Developments in wave function-based approaches to two-dimensional materials

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King's College London

Conference on Frontiers in Two-dimensional Quantum Systems

Trieste, Italy

14/11/17

An enduring legacy of lattice model research…

Hubbard model in infinite dimensions

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(Received 23 September 1991)

present an exact mapping of the Hubbard model in infinite dimensions onto a single-impurity
.on (or Wolff) model supplemented by a self-consistency condition. This provides a mean-field
of strongly correlated systems, which becomes exact as $d \to \infty$. We point out a special integr-
ıse of the mean-field equations, and study the general case using a perturbative renormalization
ıround the atomic limit. Three distinct Fermi-liquid regimes arise, corresponding to the Kondo,
valence, and empty-orbitals regimes of the single-impurity problem. The Kondo resonance and
ellite peaks of the single-impurity model correspond to the quasiparticle and Hubbard-bands
s of the Hubbard model, respectively.

VOLUME 69, NUMBER 19 PHYSICAL REVIEW LETTERS 9 NOVEMBER 1992

Density Matrix Formulation for Quantum Renormalization Groups

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(Received 22 May 1992)

A generalization of the numerical renormalization-group procedure used first by Wilson for the Kondo problem is presented. It is shown that this formulation is optimal in a certain sense. As a demonstration of the effectiveness of this approach, results from numerical real-space renormalization-group calculations for Heisenberg chains are presented.

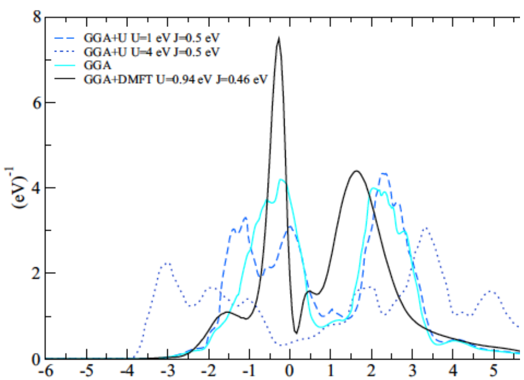
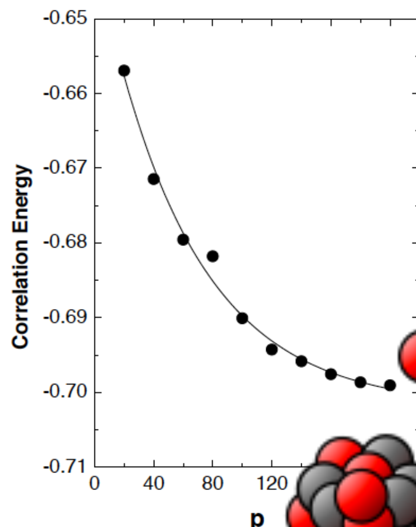
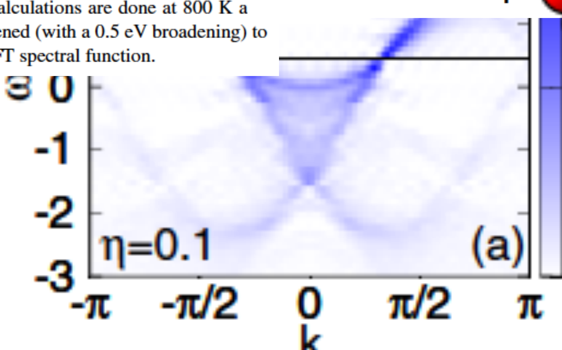
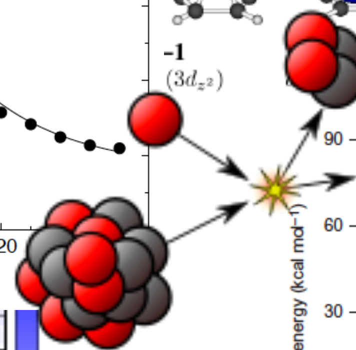
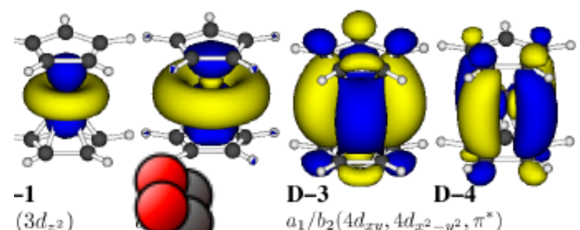


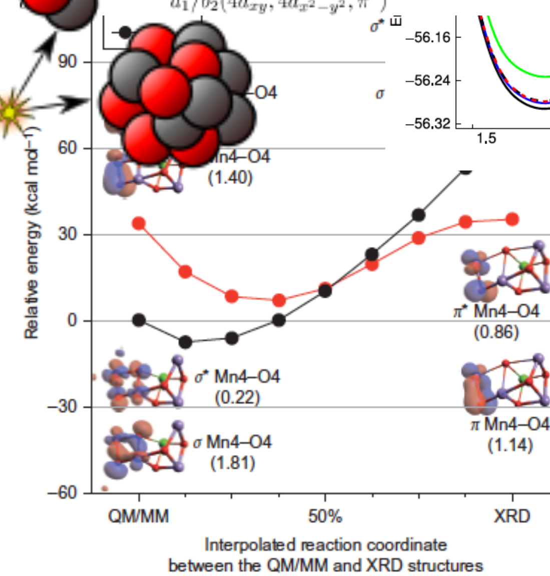
FIG. 8. DFT+DMFT 5f spectral functions of δ-Pu compared the GGA and GGA+U 5f projected density of states (DOS) us for the cRPA calculation of U. Calculations are done at 800 K a GGA+U and GGA DOS are widened (with a 0.5 eV broadening) to be easily compared to DFT+DMFT spectral function.

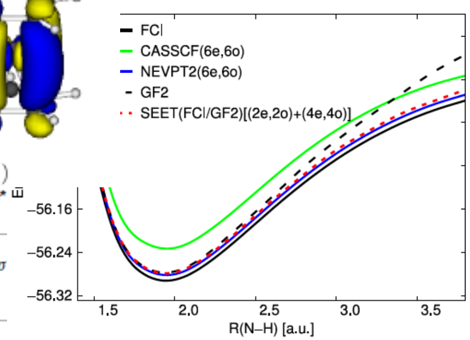












Materials Science

Nuclear Structure

Quantum Chemistry

Wavefunction **(ground state) approaches to lattice models:**

- Long history: **Gutzwiller, RVB, …**
- More recently:
  - Tensor Networks: **MPS, PEPS**
    (White, Cirac, Verstrate, Corboz,...)
  - Wfn-QMC: **VMC, AFQMC, GFMC**
    (Sorella, Becca, Zhang...)

$$|\psi\rangle = \sum_{q_1 q_2 q_3 \cdots q_m} C^{q_1 q_2 q_3 \cdots q_m} |q_1 q_2 q_3 \dots q_m\rangle$$

Exponential memory

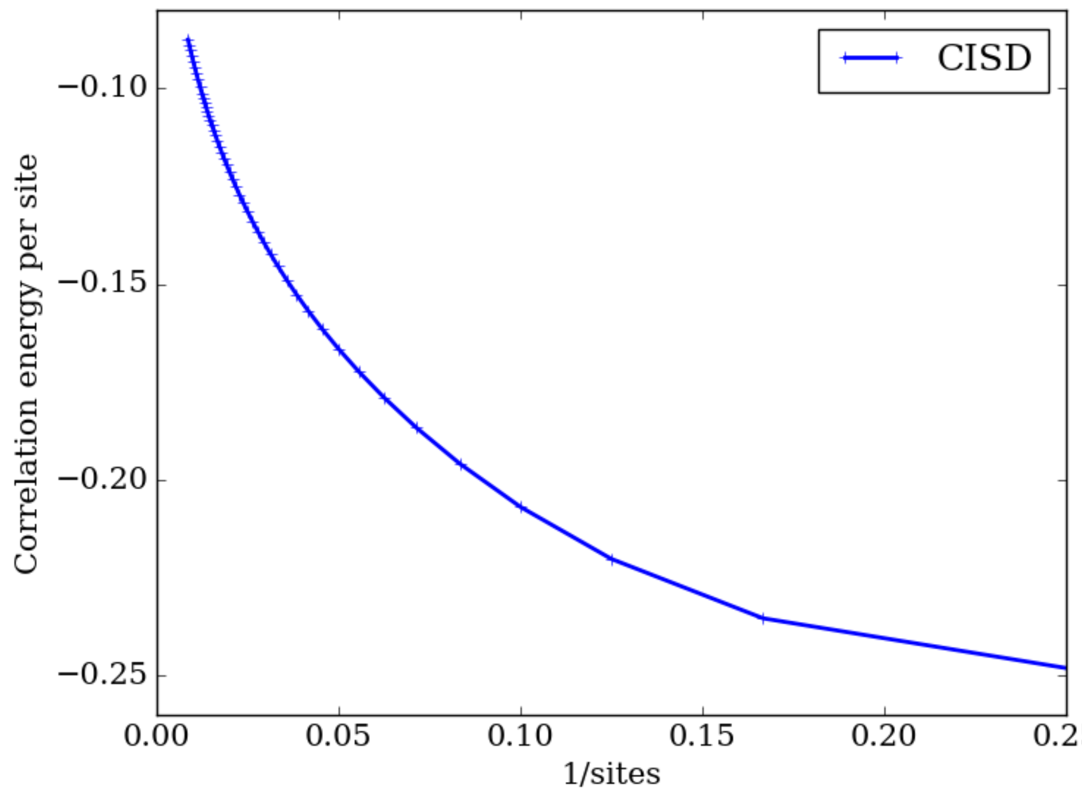
Exponential time

$$|\psi\rangle = \sum_{q_1 q_2 q_3 \cdots q_m} C^{q_1 q_2 q_3 \cdots q_m} |q_1 q_2 q_3 \ldots q_m\rangle$$

Choose subset?

✓ Linear problem

✗ Zero correlation in thermodynamic limit



$$|\psi\rangle = \sum_{q_1 q_2 q_3 \ldots q_m} C^{q_1 q_2 q_3 \ldots q_m} |q_1 q_2 q_3 \ldots q_m\rangle$$

Projector QMC

$$\Psi = e^{-\beta H} |\psi_0\rangle$$

- Stochastically apply projector
- Discretize and sample from amplitudes

Various flavors

(Choice of projector, Hilbert space):
AFQMC, GFMC, FCIQMC, DMC,…

✗ Sign problem

$$\left|\psi\right\rangle = \sum_{q_1 q_2 q_3 \cdots q_m} C^{q_1 q_2 q_3 \cdots q_m} \left|q_1 q_2 q_3 \ldots q_m\right\rangle$$

Variational QMC

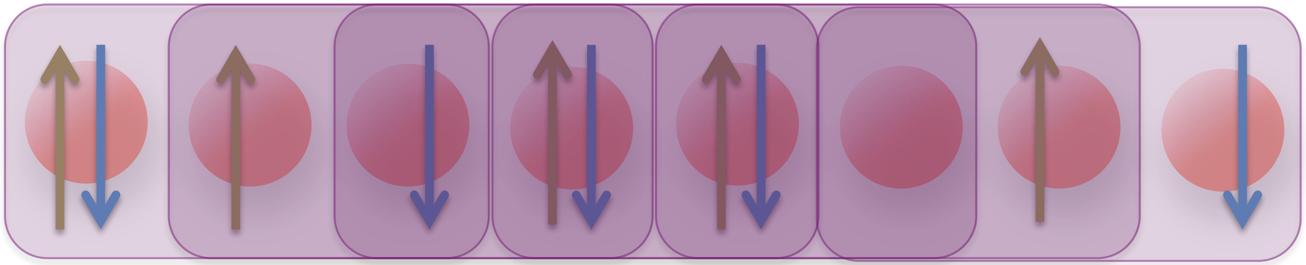
$$\left|\psi\right\rangle = \sum_{q_1 q_2 q_3 \cdots q_m} f(q_1 q_2 q_3 \ldots q_m; \underline{X}) \left|q_1 q_2 q_3 \ldots q_m\right\rangle$$

- Choose an explicit *non-linear* parameterization
- Optimize parameters via Metropolis sampling

?

- How to choose parameterization?
- How to optimize variables with MC?
- How to reduce parameter space?

