Flavour-selective Mott transitions of ultracold quantum gases on optical lattices

Nils Blümer, Univ. Mainz

Outline

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

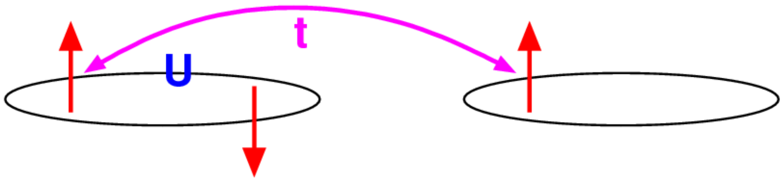
New method: multigrid Hirsch-Fye quantum Monte Carlo algorithm

Summary and outlook

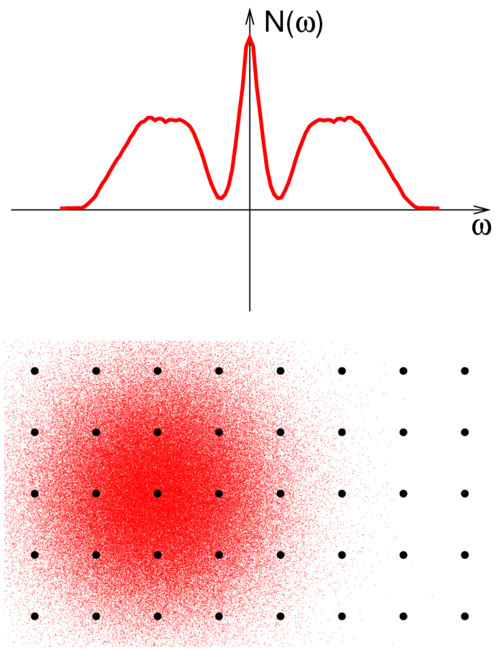
Introduction

"Regular" Mott transition in frustrated 1-band Hubbard model

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

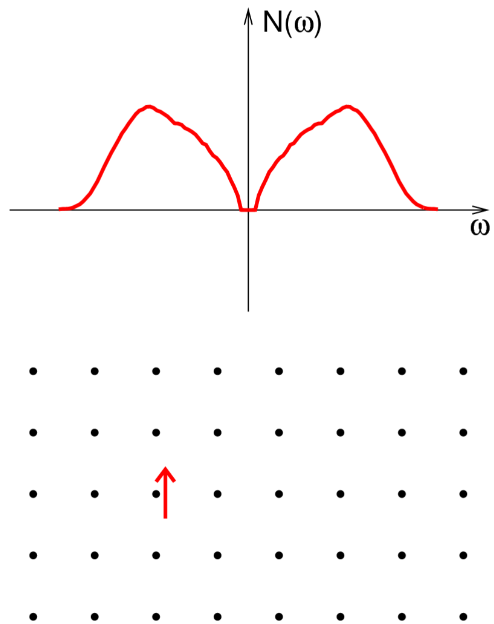


localization by interactions



$U > U_c$

$\Longrightarrow$



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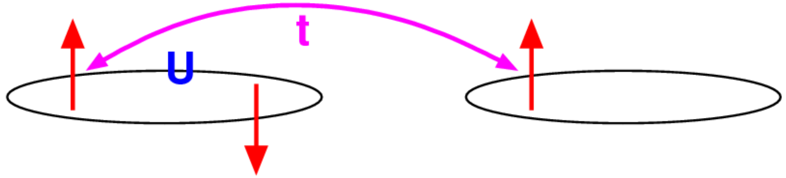

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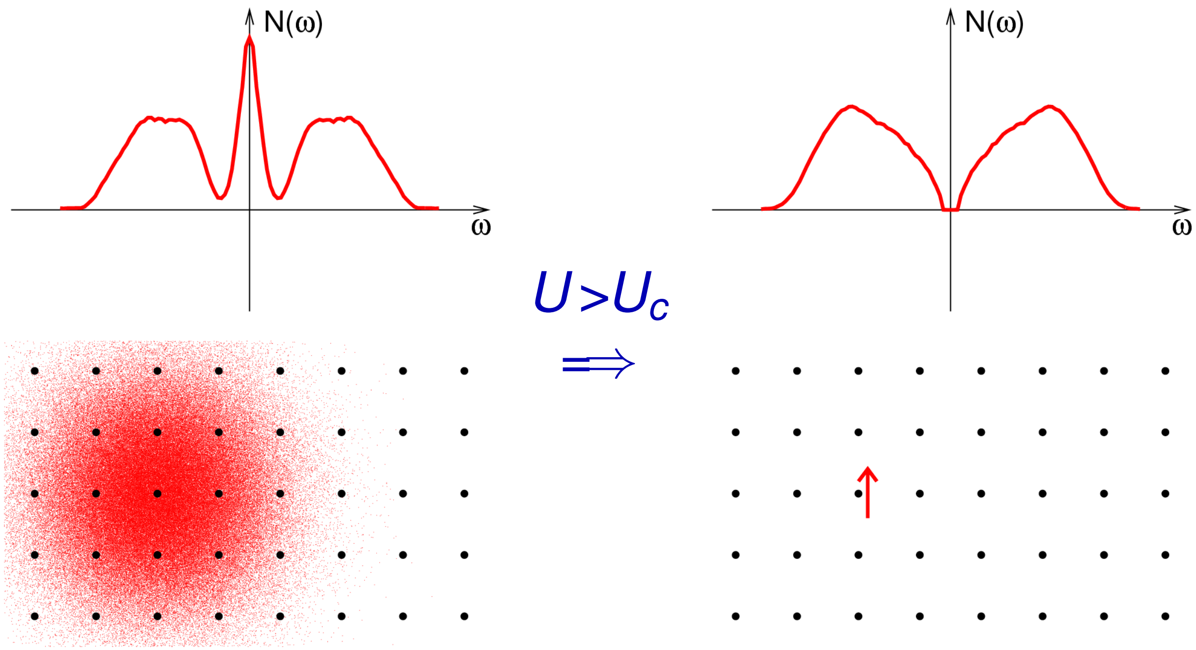

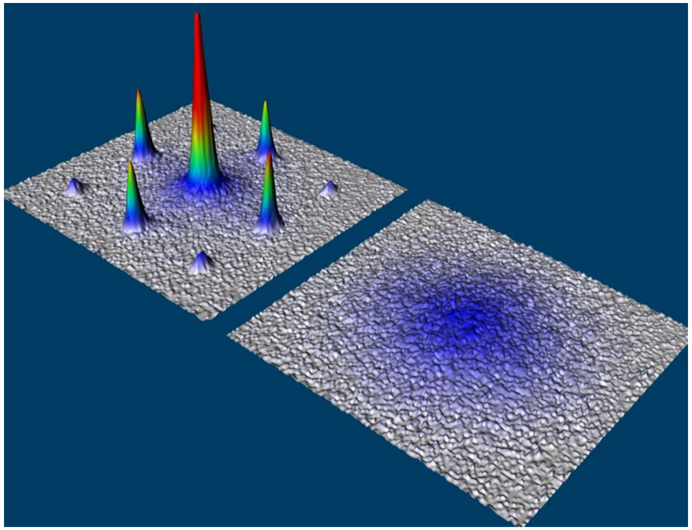

Localization (= decoherence) of ultracold bosons on optical lattice (Bloch group, 2002)

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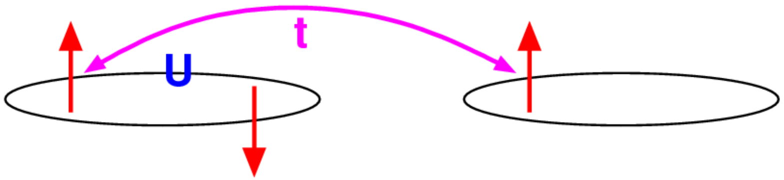

