Eigenvector continuation in nuclear physics

Sebastian König, TU Darmstadt

TRIUMF Nuclear Theory Workshop, Vancouver, BC

March 1, 2019

SK, A. Ekström, K. Hebeler, A. Sarkar, D. Lee, A. Schwenk, in preparation

Motivation

Many physics problems are tremendously difficult…

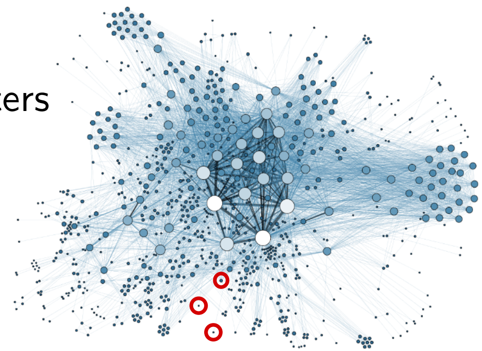
- huge matrices, possibly too large to store
  - ever more so given the evolution of typical HPC clusters
- most exact methods suffer from exponential scaling
- **interest only in a few (lowest) eigenvalues**

Martin Grandjean, via Wikimedia Commons (CC-AS 3.0)

Motivation

Many physics problems are tremendously difficult…

- huge matrices, possibly too large to store
  - ever more so given the evolution of typical HPC clusters
- most exact methods suffer from exponential scaling
- **interest only in a few (lowest) eigenvalues**



Martin Grandjean, via Wikimedia Commons (CC-AS 3.0)

Introducing eigenvector continuation

D. Lee, TRIUMF Ab Initio Workshop 2018; Frame et al., PRL **121** 032501 (2018)

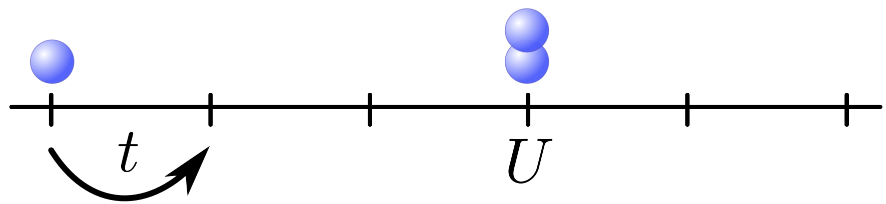
KDE Oxygen Theme

- novel numerical technique
- can solve otherwise untractable problems
- amazingly simple in practice
- broadly applicable
- **this talk: look for nuclear nails**

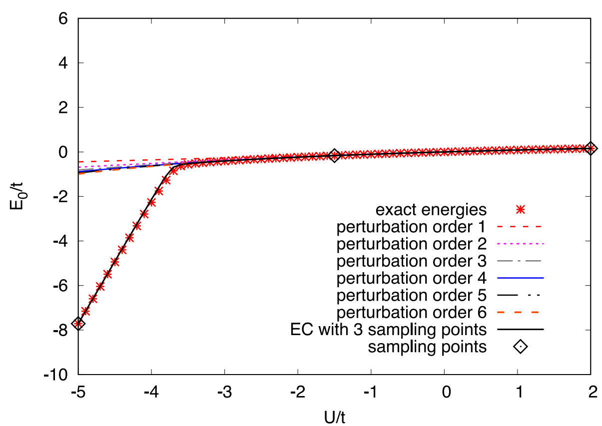
Hubbard model

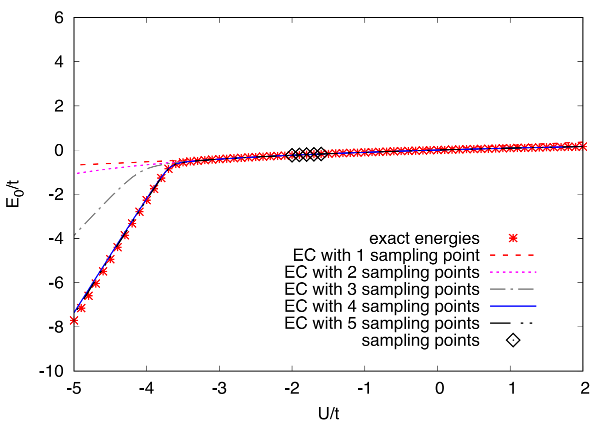
Frame et al., PRL **121** 032501 (2018)

