Quantum Monte Carlo S
Triangular Hubb

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In

- Importance of the Hubbard Model on a
- Methods
- Results
- Future Work

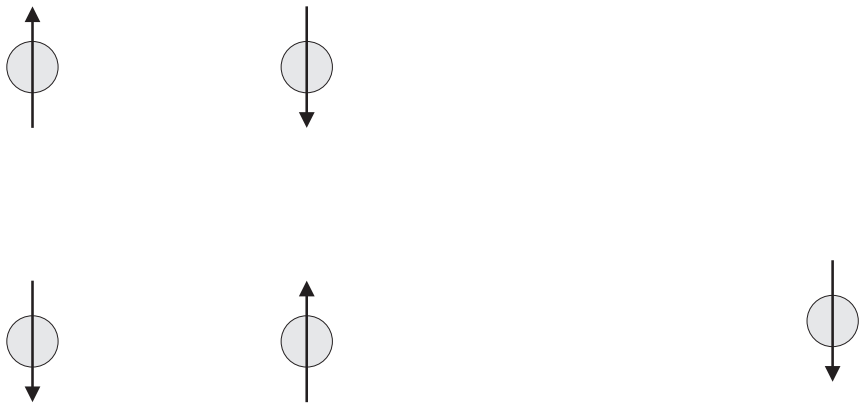
Hubb

$$\hat{H} = -t \sum_{\langle \mathbf{ij} \rangle \sigma} \left(c^{\dagger}_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} + \text{h.c.} \right) - \mu \sum_{\mathbf{i}\sigma} n_{\mathbf{i}\sigma} + U \sum_{\mathbf{i}}$$

- $c^{\dagger}_{\mathbf{i}\sigma}(c_{\mathbf{i}\sigma})$: Fermion creation(destruction) o
- t: Inter-site hopping parameter
- U: On-site Coulomb repulsion
- μ: Chemical potential

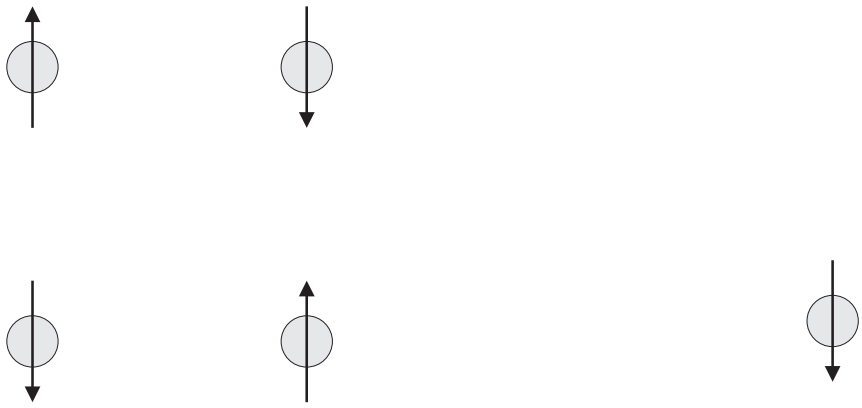
Triangu

- Anti-ferromagnetism is frustrated.



Triangu

- Anti-ferromagnetism is frustrated.



- Superconductivity in $Na_xCoO_2 \cdot yH_2O$
- Metal-insulator transition in $\kappa-$(BEDT-

K. Takada Nature , 53 (2003).

Determinant Quantum Monte Carlo (DQMC)

