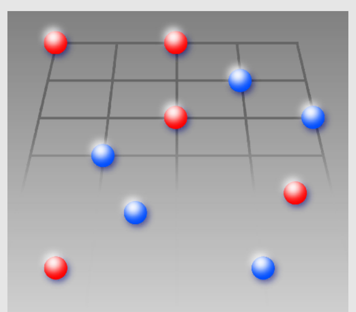
Multigrid Hirsch-Fye QMC method for DMFT

Nils M. Blümer

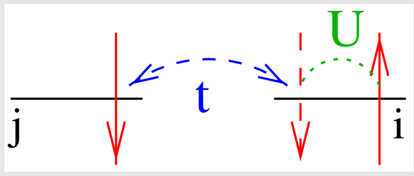
Institut für Physik, Johannes Gutenberg-Universität Mainz



Introduction

Hubbard model

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

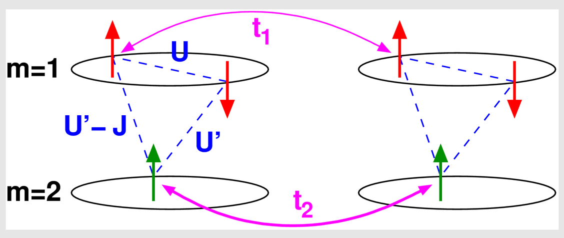


Captures important strong-correlation phenomena: Mott metal-insulator transition, (anti-) ferromagnetism, heavy fermions, high-T_c superconductivity (?), ...

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

(ii) Multi-band model, e.g., with 2 inequivalent bands:

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

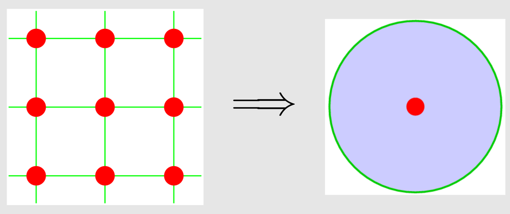


More complexity, more realistic: OSMT, spin+orbital order, LDA+DMFT, ...

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

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

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

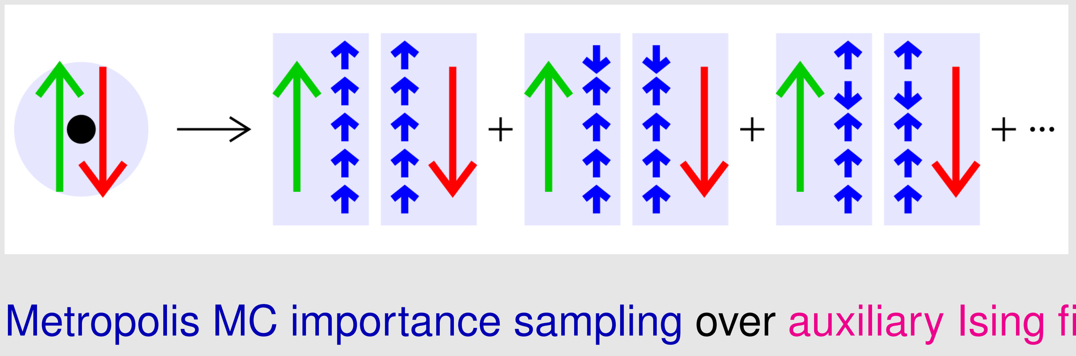


Conventional Hirsch-Fye quantum Monte Carlo

Green function G in imaginary time (fermionic Grassmann variables ψ, ψ^*):

$$G_\sigma(\tau_2-\tau_1) = \frac{1}{\mathcal{Z}}\int \mathcal{D}[\psi]\,\mathcal{D}[\psi^*]\;\psi_\sigma(\tau_1)\psi^*_\sigma(\tau_2)\;\exp\Big[\mathcal{A}_0 - U\sum_{\sigma\sigma'}\int_0^\beta d\tau\;\psi^*_\sigma\psi_\sigma\psi^*_{\sigma'}\psi_{\sigma'}\Big]$$

