Efficiency of QMC DMFT solvers

Nils Blümer, Univ. Mainz

Motivation

room B2
Material consious theories of strongly correlated electrons
O. Andersen
M. Capone
K. I. Kugel
N. Bluemer
A. J. Freeman

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room A
00 - 10:30)
Symposium: Numerical approaches to quantum spin systems
A. Sandvik
M. Troyer
U. J. Schollwoeck

Towards ab-initio simulations of the properties of quantum magnets in the ALPS project

M. Troyer[1], A. Kozhevnikov[2], V.I. Anisimov[2], P. Werner[3] and E. Gull [1]

[1] Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland; [2] Institute of Metal Physics, Ekaterinburg GSP-170, Russia; [3] Columbia University, 538 West, 120th Street, New York, NY 10025, USA

The ALPS project (Algorithms and Libraries for Physics Simulations) [1,2] provides open-source software for the simulation of classical and quantum lattice models. The current release 1.3 provides flexible programs for the simulation of classical and quantum lattice models of quantum magnets with anisotropies, disorder, and impurities. It can be used to quantitatively simulate a quantum magnet as long as the microscopic Hamiltonian is known. To derive the microscopic coupling constants, we have in the past used the method of Ref. [3] in an LDA+U [4] calculation to calculate, e.g. the magnetic properties of a series of planar vanadates, and then manually set up a lattice model simulation to calculate the magnetic properties [5]. A recent implementation of XML I/O into the TB-LMTO-ASA band structure code now allows the nearly seamless integration of ab-initio band structure codes with the ALPS simulations to allow for direct ab-initio simulations of quantum magnets. A second recent development in the ALPS project is the development of a framework for dynamical mean field theory (DMFT) solvers within the ALPS project for the simulation of fermionic models. In the second part of this talk we will present a comparison of two new quantum Monte Carlo solvers [6,7] for the DMFT impurity problem done within this framework – both methods perform orders of magnitudes faster than the standard Hirsch-Fye algorithm [8], with the method of Ref. [7] being the best near the Mott transition.

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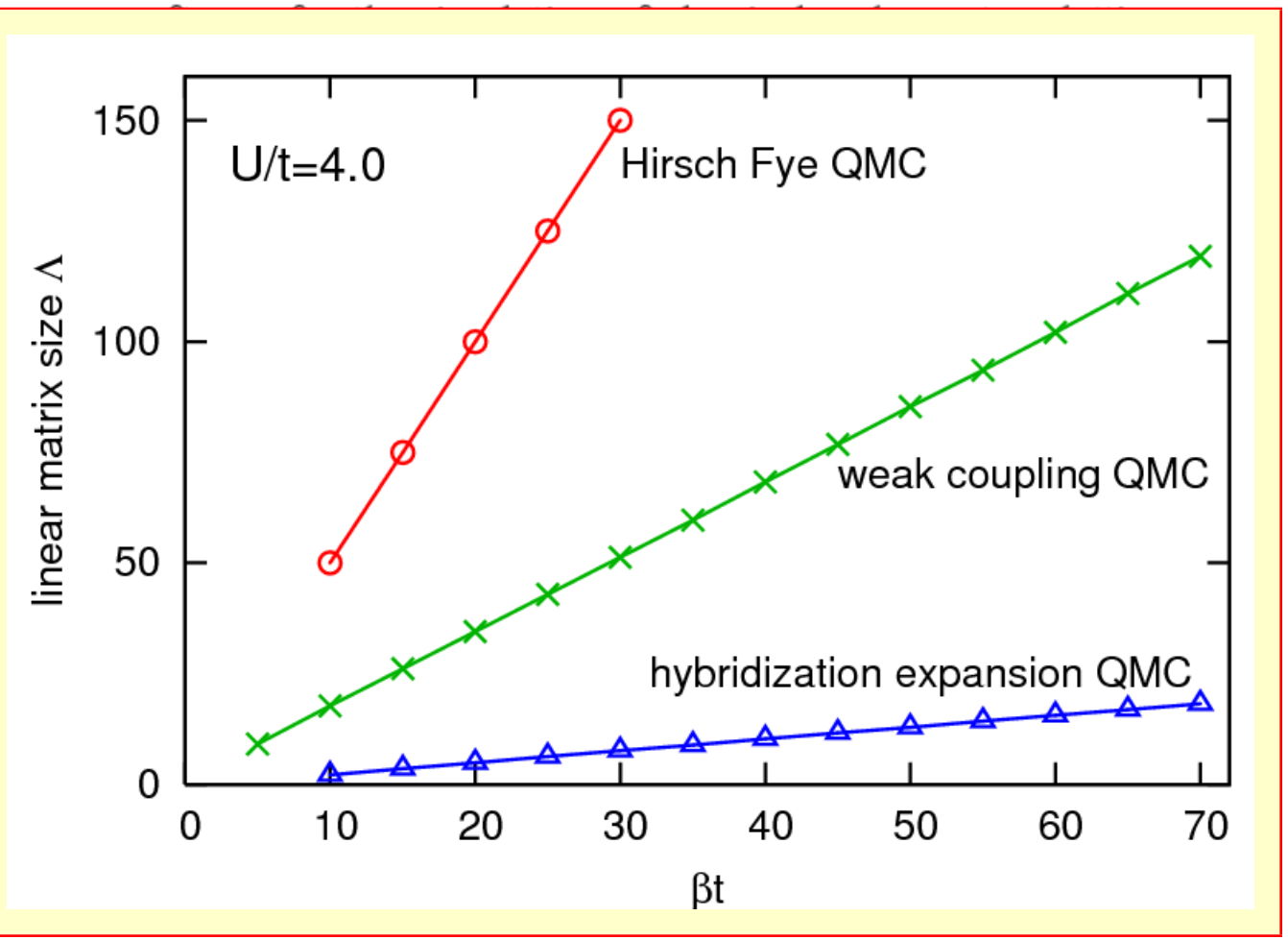

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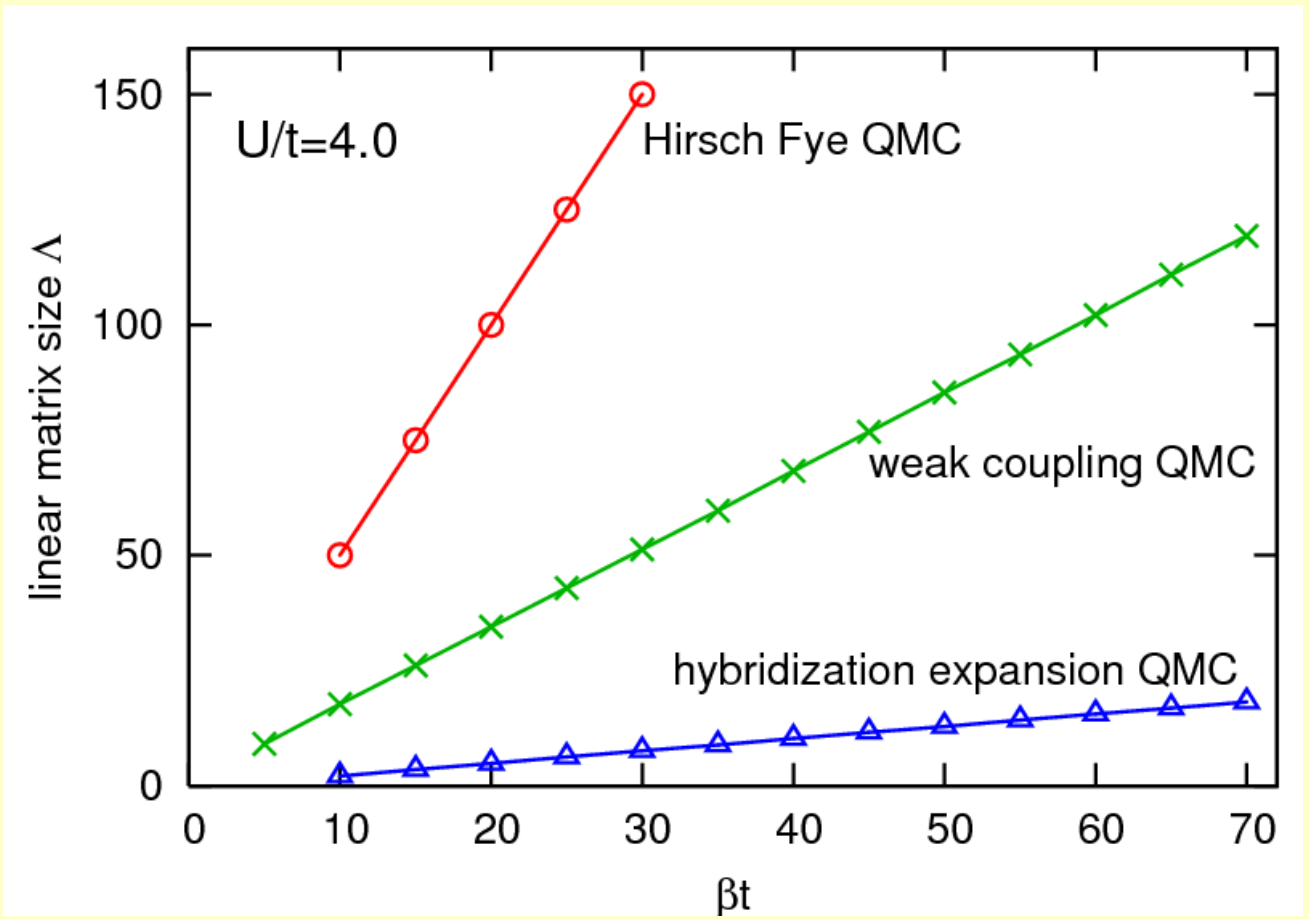

problem:

numerical cost scales as Λ^3

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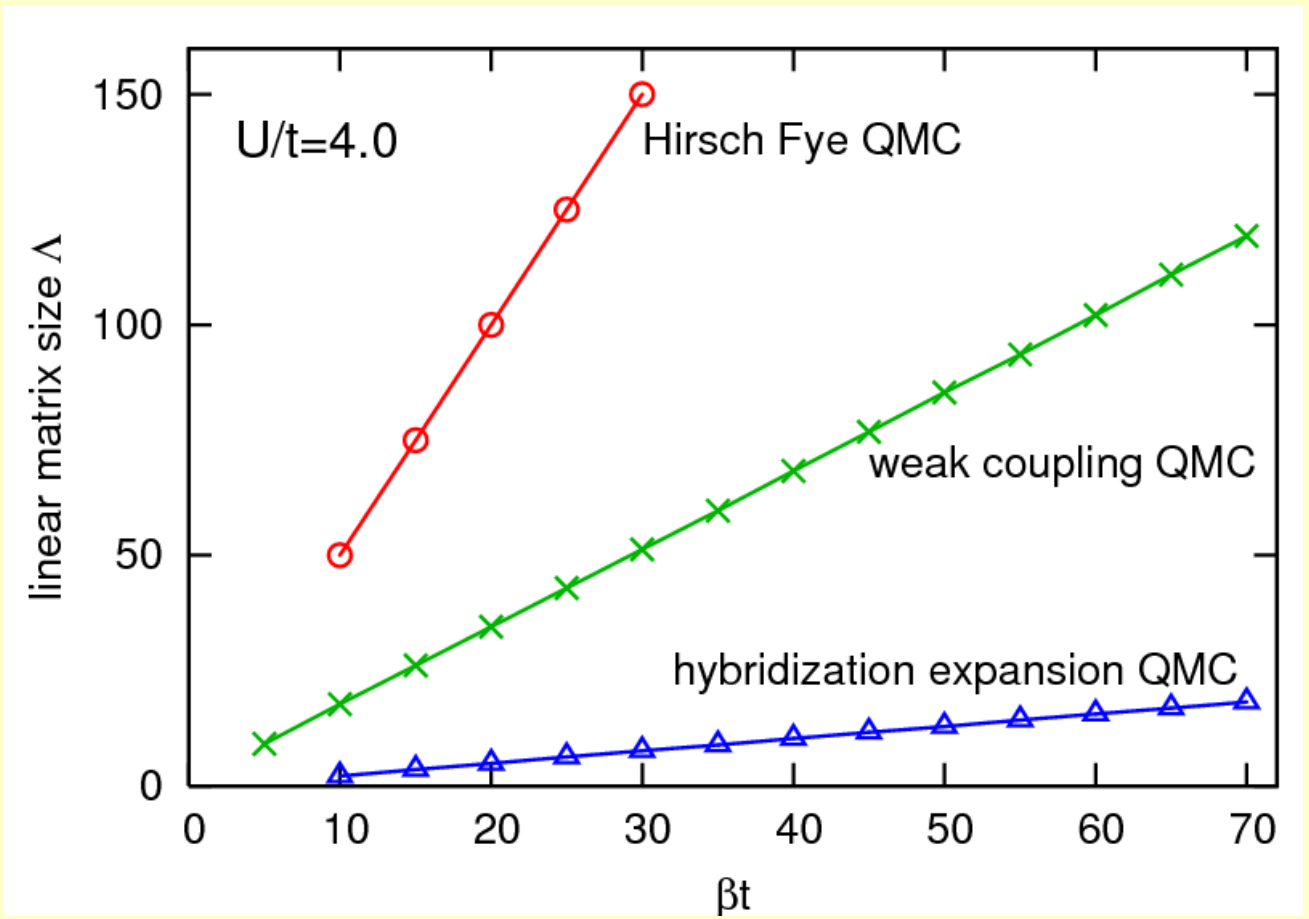

problem:

numerical cost scales as Λ^3

HF-QMC dead!

