Numerical linked-cluster expansion approach for strongly-correlated electronic systems

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Mardi Gras Conference

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Baton Rouge, LA

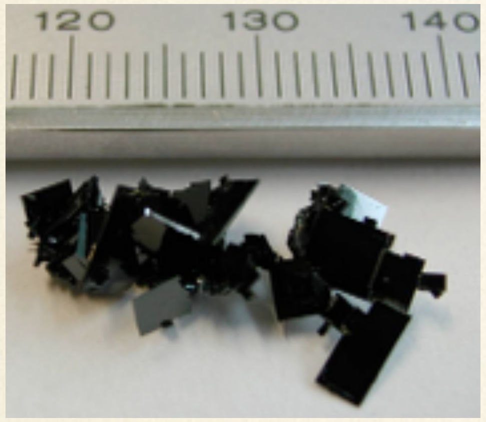
Outline

- Introduction
  - Strongly-correlated electronic systems
  - Common methods for quantum lattice models

- The Numerical Linked-Cluster Expansion

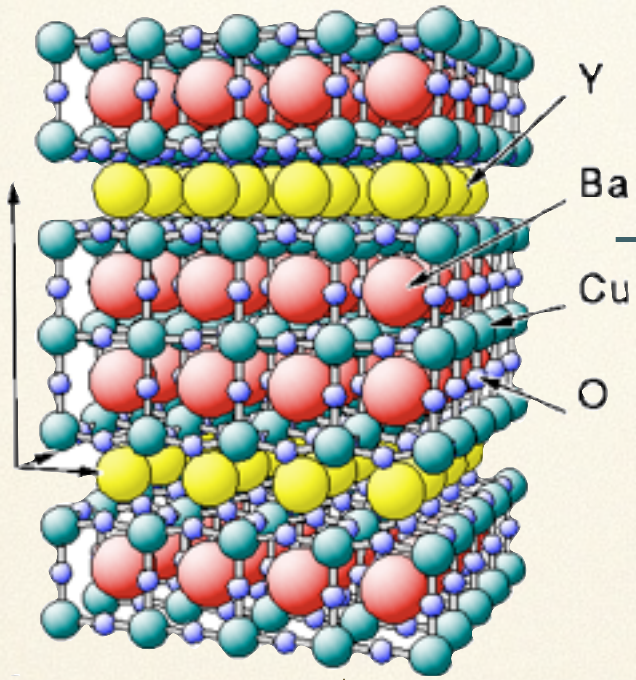
- Results for the Fermi-Hubbard model
  - Thermodynamic properties
  - Superconducting correlations

Quantum lattice models

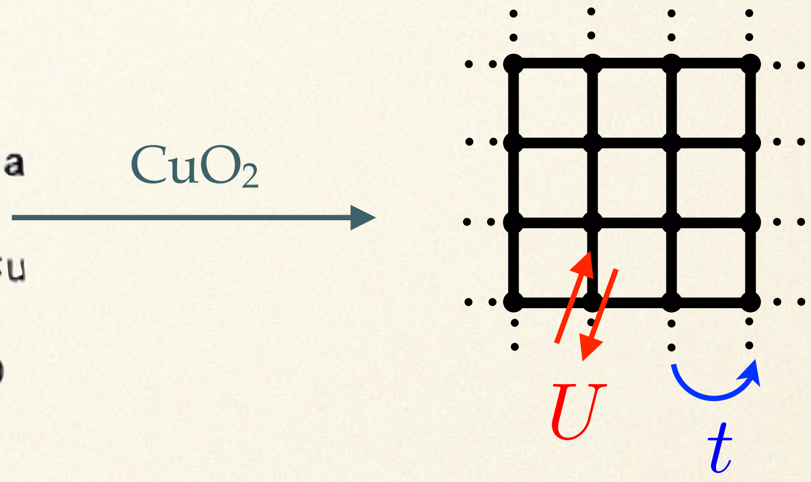


UBC Physics

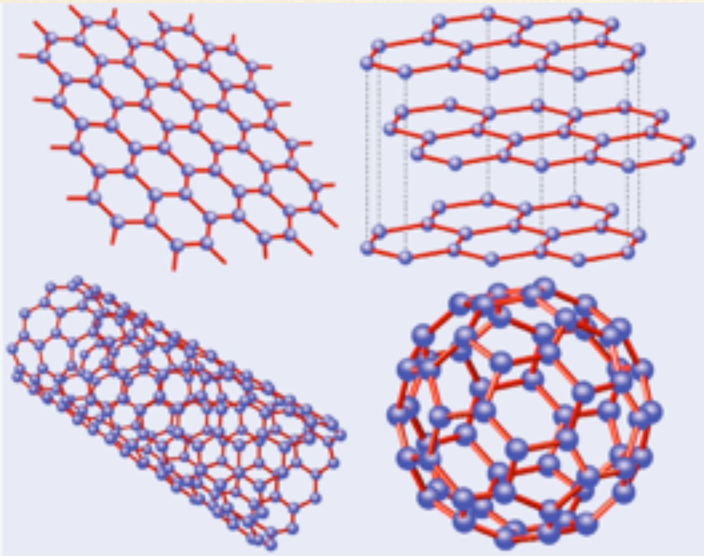
YBCO



K. Hermann / Fritz Haber Institute

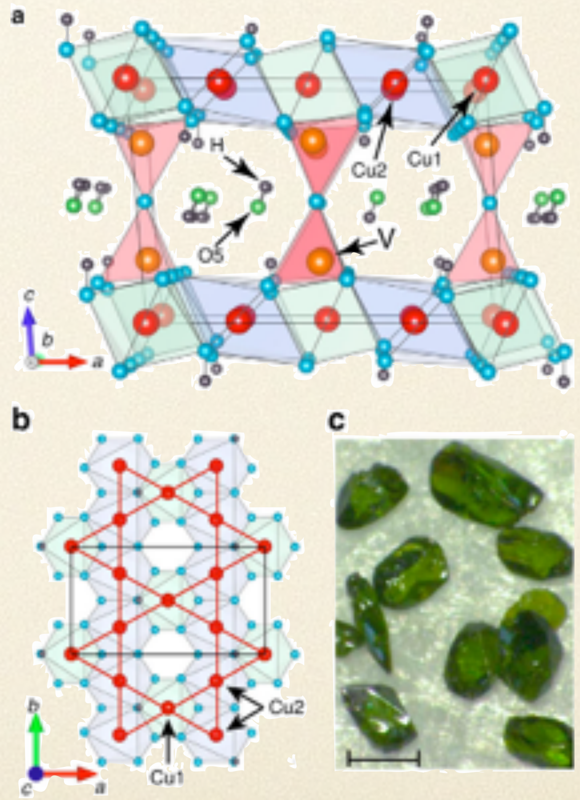


Graphene



Physics World 19, 33–37 (2006)

Volborthite, $Cu_3V_2O_7(OH)_2{\cdot}2H_2O$



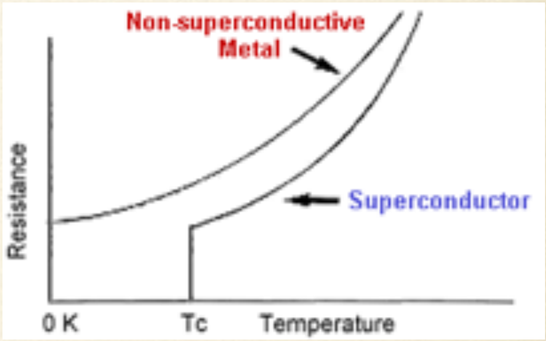
Yoshida et al., Nature Communications 3, 860 (2012)

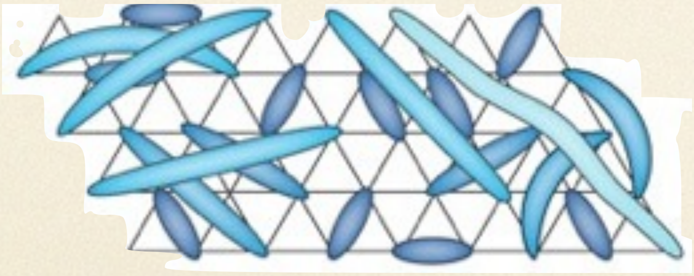
Strongly-correlated electronic systems

- When the Coulomb interaction between electrons plays an important role.

- Exotic phenomena:
  - Mott insulating
  - Superconductivity
  - Superfluidity
  - Spin liquid
  - :

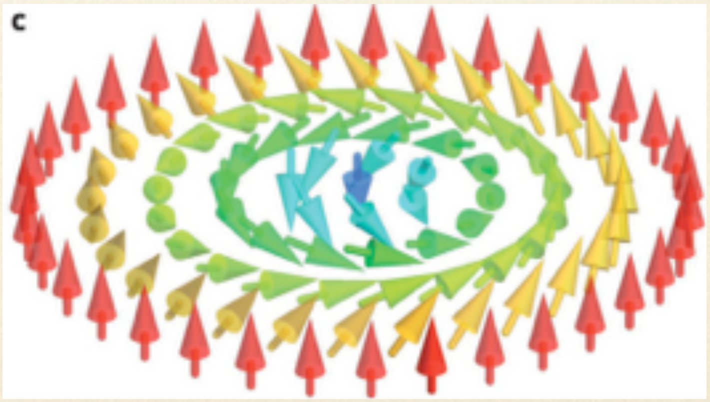
Superconductor





L. Balents, Nature **464**, 199 (2010)

Skyrmion



Nature Physics **7**, 673 (2011)

Superfluid

Computational methods

- Quantum Monte Carlo based simulations

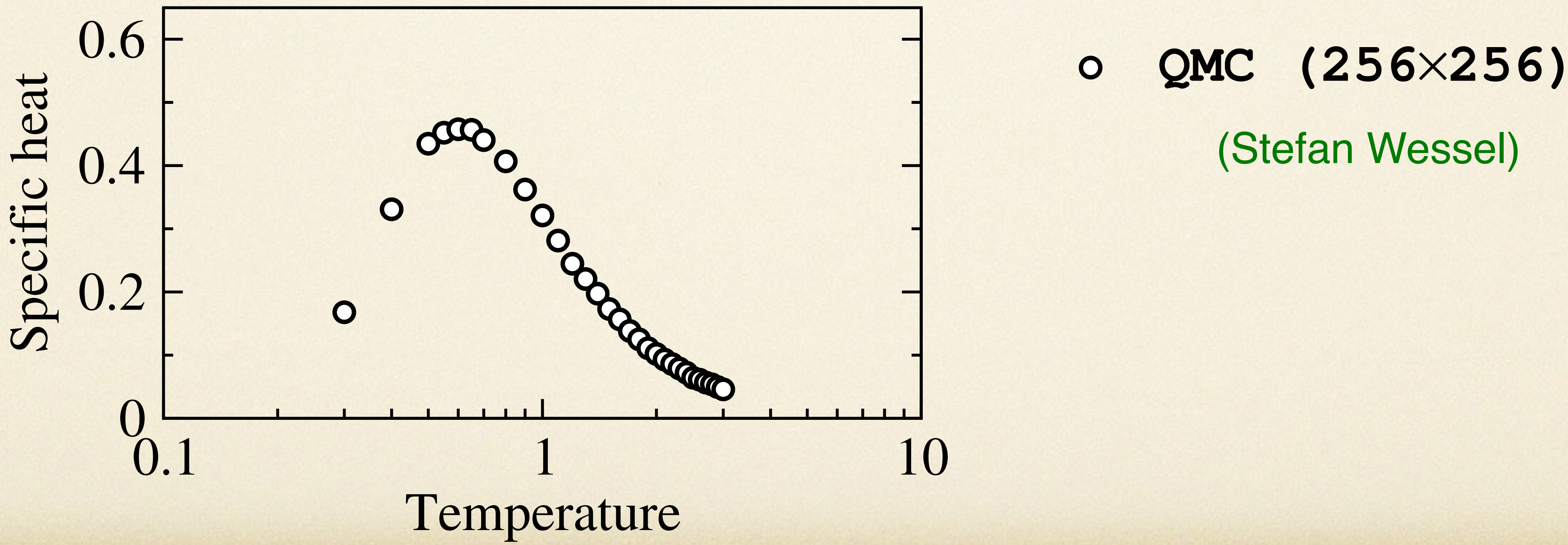
Large system sizes because of the polynomial scaling => Finite size scaling

Limited number of models

Sign problem (less severe with mean-field)

AF Heisenberg model on square lattice:

$$H = \sum_{<ij>} \mathbf{S}_i \cdot \mathbf{S}_j$$



Computational methods

- High-temperature expansions (HTE)