- Discretization $\beta = \Lambda\,\Delta\tau$,
- Trotter decoupling $e^{-\beta(\hat{T}+\hat{V})} = \lim_{\Lambda\to\infty}\left[e^{-\Delta\tau\hat{T}}e^{-\Delta\tau\hat{V}}\right]^\Lambda$
- Discrete Hubbard-Stratonovich transformation $e^{\Delta\tau U(\hat{n}_\uparrow-\hat{n}_\downarrow)^2/2} = \frac{1}{2}\sum_{s=\pm1} e^{\lambda s(\hat{n}_\uparrow-\hat{n}_\downarrow)}$



Wick theorem:

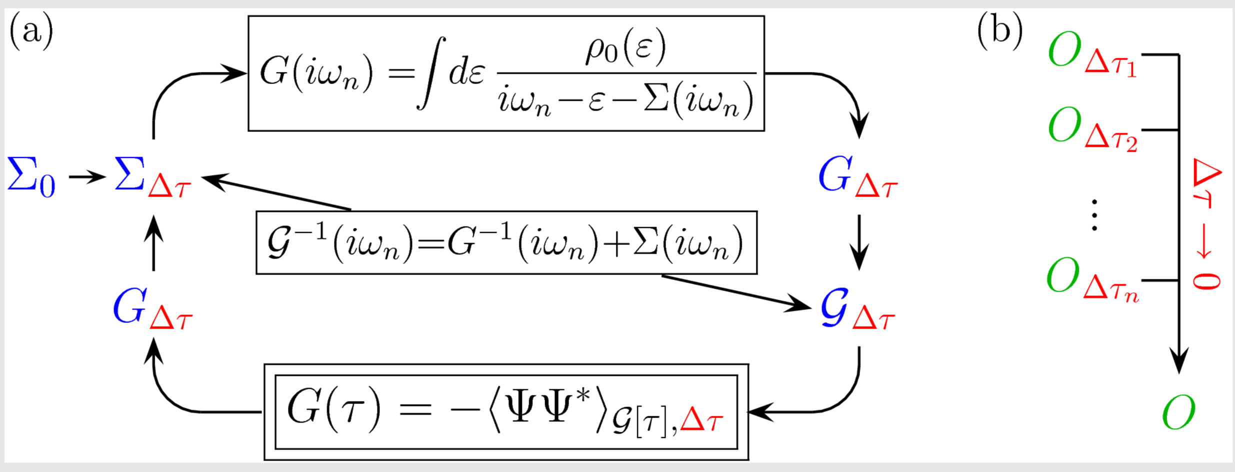
$$G = \frac{\sum M \det\{M\}}{\sum \det\{M\}}$$

Metropolis MC importance sampling over auxiliary Ising field $\{s\}$: 2^Λ configurations

$+$ numerically exact, $+$ no sign problem (density-type int.), $-$ effort scales as T^{-3}

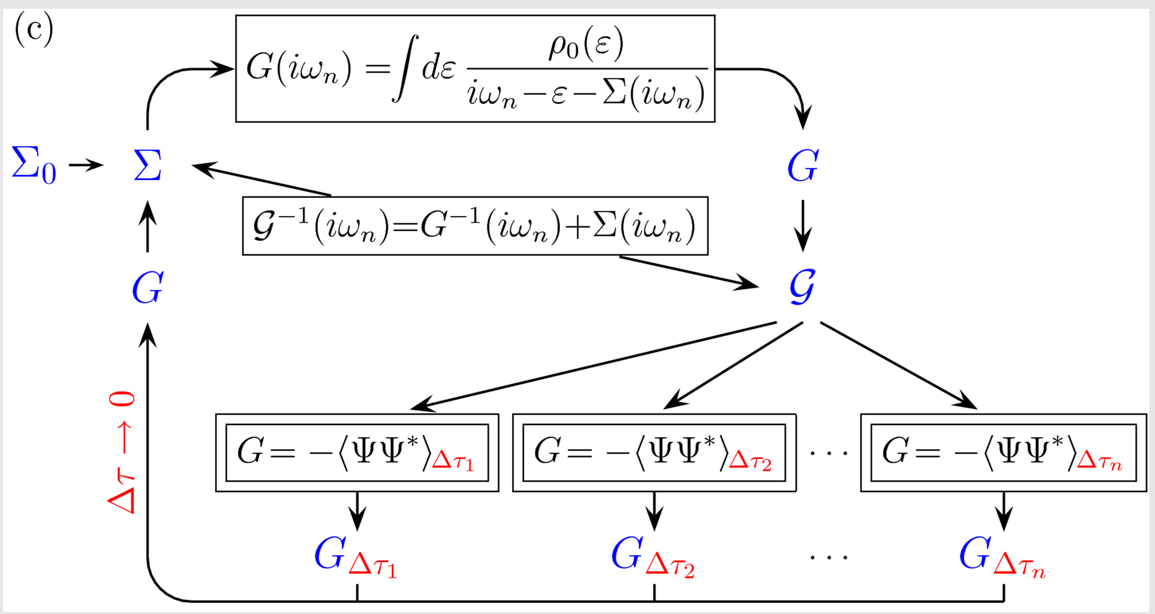
State of the art: (a) conventional HF-QMC – systematic errors from discretization $\Delta\tau$

