江南大学
JIANGNAN UNIVERSITY

蒙特卡洛壳模型的误差和外推

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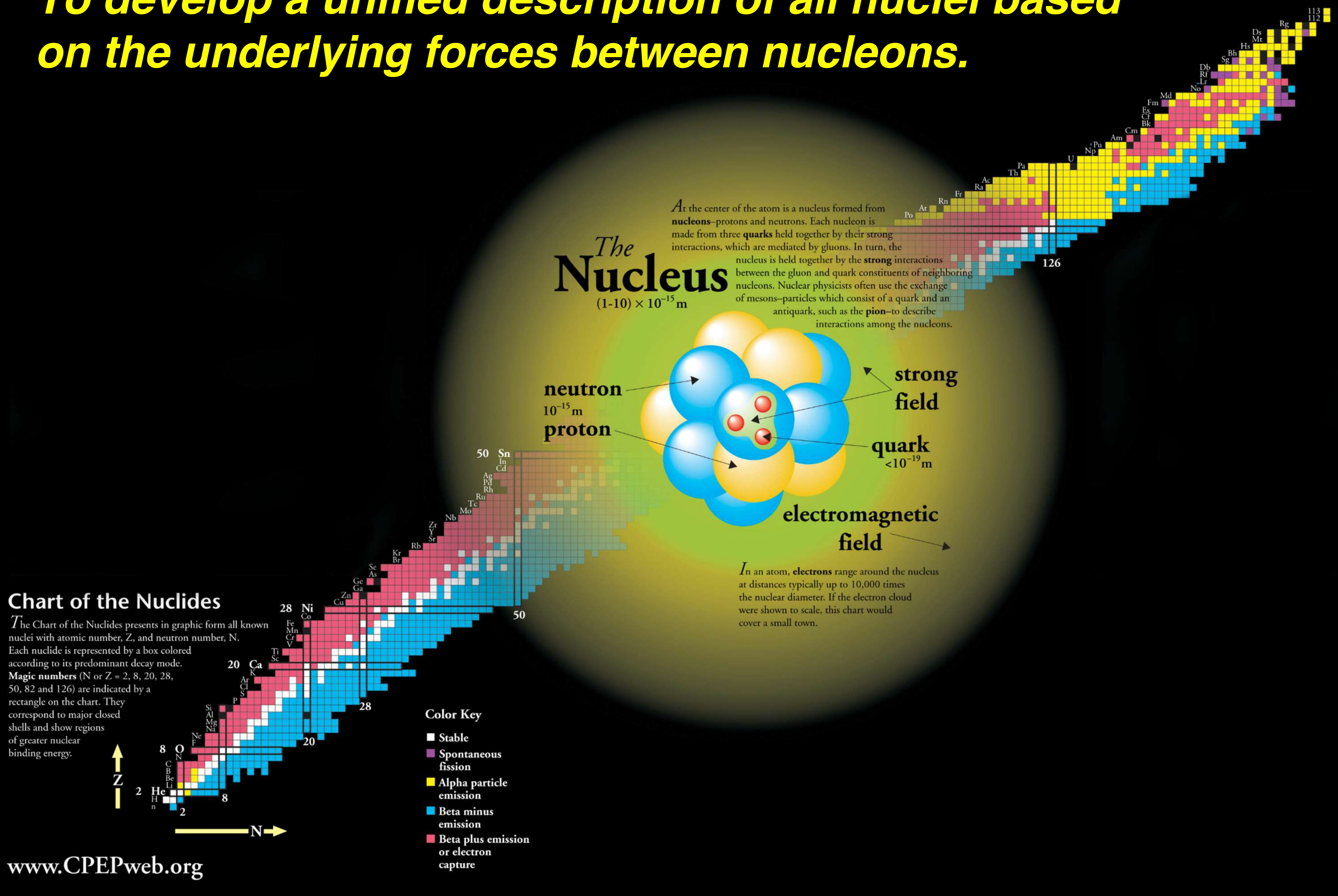
无中微子双贝塔衰变研讨会

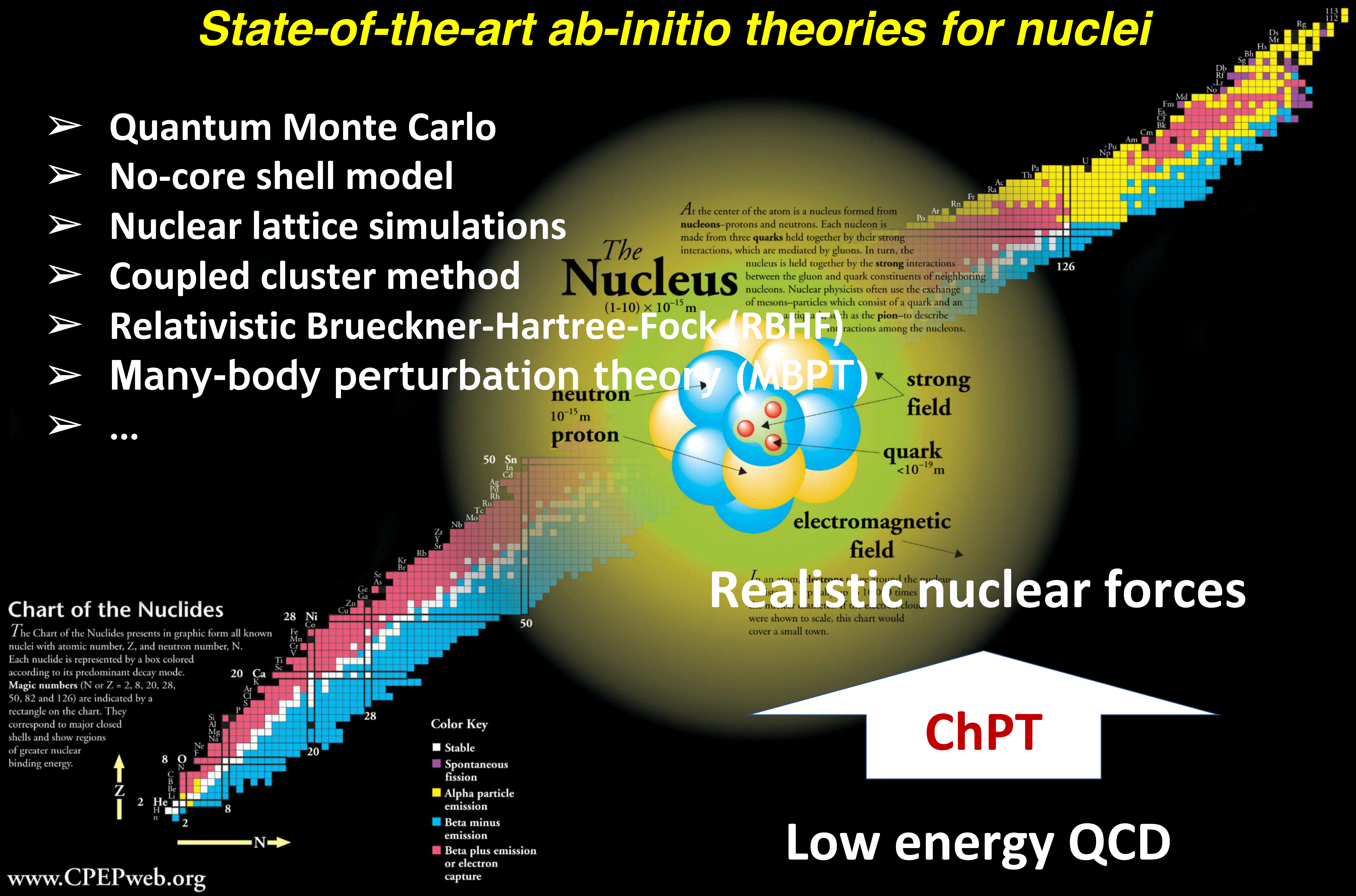
2021/05@珠海

To develop a unified description of all nuclei based on the underlying forces between nucleons.



State-of-the-art ab-initio theories for nuclei

- ➢ Quantum Monte Carlo
- ➢ No-core shell model
- ➢ Nuclear lattice simulations
- ➢ Coupled cluster method
- ➢ Relativistic Brueckner-Hartree-Fock (RBHF)
- ➢ Many-body perturbation theory (MBPT)
- ➢ …



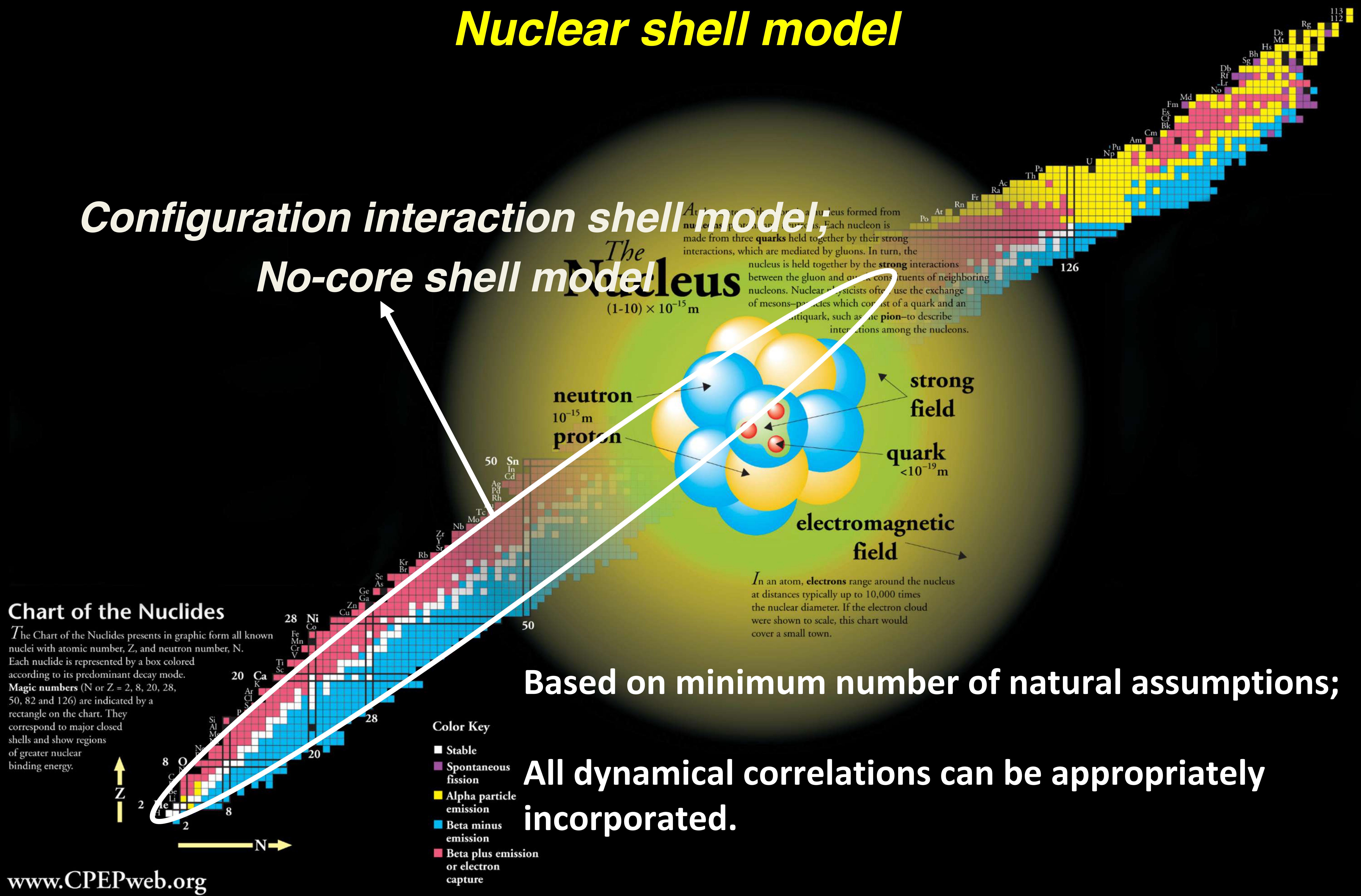
Realistic nuclear forces

ChPT

Low energy QCD

Nuclear shell model

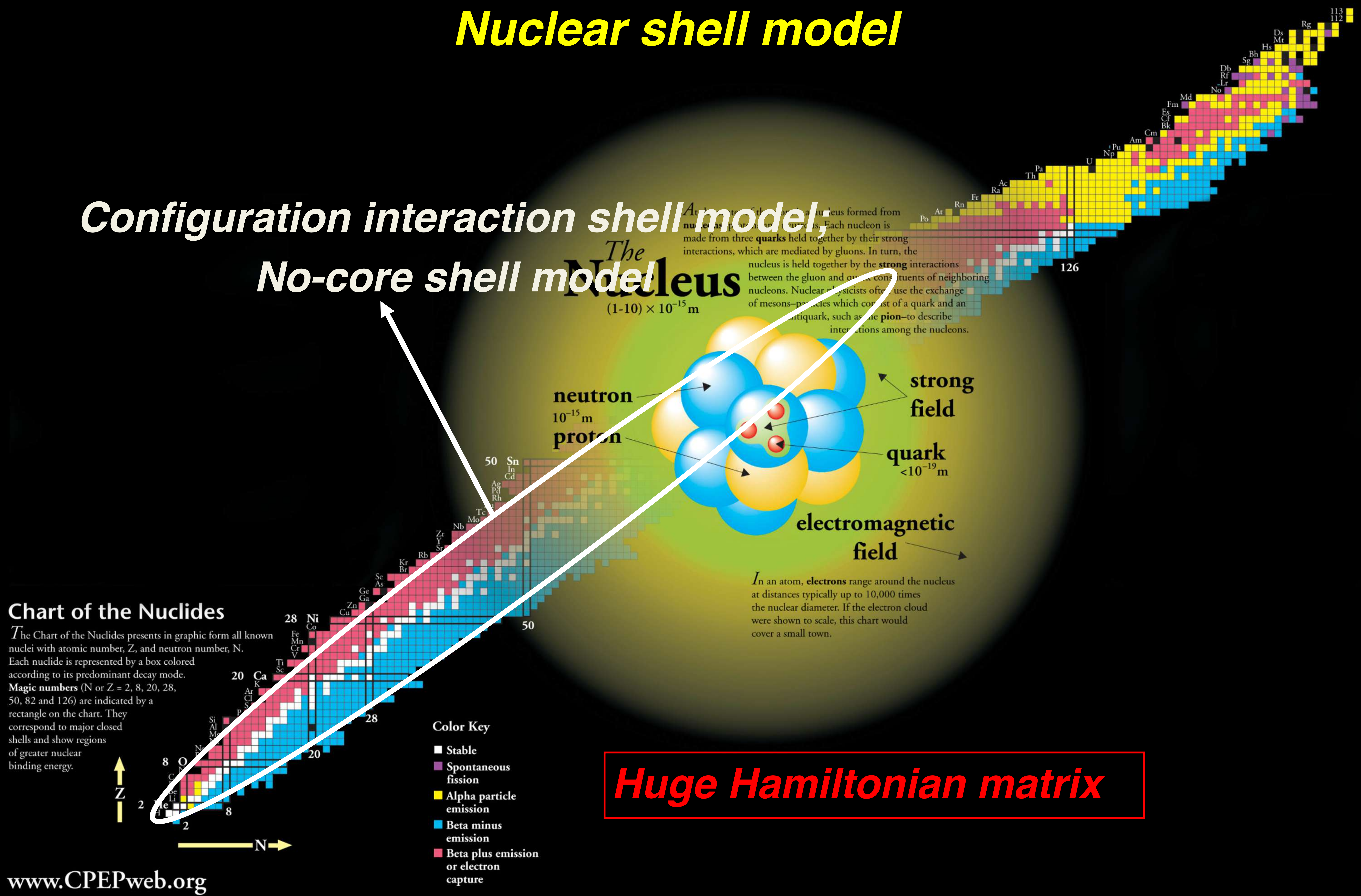
Configuration interaction shell model;
No-core shell model



Based on minimum number of natural assumptions;

All dynamical correlations can be appropriately incorporated.

Nuclear shell model



Configuration interaction shell model;

No-core shell model

Huge Hamiltonian matrix

Nuclear Shell Model

- Eigenvalue problem of large sparse Hamiltonian matrix

$$H|\Psi\rangle = E|\Psi\rangle$$

$$\begin{pmatrix} H_{11} & H_{12} & H_{13} & H_{14} & H_{15} & \cdots \\ H_{21} & H_{22} & H_{23} & H_{24} & & \\ H_{31} & H_{32} & H_{33} & & & \\ H_{41} & H_{33} & & \ddots & & \\ H_{51} & & & & & \\ \vdots & & & & & \end{pmatrix} \begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \\ \Psi_4 \\ \Psi_5 \\ \vdots \end{pmatrix} = \begin{pmatrix} E_1 & & & & 0 \\ & E_2 & & & \\ & & E_3 & & \\ & & & \ddots & \\ 0 & & & & \end{pmatrix} \begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \\ \Psi_4 \\ \Psi_5 \\ \vdots \end{pmatrix}$$

Large sparse matrix (in M-scheme)

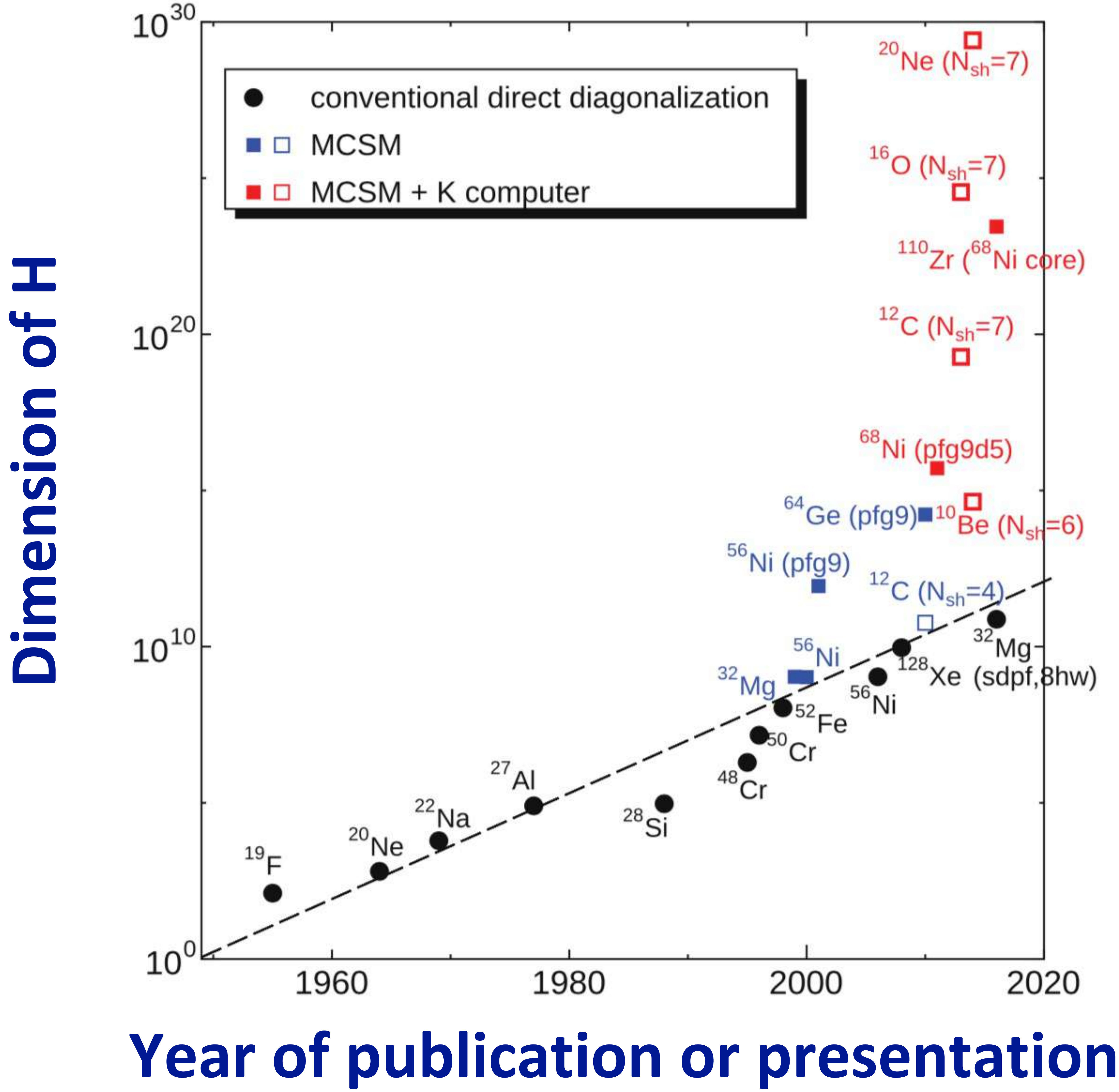
$$\sim \mathcal{O}(10^{10})$$

\# non-zero MEs $\sim \mathcal{O}(10^{13-14})$

$$\left\{ \begin{array}{lcl} |\Psi_1\rangle & = & a^\dagger_\alpha a^\dagger_\beta a^\dagger_\gamma \cdots |-\rangle \\ |\Psi_2\rangle & = & a^\dagger_{\alpha'} a^\dagger_{\beta'} a^\dagger_{\gamma'} \cdots |-\rangle \\ |\Psi_3\rangle & = & \cdots \\ \vdots & & \end{array} \right.$$

