Alternative Generators for the Similarity Renormalization Group

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Ab initio Nuclear Structure

Nucleon Interaction

- Chiral Effective Field Theory
- NN and 3N

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Similarity Renormalization Group (SRG)

- Decoupling of high and low-energy physics

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Many-Body Methods

- No-Core Shell Model
- In-Medium SRG
- Coupled Cluster

Similarity Renormalization Group

- Continuous unitary transformation with flow parameter α

$$\boldsymbol{H}_\alpha = \boldsymbol{U}_\alpha^\dagger \boldsymbol{H}_0 \boldsymbol{U}_\alpha \qquad \Rightarrow \qquad \frac{\mathrm{d}\boldsymbol{H}_\alpha}{\mathrm{d}\alpha} = [\boldsymbol{\eta}_\alpha, \boldsymbol{H}_\alpha]$$

- Antihermitian dynamic generator

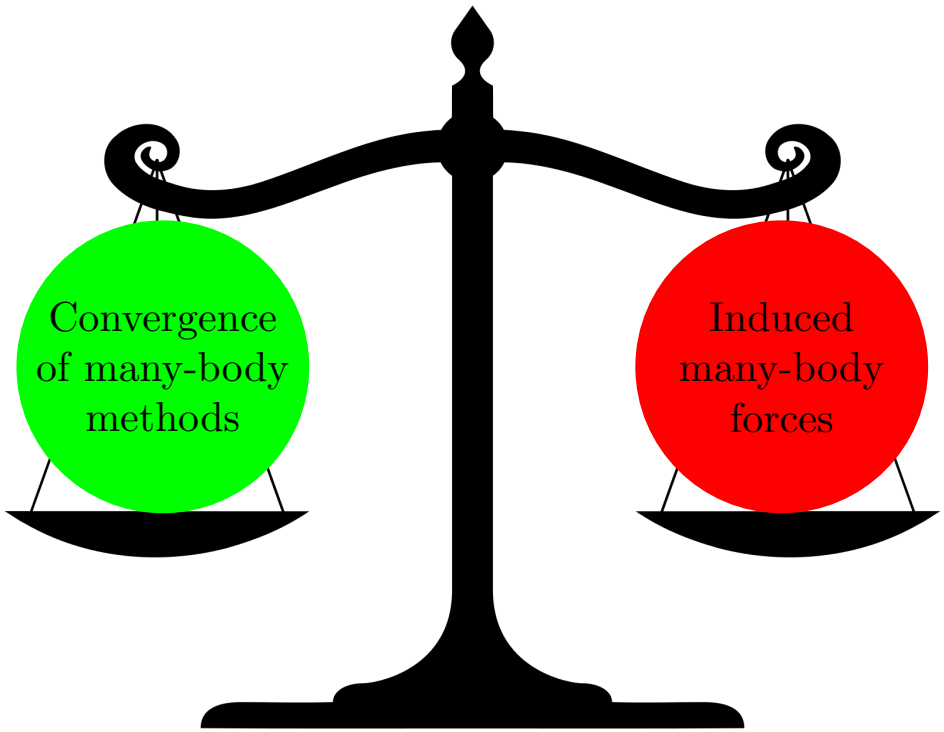
$$\boldsymbol{\eta}_\alpha = (2\mu)^2 [\boldsymbol{G}_\alpha, \boldsymbol{H}_\alpha]$$

- Generator choices

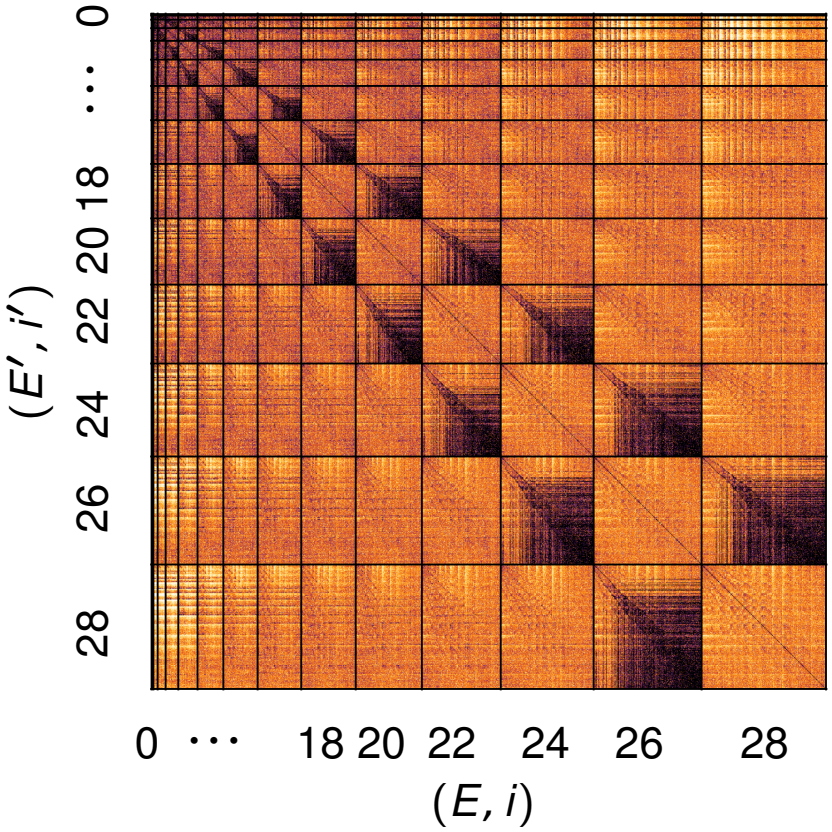
  Wegner $\quad \boldsymbol{G}_\alpha \sim \mathrm{diag}(\boldsymbol{H}_\alpha)$

  Standard $\quad \boldsymbol{G}_\alpha = \boldsymbol{T}_{\mathrm{int}}$

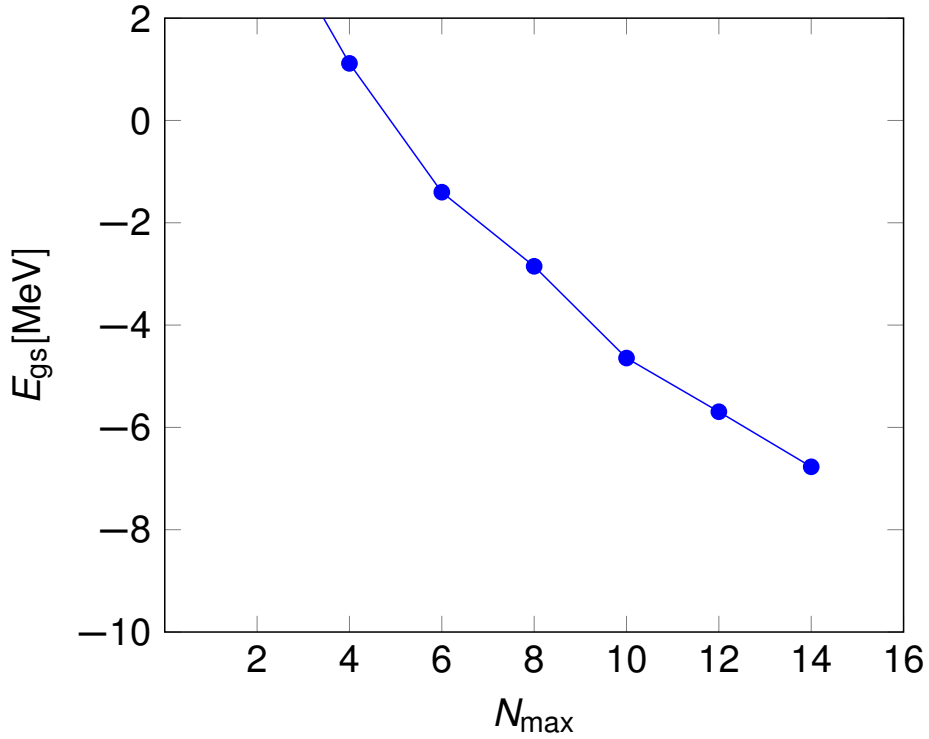
- SRG induces forces with higher particle rank
- Generator with better balance?



^{3}H SRG Evolution with α =0.0 fm^4

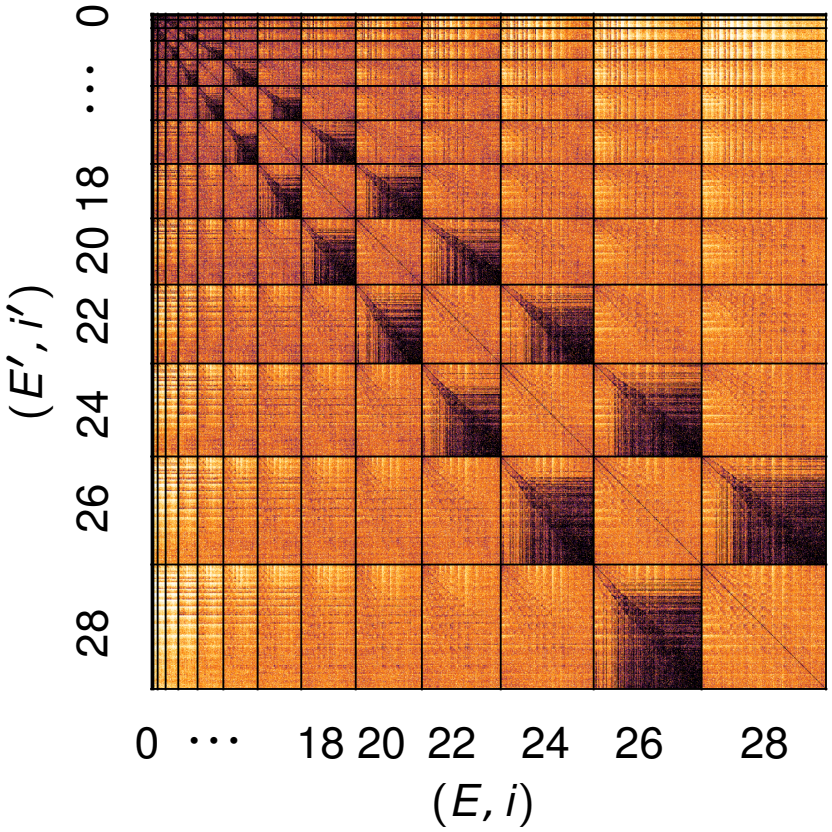


^{3}H channel (T=1 J=1 P=1) in antisymmetrized Jacobi HO basis



^{3}H NCSM calculation
$\hbar\omega = 20$ MeV

^{3}H SRG Evolution with α =0.01 fm^4



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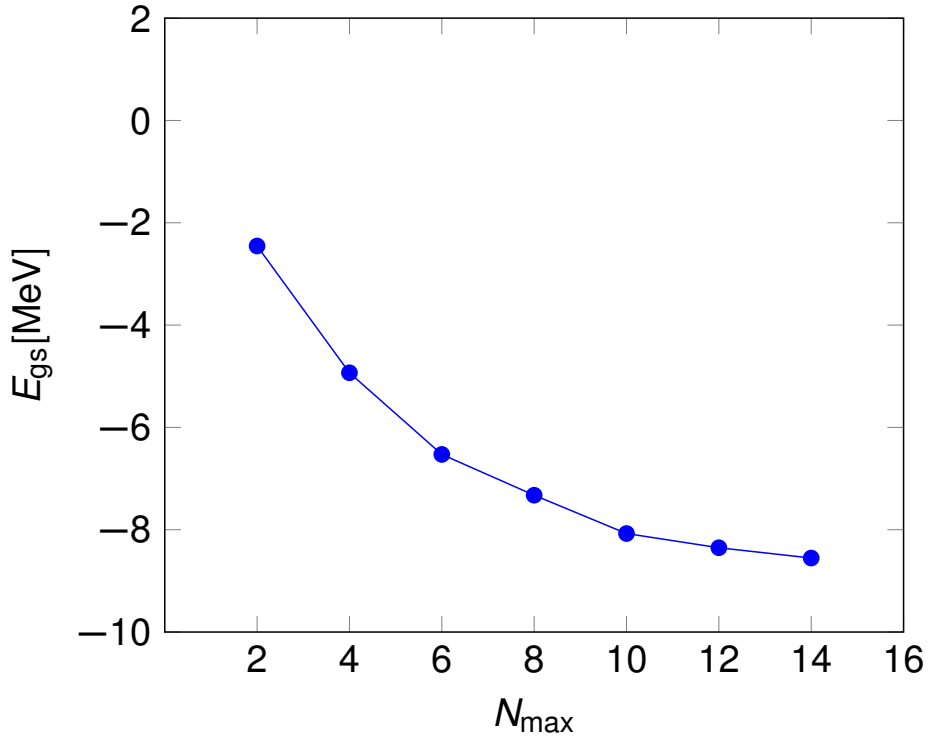
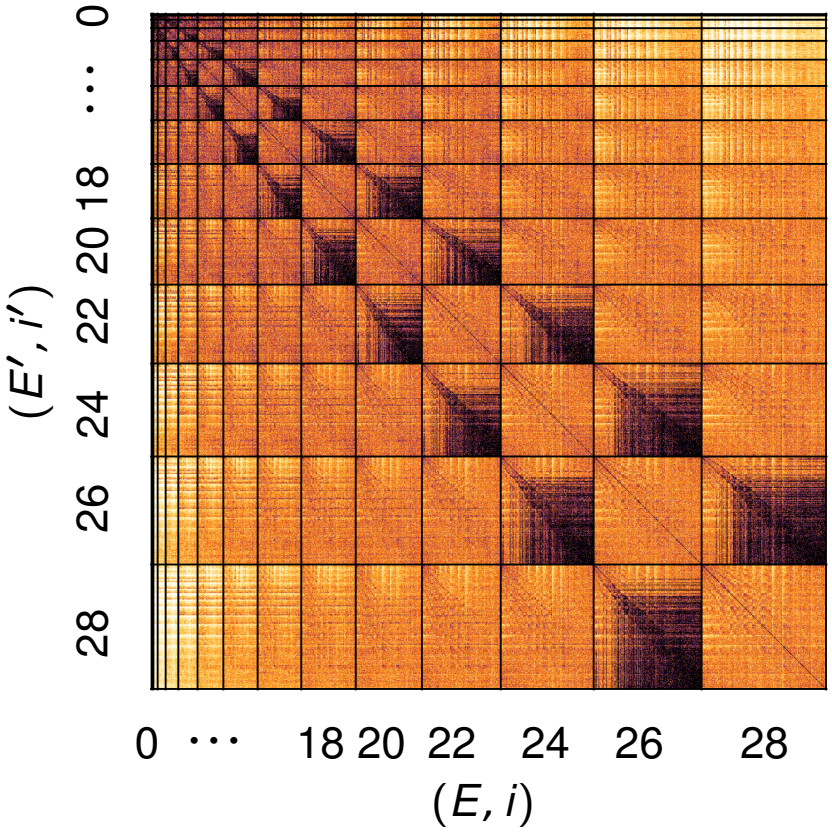
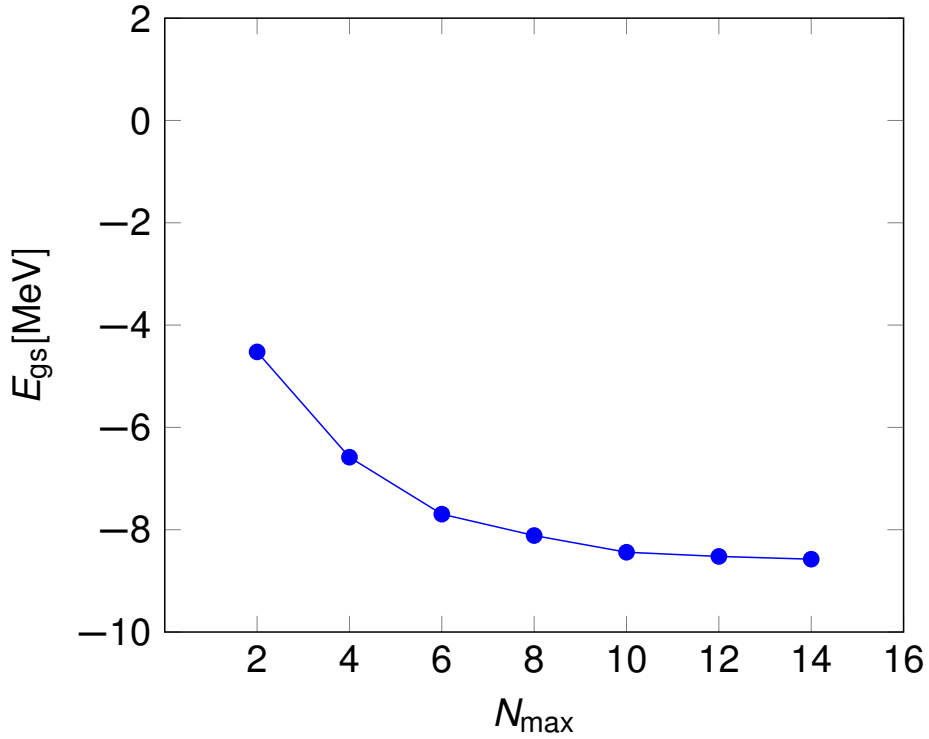