- Partition Function

$$Z = \mathrm{Tr}\, e^{-\beta \hat{H}}$$

$$\rightarrow \det\left[1 + e^{-\beta h}\right]$$

- Self-energy

$$\Sigma(r, \tau) = \Sigma(r \quad, \tau)$$

- Sign problem

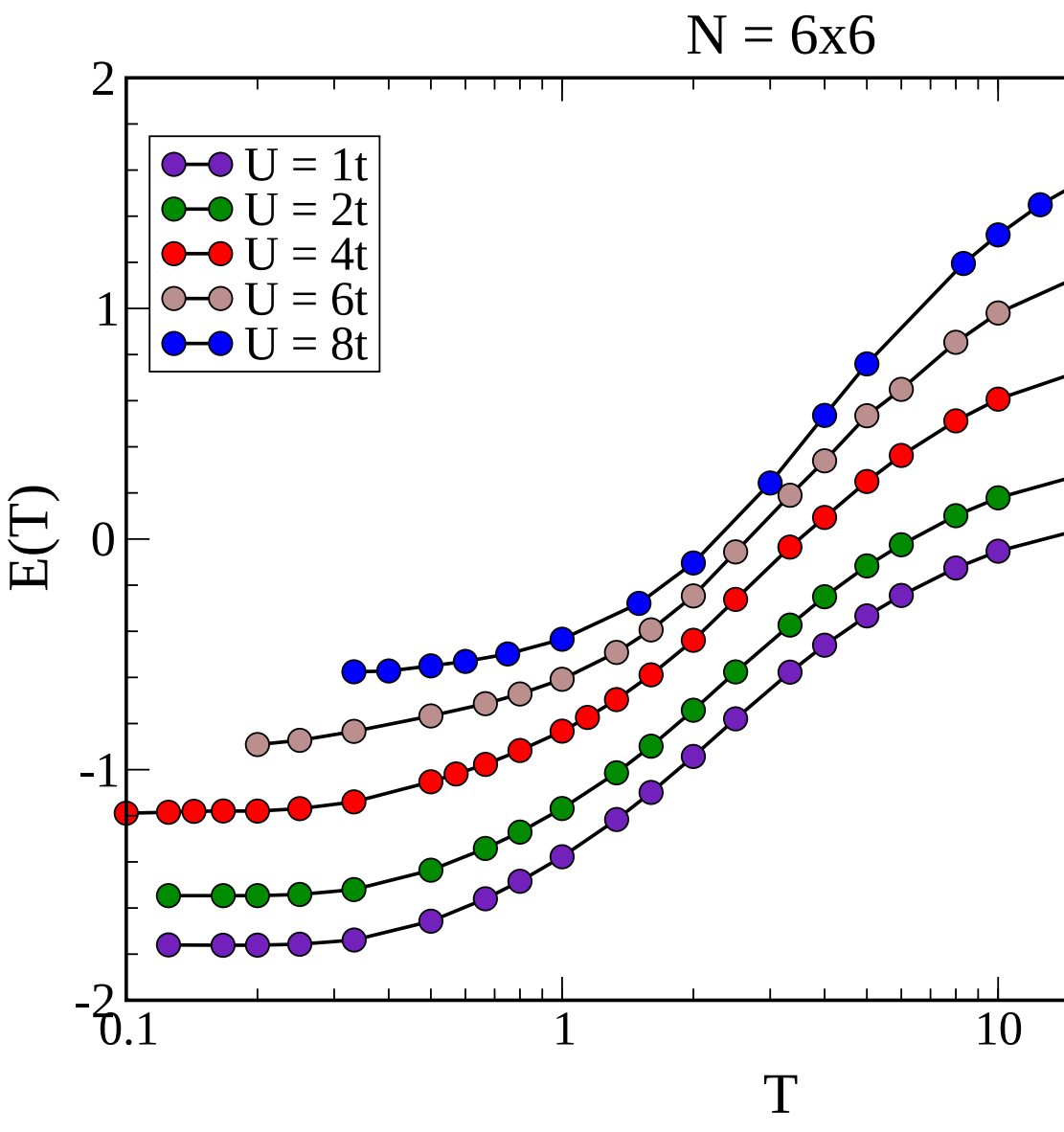
Dynamical M (DMFT)