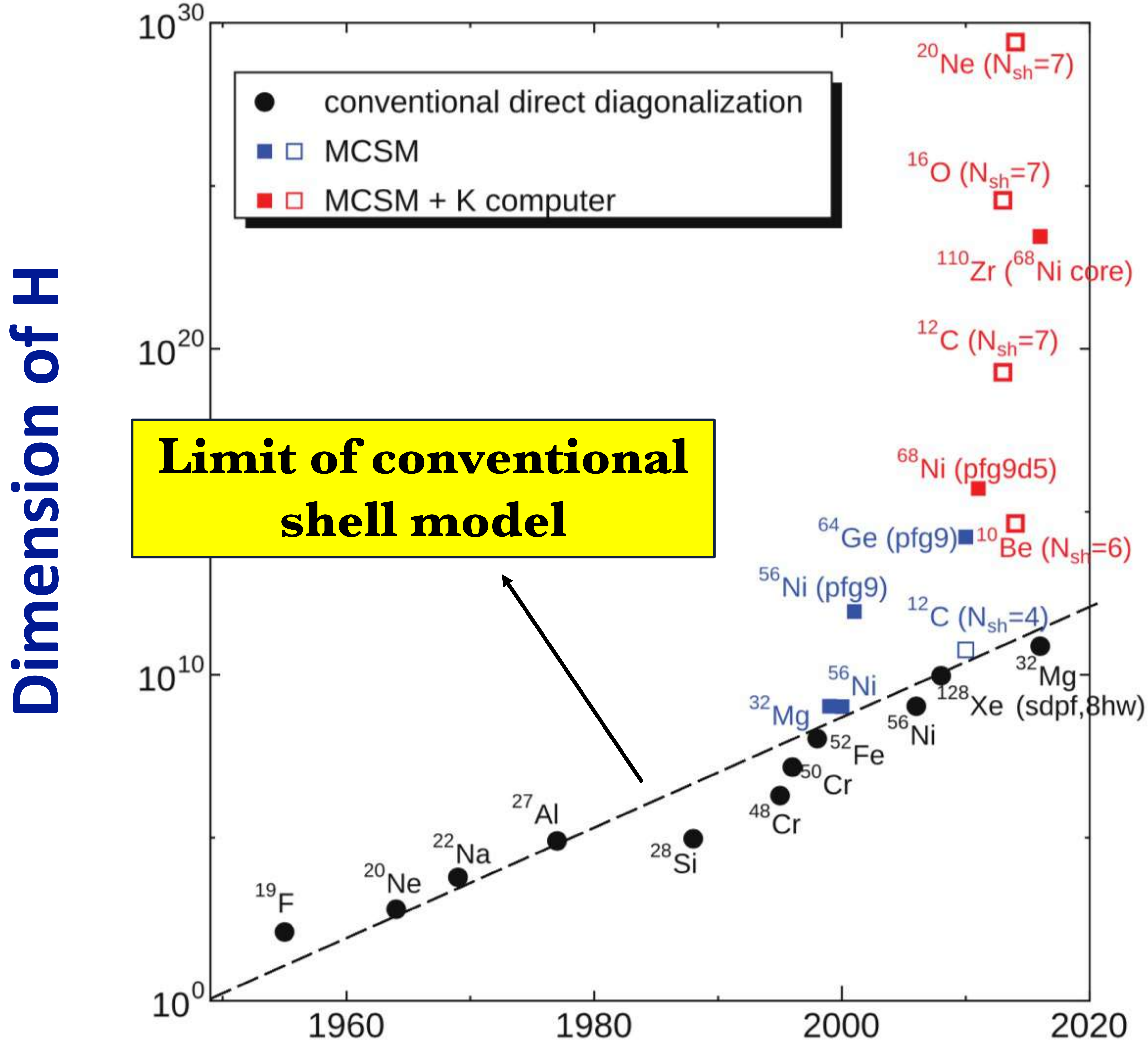
from T. Abe@UT

Historical Evolution of the Shell Model



N. Shimizu et al., Phys. Scr. 92, 063001 (2017).

Historical Evolution of the Shell Model



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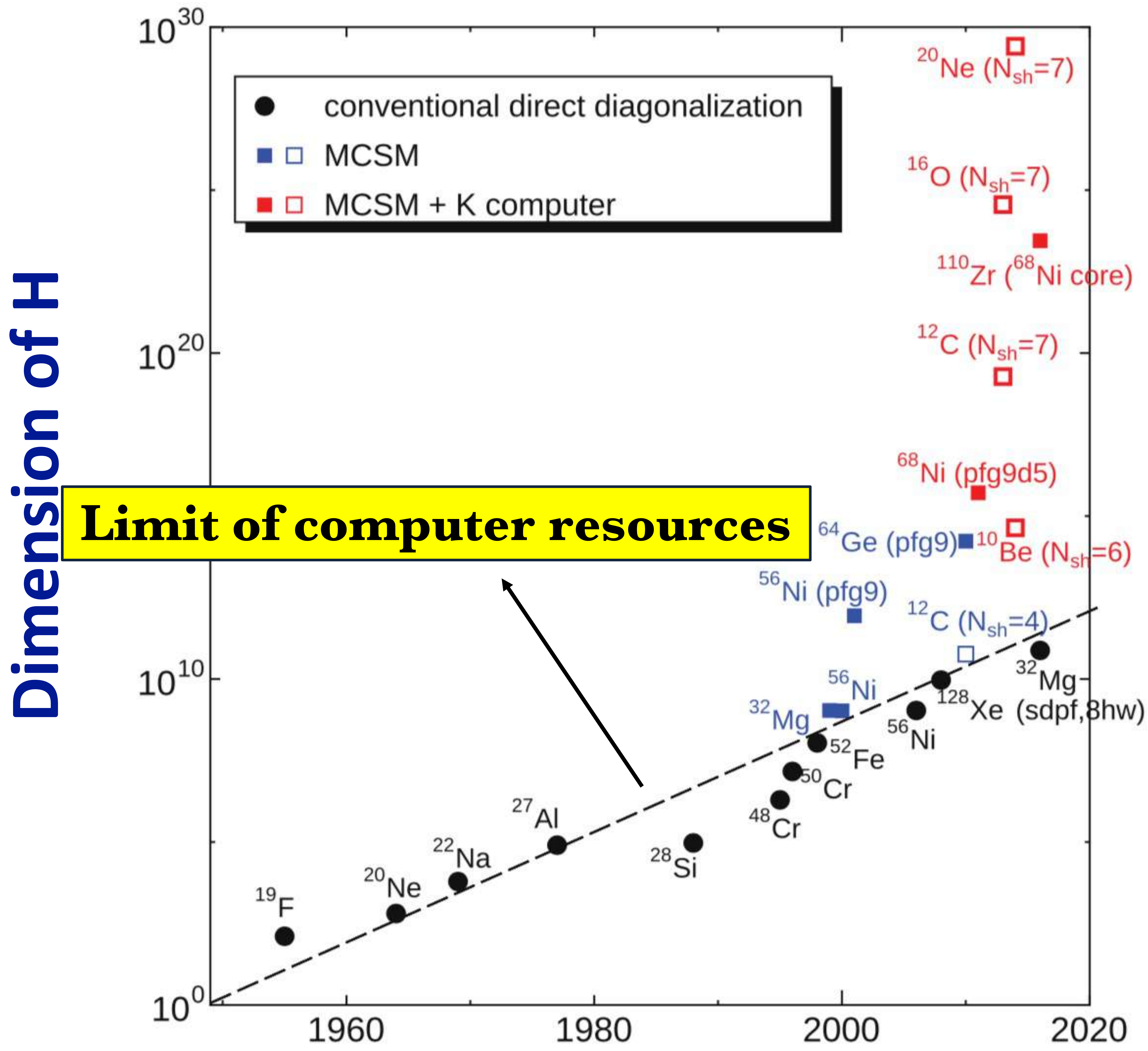
Historical Evolution of the Shell Model



N. Shimizu et al., Phys. Scr. 92, 063001 (2017).

Dimension of H matrix for MCSM

Standard shell model

$$H = \begin{pmatrix} \star & \star & \star & \star & \star & \cdots \\ \star & \star & \star & \star & & \\ \star & \star & \star & & & \\ \star & \star & & \ddots & & \\ \star & & & & & \\ \vdots & & & & & \end{pmatrix} \Longrightarrow \begin{pmatrix} E_0 & & & & 0 \\ & E_1 & & & \\ & & E_2 & & \\ & & & \ddots & \\ 0 & & & & \end{pmatrix}$$

Diagonalization

Large sparse matrix $\sim \mathcal{O}(10^{10})$

non-zero MEs $\sim \mathcal{O}(10^{13-14})$

Monte Carlo shell model

T. Otsuka *et al*., Prog. Part. Nucl. Phys. 47, 319 (2001)

Importance truncation

$$H \sim \begin{pmatrix} \star & \star & \cdots \\ \star & \ddots & \\ \vdots & & \end{pmatrix} \Longrightarrow \begin{pmatrix} E'_0 & & 0 \\ & E'_1 & \\ 0 & & \ddots \end{pmatrix}$$

Diagonalization

Important bases stochastically selected **~ O(100)**

MCSM — Starting Point

- **imaginary-time evolution operator**

$$e^{-\beta \hat{H}}$$

β : inverse of the temperature T

$\hat{H}$: a general time-independent Hamiltonian

- **an initial state**

$$|\Psi^{(0)}\rangle = \sum_i c_i |\phi_i\rangle$$

$|\phi_i\rangle$: $\hat{H}$'s eigenfunction

c_i : amplitude

$$e^{-\beta \hat{H}} |\Psi^{(0)}\rangle = \sum_i e^{-\beta E_i} c_i |\phi_i\rangle$$

E_i: the i-th eigenvalue of $\hat{H}$

β big enough —> only the ground state and low-lying excited states survive

MCSM — General Idea

- **a general Hamiltonian**

$$\hat{H} = \sum_{i,j=1}^{N_{s.p.}} \epsilon_{ij} c_i^\dagger c_j + \frac{1}{4} \sum_{i,j,k,l=1}^{N_{s.p.}} v_{i,j,k,l}\, c_i^\dagger c_j^\dagger c_l c_k$$

i, j : the single particle states.

$N_{s.p.}$: the number of the single particle states.

- **Hamiltonian in a quadratic form**

$$\hat{H} = \sum_{\alpha=1}^{N_f} (E_\alpha \hat{O}_\alpha + \frac{1}{2} V_\alpha \hat{O}_\alpha^2)$$

$\hat{O}_\alpha$: one-body operators

N_f : the number of the O_α's

$$e^{-\beta \hat{H}} = \int_{-\infty}^{\infty} \prod_\alpha \mathrm{d}\sigma_\alpha \sqrt{\frac{\beta |V_\alpha|}{2\pi}} \cdot e^{-\frac{\beta}{2}|V_\alpha|\sigma_\alpha^2} \cdot e^{-\beta |V_\alpha| \sigma_\alpha \hat{O}_\alpha}$$

MCSM — General Cases

- **a general Hamiltonian**

$$\hat{H} = \sum_{i,j=1}^{N_{s.p.}} \epsilon_{ij} c_i^\dagger c_j + \frac{1}{4} \sum_{i,j,k,l=1}^{N_{s.p.}} v_{i,j,k,l}\, c_i^\dagger c_j^\dagger c_l c_k$$

i, j : the single particle states.

$N_{s.p.}$: the number of the single particle states.

- **Hamiltonian in a quadratic form**

$$\hat{H} = \sum_{\alpha=1}^{N_f} (E_\alpha \hat{O}_\alpha + \frac{1}{2} V_\alpha \hat{O}_\alpha^2)$$

$\hat{O}_\alpha$: one-body operators

N_f : the number of the O_α's

$$e^{-\beta \hat{H}} ✖ \int_{-\infty}^{\infty} \prod_\alpha d\sigma_\alpha \sqrt{\frac{\beta |V_\alpha|}{2\pi}} \cdot e^{-\frac{\beta}{2}|V_\alpha|\sigma_\alpha^2} \cdot e^{-\beta |V_\alpha| \sigma_\alpha \hat{O}_\alpha}$$

Ĥ contains many-body term,
Ôα's do not commute with each other !

MCSM — Hubbard-Stratonovich (HS) Transformation

- "time" slices of β

$$e^{-\beta\hat{H}} = \left[e^{-\Delta\beta\hat{H}}\right]^{N_t}$$

- HS transformation

$$e^{-\beta\hat{H}} \simeq \prod_{n=1}^{N_t}\int_{-\infty}^{\infty}\prod_{\alpha} d\sigma_{\alpha n}\sqrt{\frac{\Delta\beta|V_\alpha|}{2\pi}}\cdot e^{-\frac{\Delta\beta}{2}|V_\alpha|\sigma_{\alpha n}^2}\cdot e^{-\Delta\beta(E_\alpha + s_\alpha V_\alpha \sigma_{\alpha n})\hat{O}}$$

- Gaussian weight factor

$$G(\sigma_\alpha) = e^{-\frac{\Delta\beta}{2}|V_\alpha|\sigma_{\alpha n}^2}$$

- one-body Hamiltonian

$$\hat{h}(\sigma_n) = \sum_{\alpha}(E_\alpha + s_\alpha V_\alpha \sigma_{\alpha n})\hat{O}_\alpha$$

$s_\alpha = \pm 1\ (\pm i)$ if $V_\alpha < 0\ (> 0)$

- HS transformation

$$e^{-\beta\hat{H}} \simeq \prod_{n=1}^{N_t}\int_{-\infty}^{\infty}\prod_{\alpha} d\sigma_{\alpha n}\sqrt{\frac{\Delta\beta|V_\alpha|}{2\pi}}\cdot G(\sigma_\alpha)\cdot e^{-\Delta\beta\hat{h}(\sigma_\alpha)}$$

R. L. Stratonovich, Dokl. Akad. Nauk SSSR **115**, 1097 (1957) [Sov. Phys. Dokl. **2**, 416 (1958)].

SMMC and MCSM

- **HS transformation**

$$e^{-\beta \hat{H}} \simeq \prod_{n=1}^{N_t} \int_{-\infty}^{\infty} \prod_{\alpha} \mathrm{d}\sigma_{\alpha,n} \sqrt{\frac{\beta |V_\alpha|}{2\pi}} \cdot G(\sigma_\alpha) \cdot e^{-\Delta\beta \hat{h}(\sigma_\alpha)}$$

- **the ground state**

$$|\Phi_{g.s.}\rangle \simeq \prod_{n=1}^{N_t} \sum_{MC,\sigma} e^{-\Delta\beta \hat{h}(\sigma_n)} |\Psi^{(0)}\rangle$$

- **states with σ**

$$|\Phi(\sigma)\rangle \propto \prod_{n=1}^{N_t} e^{-\Delta\beta \hat{h}(\sigma_n)} |\Psi^{(0)}\rangle$$

- **the ground state energy**

$$E_{g.s.} = \frac{\langle \Phi_{g.s.} | \hat{H} | \Phi_{g.s.} \rangle}{\langle \Phi_{g.s.} | \Phi_{g.s.} \rangle}$$

- **generate basis;**
- **diagonalization.**

Shell Model Monte Carlo

Quantum Monte Carlo

MCSM — Generation Process for Basis

$$|\Phi^{(1)}(\sigma)\rangle$$
$$|\Phi^{(2)}(\sigma)\rangle$$
$$\vdots$$
$$|\Phi^{(m)}(\sigma)\rangle$$

$$\sigma \equiv \{\sigma_1, \sigma_2, \cdots, \sigma_{N_t}\}$$

$$|\Phi(\sigma)\rangle \propto \prod_{n=1}^{N_t} e^{-\Delta\beta \hat{h}(\sigma_n)} \left|\Psi^{(0)}\right\rangle$$

ortho-normalizing

$$|\Phi^{(1)}(\sigma)\rangle,\ |\Phi^{(2)}(\sigma)\rangle, \cdots, |\Phi^{(m)}(\sigma)\rangle,\ |\Phi^{(k)}(\sigma)\rangle$$

diagonalize $\hat{H}$

$$E_1^{(k)},\ E_2^{(k)}, \cdots E_m^{(k)},\ E_{m+1}^{(k)}$$

MCSM — Generation Process for Basis

$$|\Phi^{(1)}(\sigma)\rangle$$
$$|\Phi^{(2)}(\sigma)\rangle$$
$$\vdots$$
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$$\sigma \equiv \{\sigma_1, \sigma_2, \cdots, \sigma_{N_t}\}$$

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ortho-normalizing

$$|\Phi^{(1)}(\sigma)\rangle,\ |\Phi^{(2)}(\sigma)\rangle, \cdots, |\Phi^{(m)}(\sigma)\rangle,\ |\Phi^{(k)}(\sigma)\rangle$$

diagonalize $\hat{H}$

$$E_1^{(k)},\ E_2^{(k)}, \cdots E_m^{(k)},\ E_{m+1}^{(k)}$$

$$\left|\Phi^{(1)}(\sigma)\right\rangle, \left|\Phi^{(2)}(\sigma)\right\rangle, \cdots, \left|\Phi^{(m)}(\sigma)\right\rangle, \left|\Phi^{(k+1)}(\sigma)\right\rangle$$

$$E_1^{(k+1)}, E_2^{(k+1)}, \cdots E_m^{(k+1)}, E_{m+1}^{(k+1)}$$

$$E_1^{(k+1)} < E_1^{(k)}, E_2^{(k+1)} < E_2^{(k)}, \cdots$$

MCSM — Generation Process for Basis

$$|\Phi^{(1)}(\sigma)\rangle$$
$$|\Phi^{(2)}(\sigma)\rangle$$
$$\vdots$$
$$|\Phi^{(m)}(\sigma)\rangle$$

$$\sigma \equiv \{\sigma_1, \sigma_2, \cdots, \sigma_{N_t}\}$$

$$|\Phi(\sigma)\rangle \propto \prod_{n=1}^{N_t} e^{-\Delta\beta \hat{h}(\sigma_n)} \left|\Psi^{(0)}\right\rangle$$

ortho-normalizing

$$|\Phi^{(1)}(\sigma)\rangle,\ |\Phi^{(2)}(\sigma)\rangle, \cdots, |\Phi^{(m)}(\sigma)\rangle,\ |\Phi^{(k)}(\sigma)\rangle$$

diagonalize $\hat{H}$

$$E_1^{(k)},\ E_2^{(k)}, \cdots E_m^{(k)},\ E_{m+1}^{(k)}$$

wave function selection

MCSM Bases

MCSM bases

MCSM dimension: the number of bases.

$$|\Phi^{(1)}(\sigma)\rangle$$

$$|\Phi^{(2)}(\sigma)\rangle$$

$$\vdots$$

$$|\Phi^{(m)}(\sigma)\rangle$$

$$|\Phi^{(m+1)}(\sigma)\rangle$$

MCSM — Restoration of Symmetry

spurious center-of-mass motion

$$|\Phi^{(1)}(\sigma)\rangle,\ |\Phi^{(2)}(\sigma)\rangle,\ \vdots,\ |\Phi^{(m)}(\sigma)\rangle,\ |\Phi^{(m+1)}(\sigma)\rangle$$

$\Rightarrow$

$$\hat{P}^J_{MK}|\Phi^{(1)}(\sigma)\rangle,\ \hat{P}^J_{MK}|\Phi^{(2)}(\sigma)\rangle,\ \vdots,\ \hat{P}^J_{MK}|\Phi^{(m)}(\sigma)\rangle,\ \hat{P}^J_{MK}|\Phi^{(m+1)}(\sigma)\rangle$$

$\Rightarrow$

$$\langle\Phi'(\sigma)|\hat{H}\hat{P}^J_{MK}|\Phi(\sigma)\rangle$$

$\Rightarrow$

$$\langle\Phi'(\sigma)|\hat{H}'\hat{P}^J_{MK}|\Phi(\sigma)\rangle$$

$$\hat{H}' = \hat{H} + \beta_{c.m.}\hat{H}_{c.m.}$$

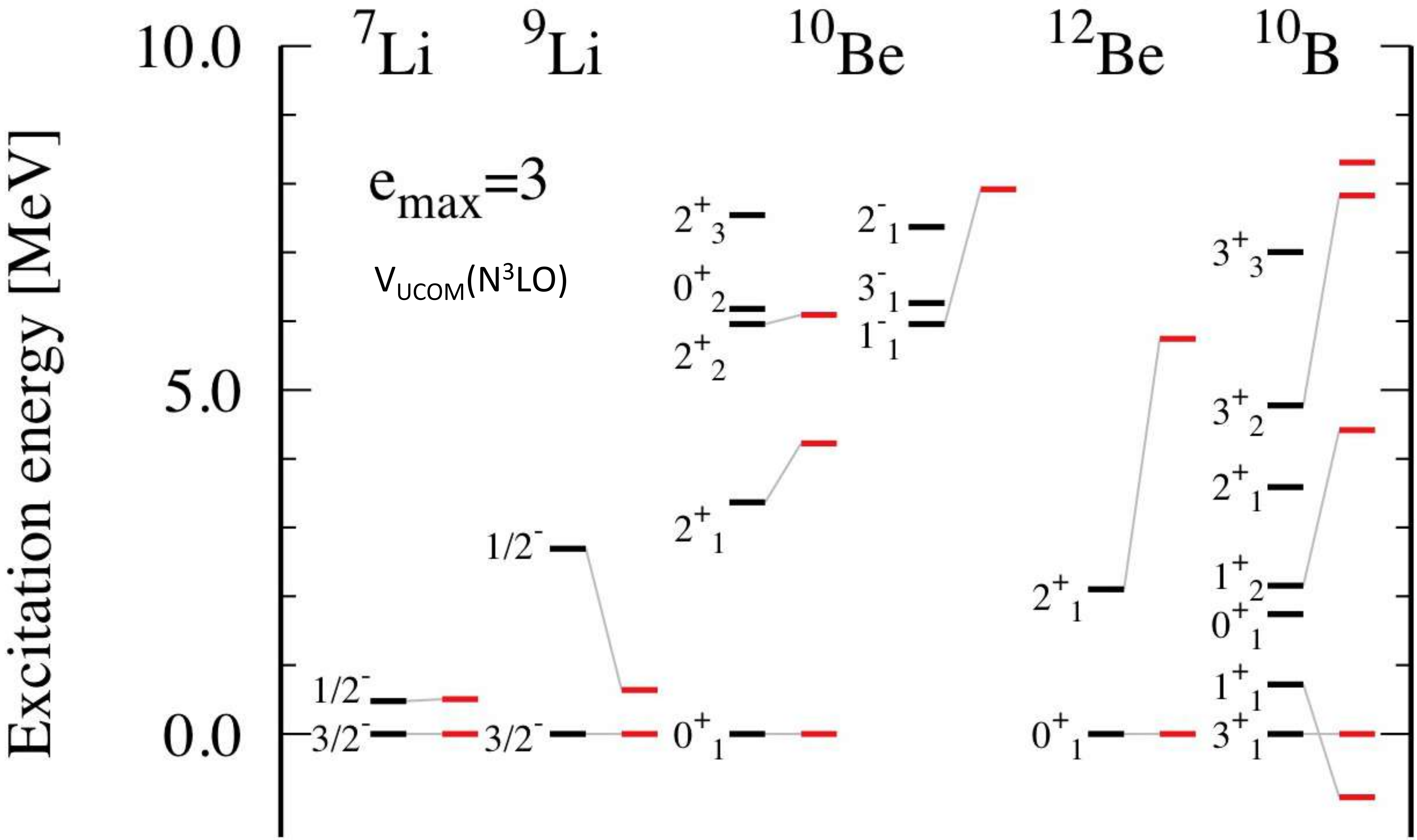
$$\hat{H}_{c.m.} = \frac{\hat{\mathbf{P}}^2}{2AM} + \frac{1}{2}MA\omega^2\hat{\mathbf{R}}^2 - \frac{3}{2}\hbar\omega$$