^{3}H NCSM calculation
$\hbar\omega = 20$ MeV

^{3}H SRG Evolution with α =0.02 fm^4

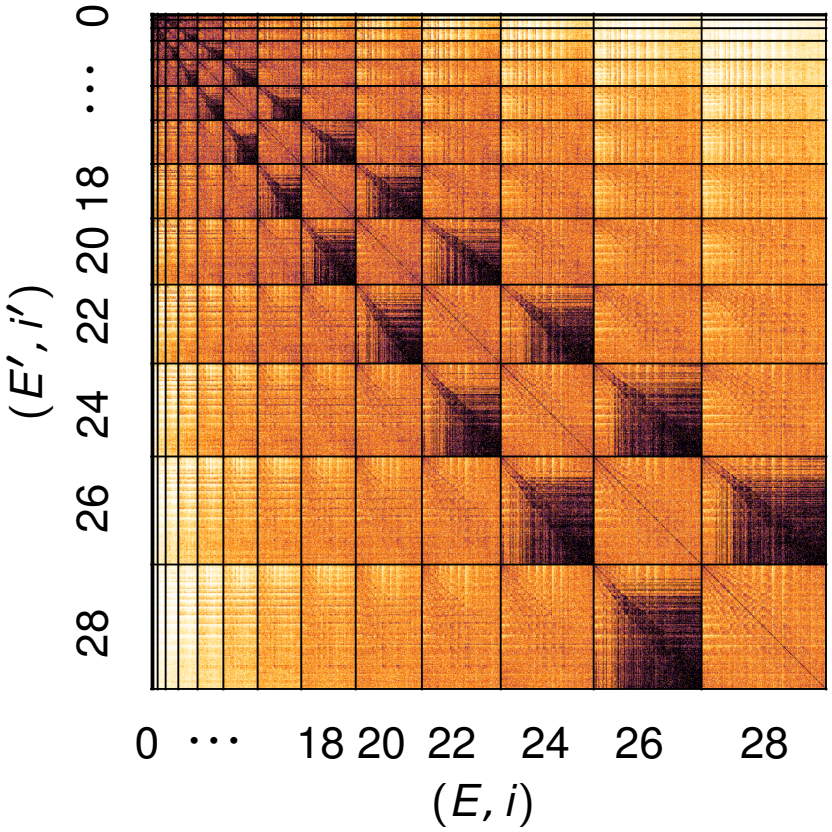


^{3}H channel (T=1 J=1 P=1) in antisymmetrized Jacobi HO basis

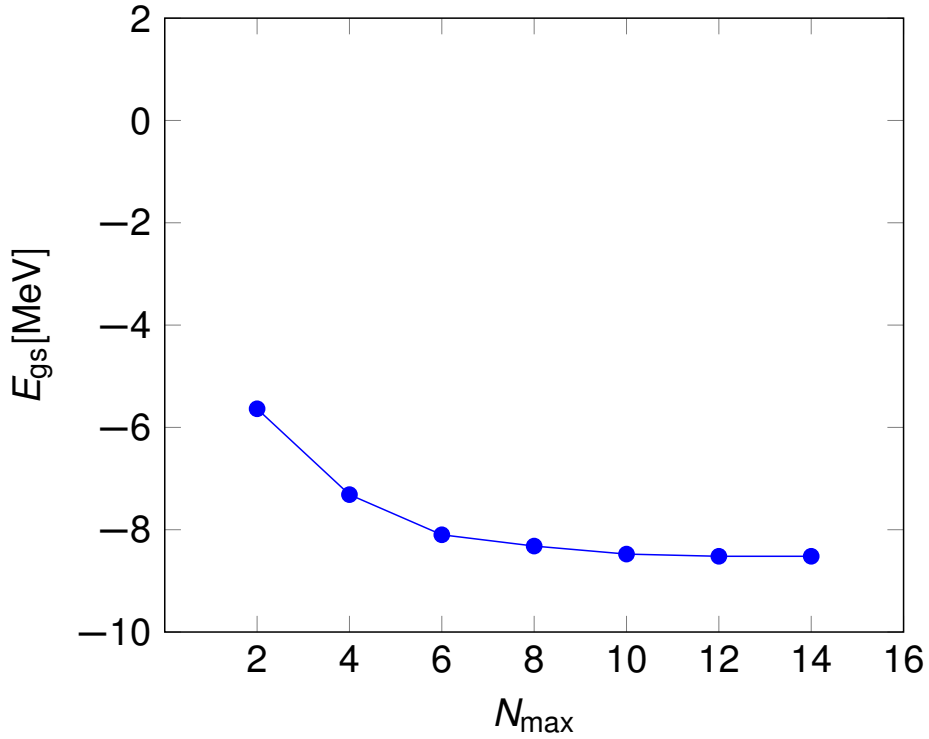


^{3}H NCSM calculation
$\hbar\omega = 20$ MeV

^{3}H SRG Evolution with α =0.04 fm^4

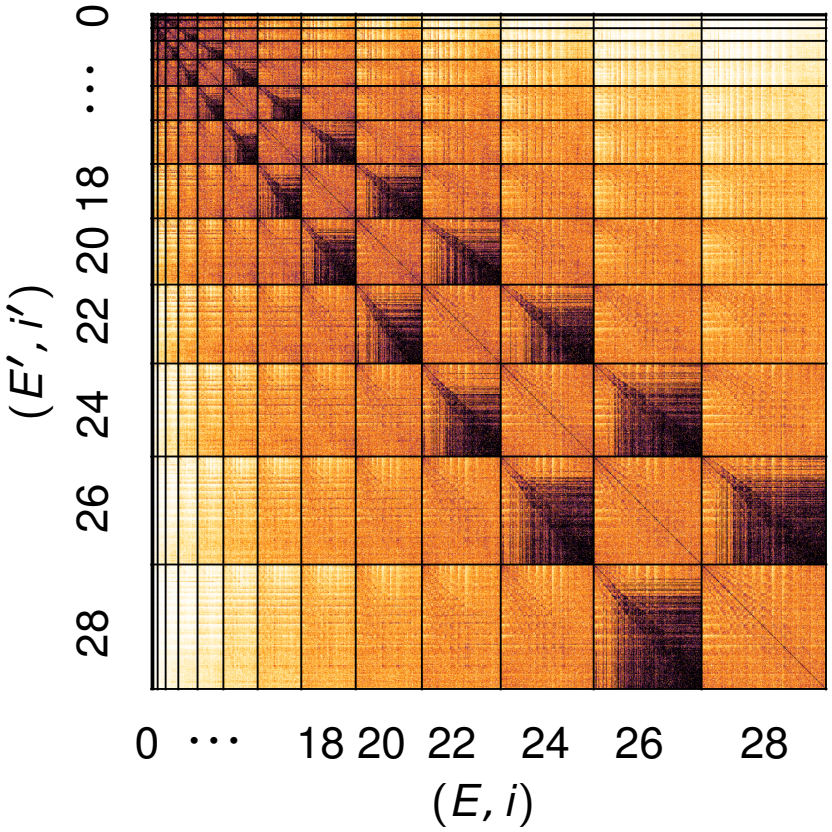


^{3}H channel (T=1 J=1 P=1) in antisymmetrized Jacobi HO basis

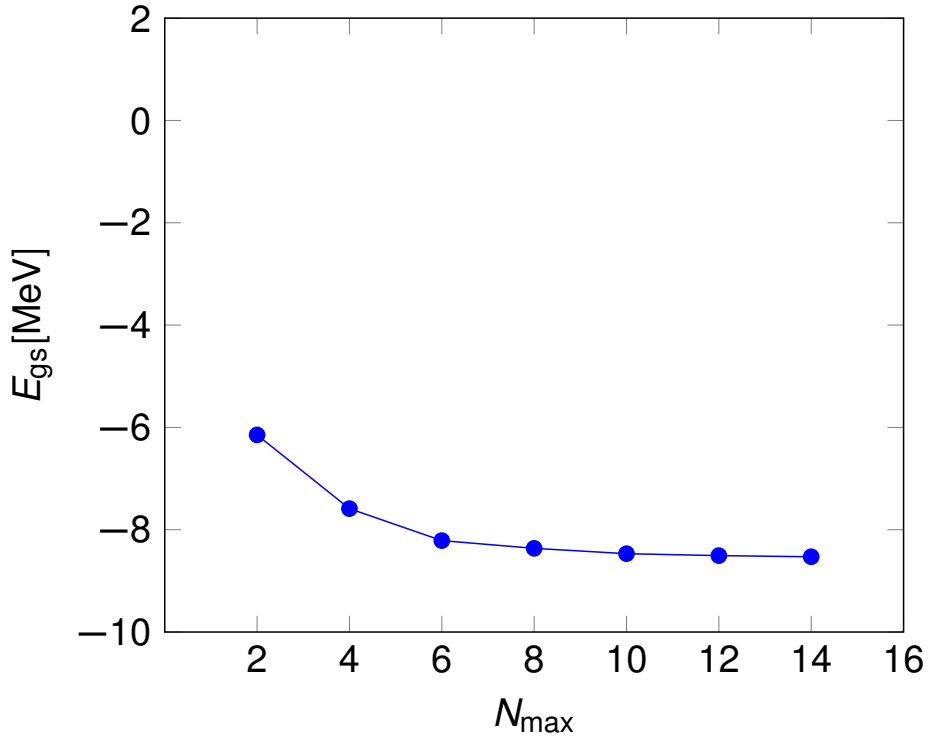


^{3}H NCSM calculation
$\hbar\omega = 20$ MeV

^{3}H SRG Evolution with α =0.0625 fm^4

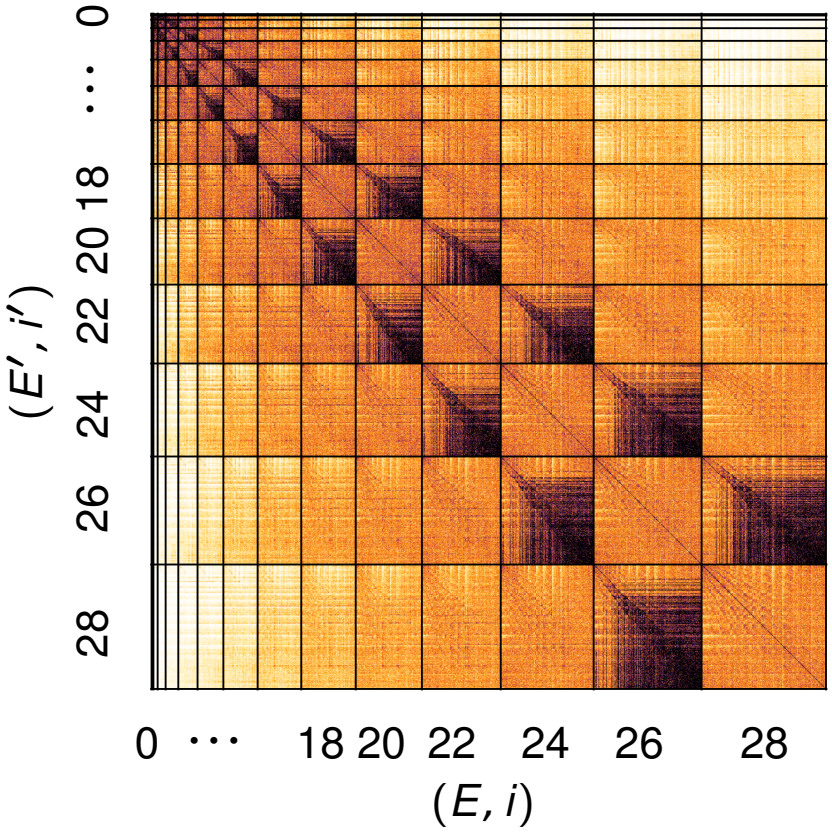


^{3}H channel (T=1 J=1 P=1) in antisymmetrized Jacobi HO basis

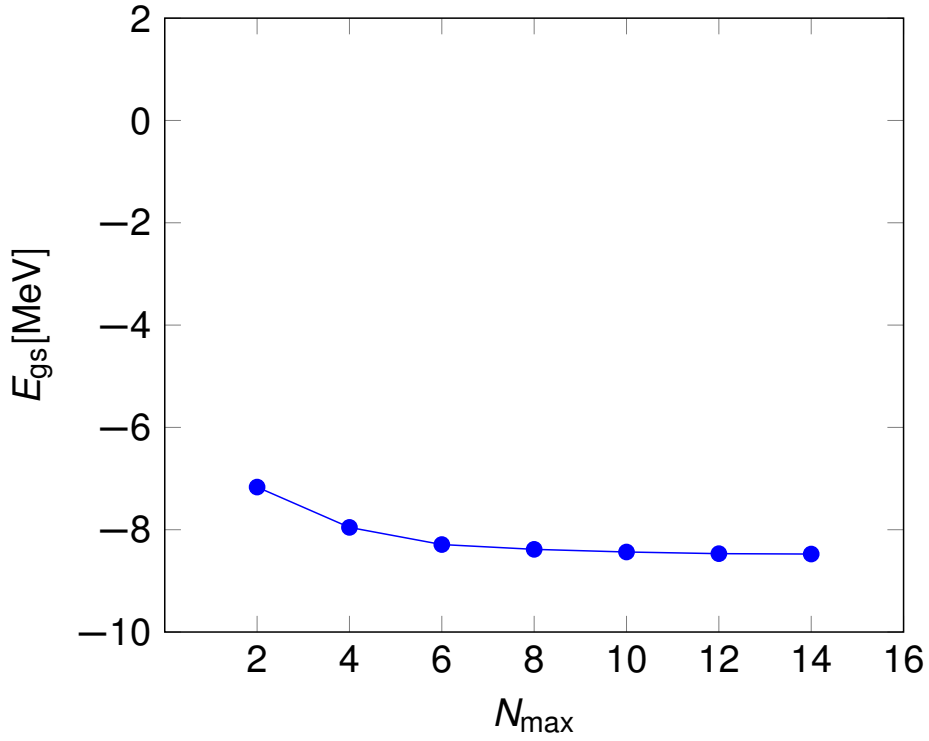


^{3}H NCSM calculation
$\hbar\omega = 20$ MeV

^{3}H SRG Evolution with α =0.08 fm^4

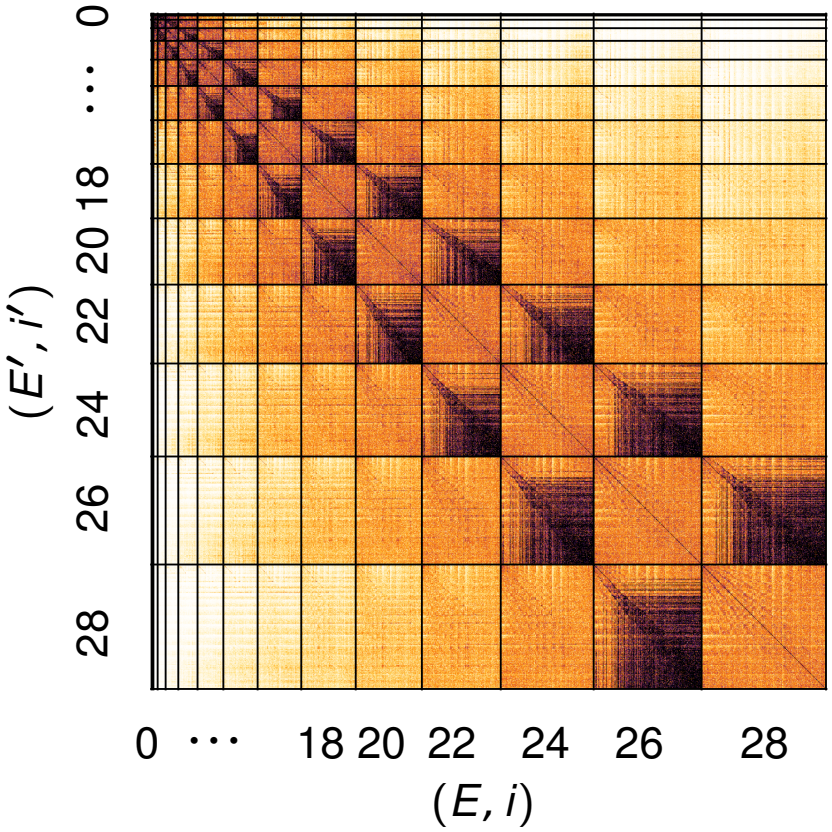


^{3}H channel (T=1 J=1 P=1) in antisymmetrized Jacobi HO basis

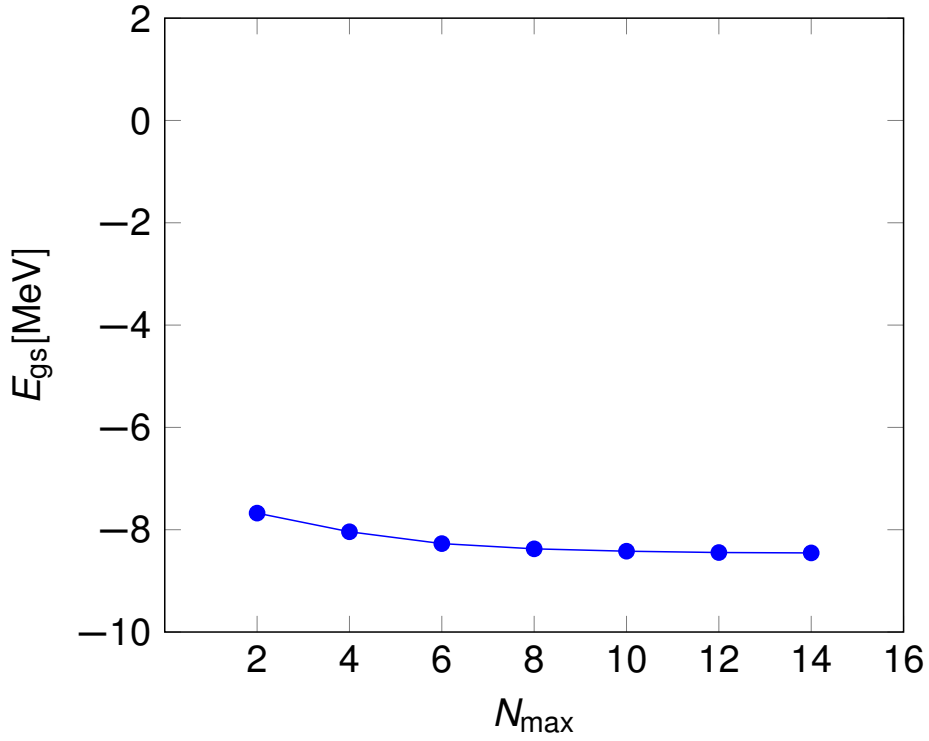


^{3}H NCSM calculation
$\hbar\omega = 20$ MeV

^{3}H SRG Evolution with α =0.16 fm^4

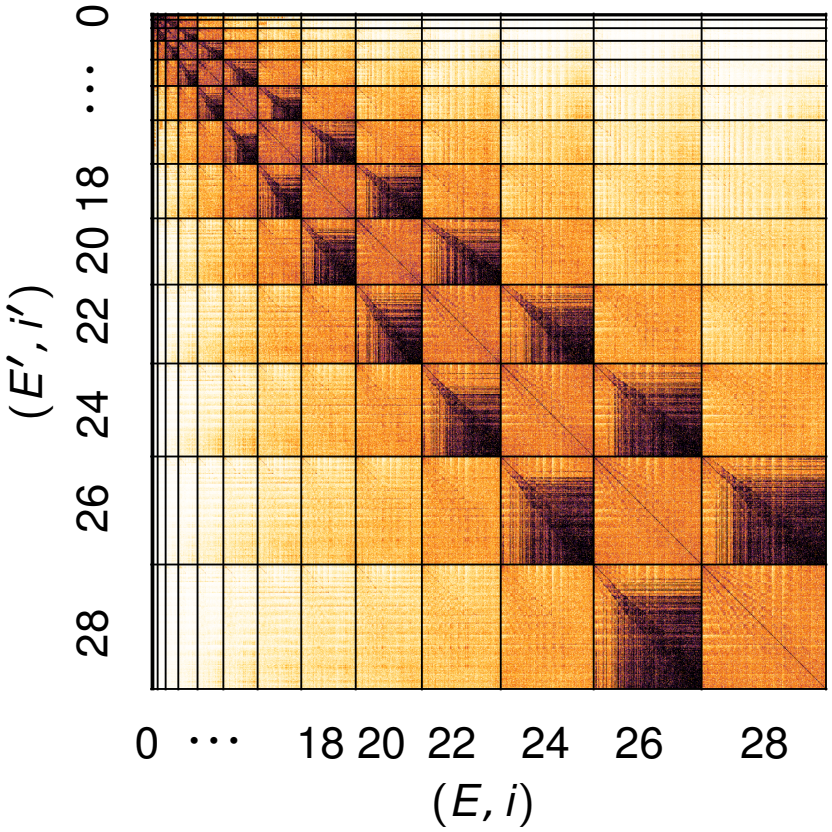


^{3}H channel (T=1 J=1 P=1) in antisymmetrized Jacobi HO basis

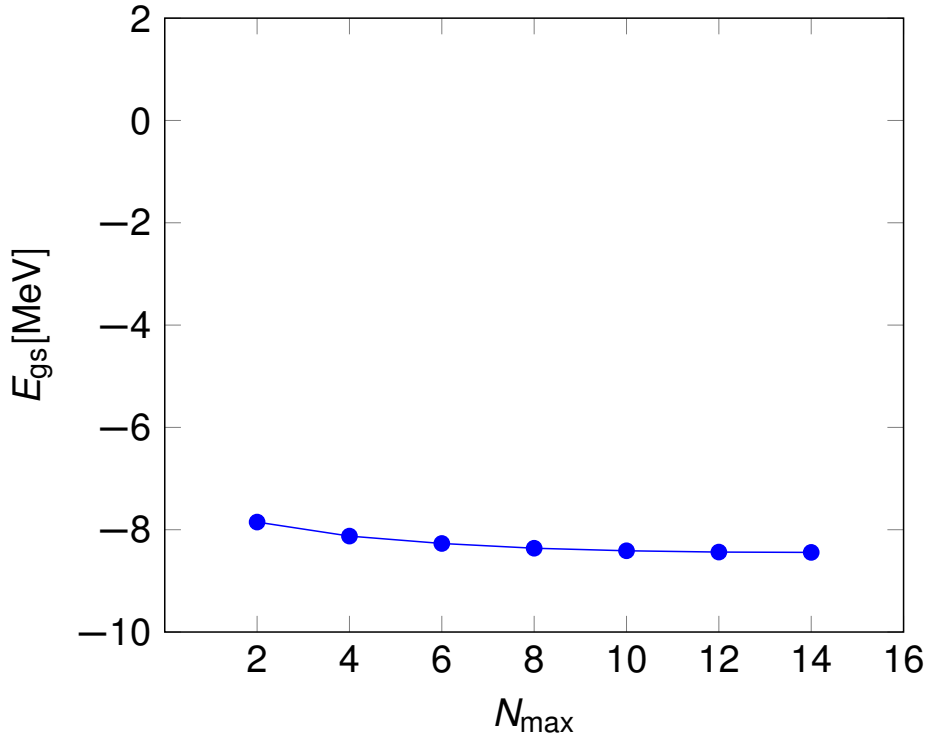


^{3}H NCSM calculation
$\hbar\omega = 20$ MeV

^{3}H SRG Evolution with α =0.32 fm^4



^{3}H channel (T=1 J=1 P=1) in antisymmetrized Jacobi HO basis



^{3}H NCSM calculation
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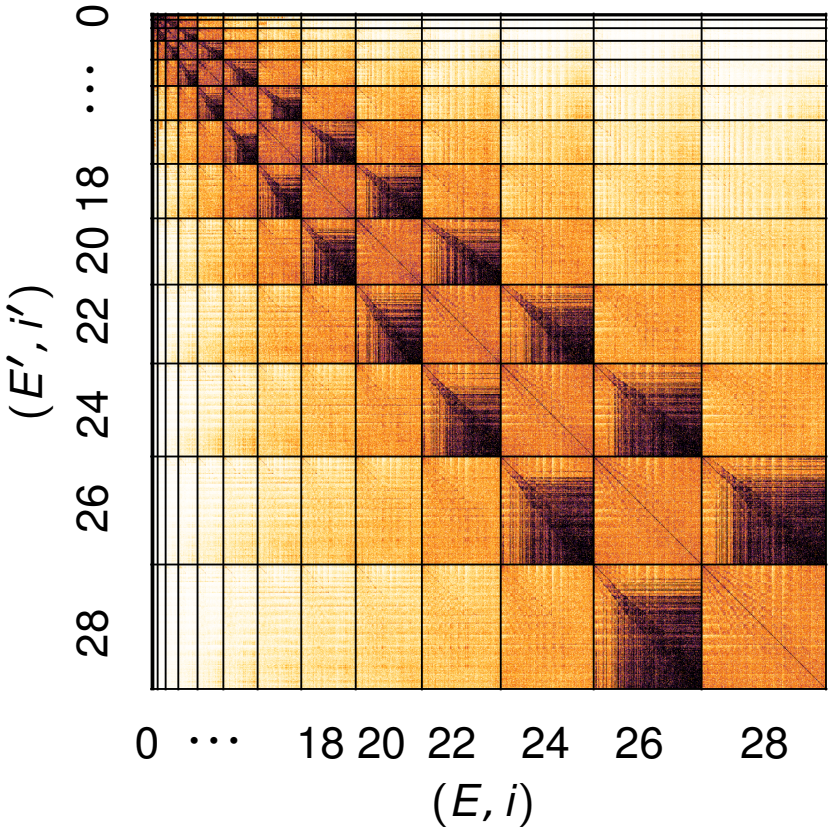
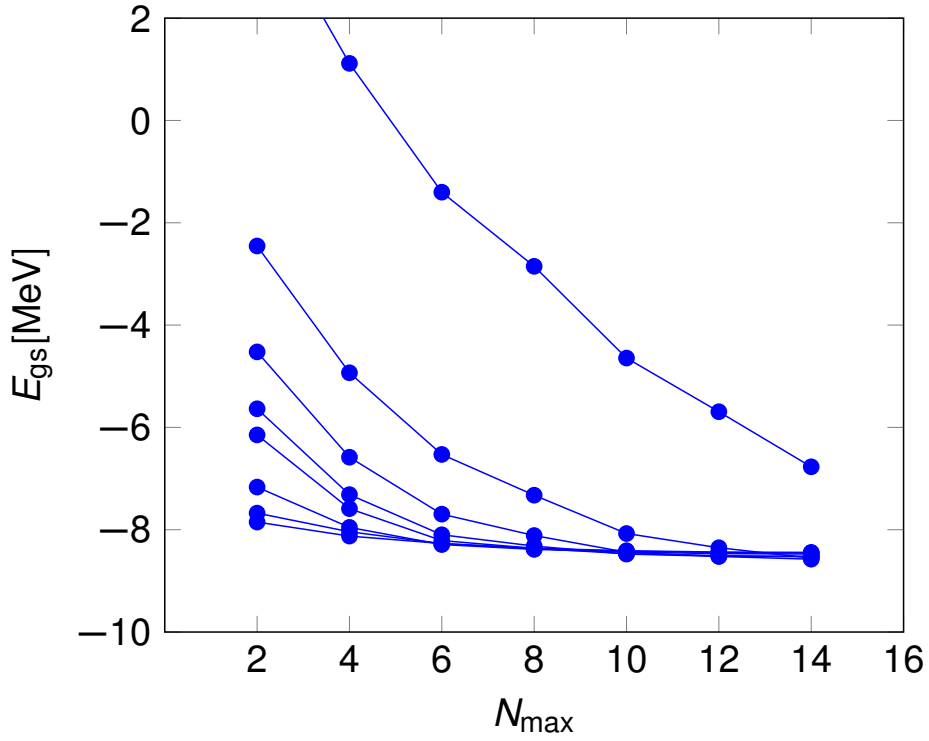
^{3}H SRG Evolution with α =0.32 fm^4



^{3}H channel (T=1 J=1 P=1) in antisymmetrized Jacobi HO basis



^{3}H NCSM calculation
$\hbar\omega = 20$ MeV

Cluster Decomposition