- three-dimensional Bose-Hubbard model (4 bosons on $4 \times 4 \times 4$ lattice)
- hopping parameter t, on-site interaction $U \rightsquigarrow H = H(c = U/t)$



- Bose gas for $c > 0$, weak binding for $-3.8 < c < 0$, tight cluster for $c < -3.8$
- **eigenvector continuation can extrapolate across regimes**





General idea

Scenario

Frame et al., PRL **121** 032501 (2018)

- consider physical state (eigenvector) in a large space
- **parametric dependence of Hamiltonian $H(c)$ traces only small subspace**

Procedure

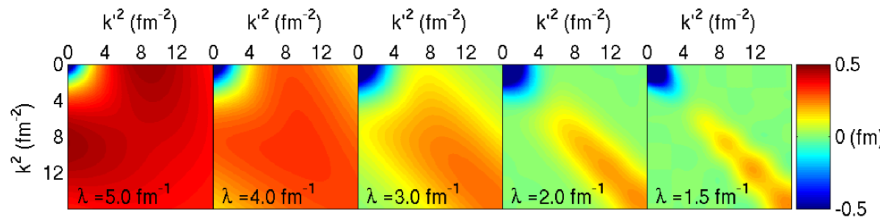
- calculate $|\psi(c_i)\rangle$, $i = 1, \ldots N_{\mathrm{EC}}$ in "easy" regime
- solve generalized eigenvalue problem $H|\psi\rangle = \lambda N|\psi\rangle$ with
  - $H_{ij} = \langle\psi_i|H(c_{\mathrm{target}})|\psi_j\rangle$
  - $N_{ij} = \langle\psi_i|\psi_j\rangle$

Prerequisite

- smooth dependence of $H(c)$ on c
- enables analytic continuation of $|\psi(c)\rangle$ from c_{easy} to c_{target}

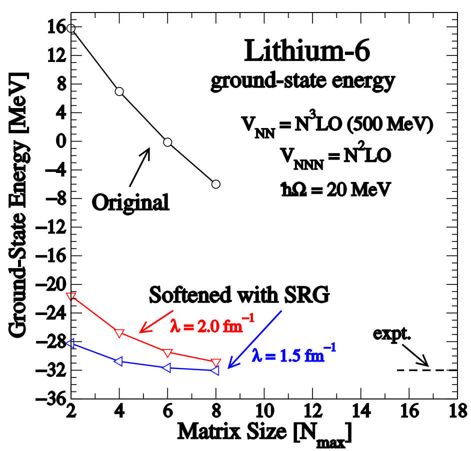
SRG evolution

- unitary transformation of Hamiltonian: $H \to H_\lambda = U_\lambda H U_\lambda^\dagger \rightsquigarrow V_\lambda$
- decouple low and high momenta at scale λ

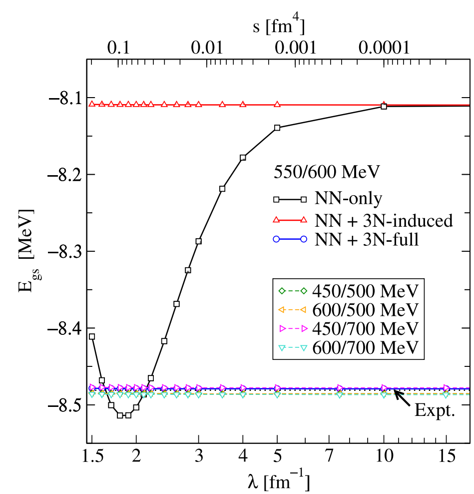


R. Furnstahl, HUGS 2014 lecture slides

- **interaction becomes more amenable to numerical methods...**
- **...at the cost of induced many-body forces!**



Bogner et al., PPNP 65 94 (2010)



Hebeler+Furnstahl, RPP **76** 126301 (2013)

