Analysis of the Dynamical Cluster Approximation for the Triangular Lattice Hubbard Model

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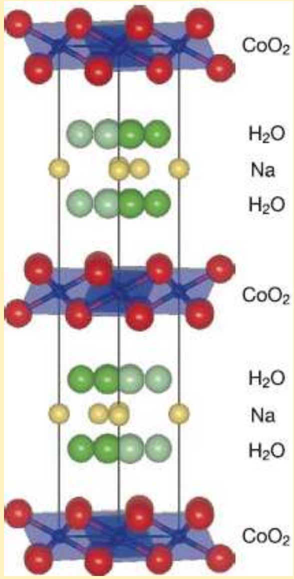
Overview

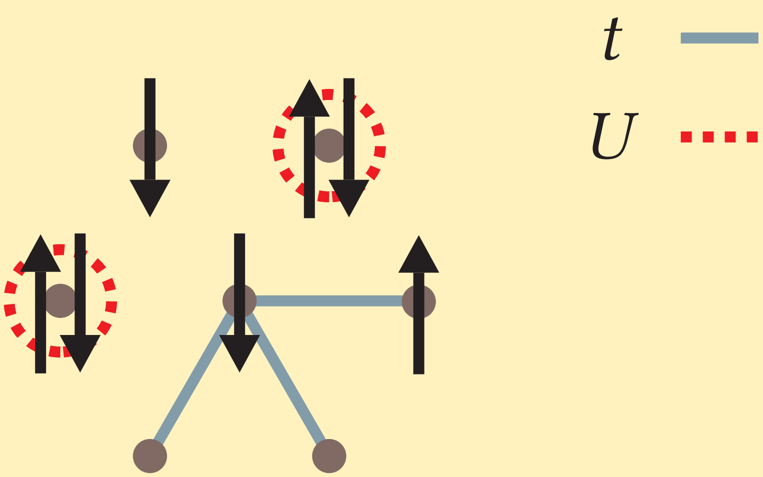
- Hubbard Model
- Dynamical Cluster Approximation
- Results
  - Energy
  - Specific Heat
  - Local Moment
- Future Work

Triangular Lattice Hubbard Model

$$H = -t \sum_{\langle \mathbf{i},\mathbf{j} \rangle} \sum_{\sigma} \left[c^{\dagger}_{\mathbf{i},\sigma} c_{\mathbf{j},\sigma} + \mathrm{H.c.} \right] + U \sum_{\mathbf{i}} n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow} - \mu \sum_{\mathbf{i}} n_{\mathbf{i}}$$

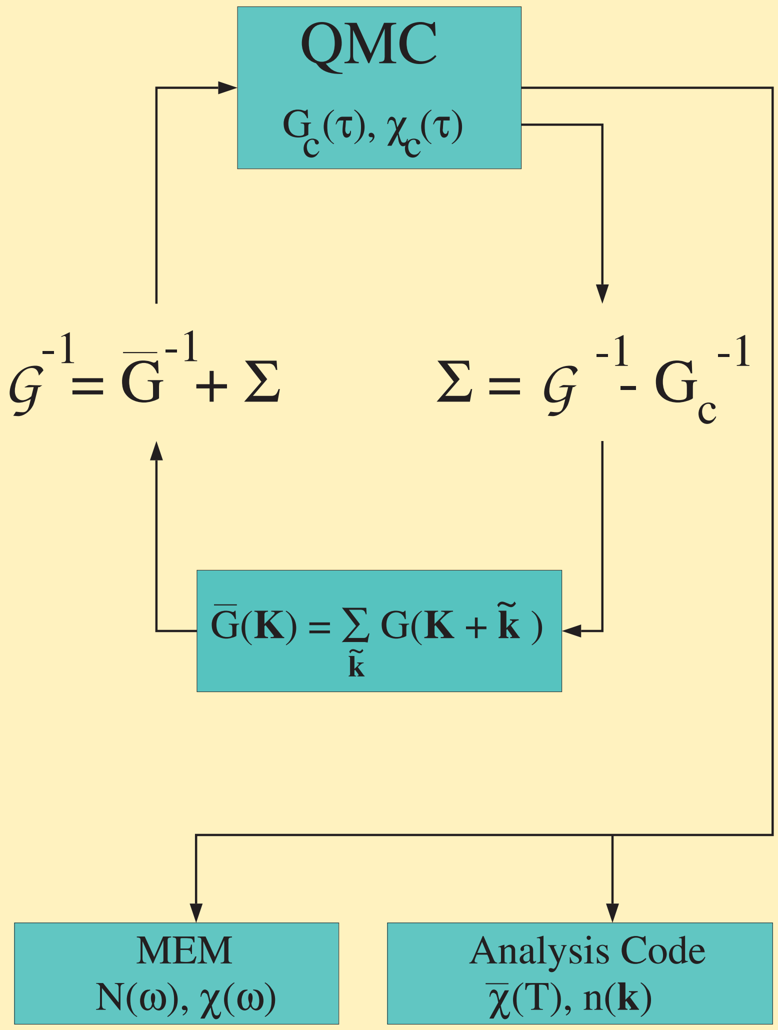
- Geometrically frustrated
- $Na_xCoO_2 \cdot yH_2O$
- κ-$(ET)_2X$