Consequences

Consequences

1) `> rm -rf /home/nils/super_HF-QMC_code`

Consequences

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2) sightseeing . . .

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Consequences

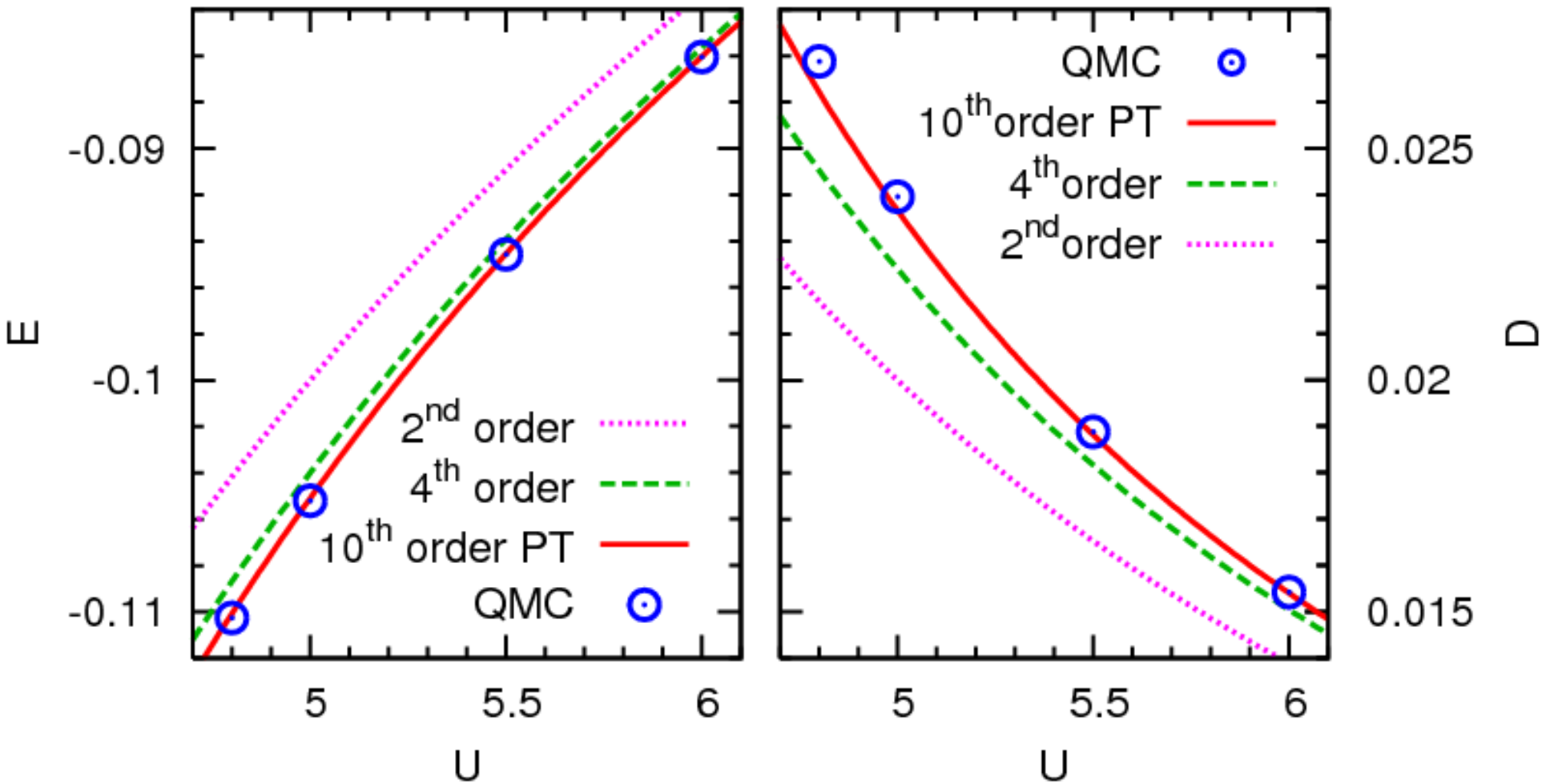
1) `> rm -rf /home/nils/super_HF-QMC_code`

2) sightseeing . . .

but . . .

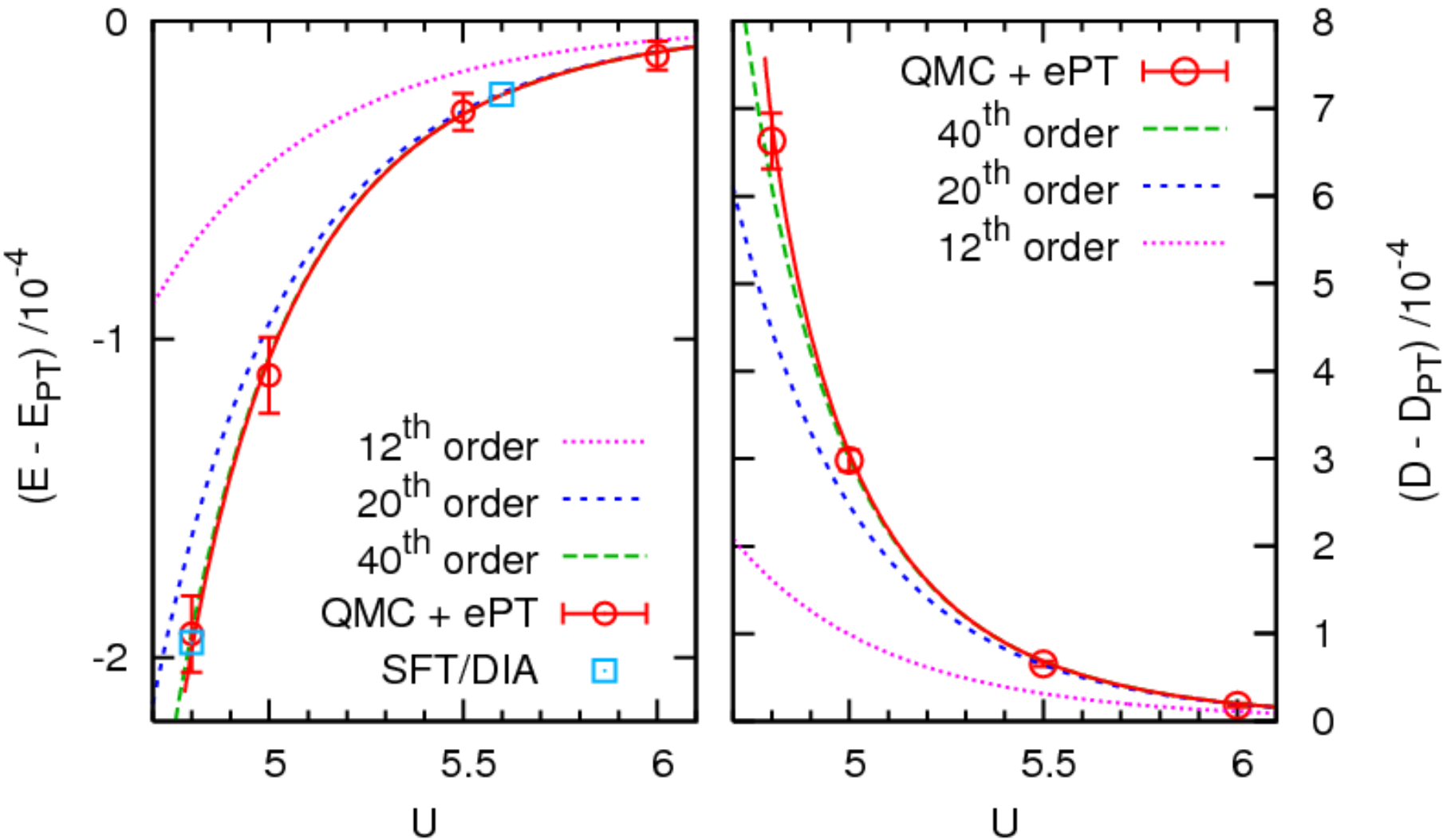
Extreme QMC precision for Mott insulator

Energy E and double occupancy D in Mott insulating ground state of 1-band Hubbard model with semi-elliptic DOS (W=4): QMC vs. perturbation theory



[N. Blümer and E. Kalinowski, Phys. Rev. B 71, 195102 (2005)]

Subtract 10^{th} order PT: perfect agreement of QMC with extrapolated PT



[N. Blümer and E. Kalinowski, Phys. Rev. B 71, 195102 (2005)]

QMC accuracy only challenged by self-energy functional theory (SFT)

Efficiency of QMC DMFT solvers

Nils Blümer, Univ. Mainz

Outline

Motivation: Gull/Troyer comparison

Introduction: DMFT and QMC

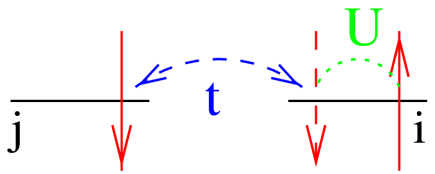
Efficiency: HF-QMC vs. CT-QMC

Precision: HF-QMC vs. ground state methods

Conclusion

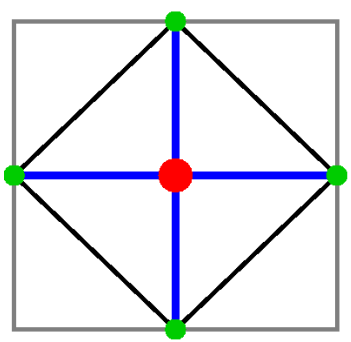
Introduction: DMFT and QMC

Hubbard model $\hat{H} = -t \sum_{\langle i,j \rangle,\sigma} (\hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + \text{h.c.}) + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$

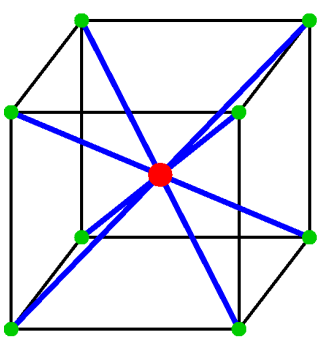


Dynamical mean-field theory (DMFT): local self-energy $\Sigma(\mathbf{k}, \omega) \equiv \Sigma(\omega)$

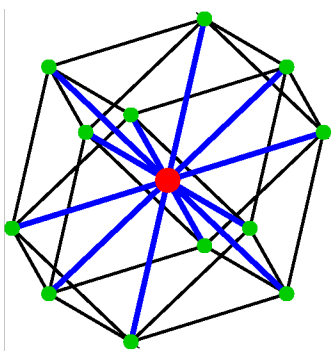
+ non-perturbative $\rightsquigarrow$ valid at MIT
+ dynamical on-site correlations preserved
+ exact for $Z \to \infty$
+ in thermodynamic limit