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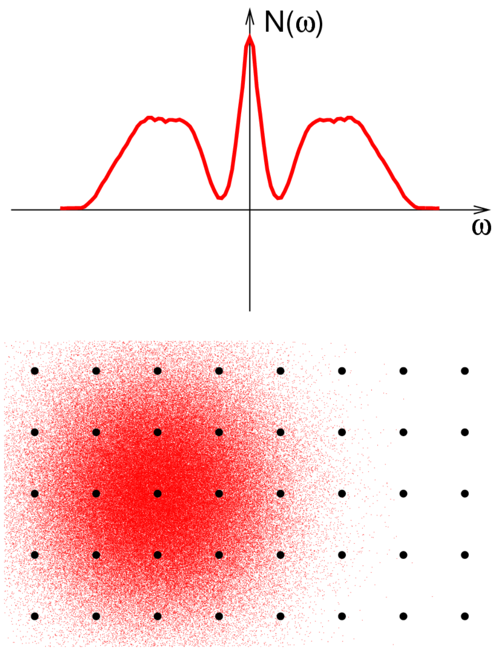

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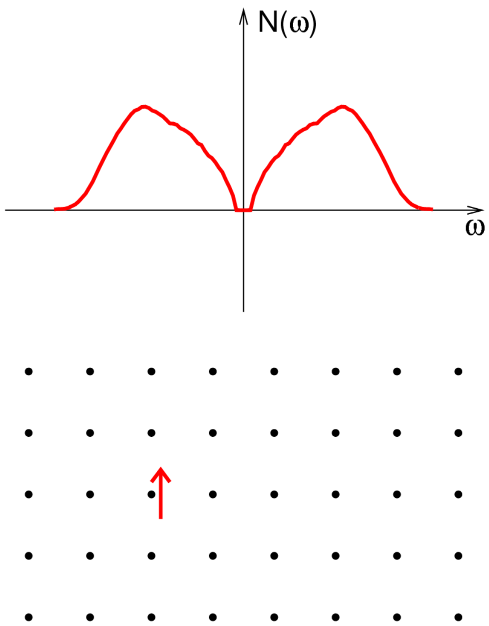

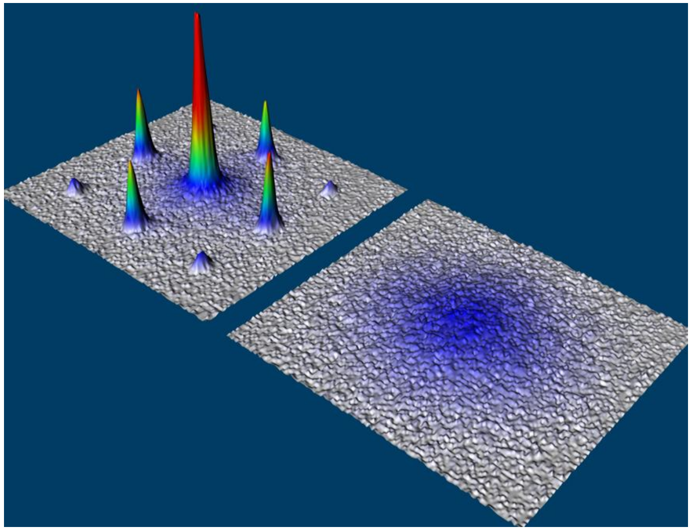

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Case of multiple inequivalent orbitals/flavors?

2-band model with orbital-dependent hopping

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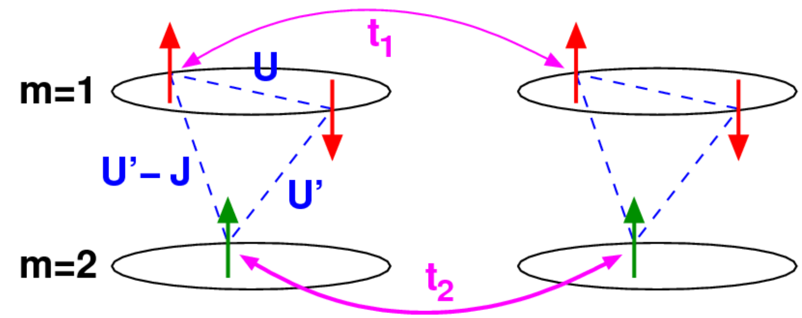

Ising-type Hund couplings [Liebsch, PRL (2003)]

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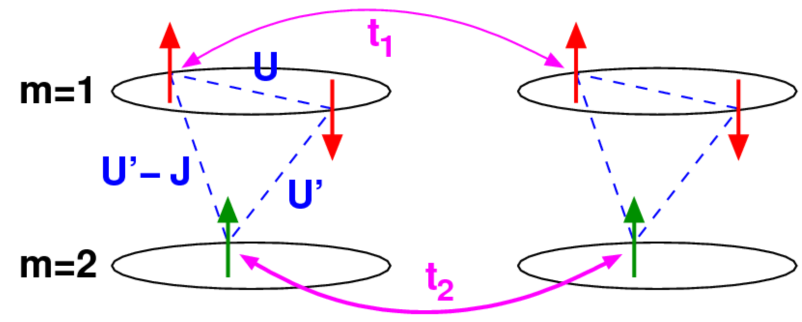

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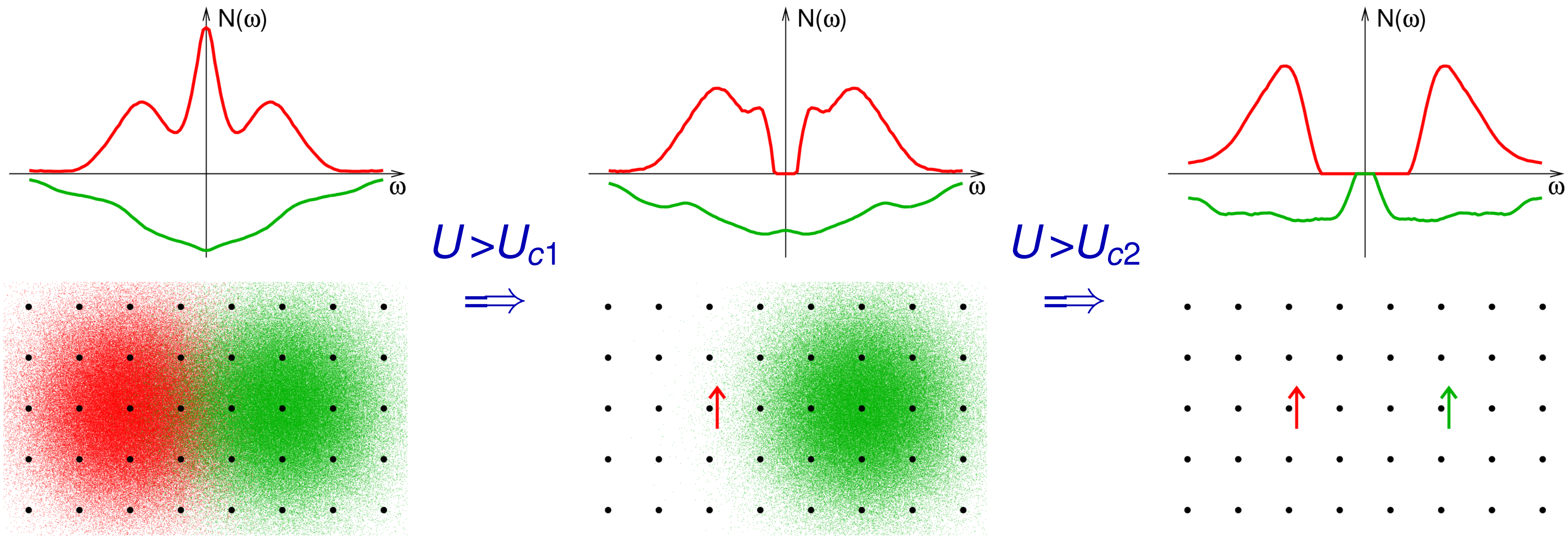
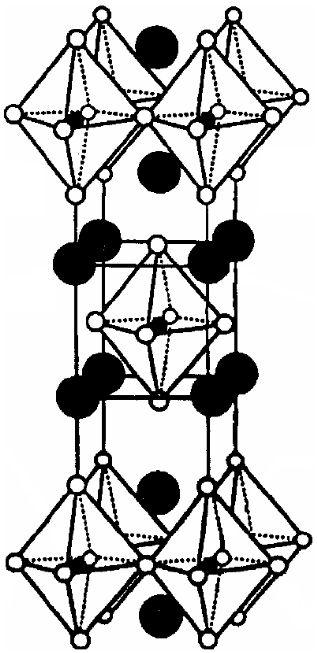


2 phase transitions [Knecht et al. (PRB 2005), de' Medici et al. (PRB 2005), Rüegg et al. (EPJB 2005)]

Experimental realizations of orbital/flavor-selective physics?