- Self-en

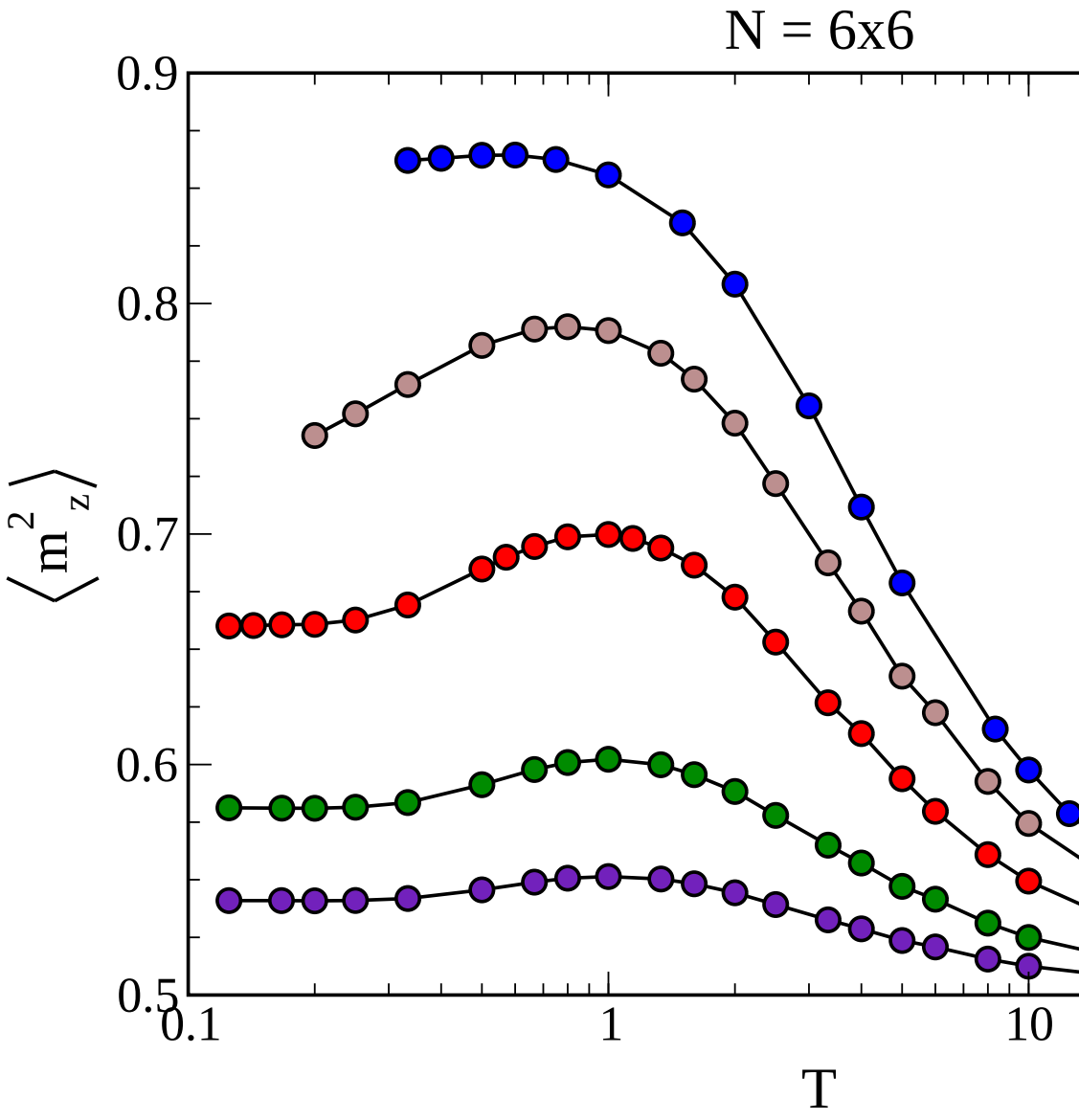
$$\Sigma($$

- Ignores fluctua
- No sig

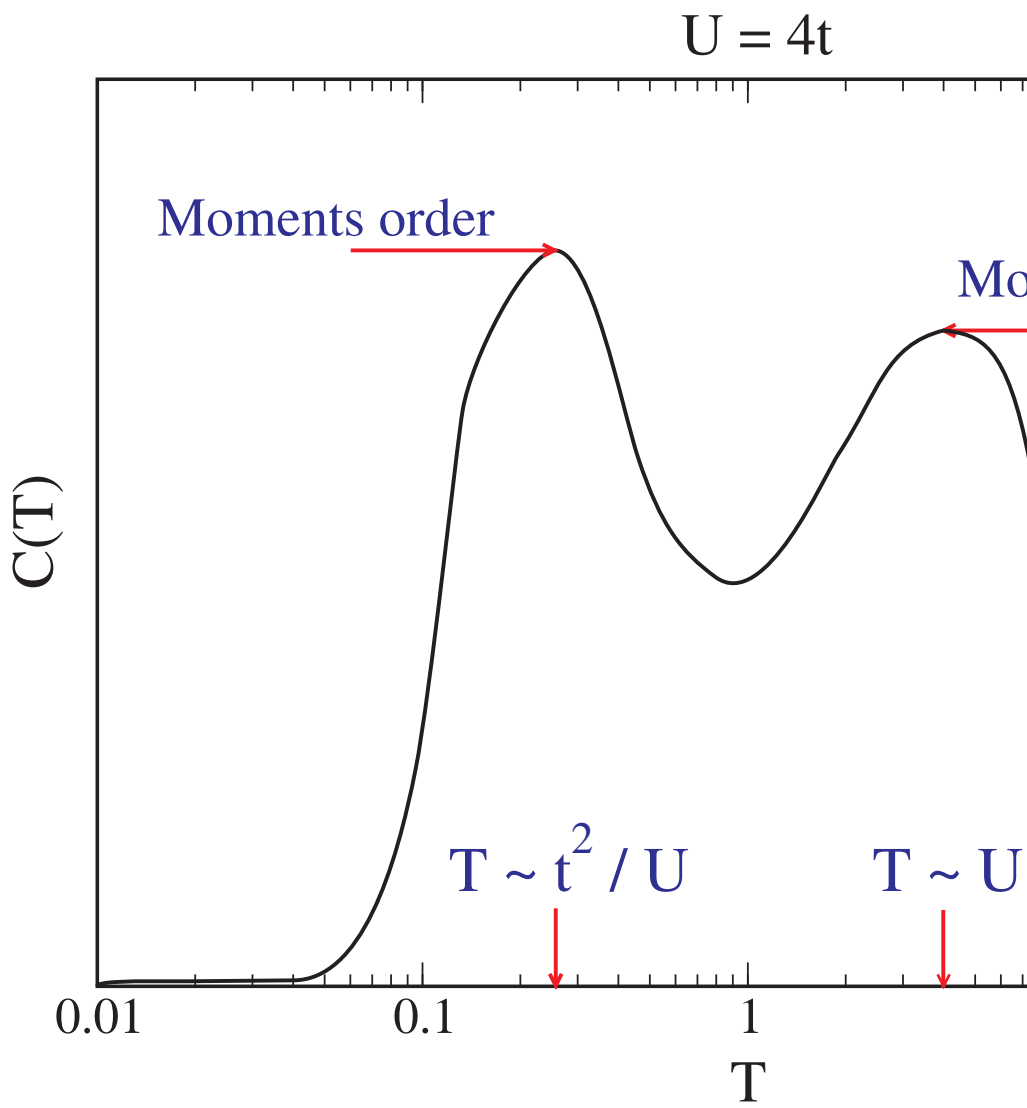
Energ



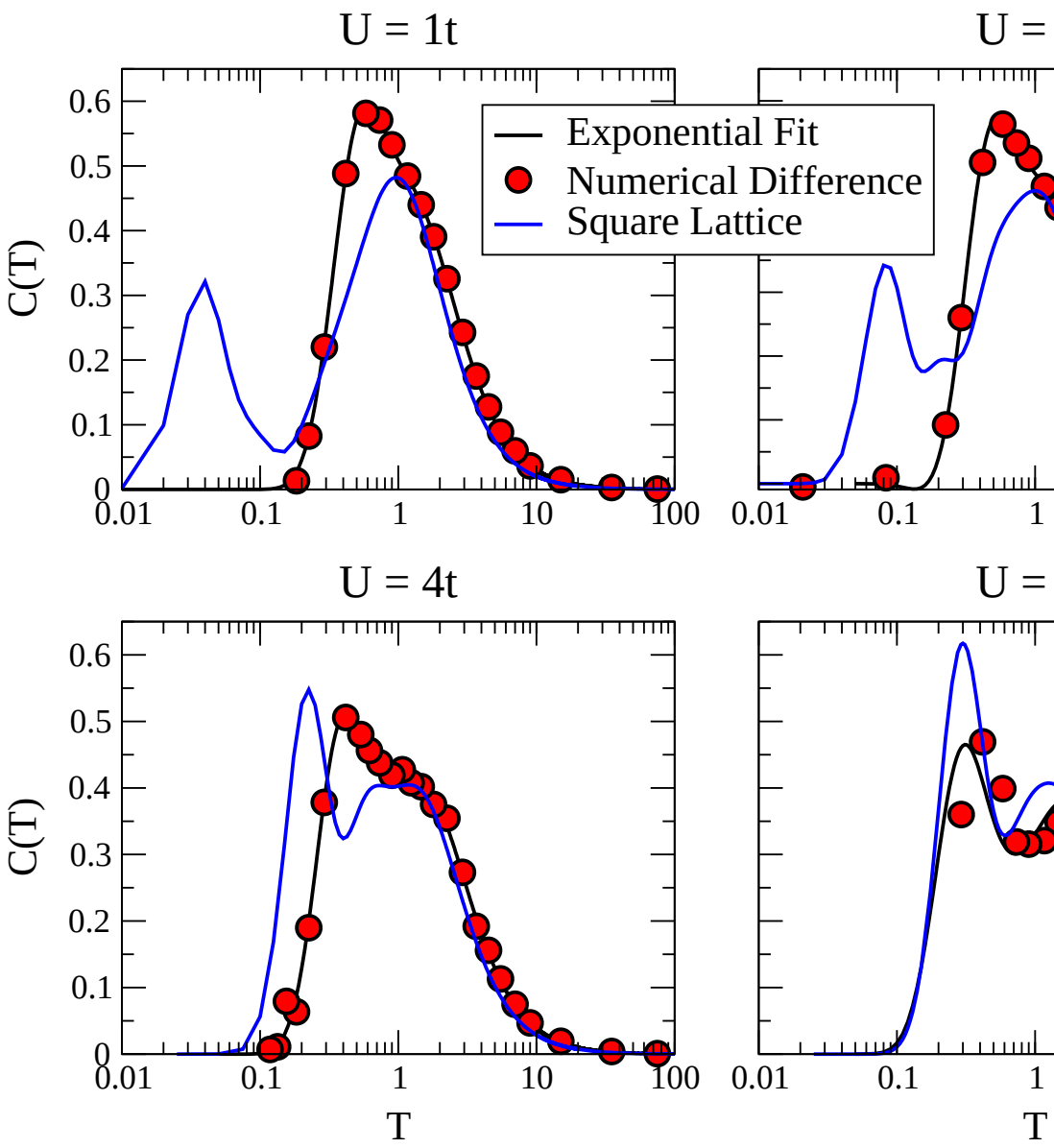