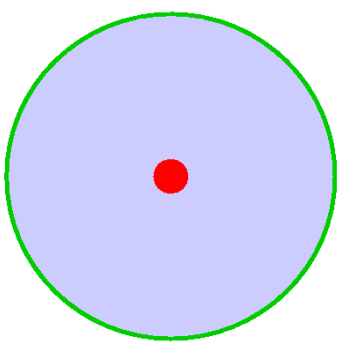
d=2: $Z = 4$



bcc: $Z = 8$

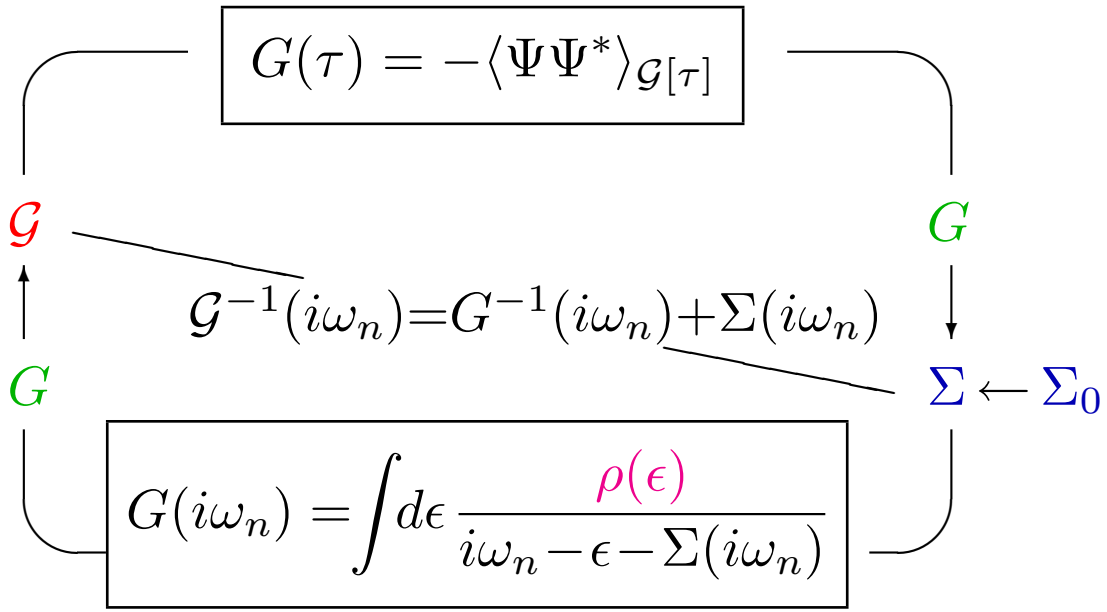


fcc: $Z = 12$



DMFT: $Z = \infty$

Iterative solution of DMFT equations



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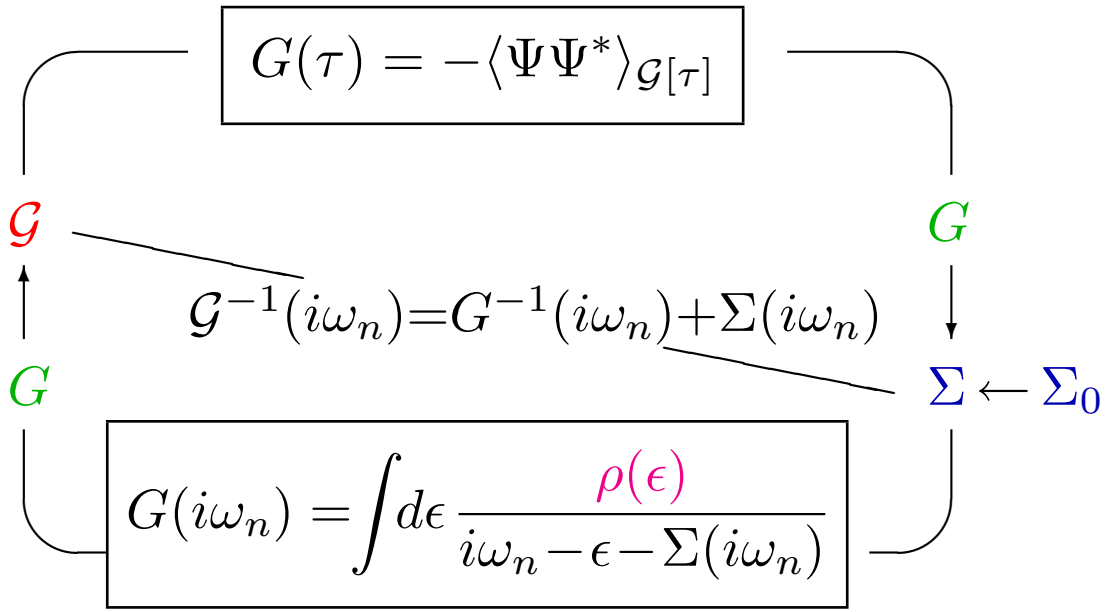


Impurity solver:

- Quanten-Monte-Carlo (QMC)
- Iterative perturbation theory (IPT)
- Non-crossing approximation (NCA)
- Exact diagonalization (ED)
- Numerical renormalization group (NRG)
- Density matrix renormalization group (DMRG)
- Self-energy functional theory (SFT) + ED

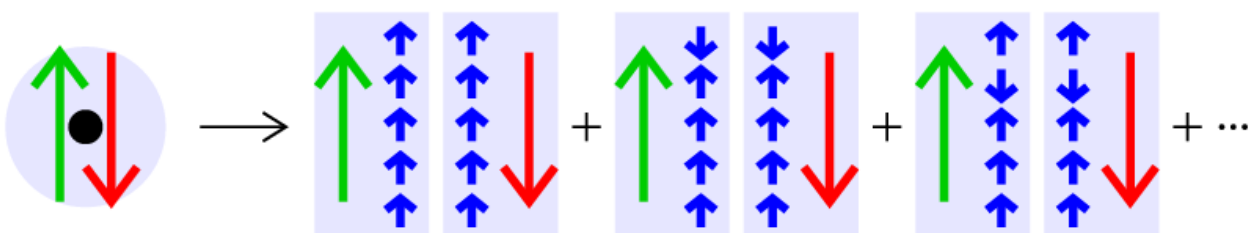
Principles of Hirsch-Fye QMC

Treatment in imaginary time using fermionic Grassmann variables ψ, ψ^*:

$$G_\sigma(\tau_2-\tau_1) = \frac{1}{\mathcal{Z}} \int \mathcal{D}[\psi]\,\mathcal{D}[\psi^*]\ \psi_\sigma(\tau_1)\psi^*_\sigma(\tau_2) \exp\left[\mathcal{A}_0 - \frac{U}{2}\sum_{\sigma\sigma'}\int_0^\beta d\tau\, \psi^*_\sigma\psi_\sigma\psi^*_{\sigma'}\psi_{\sigma'}\right]$$

discretization $\beta = \Lambda\,\Delta\tau$, Trotter decoupling

discrete Hubbard-Stratonovich transformation $e^{-\Delta\tau U(n_\uparrow - n_\downarrow)^2/2} = \frac{1}{2}\sum_{s=\pm1} e^{\lambda s(n_\uparrow - n_\downarrow)}$



Wick theorem:

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

Metropolis MC importance sampling over auxiliary Ising field: 2^Λ configurations

$+$ nonperturbative, numerically exact $\quad -$ effort scales as T^{-3}

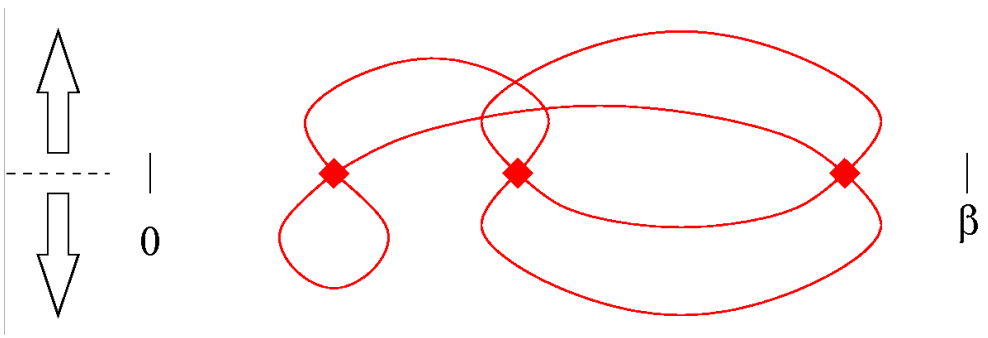
Principles of weak-coupling CT-QMC

Decouple action into quadratic part

$$S_0 = -\int_0^\beta d\tau d\tau' \sum_\sigma c_\sigma(\tau) F_\sigma(\tau - \tau') c_\sigma^\dagger(\tau') - \mu \int_0^\beta d\tau (n_\uparrow + n_\downarrow)$$

and an interaction part

$$S_U = U \int_0^\beta d\tau n_\uparrow n_\downarrow,$$



[Gull et al. cond-mat/0609438]

where $\mathcal{G}_{0,\sigma}^{-1}(i\omega) = i\omega + \mu - F_\sigma(-i\omega)$.

$$Z = \sum_k \frac{(-U)^k}{k!} \int d\tau_1 \dots d\tau_k \, Tr T_\tau e^{-S_0} \quad n_\uparrow(\tau_1) n_\downarrow(\tau_1) \dots n_\uparrow(\tau_k) n_\downarrow(\tau_k)$$

is sampled by random insertions/removals of vertices. Trick: avoid sign problem

[Rubtsov, Savkin, Lichtenstein, PRB **72**, 035122 (2005)]

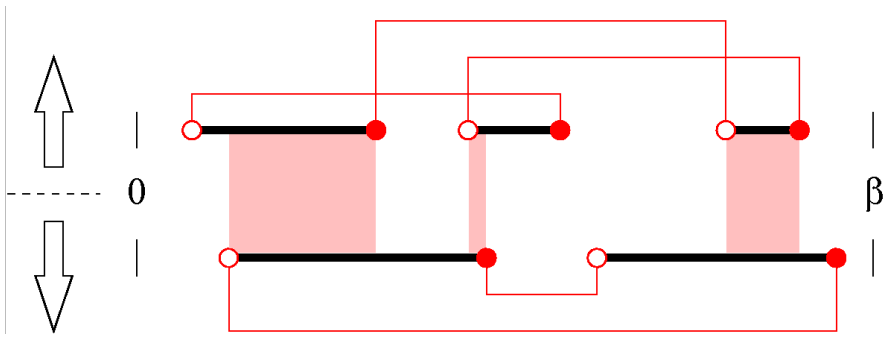
Principles of hybridization expansion CT-QMC

Decompose action into local part

$$S_L = -\mu \int_0^\beta d\tau (n_\uparrow + n_\downarrow) + U \int_0^\beta d\tau n_\uparrow n_\downarrow$$

and hybridization part

$$S_F = -\int_0^\beta d\tau d\tau' \sum_\sigma c_\sigma(\tau) F_\sigma(\tau - \tau') c_\sigma^\dagger(\tau');$$



[Gull et al. cond-mat/0609438]

expanding the partition function in powers of F_σ leads to:

$$\begin{aligned} Z &= Tr T_\tau e^{-S_L} \prod_\sigma \sum_{k_\sigma} \frac{1}{k_\sigma!} \int_0^\beta d\tau_1^\sigma \ldots d\tau_{k_\sigma}^\sigma \int_0^\beta d\tilde{\tau}_1^\sigma \ldots d\tilde{\tau}_{k_\sigma}^\sigma \\ &\quad \times \Big[c_\sigma(\tau_1) F_\sigma(\tau_1 - \tilde{\tau}_1) c_\sigma^\dagger(\tilde{\tau}_1) \ldots c_\sigma(\tau_{k_\sigma}) F_\sigma(\tau_{k_\sigma} - \tilde{\tau}_{k_\sigma}) c_\sigma^\dagger(\tilde{\tau}_{k_\sigma}) \Big]. \end{aligned}$$

Express combined weight corresponding to given collection $\{c_\sigma^\dagger(\tilde{\tau}_i), c_\sigma(\tau_i)\}_{i=1,\ldots,k_\sigma}$ of creation and annihilation operators as the determinant of a matrix $D_{F,\sigma}$, sample . . . [Werner et al., PRL **97**, 076405 (2006); Werner and Millis, PRB **76**, 1 (2006)]

Efficiency: HF-QMC vs. CT-QMC

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

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- Test case: 1-band Hubbard model (semi-elliptic DOS, $n = 1$, $W = 4$) for $U = 4$
- Focus on low temperatures: $T = 1/45$
- Additional results for doped model (also different U)

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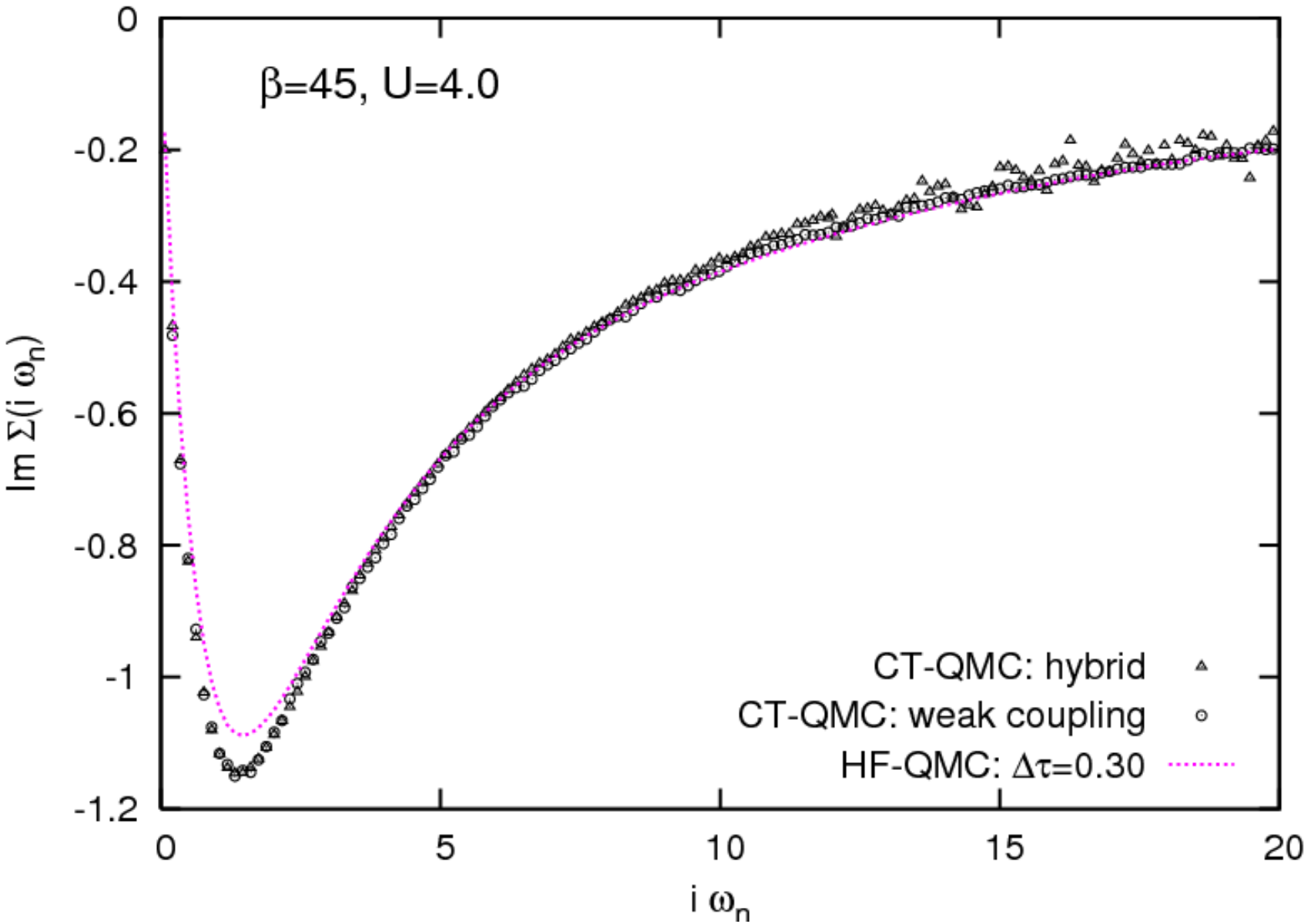
Good Hirsch-Fye implementation? Fair comparison? Precision of results?