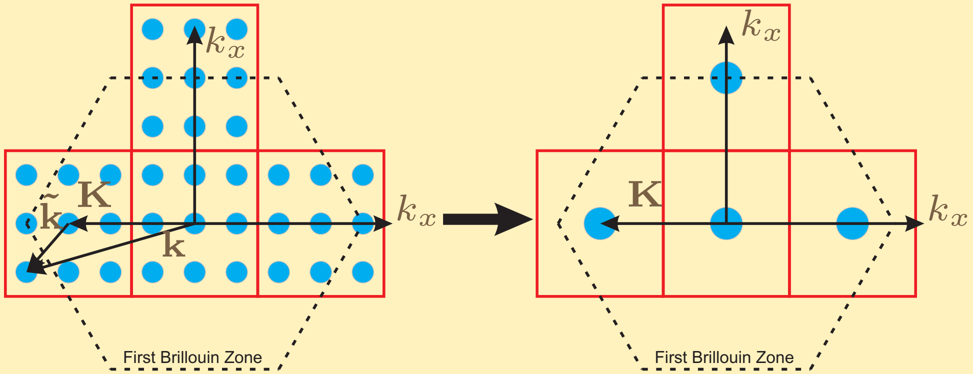


K. Takada *et al.* Nature **422**, 53 (2003).

DCA

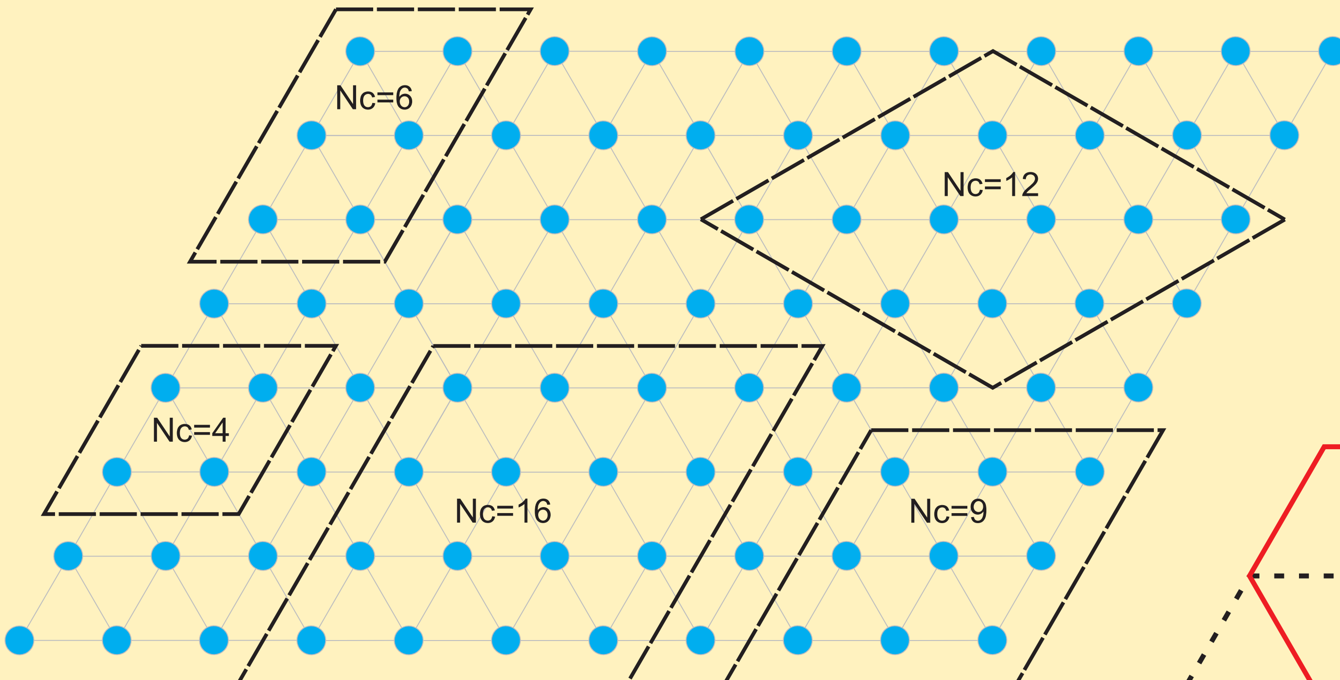


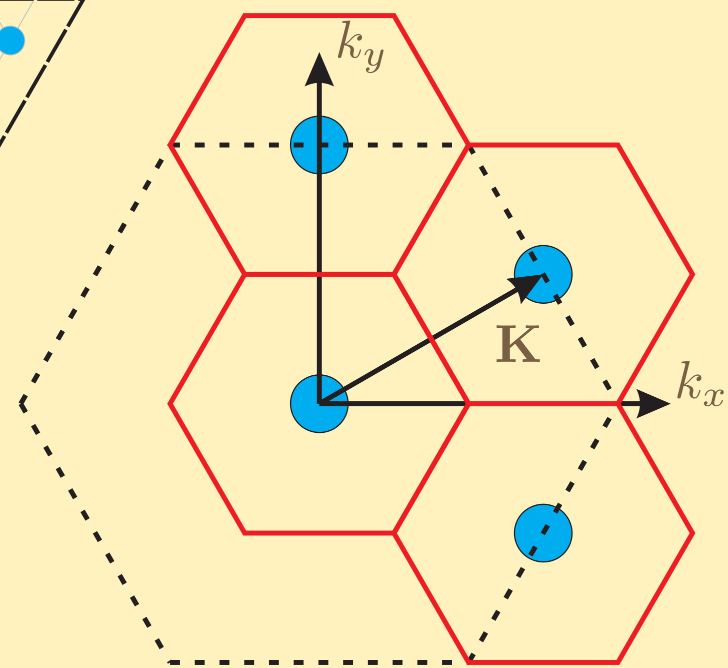
- Translationally invariant
- Exact for weak/strong-coupling, $N_c \to \infty$, $d = \infty$
- Observables are measured experimentally



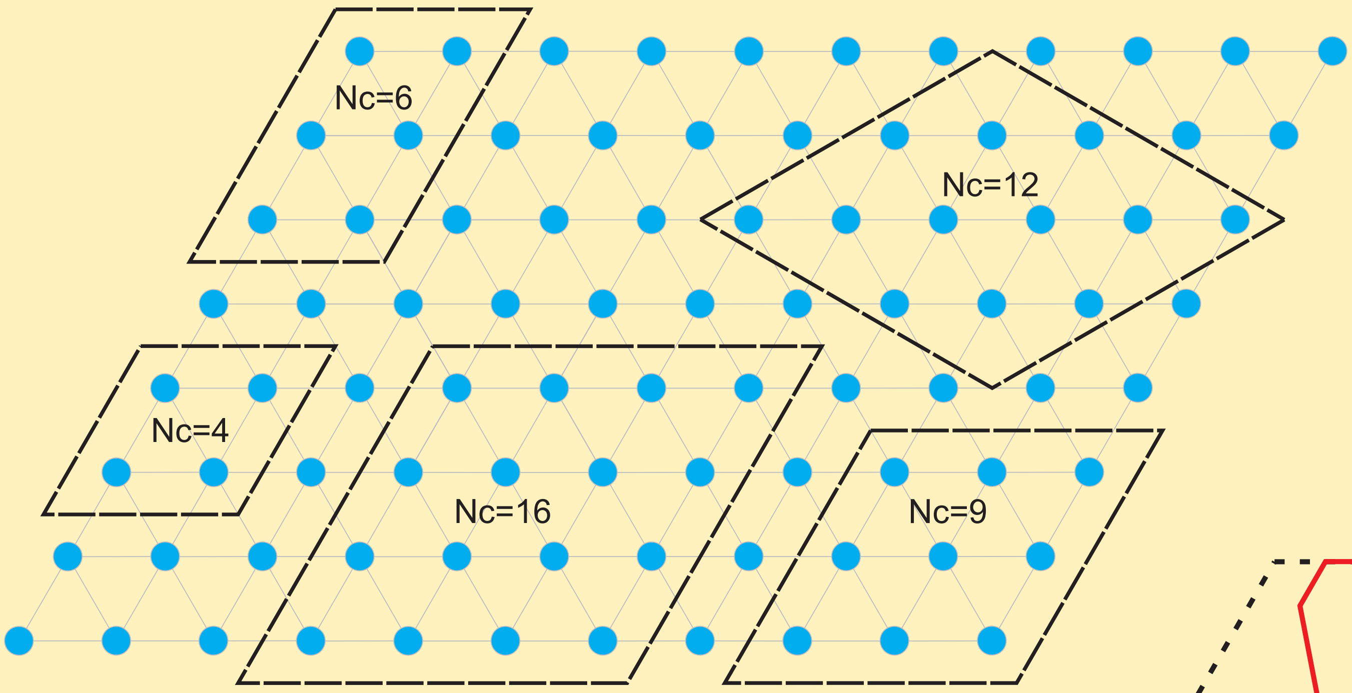
Th. Maier *et al.* Rev. Mod. Phys. **77**, 1027 (2005).