1) t_{2g} electrons
in perovskites



[Nakatsuji, Maeno,
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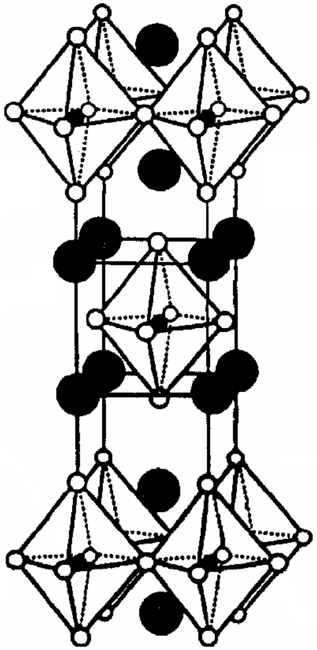
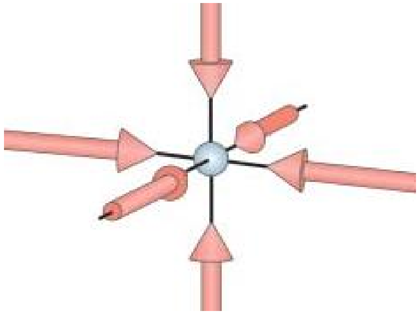
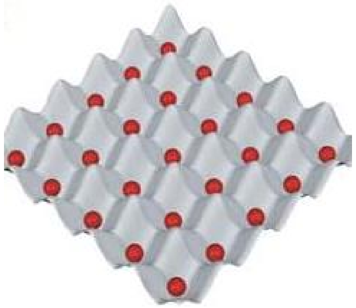


[Nakatsuji, Maeno, PRL (2000)]

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





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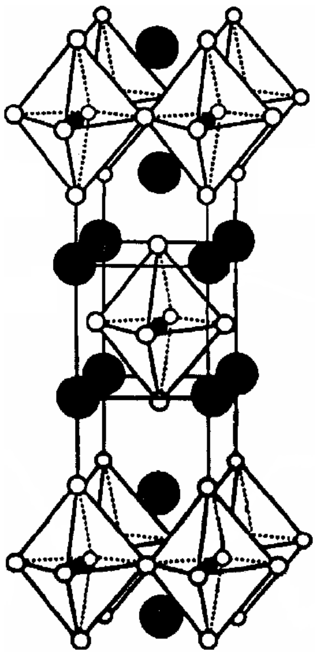

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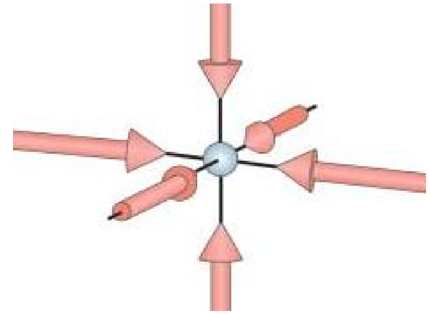
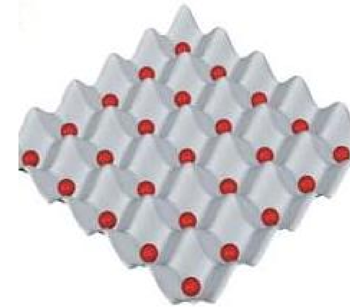
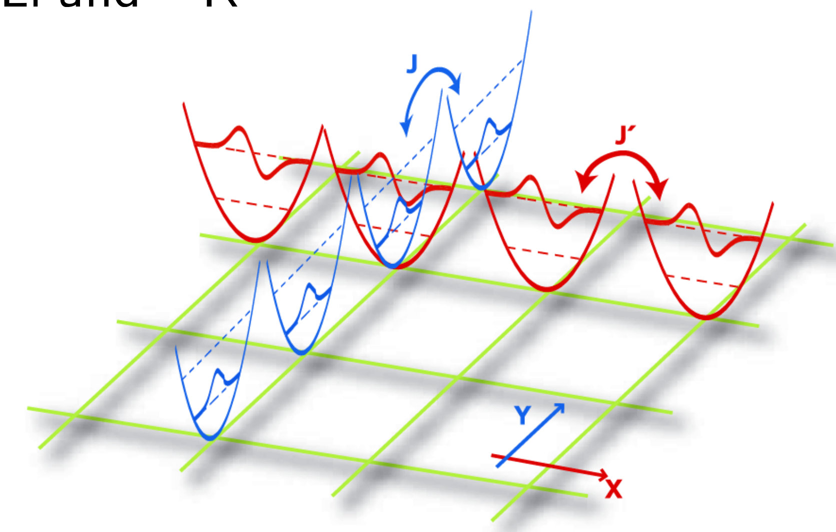




Flavors:

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

Hopping amplitudes are generically flavor dependent!



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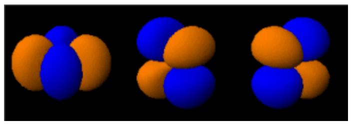

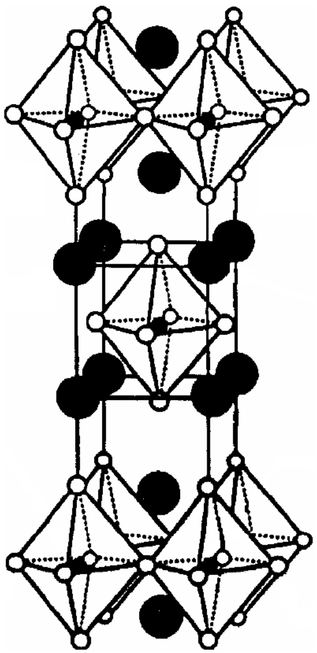

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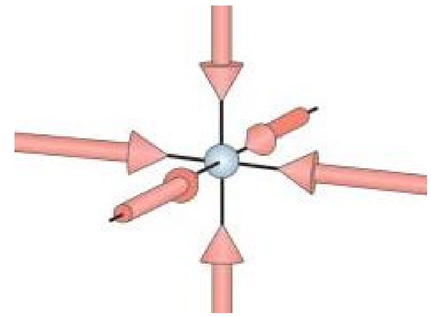

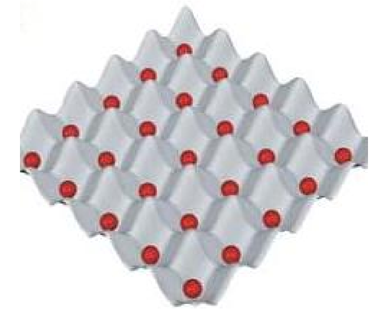

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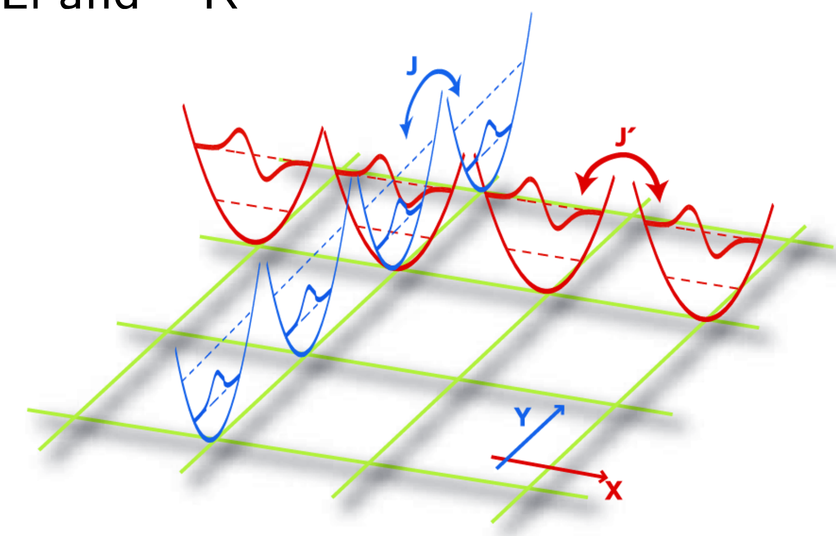