SRG evolution = ODE solving

$$\frac{\mathrm{d}H_s}{\mathrm{d}s} = \frac{\mathrm{d}V_s}{\mathrm{d}s} = [[G, H_s], H_s]\,,\ \lambda = 1/s^{1/4}$$

ordinary differential equation ensures smooth parametric dependence

$\hookrightarrow$ **SRG evolution satisfies EC prerequisites!**

Reverse SRG

Consider A = 3,4 test cases

- EMN N3LO(500) interaction, Jacobi NCSM calculation

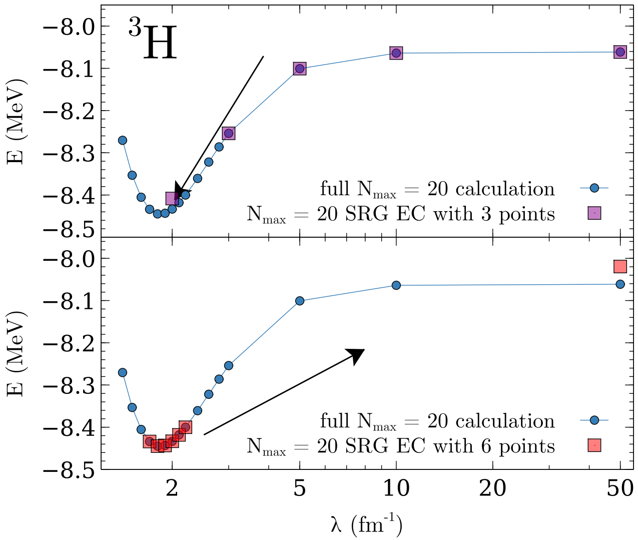
Entem et al., PRC **96** 024004 (2017); A. Ekström implementation of Navratil et al., PRC **61** 044001 (2000)

Reverse SRG

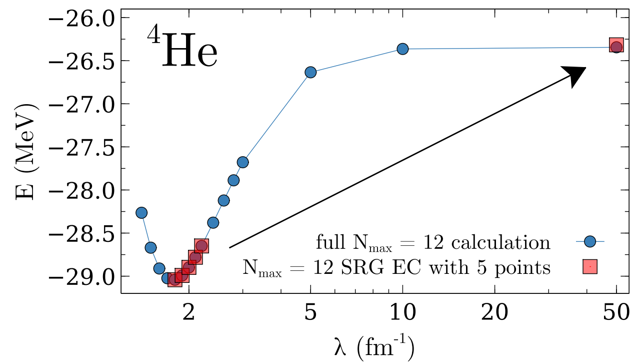
Consider A = 3,4 test cases

- EMN N3LO(500) interaction, Jacobi NCSM calculation

Entem et al., PRC **96** 024004 (2017); A. Ekström implementation of Navratil et al., PRC **61** 044001 (2000)



Not even induced 3N forces kept here!

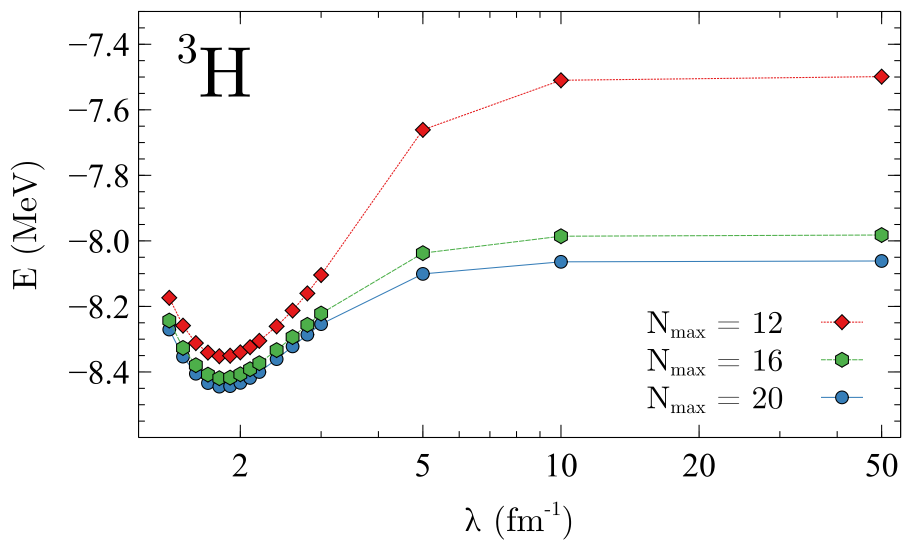


- possible to extrapolate back from small λ to bare interaction
- **information about missing many-body forces in wavefunctions**
  - not in any single wavefunction, but in how they change

Mind the gap

Still no free lunch, however...

- EC is a variational method
- **cannot go beyond what bare interaction gives in same model space!**



So now what?