Correlator Product States / Entangled Plaquette States



$$= \sum_{q_1 q_2 q_3} C^{q_1 q_2 q_3} |q_1 q_2 q_3\rangle$$

$$|\psi\rangle = \sum_{q_1 q_2 q_3 \cdots q_m} C^{q_1 q_2 q_3} C^{q_2 q_3 q_4} C^{q_3 q_4 q_5} \ldots |q_1 q_2 q_3 \ldots q_m\rangle \times \phi_{HF/DFT}$$

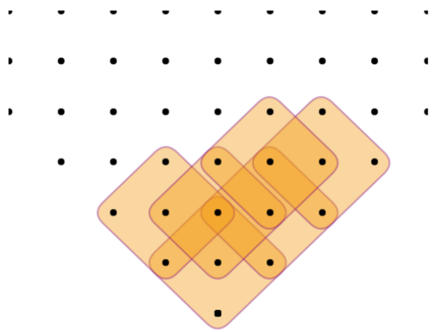
Local (correlated) entanglement

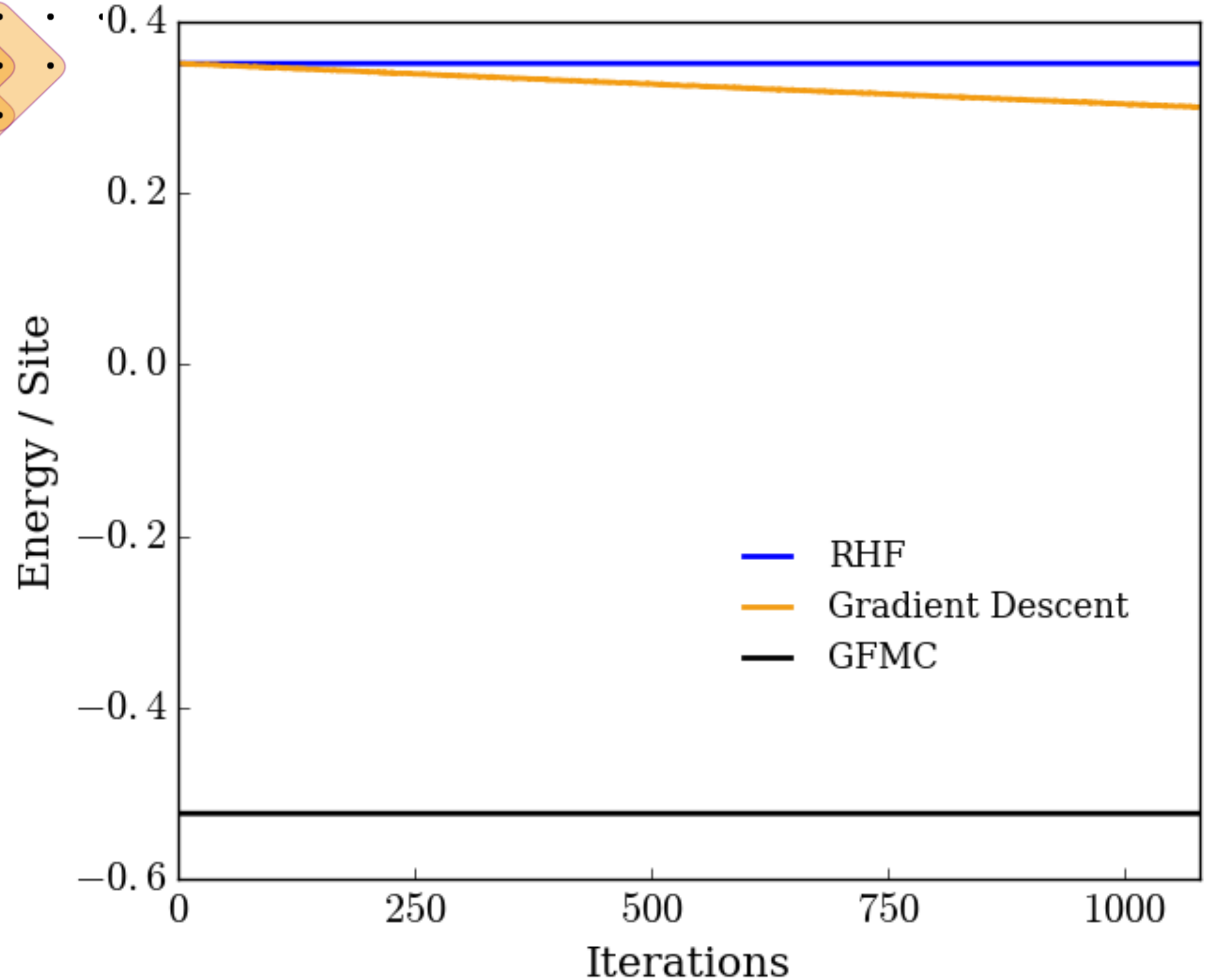
Delocalized (KE) physics

- Linear parameters with system size
- Exponential growth of parameters with correlator size

Non-linear projector Monte Carlo

Overlapping 5-site correlators x Slater determinant for 98-site, 2D Hubbard (U=8t)



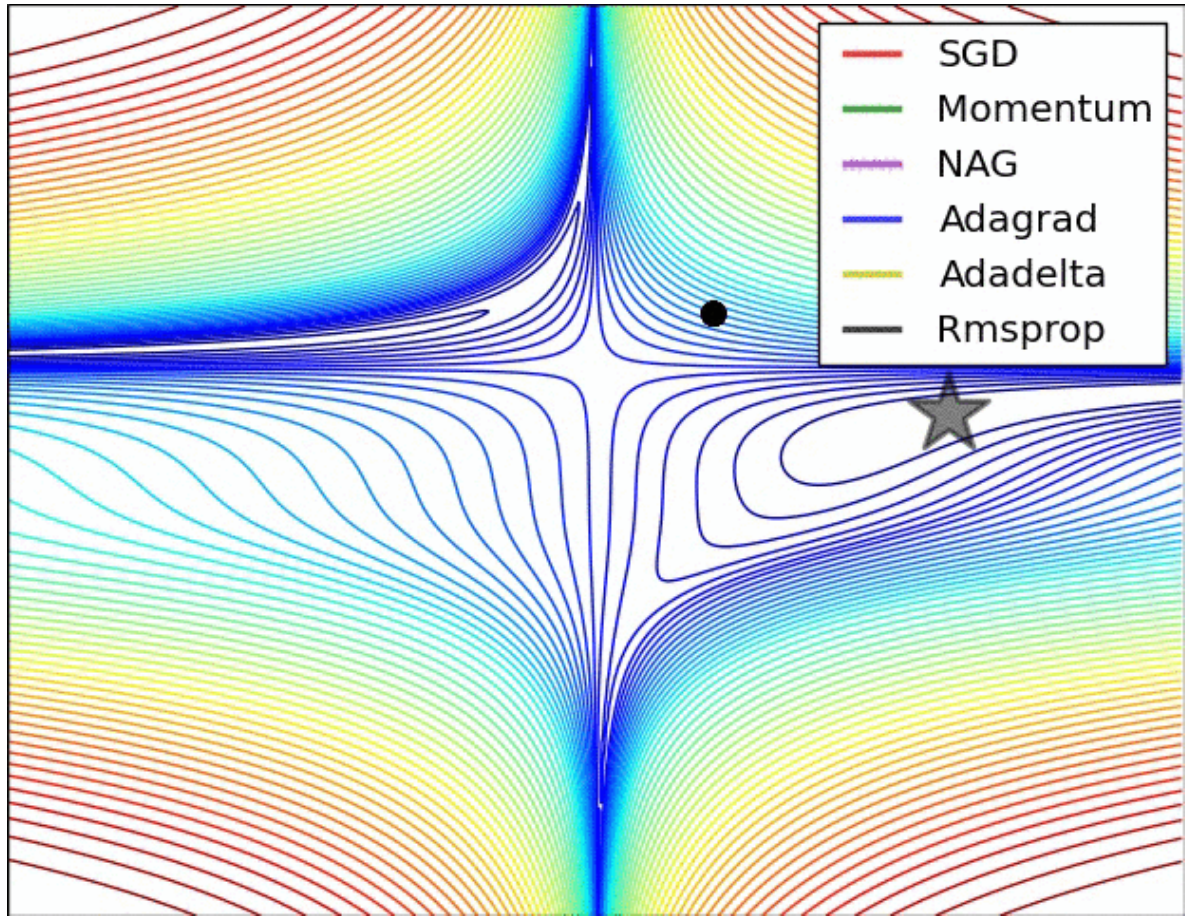


Schwarz, Alavi, Booth, *Phys. Rev. Lett*. (2017)

Similar problems found in optimization of non-linear neural networks…

$$\frac{\partial \Psi}{\partial \beta} = -(H - E)\Psi$$

$$\frac{\partial^2 \Psi}{\partial \beta^2} = -b\frac{\partial \Psi}{\partial \beta} - (H - E)\Psi$$



- Chebyshev expansion of optimal projection operator

Non-linear projector Monte Carlo

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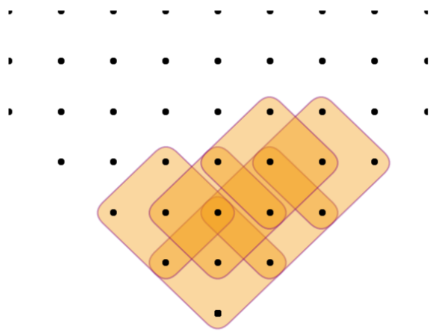