D. Gloeckner and R. Lawson, 1974

$$\hat{P}^J_{MK} = \frac{2J+1}{8\pi^2}\int \mathrm{d}\Omega\, {D^J_{MK}}^*(\Omega)\, e^{i\alpha\hat{J}_z}\, e^{i\beta\hat{J}_y}\, e^{i\gamma\hat{J}_z}$$

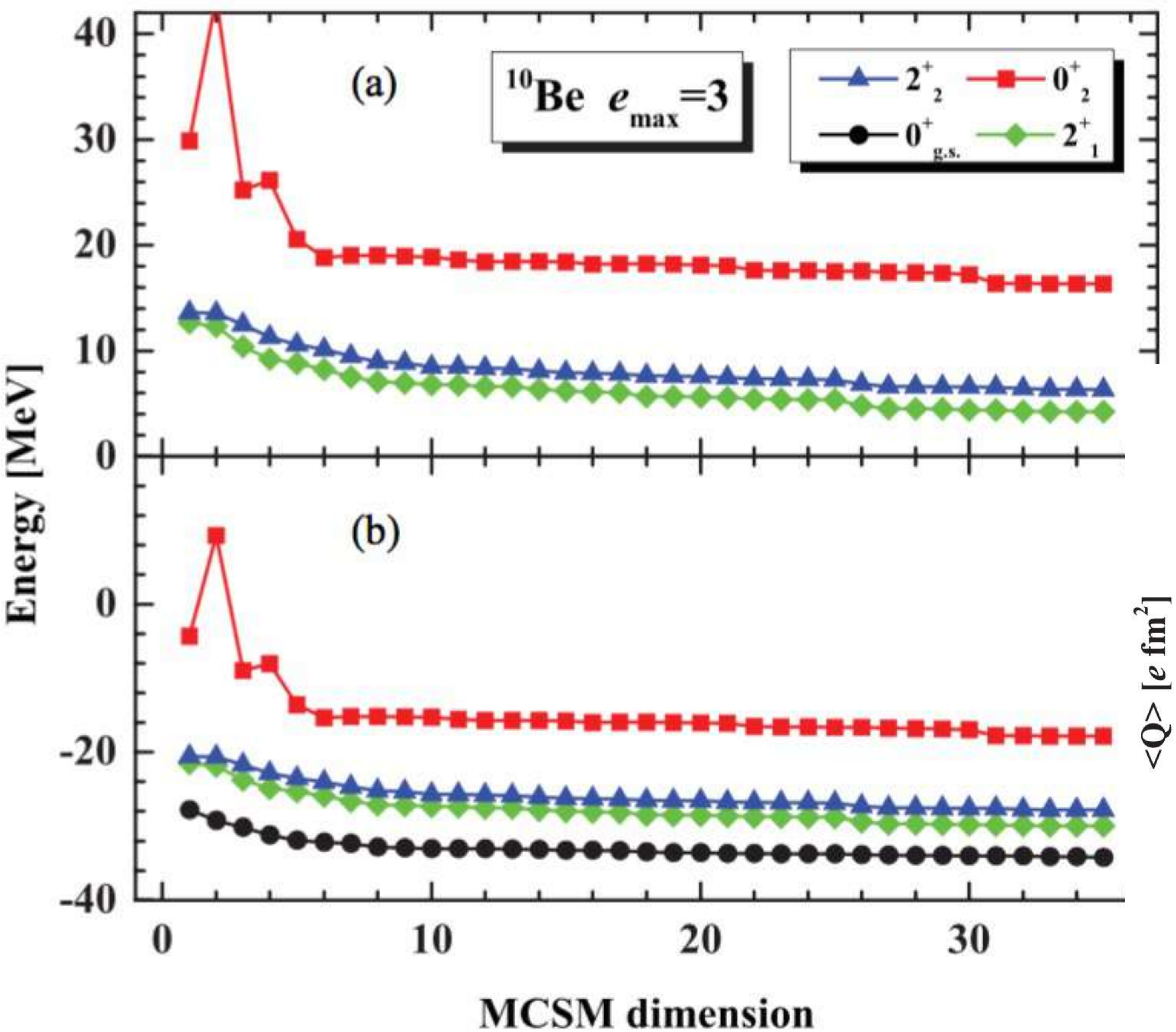
Ring & Schuck, "The Nuclear Many-Body Problem", Springer

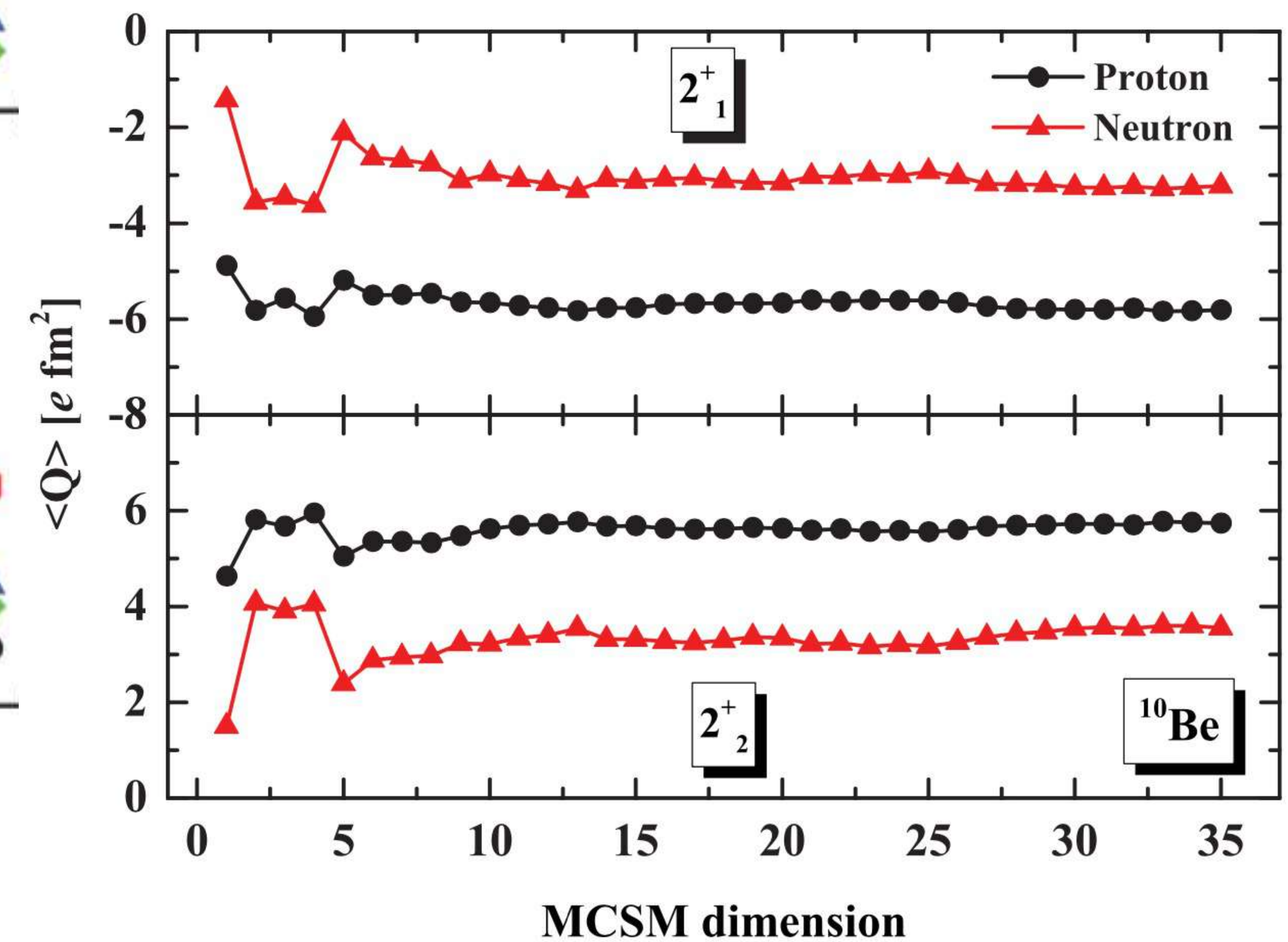
Low-lying Spectra for Light Nuclei



Beryllium Low-lying Spectra

- *The convergence of energy and Q for ^{10}Be as the function of MCSM dimension.*





L. Liu, *et al.* 2012

^{10}Be E2 Transition

Unit: Q(e fm^2), B(E2) (e^2 fm^4)

❖ ***MCSM***

	Q	B(E2;$2^+_1 \rightarrow 0^+_1$)	B(E2;$2^+_2 \rightarrow 0^+_1$)	B(E2;$2^+_2 \rightarrow 2^+_1$)
Exp.		9.2(3)	0.11(2)	
MCSM	-7.71	9.29	0.32	3.28

E.A. McCutchan, C. J. Lister, R. B. Wiringa, *et al.* Phys. Rev. Lett. **103**, 192501 (2009)

❖ ***GFMC***

H	AV18	AV18+UIX	AV18+IL2	AV18+IL7	Expt.
$\|E_{gs}(0^+)\|$	50.1(2)	59.5(3)	66.4(4)	64.3(2)	64.98
$E_x(2_1^+)$	2.9(2)	3.5(3)	5.0(4)	3.8(2)	3.37
$E_x(2_2^+)$	2.7(2)	3.8(3)	5.8(4)	5.5(2)	5.96
$B(E2; 2_1^+ \rightarrow 0^+)$	10.5(3)	17.9(5)	8.1(3)	8.8(2)	9.2(3)
$B(E2; 2_2^+ \rightarrow 0^+)$	3.3(2)	0.35(5)	3.3(2)	1.7(1)	0.11(2)
$\Sigma B(E2)$	13.8(4)	18.2(6)	11.4(4)	10.5(3)	9.3(3)

M. Pervin, S. C. Pieper, and R.B. Wiringa, Phys. Rev. C. **76**, 064319 (2007).

❖ ***NCSM***

with the CD-BONN: **B(E2; $2^+_1 \rightarrow 0^+_{g.s.}$) = 6.5 e^2 fm^4**
with the CDB2K: **B(E2; $2^+_1 \rightarrow 0^+_{g.s.}$) = 9.8 e^2 fm^4**

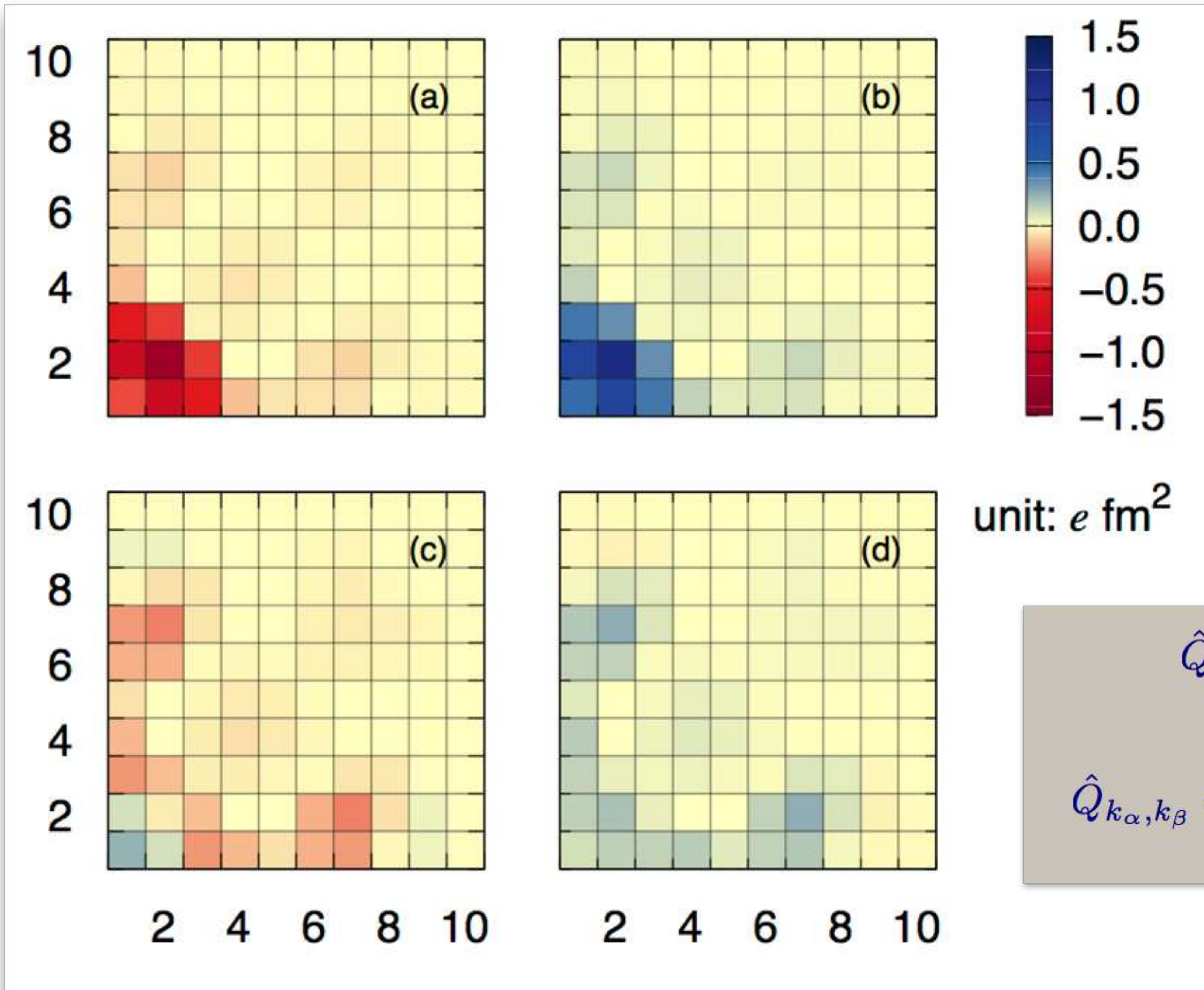
E. Caurier, P. Navr´atil, W.E. Ormand, and J.P Vary, Phys. Rev. C **66**, 024314 (2002).

Contribution of Single Particle Orbit to Q

$\langle 2^+_1 \| Q_{k_\alpha, k_\beta} \| 2^+_1 \rangle$ $\langle 2^+_2 \| Q_{k_\alpha, k_\beta} \| 2^+_2 \rangle$

proton

neutron



$$\hat{Q} = \sum_{k_\alpha, k_\beta} \hat{Q}_{k_\alpha, k_\beta}$$

$$\hat{Q}_{k_\alpha, k_\beta} = \sum_{m_\alpha, m_\beta} \langle \alpha | \hat{Q} | \beta \rangle a^\dagger_\alpha a_\beta$$

$0s1/2$, $0p3/2$, $0p1/2$, $0d5/2$, $0d3/2$, $1s1/2$, $0f7/2$, $0f5/2$, $1p3/2$ and $1p1/2$

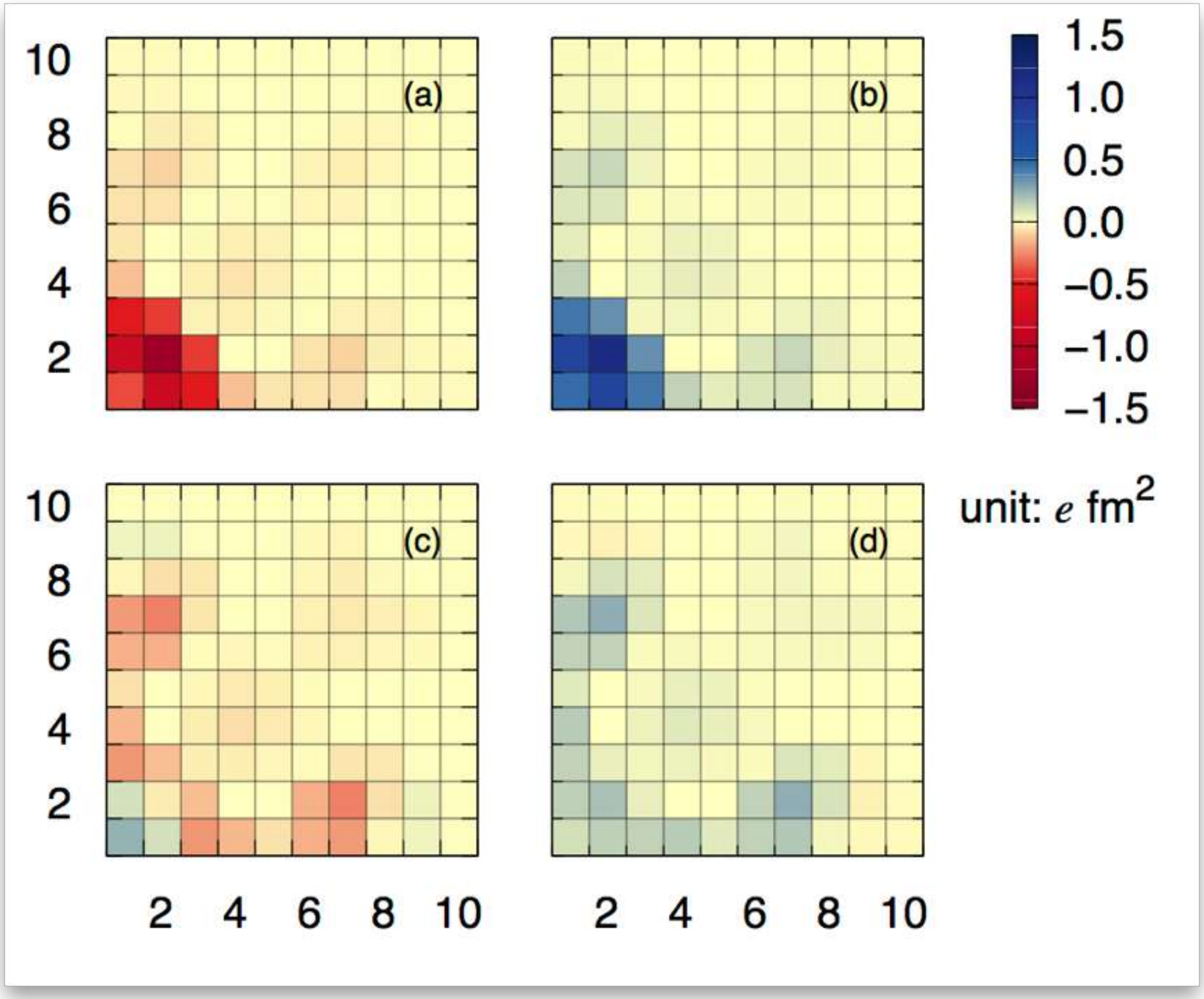
L. Liu, 2015

Contribution of Single Particle Orbit to Q

$\langle 2^+_1 \| Q_{k_\alpha, k_\beta} \| 2^+_1 \rangle$ $\langle 2^+_2 \| Q_{k_\alpha, k_\beta} \| 2^+_2 \rangle$