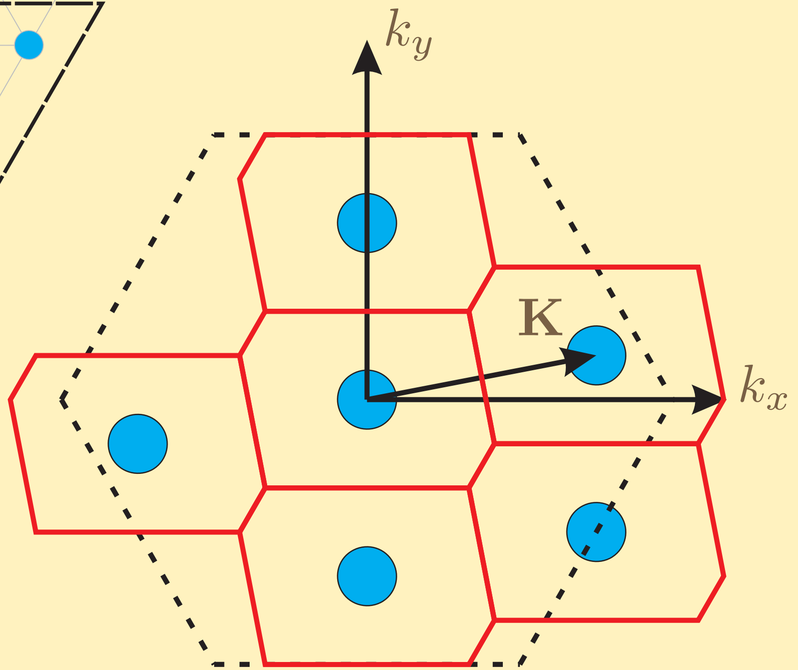
Clusters



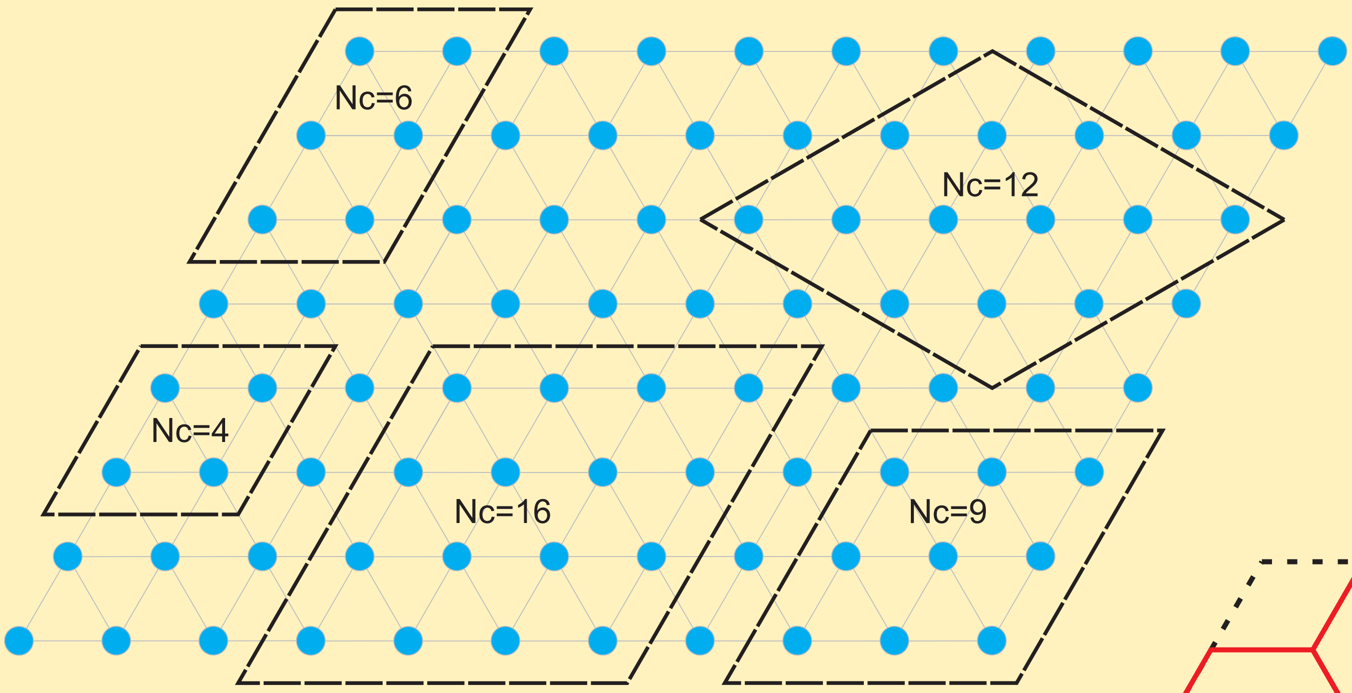


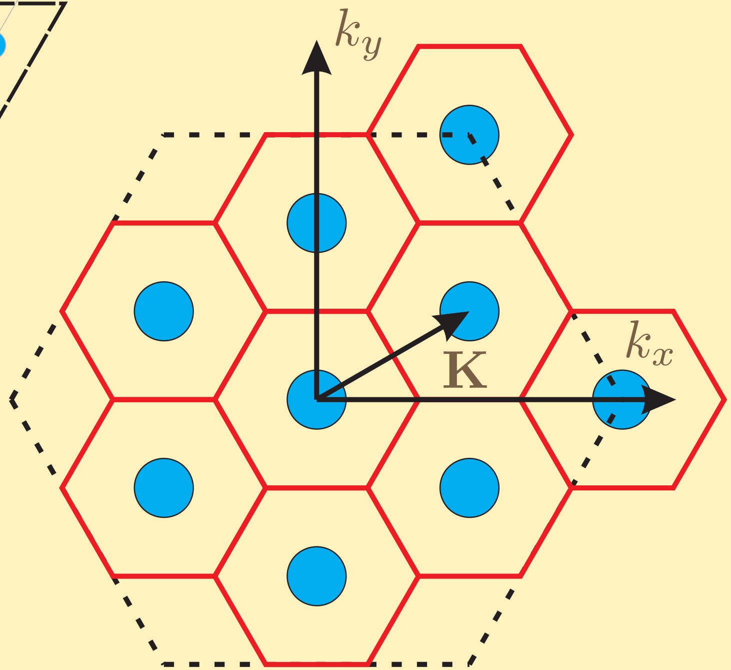
Clusters



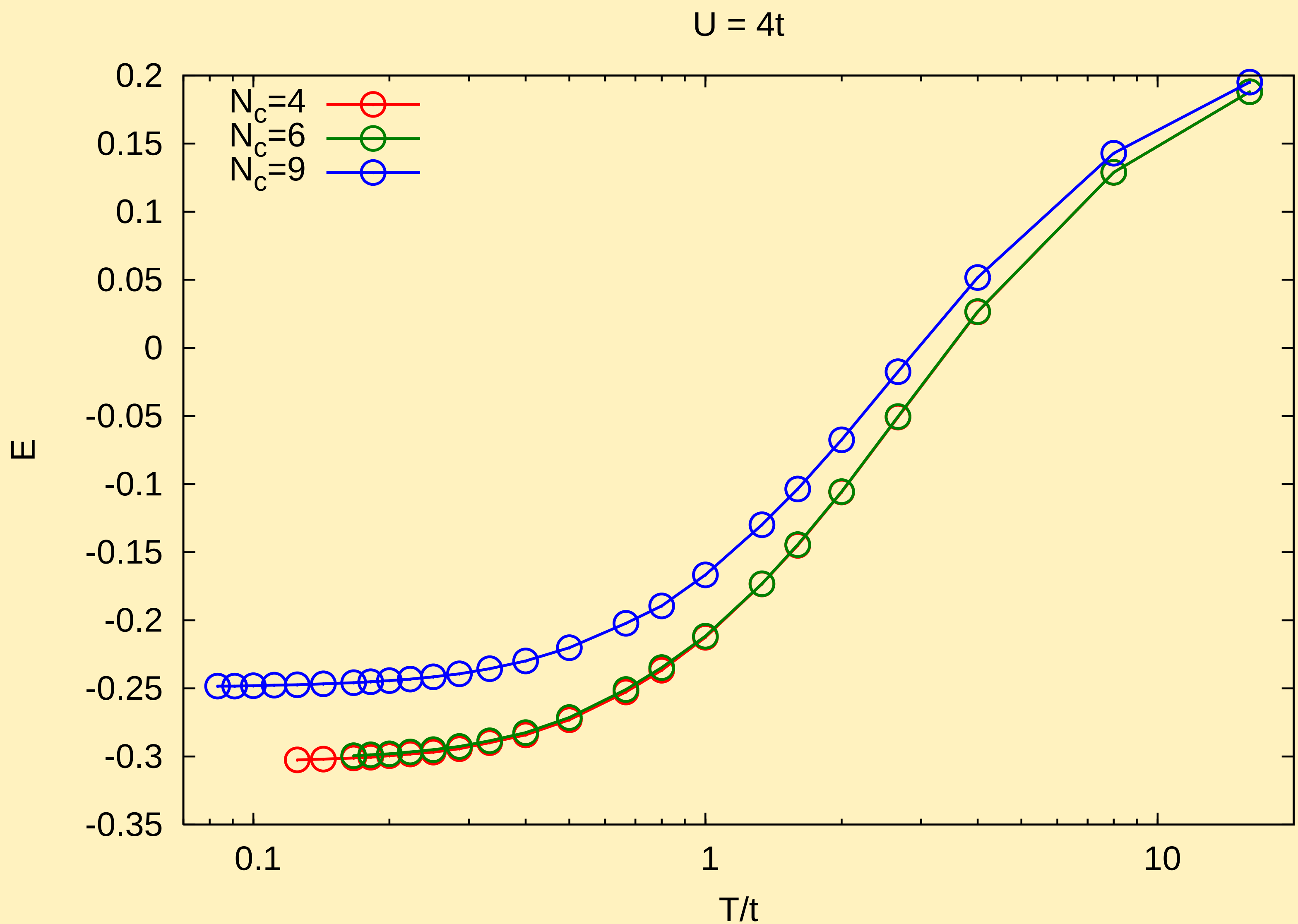