- SRG induces contributions up to the A-body rank

$$\boldsymbol{H}_\alpha = \boldsymbol{H}_\alpha^{[1]} + \boldsymbol{H}_\alpha^{[2]} + \boldsymbol{H}_\alpha^{[3]} + \boldsymbol{H}_\alpha^{[4]} + \cdots + \boldsymbol{H}_\alpha^{[A]}$$

- SRG in two-body space

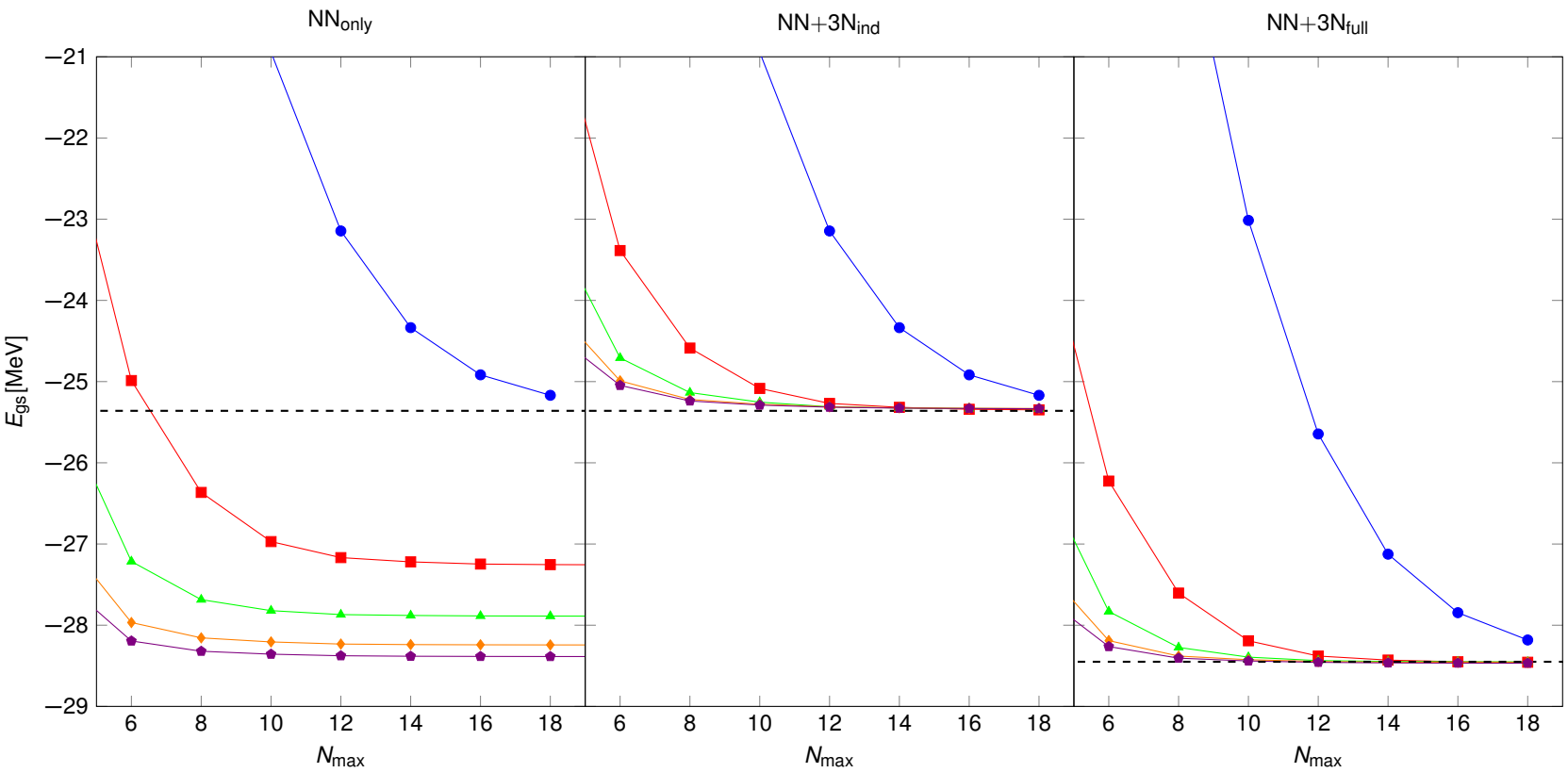
$$\boldsymbol{H}_{\mathrm{NN_{only}},\alpha} = \boldsymbol{T}_{\mathrm{int}} + \boldsymbol{V}_{\mathrm{NN},\alpha}^{[2]}$$

- SRG in three-body space

$$\boldsymbol{H}_{\mathrm{NN+3N_{ind}},\alpha} = \boldsymbol{T}_{\mathrm{int}} + \boldsymbol{V}_{\mathrm{NN},\alpha}^{[2]} + \boldsymbol{V}_{\mathrm{NN},\alpha}^{[3]}$$

$$\boldsymbol{H}_{\mathrm{NN+3N_{full}},\alpha} = \boldsymbol{T}_{\mathrm{int}} + \boldsymbol{V}_{\mathrm{NN},\alpha}^{[2]} + \boldsymbol{V}_{\mathrm{NN},\alpha}^{[3]} + \boldsymbol{V}_{\mathrm{NNN},\alpha}^{[3]}$$

NCSM ^{4}He: SRG Evolution with $T_{\rm int}$



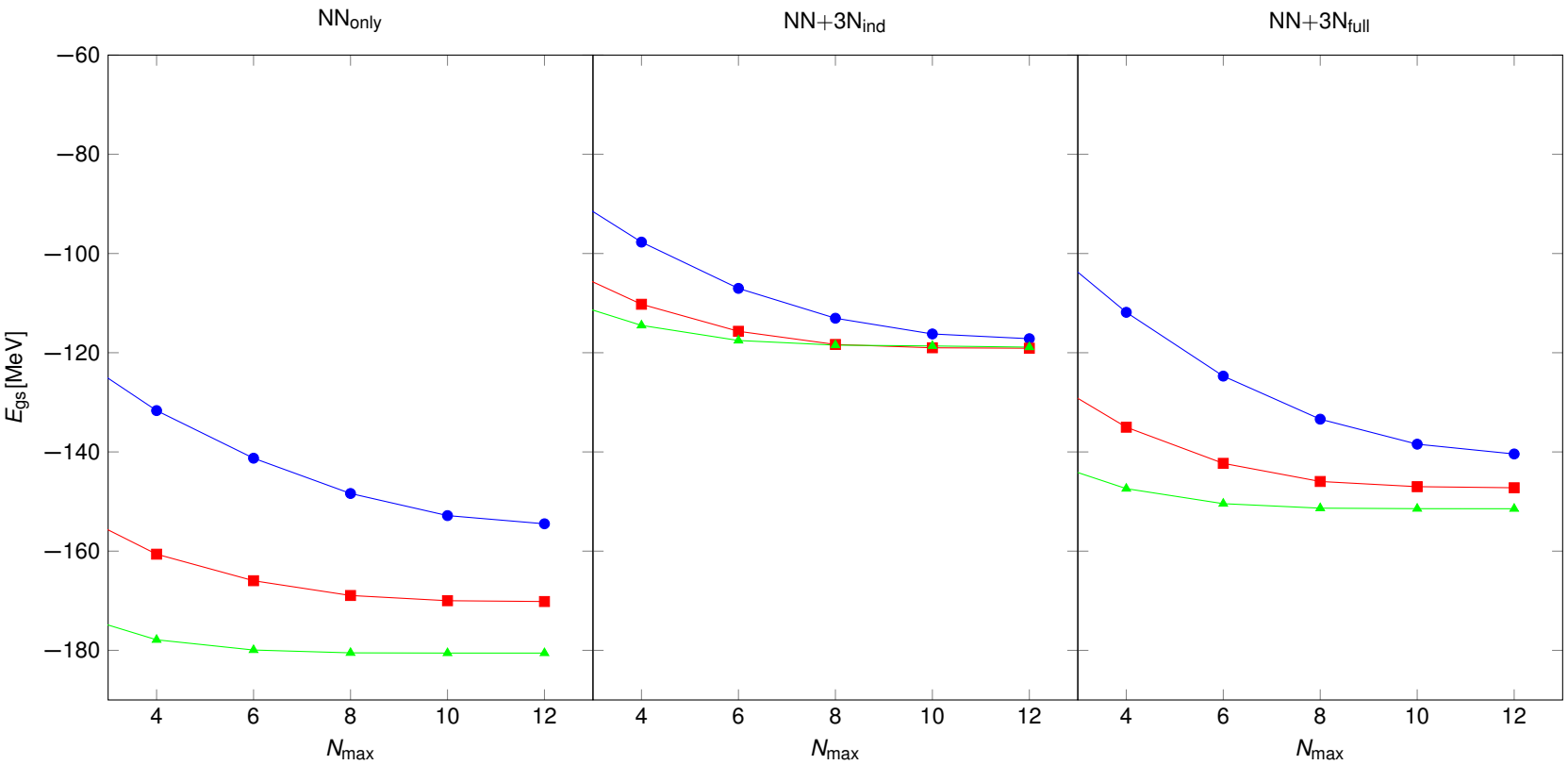
^{4}He

$\hbar\omega = 28$ MeV

$T_{\rm int}$

Bare Exact α[fm^4] 0.02 0.04 0.0625 0.08

IT-NCSM ^{16}O: SRG Evolution with $T_{\rm int}$



^{16}O

$\hbar\omega = 20$ MeV

$T_{\rm int}$

Exact α[fm^4] 0.04 0.08 0.16

Block Generator

- Block generator

$$\boldsymbol{G}_\alpha = \boldsymbol{T}_{\text{int}} + \boldsymbol{P}_{\text{gen}}\boldsymbol{V}_{\text{NN},\alpha}\boldsymbol{P}_{\text{gen}}$$

- In harmonic-oscillator (HO) basis

Dicaire *et al.* PhysRevC.90.034302.

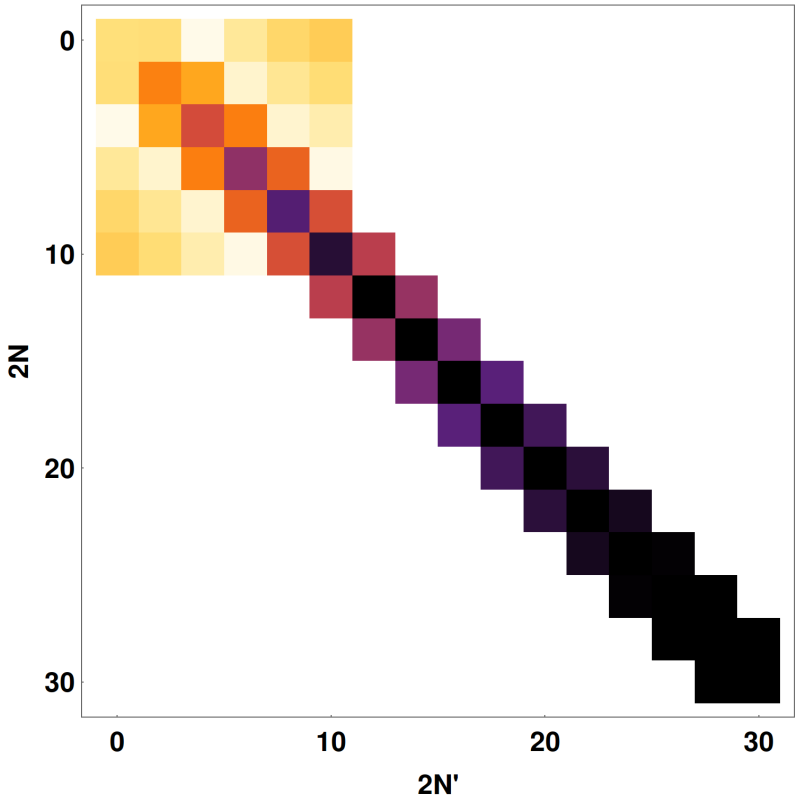
$$\boldsymbol{P}^{\text{HO}}_{\text{gen}} = \begin{cases} 1\,, & 2N + L \leq E_{\text{gen}} \\ 0\,, & \text{else} \end{cases}$$

- In momentum basis

$$\boldsymbol{P}^{\text{Q}}_{\text{gen}} = \begin{cases} 1\,, & q \leq q_{\text{gen}} \\ 0\,, & \text{else} \end{cases}$$