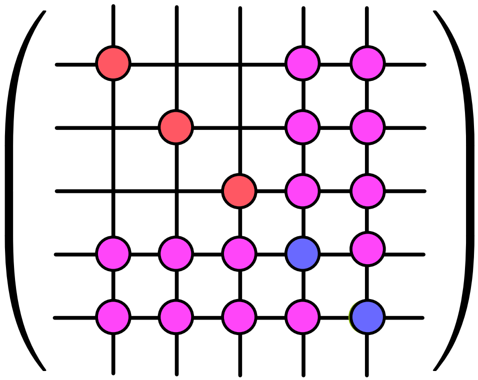
Perturbation theory

- **consider a Hamiltonian diagonalized in a (small) subspace**

$$H = \begin{pmatrix} H_{\phi\phi} & H_{\phi\psi} \\ H_{\psi\phi} & H_{\psi\psi} \end{pmatrix}$$

$$N_0 = \dim H_{\phi\phi} \ll \dim H = N_1$$

$$H_{\phi\phi} = \mathrm{diag}(\{\lambda_i\}_{i=1,..N_0})$$



- factor out large number X from diagonal entries of $H_{\psi\psi}$
- perturbative expansion for lowest eigenvalue and vector

$$|\psi_1\rangle = \sum_{n=0}^{\infty} X^{-n} \left(\sum_{i=1}^{N_0} x_i^{(n)} |\phi_i\rangle + \sum_{j=N_0+1}^{N_1} x_j^{(n)} |\psi_j\rangle \right) \ , \ \lambda_1^{\mathrm{full}} = \sum_{n=0}^{\infty} X^{-n} \lambda_1^{(n)}$$

  - **matching powers gives coupled recursive expressions for $x_j^{(n)}$ and $\lambda_1^{(n)}$**

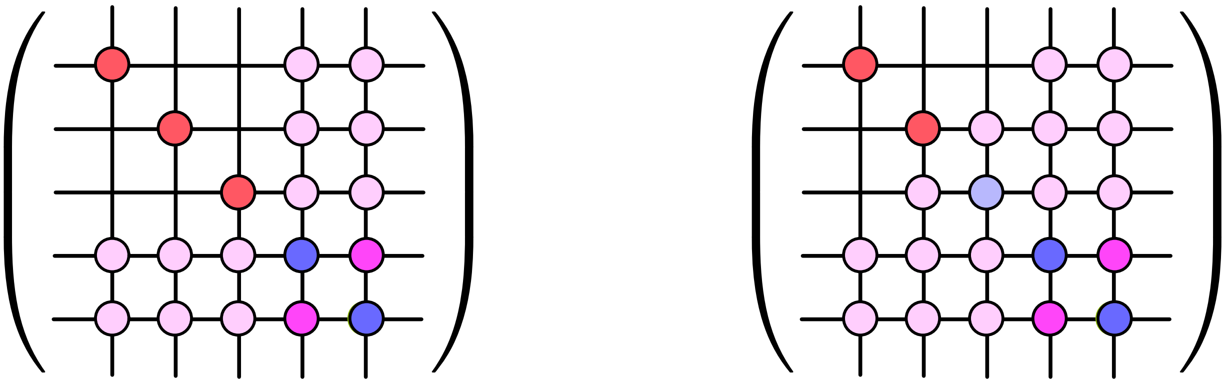
Perturbation theory (continued)

Diagonalizing a small space can still be too expensive...

Perturbation theory (continued)

Diagonalizing a small space can still be too expensive...

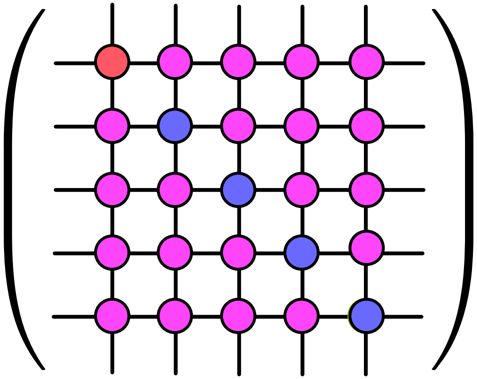
- actually, a partial diagonalization per se is ok ($\rightarrow$ Lanczos)
- but transforming the Hamiltonian is problematic...