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Project A6: predict phases/properties of systems with inequivalent flavors
find experimentally accessible signatures

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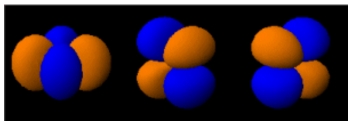

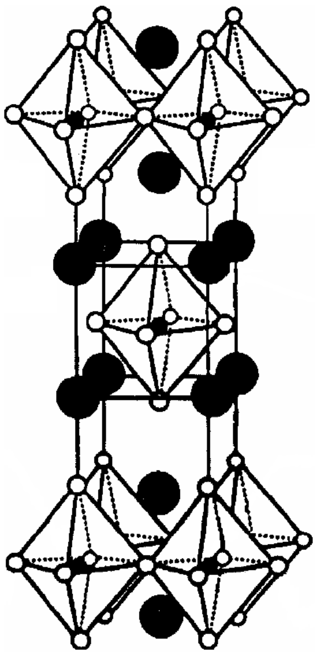

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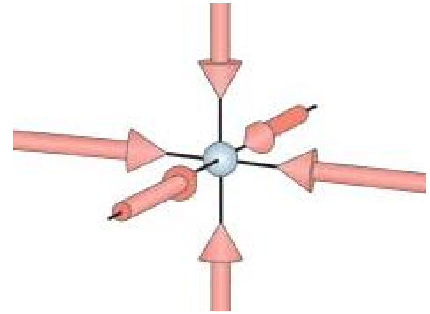

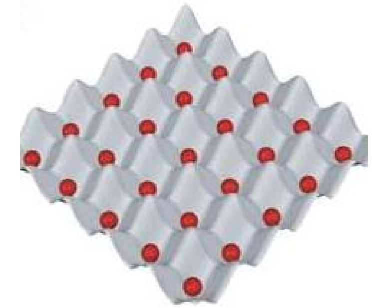

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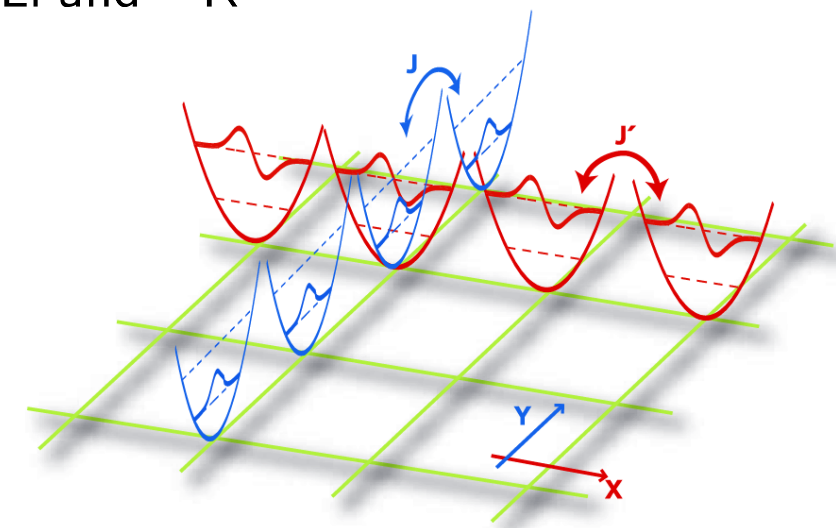
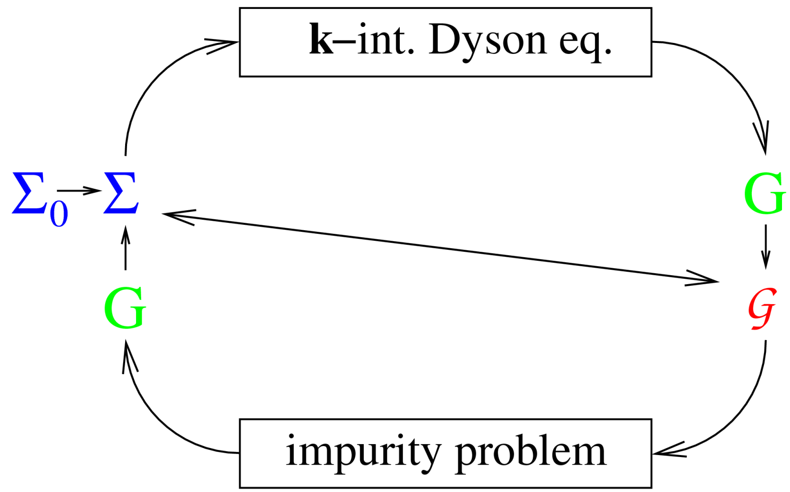


Project A6: predict phases/properties of systems with inequivalent flavors
find experimentally accessible signatures how?

Methods

Iterative solution of DMFT equations

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



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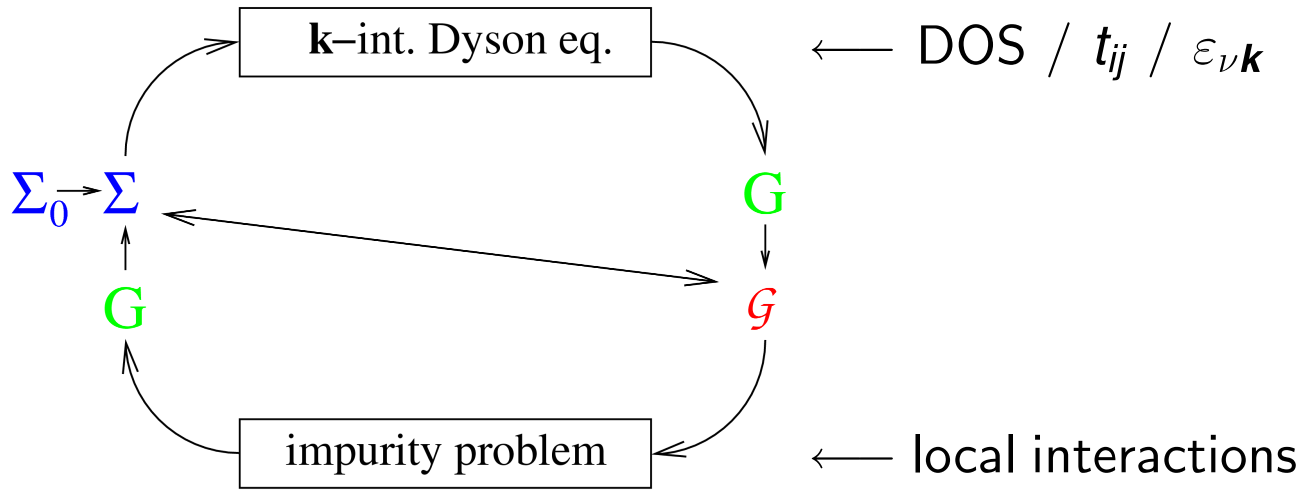