Clusters

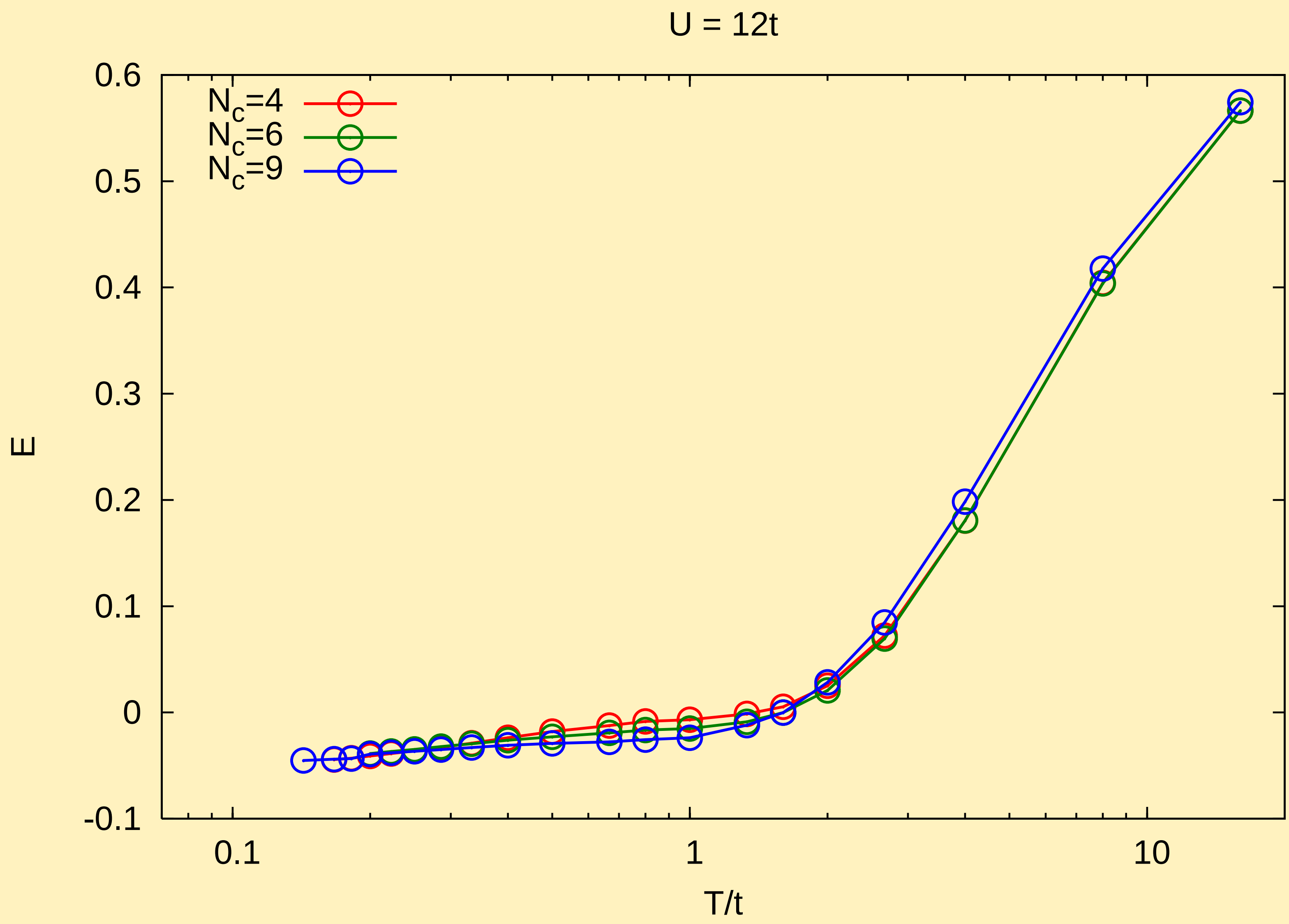




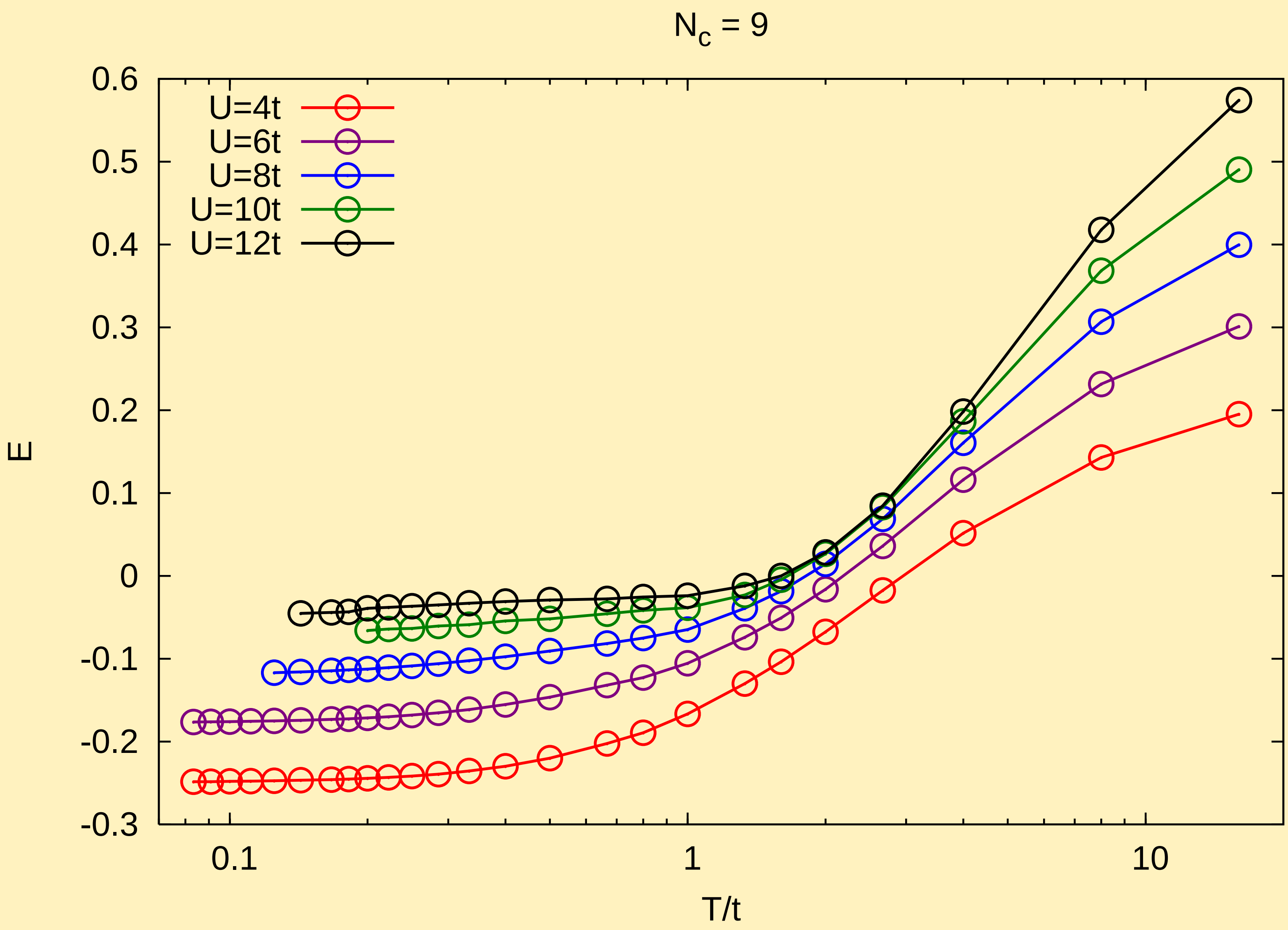
Energy



Energy



Energy



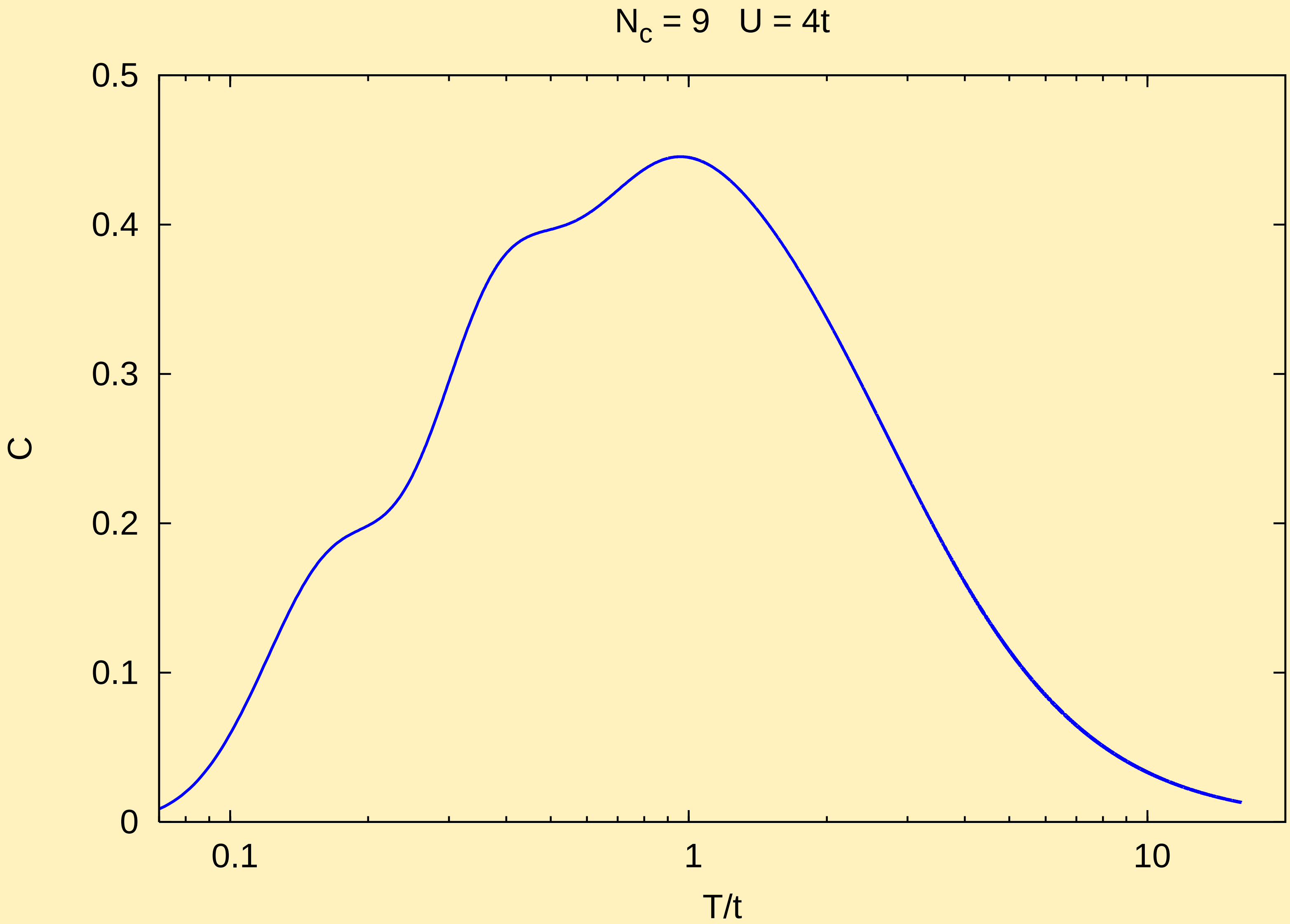
Fit