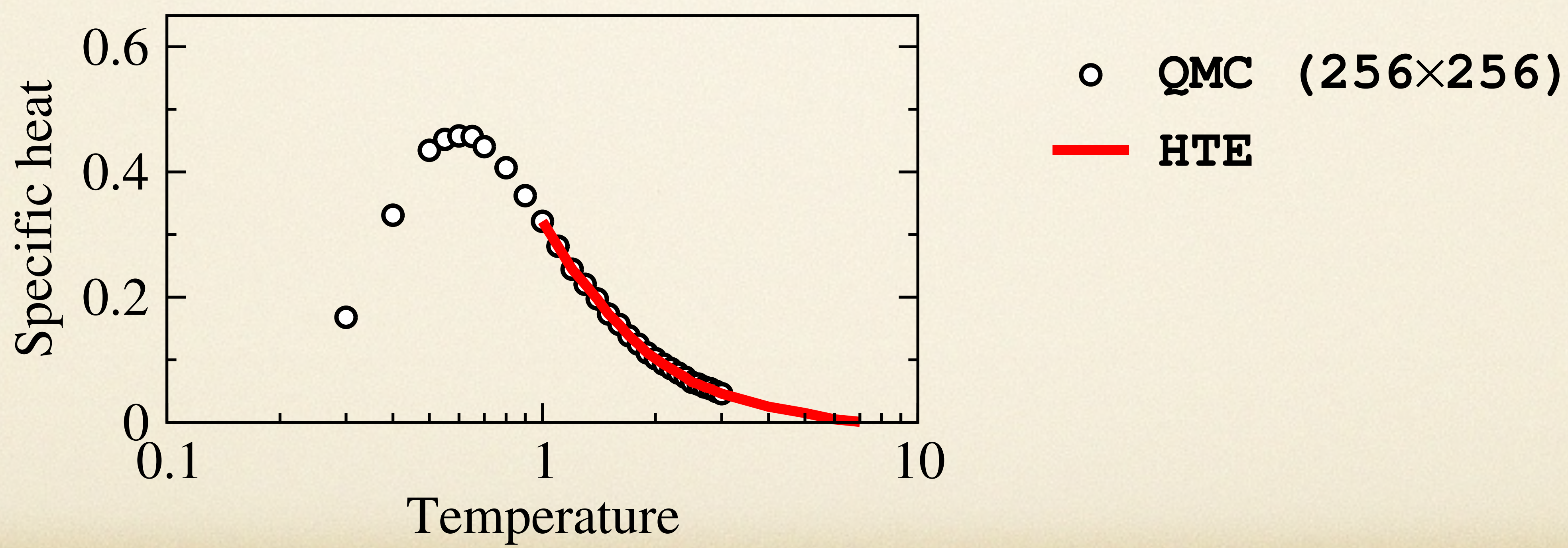
Can be used for any model
In the thermodynamic limit

Exponential problem => Can fail at low T even when correlations are short ranged

Pade approximations (even down to T=0)

AF Heisenberg model on square lattice:

$$H = \sum_{<ij>} \mathbf{S}_i \cdot \mathbf{S}_j$$

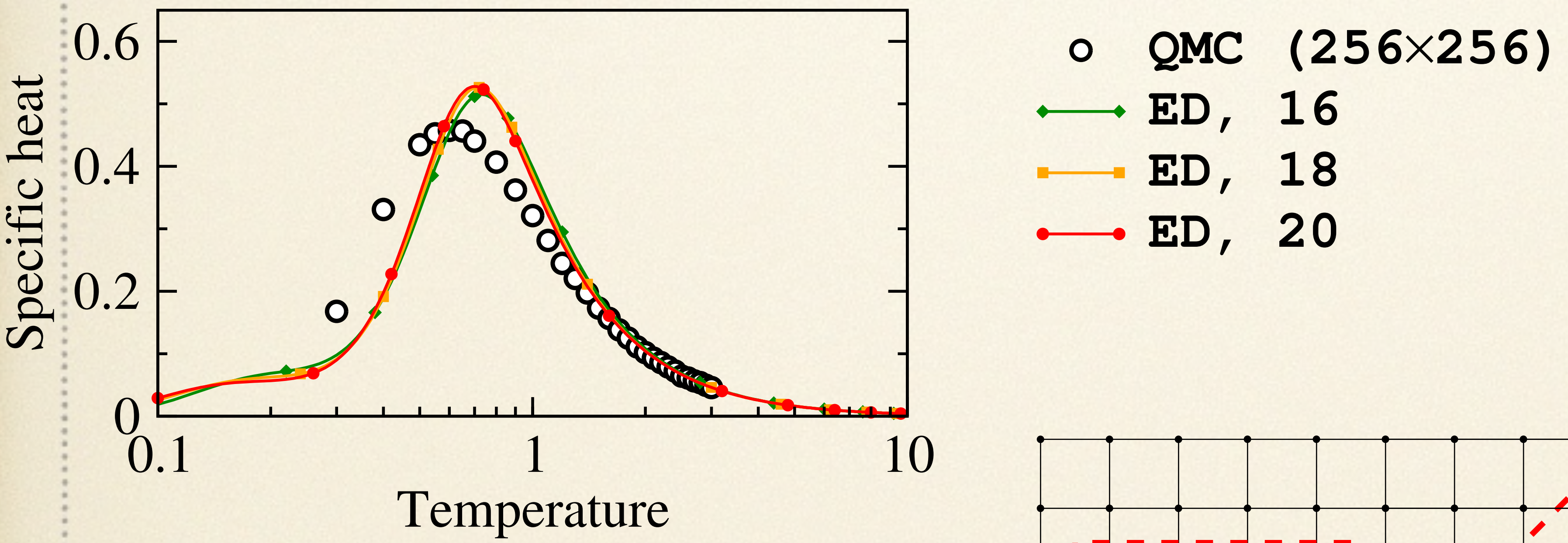


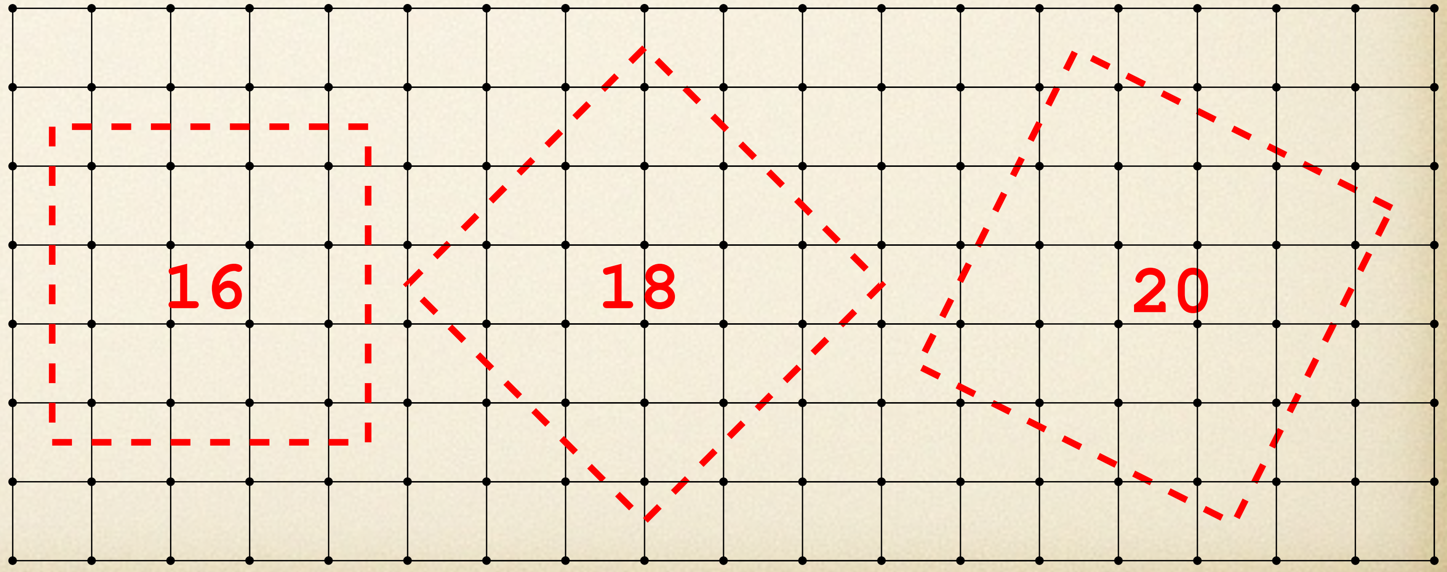
Computational methods

- Exact diagonalization

Can be used for any model

Exponential problem (small systems) => Finite size effects





Computational methods

- Density-matrix renormalization group
- Multi-scale entanglement renormalization ansatz
- Projected entangled pair states
- Methods for bosonic systems

  :
  :

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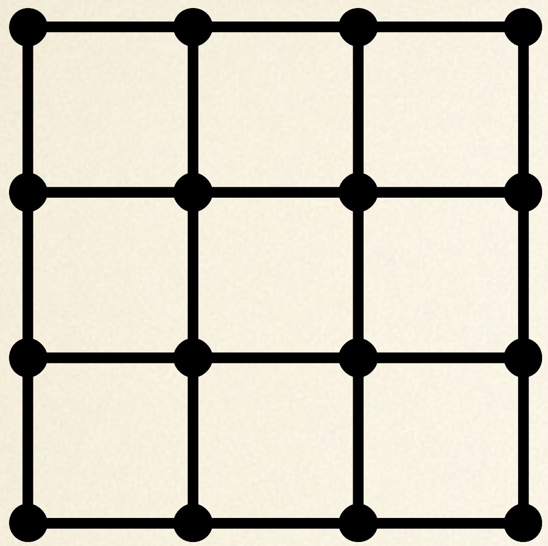
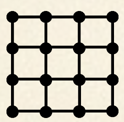
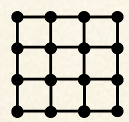
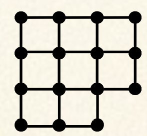
Cluster Expansions



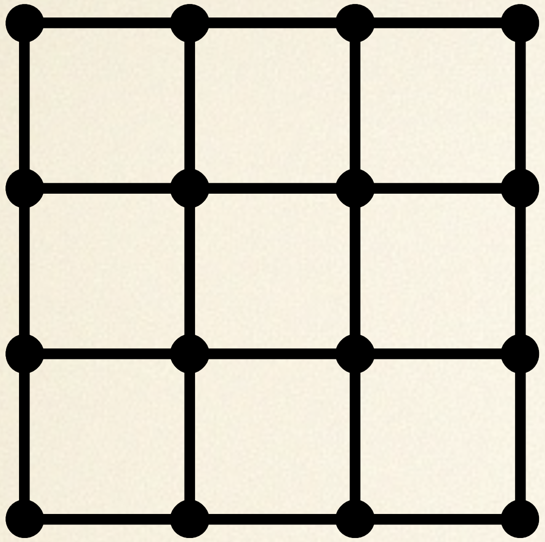
We express an extensive property of the model in terms of contributions from all clusters that can be embedded in the lattice:

$P($  $) = W_P($  $) + 4W_P($  $) + \ldots + 24W_P(\bullet\!\!-\!\!\bullet) + 16W_P(\bullet)$

Sykes et al.,
J. Math. Phys. **7**,
1557 (1966)

M. Rigol, T. Bryant, and R. R. P. Singh, PRL **97**, 187202 (2006); PRE **75**, 061118 (2007)

Cluster Expansions



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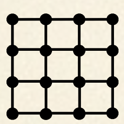
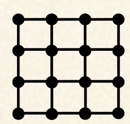
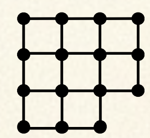
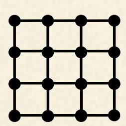
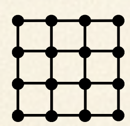
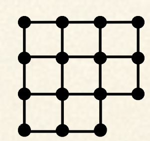
$P($  $) = W_P($  $) + 4W_P($  $) + \ldots + 24W_P(\bullet\!\!-\!\!\bullet) + 16W_P(\bullet)$

$W_P($  $) = P($  $) - 4W_P($  $) - \ldots - 24W_P(\bullet\!\!-\!\!\bullet) - 16W_P(\bullet)$

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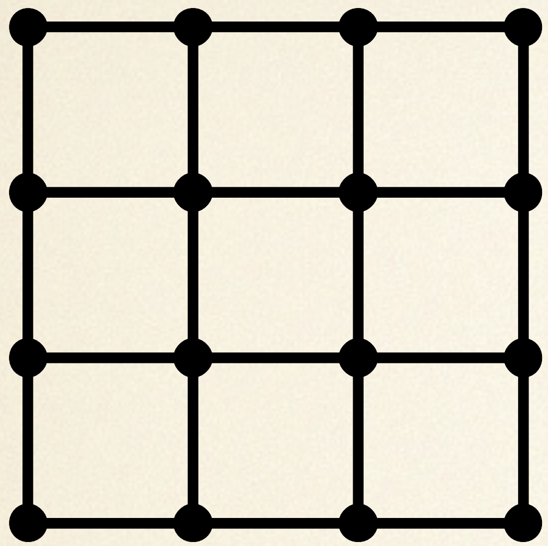

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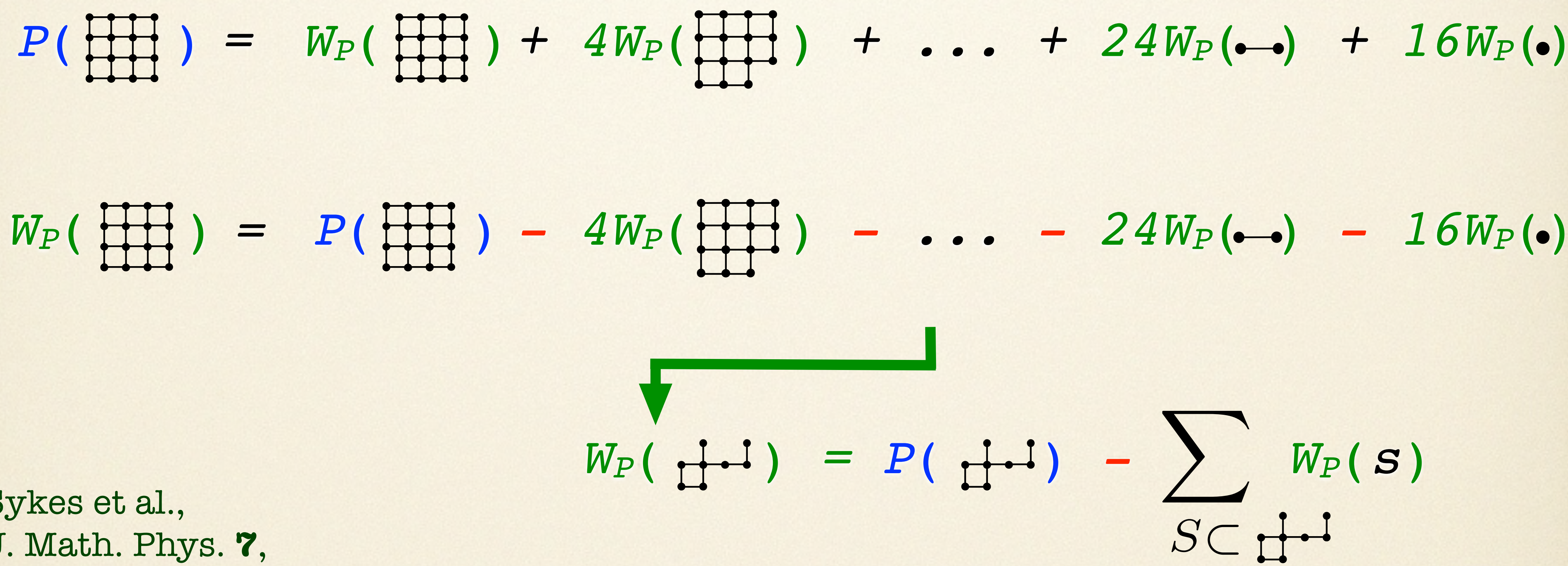