(b) *a posteriori* extrapolation of selected observables



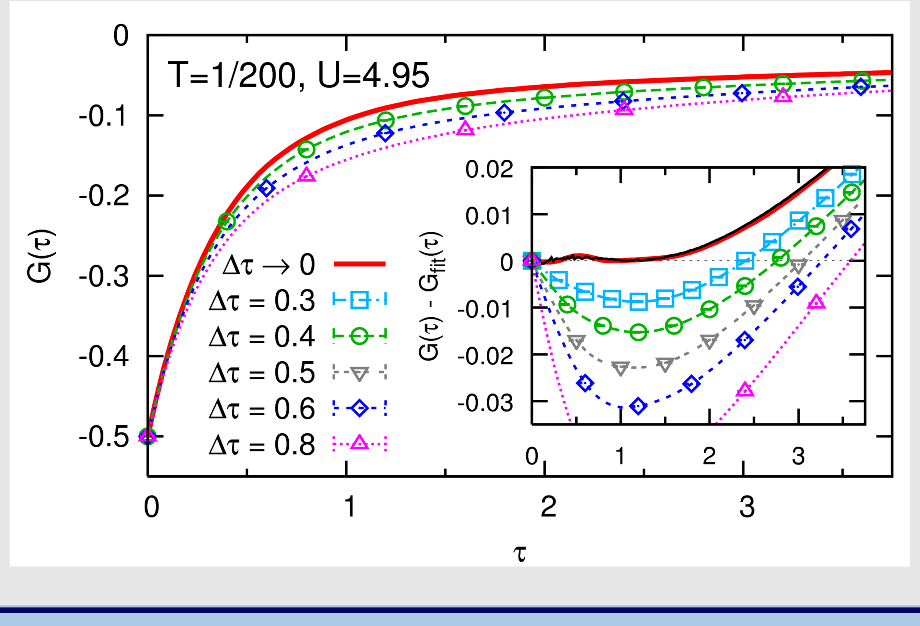
Multigrid Hirsch-Fye quantum Monte Carlo

Internal elimination of Trotter error ⇝ quasi continuous time algorithm [NB, arXiv:0801.1222]



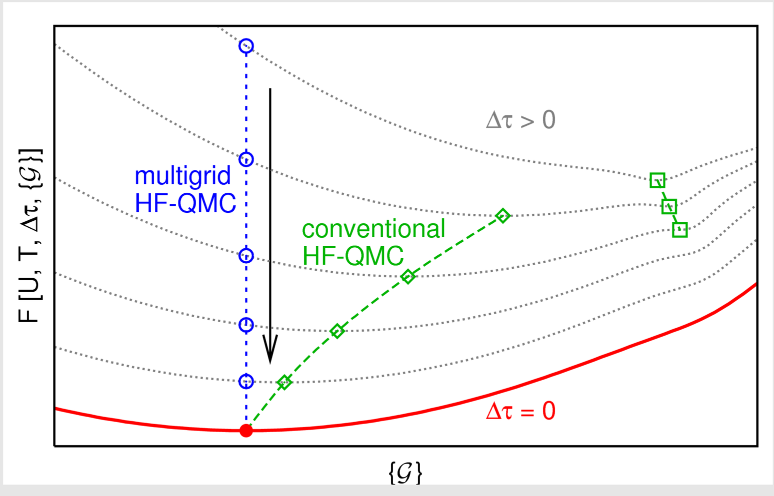
Important/difficult ingredient: Green function extrapolation [NB, arXiv:0712.1290]

Excellent agreement with hybridization expansion CT-QMC [Werner et al., PRL (2006)]