$$E(T) = E_0 + \sum_{n=1}^{M} c_n \exp\left(-n\Delta/T\right)$$

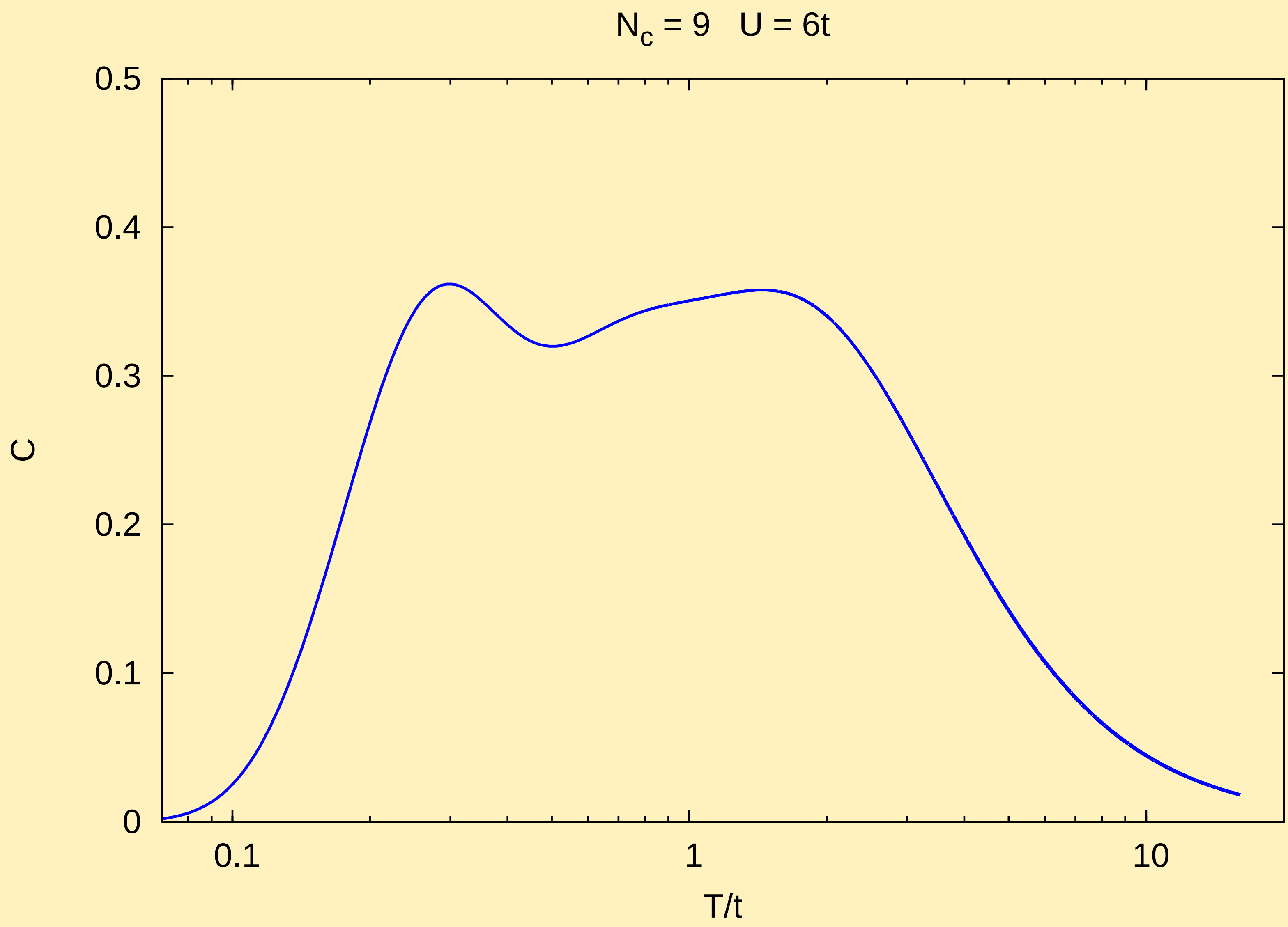
$$C(T) = \frac{\Delta}{T^2} \sum_{n=1}^{M} n c_n \exp\left(-n\Delta/T\right)$$