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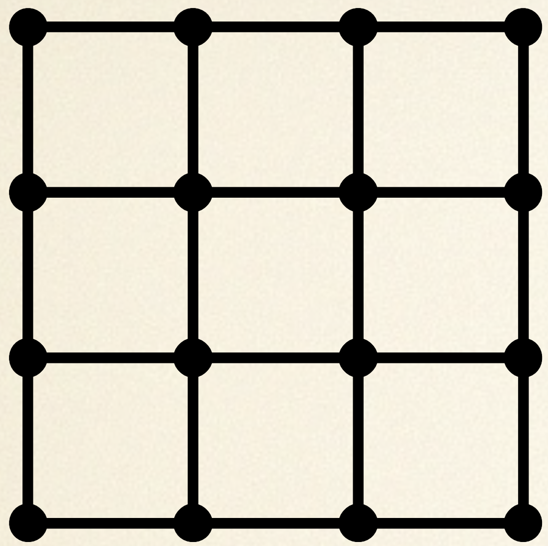

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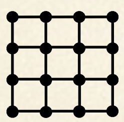
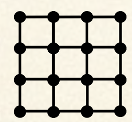
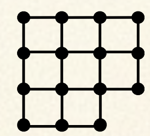
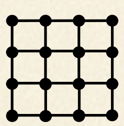
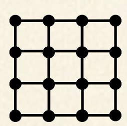
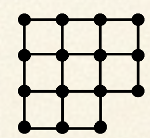
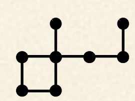
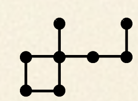
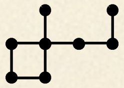
$P($  $) = W_P($  $) + 4W_P($  $) + \ldots + 24W_P(\bullet\!\!-\!\!\bullet) + 16W_P(\bullet)$

$W_P($  $) = P($  $) - 4W_P($  $) - \ldots - 24W_P(\bullet\!\!-\!\!\bullet) - 16W_P(\bullet)$

$W_P($  $) = P($  $) - \sum_{S \subset}$  $W_P(s)$

$\vdots$

$W_P(\bullet) = P(\bullet)$

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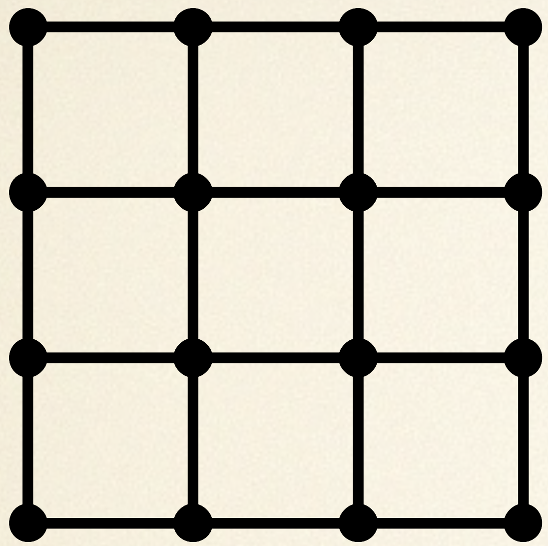
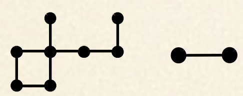
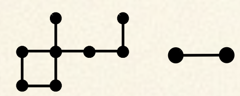
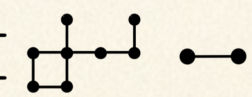
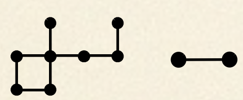
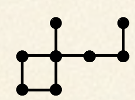
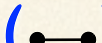
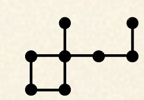
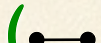
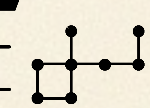
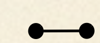
Cluster Expansions



Disconnected clusters do not contribute:

$W_P($  $) \; = \; P($  $) \; - \sum_{S \subset}$  $W_P(s)$

$W_P($  $) \; = \; P($  $) + P($  $) \; - \; W_P($  $) \; - \; W_P($  $)$

$- \sum_{S \subset}$  $W_P(s) \; - \sum_{S \subset}$  $W_P(s)$

$= \; 0$

Sykes et al.,
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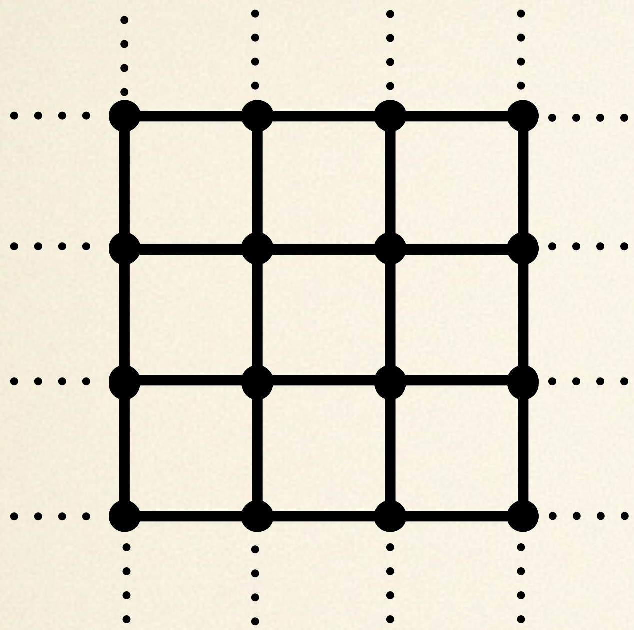
Cluster Expansions (TL)

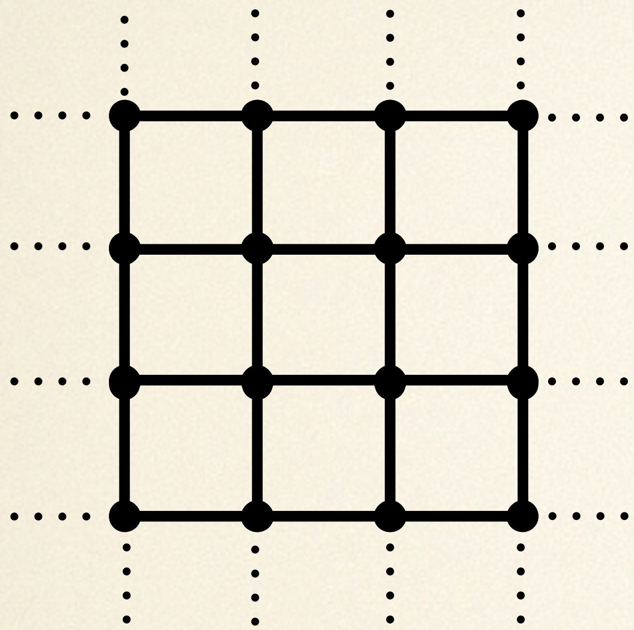


Similarly, an expansion can be written in the thermodynamic limit (TL).

But, we have to truncate the series.

$$P(\infty)/L = W_P(\bullet) + 2W_P(\bullet\!-\!\bullet) + 6W_P(\lrcorner) + 4W_P(\perp) + \ldots$$

Cluster Expansions (TL)



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$$W_P(\bullet) \;=\; P(\bullet)$$

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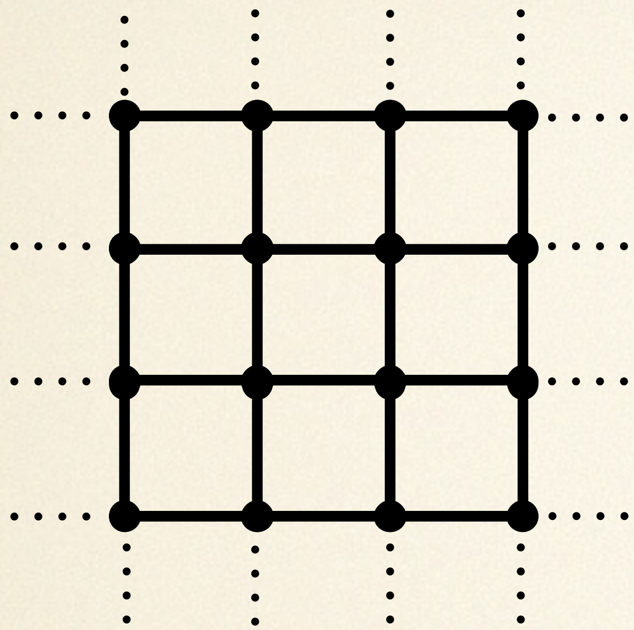

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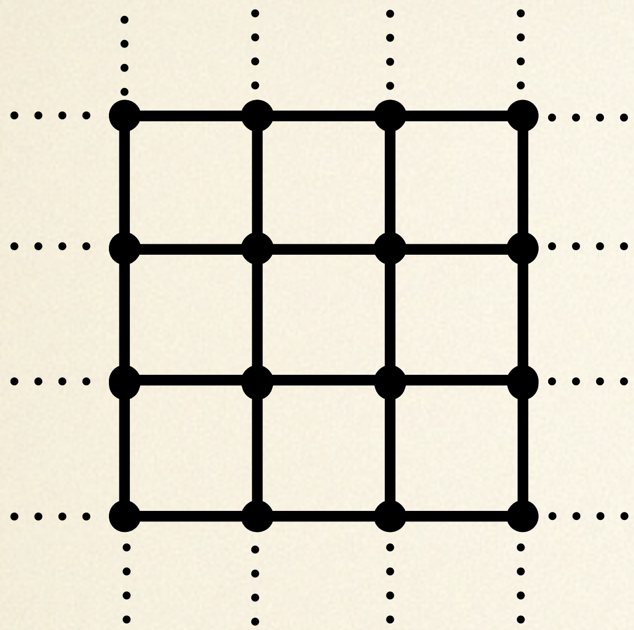
$$W_P(\bullet) = P(\bullet)$$

$$W_P(\bullet\!\!-\!\!\bullet) = P(\bullet\!\!-\!\!\bullet) - 2W_P(\bullet) = P(\bullet\!\!-\!\!\bullet) - 2P(\bullet)$$

$$\vdots$$

Cluster Expansions (TL)



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$$P(\infty)/L = W_P(\bullet) + 2W_P(\bullet\!-\!\bullet) + 6W_P(\lrcorner) + 4W_P(\perp) + \ldots$$

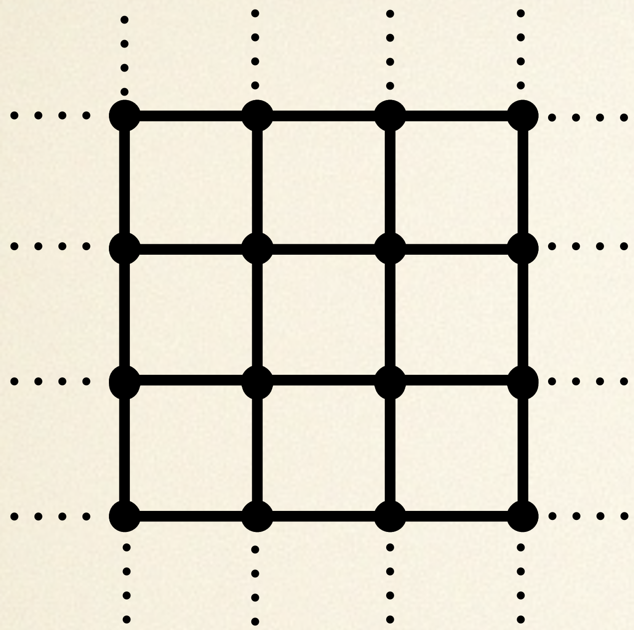
$$W_P(\bullet) = P(\bullet)$$

$$W_P(\bullet\!-\!\bullet) = P(\bullet\!-\!\bullet) - 2W_P(\bullet) = P(\bullet\!-\!\bullet) - 2P(\bullet)$$

$$\vdots$$

Calculated using
Exact Diagonalization

Cluster Expansions (TL)



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$$W_P(\bullet) \;=\; P(\bullet)$$

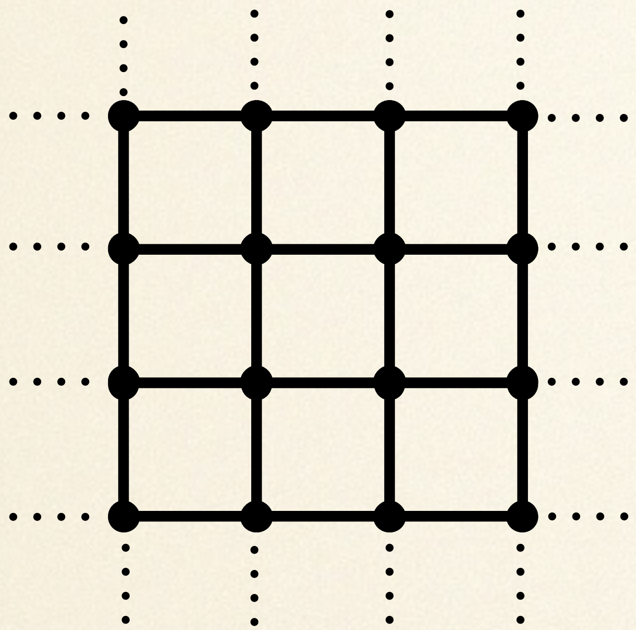
$$W_P(\bullet\!\!-\!\!\bullet) \;=\; P(\bullet\!\!-\!\!\bullet) \;-\; 2W_P(\bullet) \;=\; P(\bullet\!\!-\!\!\bullet) \;-\; 2P(\bullet)$$

$$\vdots$$

$$P(\infty)/\mathrm{L} \;=\; -3P(\bullet) \;+\; 2P(\bullet\!\!-\!\!\bullet) \;+\; \ldots$$