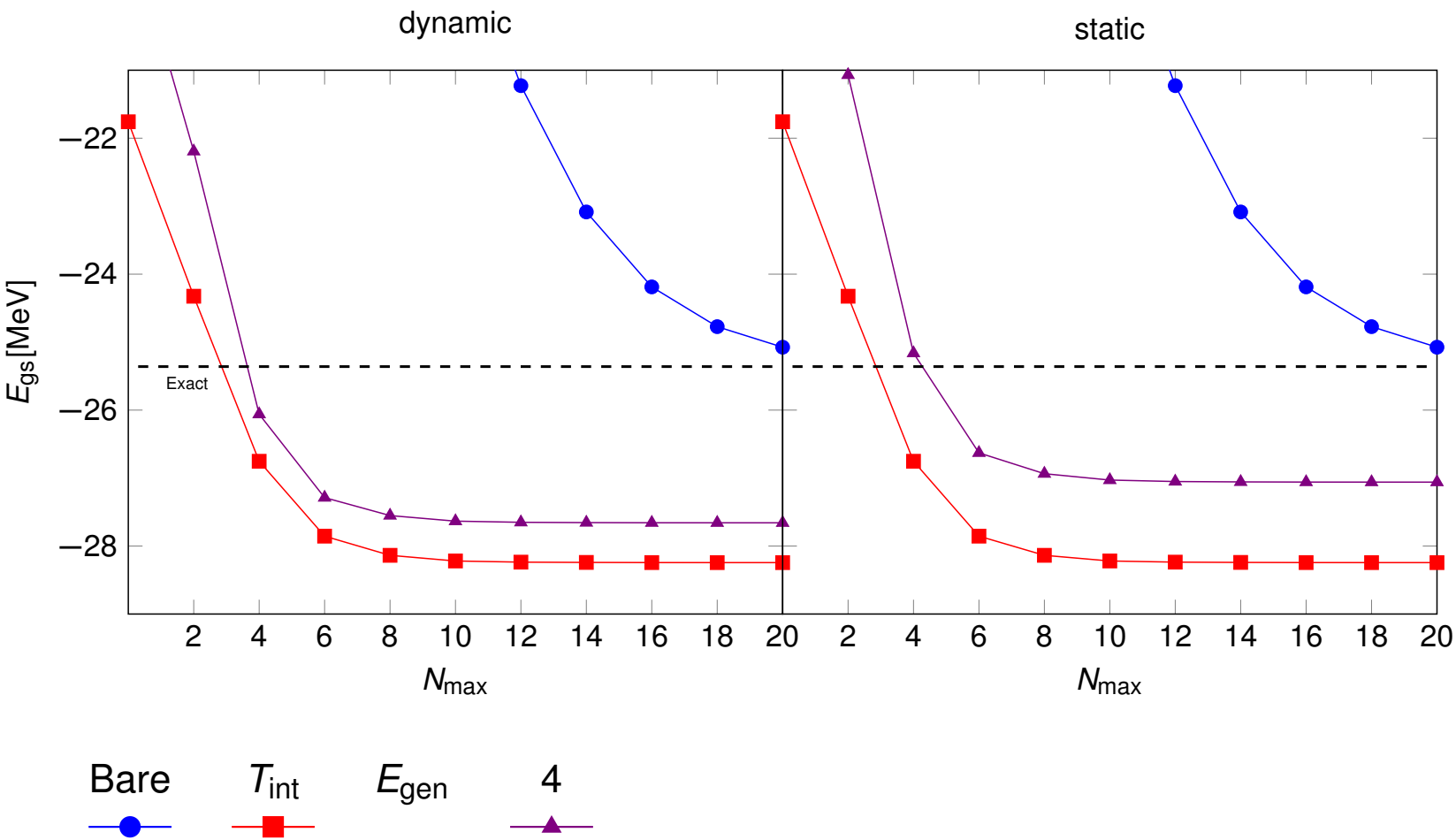
- Additional static versions

$$\boldsymbol{G}_\alpha = \boldsymbol{G}_0$$



$\boldsymbol{G}^{\text{HO}}_0$ in the $^3S_1$−channel with $E_{\text{gen}} = 10$

NCSM ^{4}He : Two-Body Evolution with HO Block



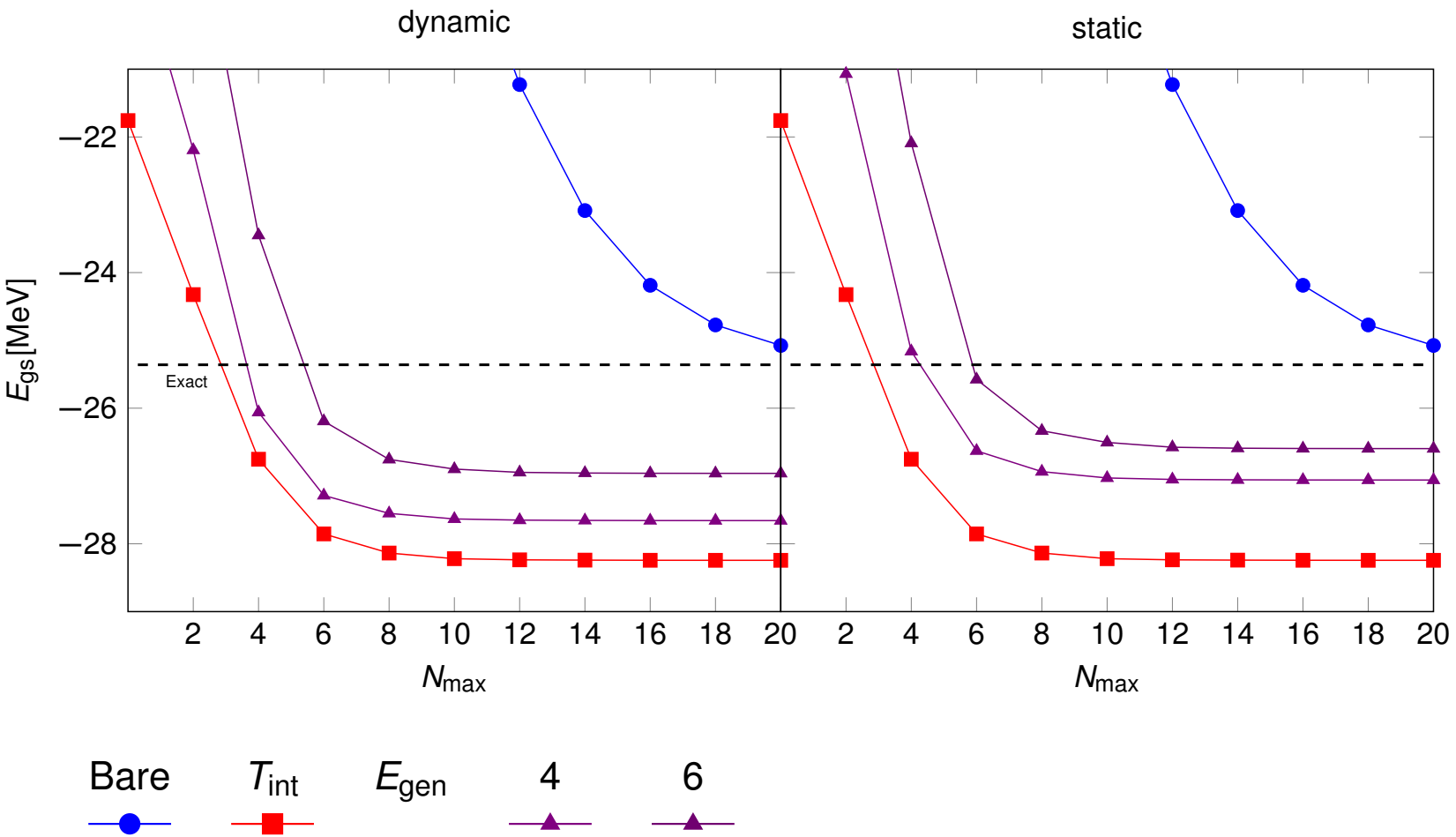
^{4}He

$\hbar\omega = 24$ MeV

$\alpha = 0.0625$ fm^4

NN_{only}

NCSM ^{4}He : Two-Body Evolution with HO Block



^{4}He

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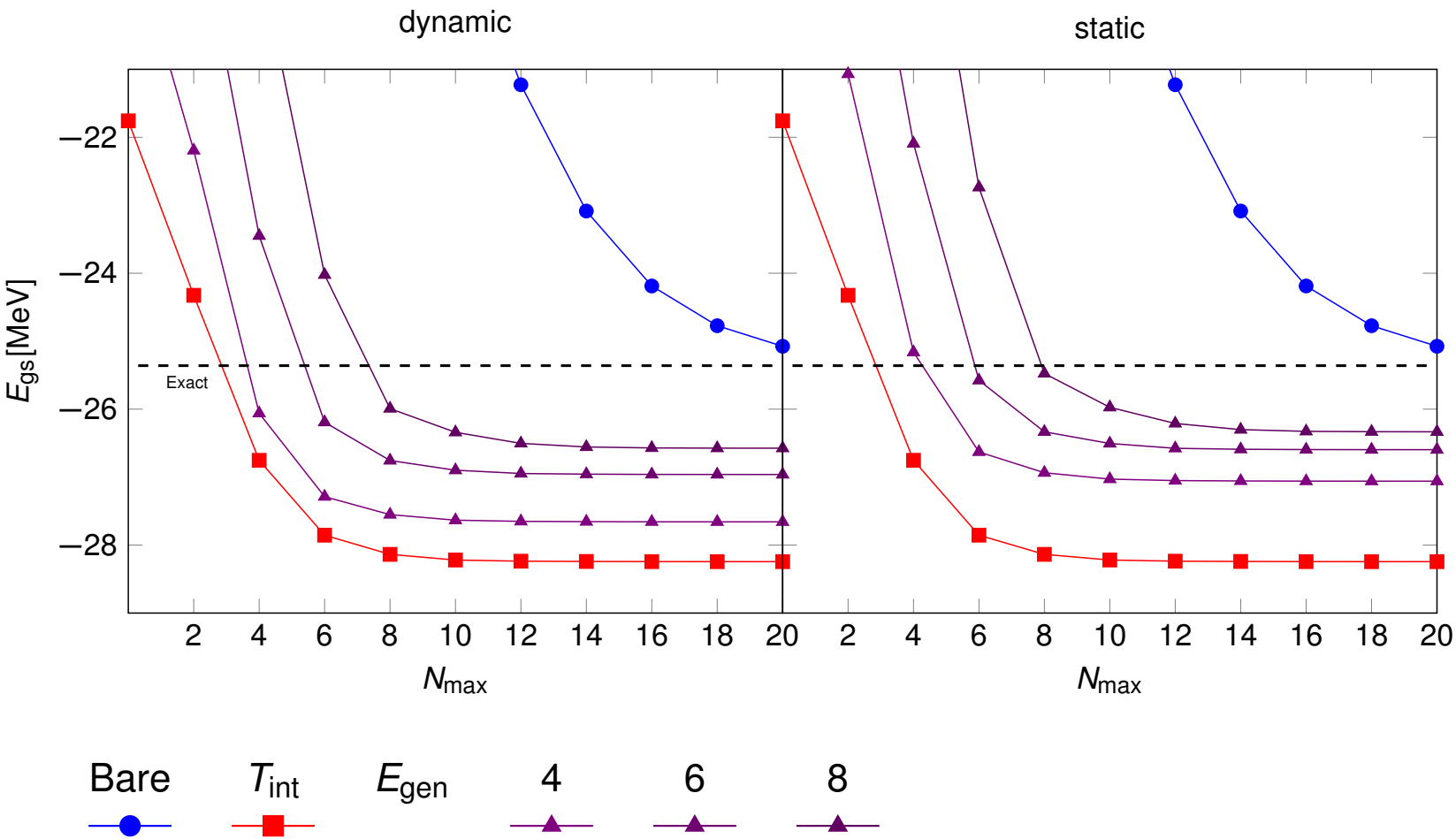
NN_{only}

NCSM ^{4}He : Two-Body Evolution with HO Block



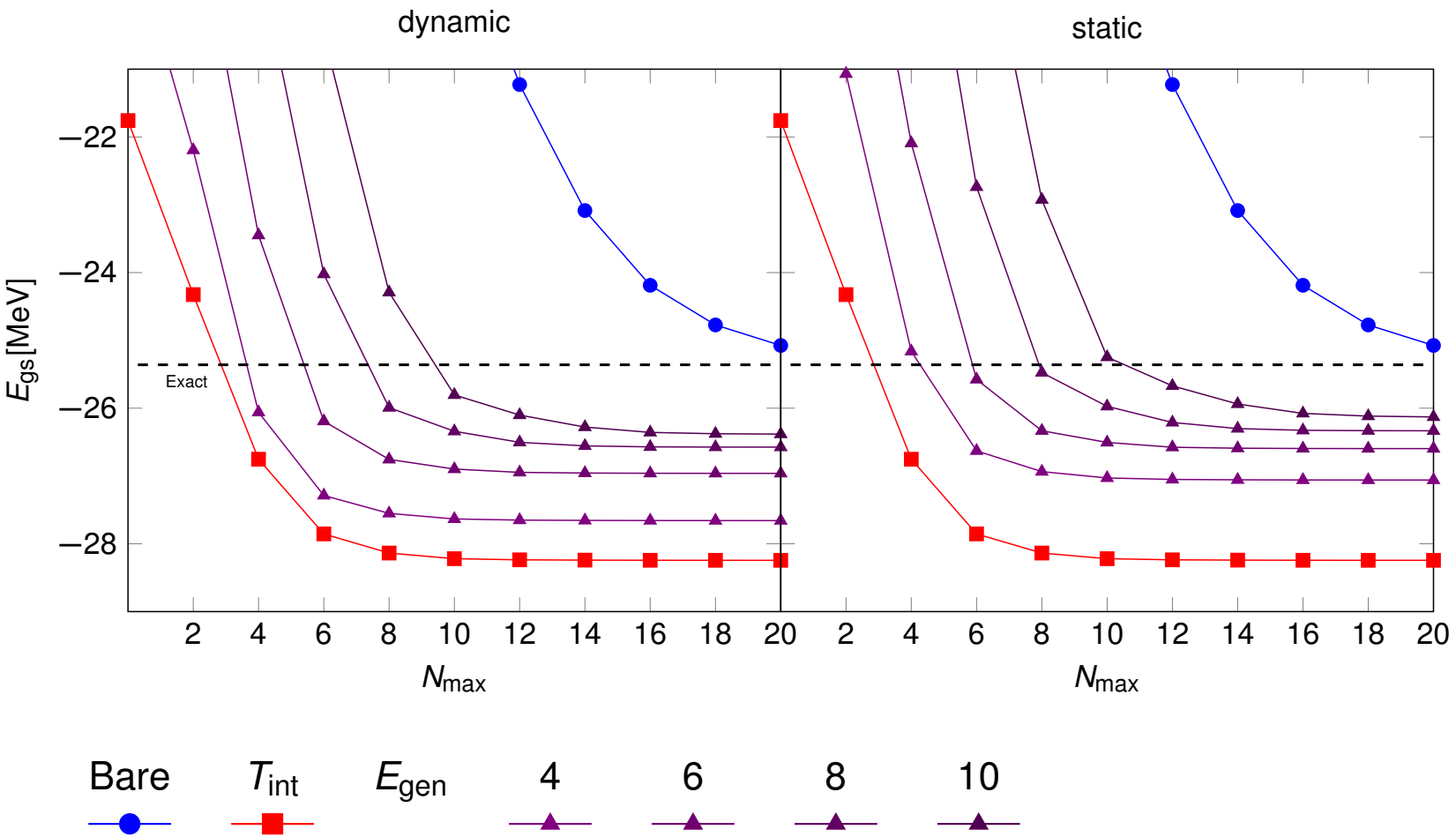
^{4}He

$\hbar\omega = 24$ MeV

$\alpha = 0.0625$ fm^4

NN_{only}

NCSM ^{4}He : Two-Body Evolution with HO Block



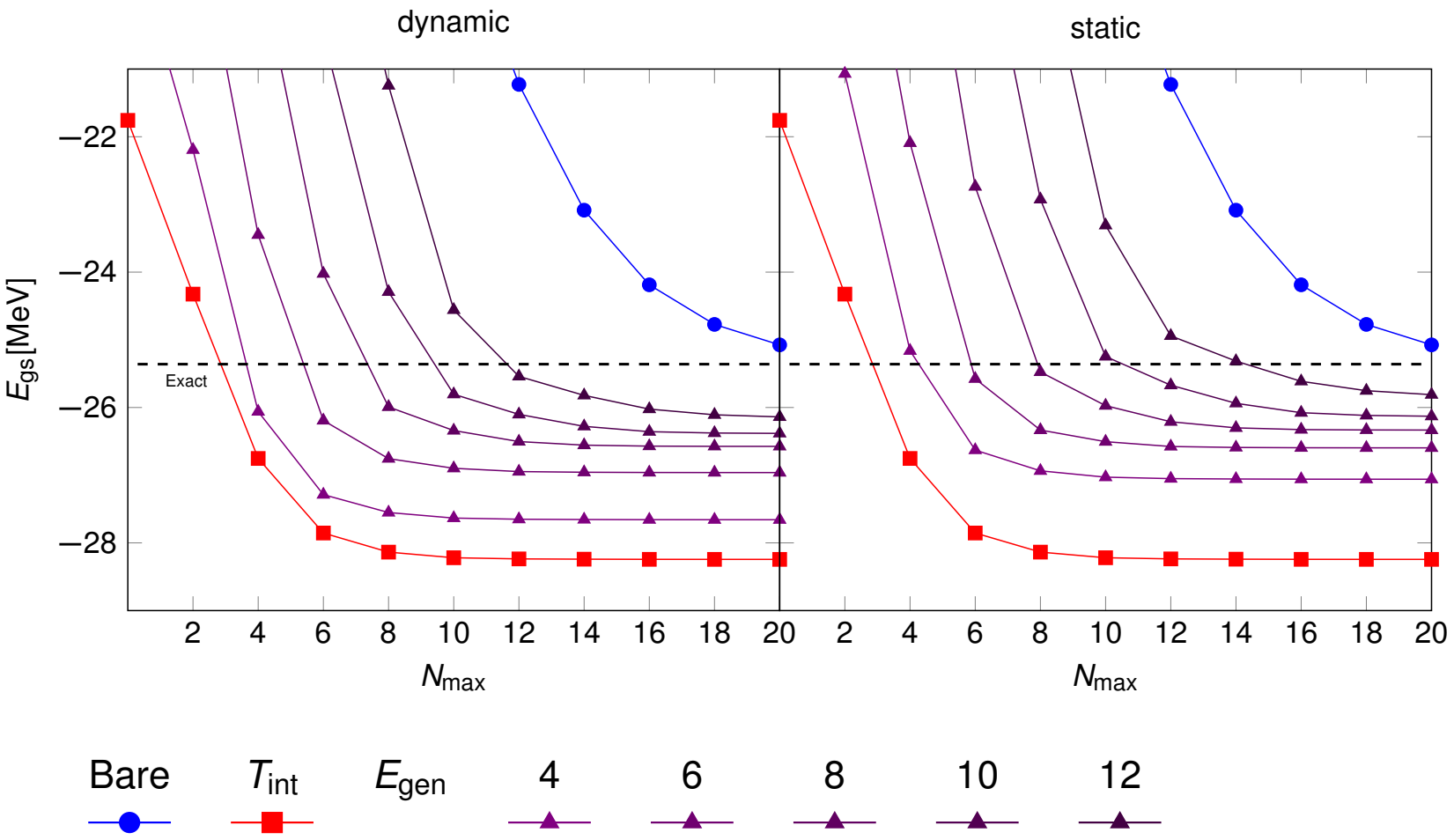
^{4}He

$\hbar\omega = 24$ MeV

$\alpha = 0.0625$ fm^4

NN_{only}

NCSM ^{4}He : Two-Body Evolution with HO Block



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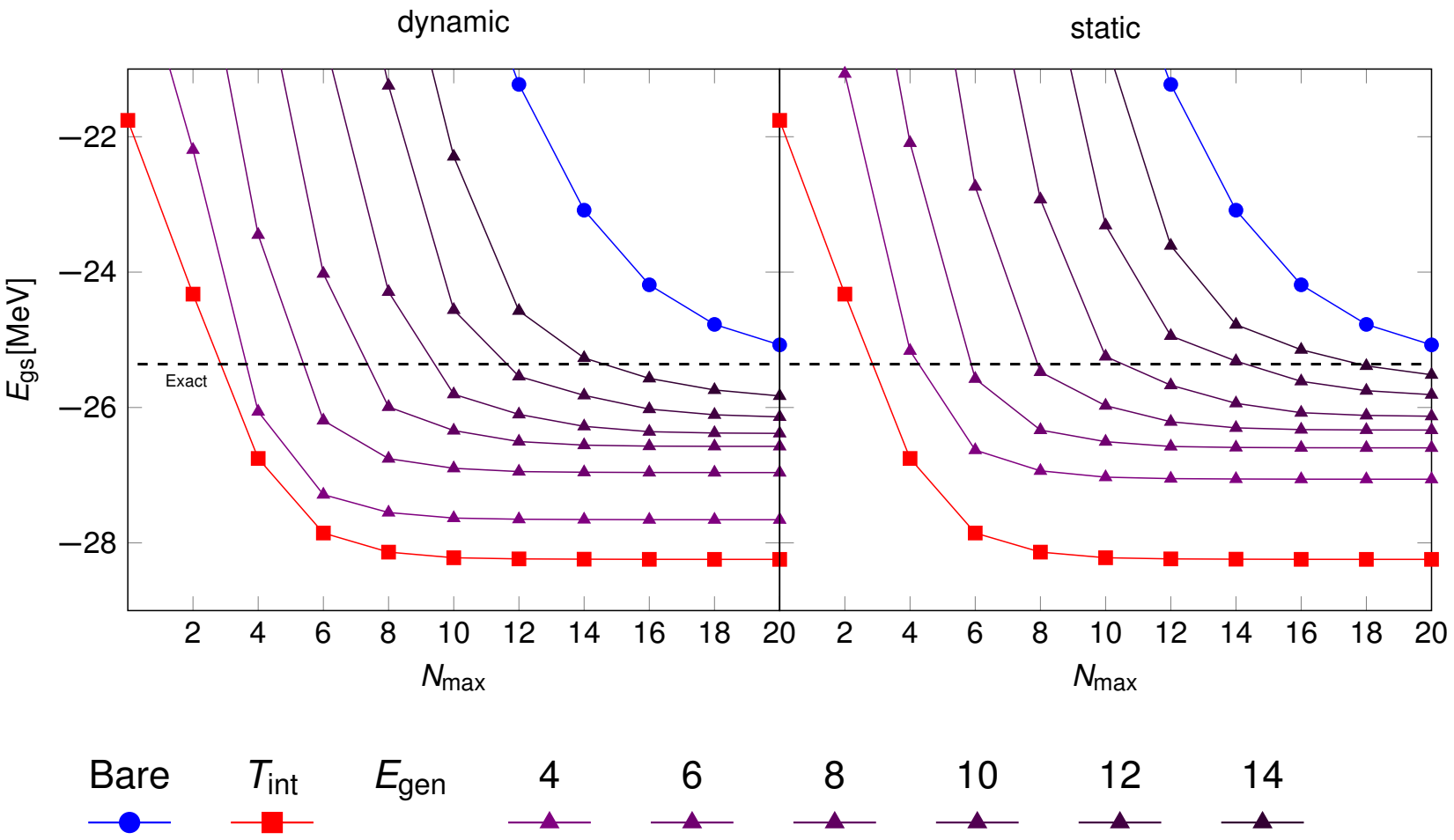