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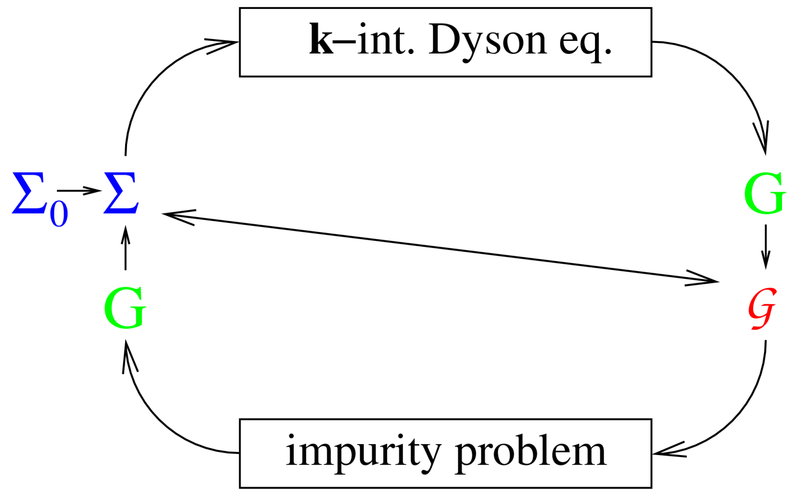

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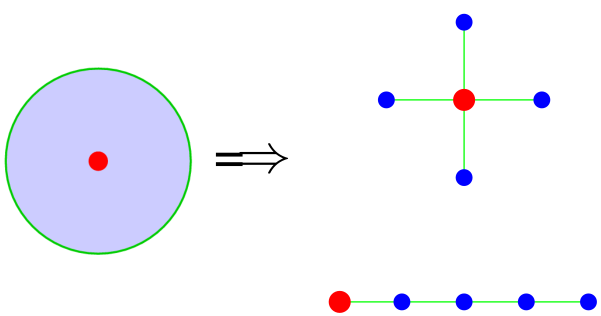
Impurity solver:

- 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

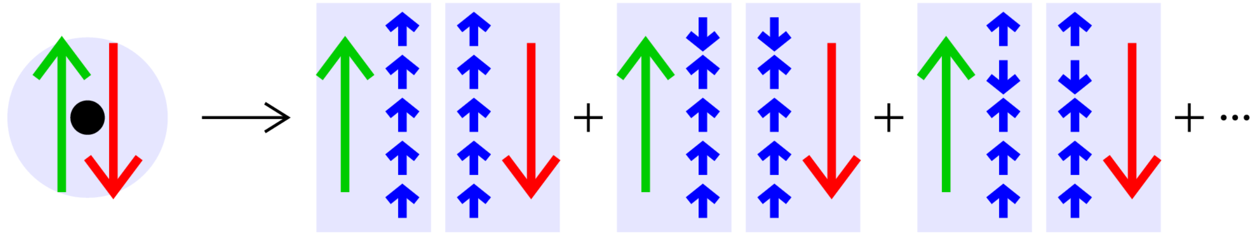


Auxiliary-field QMC algorithm [Hirsch, Fye (1986)]

Wanted: Green function $G(\omega)$

Treatment in imaginary time $\tau \in [0, \beta]$

discretization $\beta = \Lambda\,\Delta\tau$, Trotter decoupling, Hubbard-Stratonovich trafo



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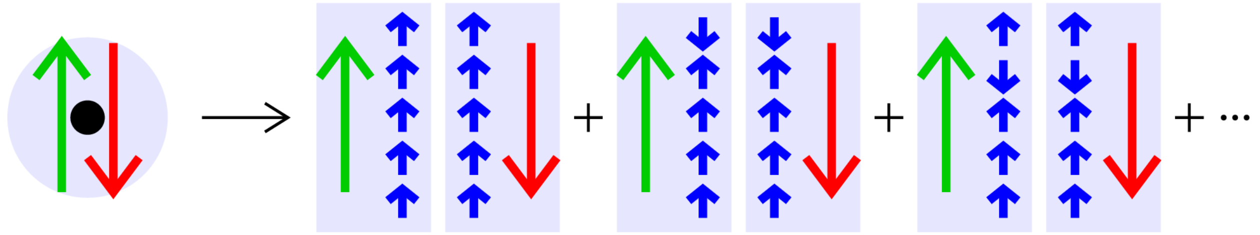

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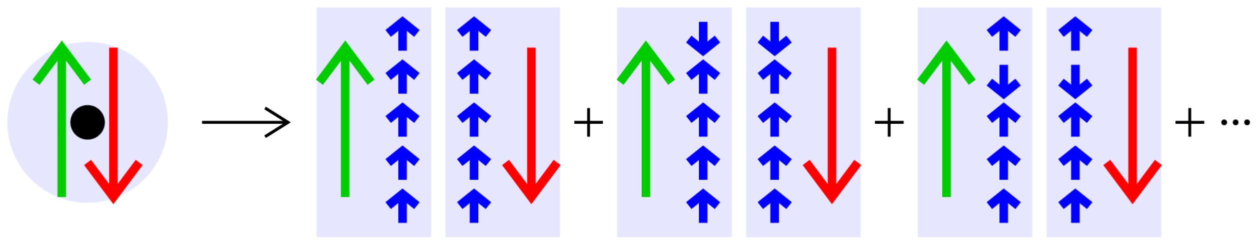

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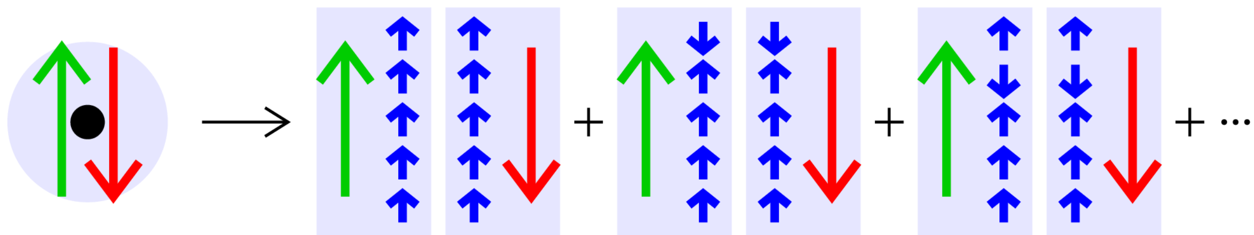

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New developments: exact Green functions multigrid HF-QMC

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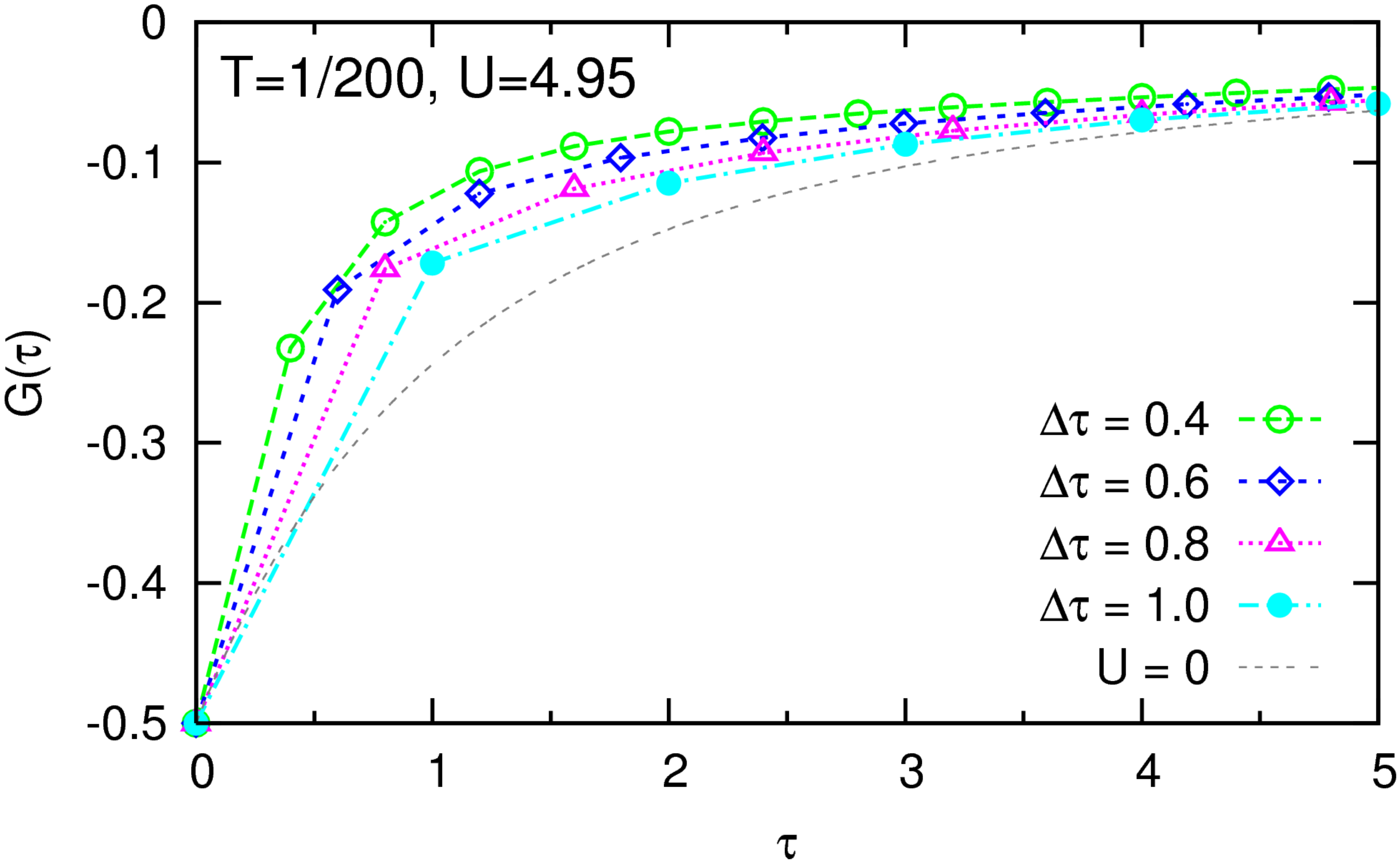