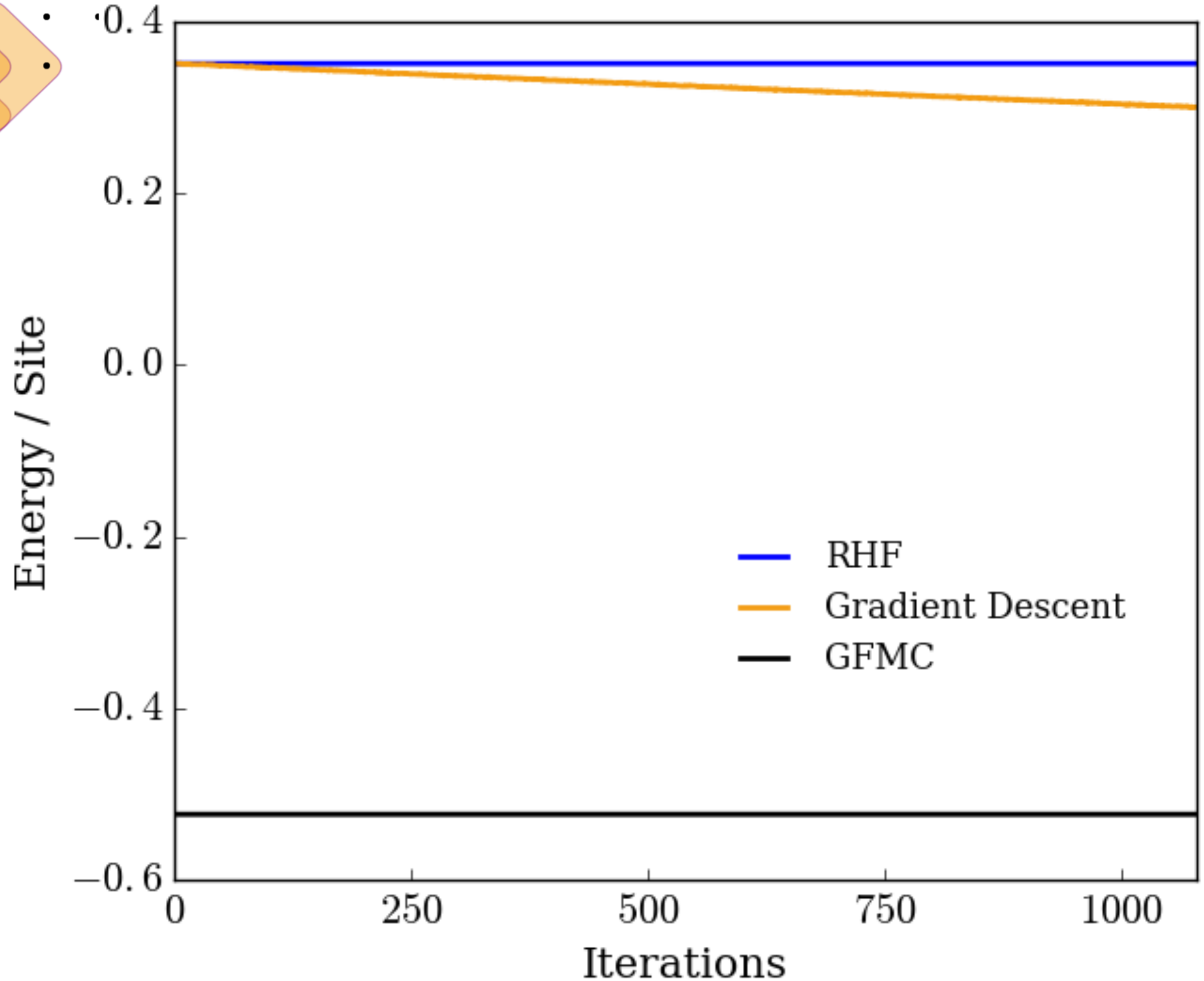

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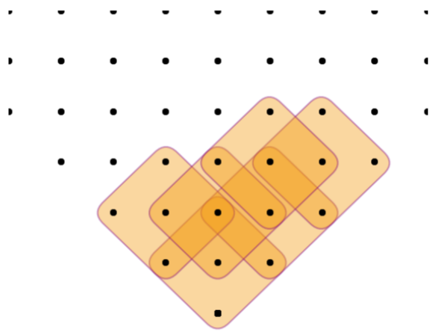
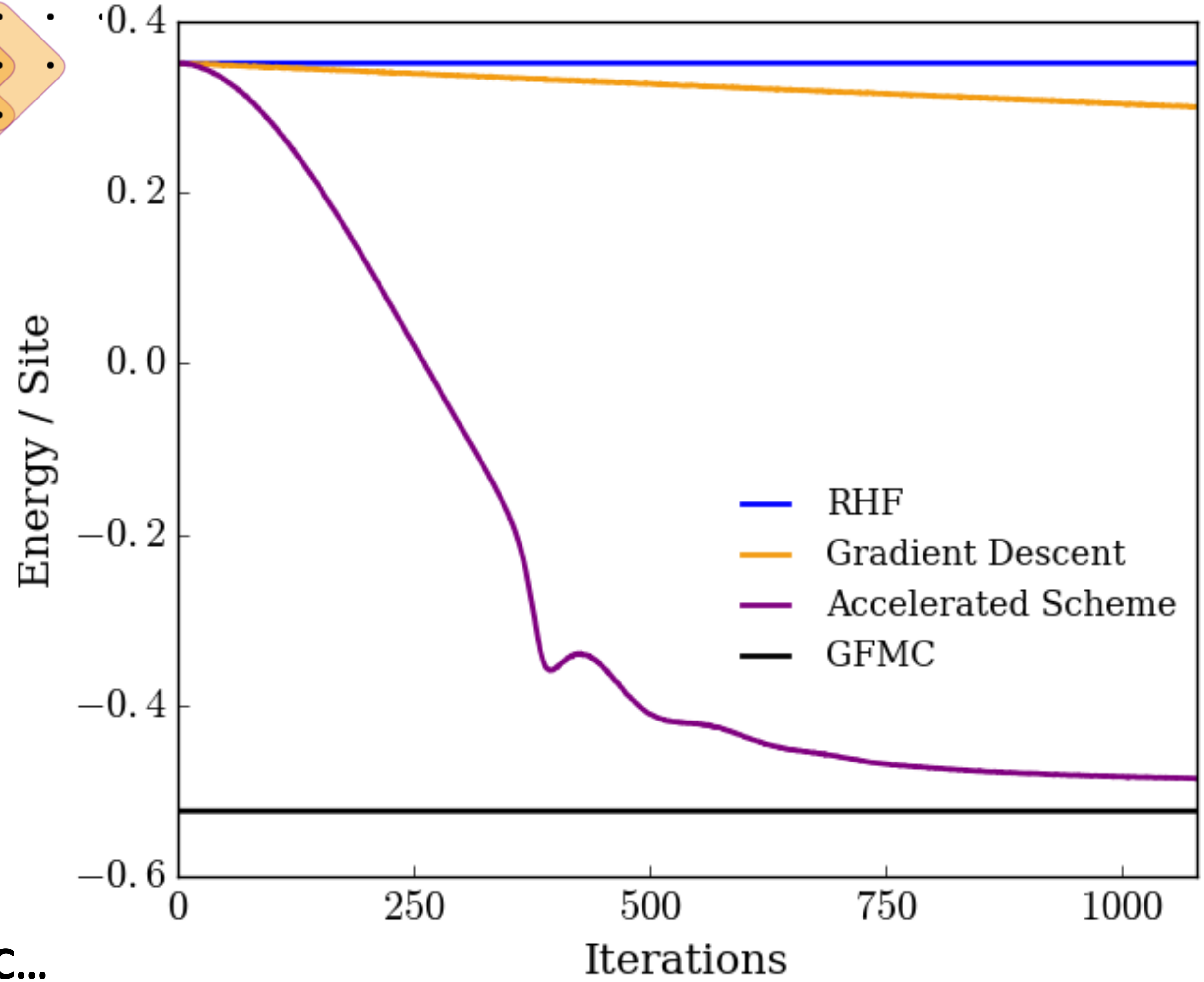
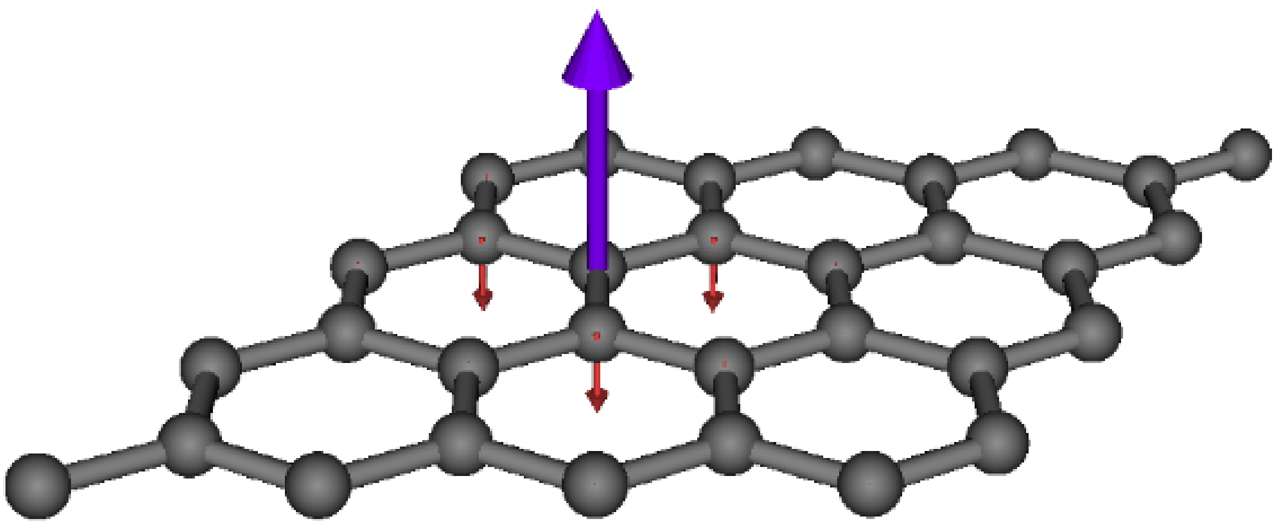




Million+ parameter VMC…

Non-linear projector Monte Carlo

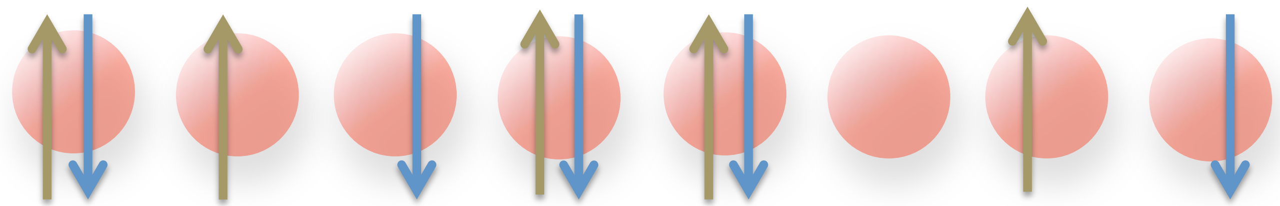
4 x 4 Graphene sheet
Local p-space Gaussian functions from VASP



Low-energy correlated spin-fluctuations

?

- How to choose parameterization?
- How to optimize variables with MC?
- How to reduce parameter space?

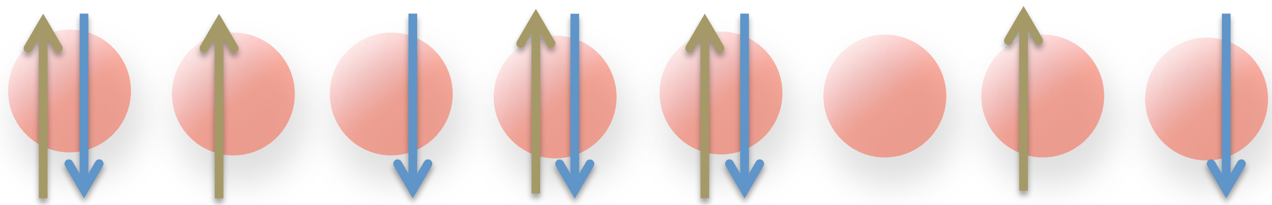


‘Parameter-space’ → **‘Data-space’**

Modern fitting of Potential Energy Surfaces $E(r_1, r_2, r_3, \ldots, r_N)$

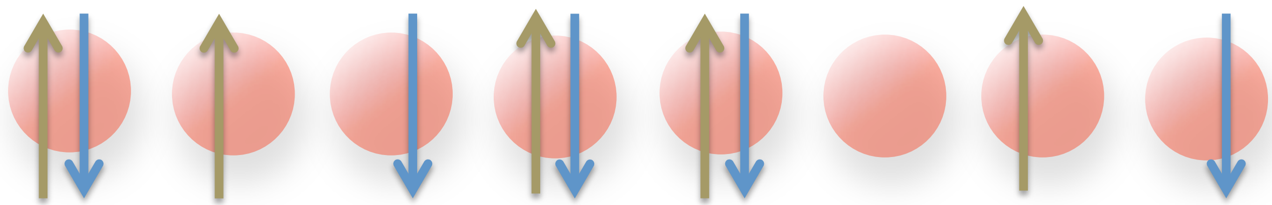
Statistical inference
(Gaussian Process Regression)

Aldo Glielmo



‘Parameter-space’ → **‘Data-space’**

f(plaquette parameters)	*f*(*distance* from *data* points)
• Explicit parameters	• Implicit parameters (never referenced directly)
• Iterative Non-linear fitting	• Analytic optimal fitting without expanding in variables
• Restricted to ‘small’ numbers of parameters	• No restriction in number of parameters
• Optimize parameters	• Optimize datapoints



‘Parameter-space’ → **‘Data-space’**

$$\Psi(\mathbf{r}) = e^{\left(\sum_{\mathbf{d}} k_{\mathbf{rd}} \alpha_{\mathbf{d}}\right)} \phi_{SD}(\mathbf{r}) |\mathbf{r}\rangle$$

“Distance” to data points

Weight of data points

- Independent of number of underlying parameters
- Linear with number of “data” configurations

Data:

Subset of configurations and their amplitudes

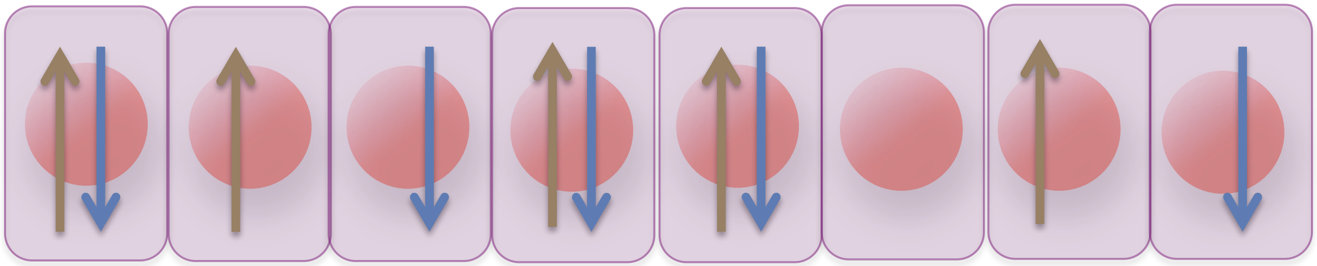
e.g. All configurations on ‘small’ system, then infer amplitudes on ‘large’ system

Distance “Covariance Kernel”:

Quantify ‘similarity’ (covariance) between two configurations:

How likely is it that their amplitudes are similar?