^{4}He

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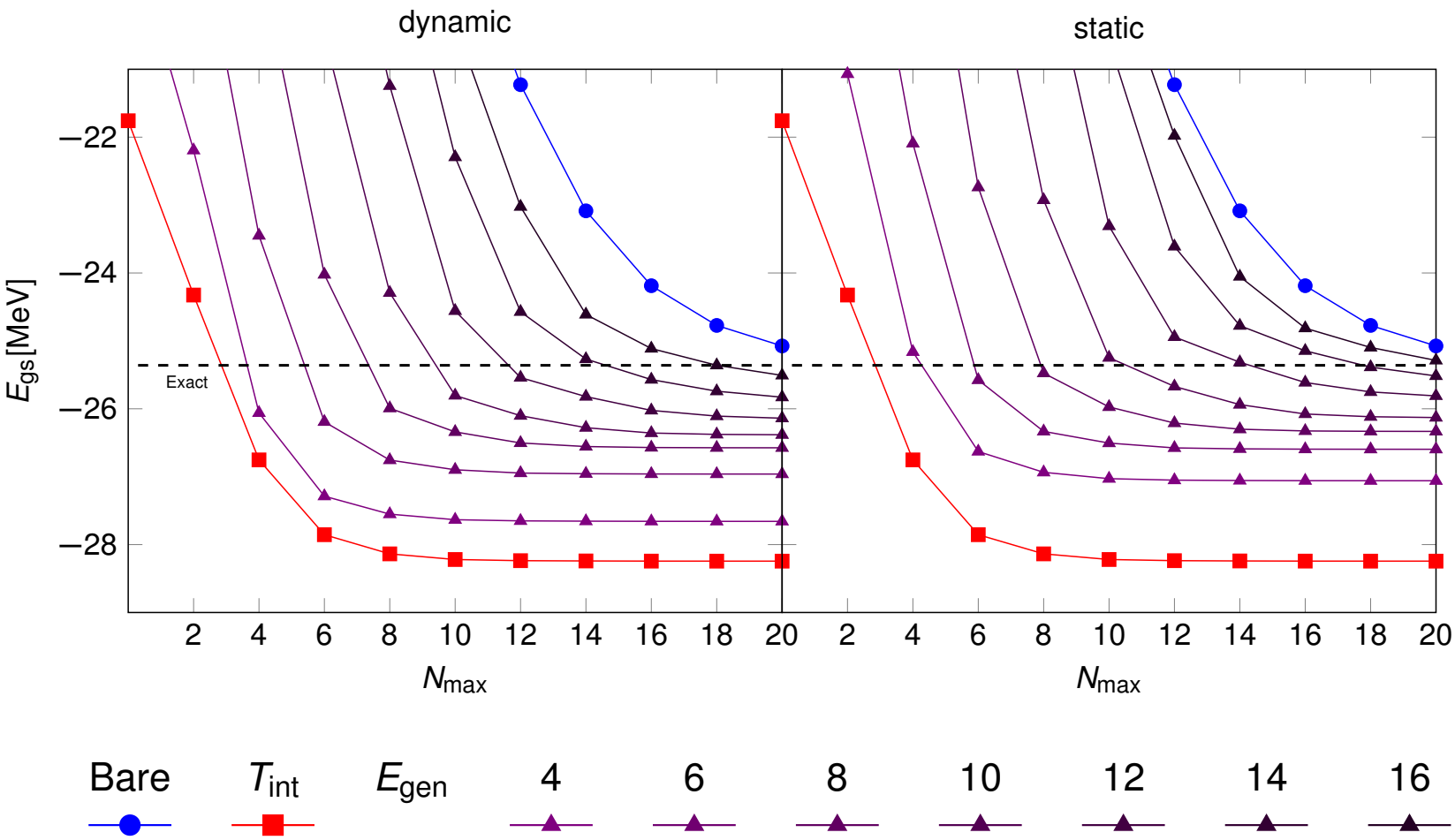
NN_{only}

