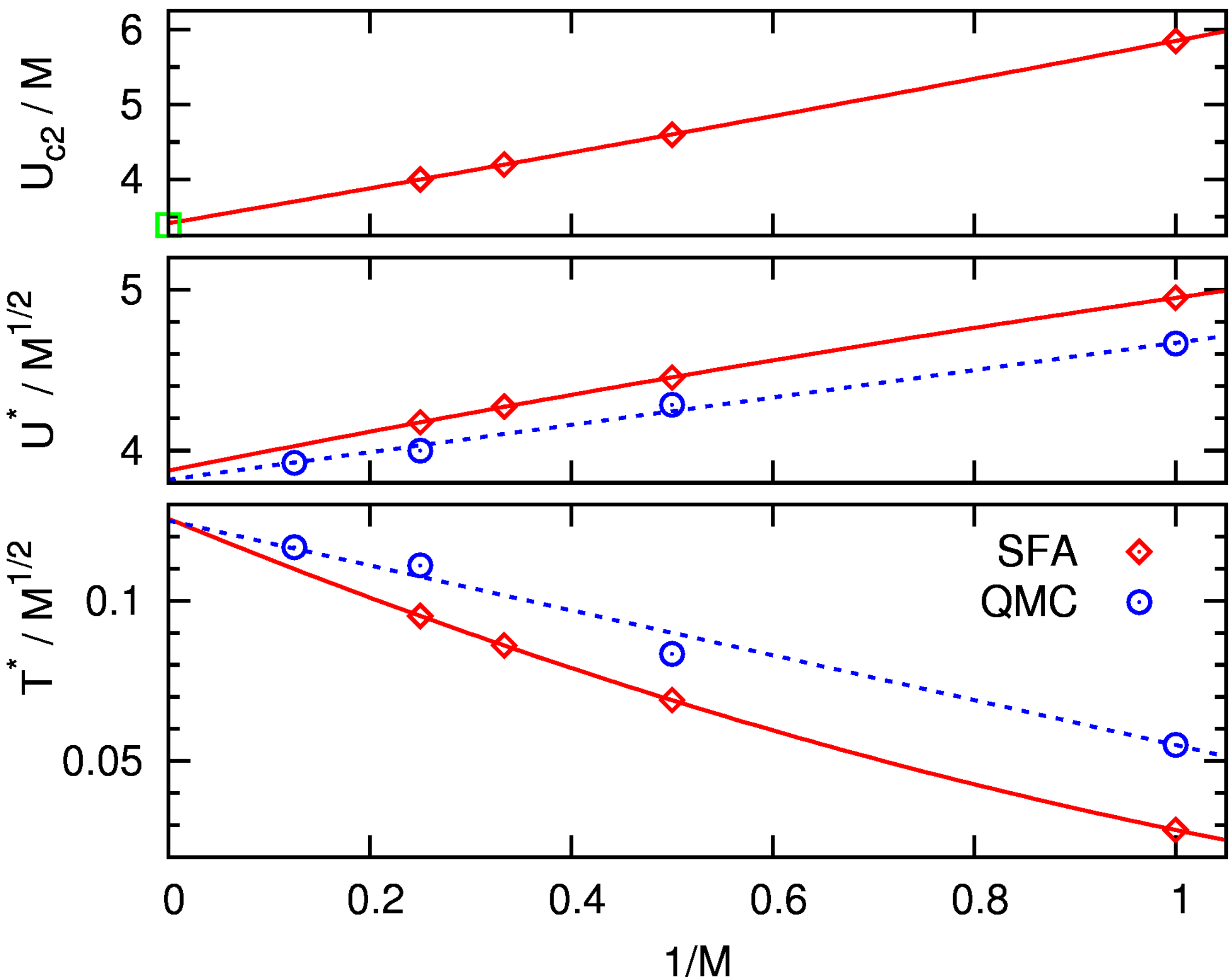


Perfect agreement for $U_{c2}(T)$, improving (with M) agreement for $U_{c1}(T)$ and T^*

Not shown: multigrid-HF calculations for $M = 8$ (beyond SFA+ED) . . .