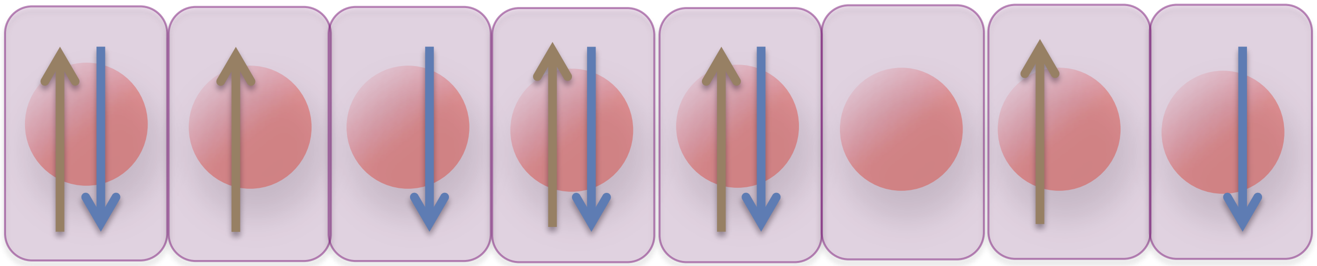
Many-body expansion



K1: How many unoccupied (Holons), up, down, Doubly-occupied (Doublons)?

$$\begin{pmatrix} \#unocc \\ \#up \\ \#down \\ \#doub \end{pmatrix}$$

Many-body expansion

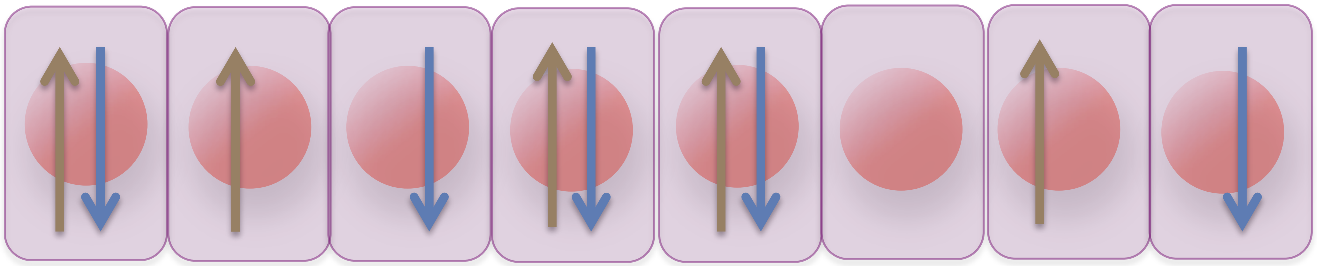


K1: How many unoccupied (Holons), up, down, Doubly-occupied (Doublons)?

$$k_{1,2} = \begin{pmatrix} \#unocc \\ \#up \\ \#down \\ \#doub \end{pmatrix}_1 \cdot \begin{pmatrix} \#unocc \\ \#up \\ \#down \\ \#doub \end{pmatrix}_2$$

Does not need to refer to the same sized system

Many-body expansion



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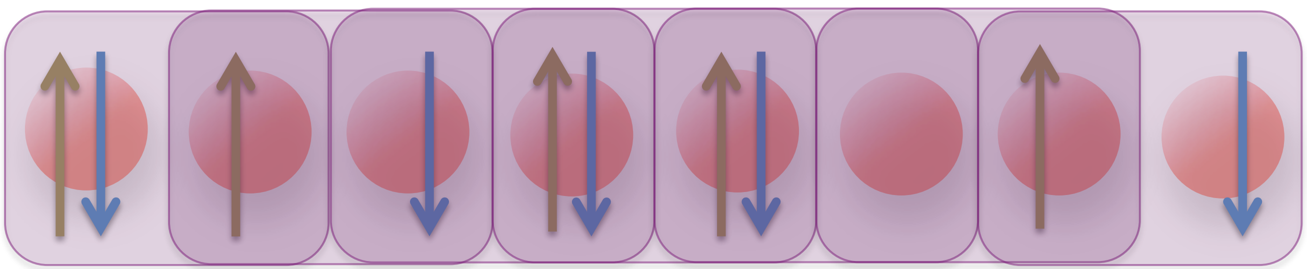
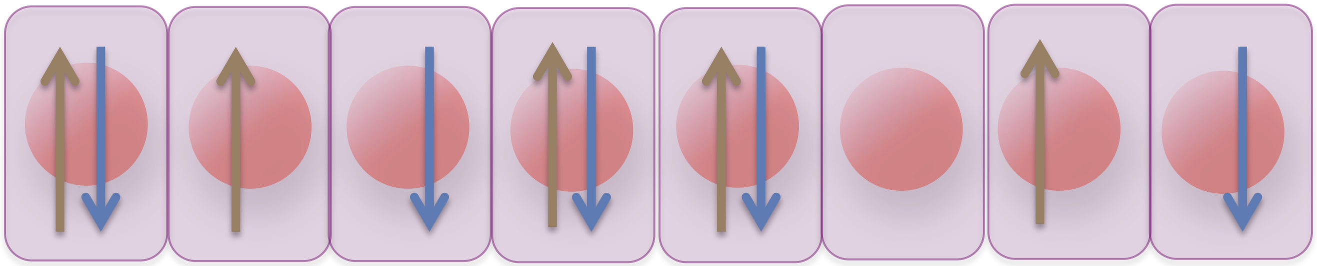


K2: Start to build in (local) anti-ferromagnetic correlation, Holon-Doublon binding

16-dimensional 'feature' space

Many-body expansion



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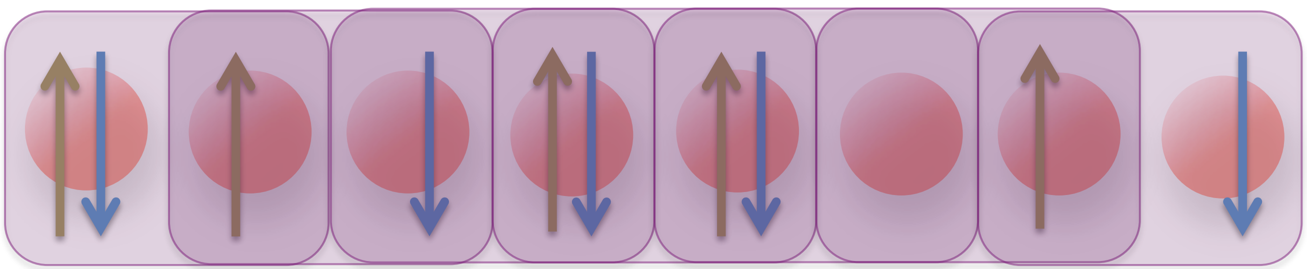

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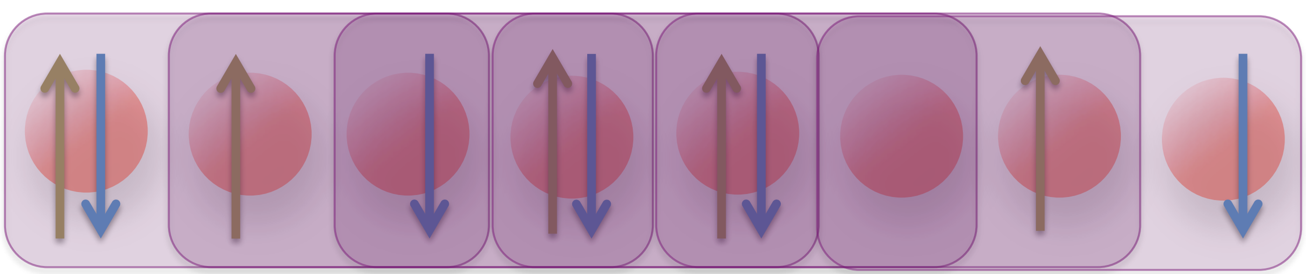
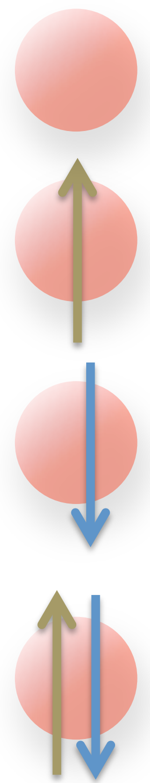


K3: 3-site descriptors

Gutzwiller Projection:



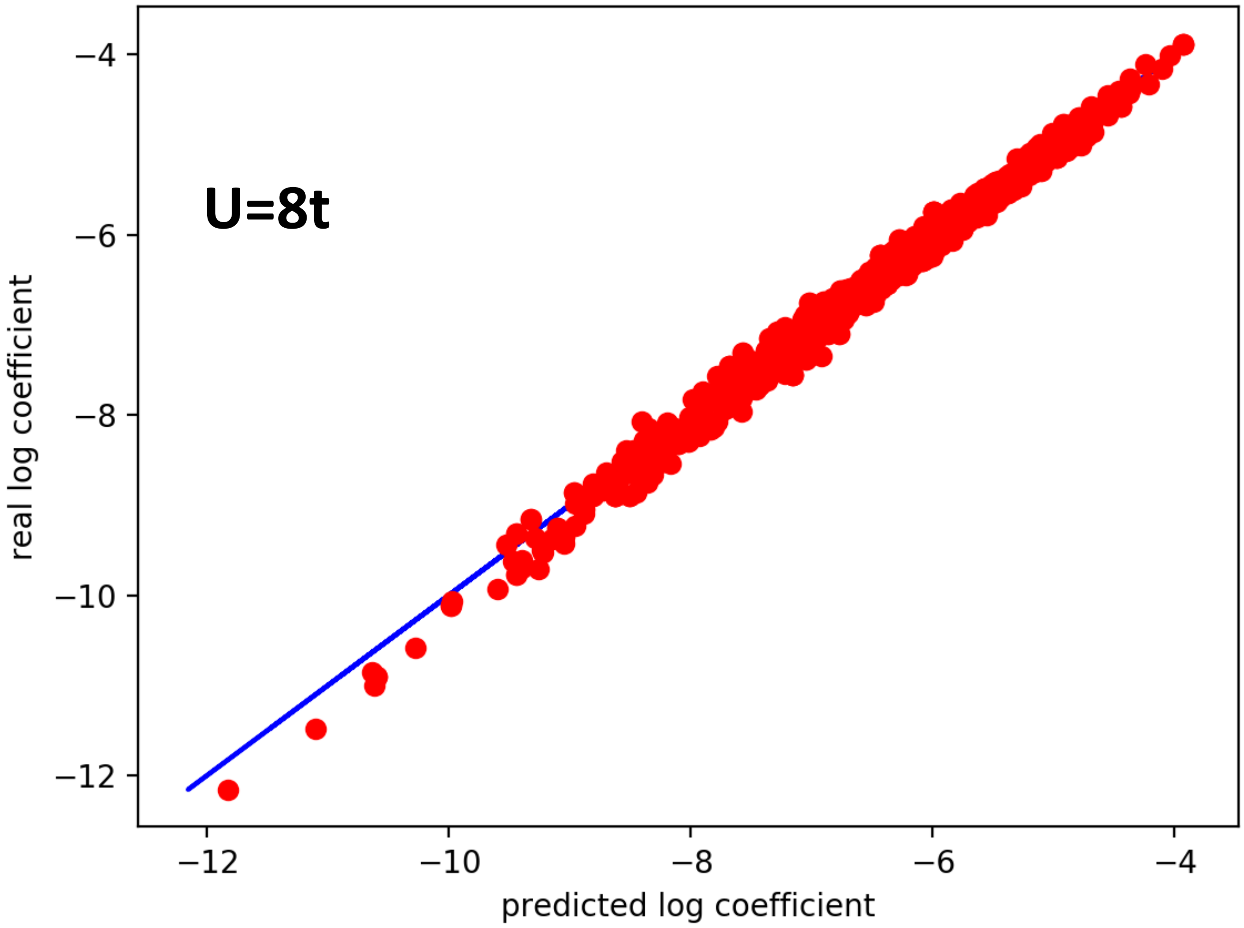
= 1.0

= 1.0

= 1.0

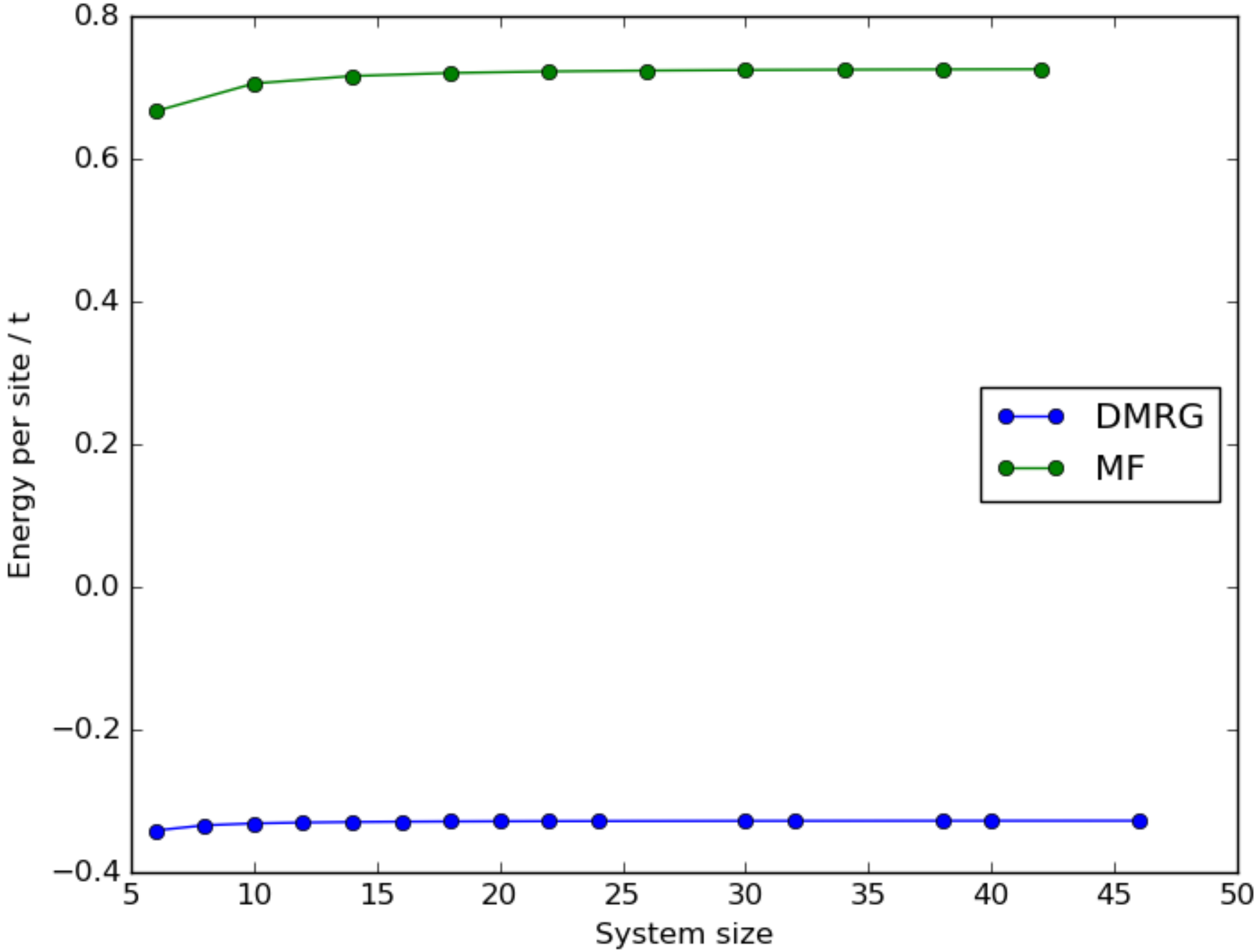
= 0.0

Extrapolation errors: Can we reproduce **10-site wave function from 6-site data**?



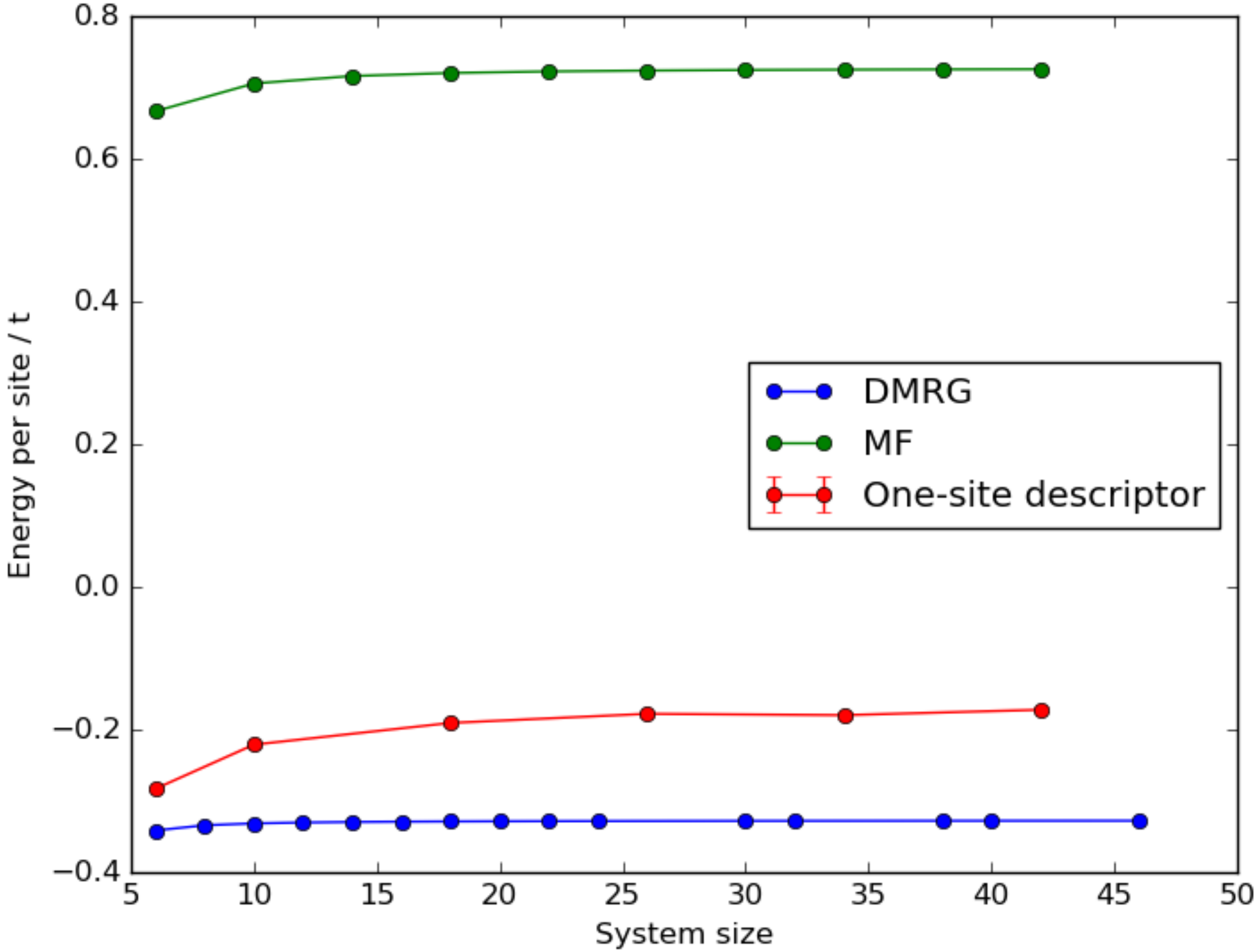
All 6-site fluctuations with all symmetries conserved

1D Hubbard Model, U=8t



400 linear coefficients from 6-site model

1D Hubbard Model, U=8t



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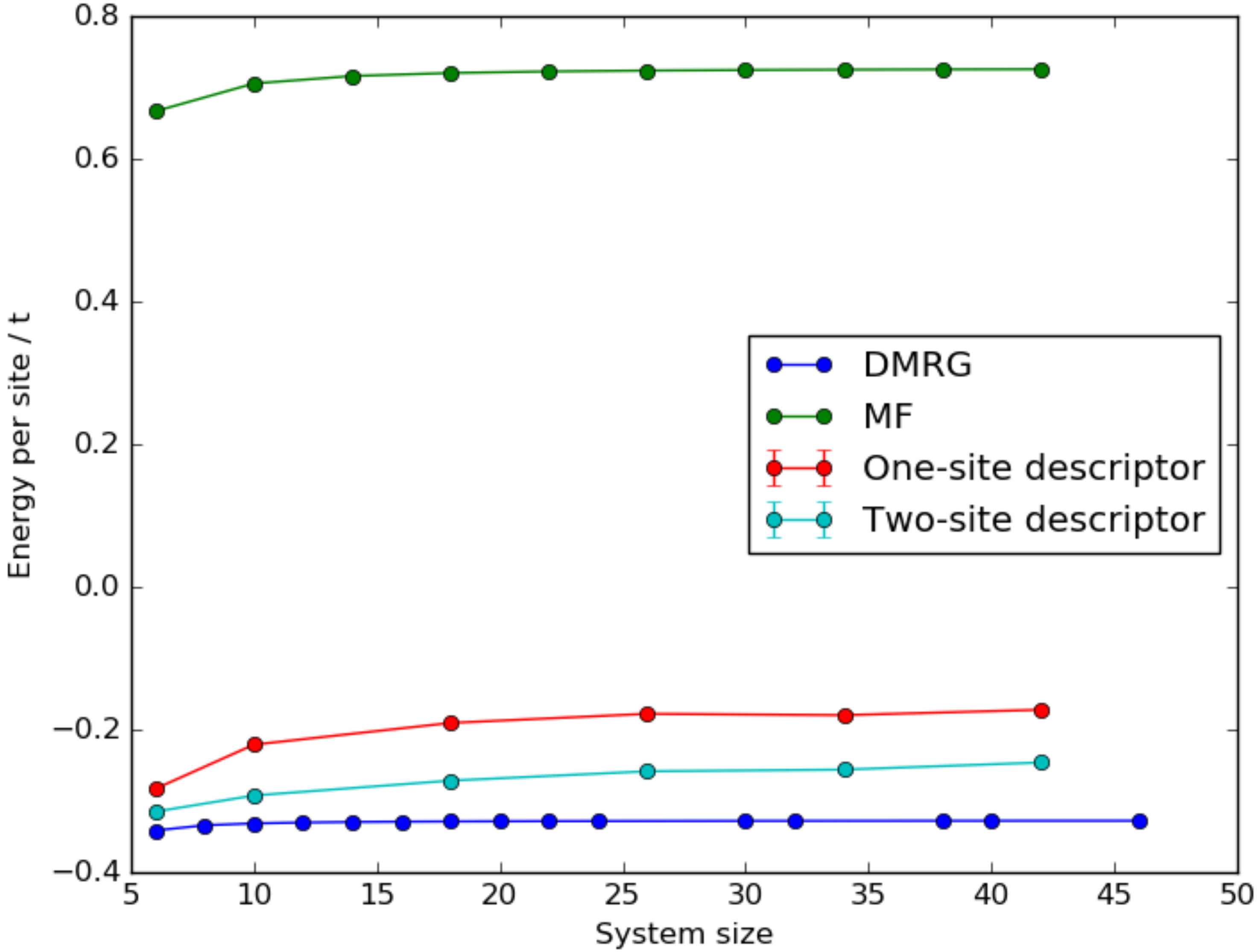