Self-energy for $U = W = 4$ and $T = 1/45$



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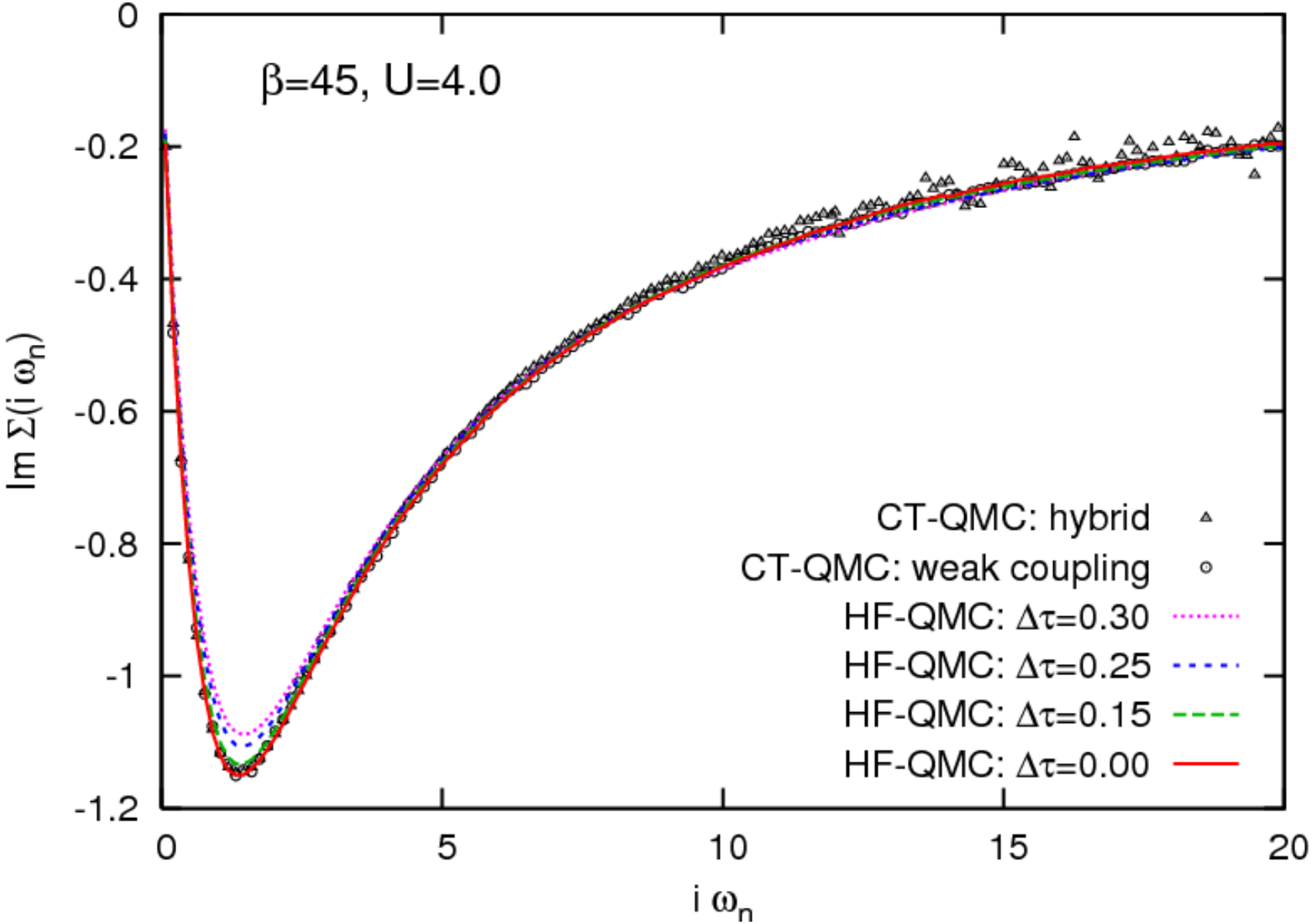

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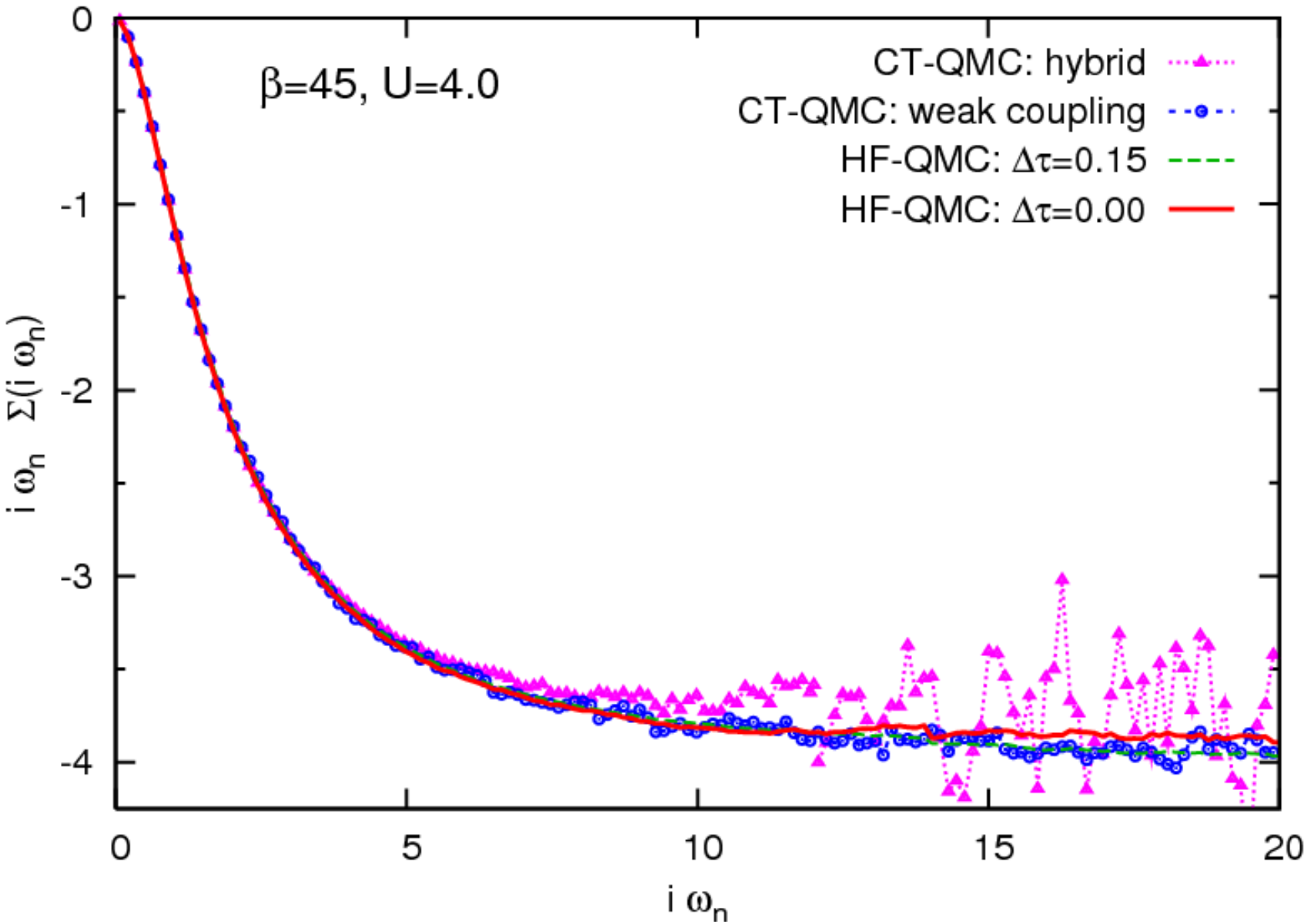
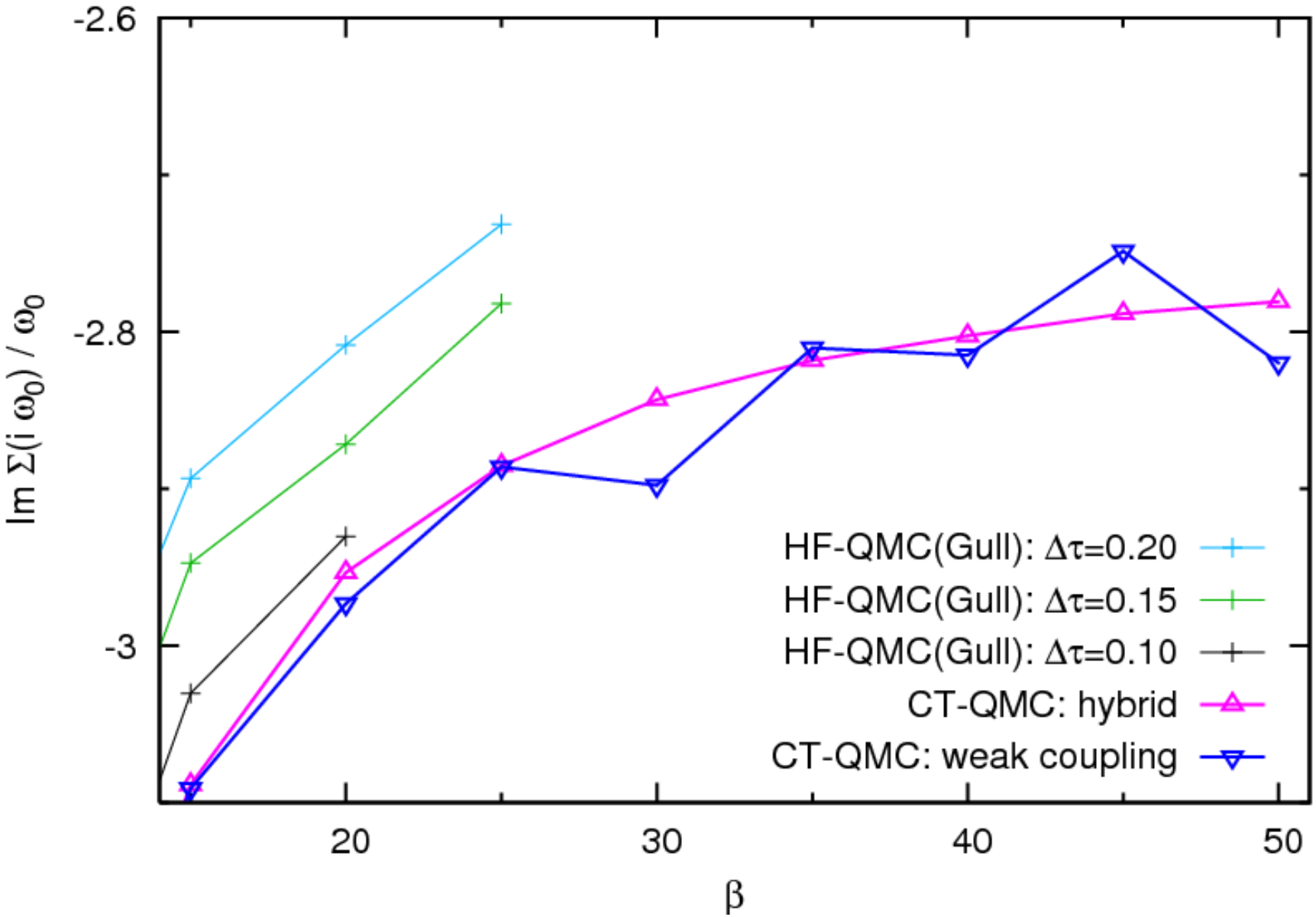