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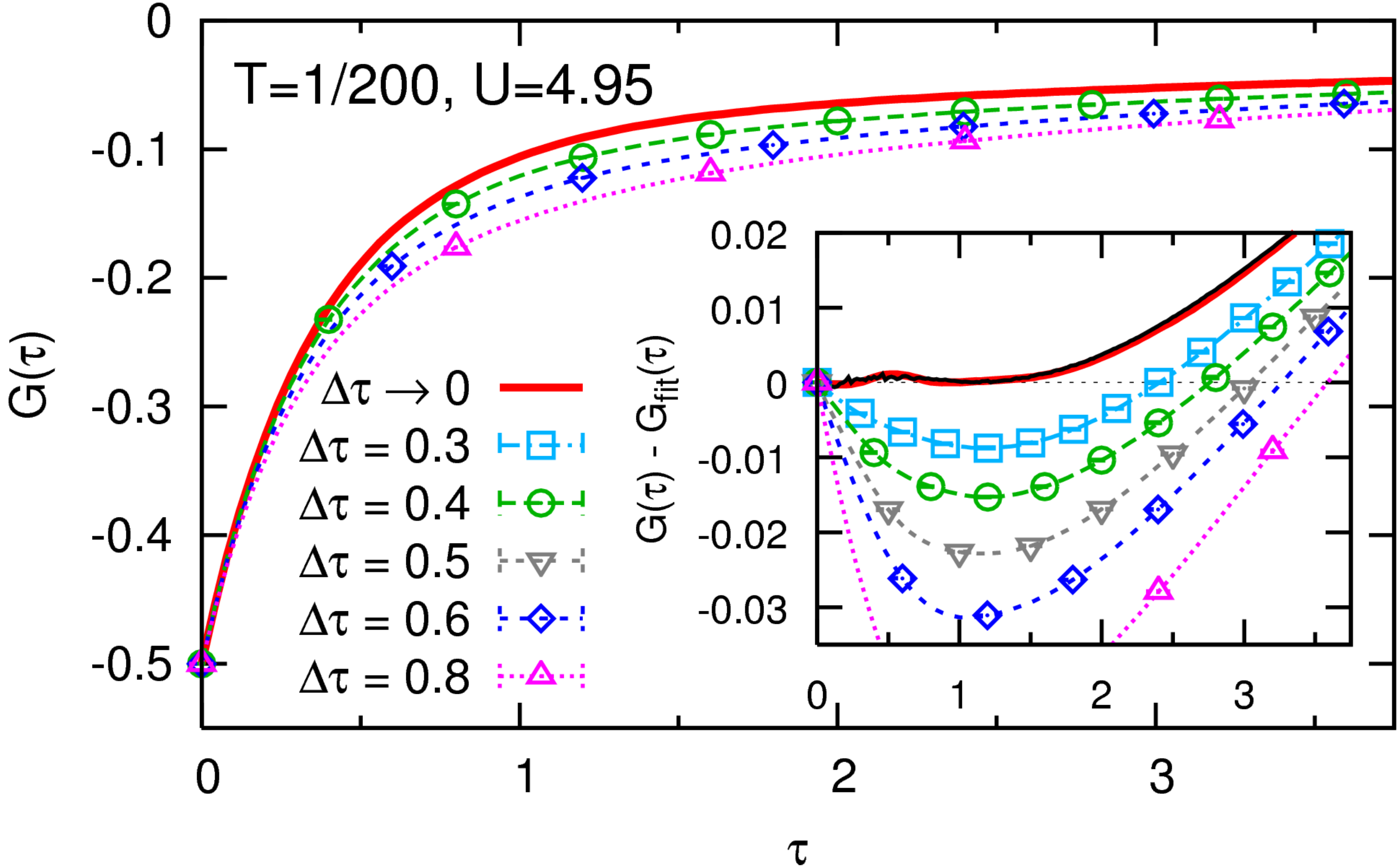

Perfect agreement with continuous-time QMC (black line)