Calculated using
Exact Diagonalization

Numerical Linked-Cluster Expansion (NLCE)



$$\begin{cases} P(c) = \dfrac{\mathrm{Tr}\ \hat{P}e^{-\beta\hat{H}_c}}{\mathrm{Tr}\ e^{-\beta\hat{H}_c}} \\ W_P(c) = P(c) - \sum_{s\subset c} W_P(s) \\ P(\infty)/L = \sum_c L(c) W_P(c) \end{cases}$$

Number of embeddings per site for cluster '*c*'

J. Oitmaa et al. "Series Expansion Methods for Strongly Interacting Lattice Models"

M. Rigol, T. Bryant, and R. R. P. Singh, PRL **97**, 187202 (2006); PRE **75**, 061118 (2007)

Site Expansion (Square Lattice)

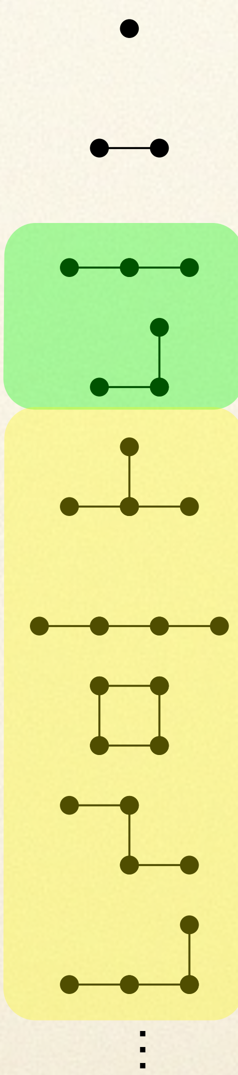
- ☑ Generate all possible clusters
- ☑ Identify their symmetries and topologies
- ☑ Identify their sub-clusters

$$S_i = \sum_{c_i} L(c_i) \times W_P(c_i)$$

(all the clusters that share a characteristic)

$$P_n = \sum_{i=0}^{n} S_i$$

Site expansion for the square lattice:



c	$L(c)$
1	1
2	2
3	2
4	4
5	4
6	2
7	1
8	4
9	8
⋮	

# of sites	# of clusters
1	1
2	1
3	1
4	3
5	4
6	10
7	19
8	51
9	112
10	300
11	746
12	2042
13	5450
14	15 197
15	42 192
16	119 561

Parallelization

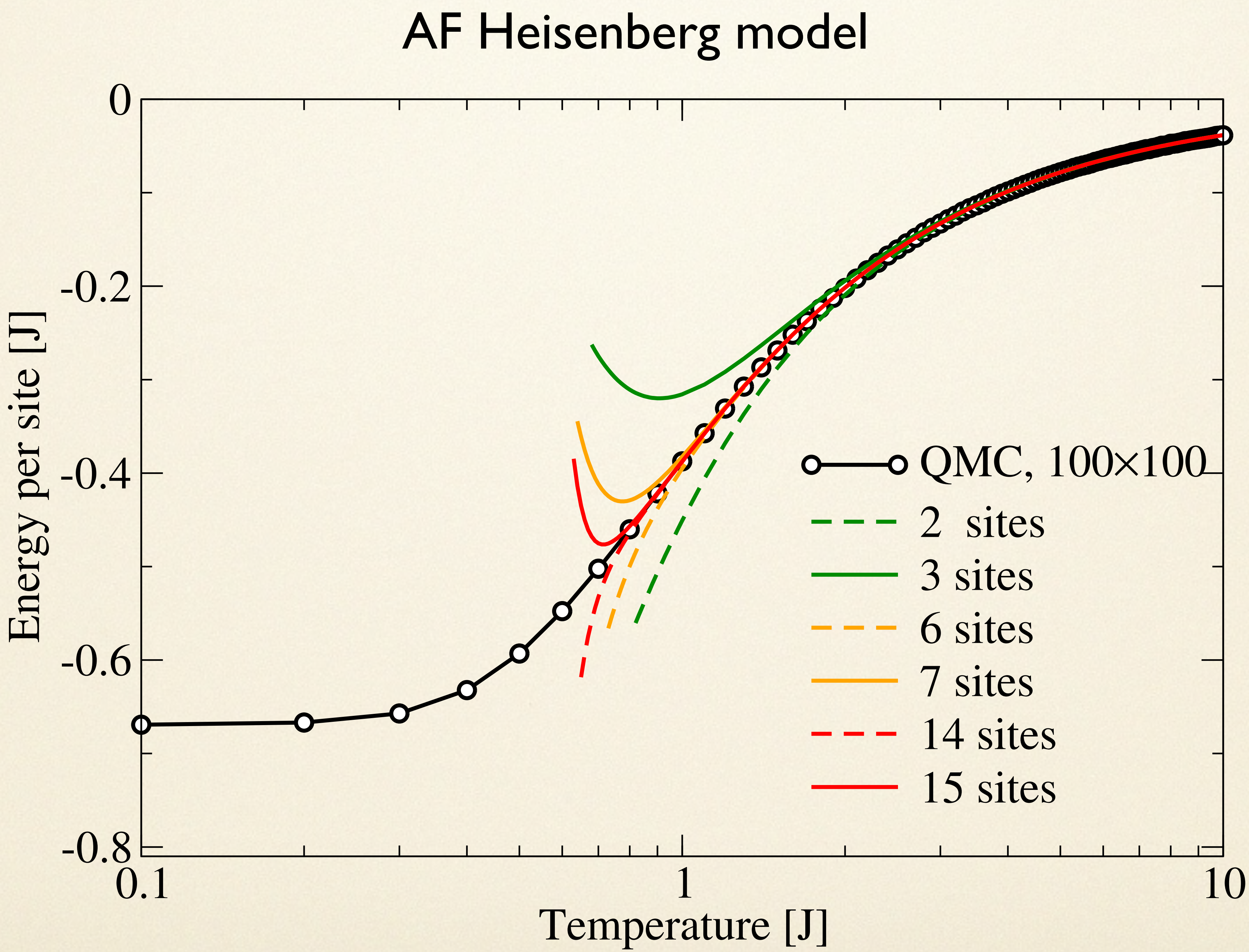
- Embarrassingly parallel (sending groups of clusters to each processor)
- We use <u>MPI</u> to assign every cluster to a different node.
- We use <u>OpenMP</u> to parallelize loops using processors on each node.

B. Tang, EK and M. Rigol, Computer Physics Communications **184**, 557 (2013)

# of sites	# of clusters
1	1
2	1
3	1
4	3
5	4
6	10
7	19
8	51
9	112
10	300
11	746
12	2042
13	5450
14	15 197
15	42 192
16	119 561

Kraken
National Institute for Computational Sciences
University of Tennessee

AF Heisenberg model on the square lattice



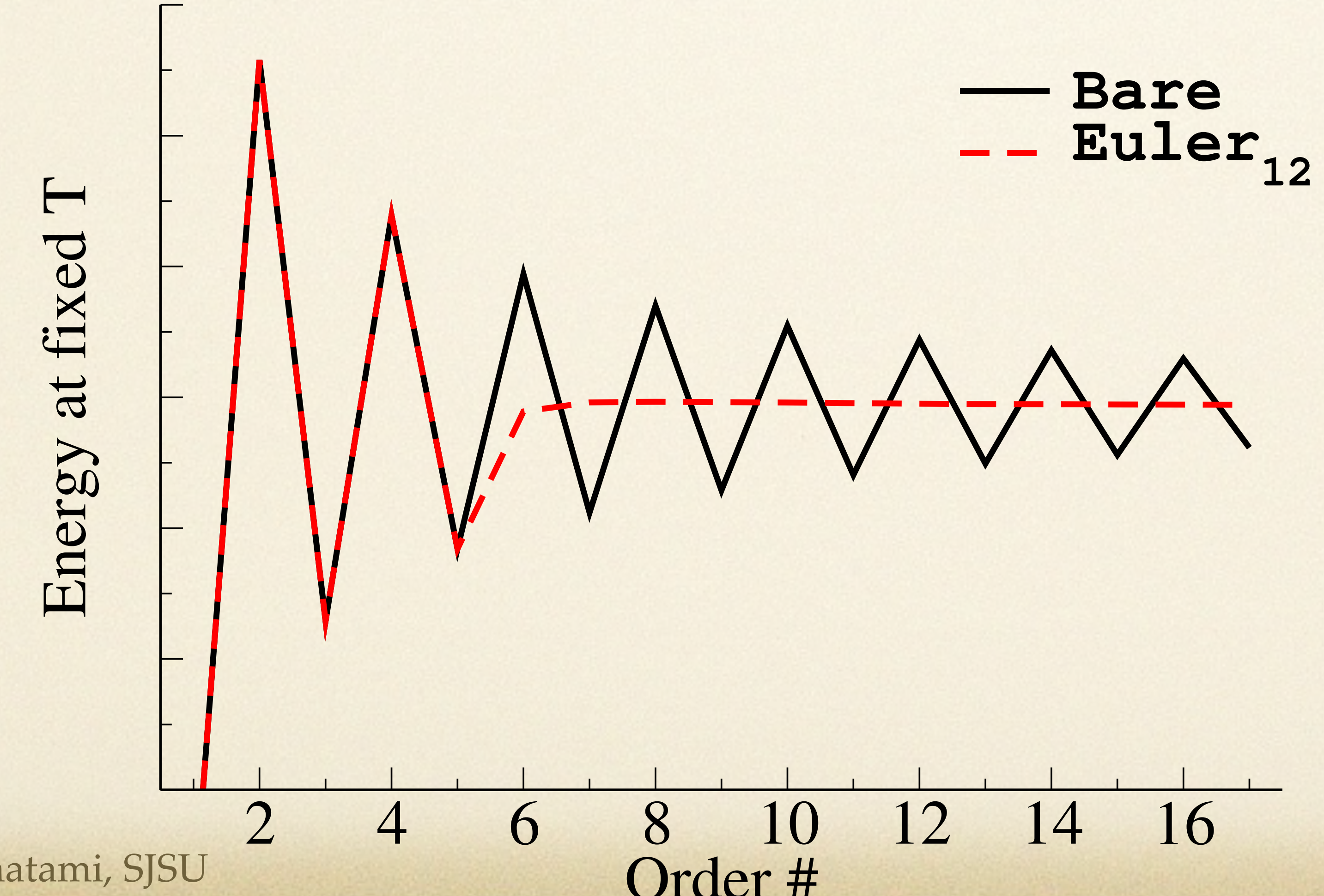
Numerical Re-summation

$$S_i = \sum_{c_i} L(c_i) \times W_P(c_i)$$

where all c_i share a given characteristic (# of bonds, sites ...)

Bare sum: $P_n = \sum_{i=0}^{n} S_i$ $\Rightarrow$ $P(\infty) = \lim_{\ n\to\infty} P_n$

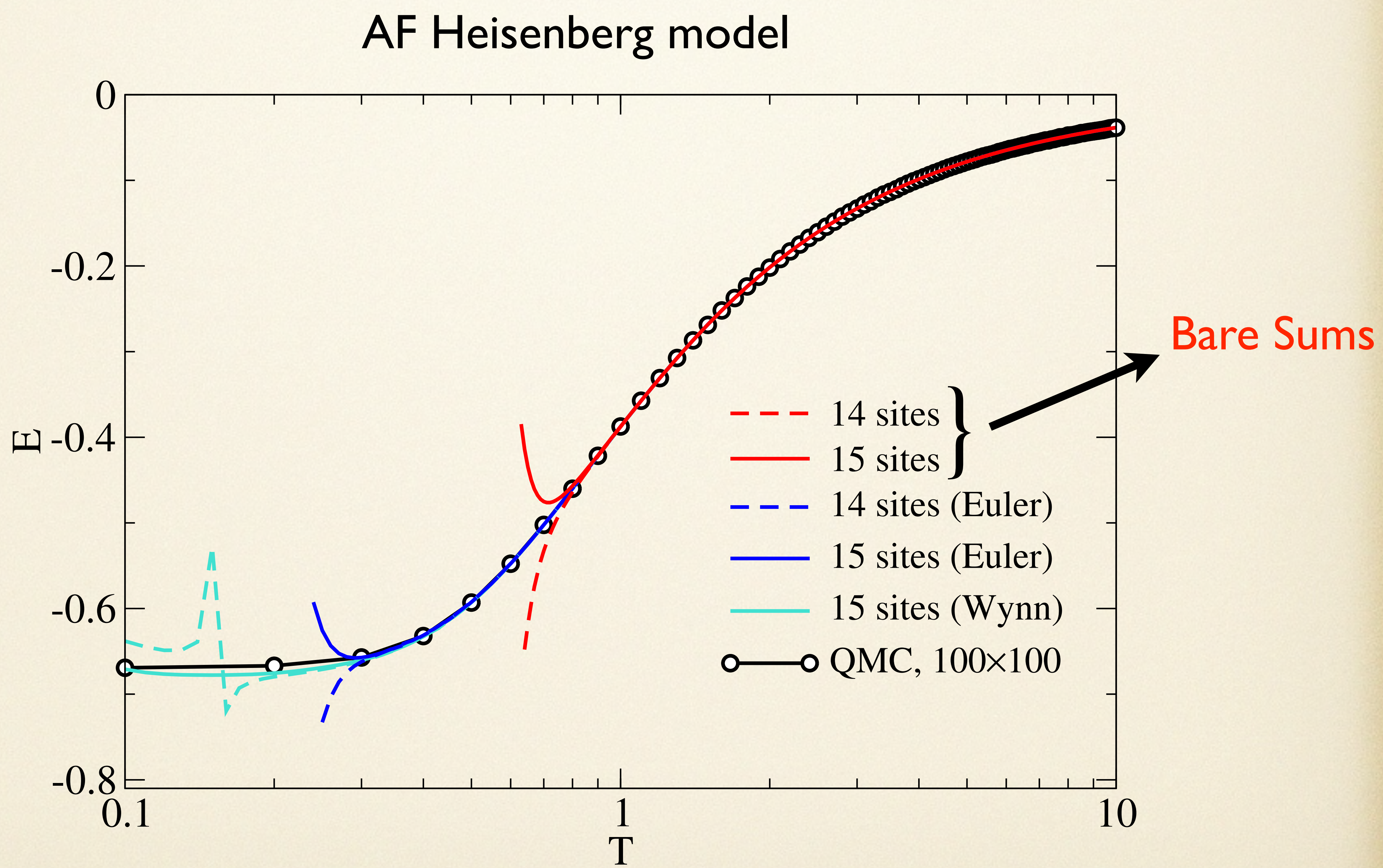
We can take advantage of numerical re-summation algorithms such as, Euler and Wynn to perform the above sum:



Numerical Recipes in Fortran

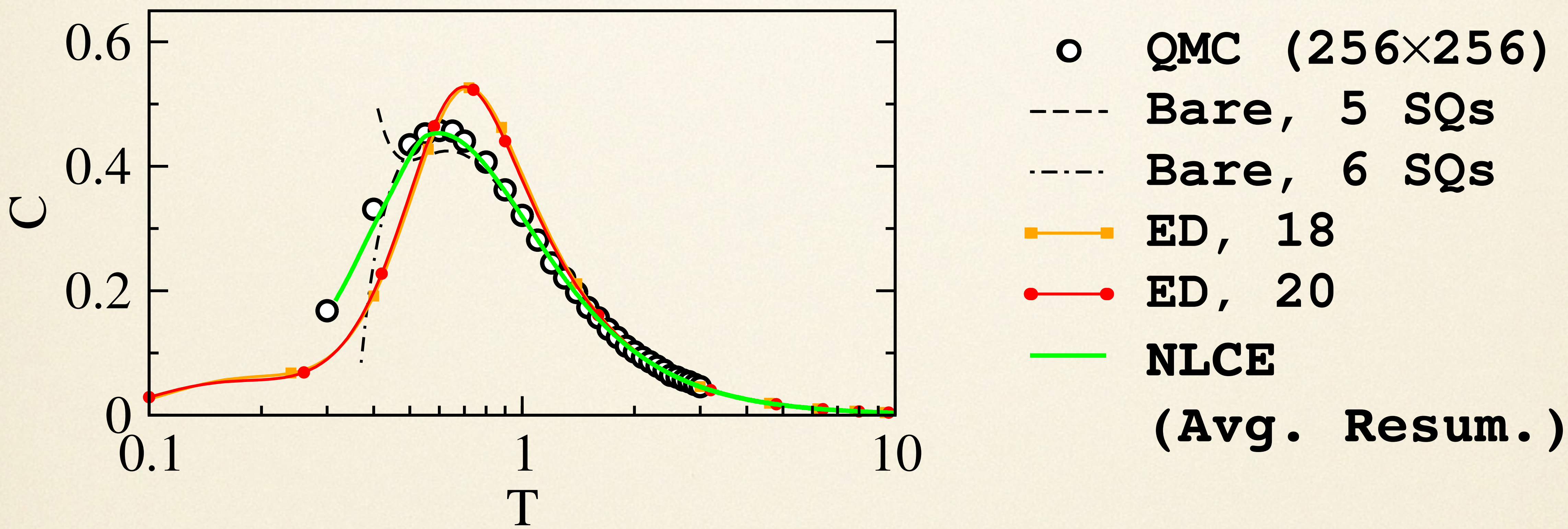
A. J. Guttmann, in Phase Transitions and Critical Phenomena edited by C. Domb and J. Lebowitz, Vol. **13**

Numerical Re-summation



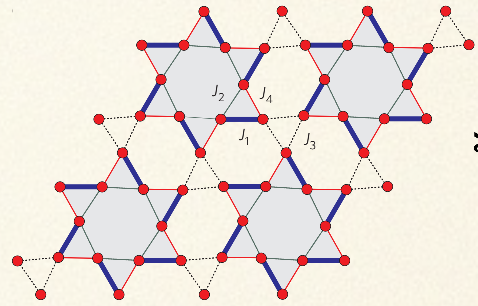
Numerical Re-summation

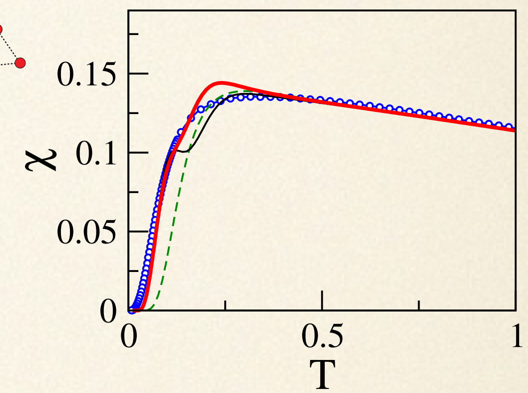
AF Heisenberg model



Numerical linked-cluster expansions

- Spin models (frustrated magnets)



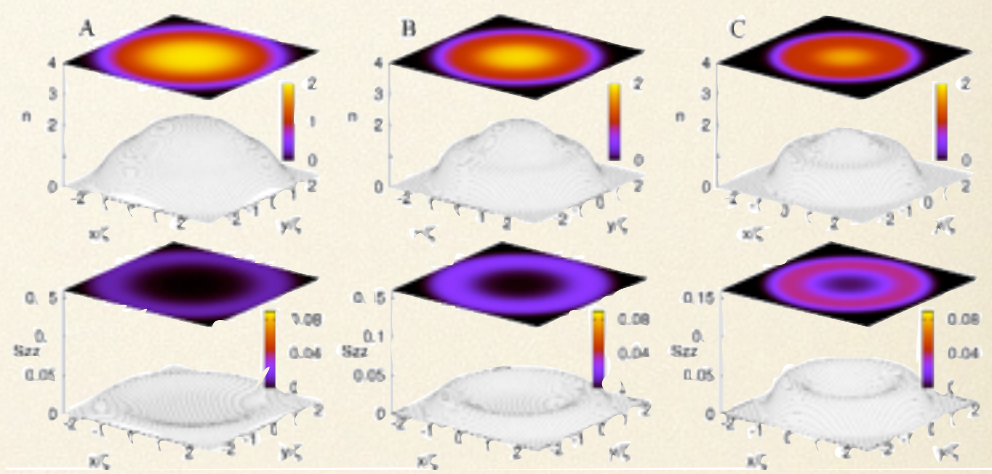


M. Rigol, T. Bryant, R. R. P. Singh, PRL **97**, 187202 (2006); **98**, 207204 (2007).

EK and M. Rigol, PRB **83**, 134431 (2011); **85**, 064401 (2012)

⋮

- Itinerant electron models

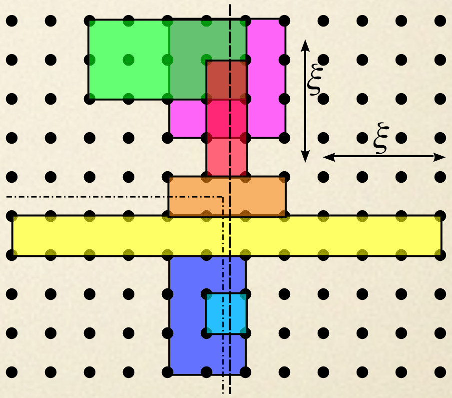


EK and M. Rigol, PRA **84**, 053611 (2011); **86**, 023633 (2012)

B. Tang, T. Paiva, EK, M. Rigol, PRL **109**, 205301 (2012); PRB **88**, 125127 (2013)

⋮

- Entanglement



A. Kallin, K. Hyatt, R. Singh, R. Melko, PRL **110**, 135702 (2013)

A. Kallin, E. M. Stoudenmire, P. Fendley, R. R. P. Singh, R. G. Melko, J Stat. Mech. **2014**, 06009 (2014) ...

- Thermalization of isolated quantum systems

M. Rigol, PRL **112**, 170601 (2014); PRE **90**, 031301(R) (2014) ...

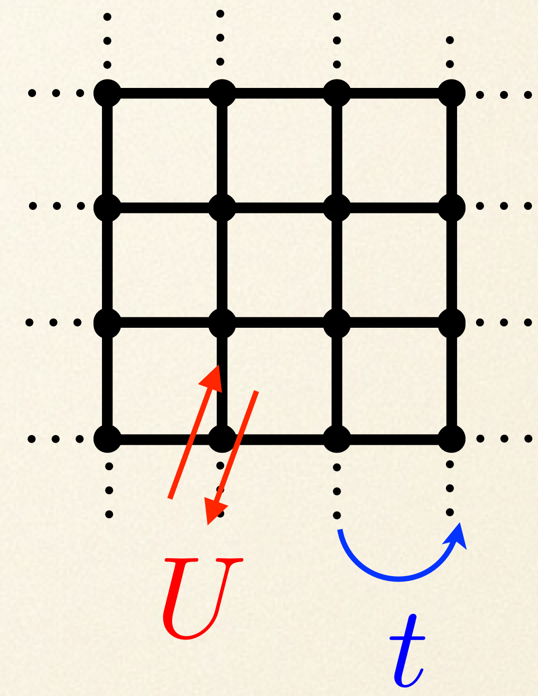
Square Lattice Hubbard Model

The Fermi-Hubbard model:

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

Kinetic energy (nearest neighbor hopping)

Potential energy (Coulomb interaction)

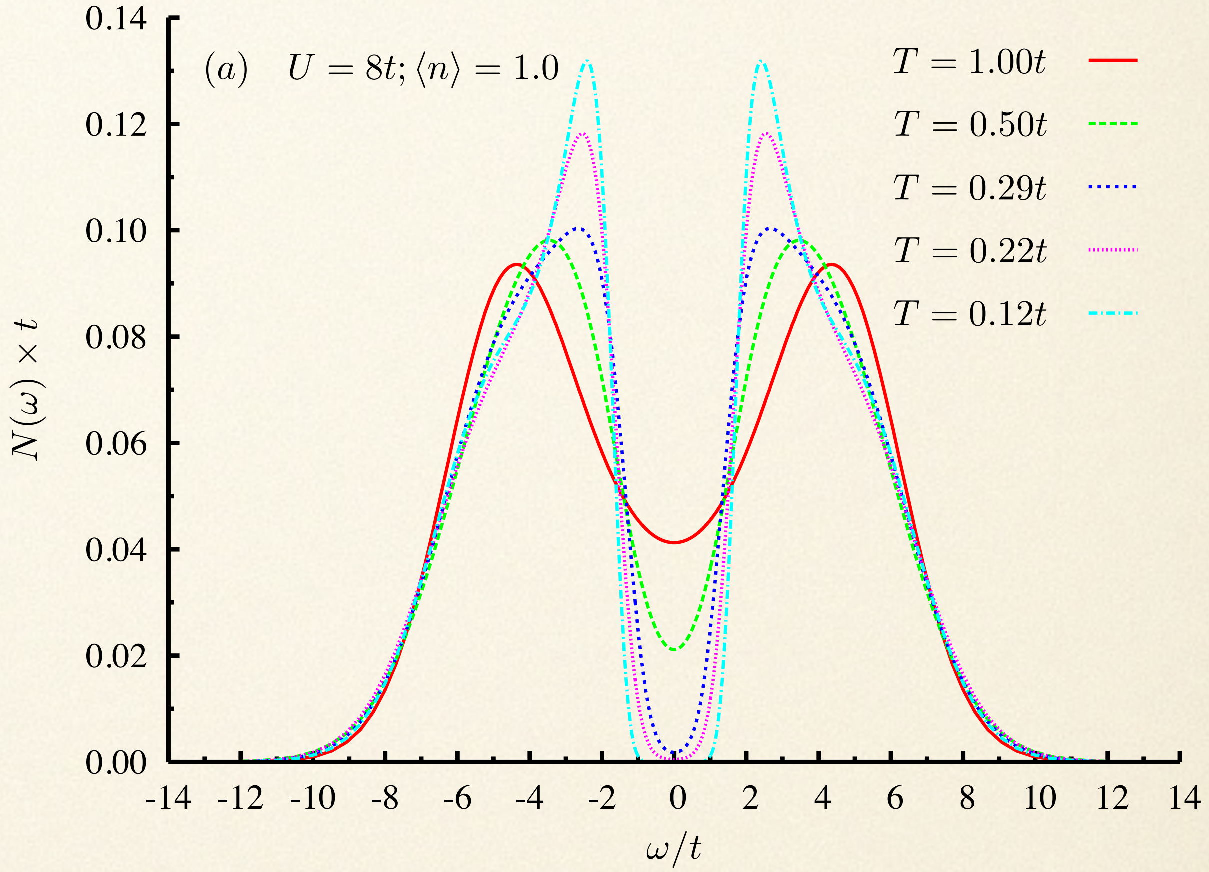


$t = 1$ *(unit of energy)*

Mott insulator at half filling

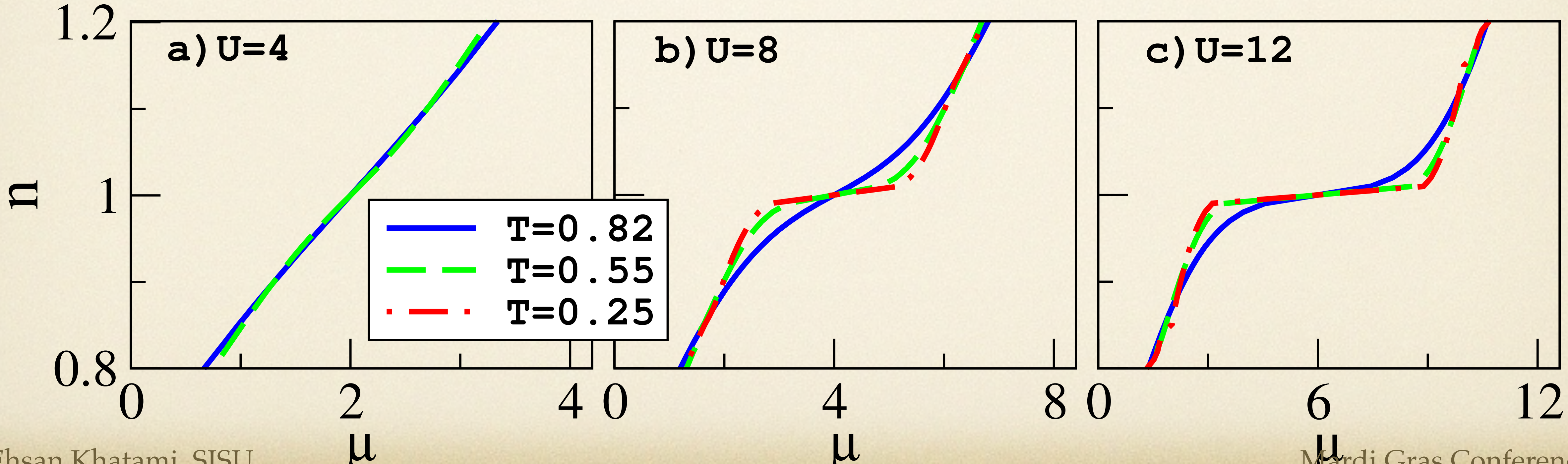
From the density of states

T.A. Maier, M. Jarrell, D.J. Scalapino, (2006)