Self-energy: $\mathrm{Im}\Sigma(i\omega_0)/\omega_0 = 1 - 1/Z$ for $U = 4$



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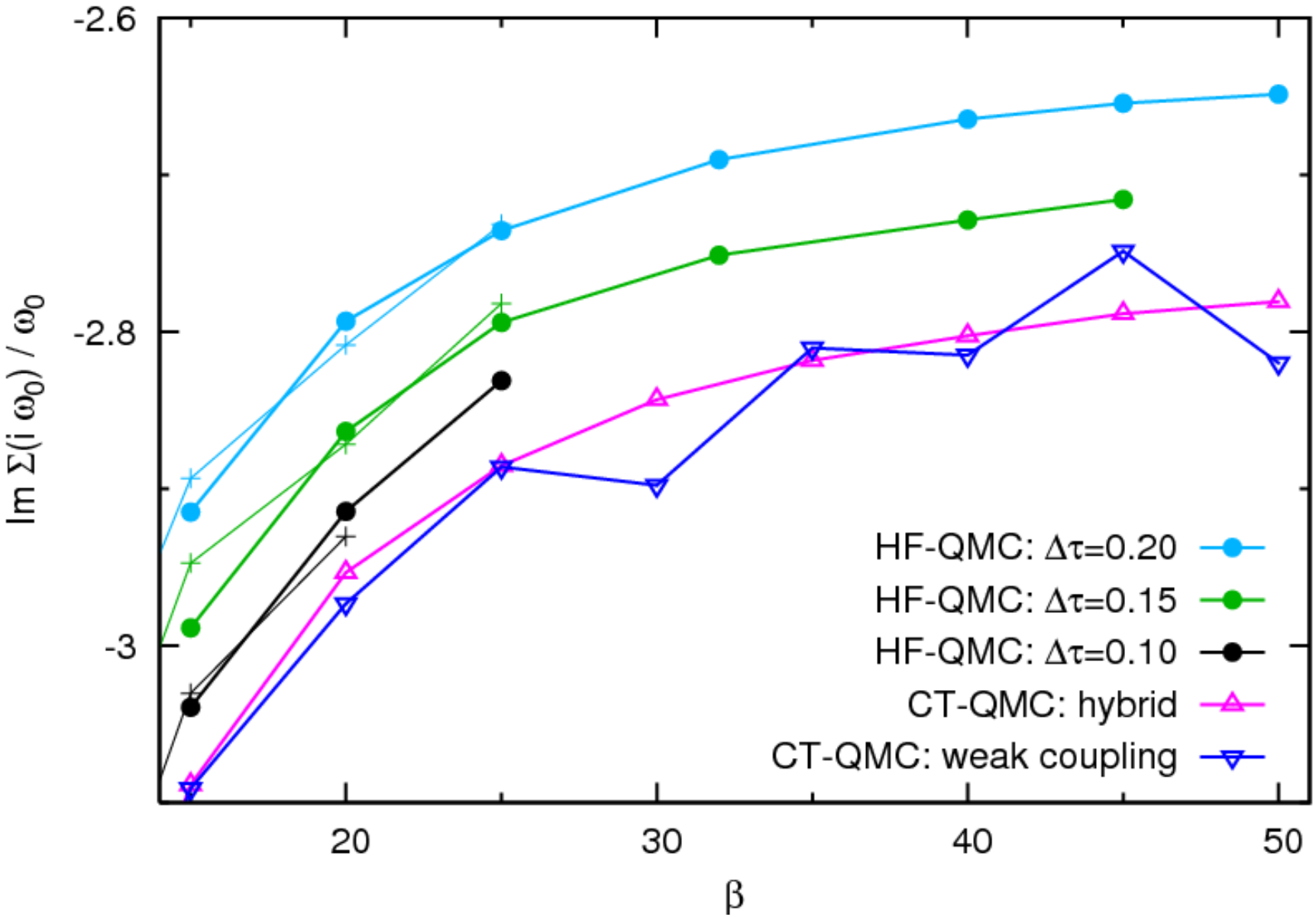

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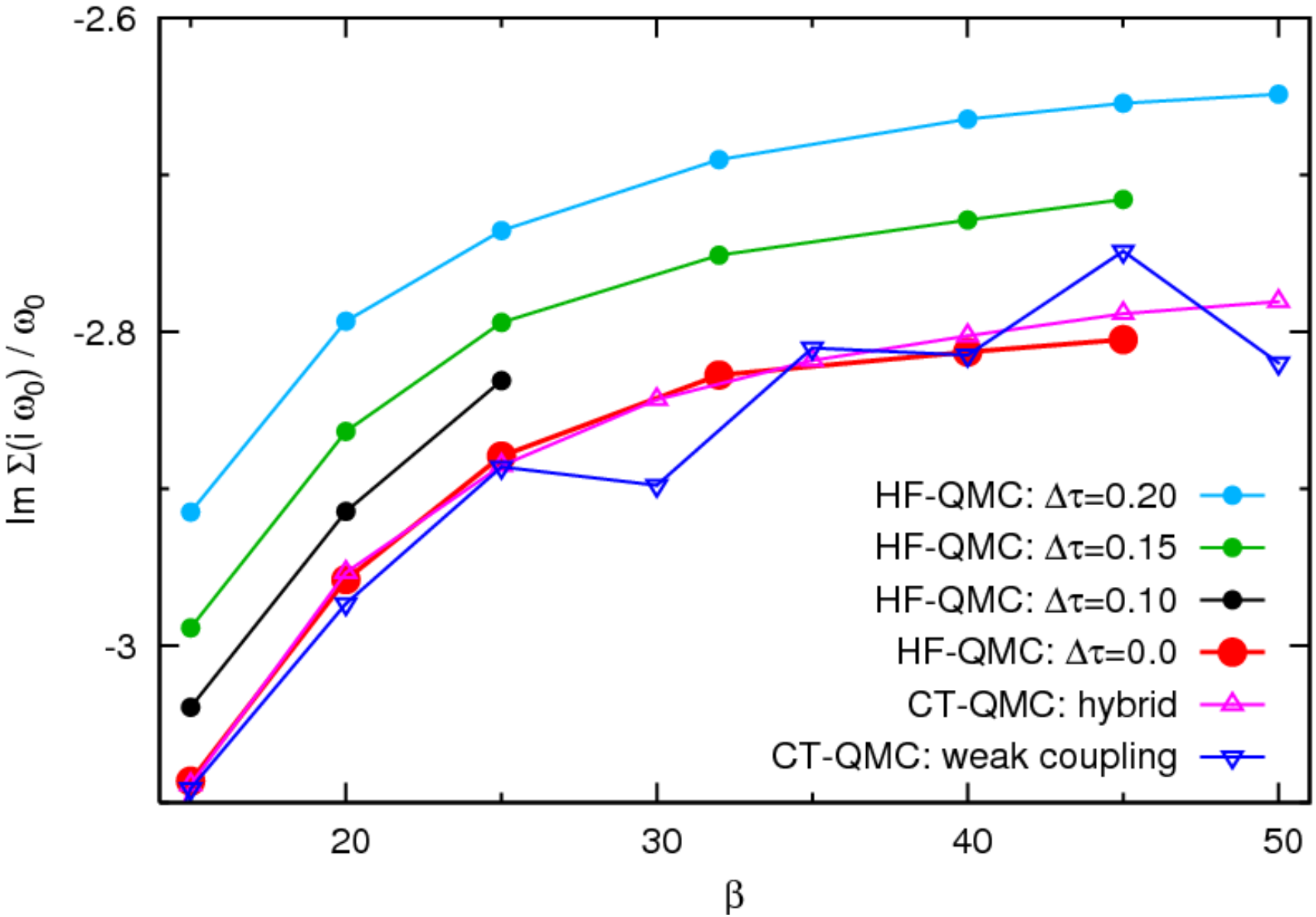
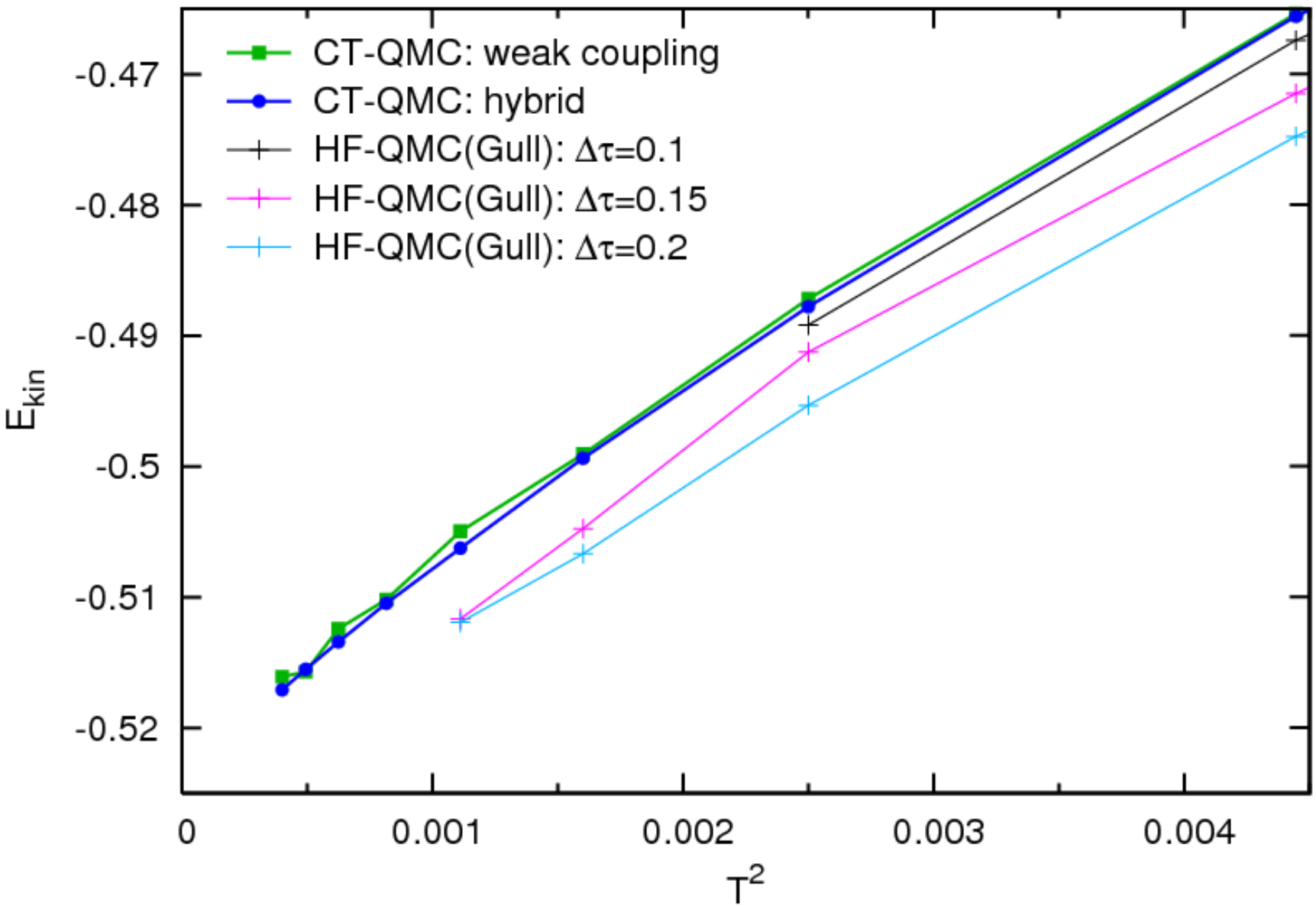