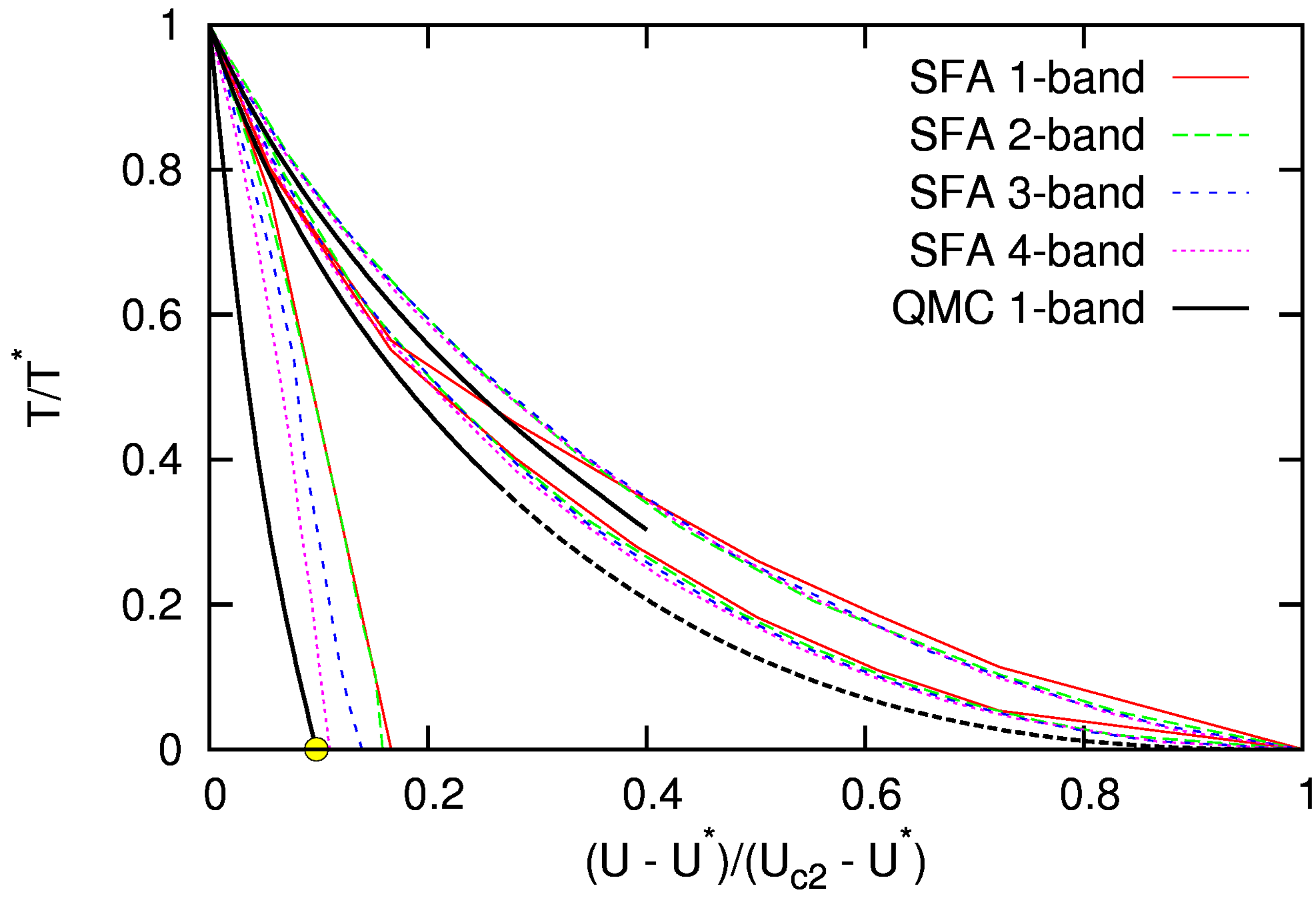
Scaling of the critical parameters



Multigrid HF-QMC: numerically exact (all M), SFA: extrapolates to $M \to \infty$

$\rightsquigarrow$ Phase diagram for arbitrary M

Scaled phase diagram (preliminary)



Note: here scaling parameters T^*, U^*, U_{c2} specific to each data set

SFA estimates of U_c, U_{c2} collapse for $M \geq 2$; but trend in U_{c1}

Summary

Mott transition at large spin/orbital degeneracy:

- SU(2M) symmetric Hubbard model, paramagnetic phase, $n = M$
- first (numerically) exact results and scaling analysis
- phase diagram (at half filling) for arbitrary M