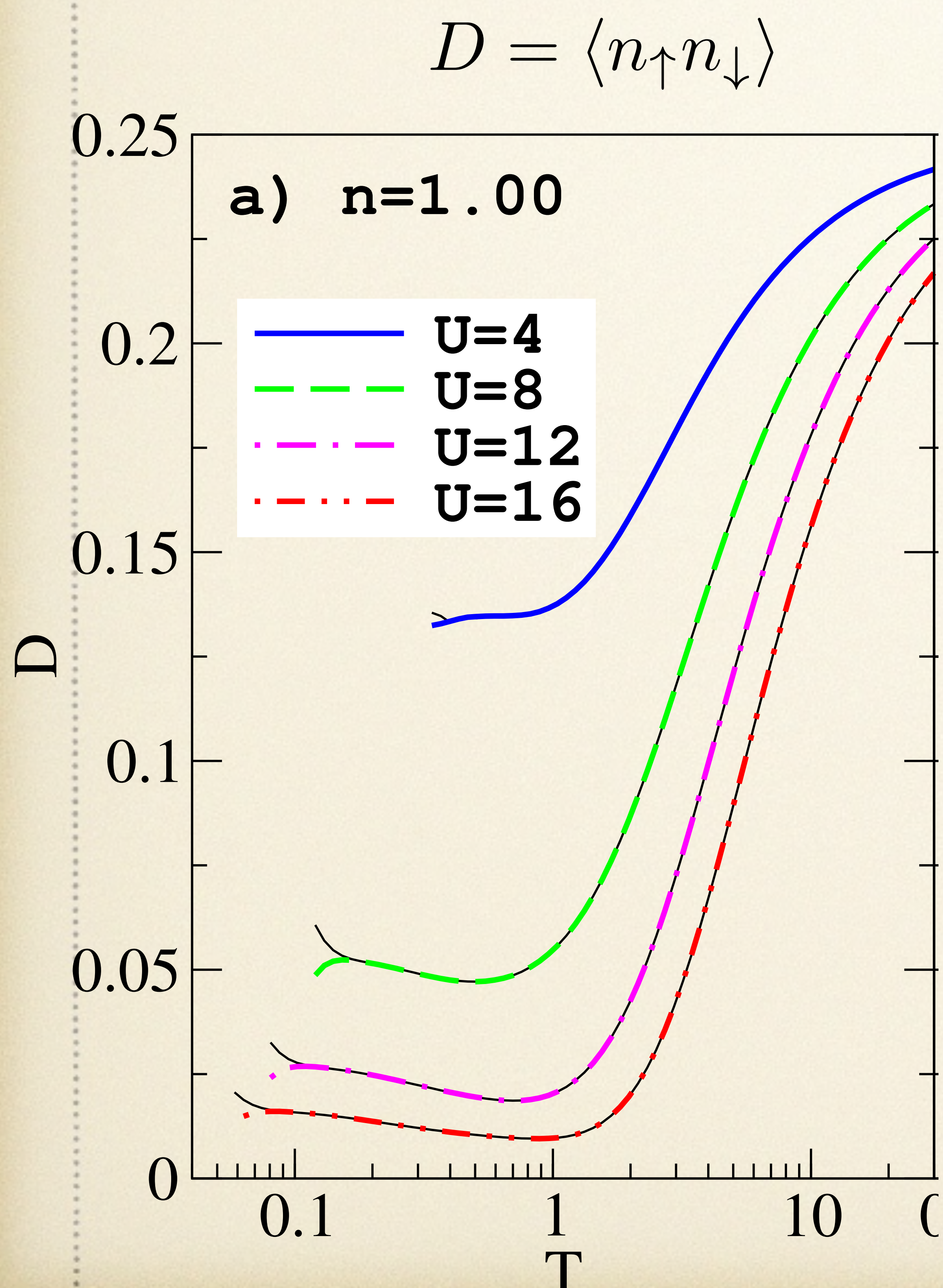


From the equation of state (NLCE)

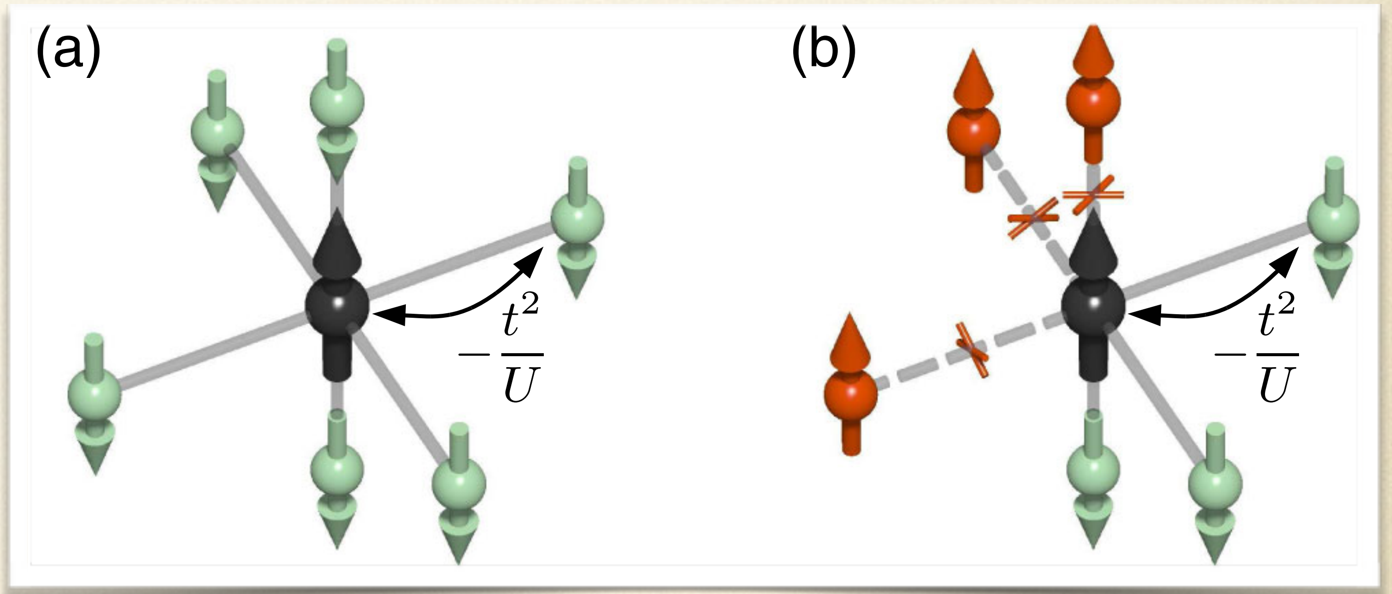
EK and M. Rigol, PRA **84**, 053611 (2011)



Double Occupancy



- Double occupancy decreases by increasing the interaction.
- For large interactions, it rises at low temperatures.
- The rise can be explained by enhanced virtual hoppings to allowed neighboring sites due to AF ordering.

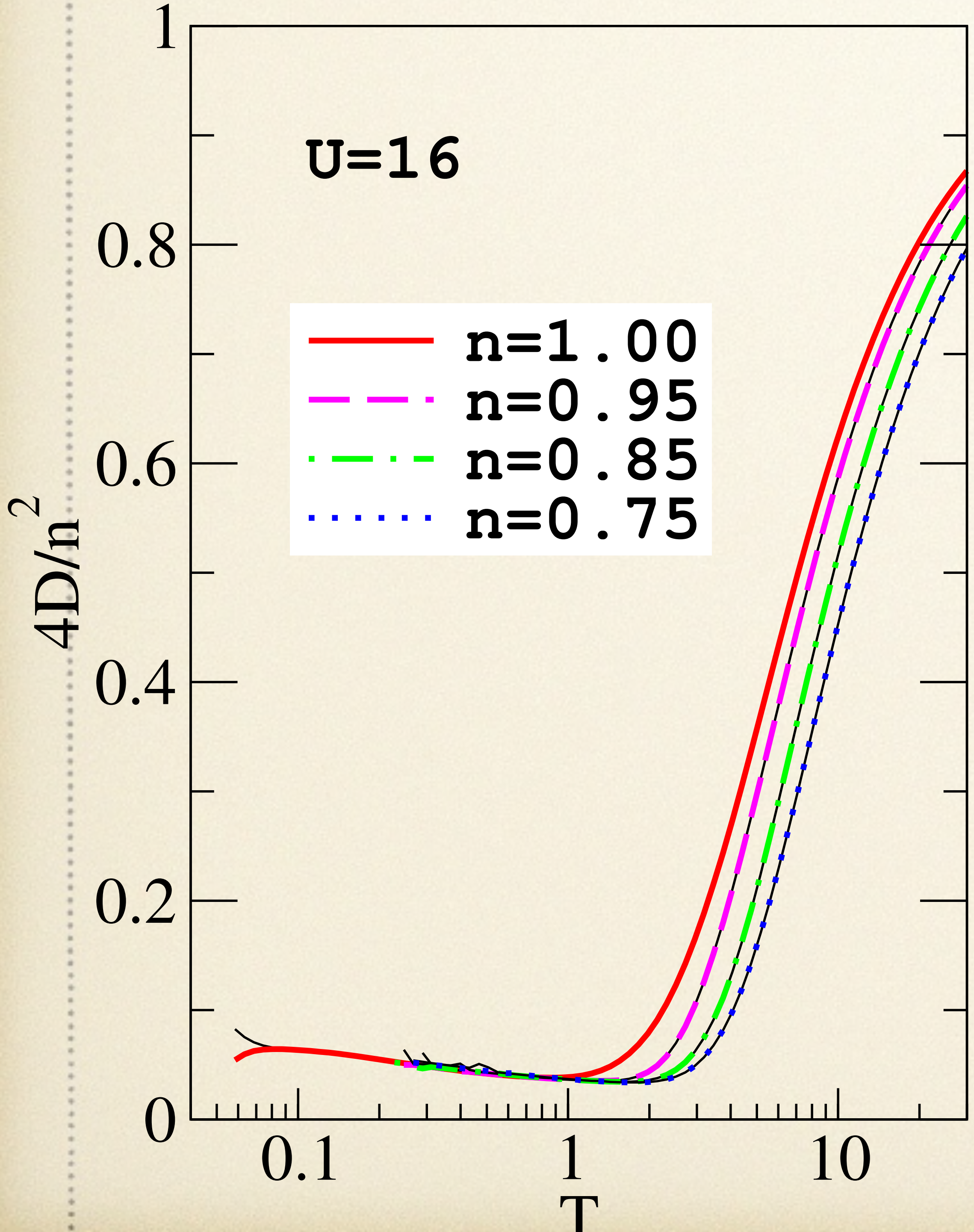


Gorelik et. al., PRL **105**, 065301 (2010)

Double Occupancy

(uncorrelated)

$$D = \langle n_\uparrow \rangle \langle n_\downarrow \rangle = \langle n \rangle^2 / 4$$