Fundamental advantages of multigrid Hirsch-Fye QMC

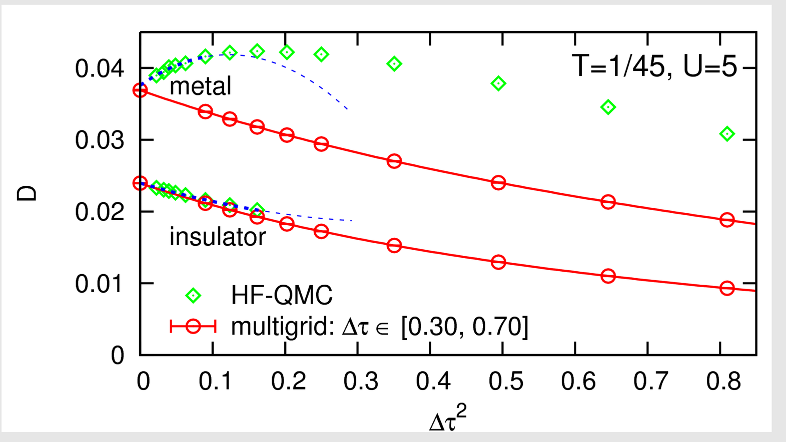
Schematic comparison via generalized Ginzburg-Landau functionals



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 $\Delta\tau$

Applications

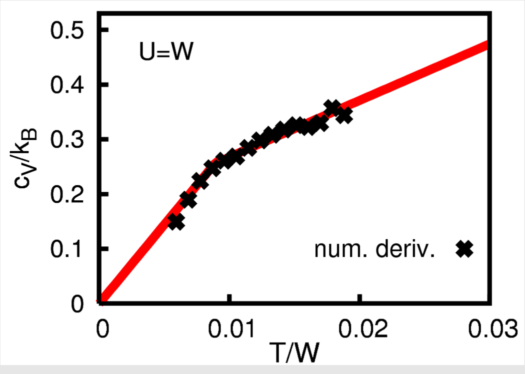
Thermal breakdown of a Fermi liquid

Fermi liquid theory: (for "low enough" T)

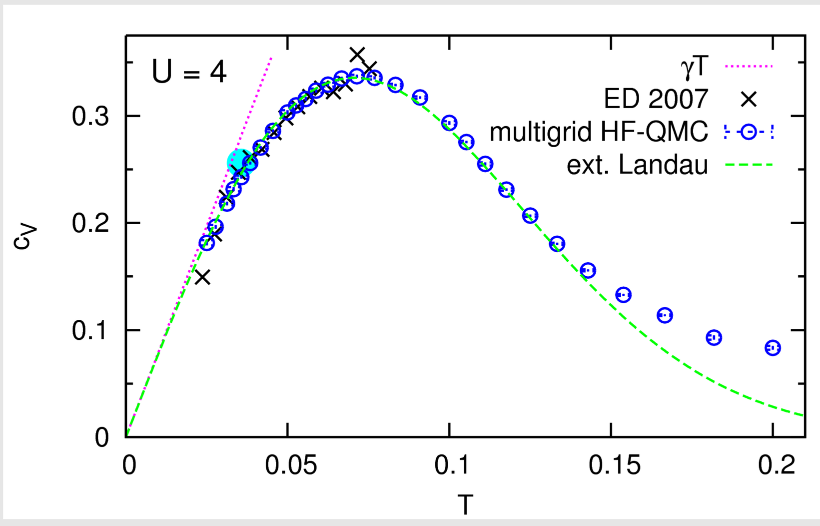
linear specific heat	$c_V = \gamma T$	
linear entropy	$S = \gamma T$	
quadratic resistivity	$\rho \propto T^2$	