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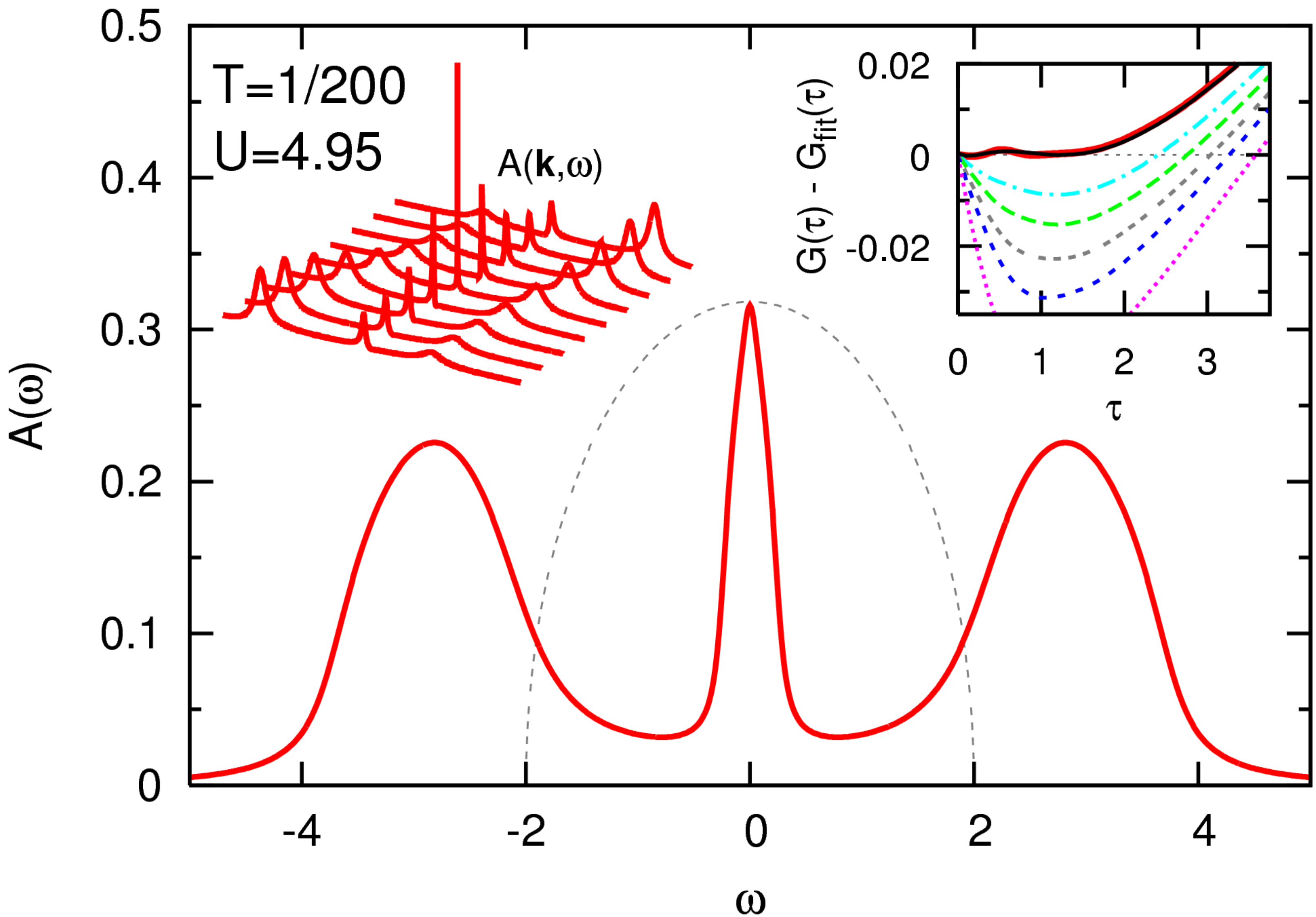
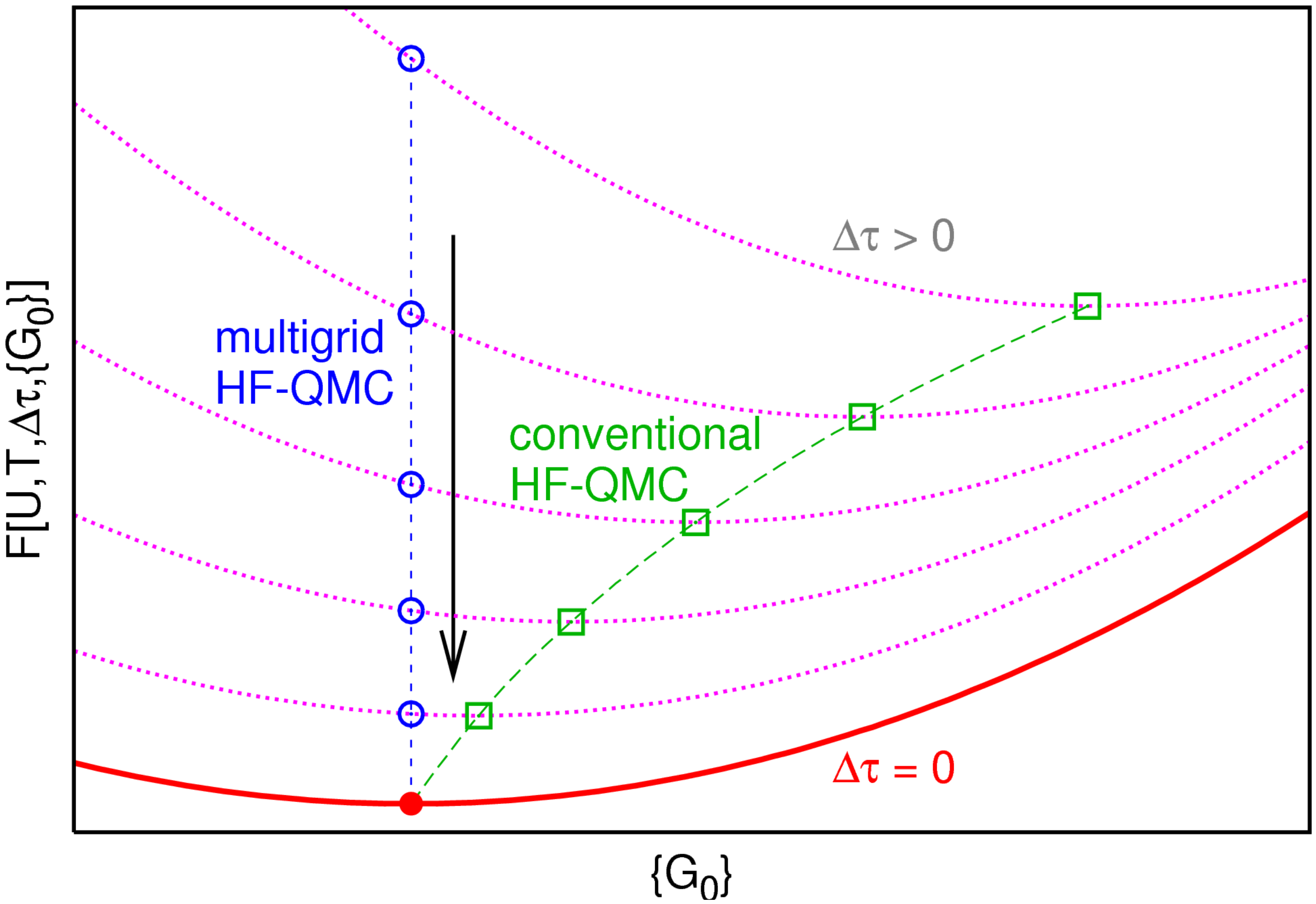


First spectra without discretization error from HF-QMC

New: multigrid DMFT solver based on HF-QMC



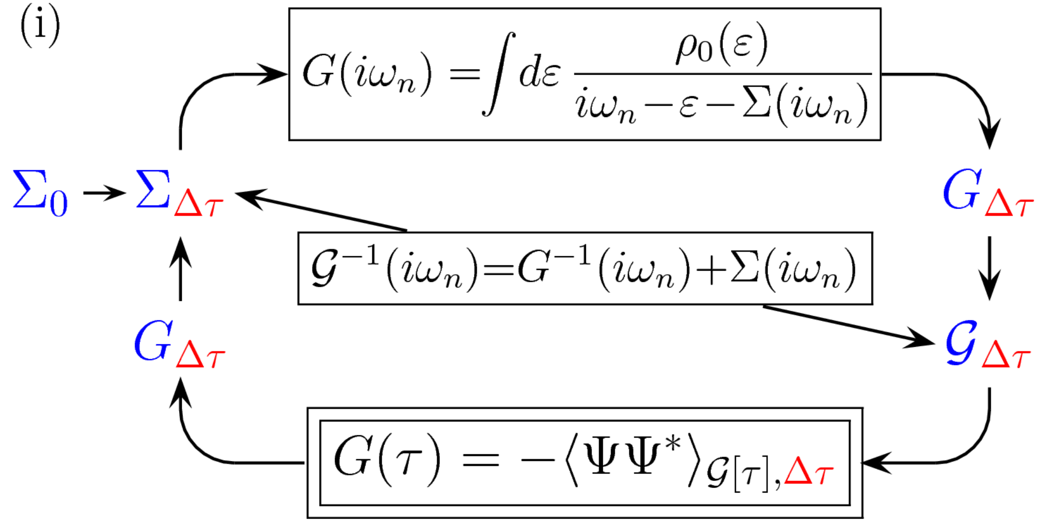
conventional Hirsch-Fye QMC: DMFT fixed point shifts with $\Delta\tau$

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

Comparison of schemes

(a) conventional HF-QMC with extrapolation

(i)