proton

neutron

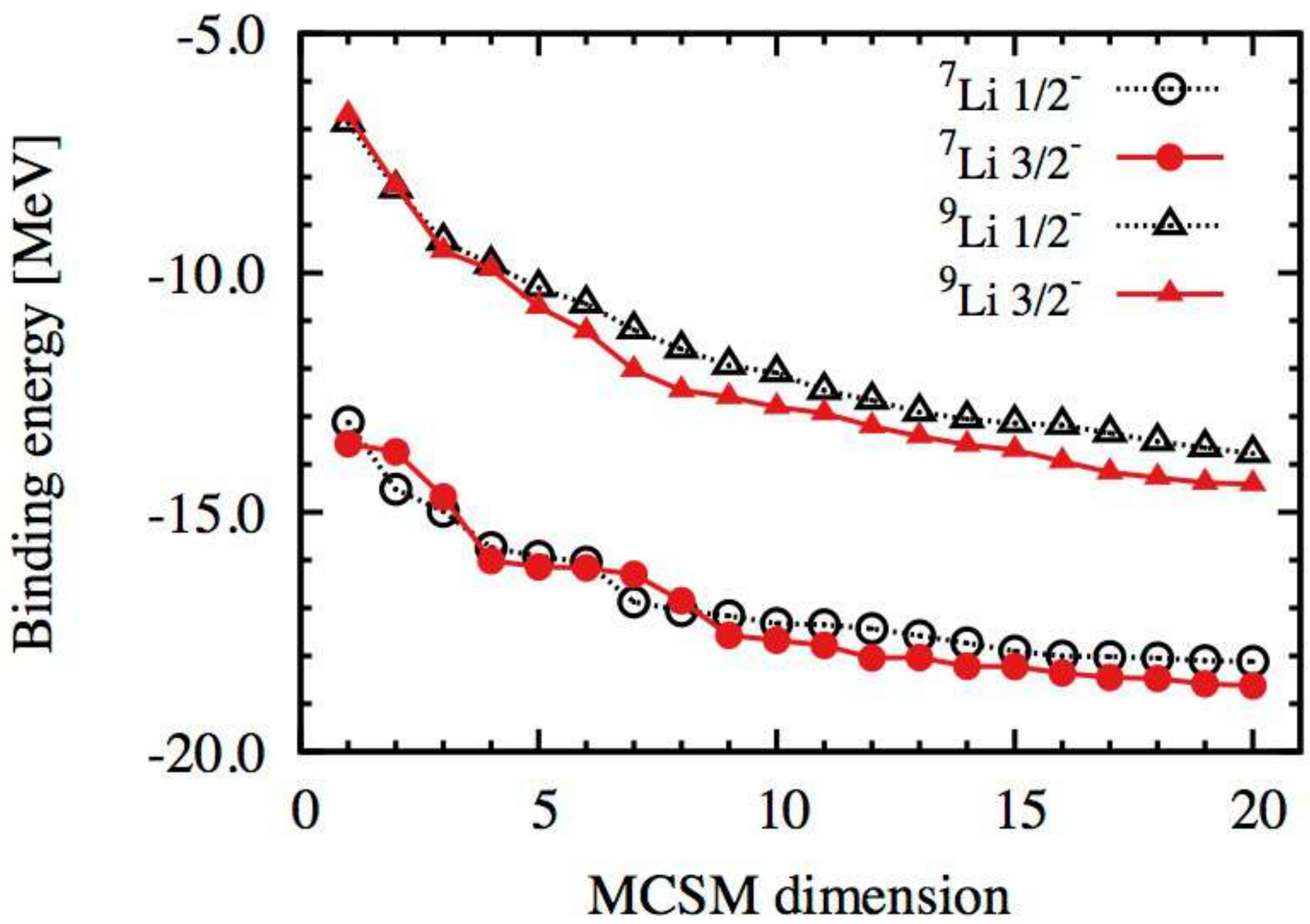


p shell dominant
Single particle

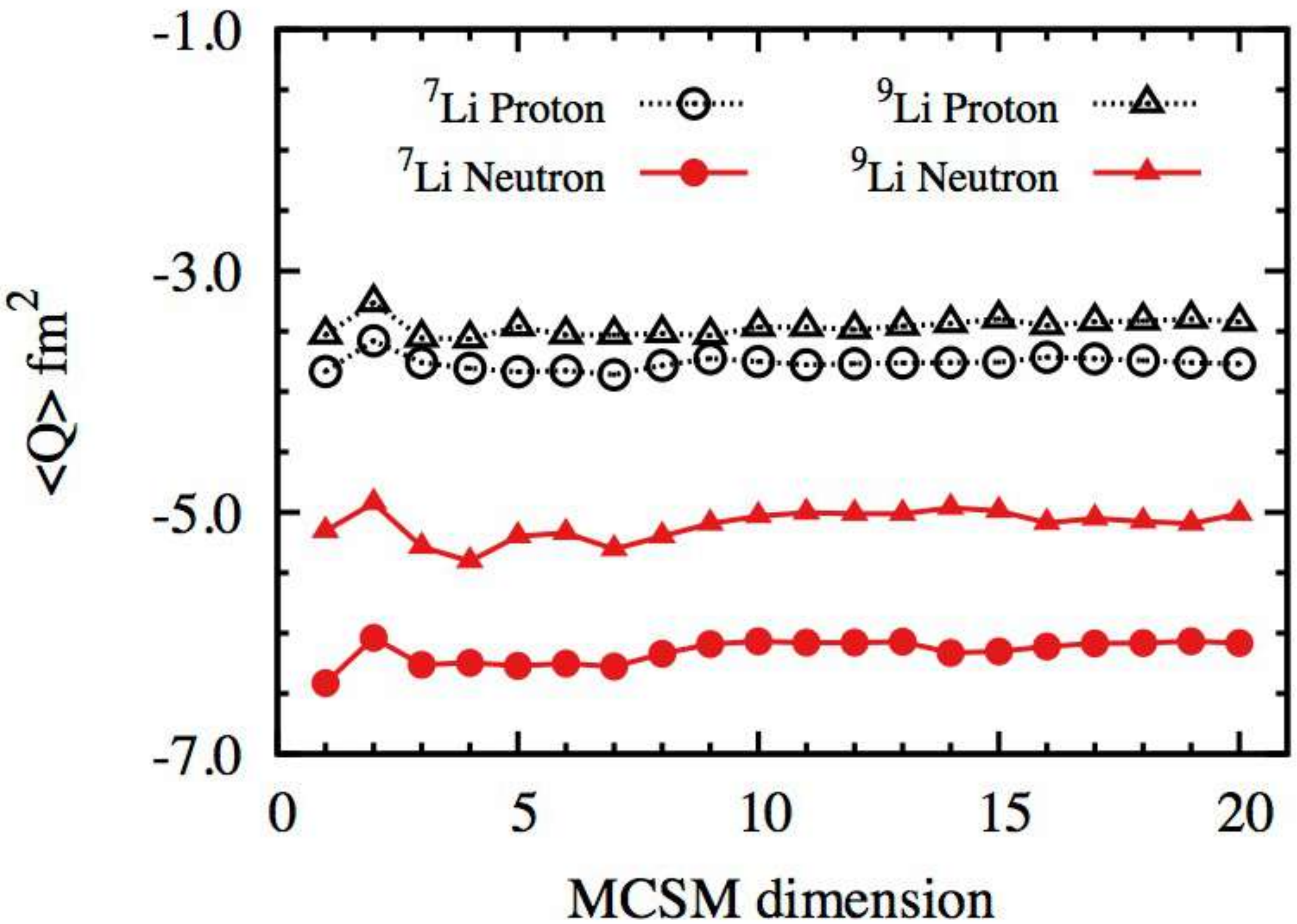
Average
collective

$0s1/2$, $0p3/2$, $0p1/2$, $0d5/2$, $0d3/2$, $1s1/2$, $0f7/2$, $0f5/2$, $1p3/2$ and $1p1/2$

^{7}Li and ^{9}Li: MCSM Dimension Convergence



- ***MCSM dimension ~ 20***



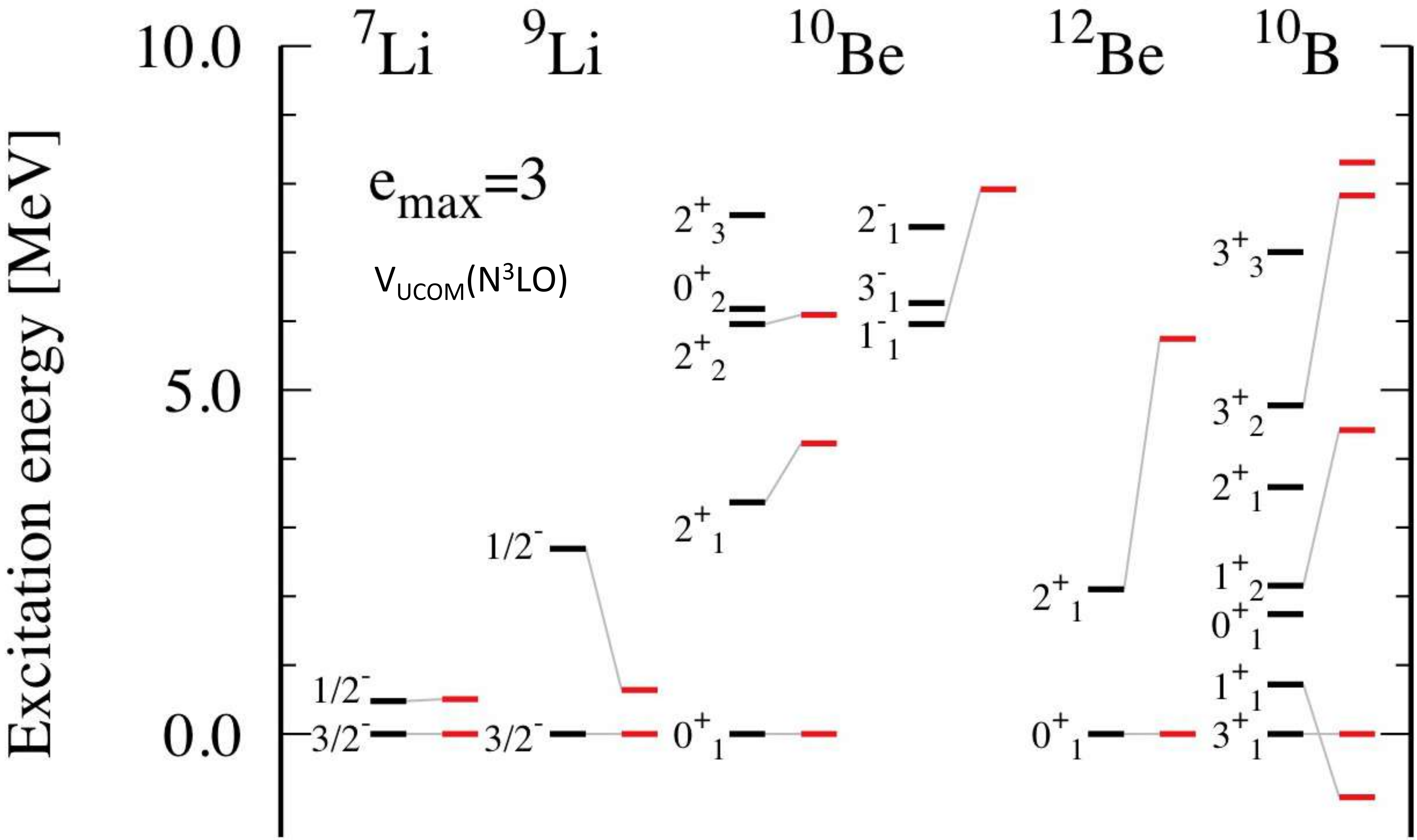
L. Liu, 2015

^{7}Li and ^{9}Li: Magnetic Moments

Isotopes	Exp.	MCSM	NCSM
		μ [μ_N]	
^{7}Li	3.256427(2)	3.116	3.01(2)
^{9}Li	3.434(5)	3.183	2.89(2)
		Q [e fm^2]	
^{7}Li	-4.00(3)	-3.770	-3.20(22)
^{9}Li	-3.06(2)	-3.452	-2.66(22)

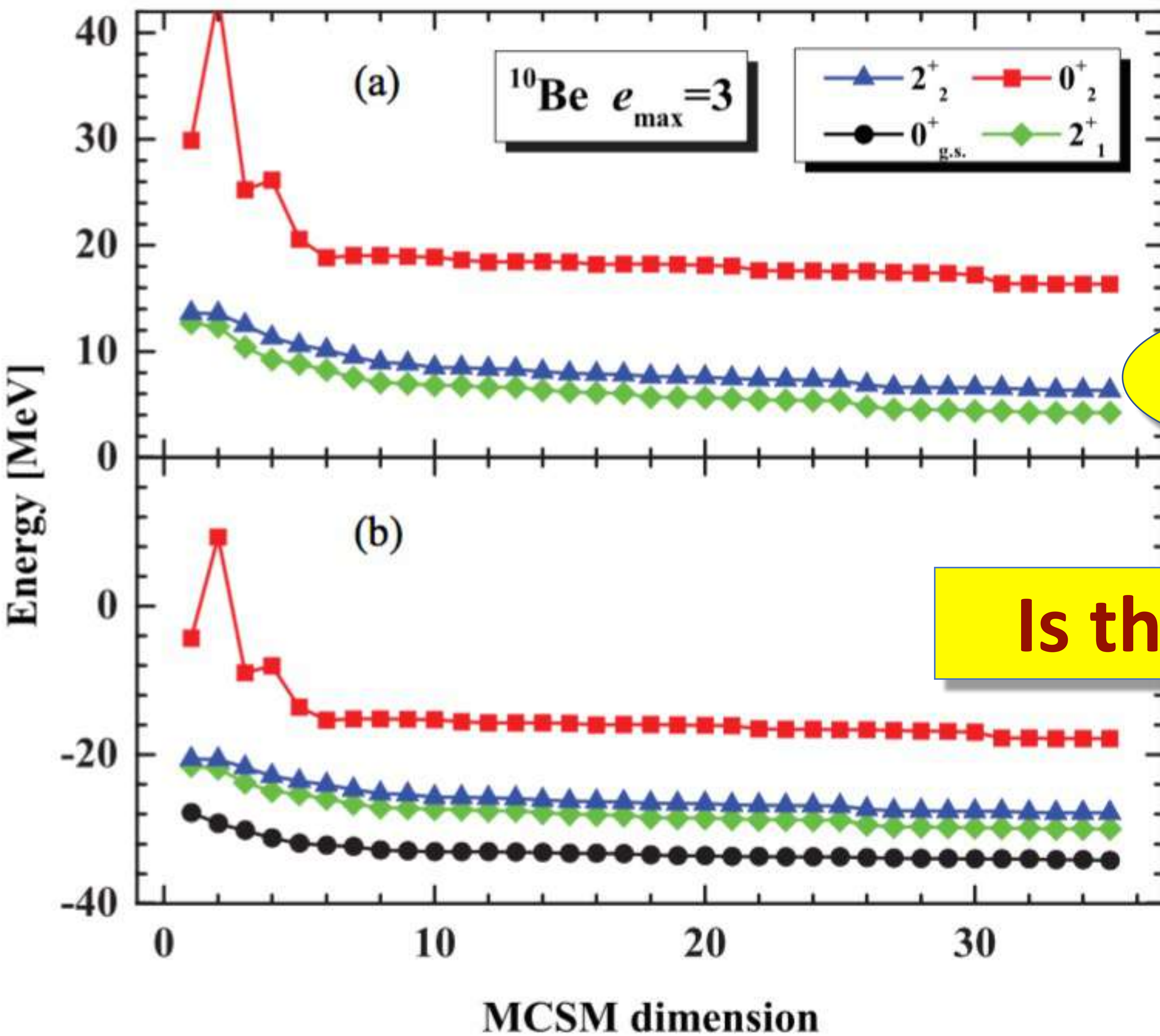
L. Liu and J. Li 2015

Low-lying Spectra for Light Nuclei



Beryllium Low-lying Spectra

The convergence of energy for ^{10}Be as the function of MCSM dimension.



$$\epsilon = |E_n - E_{n-1}|/E_n$$

< 0.7%

Is this accurate enough ?

L. Liu, *et al.* 2012

Beyond shell model limit ?

MCSM Error ?

Beyond shell model limit ?

MCSM Error ?

$$\overline{\Delta O^2} = \overline{(\hat{O} - \bar{O})^2} = \int \psi^* (\hat{O} - \bar{O})^2 \psi \mathrm{d}\tau$$

$$\langle \Delta H^2 \rangle = \langle (\hat{H} - \bar{H})^2 \rangle = \langle \hat{H^2} \rangle - \langle H \rangle^2$$

<H^2> in MCSM

$$H = \sum_{ij} t_{ij} c_i^\dagger c_j + \sum_{i<j,k<l} \bar{v}_{ijkl} c_i^\dagger c_j^\dagger c_l c_k$$

t_{ij}: one-body matrix element

$\bar{v}$: antisymmetrized two-body matrix element

$$\bar{v}_{ijkl} = -\bar{v}_{ijlk} = -\bar{v}_{jikl} = \bar{v}_{jilk}$$

the matrix element of H^2 of two Slater determinants

$$\frac{\langle\phi|H^2|\phi'\rangle}{\langle\phi|\phi'\rangle} = \sum\nolimits_{i<j,k<l} \overline{\rho'\rho' v_{ijkl}}\,\overline{\rho\rho v}_{klij}$$
$$+ \mathrm{Tr}((t+\Gamma)(1-\rho)(t+\Gamma)\rho) + \left(\mathrm{Tr}\left(\rho(t+\tfrac{1}{2}\Gamma)\right)\right)^2$$

$$\Gamma_{ik}^{(\lambda)} = \sum_{jl} \bar{v}_{ijkl} \rho_{lj}^{(\lambda)}$$

$$\overline{\rho\rho v}_{ijkl} \equiv \sum_{m<n} (\rho_{im}\rho_{jn} - \rho_{in}\rho_{jm}) \bar{v}_{mnkl}$$

$$\overline{\rho'\rho' v_{ijkl}} \equiv \sum_{m<n} ((1-\rho)_{im}(1-\rho)_{jn} - (1-\rho)_{in}(1-\rho)_{jm}) \bar{v}_{mnkl}.$$

<H²> in MCSM

$$H=\sum_{ij}t_{ij}c_i^\dagger c_j+\sum_{i<j,k<l}\bar{v}_{ijkl}c_i^\dagger c_j^\dagger c_l c_k$$

t_{ij}: one-body matrix element

$\bar{v}$: antisymmetrized two-body matrix element

$$\bar{v}_{ijkl}=-\bar{v}_{ijlk}=-\bar{v}_{jikl}=\bar{v}_{jilk}$$

the matrix element of H² of two Slater determinants

$$\frac{\langle\phi|H^2|\phi'\rangle}{\langle\phi|\phi'\rangle}=\boxed{\sum_{i<j,k<l}\overline{\rho'\rho' v}_{ijkl}\overline{\rho\rho v}_{klij}}$$

$$+\,\mathrm{Tr}((t+\Gamma)(1-\rho)(t+\Gamma)\rho)+\left(\mathrm{Tr}\left(\rho(t+\tfrac{1}{2}\Gamma)\right)\right)^2$$

Extreme time consuming !

$$\overline{\rho\rho v}_{ijkl}\equiv\sum_{m<n}(\rho_{im}\rho_{jn}-\rho_{in}\rho_{jm})\bar{v}_{mnkl}$$

$$\overline{\rho'\rho' v}_{ijkl}\equiv\sum_{m<n}((1-\rho)_{im}(1-\rho)_{jn}-(1-\rho)_{in}(1-\rho)_{jm})\bar{v}_{mnkl}.$$

<H²> in MCSM

the matrix element of H^2 of two Slater determinants

$$\frac{\langle\phi|H^2|\phi'\rangle}{\langle\phi|\phi'\rangle} = \sum_{i<j,k<l} \overline{\rho'\rho' v_{ijkl}}\,\overline{\rho\rho v}_{klij}$$

$$+ \mathrm{Tr}((t+\Gamma)(1-\rho)(t+\Gamma)\rho) + \left(\mathrm{Tr}\left(\rho(t+\tfrac{1}{2}\Gamma)\right)\right)^2$$

Puddu G 2012 *J. Phys. G: Nucl. Part. Phys.* 39 085108

$$\rho_{ij} = \sum_{\alpha=1}^{N_f} W_{i\alpha} D^\dagger_{\alpha j}$$

$$W_{i\alpha} \equiv \sum_{\beta=1}^{N_f} D'_{i\beta}\left(D^\dagger D'\right)^{-1}_{\beta\alpha}$$

$$\sum_{i<j,k<l} \overline{\rho'\rho' v_{ijkl}}\,\overline{\rho\rho v}_{klij} = \sum_{\alpha<\beta,\gamma<\delta} \overline{DDvWW}_{\alpha\beta\gamma\delta}\overline{DDvWW}_{\gamma\delta\alpha\beta}$$
$$- \sum_{\alpha<\beta k,\delta}\left(\sum_l \overline{DDv}_{\alpha\beta kl} W_{l\delta}\right)\left(\sum_b D^\dagger_{\delta b}\overline{vWW}_{kb\alpha\beta}\right)$$
$$+ \sum_{\alpha<\beta i<j} \overline{DDv}_{\alpha\beta ij}\overline{WW}_{ij\alpha\beta}$$

$$|\phi\rangle = \prod_{\alpha=1}^{N_f}\left(\sum_{i=1}^{N_{sp}} D_{i\alpha} c_i^\dagger\right)|-\rangle$$

$$\overline{DDv}_{\alpha\beta kl} = \sum_{i<j}\left(D^\dagger_{\alpha i}D^\dagger_{\beta j} - D^\dagger_{\alpha j}D^\dagger_{\beta i}\right)\bar{v}_{ijkl}$$

$$\overline{vWW}_{ij\gamma\delta} = \sum_{k<l}\bar{v}_{ijkl}(W_{k\gamma}W_{l\delta} - W_{k\delta}W_{l\gamma})$$

$$\overline{DDVWW}_{\alpha\beta\gamma\delta} = \sum_l\left(\sum_k \overline{DDv}_{\alpha\beta kl}W_{k\gamma}\right)W_{l\delta}$$