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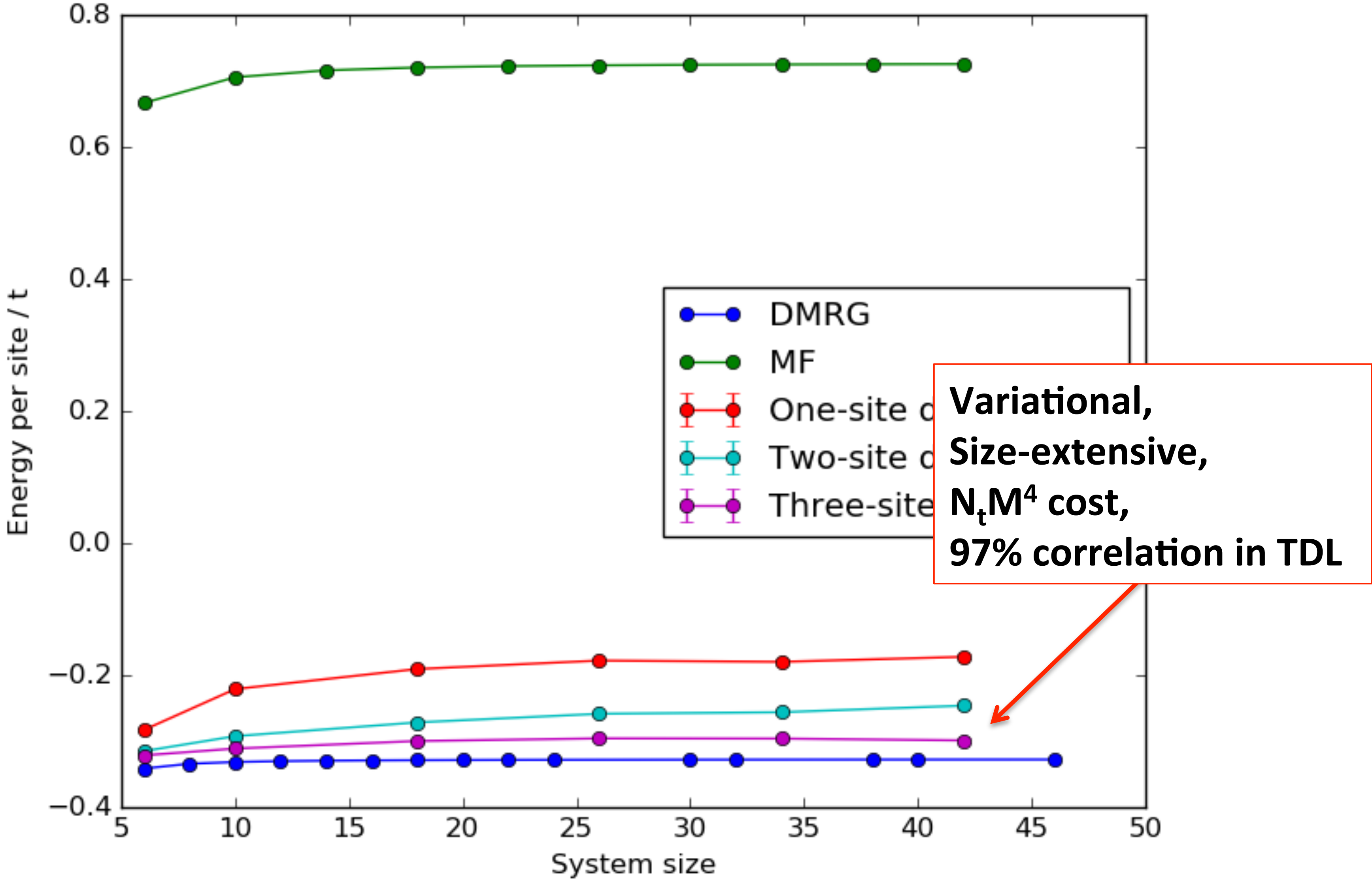
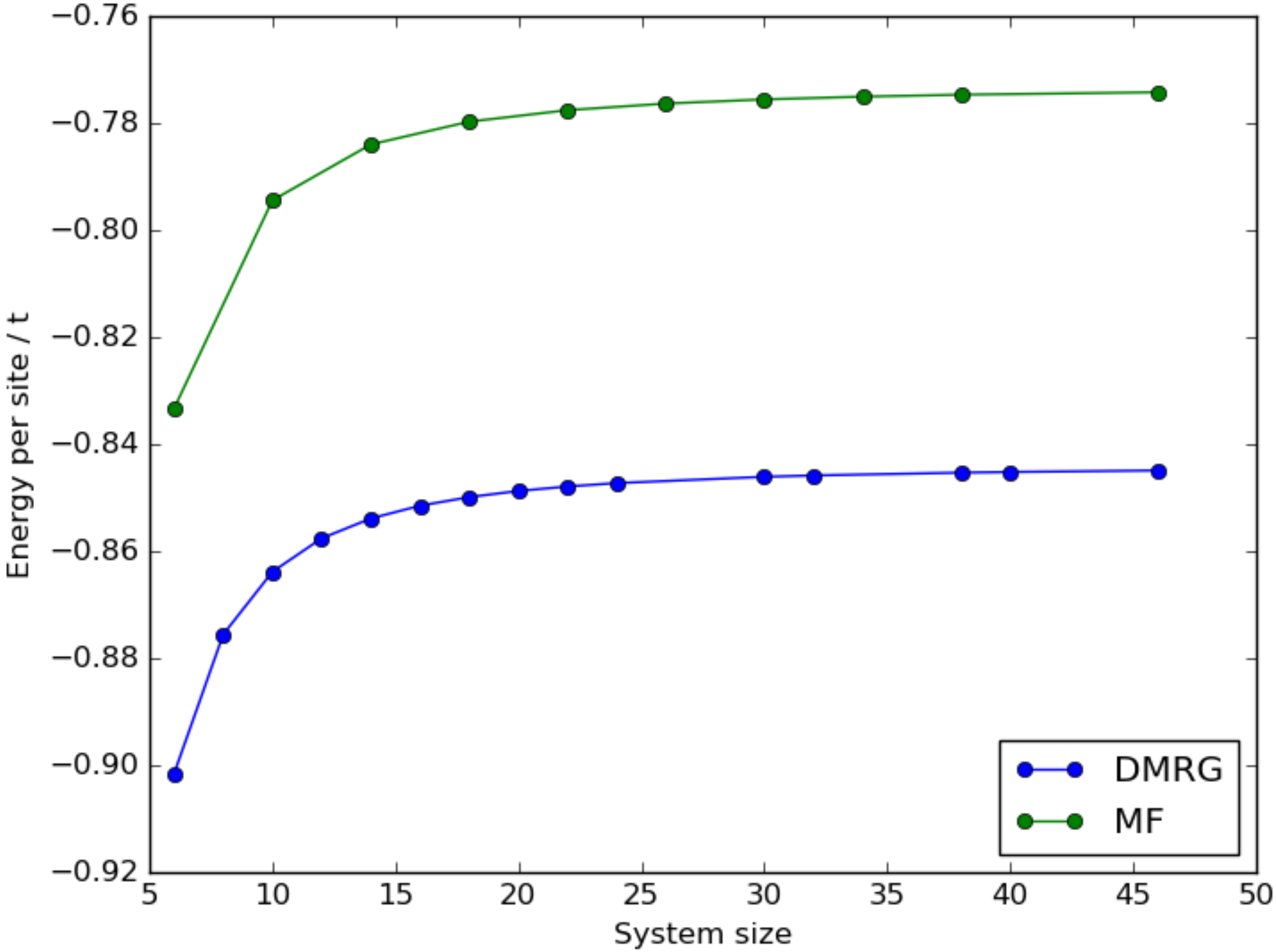


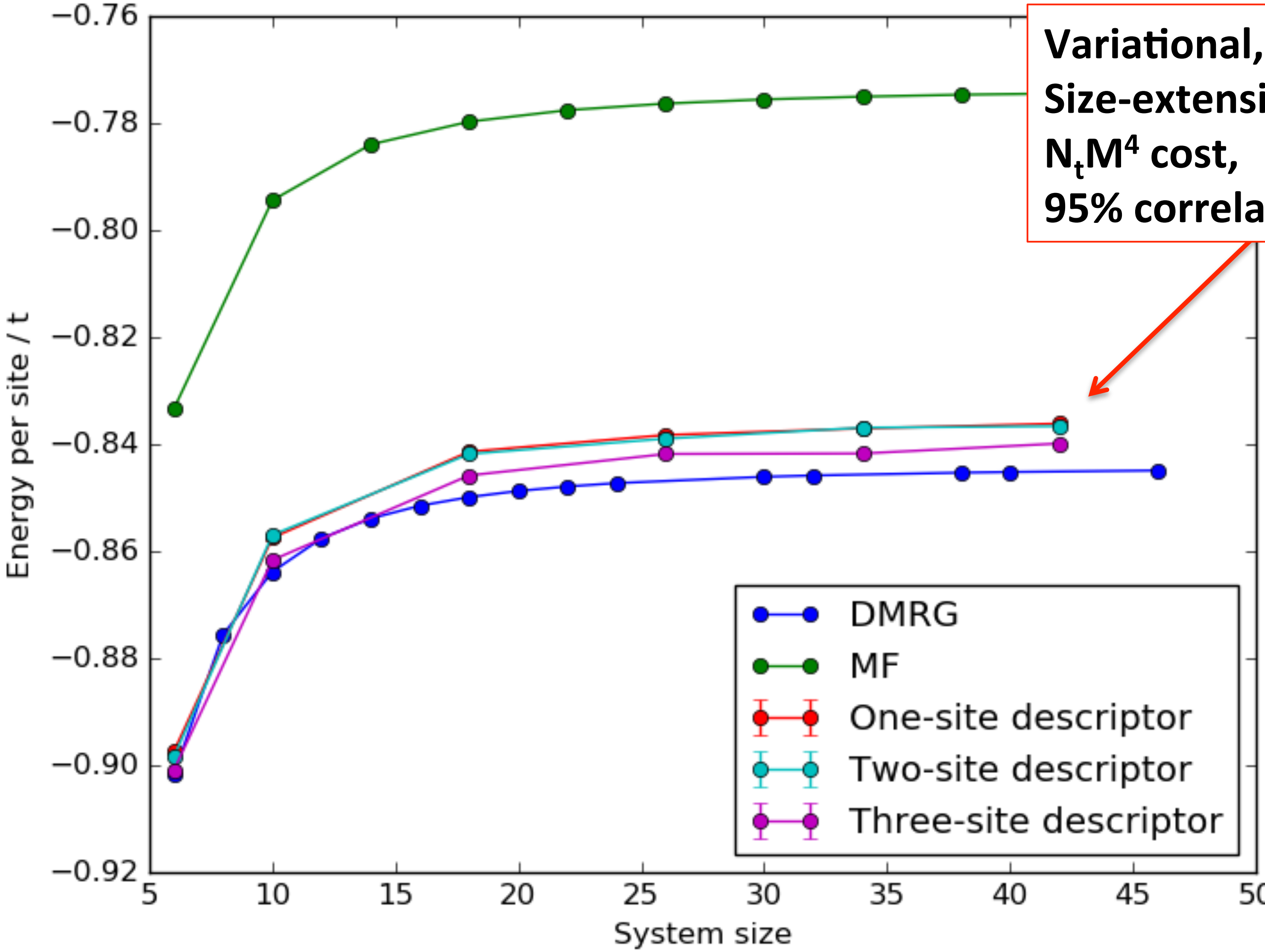
400 linear coefficients from 6-site model