NCSM ^{4}He : Two-Body Evolution with HO Block



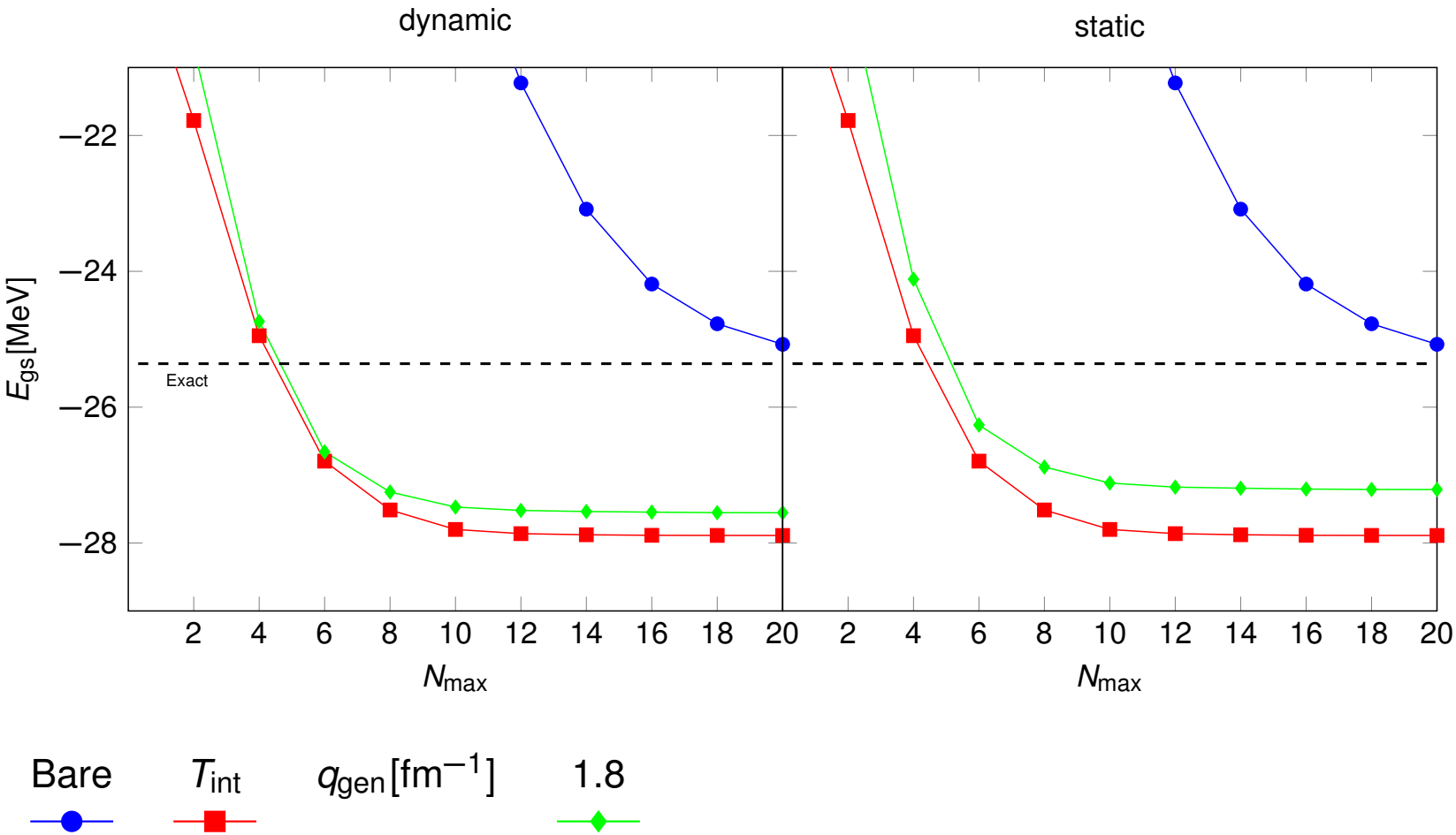
^{4}He

$\hbar\omega = 24$ MeV

$\alpha = 0.0625$ fm^4

$\mathrm{NN}_{\mathrm{only}}$

NCSM ^{4}He : Two-Body Evolution with Q Block



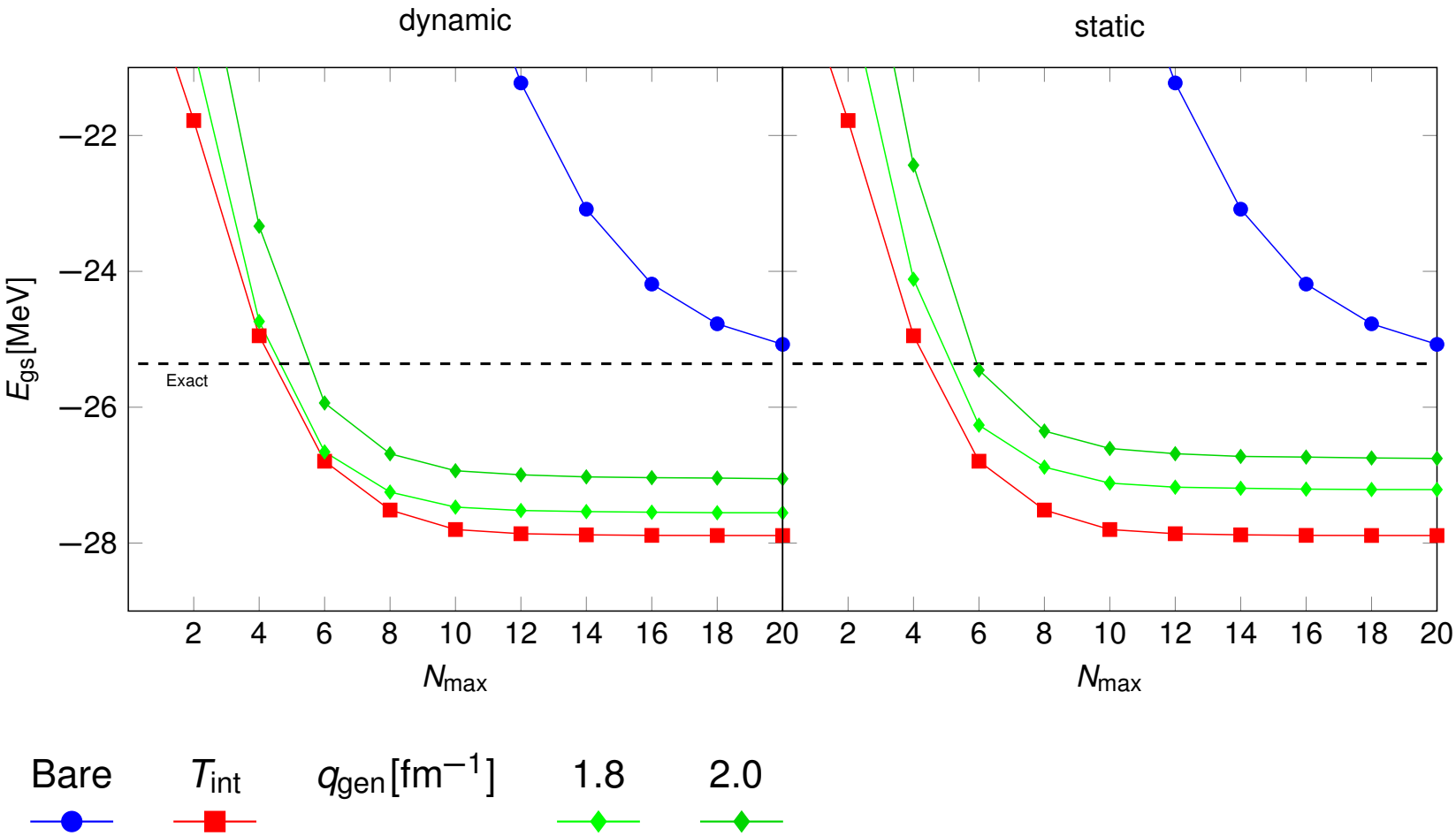
^{4}He

$\hbar\omega = 24$ MeV

$\alpha = 0.04$ fm^4

NN_{only}

NCSM ^{4}He : Two-Body Evolution with Q Block



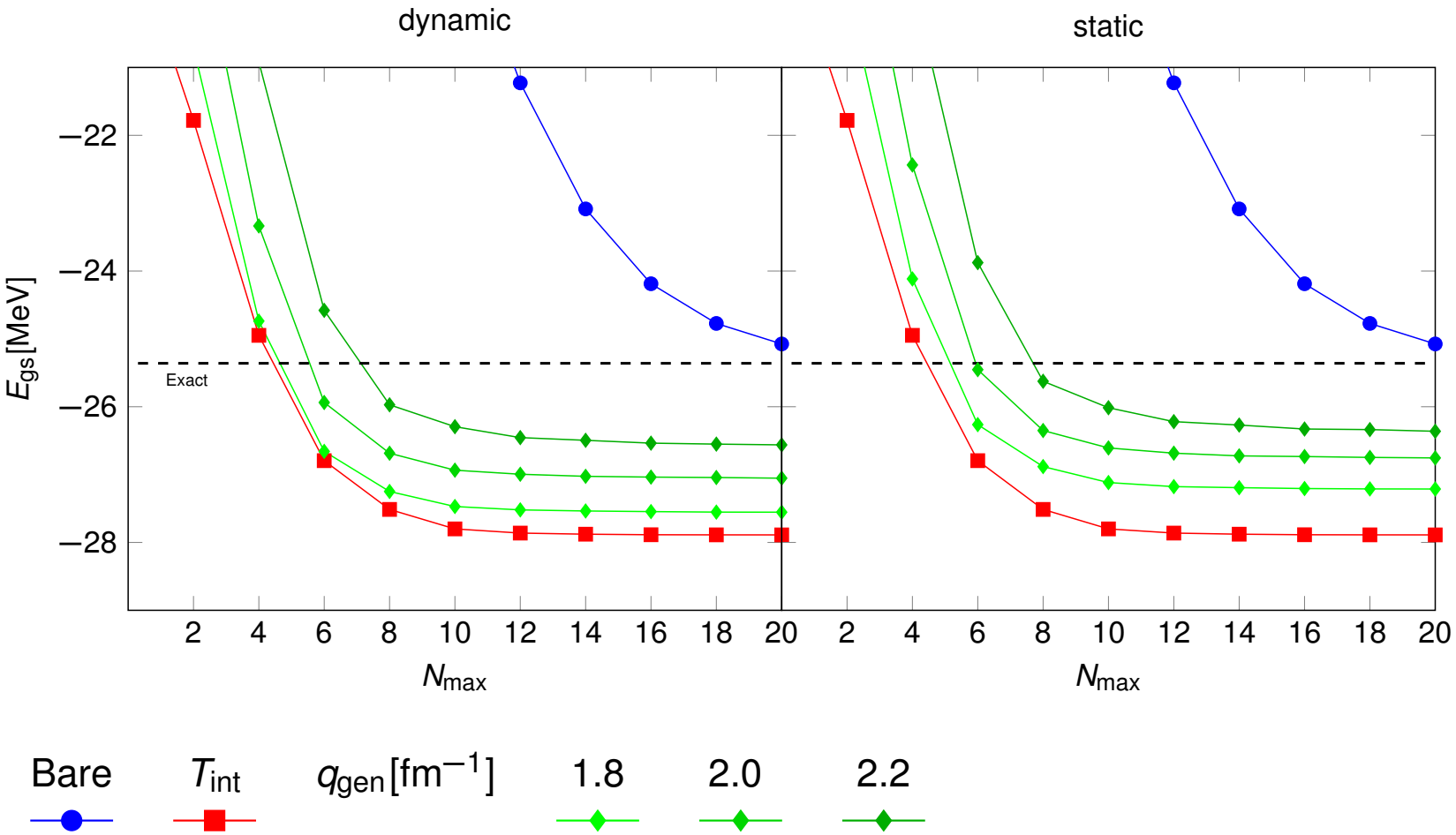
^{4}He

$\hbar\omega = 24$ MeV

$\alpha = 0.04$ fm^4

$\mathrm{NN}_{\mathrm{only}}$

NCSM ^{4}He : Two-Body Evolution with Q Block



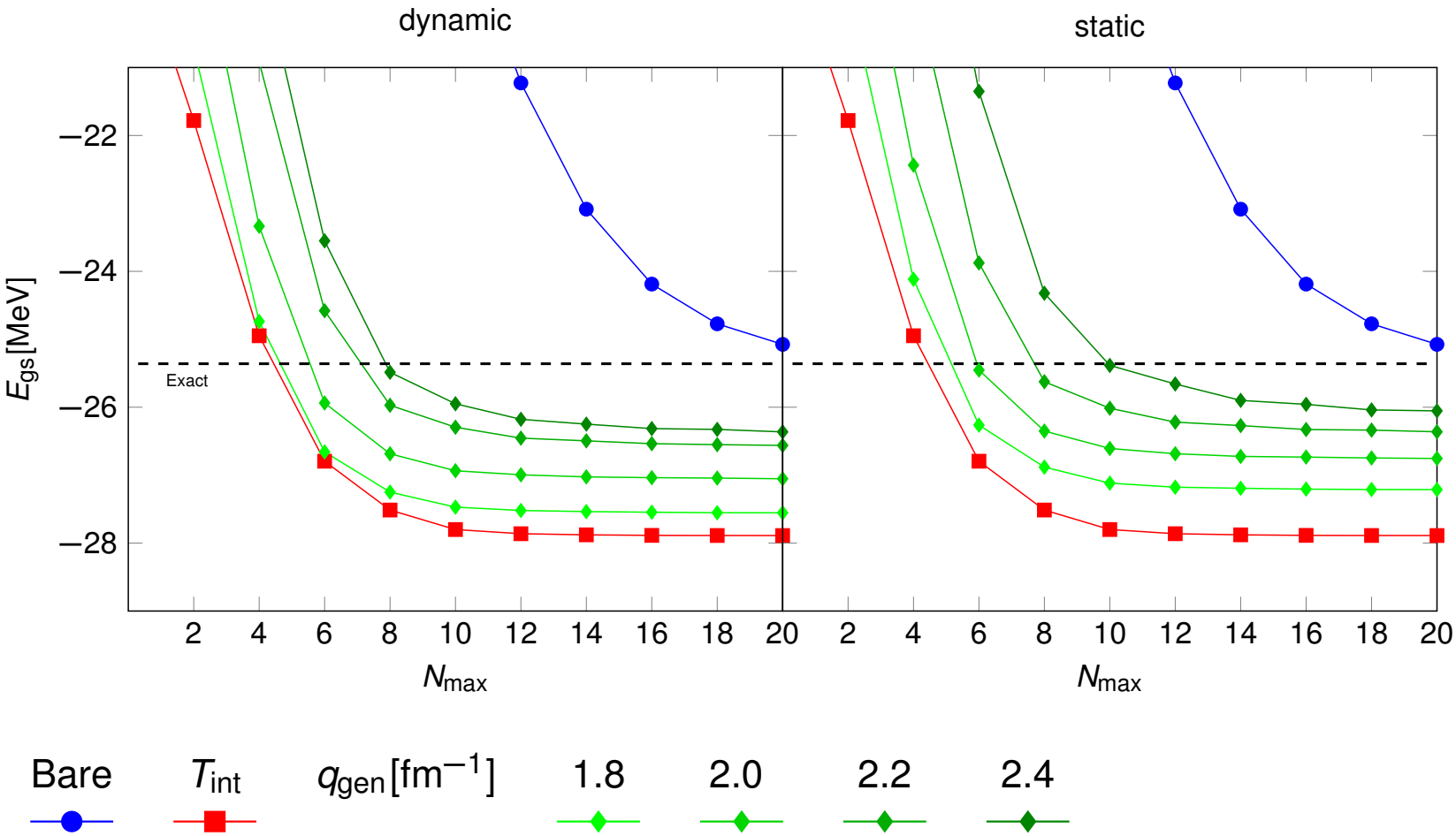
^{4}He

$\hbar\omega = 24$ MeV

$\alpha = 0.04$ fm^4

NN_{only}

NCSM ^{4}He : Two-Body Evolution with Q Block



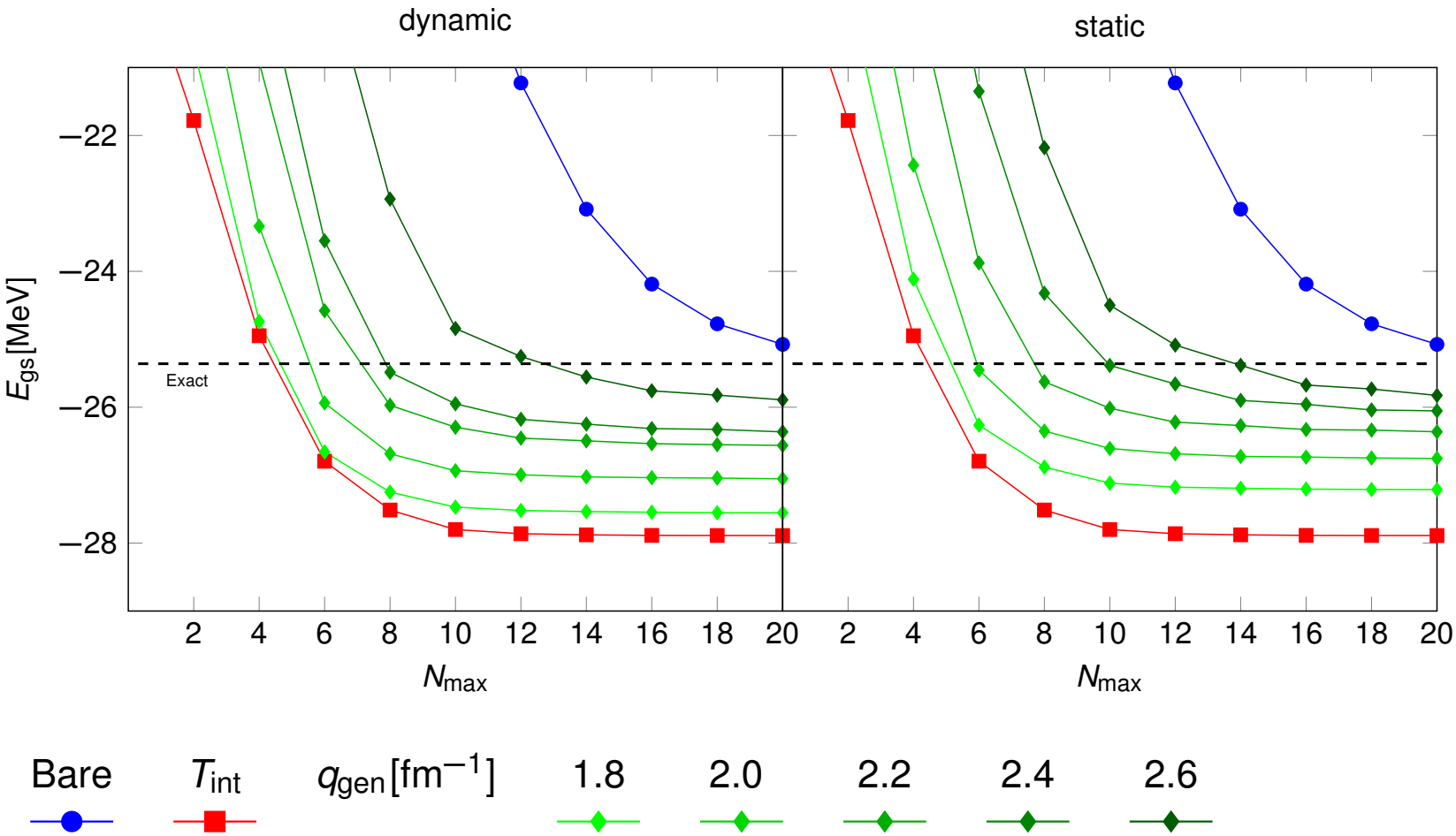
^{4}He

$\hbar\omega = 24$ MeV

$\alpha = 0.04$ fm^4

NN_{only}

NCSM ^{4}He : Two-Body Evolution with Q Block



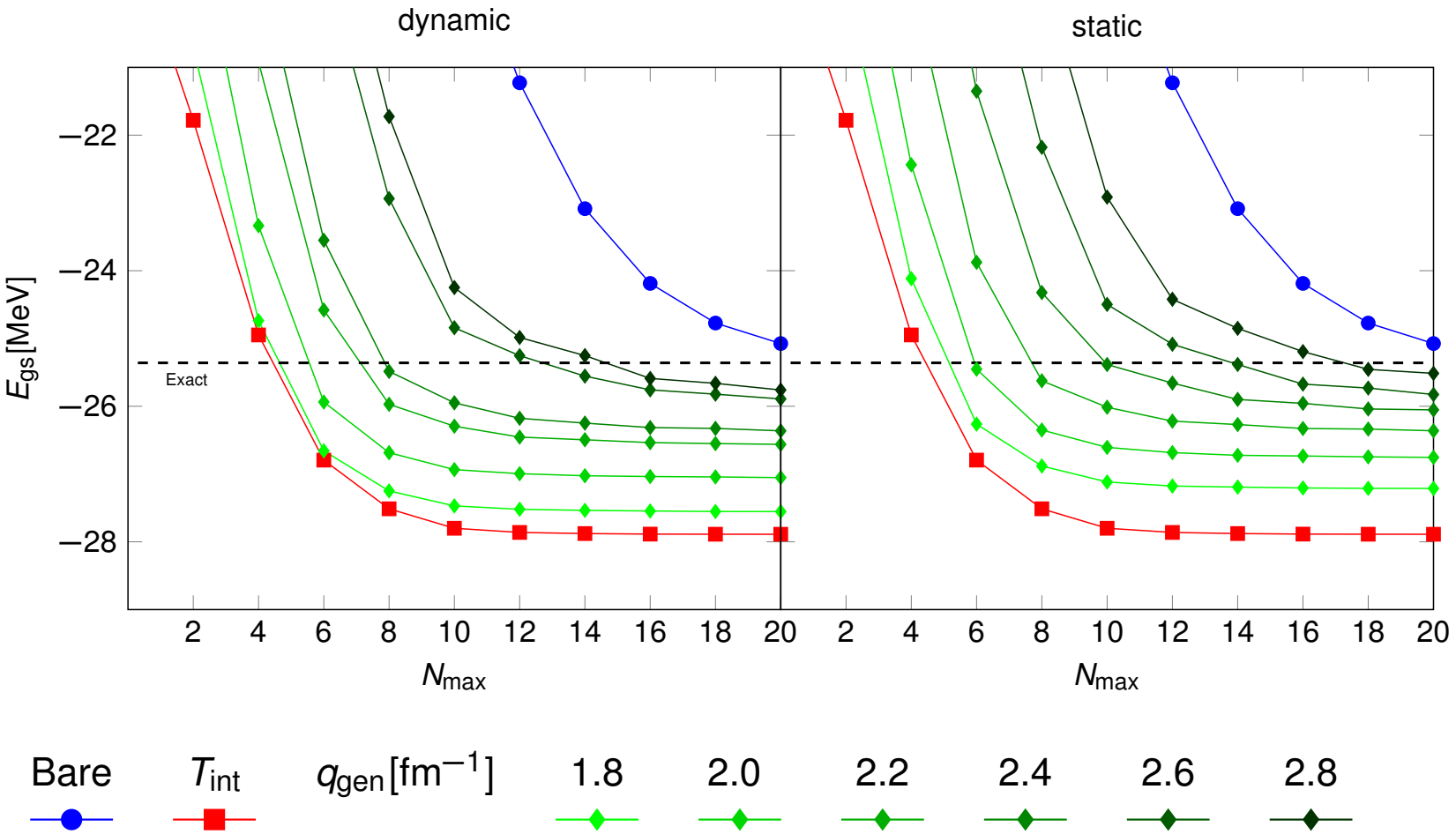
^{4}He

$\hbar\omega = 24$ MeV

$\alpha = 0.04$ fm^4

NN_{only}

NCSM ^{4}He : Two-Body Evolution with Q Block



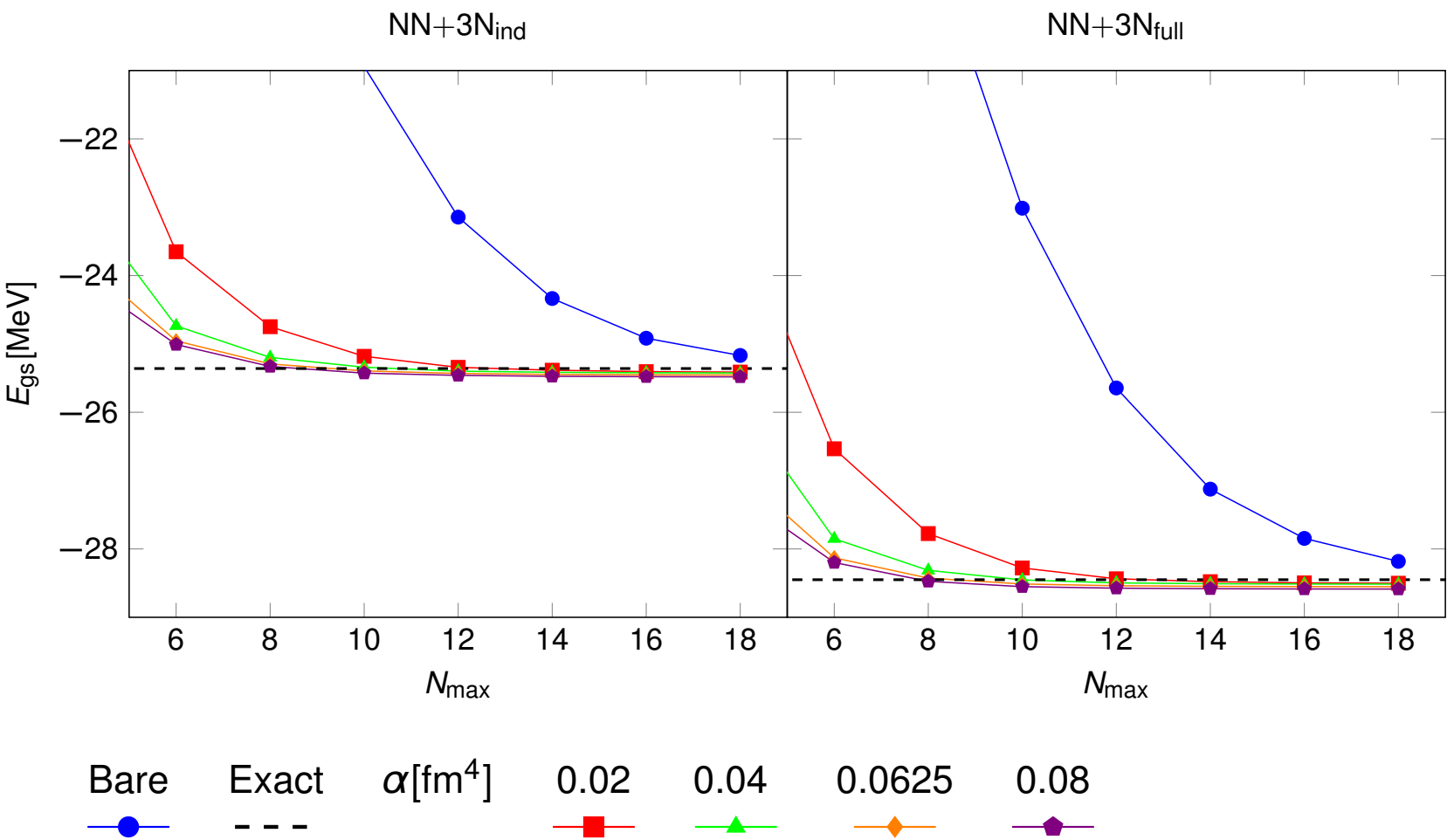
^{4}He

$\hbar\omega = 24$ MeV

$\alpha = 0.04$ fm^4

NN_{only}

NCSM ^{4}He: Three-Body Evolution with HO Block

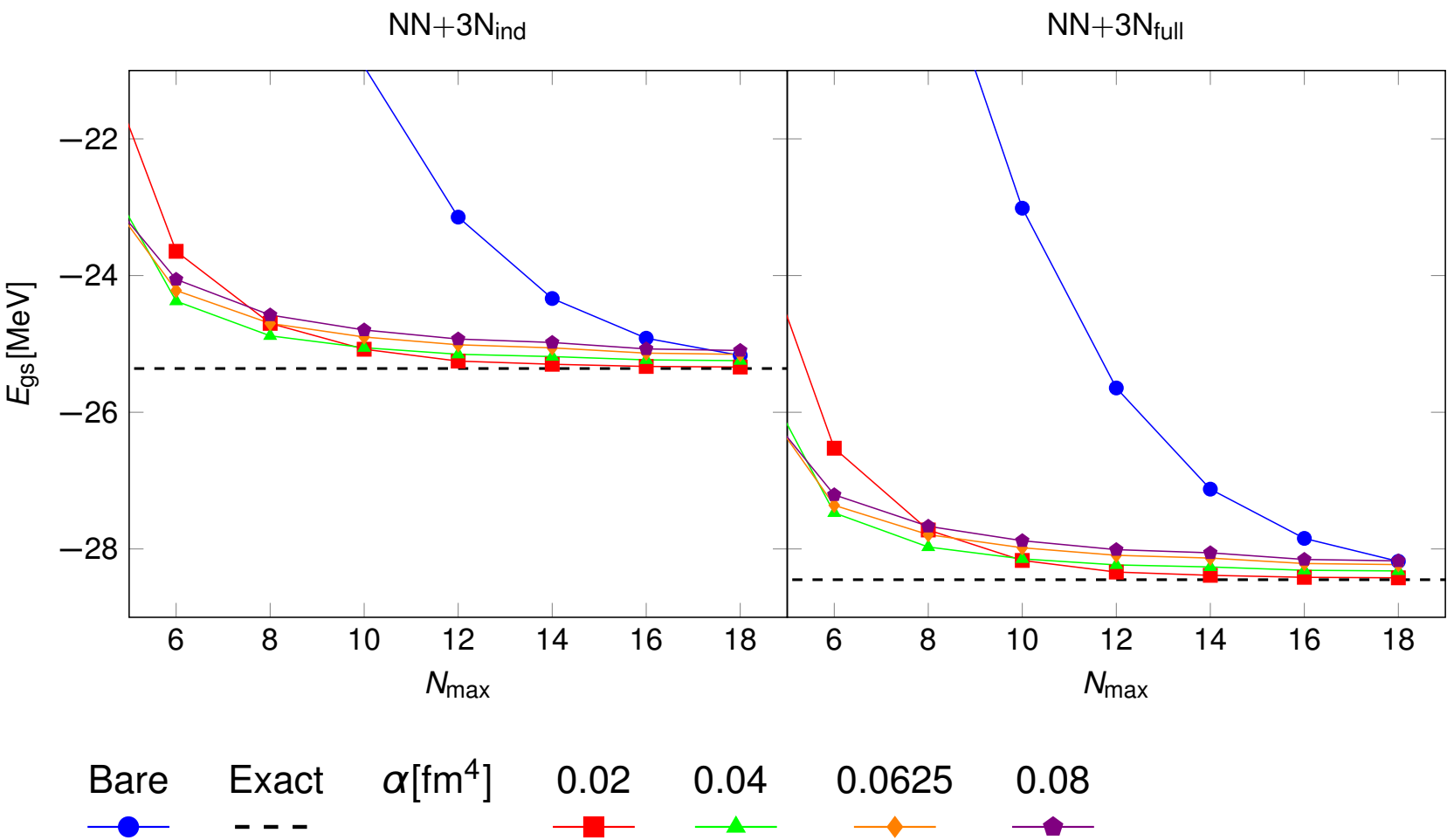


^{4}He

$\hbar\omega = 28$ MeV

E_{gen}=4

NCSM ^{4}He: Three-Body Evolution with Q Block



^{4}He

$\hbar\omega = 28$ MeV

q_{gen}=2.0 fm^{-1}

Band Generator

- Band generator

$$\boldsymbol{G}_\alpha = \boldsymbol{T}_{\text{int}} + \boldsymbol{P}_{\text{band}} \boldsymbol{V}_{\text{NN},\alpha} \boldsymbol{P}_{\text{band}}$$

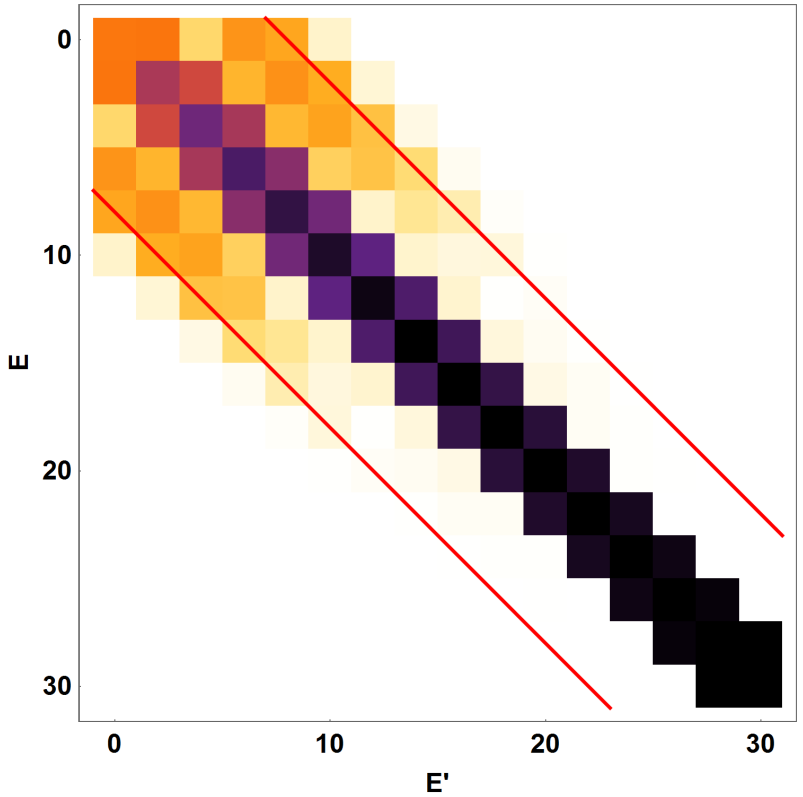
- In harmonic-oscillator (HO) basis

Coutts, Navrátil *et al.* in preparation

$$\boldsymbol{P}^{\text{HO}}_{\text{gen}} = e^{-\frac{1}{2}\left(\frac{E-E'}{E_{\text{band}}}\right)^{2n}}$$

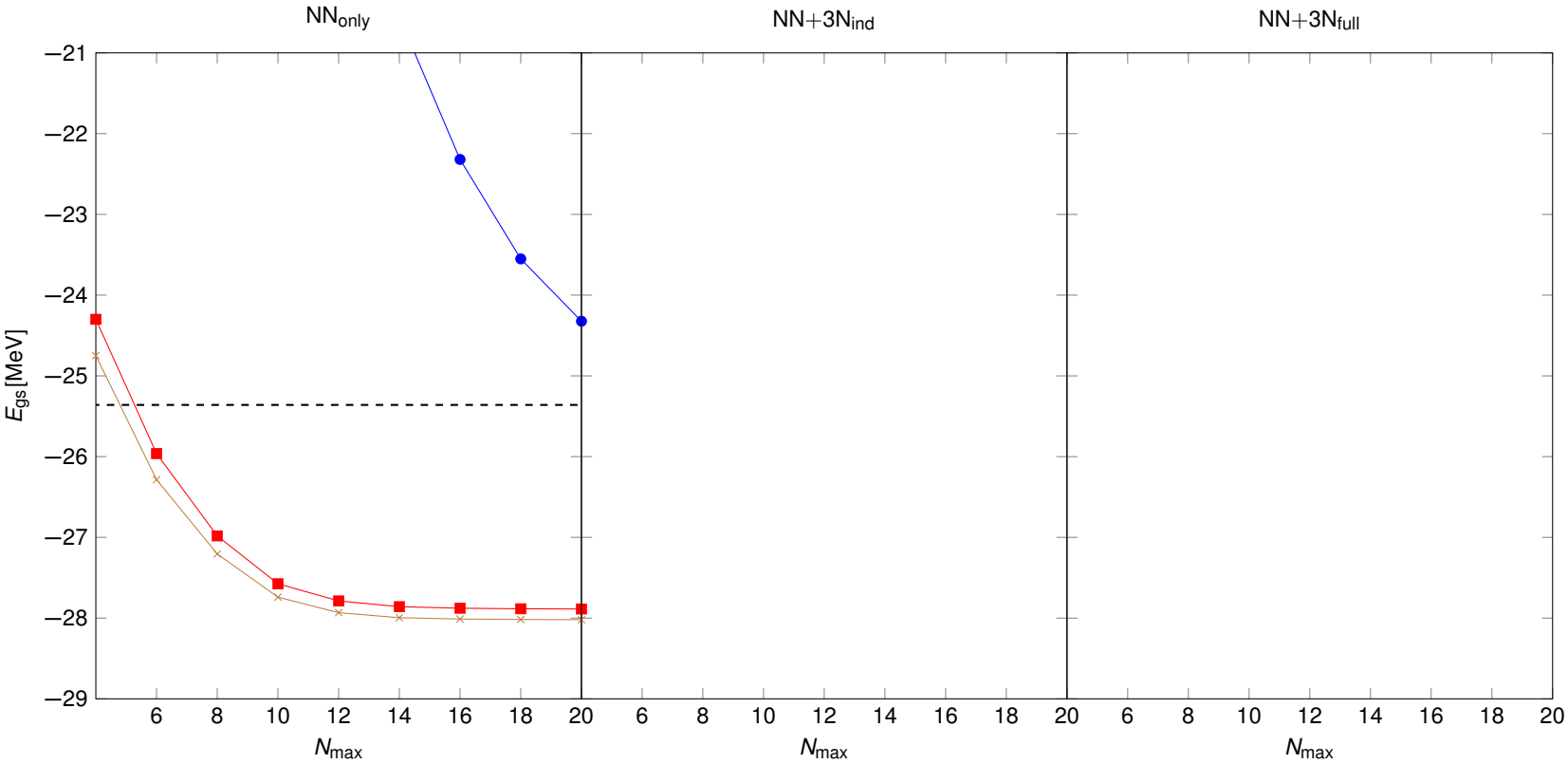
- Parameter E_{band} determines width of band
- Analog in momentum space

$$\boldsymbol{P}^{\text{Q}}_{\text{band}} = e^{-\frac{1}{2}\left(\frac{q-q'}{q_{\text{band}}}\right)^{2n}}$$