Local Momen

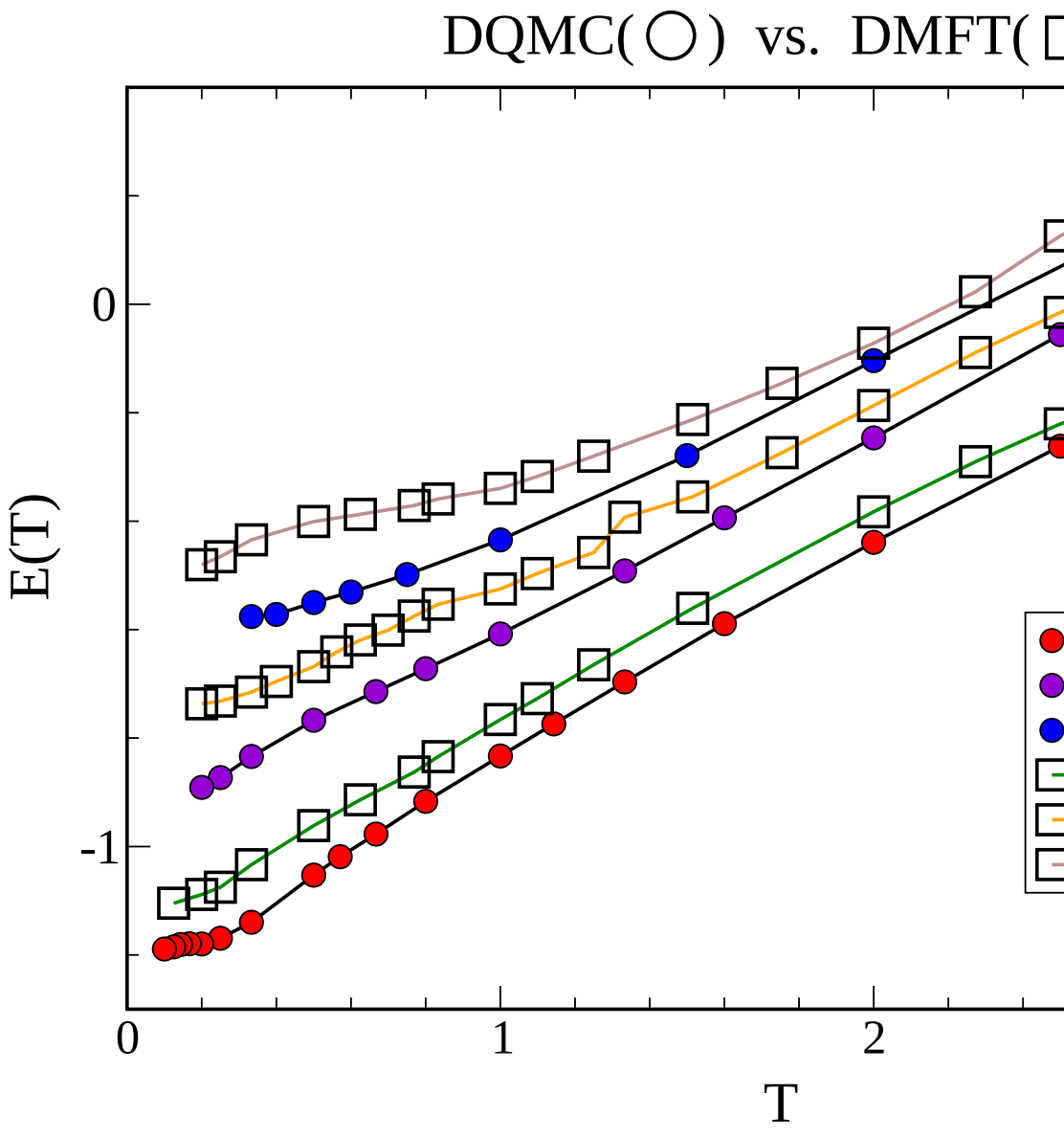


Specific Heat Comparison: □ vs △ la

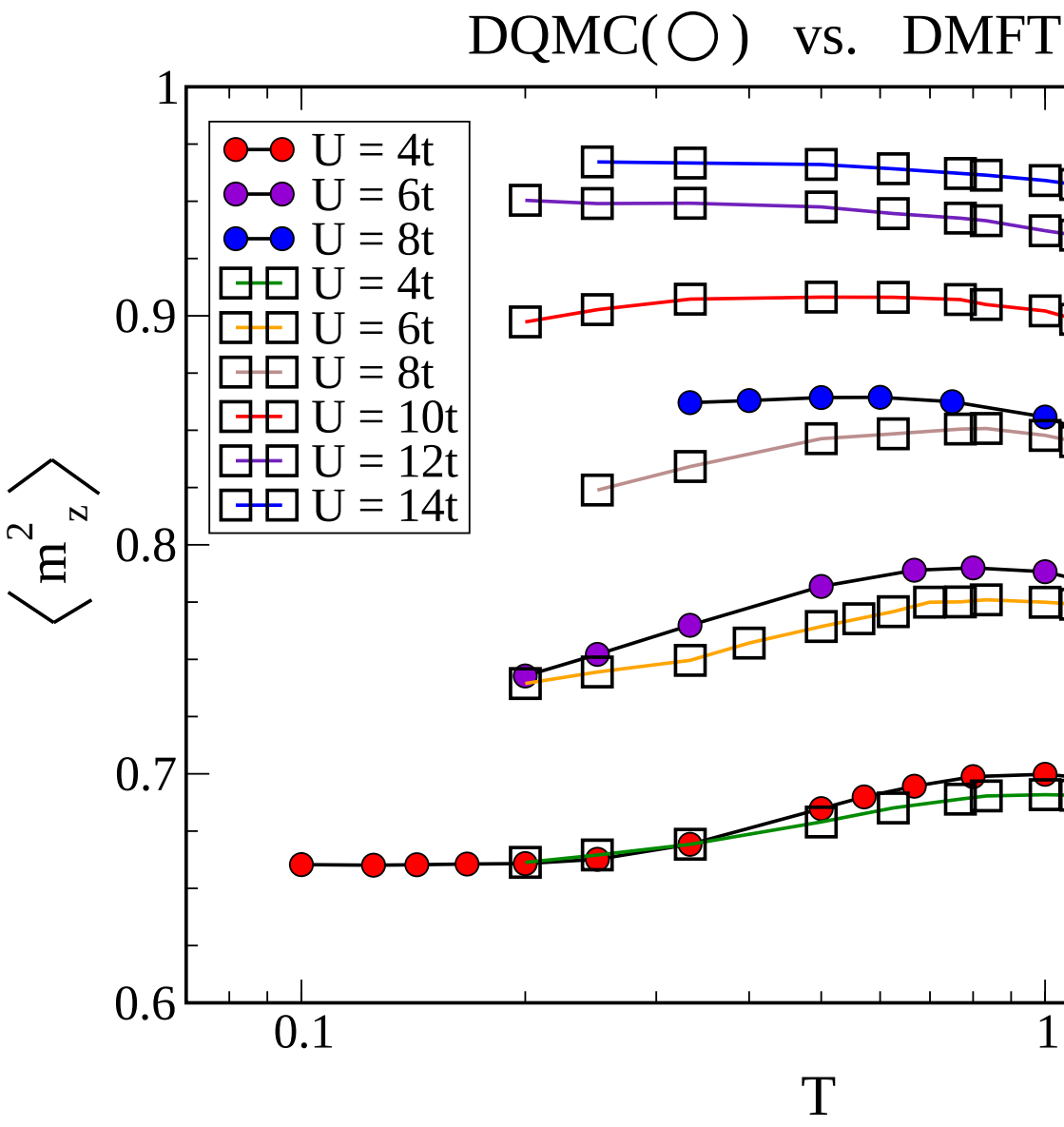


Specific Heat Comparison: □ vs △ la




DQMC(◯) vs. DMFT(□
E(T)
T
0
-1
0
1
2

Loc


DQMC(◯) vs. DMFT
U = 4t
U = 6t
U = 8t
U = 4t
U = 6t
U = 8t
U = 10t
U = 12t
U = 14t
1
0.9
0.8
0.7
0.6
0.1
1
T
⟨ m z 2 ⟩

C

- More robust moments with large U
- Vanishing moment peak in DMFT result
  - Mott transition
- Low-T specific heat behavior is less pron lattice
  - No low-T peak for small U

Fu

- Density of States calculation
  - Mott Transition
  - Spin liquid state
- DMFT → Dynamical Cluster Approxim
  - Larger systems
  - Wide range in T
  - Results away from half-filling

S.-S. Lee, P. A. Lee, cond-mat/0502139.