1D Hubbard Model, U=2t



400 linear coefficients from 6-site model

1D Hubbard Model, U=2t

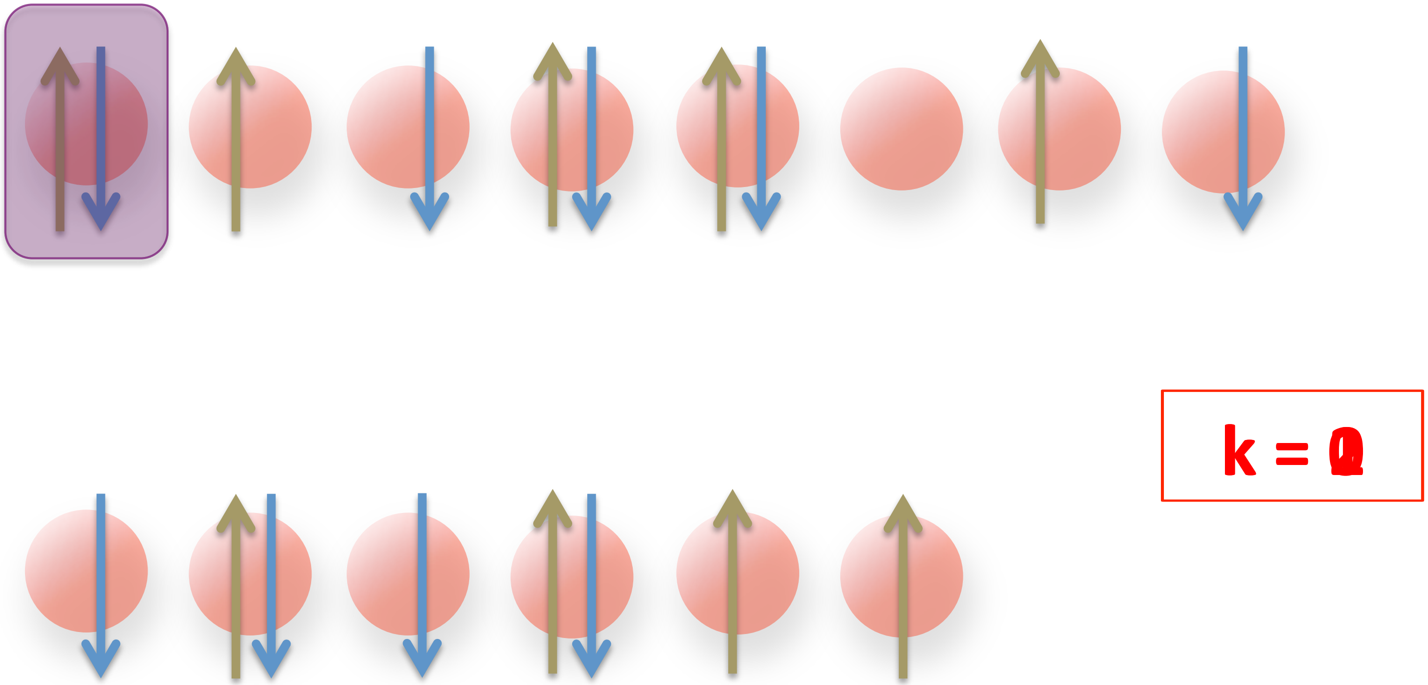


Variational,
Size-extensive,
$N_t M^4$ cost,
95% correlation in TDL

400 linear coefficients from 6-site model

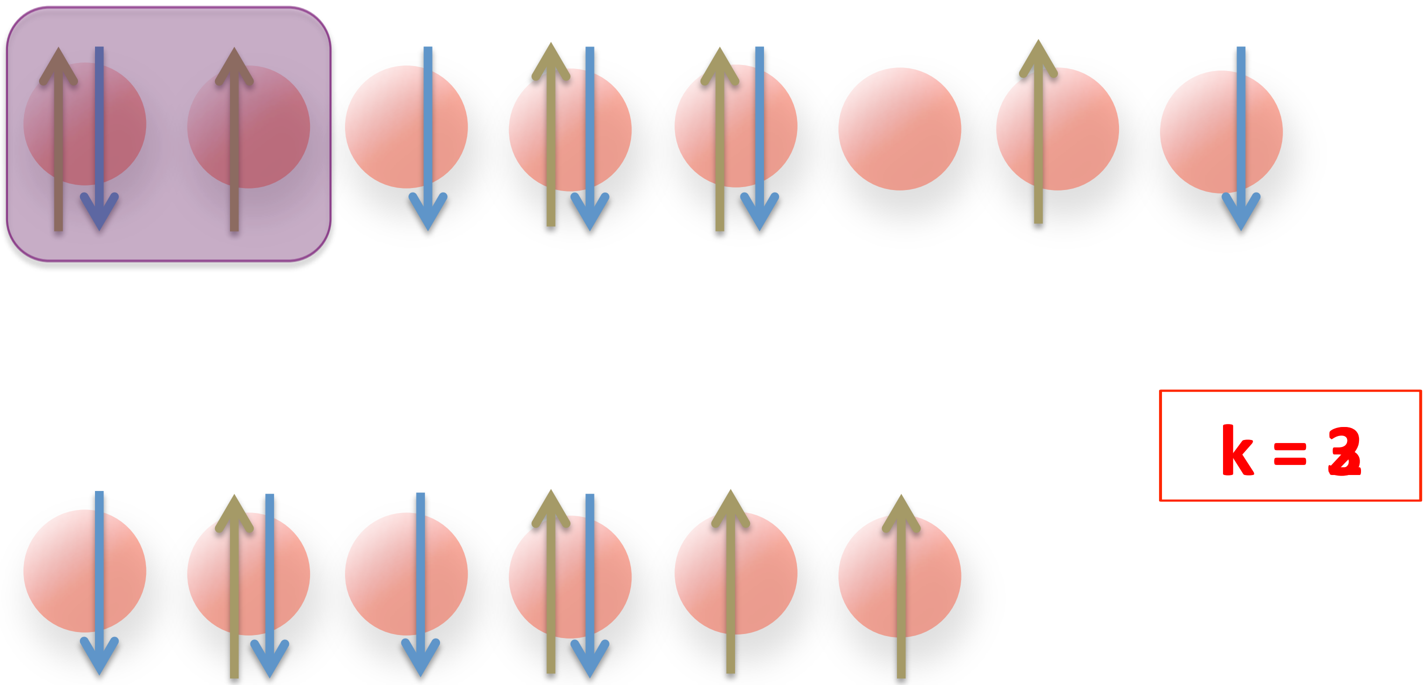
How to we avoid constructing these vectors…?

How to we avoid constructing these vectors…?



L^2 cost to evaluate contribution to kernel function **between any two configurations, for any plaquette topology, independent of size**

How to we avoid constructing these vectors…?



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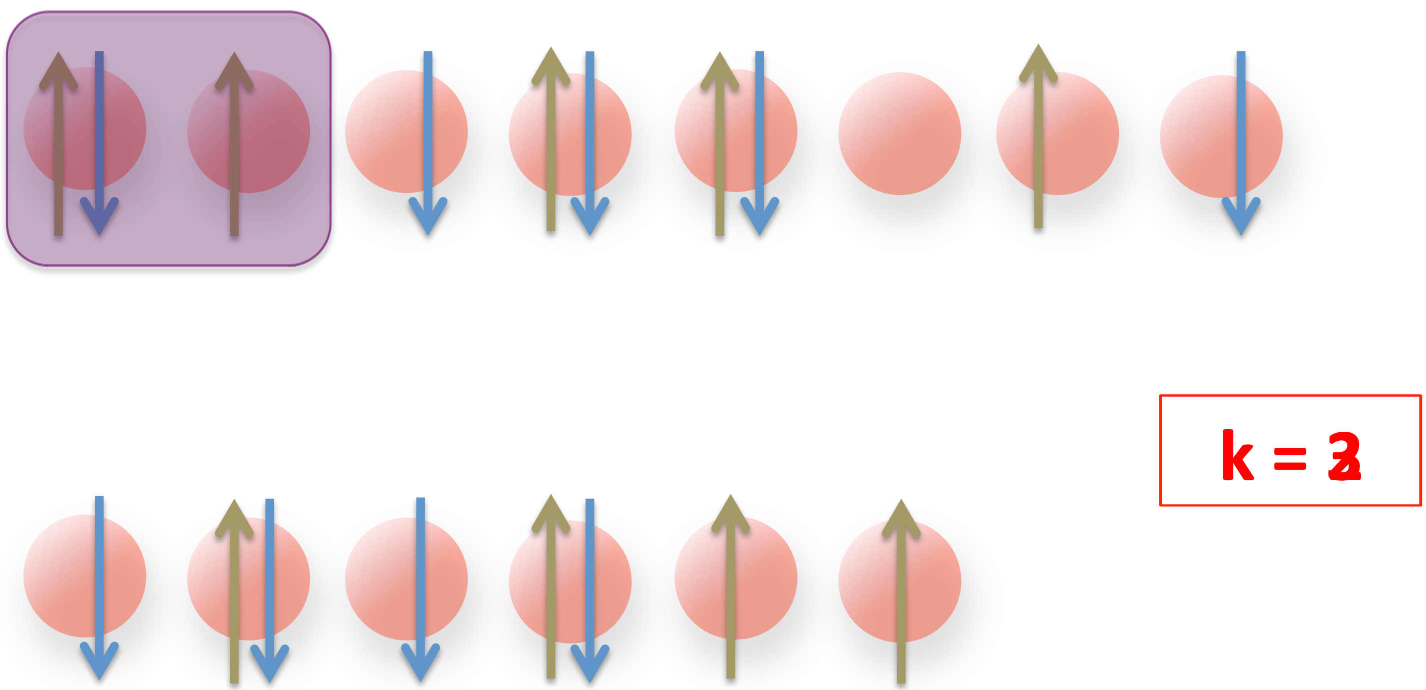
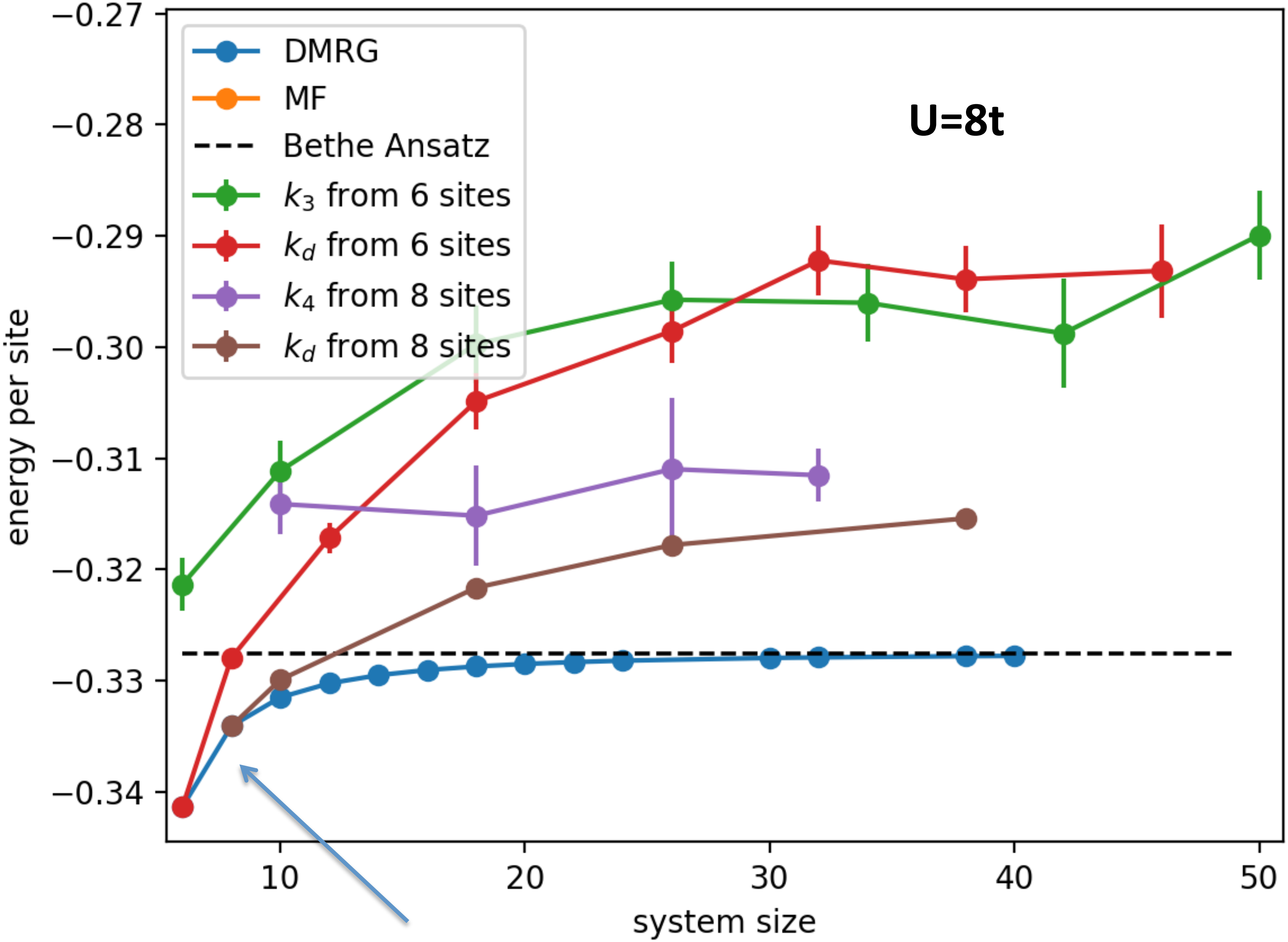
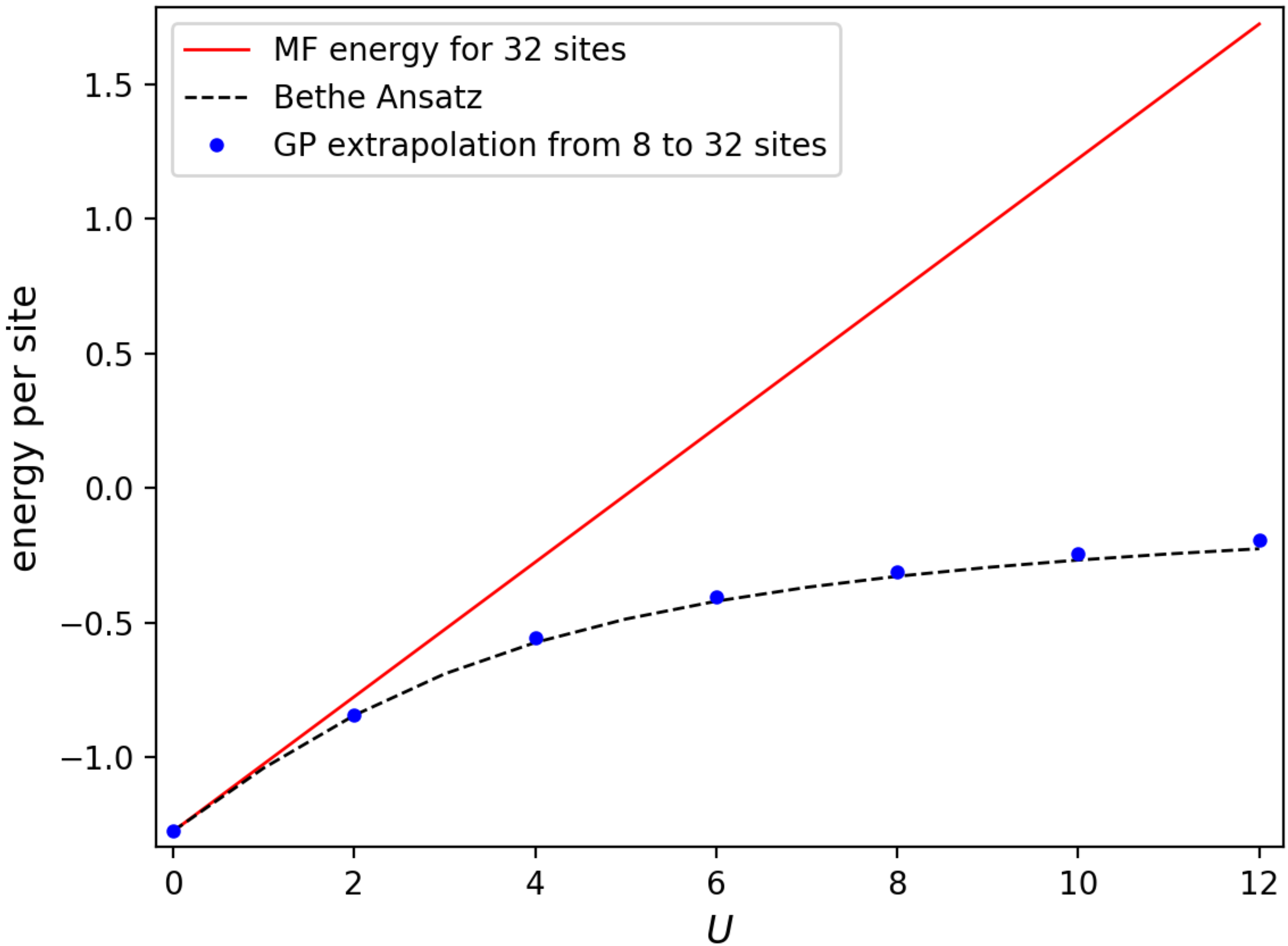