- **cost for adjusting off-diagonal elements is prohibitive**
  - scales with size of the full (large) space

Way out

Start from one-dimensional space ($N_{\max} = 0$)...



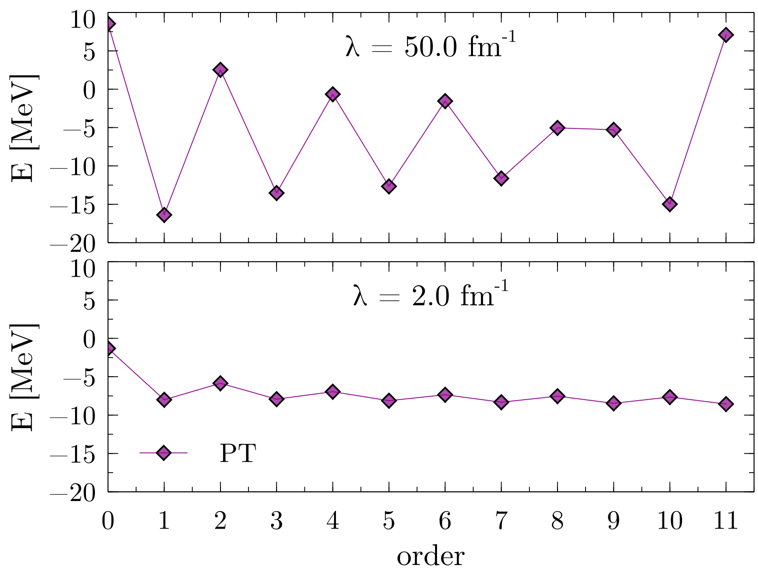
...i.e., directly use the given Hamiltonian

Failure

^{3}H NCSM calculation, $N_{\mathrm{max}} = 12$ model space

- EMN N3LO 500 interaction

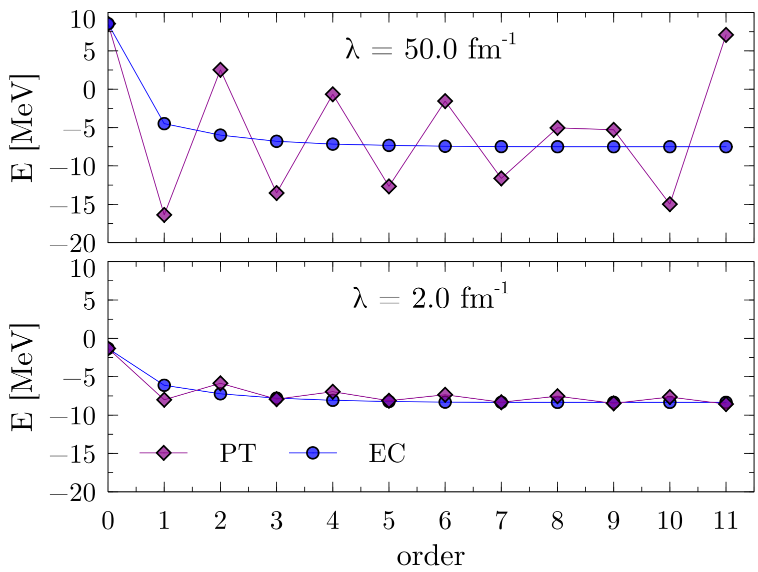
Entem et al., PRC **96** 024004 (2017)



- **perturbation theory does not converge!**
  - however, interaction clearly "more perturbative" for small SRG λ
  - convergence perhaps for very small λ

Saved by EC

- span space by the wavefunction corrections $|\psi_1^{(n)}\rangle \to x_j^{(n)}$, $n = 0, \cdots \text{order}$
- evaluate Hamiltonian between these states
- interpretation: $H = H_{\text{diag}} + c\,H_{\text{off-diag}}$, EC-extrapolate to $c = 1$