$\boldsymbol{G}^{\text{HO}}_0$ in the $^3S_1-$channel with $E_{\text{band}} = 8$

NCSM ^{4}He : Band Generator



^{4}He

$\hbar\omega = 20$ MeV

$\alpha = 0.04$ fm^4

Bare

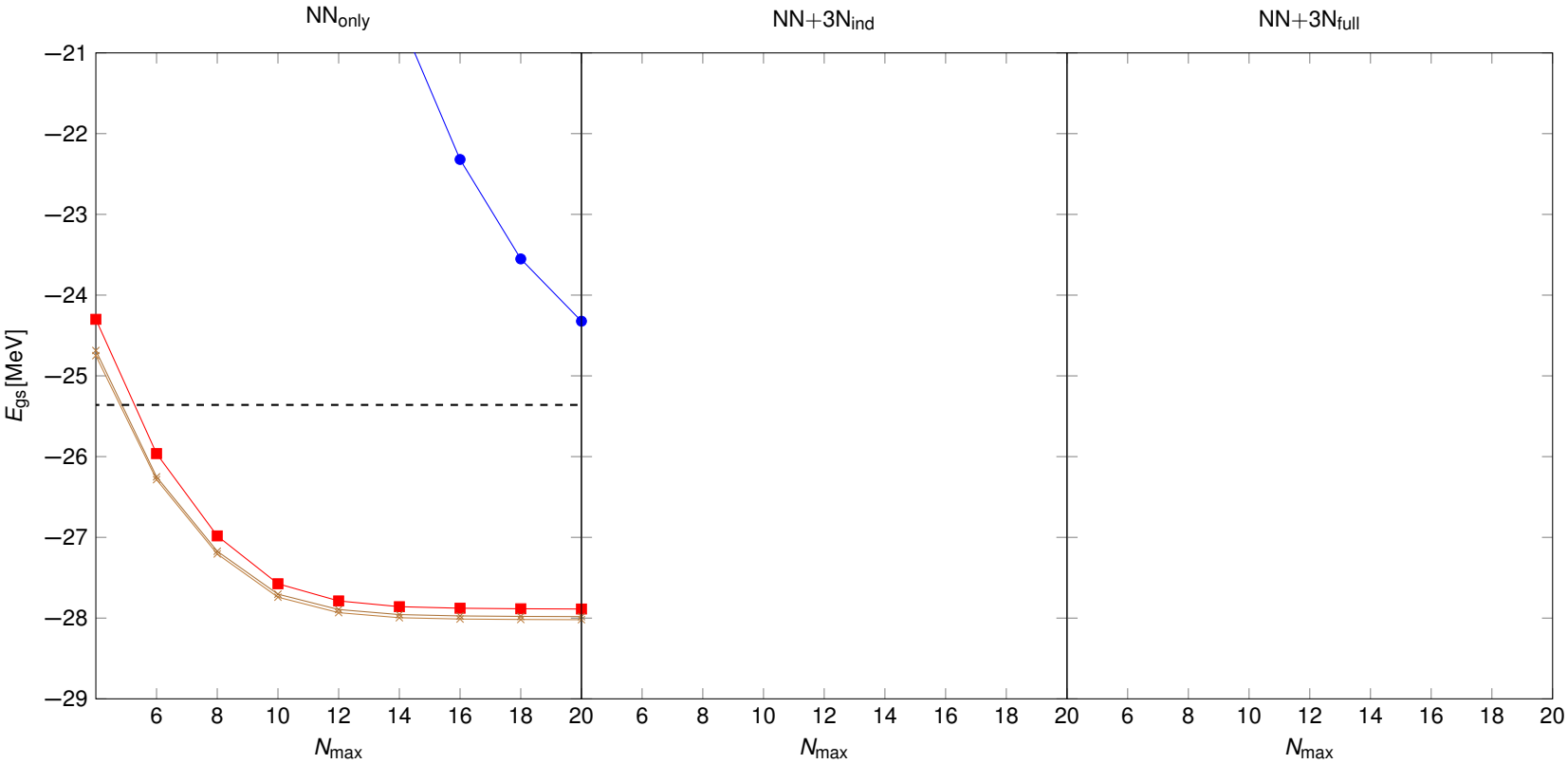
Exact

T_{int}

q_{band}[fm^{-1}]