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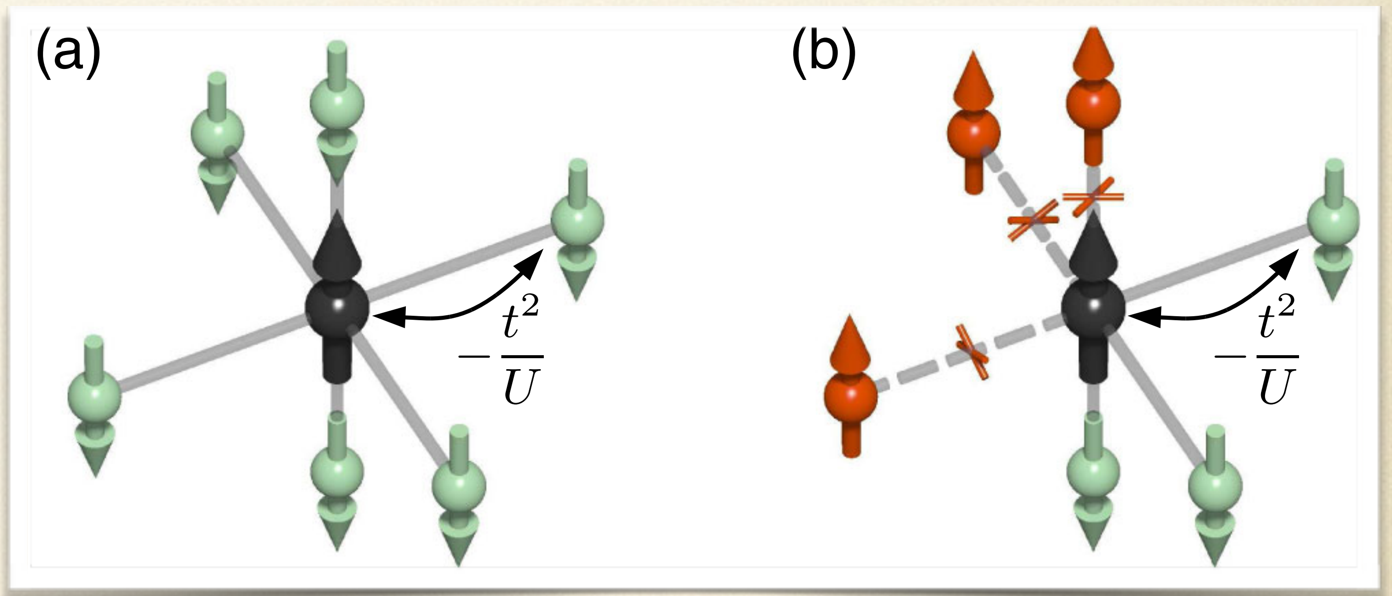


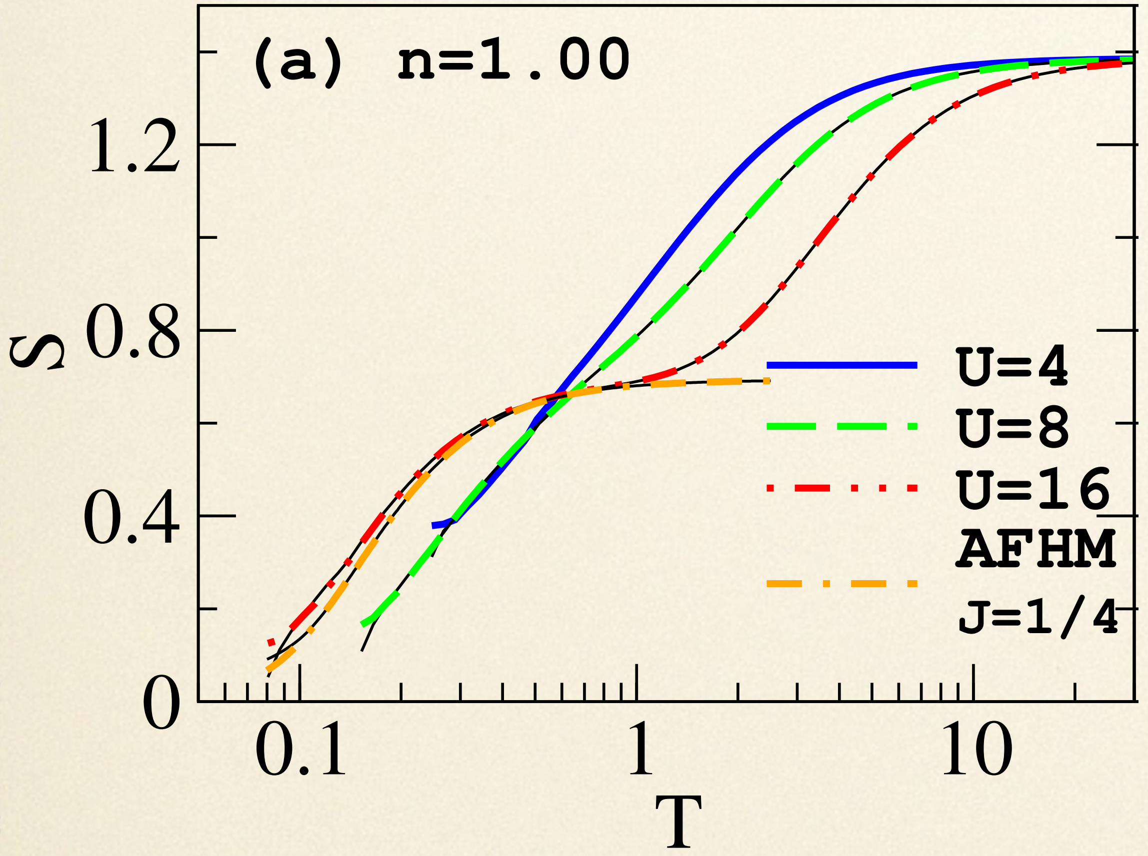
Gorelik et. al., PRL **105**, 065301 (2010)

Thermodynamic properties

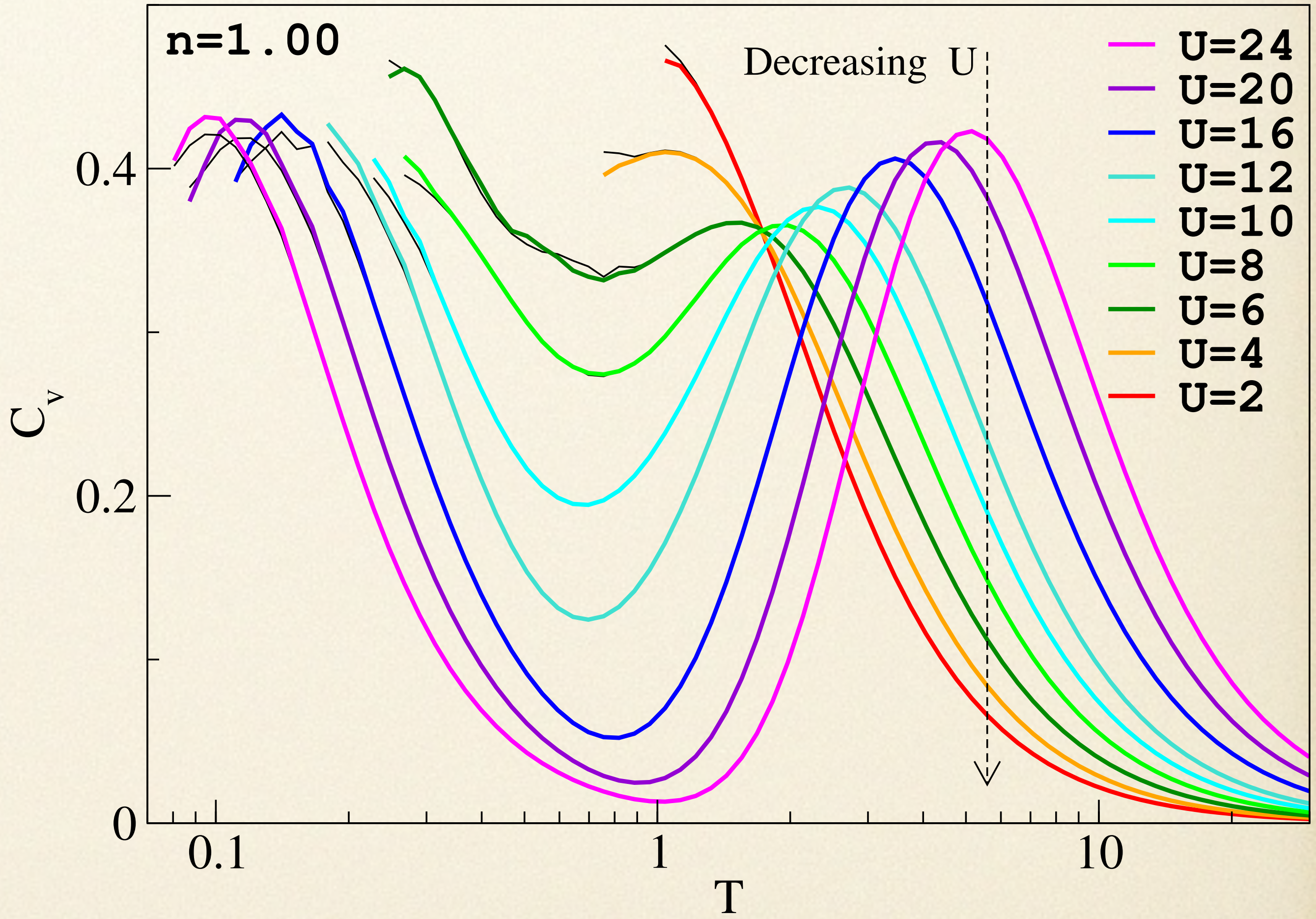
$$S = \ln(Z) + \frac{\langle \hat{H} \rangle - \mu \langle \hat{n} \rangle}{T}$$

$$C_v = \left(\frac{\partial \langle \hat{H} \rangle}{\partial T} \right)_n = \frac{1}{T^2} \left[\langle \Delta \hat{H}^2 \rangle - \frac{(\langle \hat{H} \hat{n} \rangle - \langle \hat{H} \rangle \langle \hat{n} \rangle)^2}{\langle \Delta \hat{n}^2 \rangle} \right]$$

Entropy

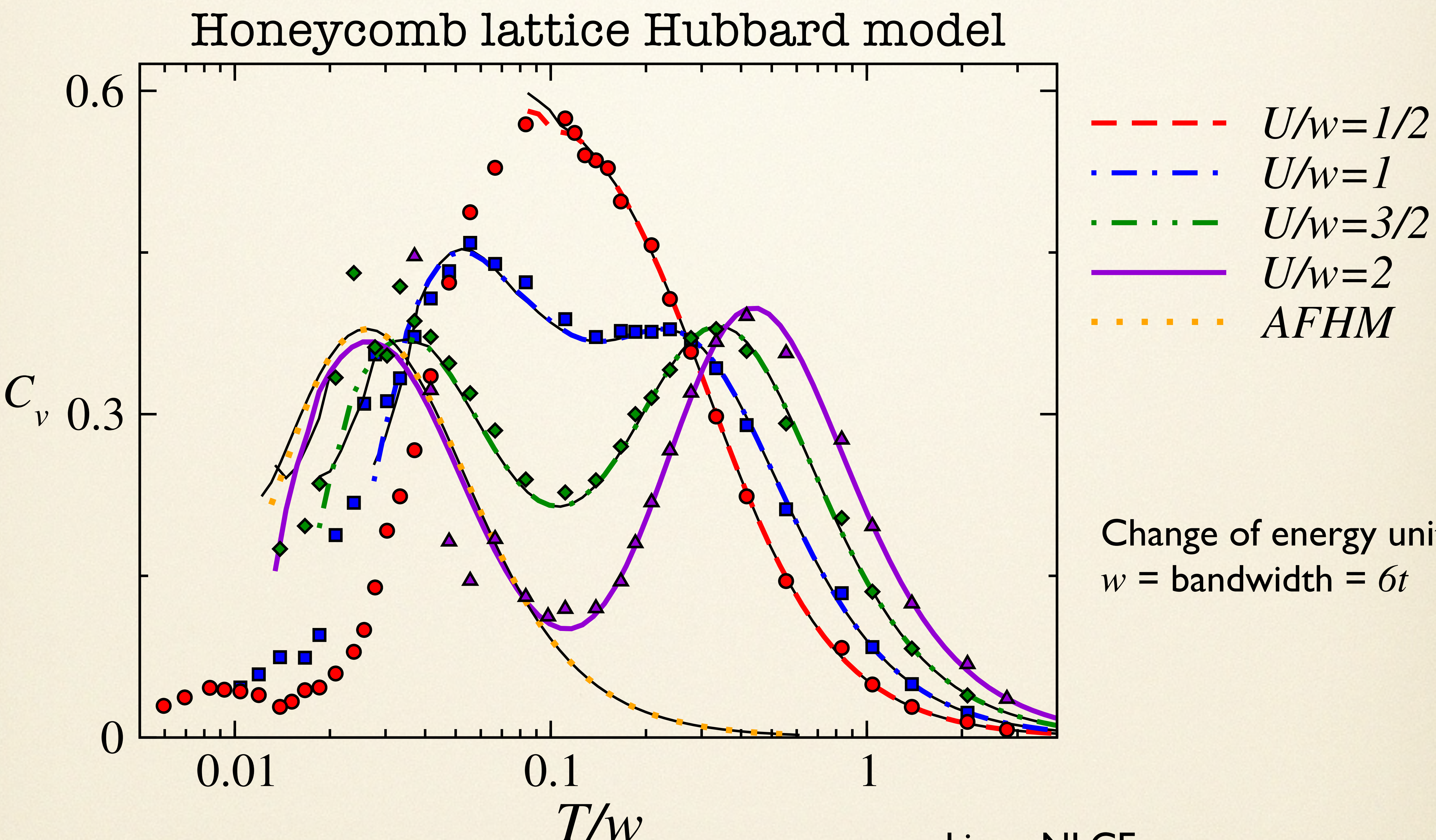


Specific heat



EK and M. Rigol, PRA **84**, 053611 (2011), ibid **86**, 023633 (2012)