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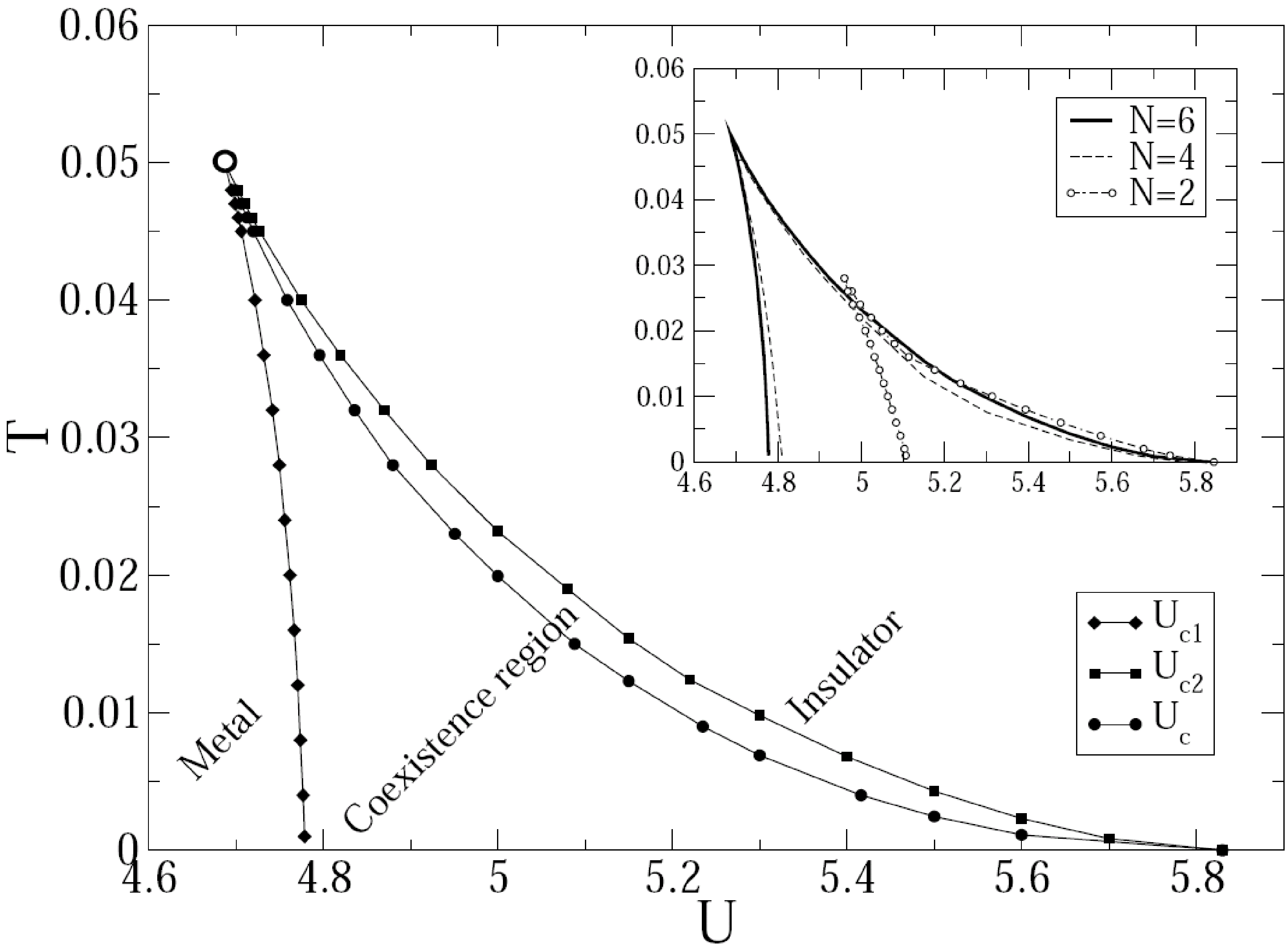
Multigrid HF-QMC method tested up to $M = 8$ (i.e. 120 binary HS fields)

SFA+ED accuracy depends on total number of (interacting + bath) orbitals

Alternative: QMC with single complex HS field [F. Assaad, PRB **71**, 075103 (2005)]

Funding by DFG within SFB/TR 49

SFA+ED: finite-size dependence in 1-band case



Here: 1 interacting orbital, $N-1$ bath sites [Pozgajcic, cond-mat/0407172v1]

Pair occupancy for $M = 8$ near critical point