- c_n, Δ are fitting parameters

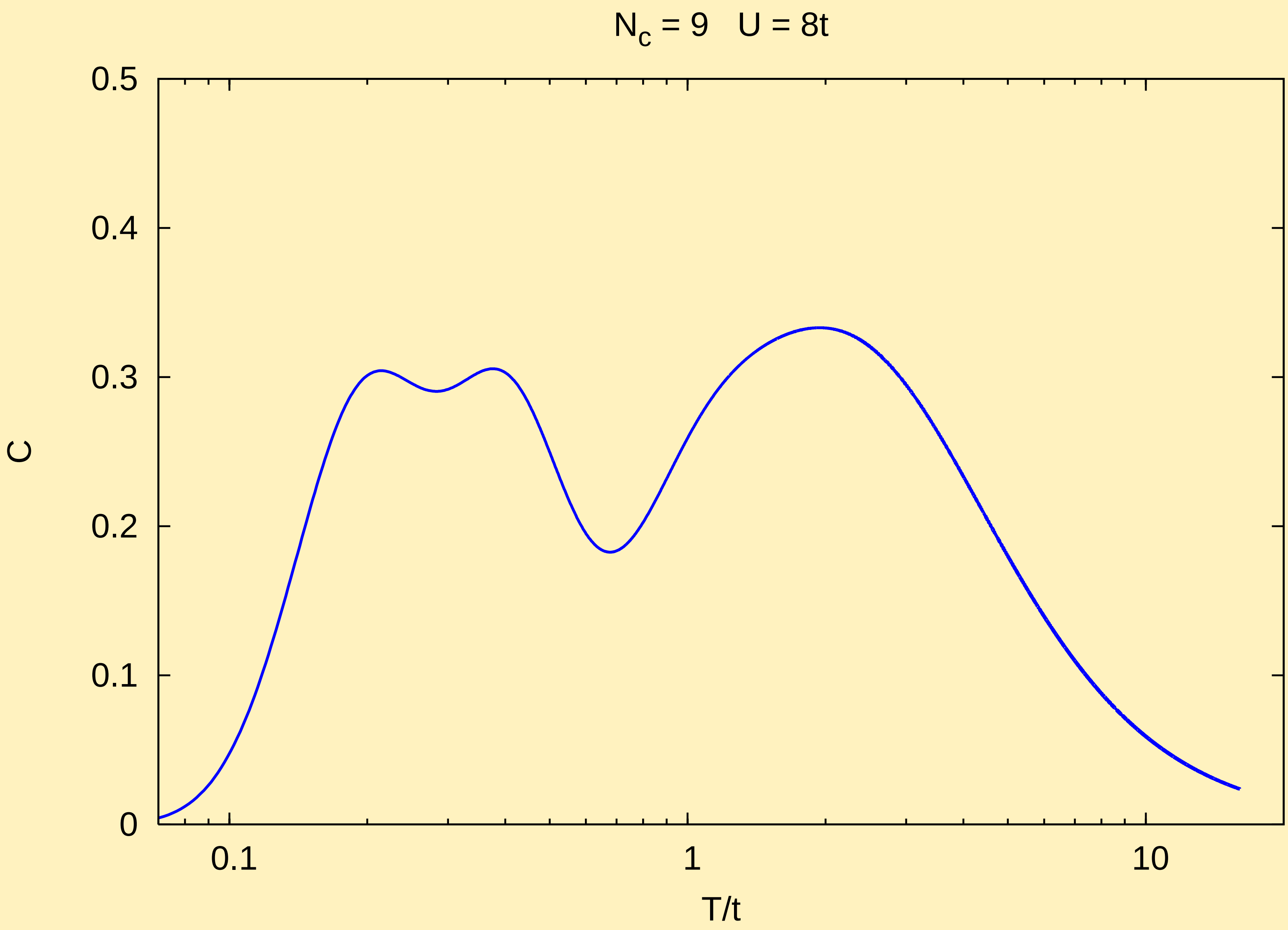
Specific Heat



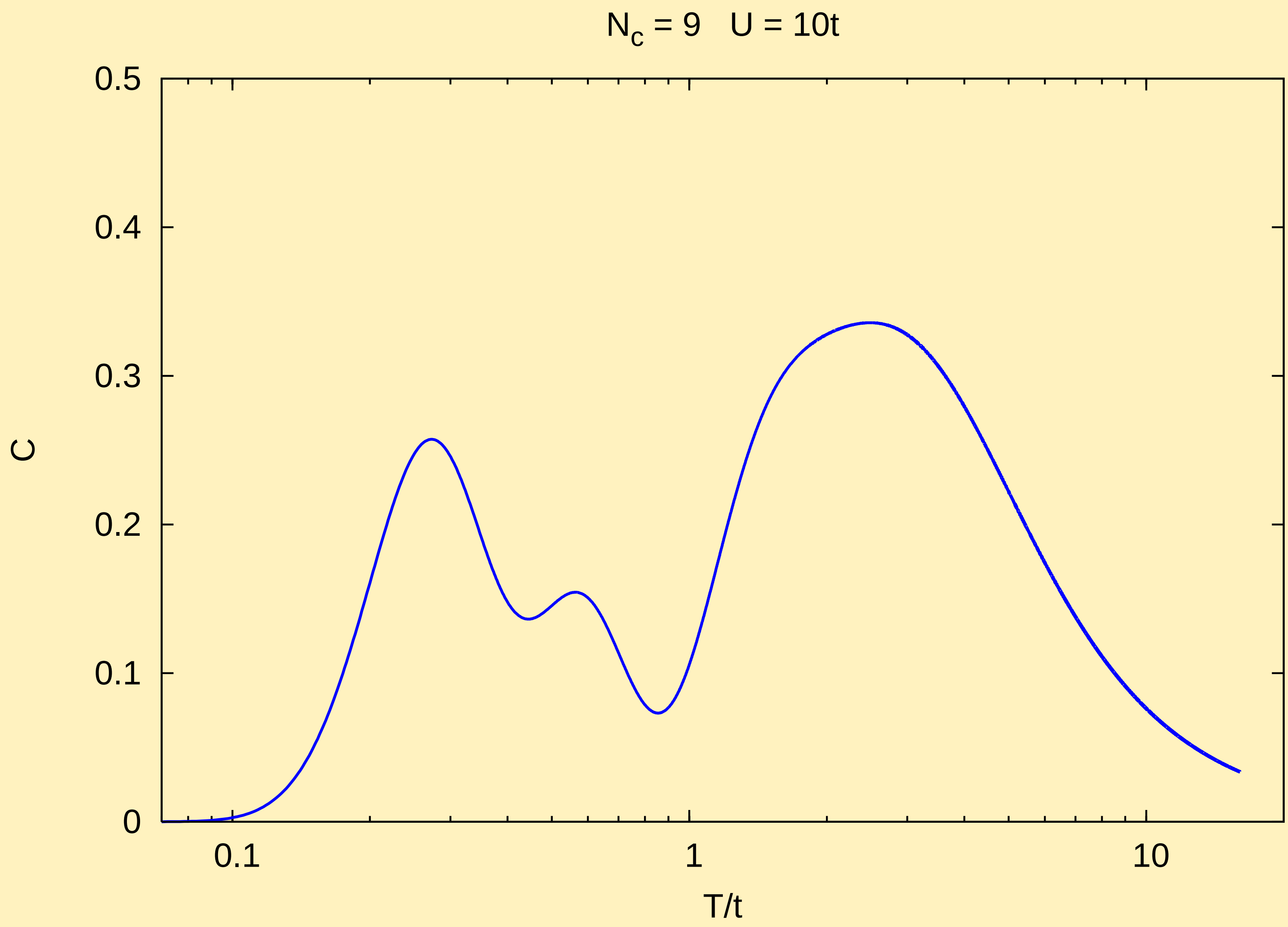
Specific Heat



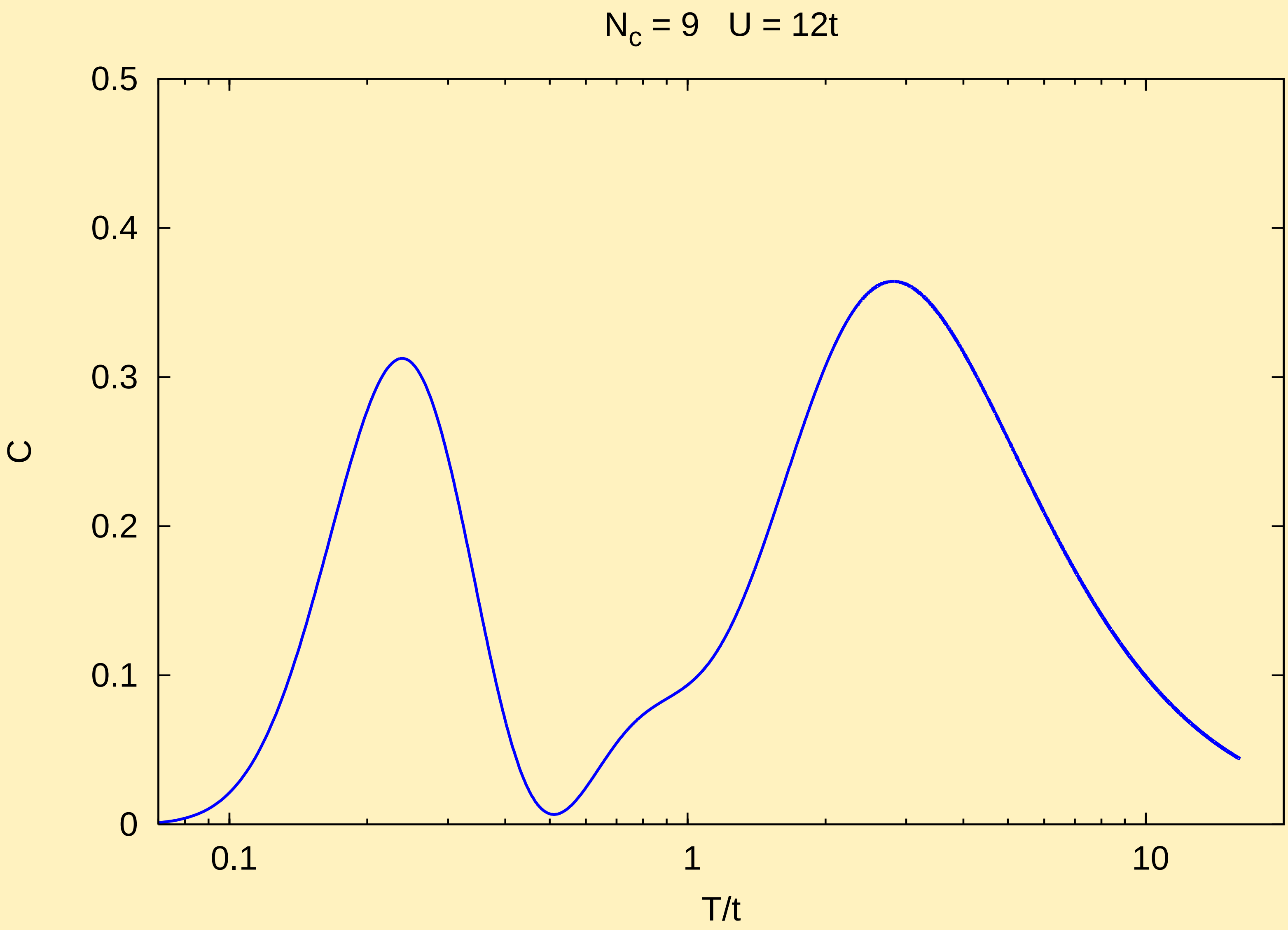
Specific Heat

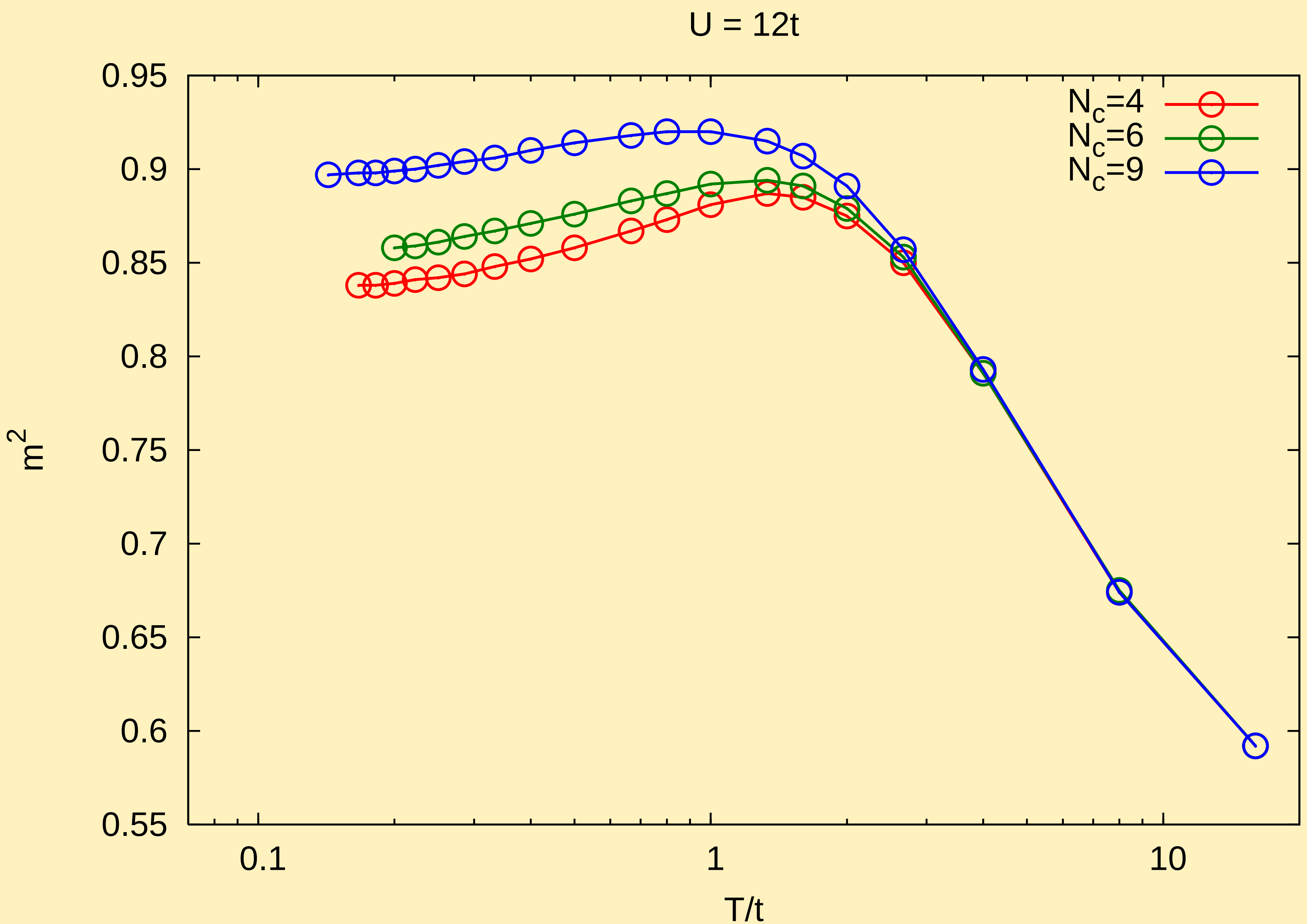


Specific Heat