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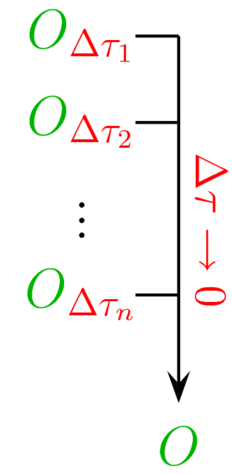
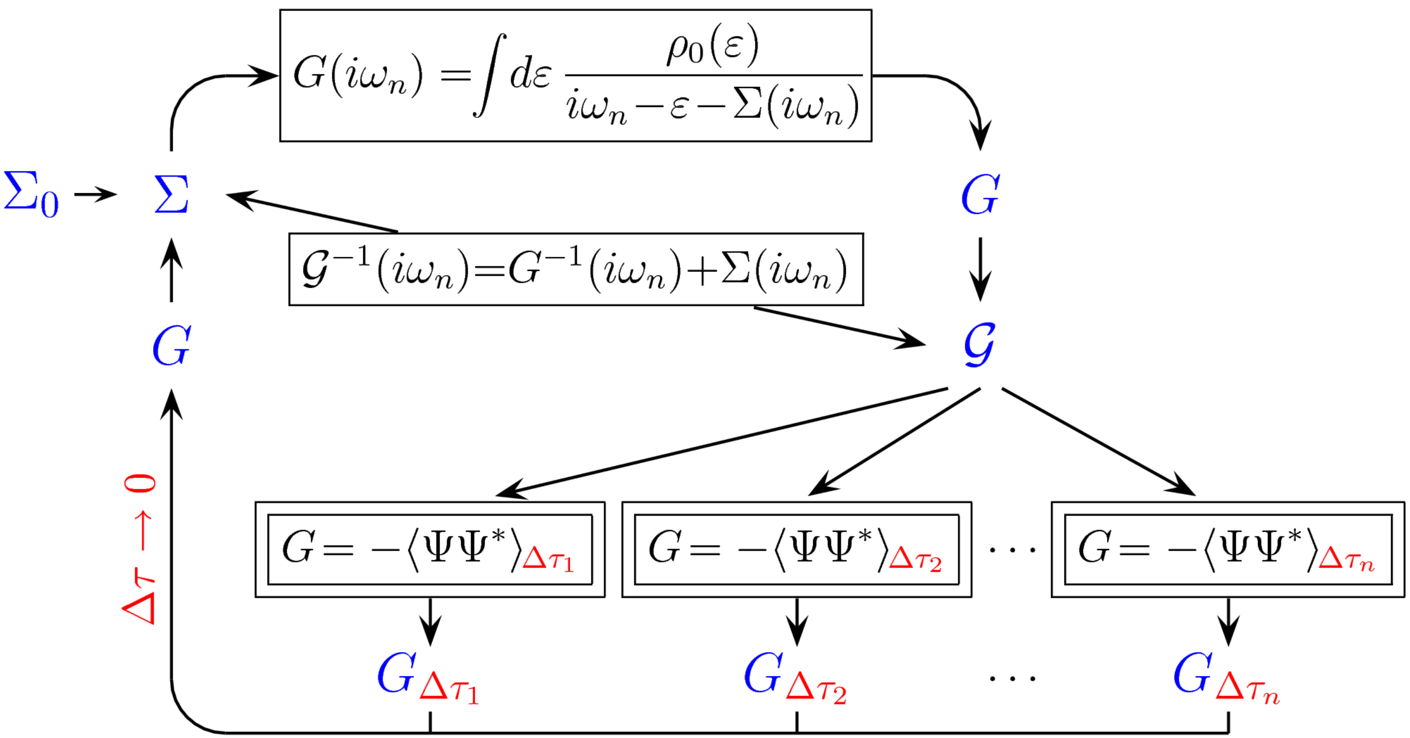
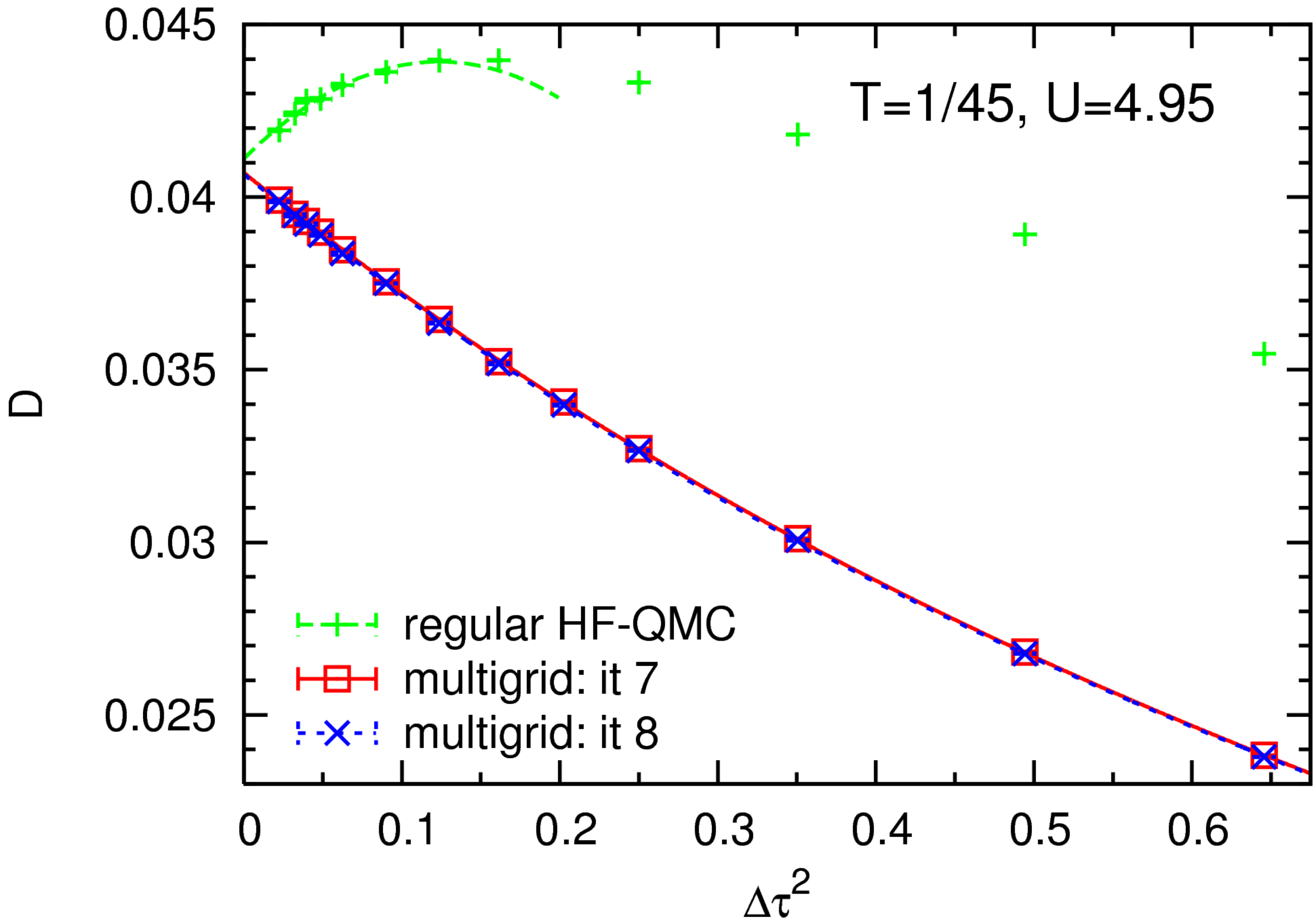




(b) multigrid HF-QMC

Preliminary study: double occupancy near Mott transition



Useful $\Delta\tau$ range vastly larger for multigrid algorithm

Summary

Orbital/flavor selective Mott transitions: interesting and challenging strong-correlation physics (solid $\leftrightarrow$ ultracold quantum gases)

Extrapolation of Green function $\rightsquigarrow$ first unbiased spectra

Multigrid algorithm: HF-QMC $\longrightarrow$ quasi-continuous-time method

more efficient than recently developed CT-QMC methods

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Multigrid algorithm: HF-QMC $\longrightarrow$ quasi-continuous-time method

more efficient than recently developed CT-QMC methods

Outlook

Publish multigrid method (still confidential!)

Tests for multiorbital cases: additional computing ressources needed

A6 project: 3-flavor mixtures of fermionic ultracold quantum gases

Fill positions: 1 PhD student, 1 postdoc

Note (inserted after talk): the methods are now documented in the preprints

Numerically exact Green functions from Hirsch-Fye quantum Monte Carlo simulations, arXiv:0712.1290 and

Multigrid Hirsch-Fye quantum Monte Carlo method for dynamical mean-field theory, arXiv:0801.1222