MCSM energy variance $\langle \Delta H^2 \rangle = \left\langle \hat{H}^2 \right\rangle - \langle \hat{H} \rangle^2$

Model space: e_{max}=1 (2 major shells) **interaction: $V_{UCOM}(N^3LO)$**

^3H		E (MeV)	$<H>^2$	$<H^2>$	$<\Delta H^2> = <H^2> - <H>^2$
MCSM	1	-1.822	3.318	7.290	**3.972**
	2	-1.823	3.323	7.274	**3.950**
	3	-1.840	3.386	6.462	**3.076**
	4	-1.894	3.587	4.009	**0.422**
	5	-1.899	3.606	3.744	**0.138**
	6	-1.900	3.610	3.700	**0.090**
	7	-1.902	3.616	3.628	**0.012**
	8	-1.902	3.616	3.628	**0.012**
	9	-1.902	3.617	3.622	**0.005**
	10	-1.902	3.617	3.617	**0.000**

Benchmark with shell model — ^{3}H

Model space: e_{max}=1 (2 major shells) **interaction: V_{UCOM}(N^3LO)**

^{3}H		E (MeV)	Occupation number					
			0s1/2	0p3/2	0p1/2	0s1/2	0p3/2	0p1/2
Shell model		-1.9019	0.9422	0.0167	0.0411	1.9172	0.0345	0.0482
MCSM	1	-1.8215	0.9431	0.0150	0.0420	1.9203	0.0315	0.0482
	2	-1.8230	0.9411	0.0162	0.0427	1.9164	0.0342	0.0494
	3	-1.8402	0.9421	0.0158	0.0421	1.9164	0.0345	0.0491
	4	-1.8939	0.9417	0.0163	0.0421	1.9179	0.0332	0.0489
	5	-1.8990	0.9425	0.0159	0.0416	1.9166	0.0341	0.0492
	6	-1.9000	0.9424	0.0164	0.0412	1.9166	0.0351	0.0482
	7	-1.9016	0.9423	0.0167	0.0410	1.9175	0.0344	0.0481
	8	-1.9016	0.9423	0.0167	0.0410	1.9175	0.0344	0.0481
	9	-1.9018	0.9422	0.0167	0.0411	1.9173	0.0345	0.0483
	10	-1.9019	0.9422	0.0167	0.0411	1.9172	0.0345	0.0482

MCSM energy variance $\langle \Delta H^2 \rangle = \left\langle \hat{H}^2 \right\rangle - \langle \hat{H} \rangle^2$

Model space: e_{max}=1 (2 major shells) **interaction: $V_{UCOM}(N^3LO)$**

^{4}He		E (MeV)	<H>^{2}	<H^2>	<ΔH^2> = <H^2> - <H>^{2}
MCSM	1	-19.589	383.732	406.949	**23.217**
	2	-19.843	393.755	412.885	**19.130**
	3	-20.027	401.068	402.373	**1.305**
	4	-20.038	401.513	401.727	**0.213**
	5	-20.040	401.594	401.603	**0.009**
	6	-20.040	401.595	401.601	**0.005**
	7	-20.040	401.596	401.600	**0.004**
	8	-20.040	401.598	401.598	**0.000**

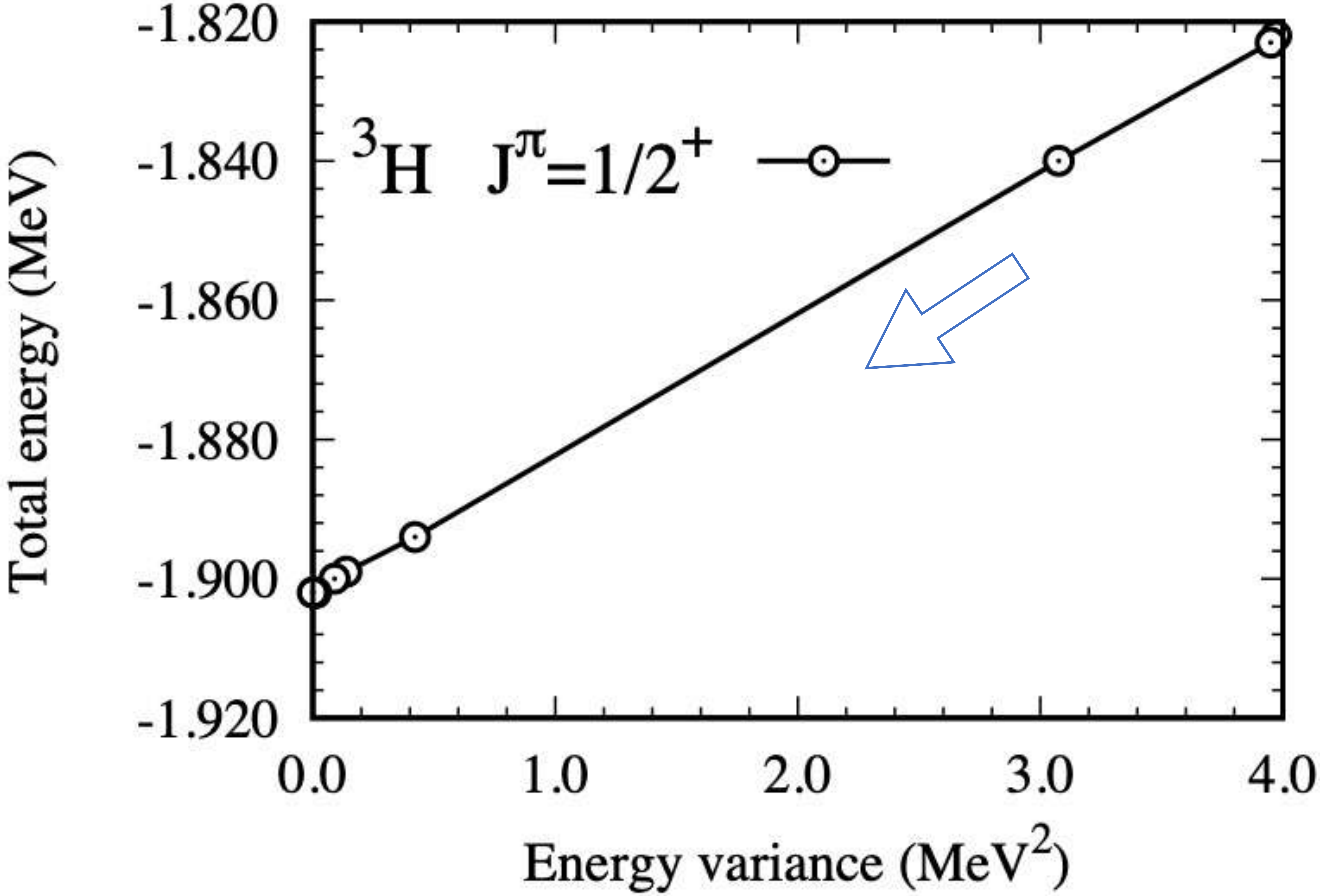
Benchmark with shell model — ^{4}He

Model space: e_{max}=1 (2 major shells) **interaction:** V_{UCOM}(N^3LO)

^{4}He		E (MeV)	Occupation number					
			0s1/2	0p3/2	0p1/2	0s1/2	0p3/2	0p1/2
Shell model		-20.0399	1.9348	0.0180	0.0472	1.9348	0.0180	0.0472
MCSM	1	-19.5891	1.9518	0.0097	0.0385	1.9518	0.0097	0.0385
	2	-19.8433	1.9456	0.0140	0.0404	1.9456	0.0140	0.0404
	3	-20.0267	1.9378	0.0169	0.0453	1.9378	0.0169	0.0453
	4	-20.0378	1.9347	0.0179	0.0474	1.9347	0.0179	0.0474
	5	-20.0398	1.9345	0.0181	0.0474	1.9345	0.0181	0.0474
	6	-20.0398	1.9347	0.0181	0.0472	1.9347	0.0181	0.0472
	7	-20.0399	1.9349	0.0179	0.0472	1.9349	0.0179	0.0472
	8	-20.0399	1.9348	0.0180	0.0472	1.9348	0.0180	0.0472

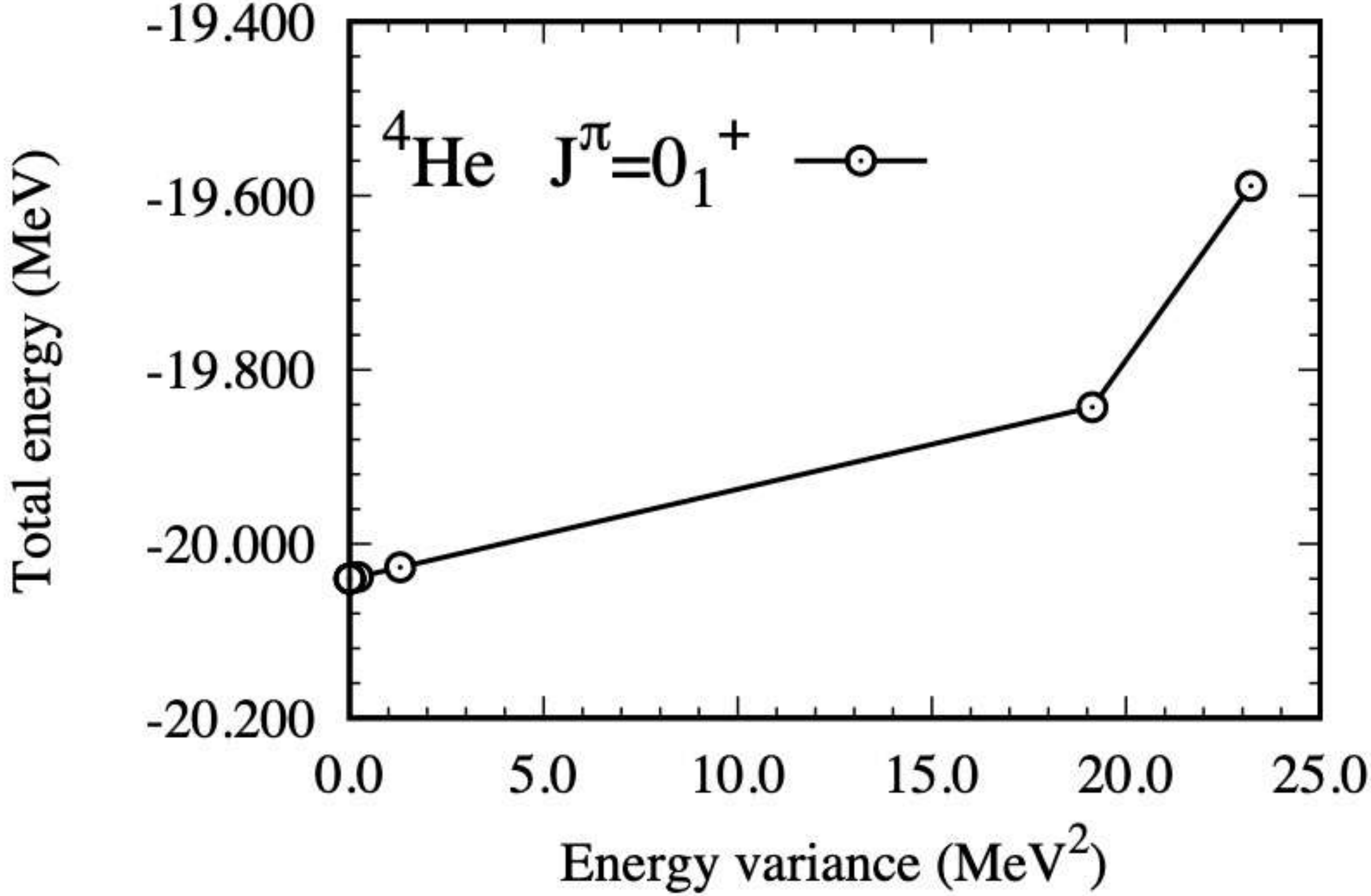
MCSM extrapolation

Model space: e_{max}=1 (2 major shells) **interaction:** $V_{UCOM}(N^3LO)$



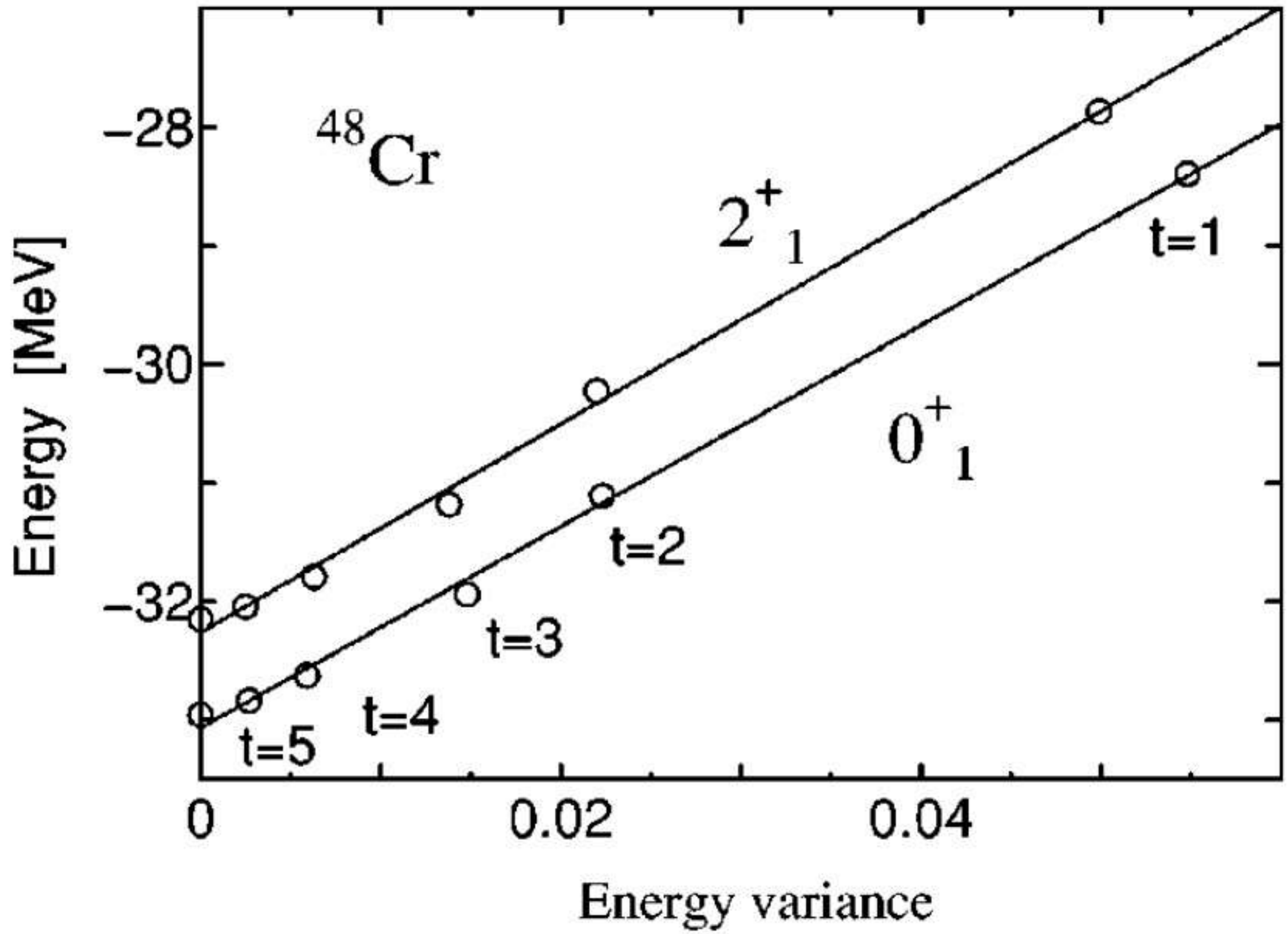
MCSM extrapolation

Model space: e_{max}=1 (2 major shells) **interaction:** $V_{UCOM}(N^3LO)$

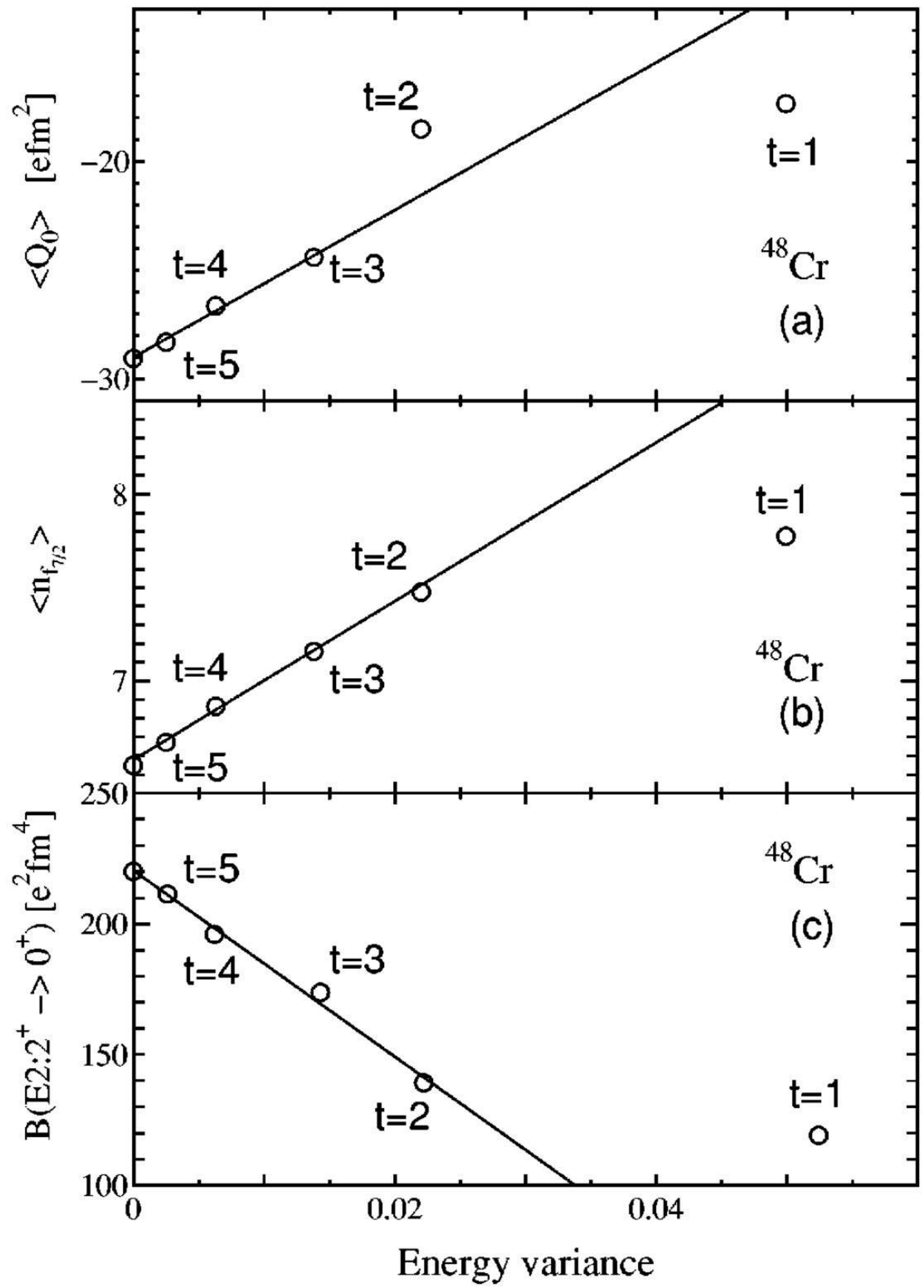


MCSM extrapolation

Sorella S 2001 *Phys. Rev.* B **64** 024512
Imada M and Kashima T 2000 *J. Phys. Soc. Jpn.* **69** 2723
Mizusaki T and Imada M 2004 *Phys. Rev.* B **69** 125110