Energetics: kinetic energy for $U = 4$



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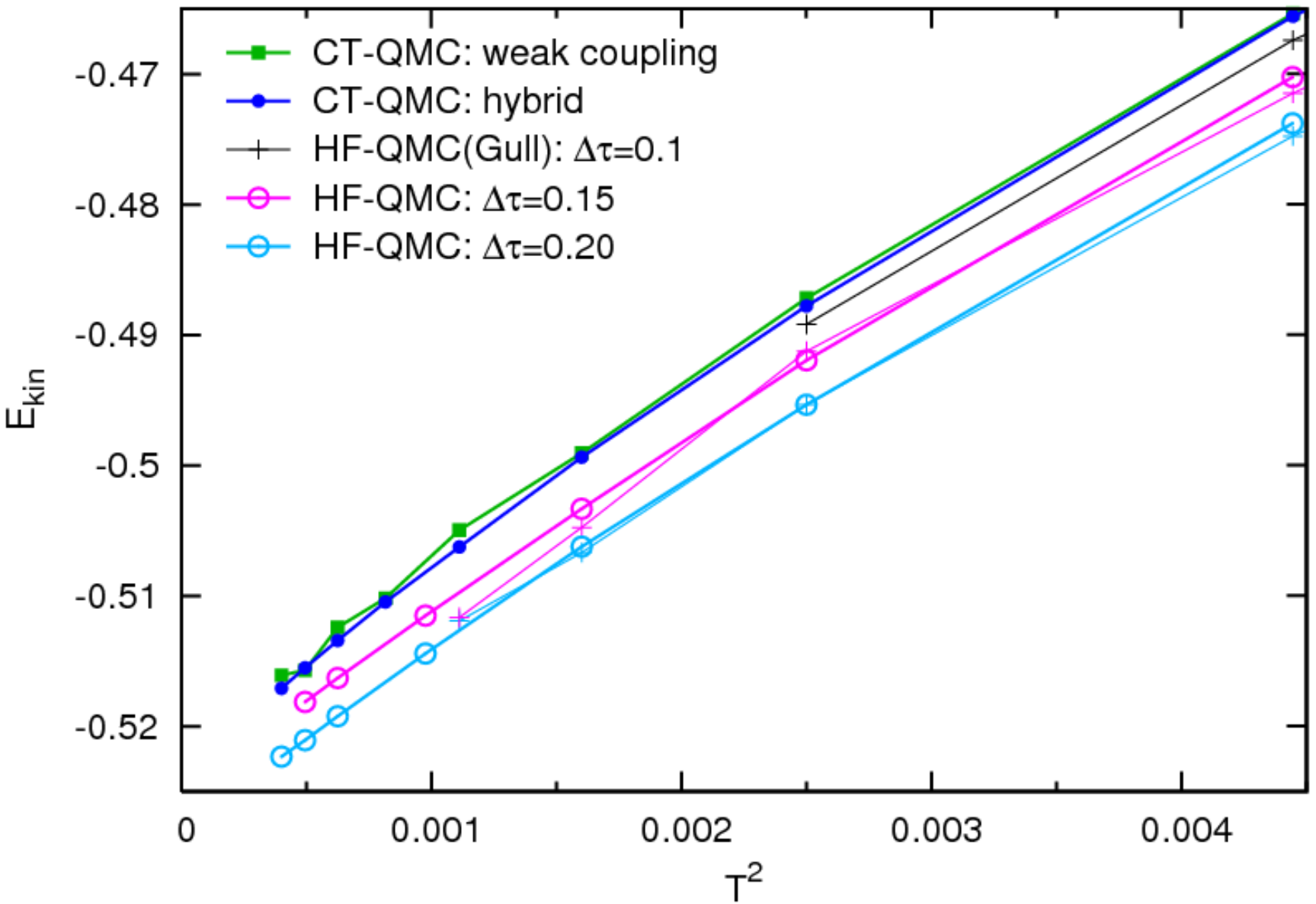

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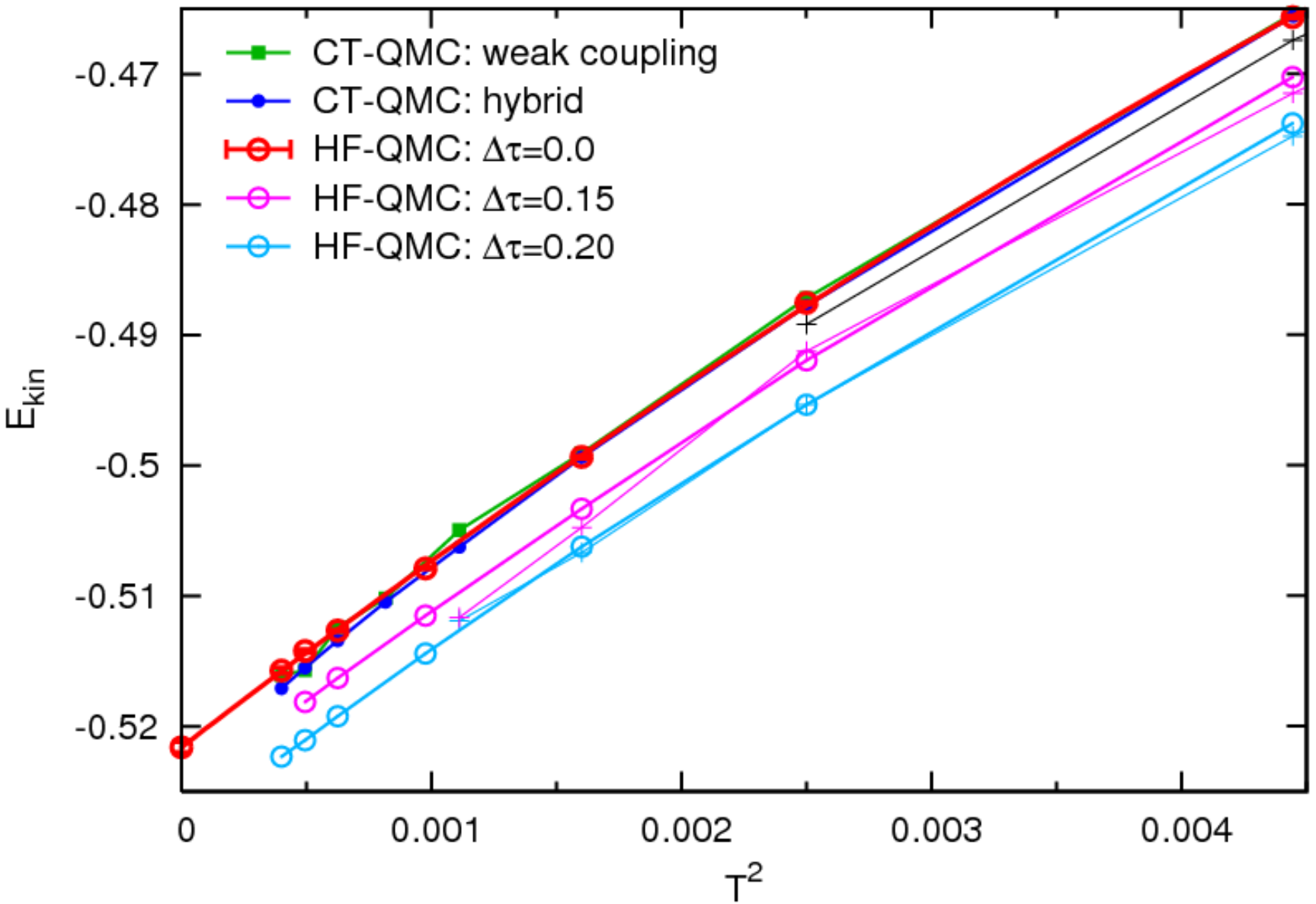

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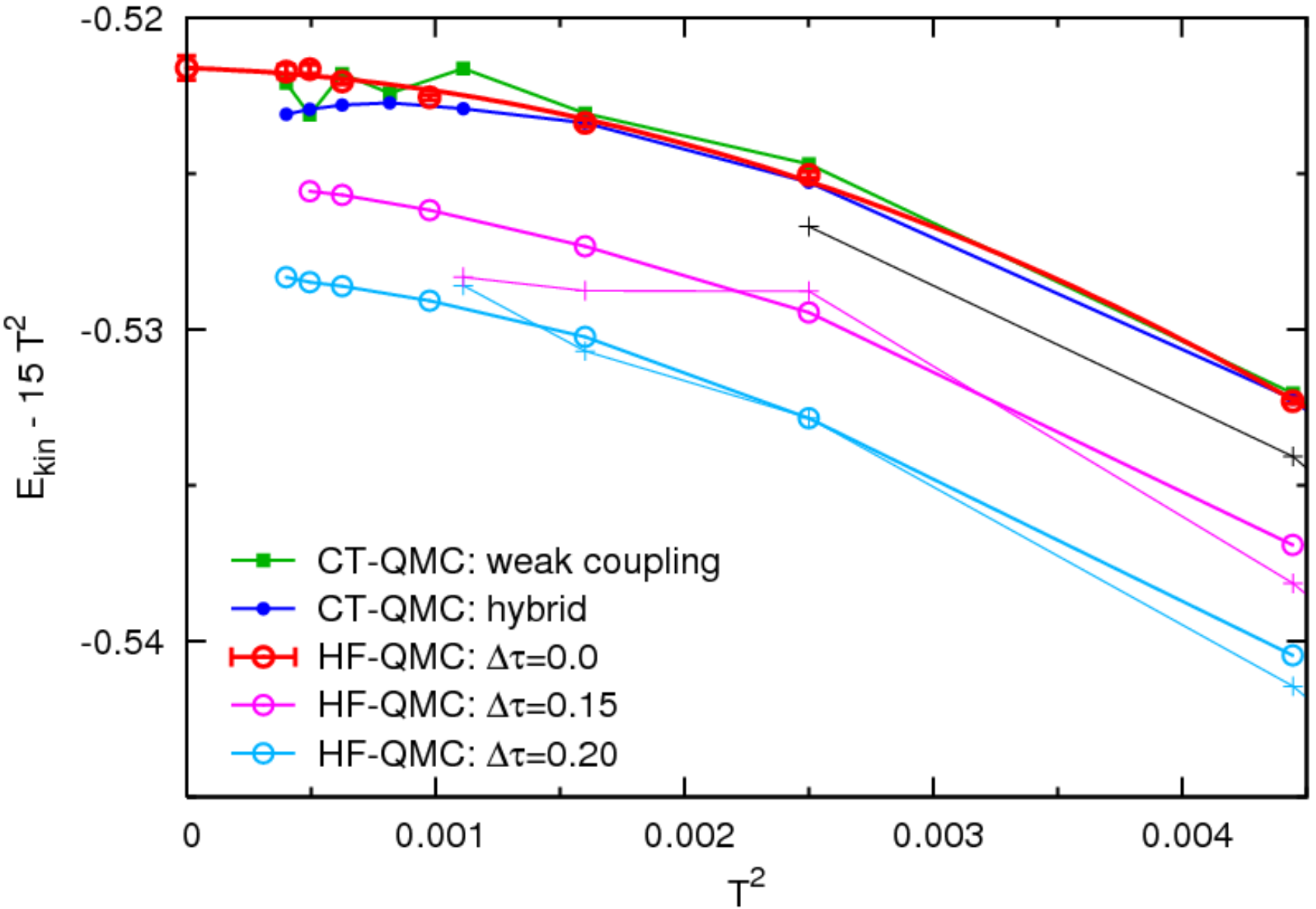
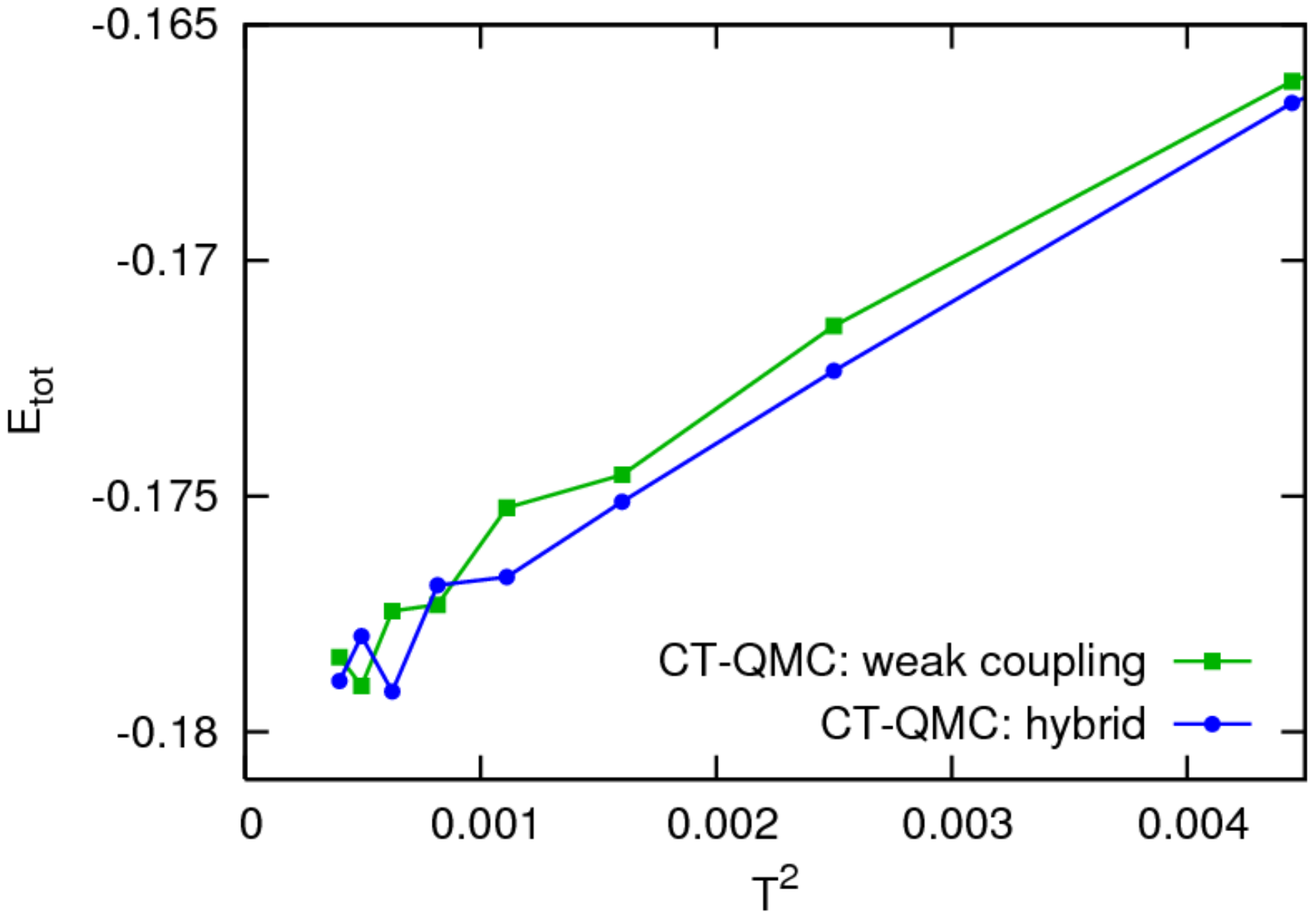