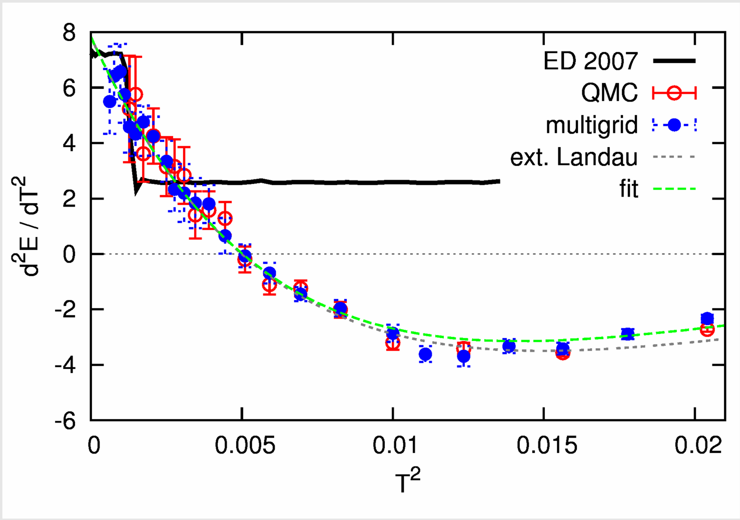
When/how do these laws break down?

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]





High-precision results ⇝ no kink!

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

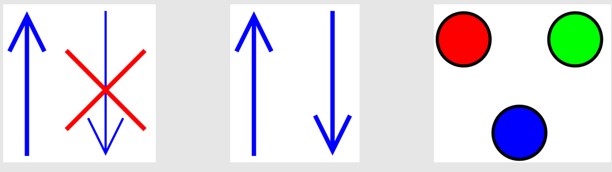
$$c_V(T) = \frac{2\pi}{3Z} T\,\exp\left[-(T/T_0)^2\right];\quad T_0 = \frac{3\log(2)}{\pi^{3/2}}Z \qquad \text{(Bethe DOS)}$$

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

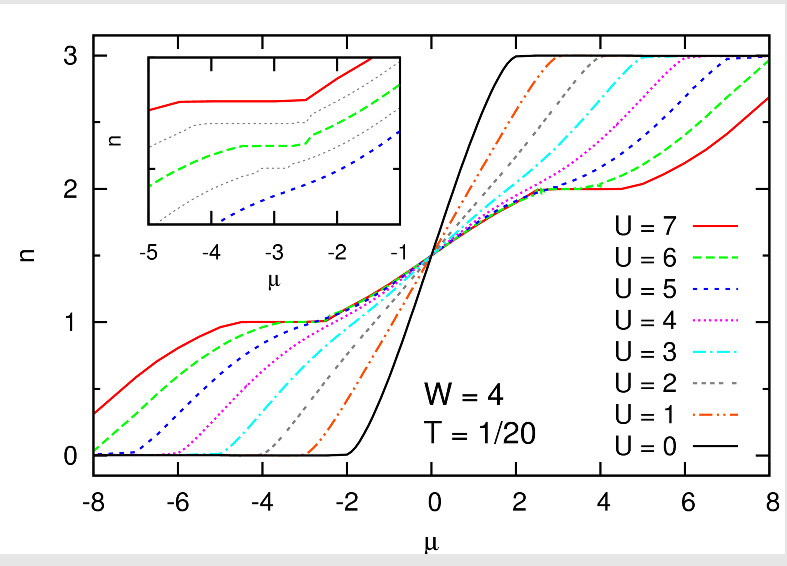
(ii) temperature dependence of $dRe\Sigma/d\omega\big|_{\omega\to0}$

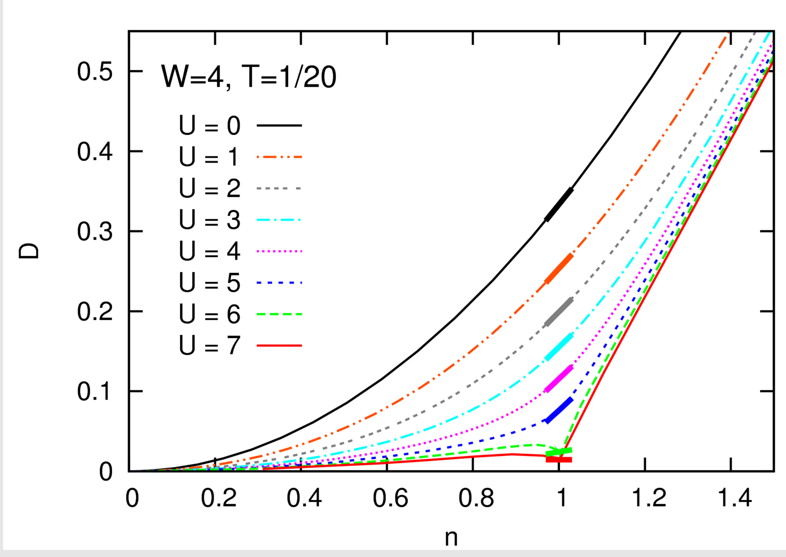
3-spin flavor mix of ultracold fermions on optical lattice