- **same input as PT, but now things converge (to the correct result!)**

Note

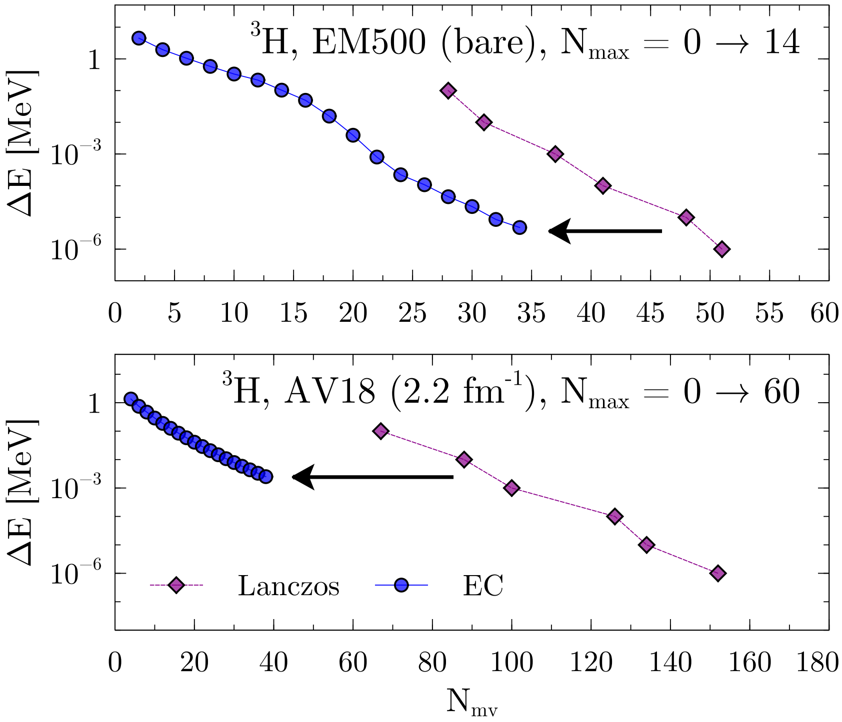
expensive part of is setting up the $x_j^{(n)}$, $j = 1, \cdots N_1$

essentially an N_1-dim. matrix-vector multiplication...

$\hookrightarrow$ compare PT-EC to Lanczos!

EC vs. Lanczos

- for EC: effective $N_{mv} = 2 \times (\text{order} - 1)$
- comparison: vanilla Lanczos in GNU Octave (i.e., ARPACK)



- **EC looks quite competitive in this benchmark!**
- **but note:** only calculating a single eigenvalue here

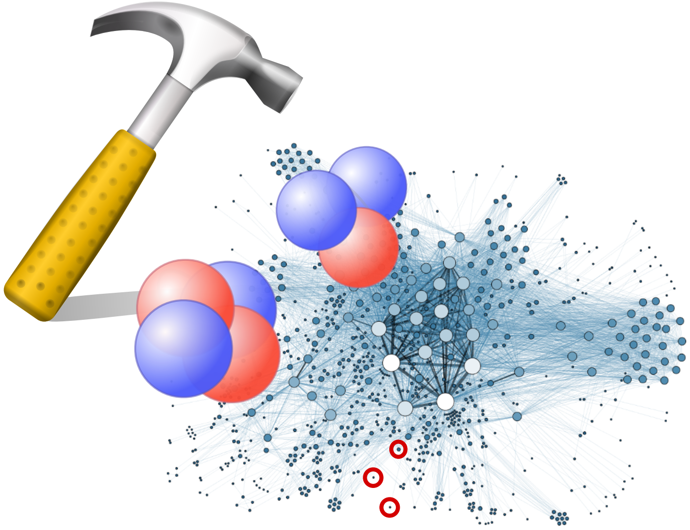
Summary and outlook

This talk

- **eigenvector continuation can be used to reverse SRG**
  - conceptually interesting: implicit information about induced forces
- **convergent perturbative model-space extension**
  - effectively tame divergent expansion coefficients
  - interesting as computational method

Future directions

- larger systems, other methods
  - in particular: m-scheme NCSM
- combined model-space and SRG EC
- other applications



Thanks...

...to my collaborators:

- A. Schwenk, K. Hebeler (TU Darmstadt)
- D. Lee, A. Sarkar (Michigan State U.)
- A. Ekström (Chalmers U.)

...for funding:

SFB 1245

DFG Deutsche Forschungsgemeinschaft

German Research Foundation

Thanks...

...to my collaborators:

- A. Schwenk, K. Hebeler (TU Darmstadt)
- D. Lee, A. Sarkar (Michigan State U.)
- A. Ekström (Chalmers U.)

...for funding:

SFB 1245

DFG Deutsche Forschungsgemeinschaft

German Research Foundation

...and to you, for your attention!