Energetics: total energy for $U = 4$



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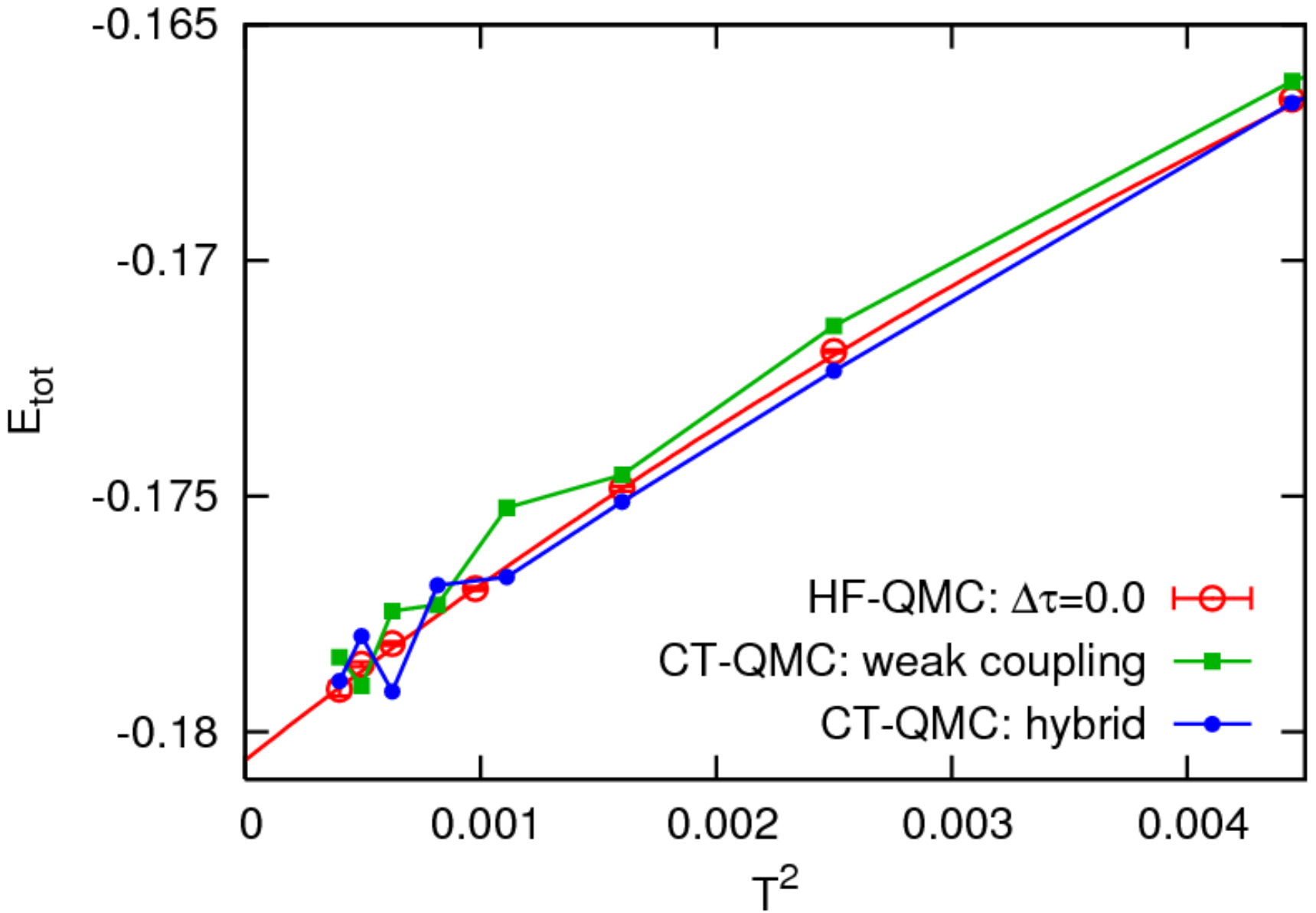
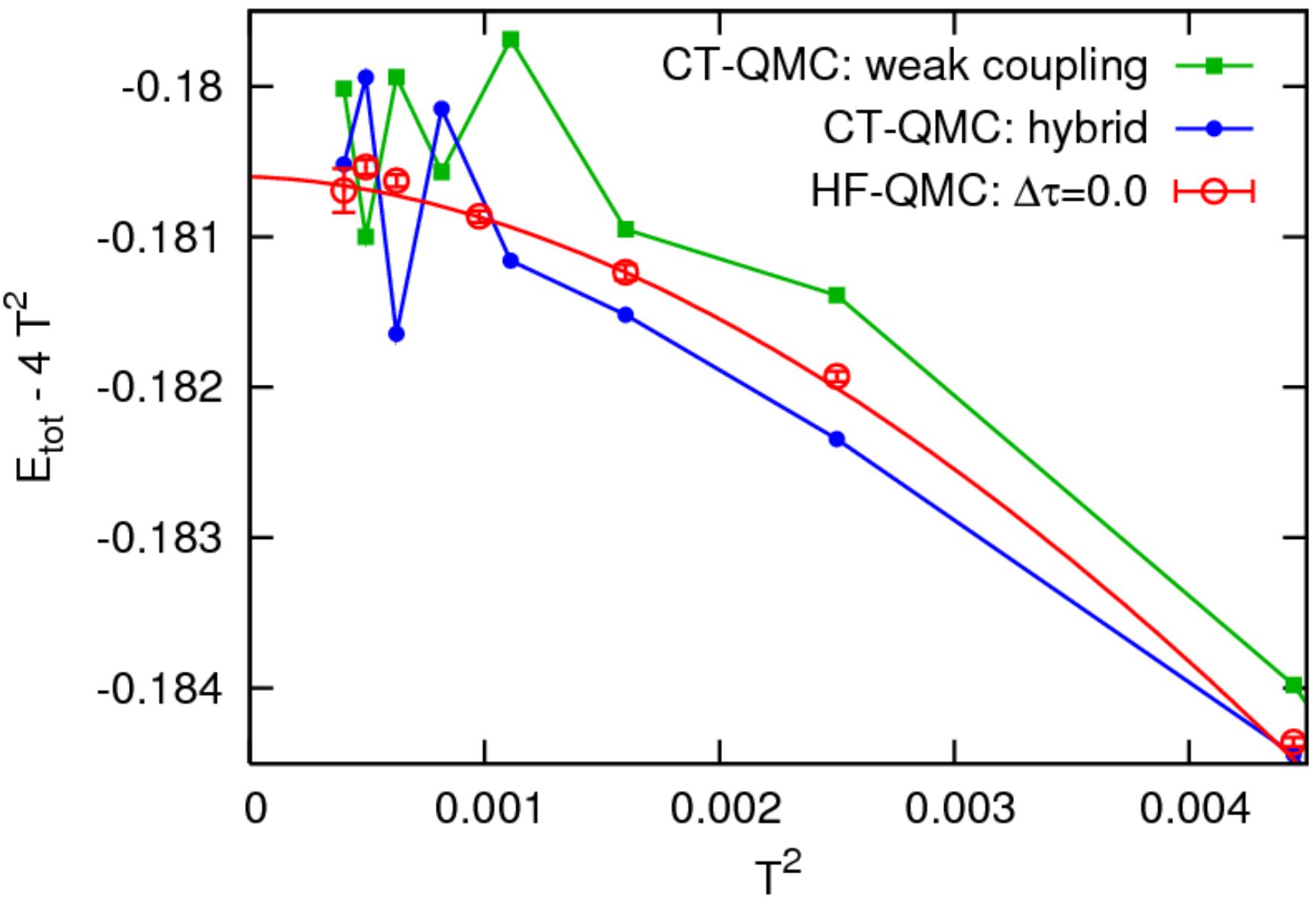


Energetics: total energy for $U = 4$



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HF-QMC cannot compete with CT-QMC without extrapolation of $\Delta\tau \to 0$.

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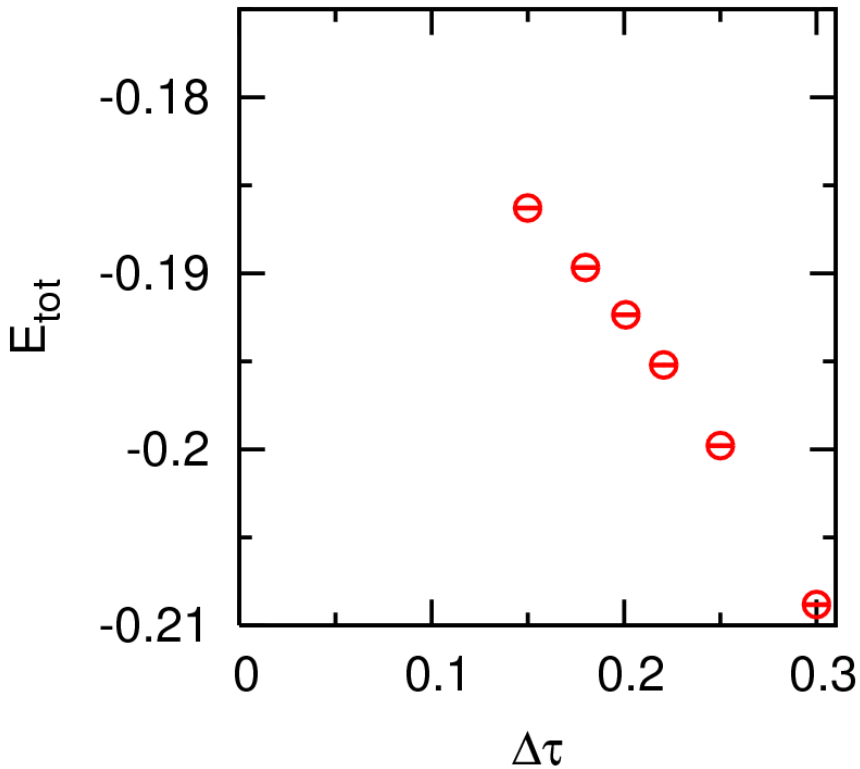

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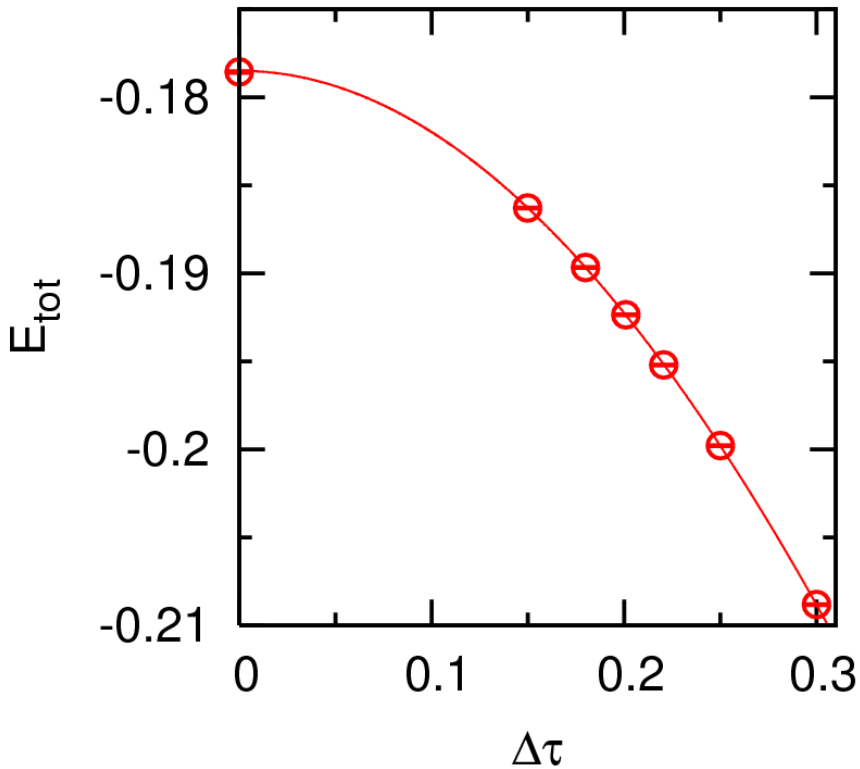