0.4

NCSM ^{4}He : Band Generator



^{4}He

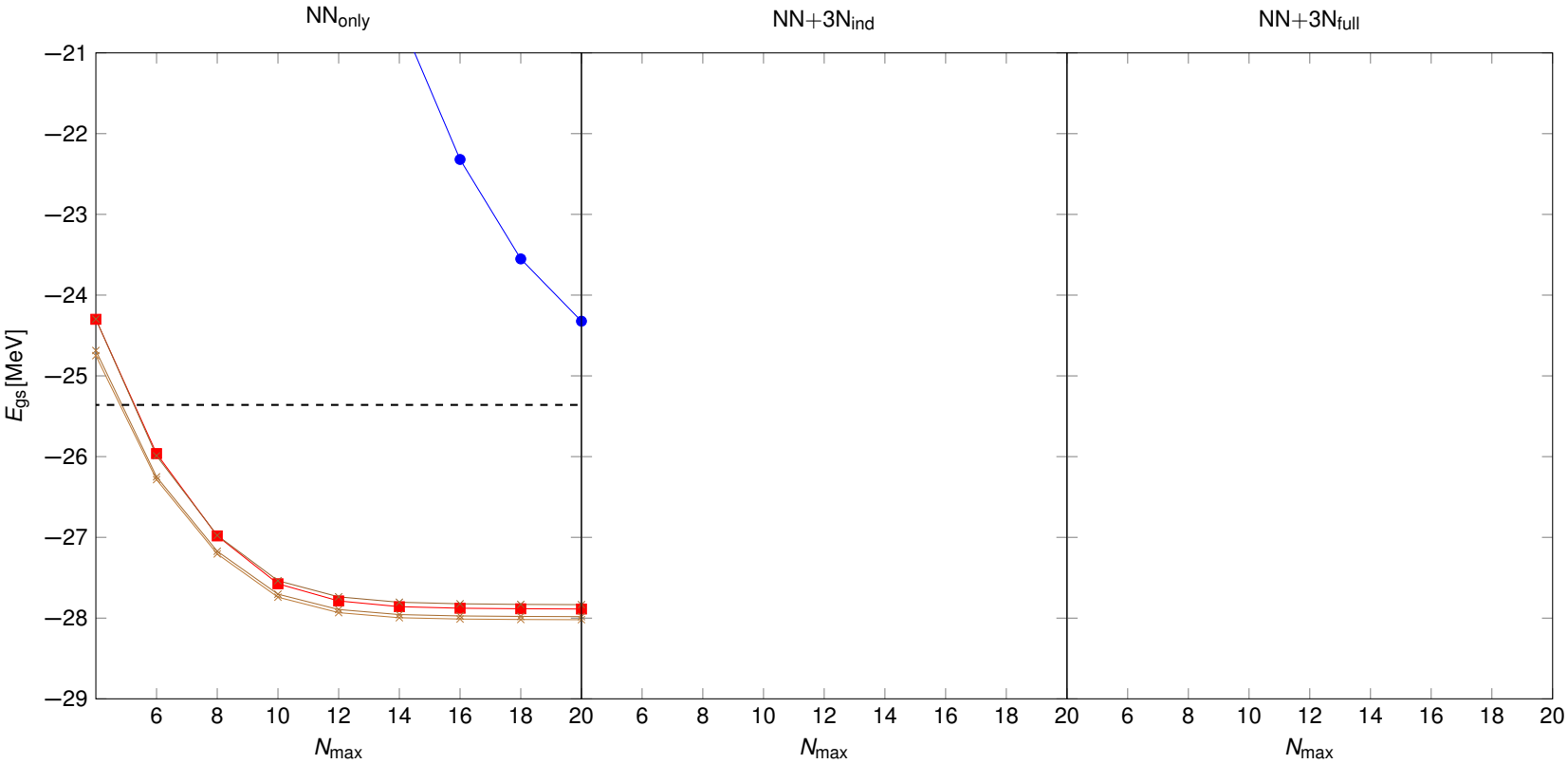
$\hbar\omega = 20$ MeV

$\alpha = 0.04$ fm^4

Bare Exact T_{int}

q_{band}[fm^{-1}] 0.4 0.6

NCSM ^{4}He : Band Generator



^{4}He

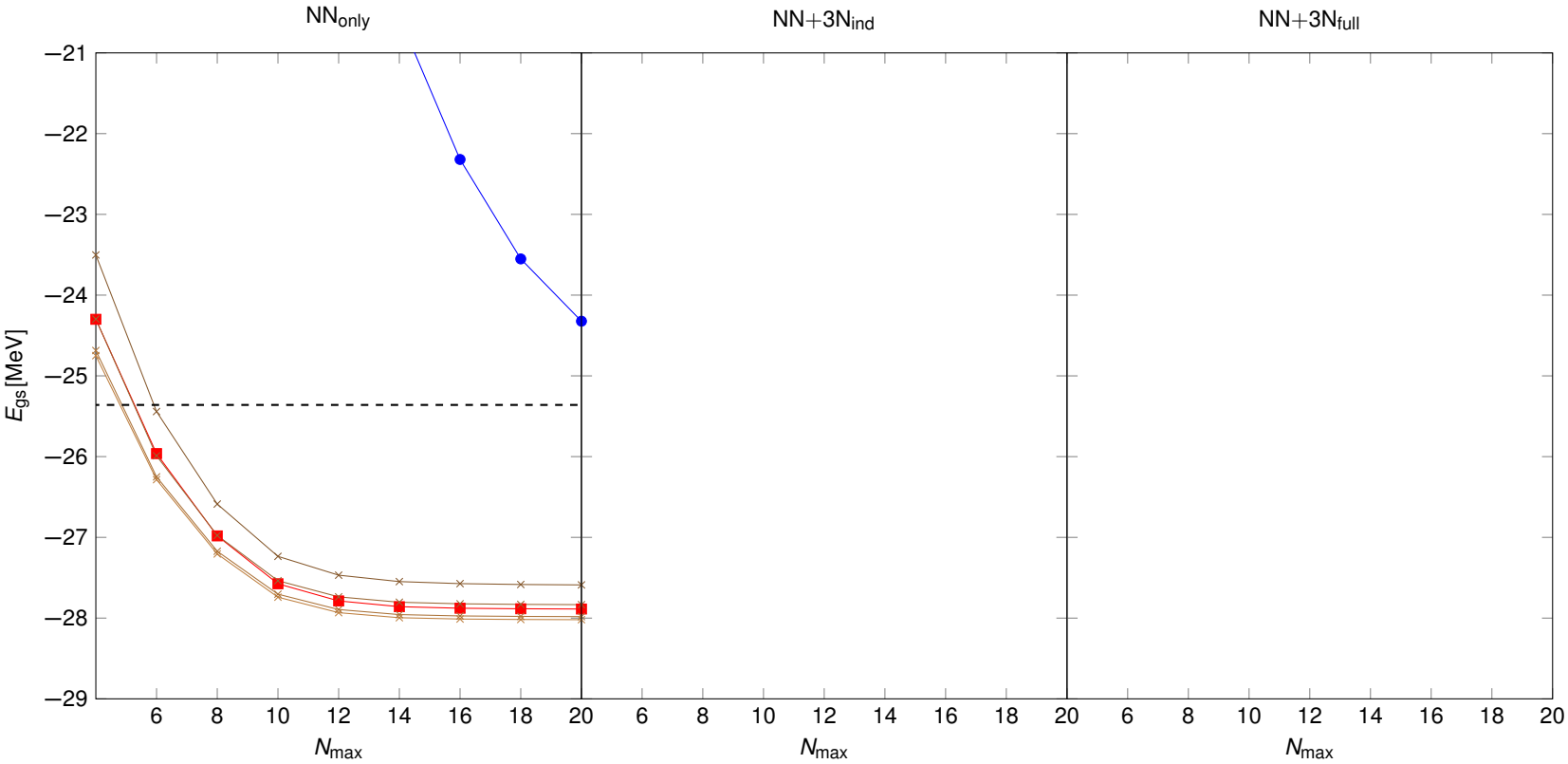
$\hbar\omega = 20$ MeV

$\alpha = 0.04$ fm^4

Bare Exact T_{int}

q_{band}[fm^{-1}] 0.4 0.6 0.8

NCSM ^{4}He : Band Generator



^{4}He

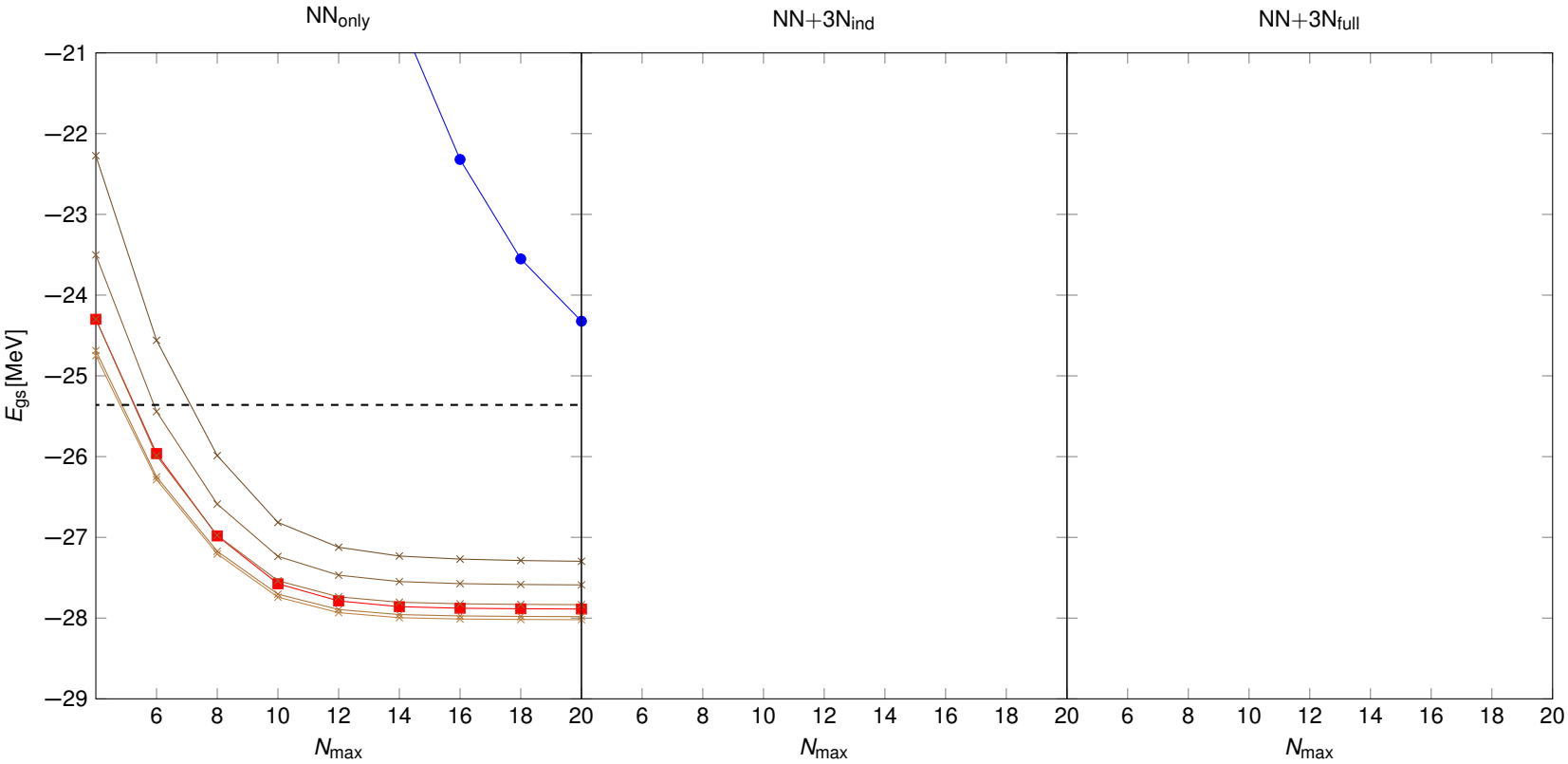
$\hbar\omega = 20$ MeV

$\alpha = 0.04$ fm^4

Bare Exact T_{int}

q_{band}[fm^{-1}] 0.4 0.6 0.8 1.0

NCSM ^{4}He : Band Generator



^{4}He

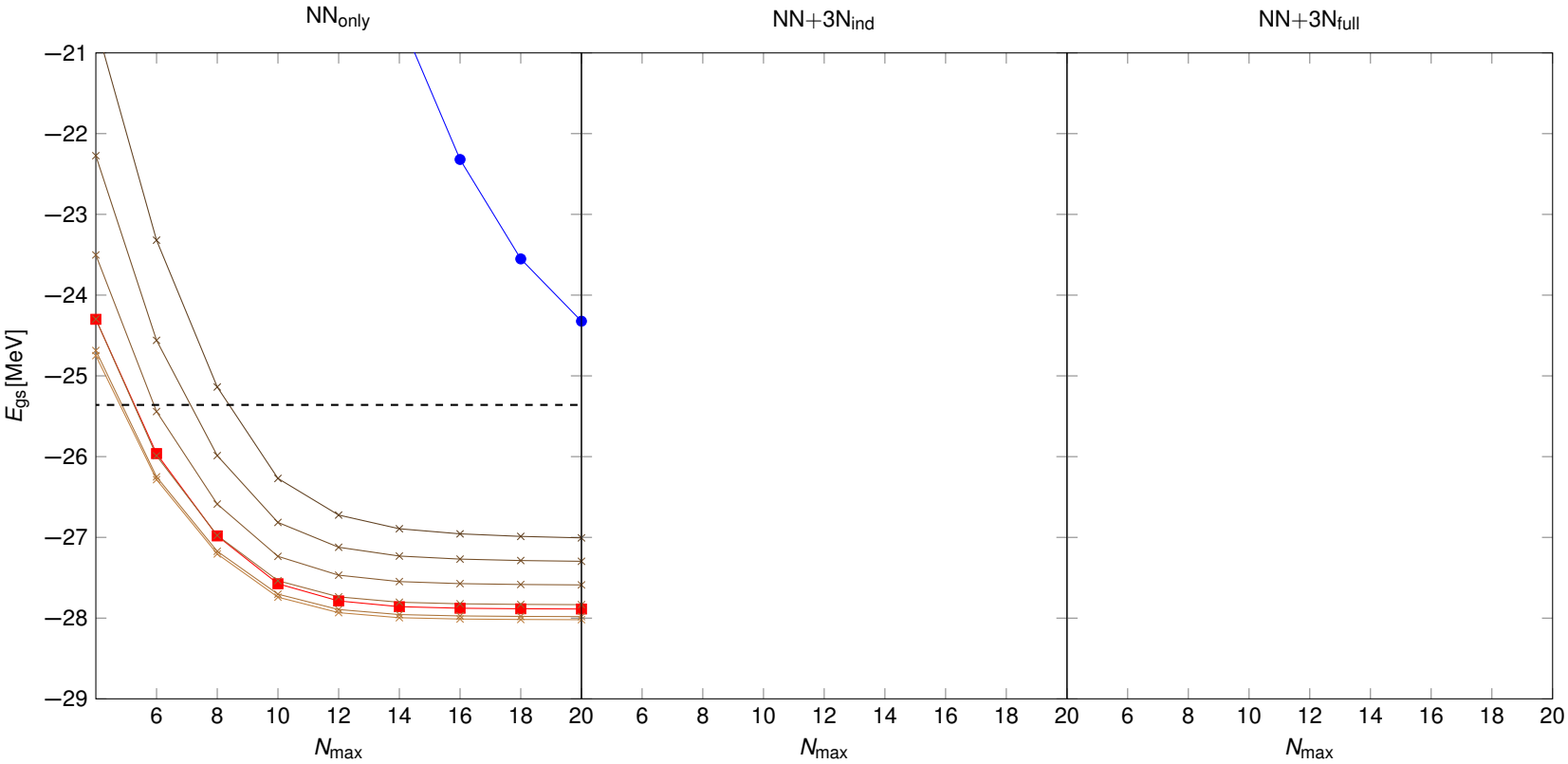
$\hbar\omega = 20$ MeV

$\alpha = 0.04$ fm^4

Bare Exact T_{int}

q_{band}[fm^{-1}] 0.4 0.6 0.8 1.0 1.2

NCSM ^{4}He : Band Generator



^{4}He

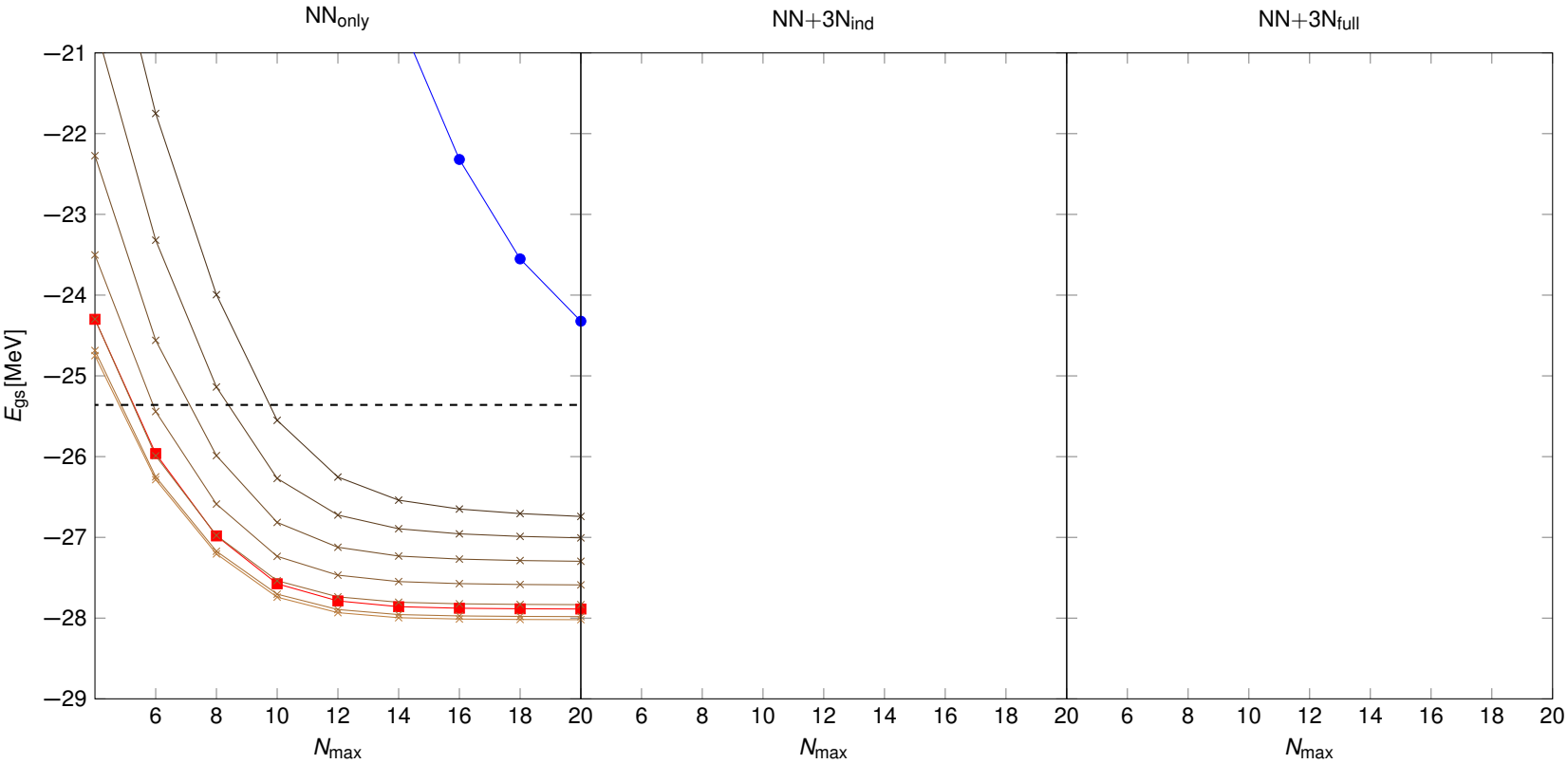
$\hbar\omega = 20$ MeV

$\alpha = 0.04$ fm^4

Bare Exact T_{int}

q_{band}[fm^{-1}] 0.4 0.6 0.8 1.0 1.2 1.4

NCSM ^{4}He : Band Generator



^{4}He

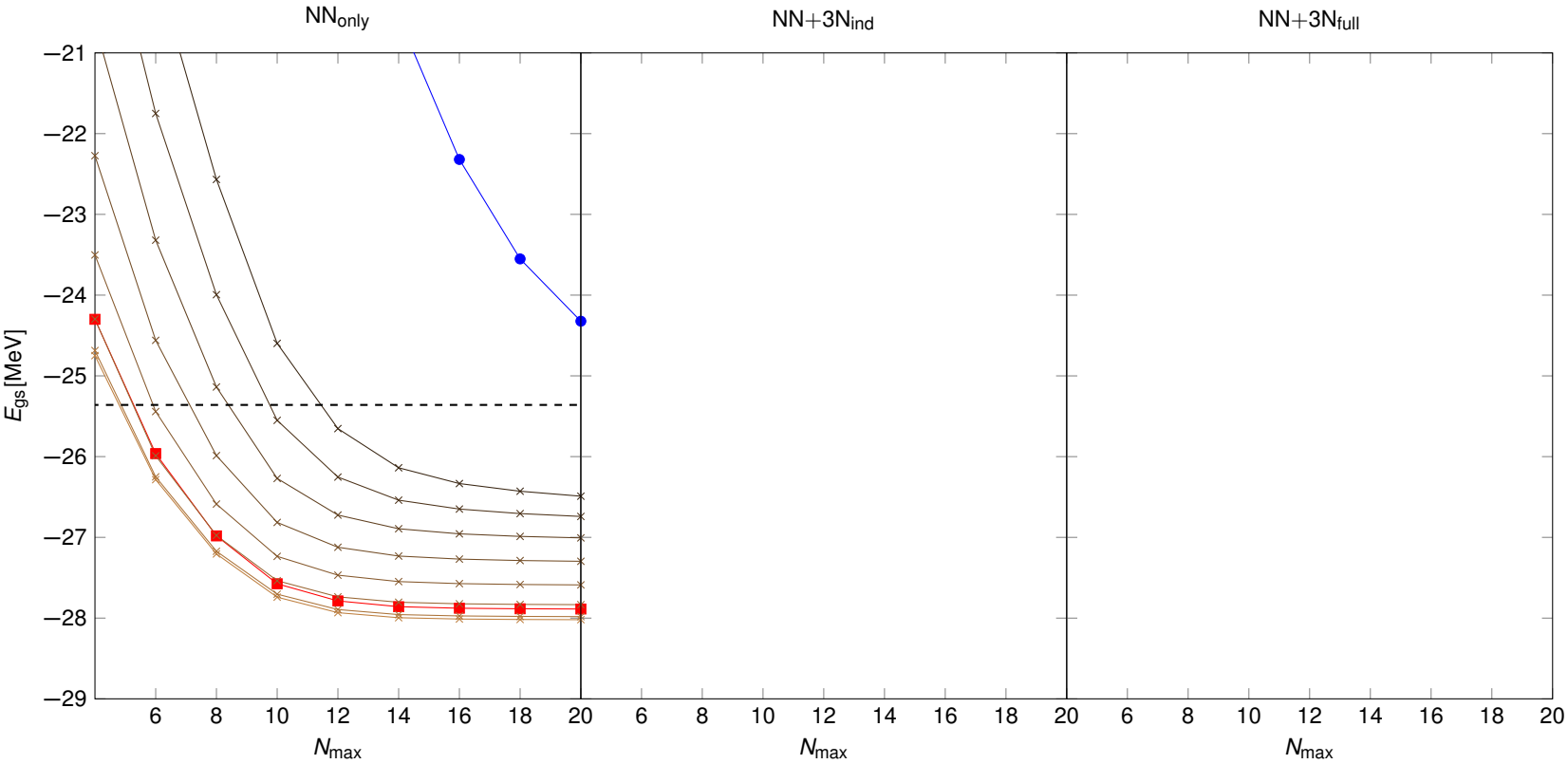
$\hbar\omega = 20$ MeV

$\alpha = 0.04$ fm^4

Bare Exact T_{int}

q_{band}[fm^{-1}] 0.4 0.6 0.8 1.0 1.2 1.4 1.6

NCSM ^{4}He : Band Generator



^{4}He

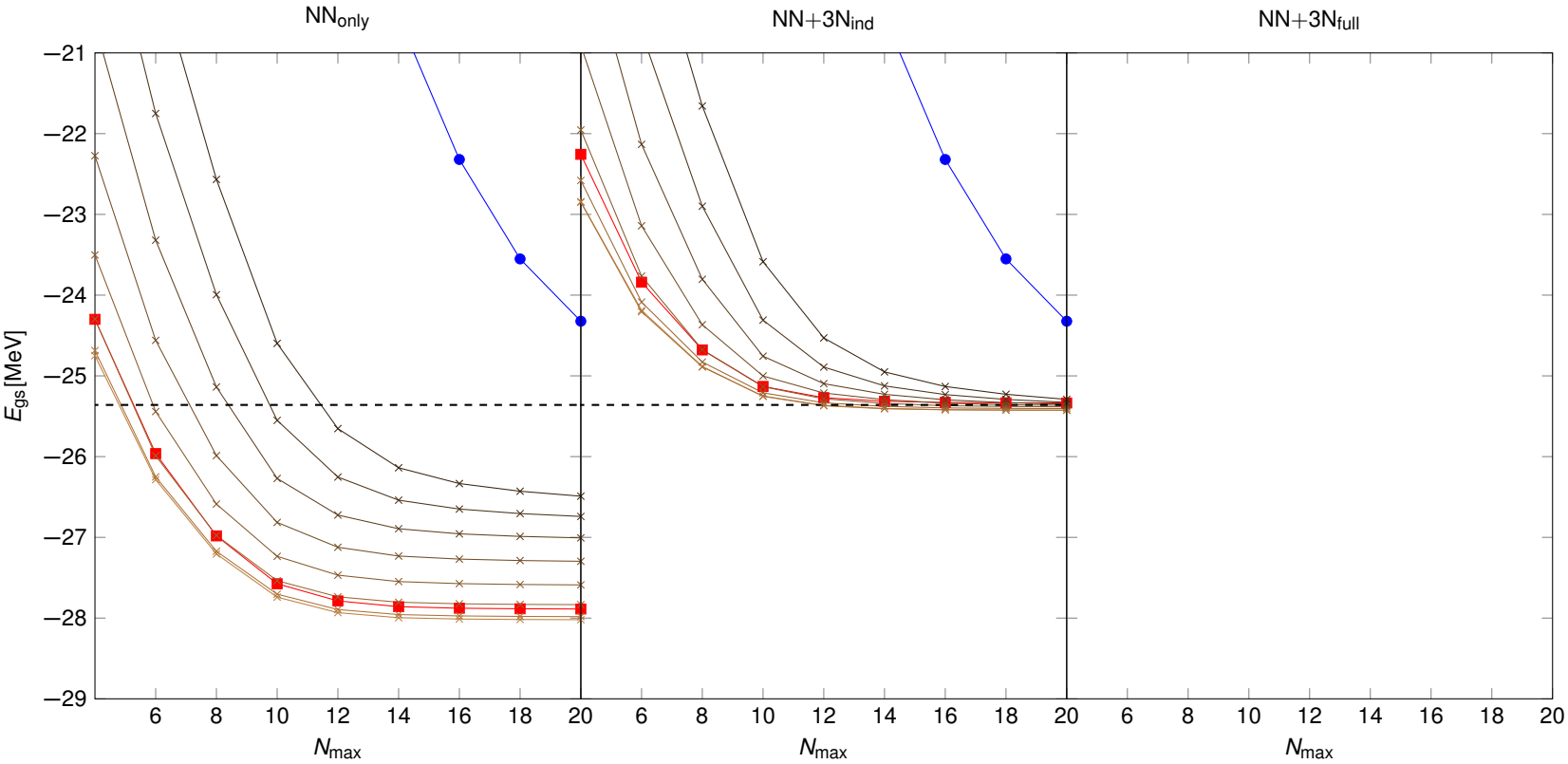
$\hbar\omega = 20$ MeV

$\alpha = 0.04$ fm^4

Bare Exact T_{int}

q_{band}[fm^{-1}]	0.4	0.6	0.8	1.0	1.2	1.4	1.6	1.8

NCSM ^{4}He : Band Generator



^{4}He

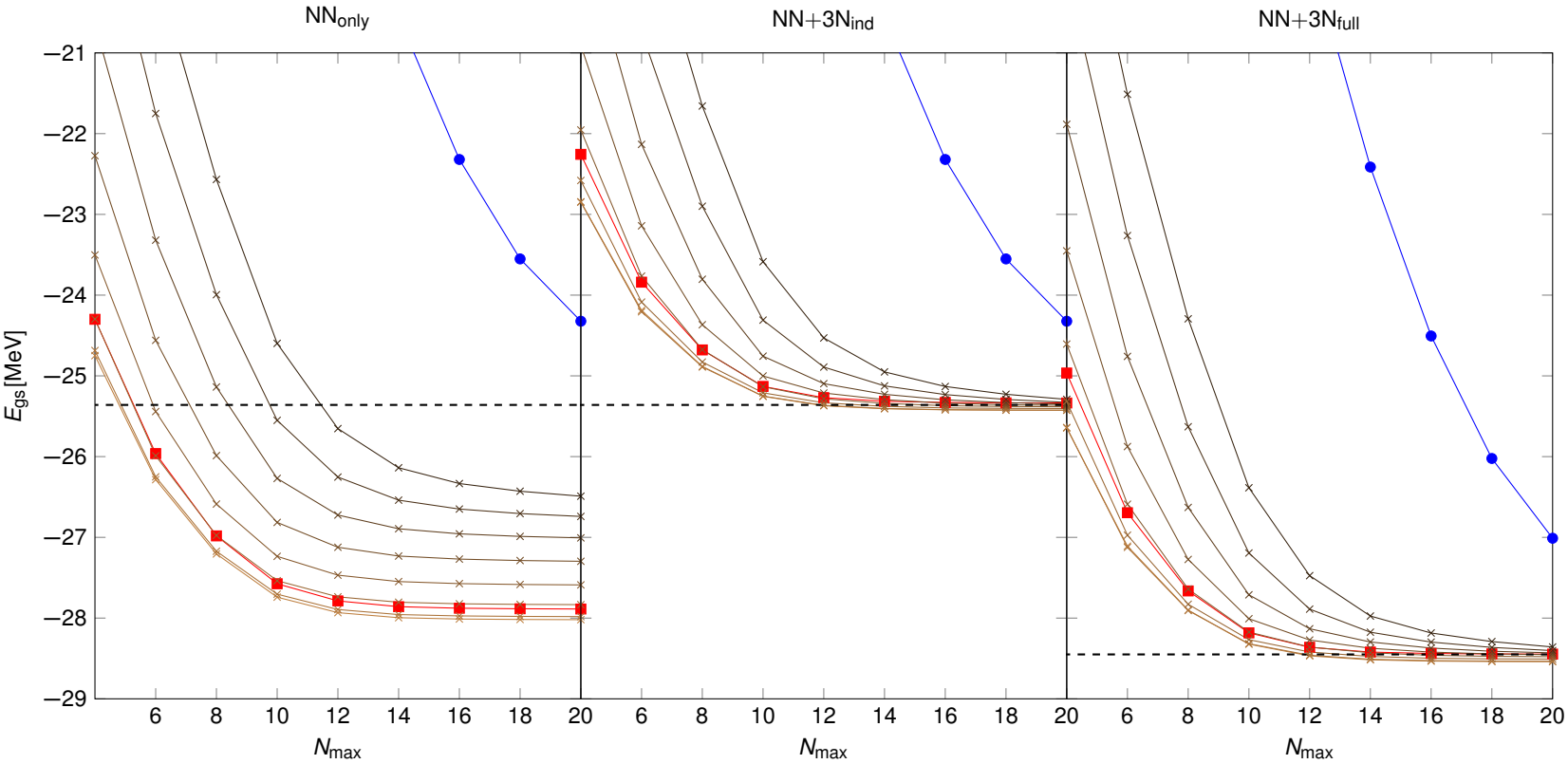
$\hbar\omega = 20$ MeV

$\alpha = 0.04$ fm^4

Bare Exact T_{int}

q_{band}[fm^{-1}] 0.4 0.6 0.8 1.0 1.2 1.4 1.6 1.8

NCSM ^{4}He : Band Generator



^{4}He

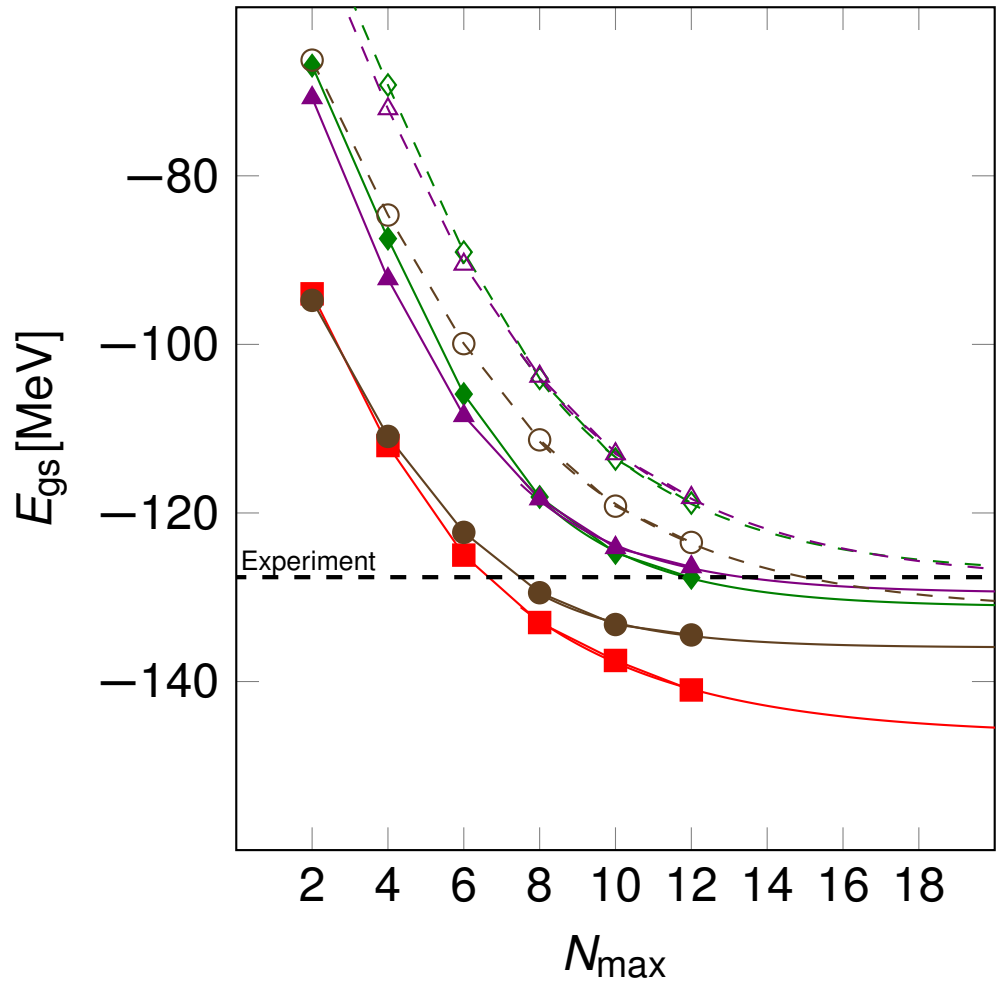
$\hbar\omega = 20$ MeV

$\alpha = 0.04$ fm^4

Bare Exact T_{int}

q_{band}[fm^{-1}] 0.4 0.6 0.8 1.0 1.2 1.4 1.6 1.8

IT-NCSM ^{16}O: Three-Body Evolution NN+3N$_{\text{full}}$



Summary and Outlook

- Explored new classes of SRG generators
- Complete implementation of the two- and three-body transformation
- Control balance between convergence and induced many-body forces

- Systematic analysis in various many-body methods
- Spectra of nuclei
- SRG transformation of observables
- Possible alternative to explicit inclusion of 4N forces in SRG framework

Epilog

- **Thanks to my group**
  - S. Alexa, S. Dentinger, E. Gebrerufael, L. Kreher, L. Mertes, **R. Roth**, S. Schulz, H. Spiess, H. Spielvogel, C. Stumpf, A. Tichai, R. Trippel, K. Vobig, R. Wirth
    Institut für Kernphysik, TU Darmstadt
- **Thanks to my collaborators**
  - **A. Calci**, **C. Coutts**, **N. Dicaire**, **P. Navráti**
    TRIUMF, Canada

- **Thank you for your attention!**

COMPUTING TIME

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