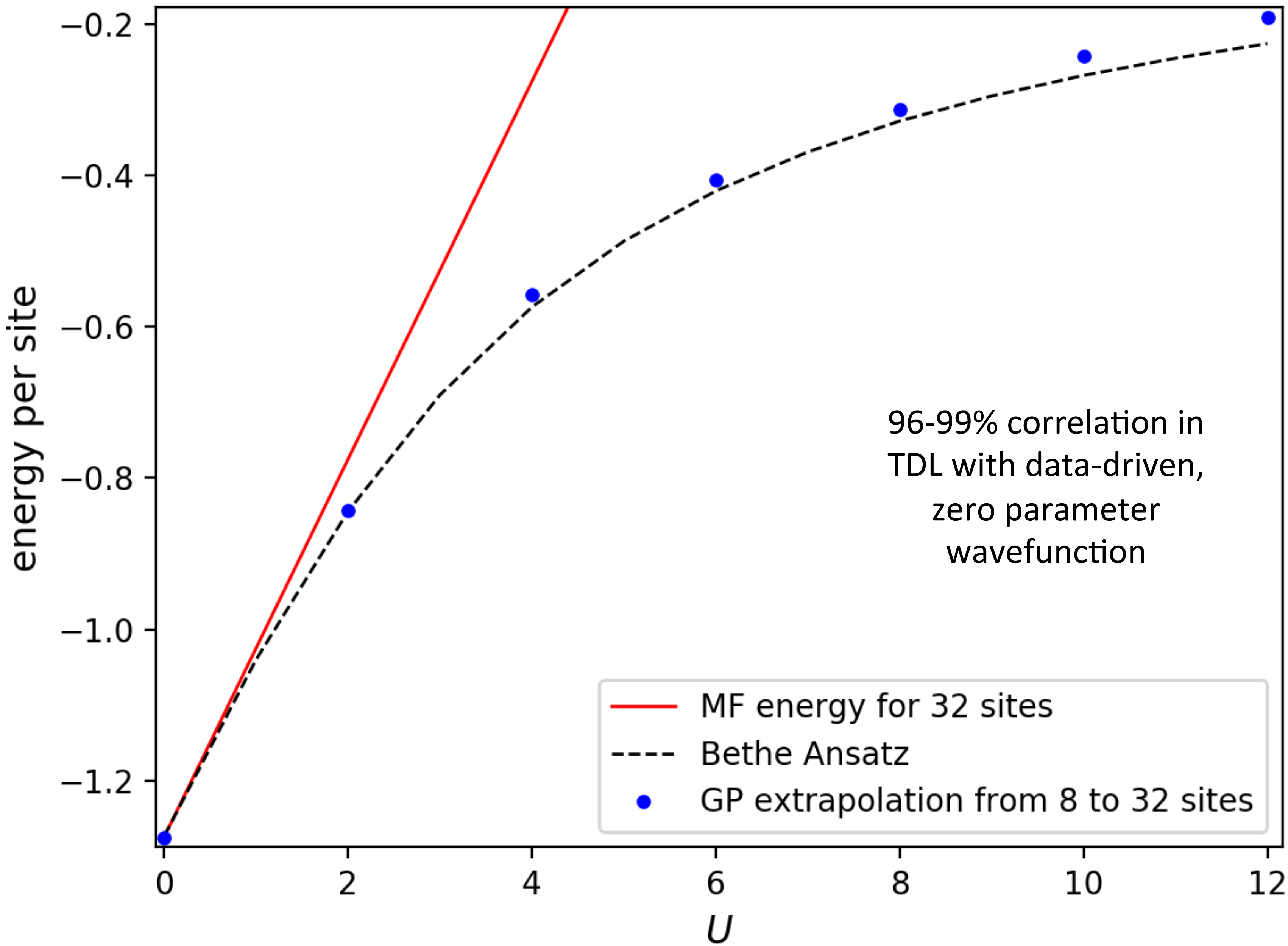
- **L^3 cost** to evaluate *all* possible plaquettes of *all* topology to quantify configurational similarity (k_d)
- **Exponentially** large 'feature' space of implicit plaquette parameters
- **Exact results with exact data**
- Beware of *overfitting*… (Hyperparameters avoid this)



Exact results for data with *complete* plaquette space

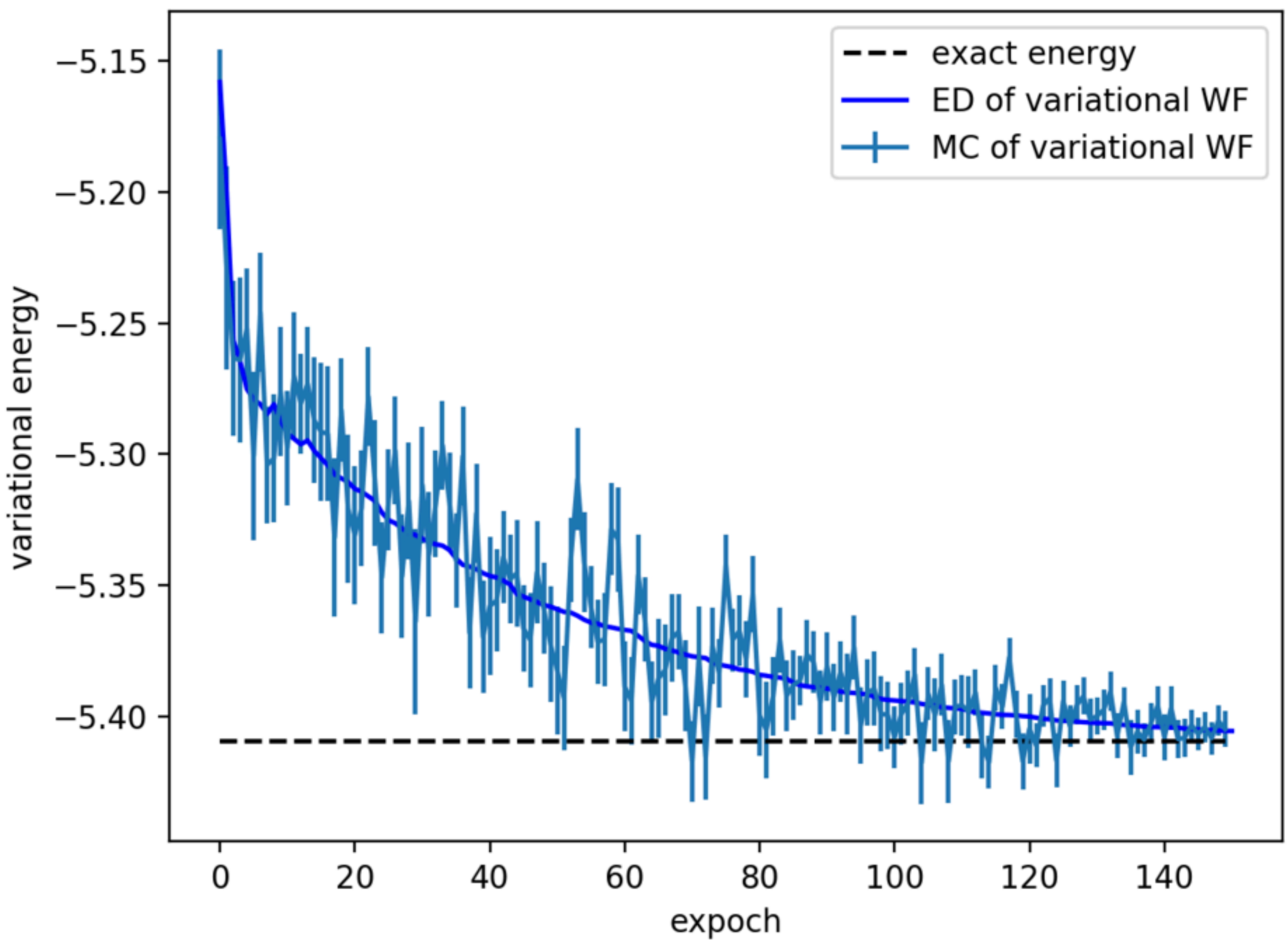


MF energy for 32 sites
Bethe Ansatz
GP extrapolation from 8 to 32 sites
energy per site
1.5
1.0
0.5
0.0
−0.5
−1.0
0
2
4
6
8
10
12
U



−0.2
−0.4
−0.6
−0.8
−1.0
−1.2
energy per site
0
2
4
6
8
10
12
U
96-99% correlation in TDL with data-driven, zero parameter wavefunction
MF energy for 32 sites
Bethe Ansatz
GP extrapolation from 8 to 32 sites

Optimize parameters → Optimize Data



Conclusions

- **Accelerated Gradient Descent** technique for combining projector and variational QMC

- **Data-driven wavefunctions** as an intriguing new approach to formulations of lattice models
  - Early development, but clear extension to 2D systems

Thanks

PhD and Postdoc positions available in the group!

Non-linear stochastic optimizations:

Lauretta Schwarz

Gaussian Process Wavefunctions:

Aldo Glielmo, Sandro de Vita, Gabor Csanyi