MCSM extrapolation



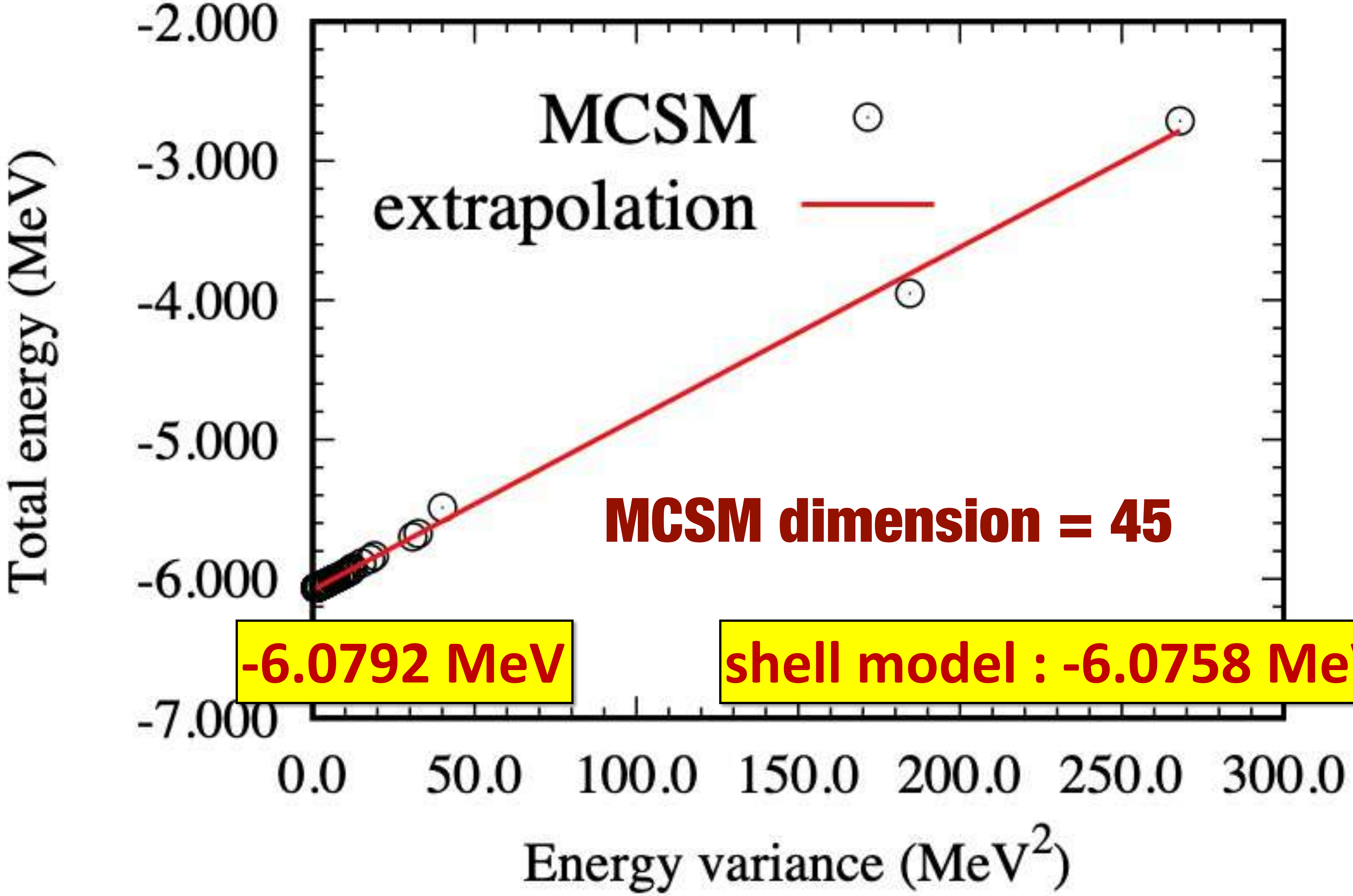
Sorella S 2001 *Phys. Rev.* B **64** 024512

Imada M and Kashima T 2000 *J. Phys. Soc. Jpn.* **69** 2723

Mizusaki T and Imada M 2004 *Phys. Rev.* B **69** 125110

MCSM extrapolation: ^{3}H

Model space: e_{max}=3 (4 major shells) **interaction:** V_{UCOM}(N^3LO)



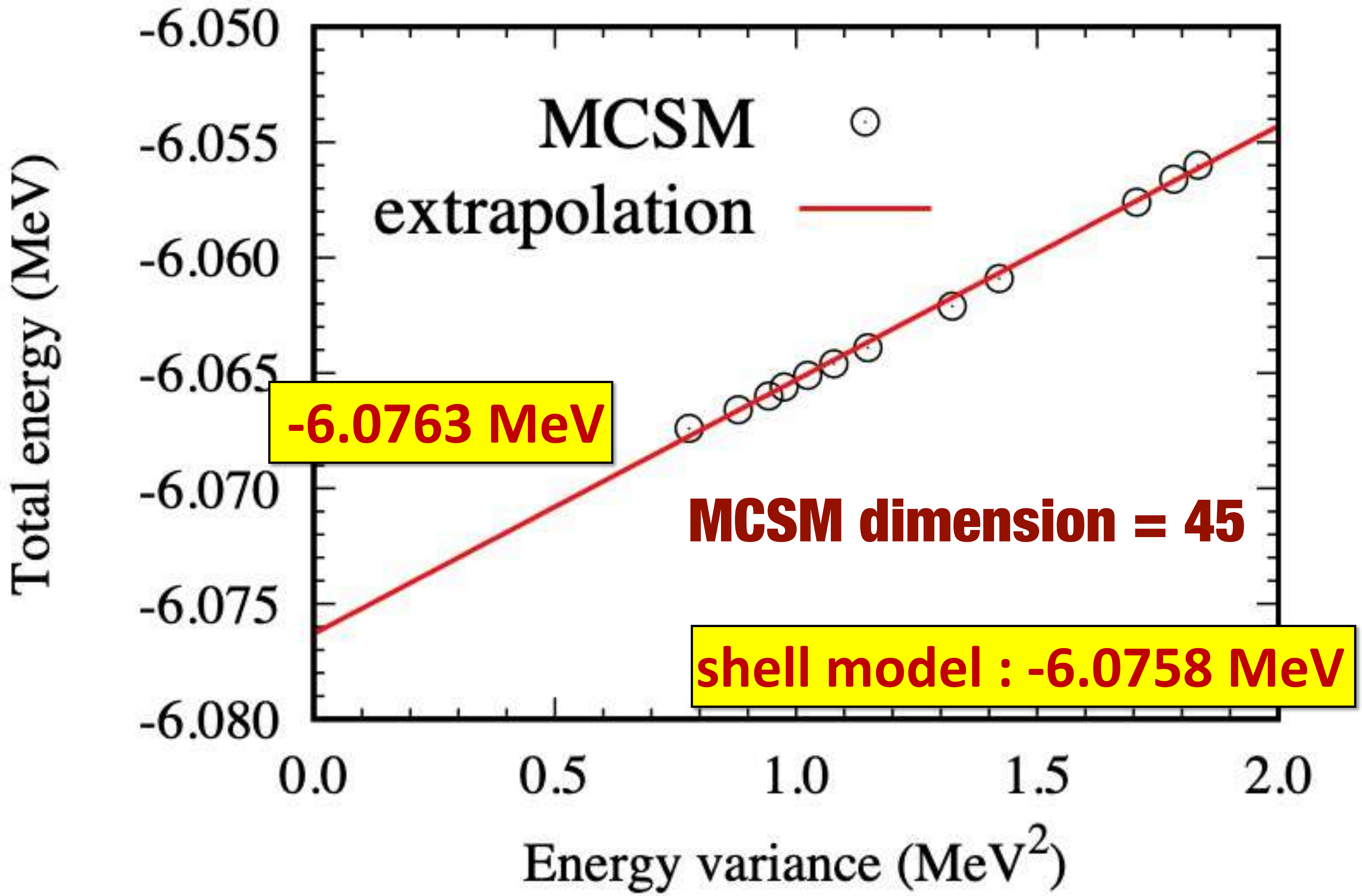
MCSM dimension = 45

-6.0792 MeV

shell model : -6.0758 MeV

MCSM extrapolation: ^{3}H

Model space: e_{max}=3 (4 major shells) **interaction:** V_{UCOM}(N^{3}LO)



Summary and Outlook

误差可控，结果可外推的蒙特卡洛壳模型。

MCSM is rather accurate for nuclear ab initio description !

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T. Otsuka@Tokyo Univ.

Y. Utsuno@JAEA

...

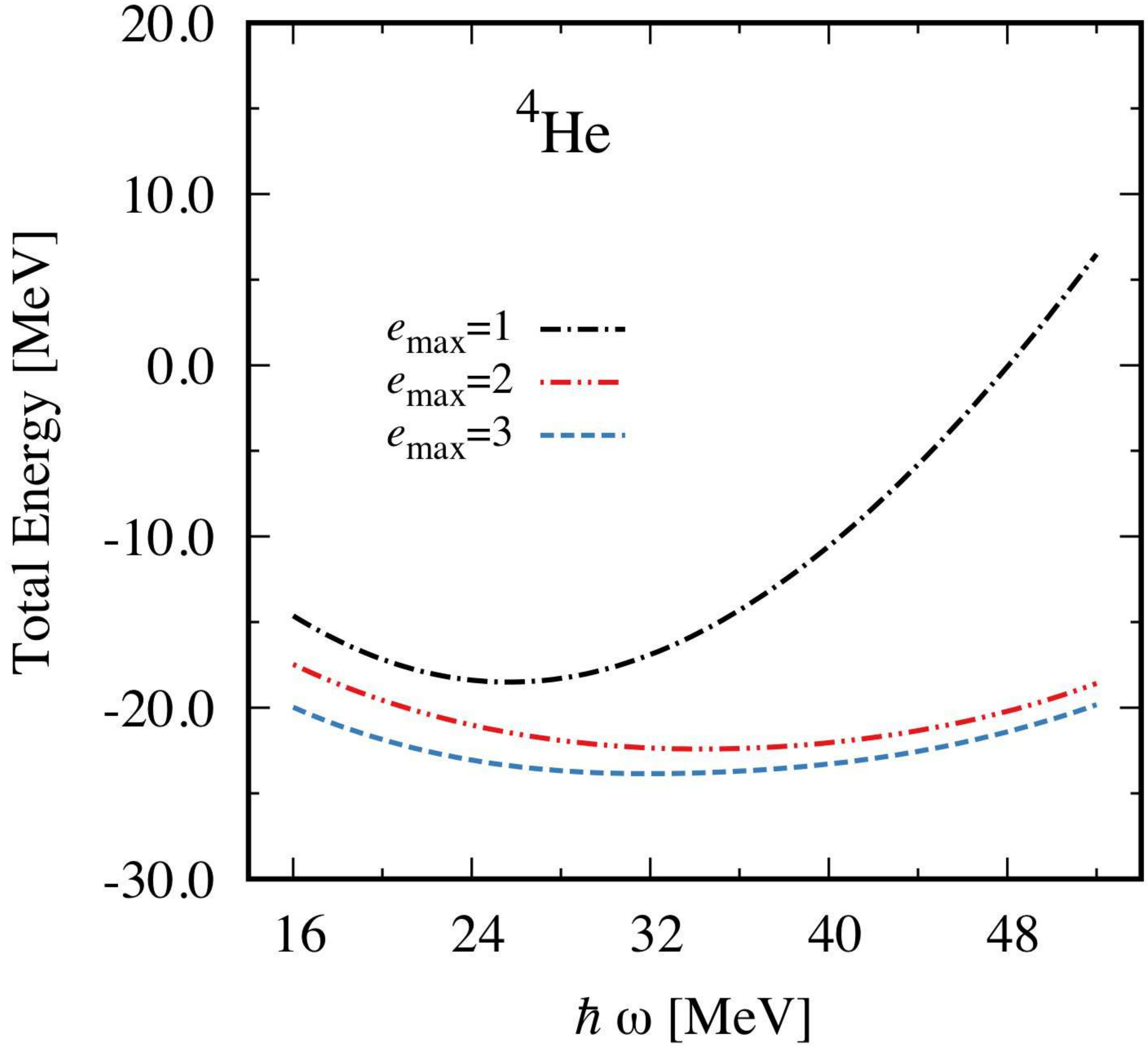
Thank you for your attention ！

Numerical Details

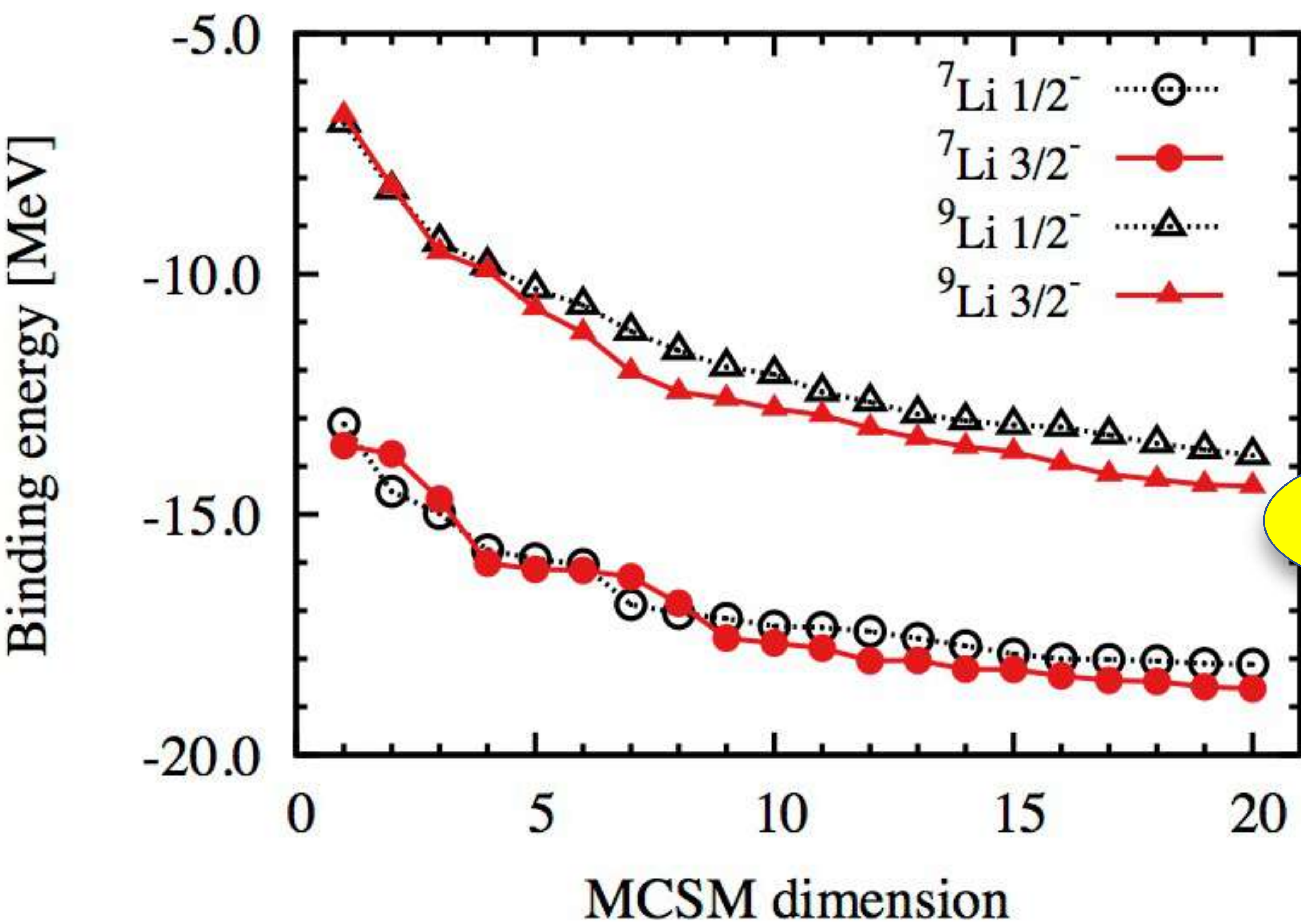
- *e_{max}=3 major shells (spsdpf-shell);*
- *The input potential is $V_{UCOM}(N^3LO)$;*
- *Coulomb interaction is not included in present calculation*

$emax$	$\langle H \rangle$ MeV	$\langle H + H_{Coulomb} \rangle$ MeV
1	-19.263	-18.857
3	-23.592	-23.152