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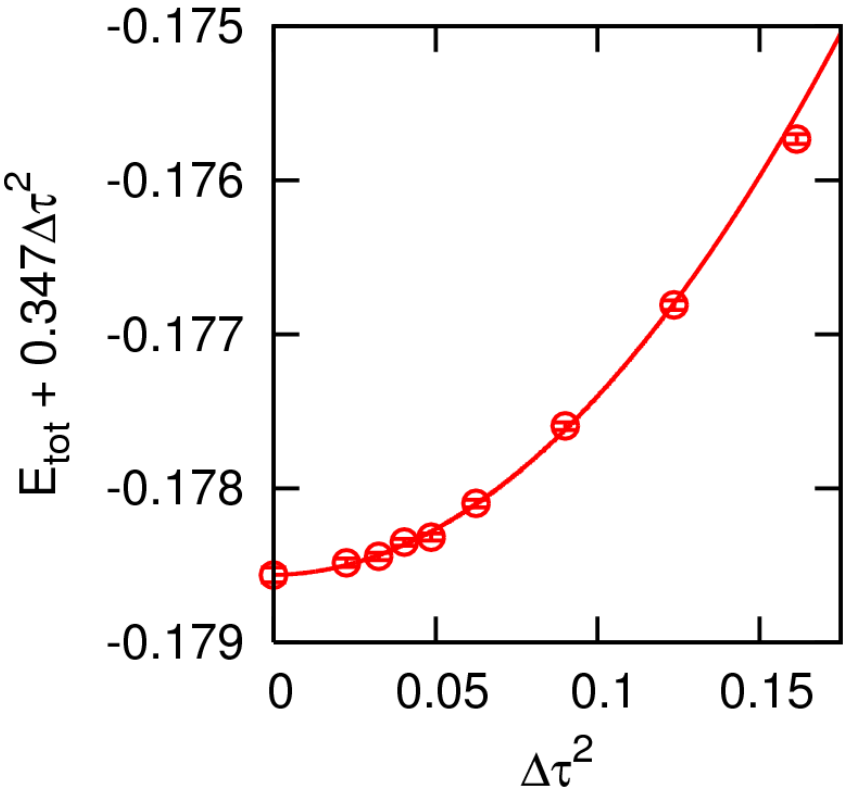

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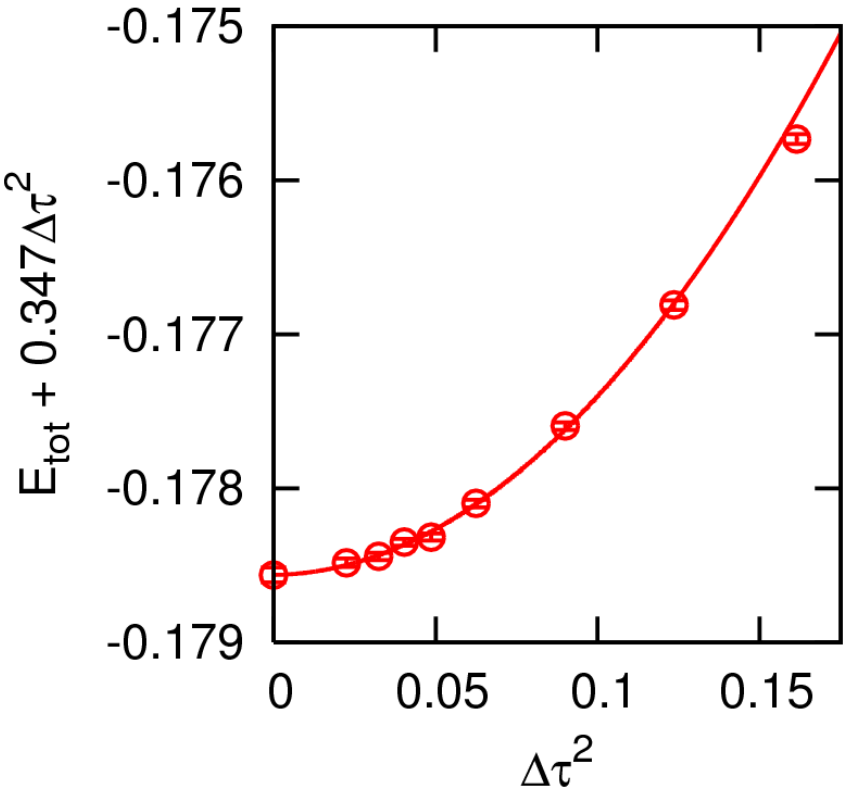


Results in comparison by Gull et al. are obtained from 20 DMFT iterations using 7 hours of CPU time on an AMD Opteron 244, starting from a converged solution, i.e. more than 140 CPU hours per data point.

My runs have used roughly an order of magnitude more (but are much more precise).

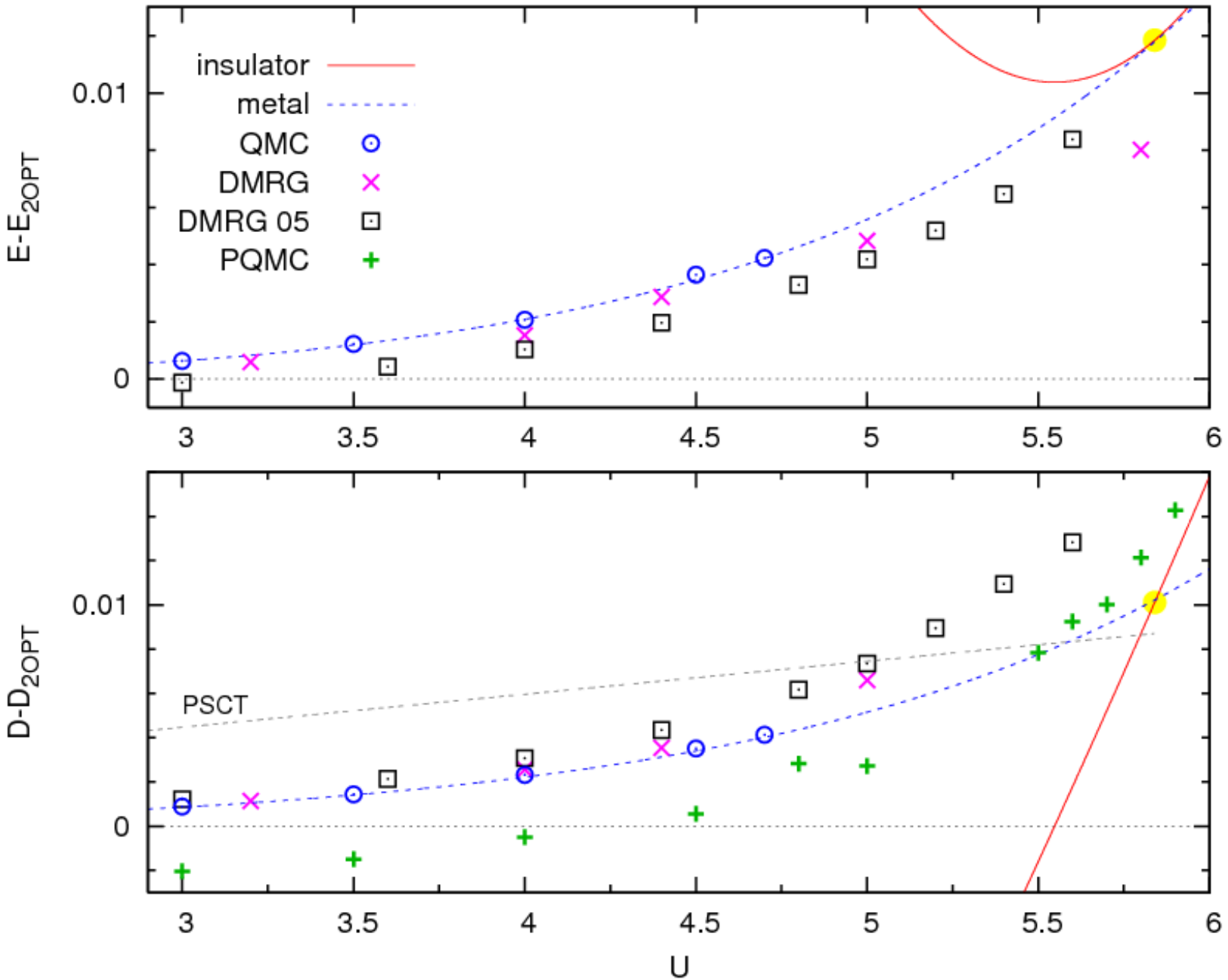
Todo: prepare exact 140 CPU-h comparison runs.

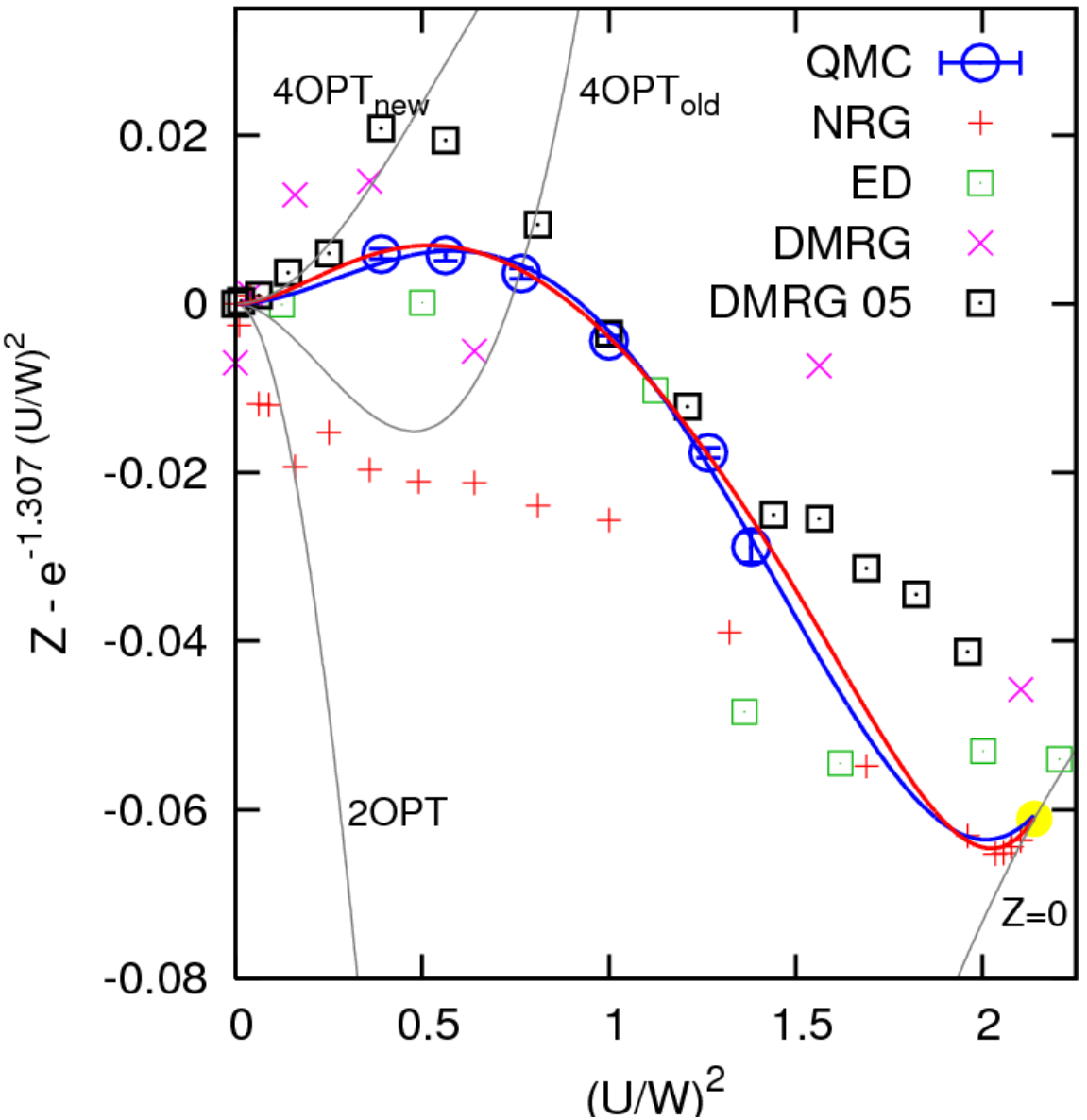
Precision: HF-QMC vs. ground state methods

Up to now: HF-QMC results extrapolated to $\Delta\tau = 0$

Extrapolate also $T \to 0$, compare with ground state methods – for metallic phase

Observables: energy, double occupancy, quasiparticle weight


insulator
metal
QMC
DMRG
DMRG 05
PQMC
E-E2OPT
0.01
0
3
3.5
4
4.5
5
5.5
6
D-D2OPT
PSCT
U



HF-QMC results:
small errors,
consistent, smooth

ground state methods:
inconsistent with PT,
strongly fluctuating

Conclusion

CT-QMC methods are promising, give easy direct access to relevant phases

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Nobody publishes precise ground state energetics - why?