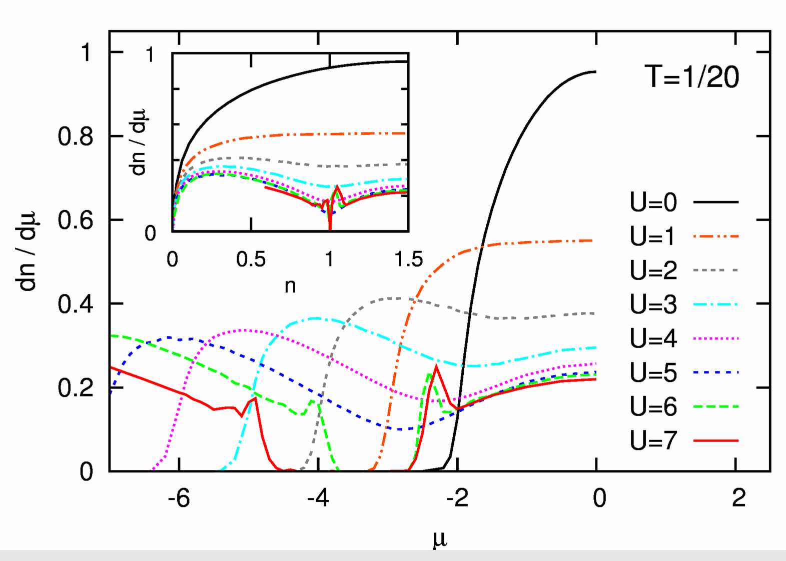
For ultracold fermions: combination of S and I into hyperfine state with angular momentum $F \geq 1/2$ ⇝ novel multiplets, e.g.: ^{40}K: $|F = 9/2, m_F = -5/7, -7/2, -9/2\rangle$



Plateaus in $n(\mu)$: incompressible Mott phase (for $U \gtrsim 6$) - not at half filling!



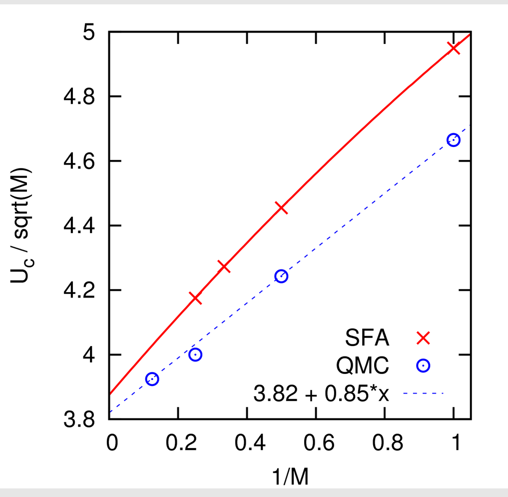


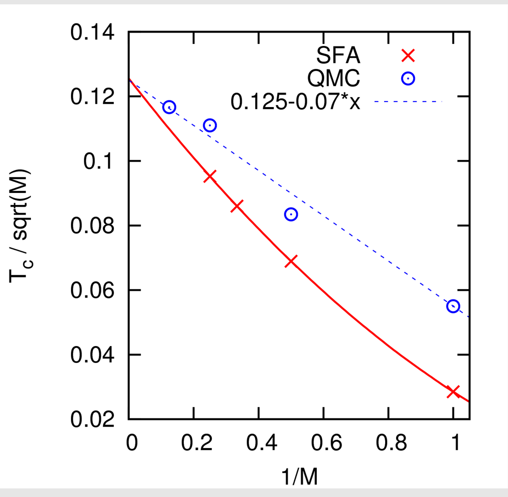


Mott transition at large degeneracy

Consider $SU(2M)$ symmetric Hubbard model

- Mott transition for any $M = 1, 2, \ldots$
- Analytic solutions for $M \to \infty$ [Florens et al., PRB (2002)]
- So far: only approximate numerical solution for $2 \leq M \leq 4$ [Inaba et al., PRB (2005)]





Multigrid HF-QMC: numerically exact results!

⟹ Phase diagram for arbitrary M