MCSM vs Conventional Shell Model



^{7}Li and ^{9}Li: MCSM Dimension Convergence

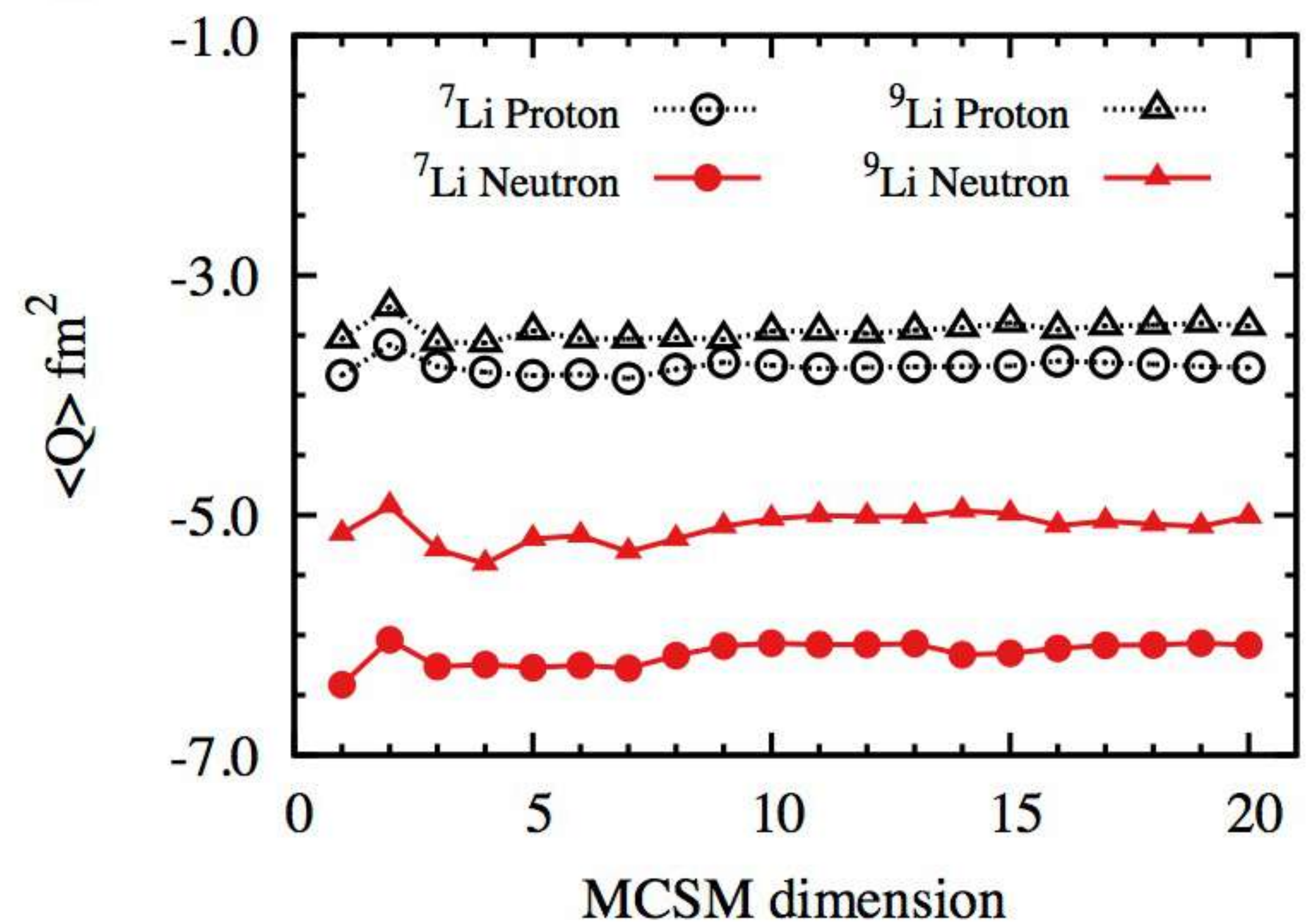


- *reliable convergence*

$$\epsilon = |E_n - E_{n-1}|/E_n$$

ϵ < 1%

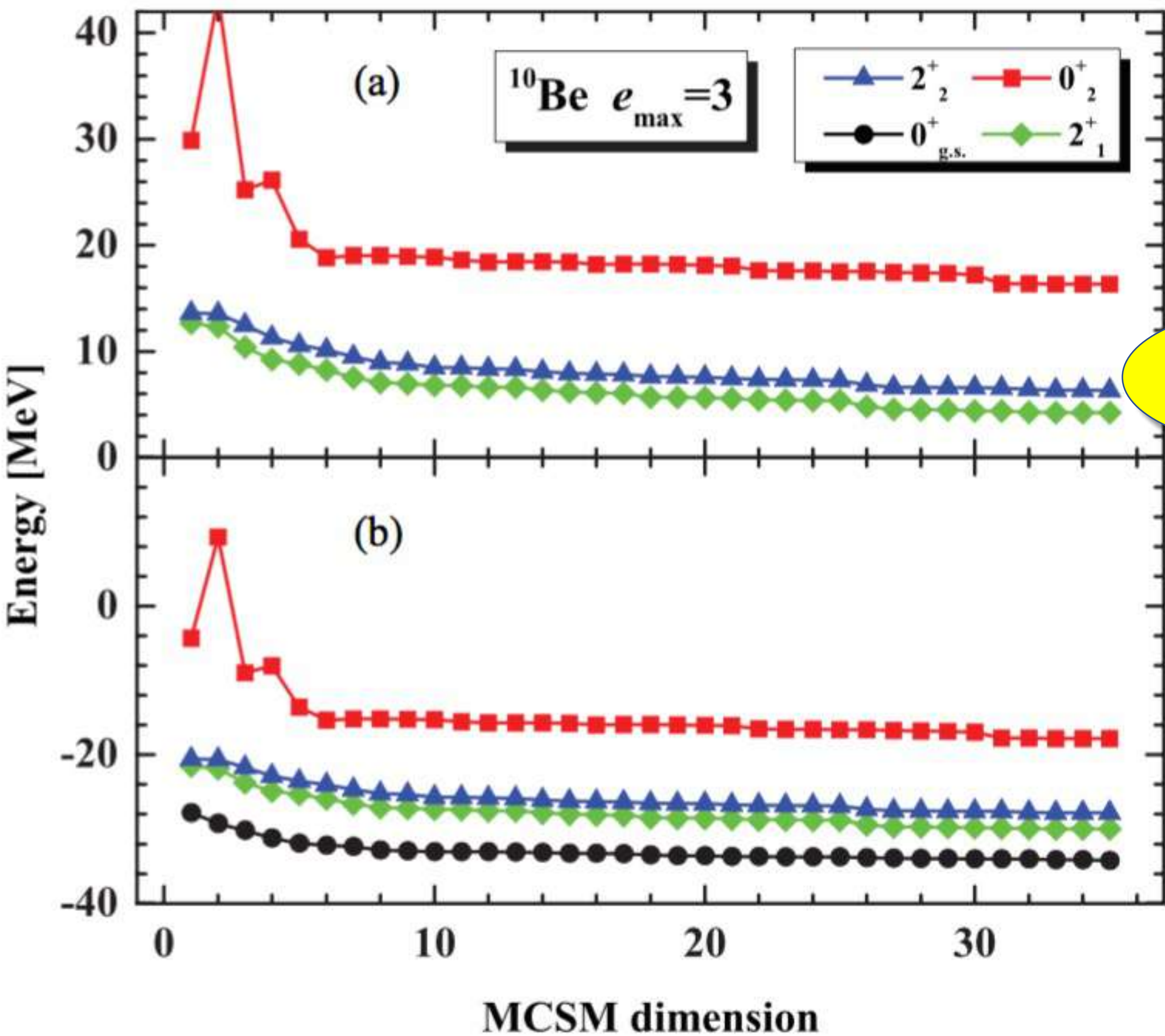
- *MCSM dimension ~ 20*



L. Liu, 2015

Beryllium Low-lying Spectra

- *The convergence of energy for ^{10}Be as the function of MCSM dimension.*

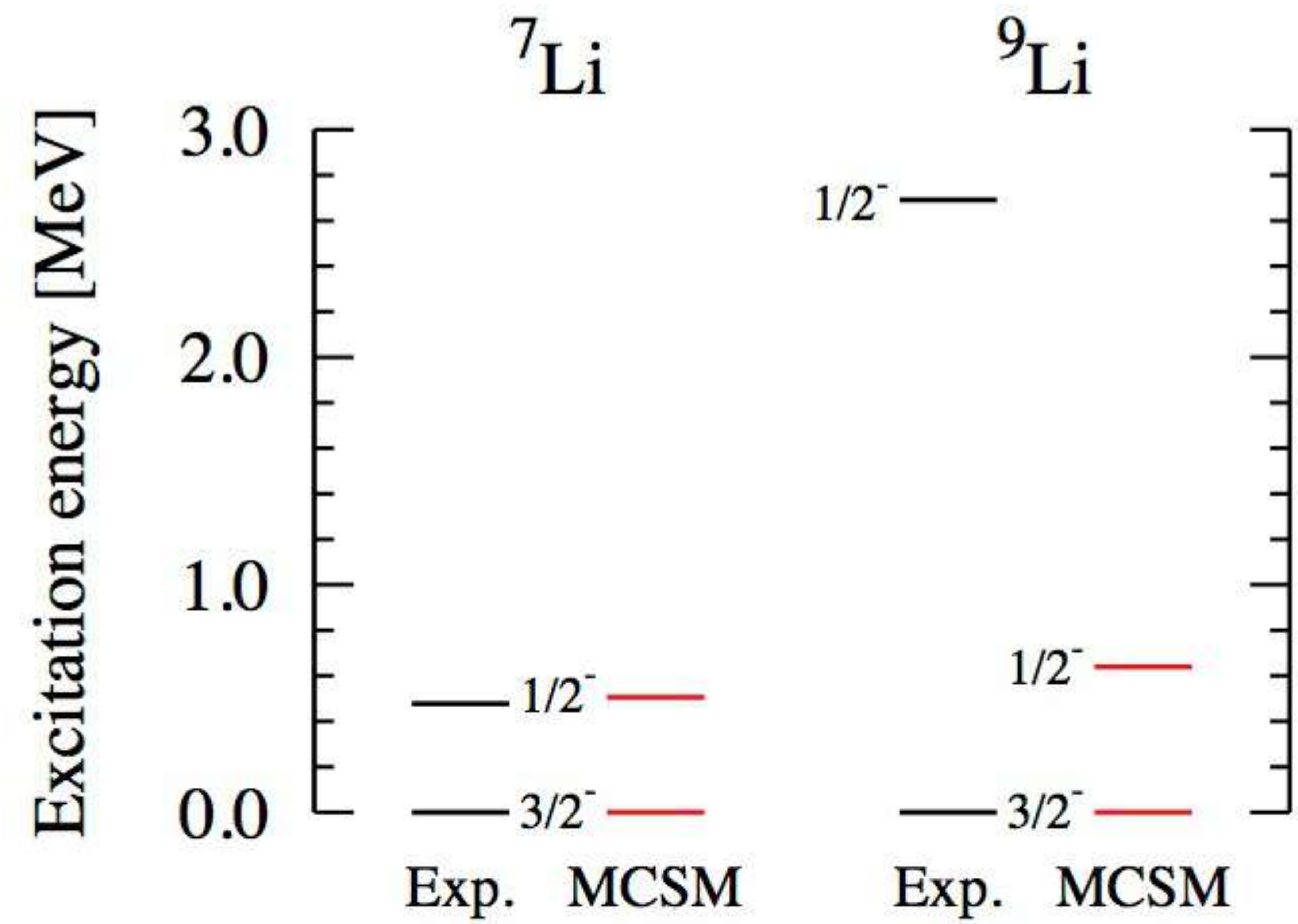


$$\epsilon = |E_n - E_{n-1}|/E_n$$

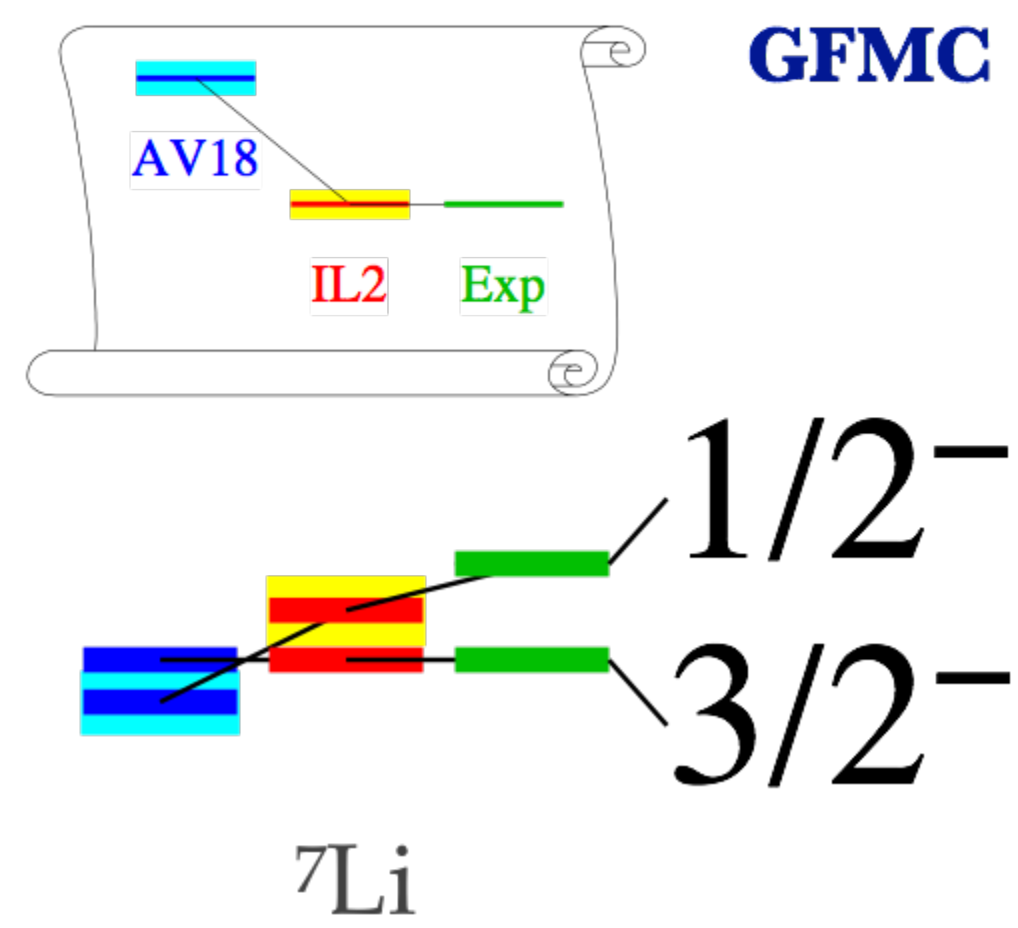
< 0.7%

L. Liu, *et al.* 2012

^7Li and ^9Li: Low-lying Spectra



L. Liu, 2015

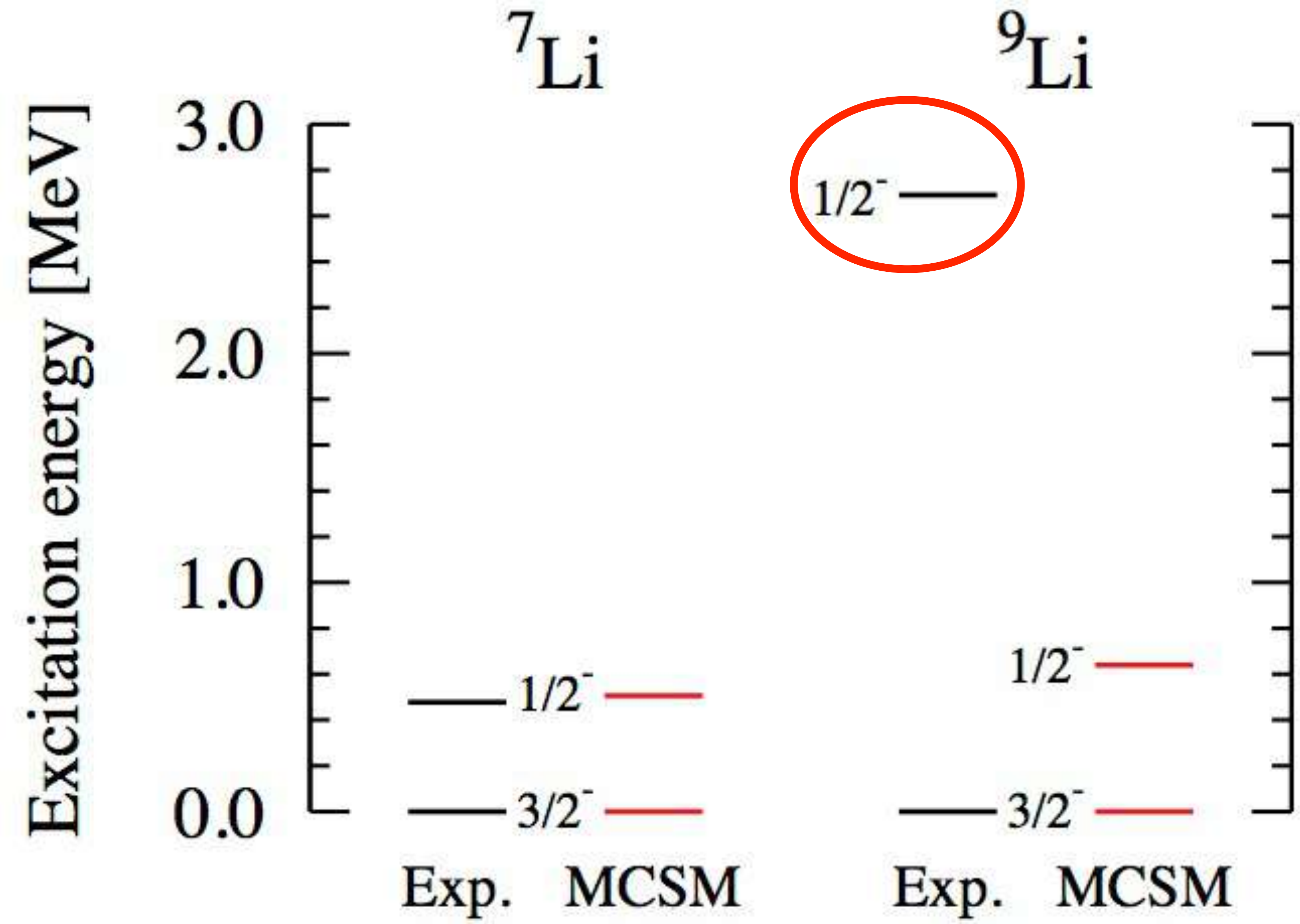


S. C. Pieper, 2005

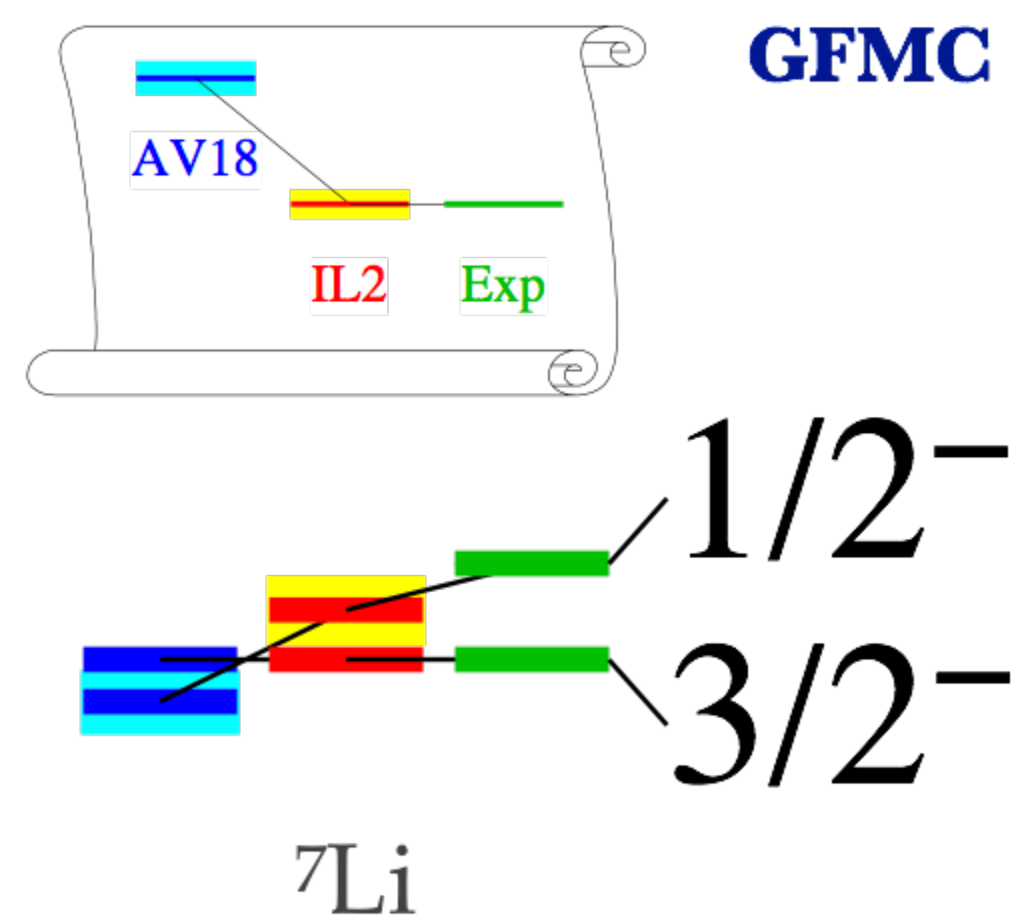
☑ ***correct level ordering;***

three-body forces or other mechanism?

^{7}Li and ^{9}Li: Low-lying Spectra



L. Liu, 2015



S. C. Pieper, 2005

☑ ***correct level ordering;***

× ***^{9}Li 1/2$^-$***

^{7}Li and ^{9}Li: Magnetic Moments

Isotopes	Exp.	MCSM	NCSM
		μ [μ_N]	
^{7}Li	3.256427(2)	3.116	3.01(2)
^{9}Li	3.434(5)	3.183	2.89(2)
		Q [e fm^2]	
^{7}Li	-4.00(3)	-3.770	-3.20(22)
^{9}Li	-3.06(2)	-3.452	-2.66(22)

L. Liu and J. Li 2015

^{10}Be E2 Transition

Unit: Q(e fm^2), B(E2) (e^2 fm^4)

❖ ***MCSM***

	Q	B(E2;$2^+_1 \to 0^+_1$)	B(E2;$2^+_2 \to 0^+_1$)	B(E2;$2^+_2 \to 2^+_1$)
Exp.		9.2(3)	0.11(2)	
MCSM	-7.71	9.29	0.32	3.28

E.A. McCutchan, C. J. Lister, R. B. Wiringa, *et al.* Phys. Rev. Lett. **103**, 192501 (2009)

❖ ***GFMC***

H	AV18	AV18+UIX	AV18+IL2	AV18+IL7	Expt.
$\lvert E_{gs}(0^+)\rvert$	50.1(2)	59.5(3)	66.4(4)	64.3(2)	64.98
$E_x(2^+_1)$	2.9(2)	3.5(3)	5.0(4)	3.8(2)	3.37
$E_x(2^+_2)$	2.7(2)	3.8(3)	5.8(4)	5.5(2)	5.96
$B(E2; 2^+_1 \to 0^+)$	10.5(3)	17.9(5)	8.1(3)	8.8(2)	9.2(3)
$B(E2; 2^+_2 \to 0^+)$	3.3(2)	0.35(5)	3.3(2)	1.7(1)	0.11(2)
$\Sigma B(E2)$	13.8(4)	18.2(6)	11.4(4)	10.5(3)	9.3(3)

M. Pervin, S. C. Pieper, and R.B. Wiringa, Phys. Rev. C. **76**, 064319 (2007).

❖ ***NCSM***

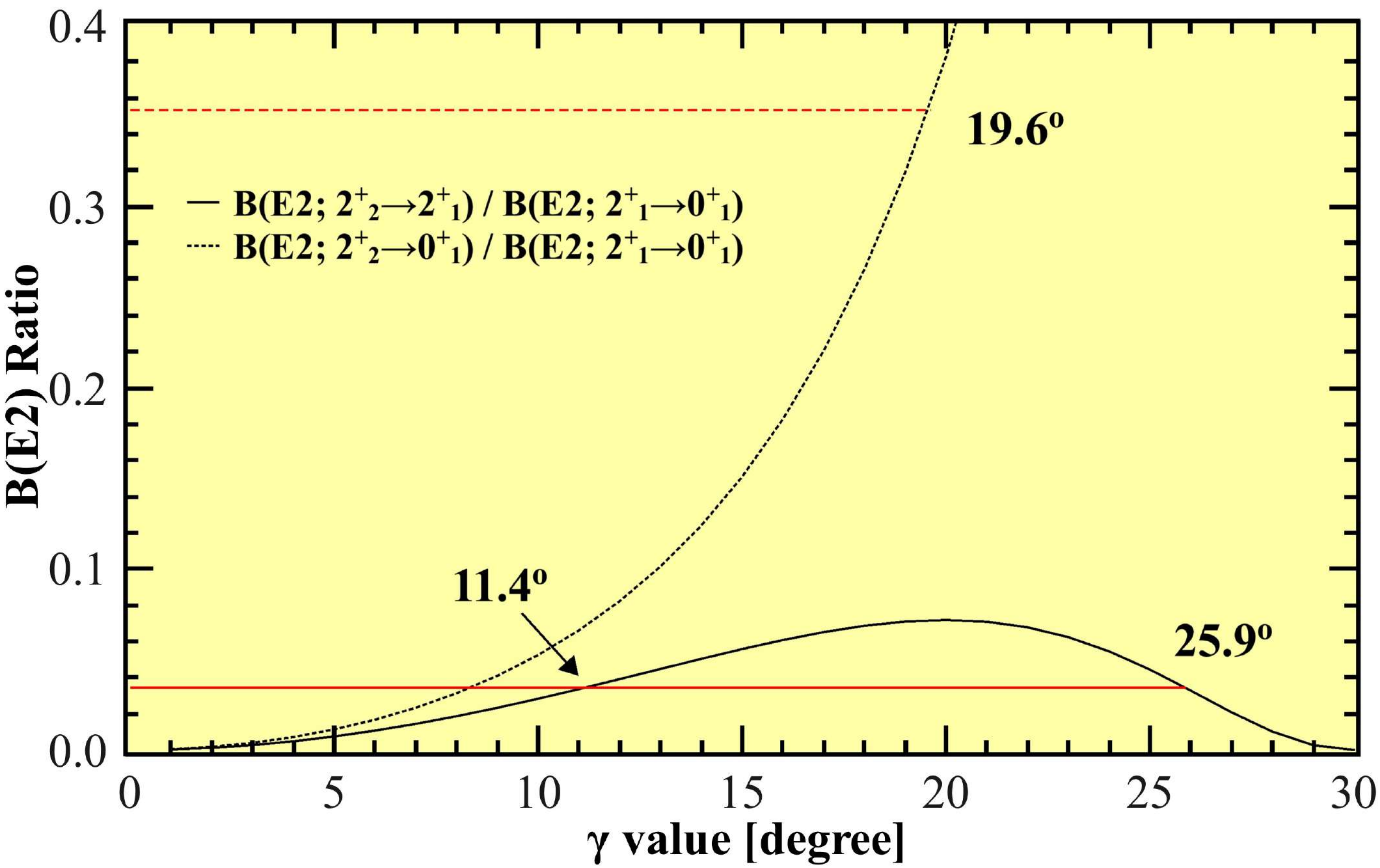
with the CD-BONN: **B(E2; $2^+_1 \to 0^+_{g.s.}$) = 6.5 e^2 fm^4**
with the CDB2K: **B(E2; $2^+_1 \to 0^+_{g.s.}$) = 9.8 e^2 fm^4**

E. Caurier, P. Navr´atil, W.E. Ormand, and J.P Vary, Phys. Rev. C **66**, 024314 (2002).

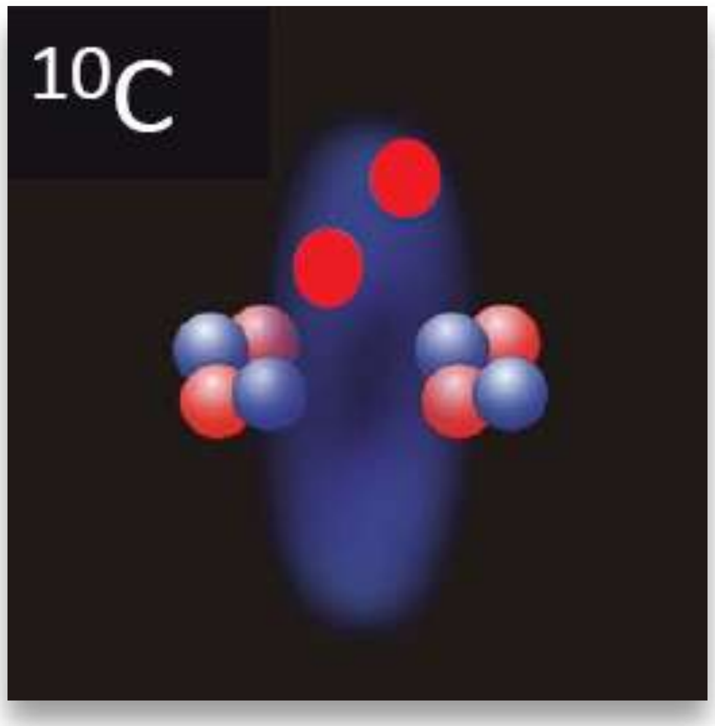
^{10}Be: Triaxial Deformation ?