Complementarity to DQMC

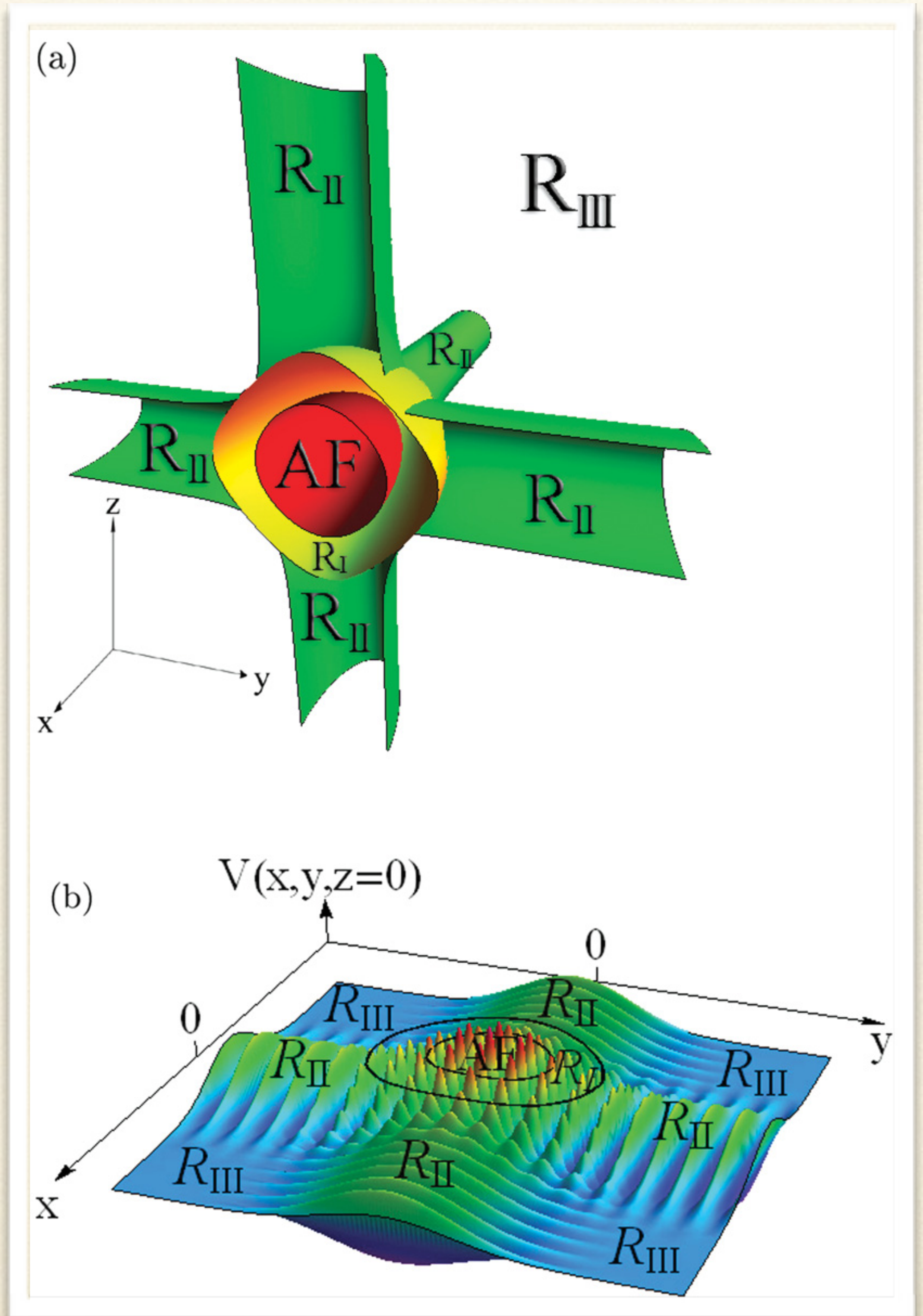


Change of energy unit:
w = bandwidth = $6t$

Lines: NLCE
Symbols: DQMC (~100 sites)

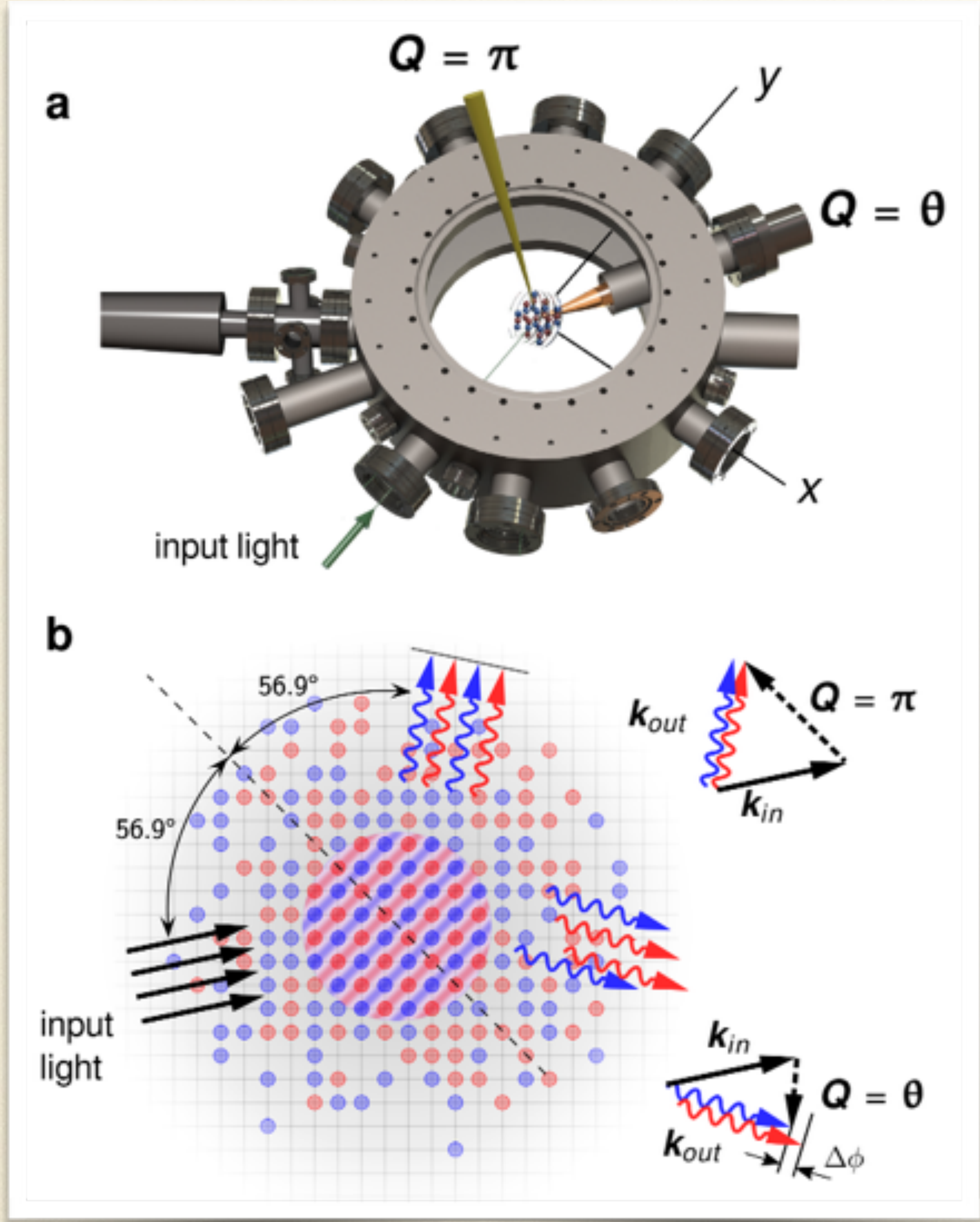
B. Tang, T. Paiva, EK and M. Rigol,
PRL **109**, 205301 (2012)

Cold atoms on optical lattices

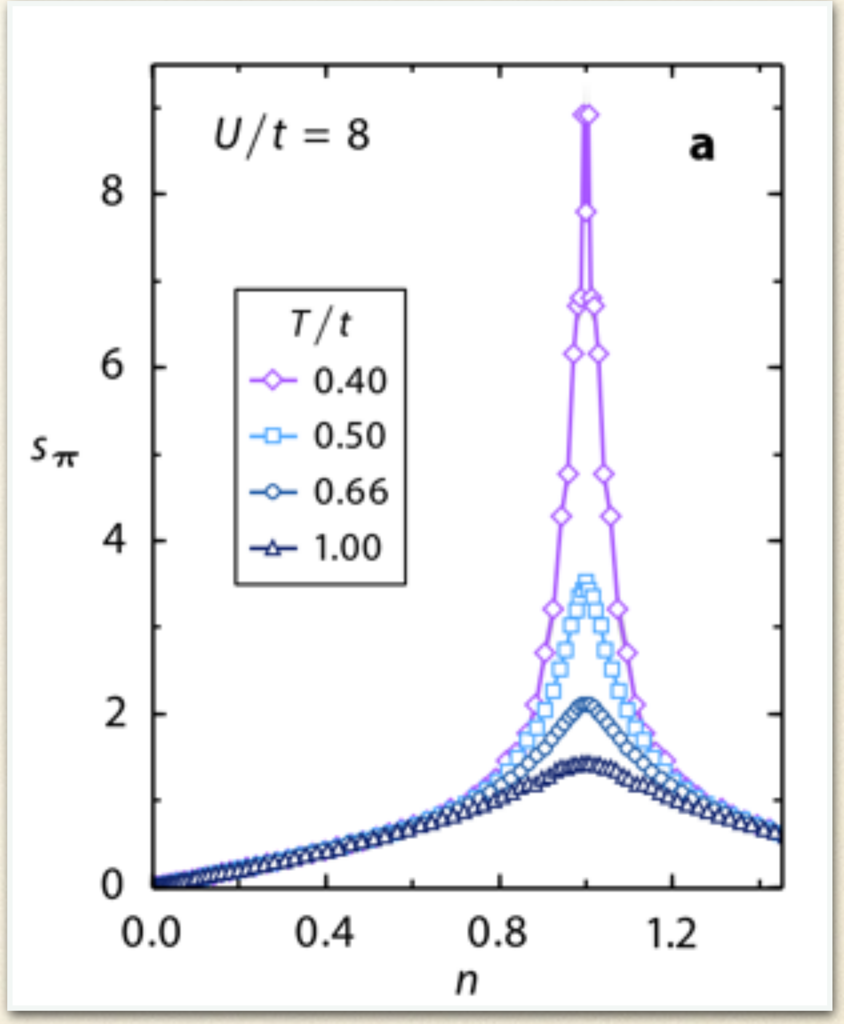


Rice group

Optical lattice experiments

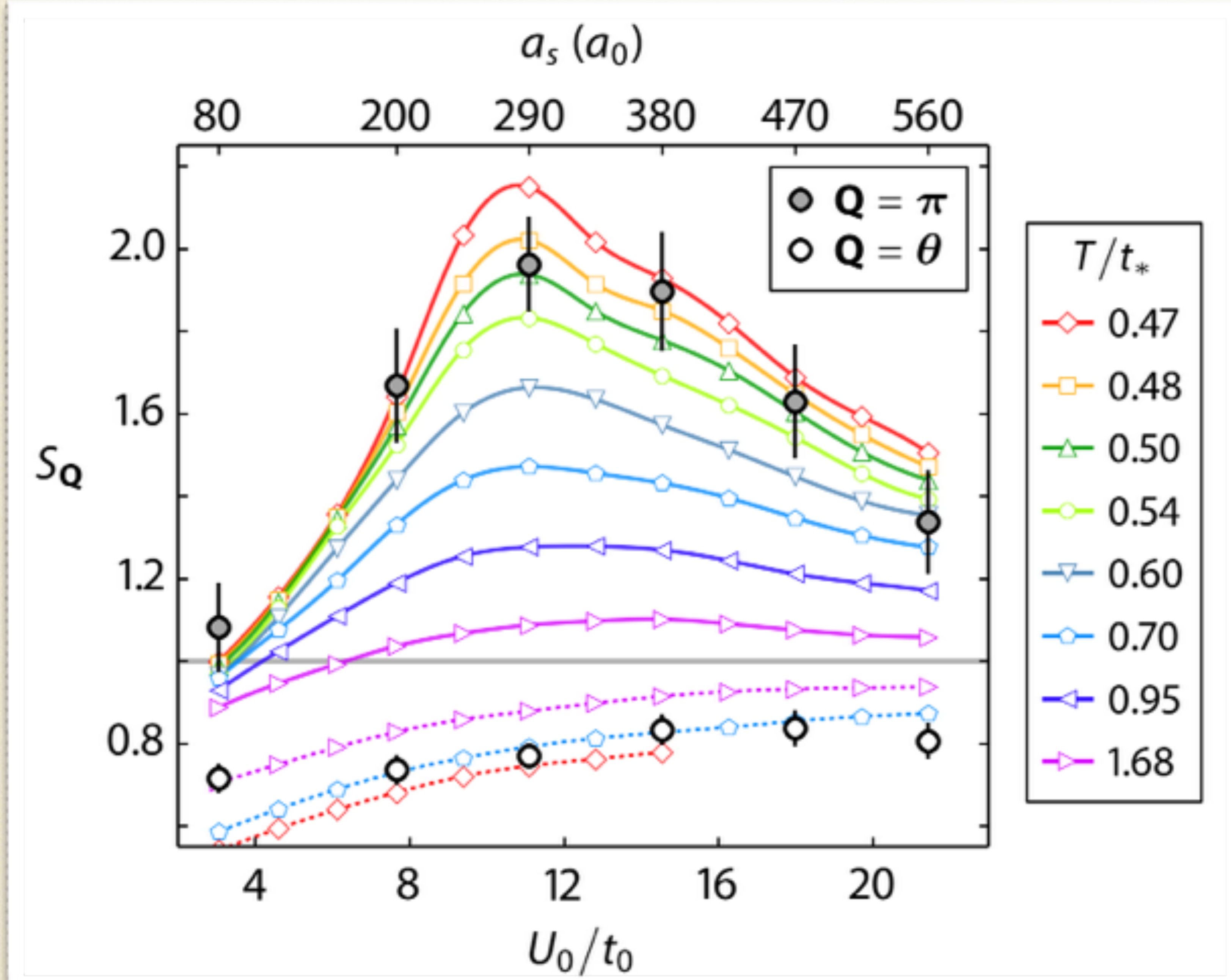


AF structure factor
DQMC + NLCE



Rice group, to appear in Nature

Optical lattice experiments



Estimating the temperature to be ~1.4T_N by comparing to theory (DQMC +NLCE)

Rice group, to appear in Nature

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Thereza Paiva
(U of Rio)

Randy Hulet
and his Group
(Rice)

Summary

* The Numerical Linked-Cluster Expansion provides a powerful tool for studying quantum lattice models in the thermodynamic limit.

* It can be used to study thermodynamic properties of the Hubbard models -- especially useful in the strong-coupling regime (complementary to QMC methods).

Thank you!