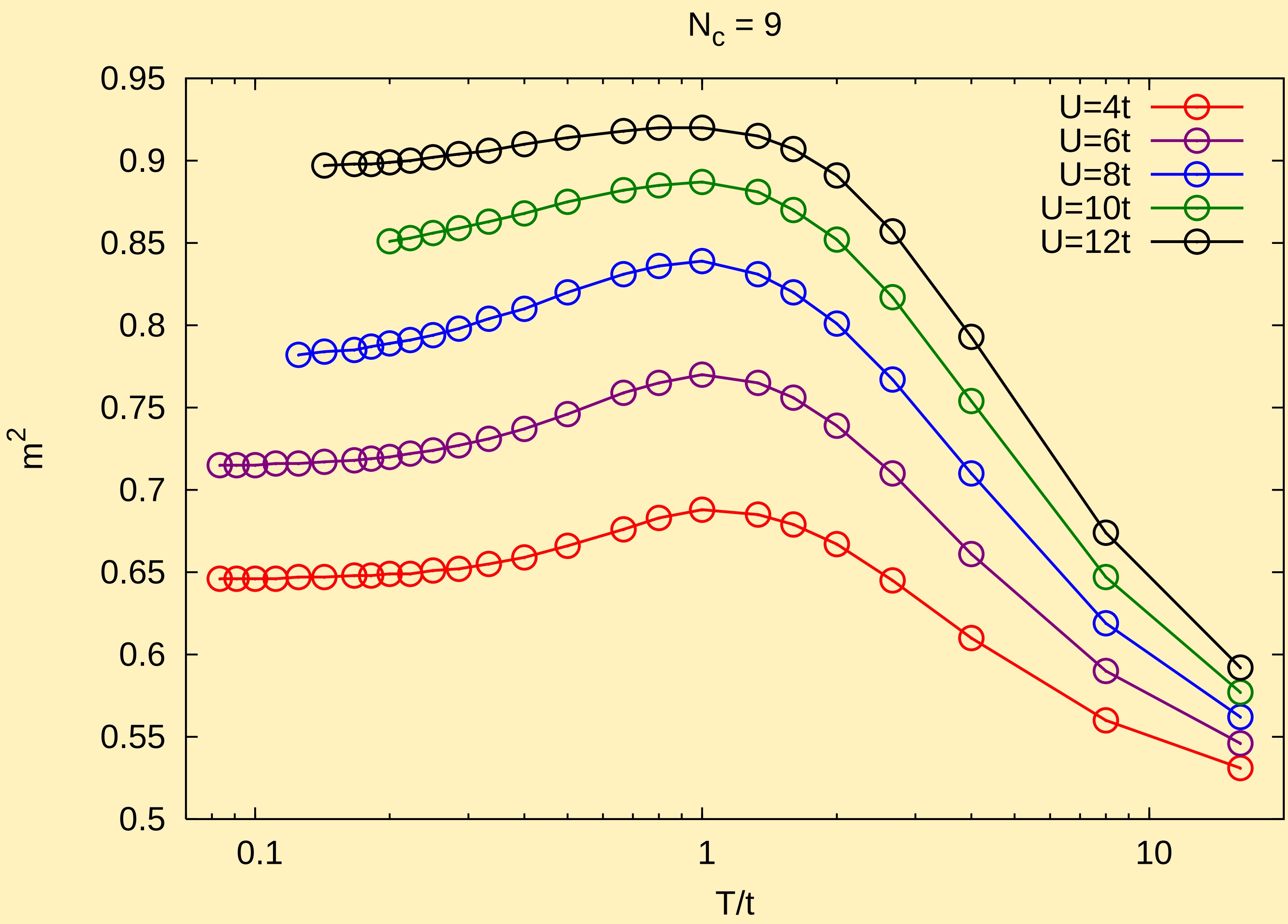


Specific Heat




U = 12t
0.95
0.9
0.85
0.8
0.75
0.7
0.65
0.6
0.55
m^2
0.1
1
10
T/t
N_c=4
N_c=6
N_c=9

Local Moment $\langle m_z^2 \rangle = \langle (n_\uparrow - n_\downarrow)^2 \rangle$



Summary

- DCA to study half-filled Hubbard model on a triangular lattice
- Large U specific heat: two peaks
- Local moment grows with cluster size.

Future Work:

- Analytic continuation

$$G(\mathbf{K},\tau) = \int \mathrm{d}\omega \frac{\mathrm{e}^{-\omega\tau}}{1+\mathrm{e}^{-\beta\omega}} A(\mathbf{K},\omega)$$

- $N_c = 12, 16$
- $\rho = 1/3, 2/3$