Davydov-Filippov model: A.S. Davydov and G.F. Filippov, 1958.

$$\frac{B(E2;2_2^+\to 0_1^+)}{B(E2;2_1^+\to 0_1^+)}=\frac{1-\frac{3-2\sin^2(3\gamma)}{\sqrt{9-8\sin^2(3\gamma)}}}{1+\frac{3-2\sin^2(3\gamma)}{\sqrt{9-8\sin^2(3\gamma)}}}\qquad \frac{B(E2;2_2^+\to 2_1^+)}{B(E2;2_1^+\to 0_1^+)}=\frac{\frac{20}{7}\cdot\frac{3-2\sin^2(3\gamma)}{9-8\sin^2(3\gamma)}}{1+\frac{3-2\sin^2(3\gamma)}{\sqrt{9-8\sin^2(3\gamma)}}}$$



B(E2) of Mirror Nuclei: ^{10}Be and ^{10}C



- **Liquid drop model**

$$B(E2) \propto Q^2 \propto (ZeR_0^2\beta)^2 \Longrightarrow \frac{^{10}\mathrm{C} : B(E2; 2_1^+ \to 0_1^+)}{^{10}\mathrm{Be} : B(E2; 2_1^+ \to 0_1^+)} = \left(\frac{6}{4}\right)^2$$

The B(E2) of ^{10}C should be LARGER than that of ^{10}Be

- **Shell model**

$$B(E2; 2_1^+ \to 0_1^+) \propto [3.2 + 0.1 \times T_z]^2$$

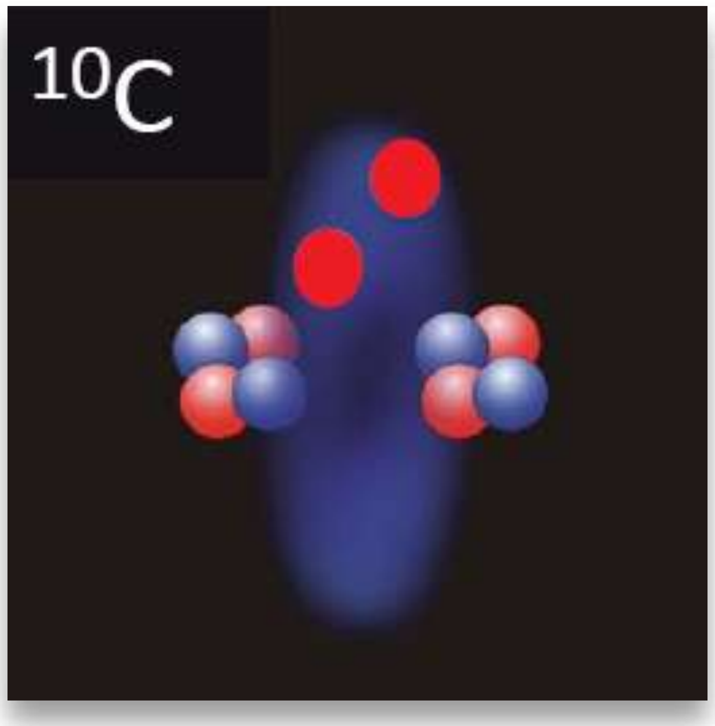
^{10}C: T_z = -1

^{10}Be: T_z=1

The B(E2) of ^{10}C should be SMALLER than that of ^{10}Be

D. E. Alburger, 1969

B(E2) of Mirror Nuclei: ^{10}Be and ^{10}C



Expt. B(E2; $2^+{}_1 \rightarrow 0^+{}_1$) = 8.8(3) e^2 fm^4

E.A. McCutchan, et al. Phys. Rev. C 86 (2012) 014312

GFMC (AV18)

B(E2; $2^+ \rightarrow 0^+$) ~ 4 e^2 fm^4

(AV18+IL2)

B(E2; $2^+ \rightarrow 0^+$) ~ 15 e^2 fm^4

E.A. McCutchan, et al. Phys. Rev. C 86 (2012) 014312 priv. com. with

MCSM

B(E2; $2^+ \rightarrow 0^+$) = 9.30 e^2 fm^4

NCSM (CD Bonn)

B(E2; $2^+ \rightarrow 0^+$) = 5.7 e^2 fm^4

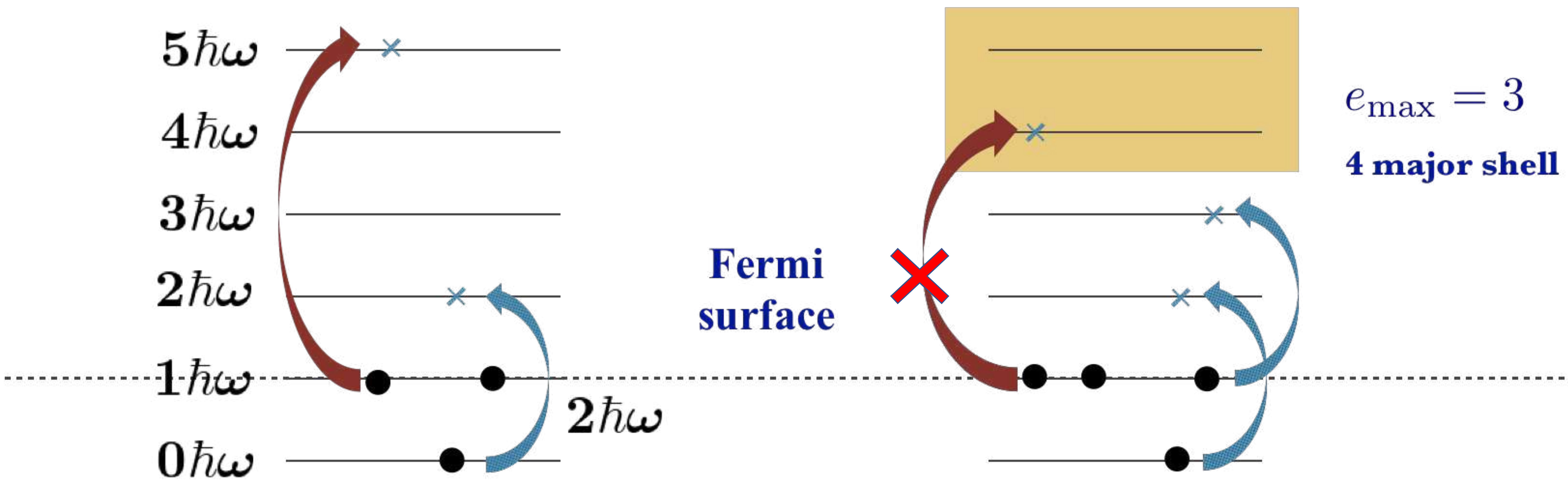
E. Caurier, P. Navratil, W. Ormand, and J. Vary, Phys. Rev. C **66**, 024314 (2002)

	^{10}Be			^{10}C		
	$B(E2;\,2_1^+ \rightarrow 0_{g.s.}^+)$	$B(E2;\,2_2^+ \rightarrow 0_{g.s.}^+)$	$B(E2;\,2_2^+ \rightarrow 2_1^+)$	$B(E2;\,2_1^+ \rightarrow 0_{g.s.}^+)$	$B(E2;\,2_2^+ \rightarrow 0_{g.s.}^+)$	$B(E2;\,2_2^+ \rightarrow 2_1^+)$
Expt.	9.2(3)	0.11(2)		8.8(3)		
MCSM	9.29	0.32	3.28	9.30	2.15	12.81

- ***4 protons in ^{10}Be tends to be deformed rather strongly in a prolate shape and the rest (6 neutrons) tends to be deformed in a triaxial shape, and the situation is just reversed in ^{10}C.***

Truncation in Shell Model

No-Core Shell Model **MCSM**



Excitation energy up to $N_{max}\hbar\omega$

Single particle energies up to $e_{max}\hbar\omega$

$$e_{max} = 2n + l$$

SMMC and MCSM

- **HS transformation**

$$e^{-\beta \hat{H}} \simeq \prod_{n=1}^{N_t} \int_{-\infty}^{\infty} \prod_{\alpha} \mathrm{d}\sigma_{\alpha,n} \sqrt{\frac{\beta |V_\alpha|}{2\pi}} \cdot G(\sigma_\alpha) \cdot e^{-\Delta\beta \hat{h}(\sigma_\alpha)}$$

- **the ground state**

$$|\Phi_{g.s.}\rangle \simeq \prod_{n=1}^{N_t} \sum_{MC,\sigma} e^{-\Delta\beta \hat{h}(\sigma_n)} |\Psi^{(0)}\rangle$$

- **states with σ**

$$|\Phi(\sigma)\rangle \propto \prod_{n=1}^{N_t} e^{-\Delta\beta \hat{h}(\sigma_n)} |\Psi^{(0)}\rangle$$

- **the ground state energy**

$$E_{g.s.} = \frac{\langle \Phi_{g.s.} | \hat{H} | \Phi_{g.s.} \rangle}{\langle \Phi_{g.s.} | \Phi_{g.s.} \rangle}$$

- **generate basis;**
- **diagonalization.**

MCSM — Illustrative example

- **Gaussian integral**

$$\int_{-\infty}^{\infty} d\sigma\, e^{-a(\sigma+c)^2} = \sqrt{\pi/a} \qquad (a > 0)$$

or $$e^{ac^2} = \sqrt{a/\pi} \int_{-\infty}^{\infty} d\sigma\, e^{-a\sigma^2 - 2ac\sigma}$$

- **imaginary-time evolution operator**

$$e^{-\frac{1}{2}\beta V \hat{O}^2} = \int_{-\infty}^{\infty} d\sigma \sqrt{\frac{\beta|V|}{2\pi}} \cdot e^{-\frac{\beta}{2}|V|\sigma^2} \cdot e^{-\beta|V|\sigma\hat{O}}$$

- **toy Hamiltonian**

$$\hat{H} = \frac{1}{2} V \hat{O}^2$$

V: a coupling constant ($V < 0$)

$\hat{O}$: a one-body operator

- **Monte Carlo sampling**

$$e^{-\frac{1}{2}\beta V \hat{O}^2} \approx \sum_{MC:\sigma} \sqrt{\frac{\beta|V|}{2\pi}} \cdot e^{-\beta|V|\sigma\hat{O}}$$

probability weight

$$G(\sigma) = e^{-\frac{\beta}{2}|V|\sigma^2}$$

σ: auxiliary field

MCSM — Illustrative Example

- **Gaussian integral**

$$\int_{-\infty}^{\infty} d\sigma\, e^{-a(\sigma+c)^2} = \sqrt{\pi/a} \qquad (a > 0)$$

or $$e^{ac^2} = \sqrt{a/\pi} \int_{-\infty}^{\infty} d\sigma\, e^{-a\sigma^2 - 2ac\sigma}$$

- **imaginary-time evolution operator**

$$e^{-\frac{1}{2}\beta V \hat{O}^2} = \int_{-\infty}^{\infty} d\sigma \sqrt{\frac{\beta|V|}{2\pi}} \cdot e^{-\frac{\beta}{2}|V|\sigma^2} \cdot e^{-\beta|V|\sigma\hat{O}}$$

- **the ground state**

$$|\Phi_{g.s.}\rangle \sim \sum_{MC,\sigma} e^{-\beta \hat{h}(\sigma)} |\Phi^{(0)}\rangle, \quad \beta \to \infty$$

one-body Hamiltonian

$$\hat{h}(\sigma) = V\sigma\hat{O}$$

- **toy Hamiltonian**

$$\hat{H} = \frac{1}{2} V \hat{O}^2$$

V: a coupling constant ($V < 0$)

$\hat{O}$: a one-body operator

- **Monte Carlo sampling**

$$e^{-\frac{1}{2}\beta V \hat{O}^2} \approx \sum_{MC:\sigma} \sqrt{\frac{\beta|V|}{2\pi}} \cdot e^{-\beta|V|\sigma\hat{O}}$$

probability weight

$$G(\sigma) = e^{-\frac{\beta}{2}|V|\sigma^2}$$

σ: auxiliary field

MCSM — General Cases

- **a general Hamiltonian**

$$\hat{H} = \sum_{i,j=1}^{N_{s.p.}} \epsilon_{ij} c_i^\dagger c_j + \frac{1}{4} \sum_{i,j,k,l=1}^{N_{s.p.}} v_{i,j,k,l}\, c_i^\dagger c_j^\dagger c_l c_k$$

i, j : the single particle states.

$N_{s.p.}$: the number of the single particle states.

- **Hamiltonian in a quadratic form**

$$\hat{H} = \sum_{\alpha=1}^{N_f} (E_\alpha \hat{O}_\alpha + \frac{1}{2} V_\alpha \hat{O}_\alpha^2)$$

$\hat{O}_\alpha$: one-body operators

N_f : the number of the O_α's

$$e^{-\beta \hat{H}} = \int_{-\infty}^{\infty} \prod_\alpha \mathrm{d}\sigma_\alpha \sqrt{\frac{\beta |V_\alpha|}{2\pi}} \cdot e^{-\frac{\beta}{2} |V_\alpha| \sigma_\alpha^2} \cdot e^{-\beta |V_\alpha| \sigma_\alpha \hat{O}_\alpha}$$

MCSM — Decomposition of the Hamiltonian

$$\hat{H} = a_1^\dagger a_2^\dagger a_4 a_3$$

$$\hat{H} = \overbrace{a_1^\dagger a_3 \, \underbrace{a_2^\dagger a_4}}\, - a_1^\dagger a_4 \delta_{23}$$

$$= -a_1^\dagger a_4 \delta_{23} + \frac{1}{2}\left[a_1^\dagger a_3, a_2^\dagger a_4\right] + \frac{1}{4}\left(a_1^\dagger a_3 + a_2^\dagger a_4\right)^2 - \frac{1}{4}\left(a_1^\dagger a_3 - a_2^\dagger a_4\right)^2$$

one-body operator

$$\hat{H} = -\overbrace{a_1^\dagger a_4 \, \underbrace{a_2^\dagger a_3}}\, + a_1^\dagger a_3 \delta_{24}$$

$$= a_1^\dagger a_3 \delta_{24} - \frac{1}{2}\left[a_1^\dagger a_4, a_2^\dagger a_3\right] - \frac{1}{4}\left(a_1^\dagger a_4 + a_2^\dagger a_3\right)^2 + \frac{1}{4}\left(a_1^\dagger a_4 - a_2^\dagger a_3\right)^2$$

MCSM — General Cases

❖ **a general Hamiltonian**

$$\hat{H} = \sum_{i,j=1}^{N_{s.p.}} \epsilon_{ij} c_i^\dagger c_j + \frac{1}{4} \sum_{i,j,k,l=1}^{N_{s.p.}} v_{i,j,k,l}\, c_i^\dagger c_j^\dagger c_l c_k$$

i, j : the single particle states.

$N_{s.p.}$: the number of the single particle states.

❖ **Hamiltonian in a quadratic form**

$$\hat{H} = \sum_{\alpha=1}^{N_f} (E_\alpha \hat{O}_\alpha + \frac{1}{2} V_\alpha \hat{O}_\alpha^2)$$

$\hat{O}_\alpha$: one-body operators

N_f : the number of the O_α's

$e^{-\beta \hat{H}}$ ✖ $\int_{-\infty}^{\infty} \prod_\alpha \mathrm{d}\sigma_\alpha \sqrt{\frac{\beta |V_\alpha|}{2\pi}} \cdot e^{-\frac{\beta}{2}|V_\alpha|\sigma_\alpha^2} \cdot e^{-\beta |V_\alpha| \sigma_\alpha \hat{O}_\alpha}$

Ĥ contains many-body term,
Ôα's do not commute with each other !

MCSM — Hubbard-Stratonovich (HS) Transformation

- **"time" slices of β**

$$e^{-\beta\hat{H}} = \left[e^{-\Delta\beta\hat{H}}\right]^{N_t}$$

- **HS transformation**

$$e^{-\beta\hat{H}} \simeq \prod_{n=1}^{N_t}\int_{-\infty}^{\infty}\prod_{\alpha}\mathrm{d}\sigma_{\alpha n}\sqrt{\frac{\beta|V_\alpha|}{2\pi}}\cdot e^{-\frac{\beta}{2}|V_\alpha|\sigma_{\alpha n}^2}\cdot e^{-\beta(E_\alpha+s_\alpha V_\alpha\sigma_{\alpha n})\hat{O}_\alpha}$$

R. L. Stratonovich, Dokl. Akad. Nauk SSSR **115**, 1097 (1957)
[Sov. Phys. Dokl. **2**, 416 (1958)].

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❖ **Gaussian weight factor**

$$G(\sigma_\alpha) = e^{-\sum_\alpha \frac{\beta}{2}|V_\alpha|\sigma_\alpha^2}$$

❖ **one-body Hamiltonian**

$$\hat{h}(\sigma_n) = \sum_\alpha (E_\alpha + s_\alpha V_\alpha \sigma_{\alpha n})\hat{O}_\alpha$$

$s_\alpha = \pm 1\ (\pm i)$ if $V_\alpha < 0\ (>0)$

❖ **HS transformation**

$$e^{-\beta\hat{H}} \simeq \prod_{n=1}^{N_t}\int_{-\infty}^{\infty}\prod_{\alpha} d\sigma_{\alpha,n}\sqrt{\frac{\beta|V_\alpha|}{2\pi}}\cdot G(\sigma_\alpha)\cdot e^{-\Delta\beta\hat{h}(\sigma_\alpha)}$$

R. L. Stratonovich, Dokl. Akad. Nauk SSSR **115**, 1097 (1957) [Sov. Phys. Dokl. **2**, 416 (1958)].

MCSM — Generation Process for Basis

1. $E^{(0)} = \langle \Psi^{(0)} | \hat{H} | \Psi^{(0)} \rangle$

2. $\sigma \equiv \{\sigma_1, \sigma_2, \cdots, \sigma_{N_t}\}$

3. $|\Phi^{(1)}(\sigma)\rangle \propto \prod_{n=1}^{N_t} e^{-\Delta\beta \hat{h}(\sigma_n)} |\Psi^{(0)}\rangle$

4. $E^{(1)} = \langle \Phi^{(1)}(\sigma) | \hat{H} | \Phi^{(1)}(\sigma) \rangle$

5. $E^{(1)} < E^{(0)}$

Unitary Correlation Operator Method (UCOM)

Main idea

$$\langle\Psi|\hat{H}|\Psi'\rangle = \langle\Phi|\hat{C}^\dagger\hat{H}\hat{C}|\Phi\rangle = \langle\Phi|\hat{C}^{-1}\hat{H}\hat{C}|\Phi\rangle = \langle\Phi|\hat{H}_{\mathrm{UCOM}}|\Phi\rangle$$

UCOM operator

$$\hat{C} = \hat{C}_\Omega\hat{C}_r = \exp\left[-i\sum_{i<j} g_{\Omega,ij}\right]\exp\left[-i\sum_{i<j} g_{r,ij}\right]$$

UCOM potential

$$\hat{H}_{\mathrm{UCOM}} = \hat{C}^\dagger\hat{H}\hat{C} = \hat{C}^\dagger(\hat{T}+\hat{V}_{\mathrm{real.}})\hat{C} = \hat{T}^{[1]} + \hat{T}^{[2]} + \hat{V}^{[2]} = \hat{T}_{\mathrm{int.}} + \hat{V}_{\mathrm{UCOM}}$$

MCSM — General Idea

- **a general Hamiltonian**

$$\hat{H} = \sum_{i,j=1}^{N_{s.p.}} \epsilon_{ij} c_i^\dagger c_j + \frac{1}{4} \sum_{i,j,k,l=1}^{N_{s.p.}} v_{i,j,k,l}\, c_i^\dagger c_j^\dagger c_l c_k$$

i, j : the single particle states.

$N_{s.p.}$: the number of the single particle states.

- **Hamiltonian in a quadratic form**

$$\hat{H} = \sum_{\alpha=1}^{N_f} (E_\alpha \hat{O}_\alpha + \frac{1}{2} V_\alpha \hat{O}_\alpha^2)$$

$\hat{O}_\alpha$: one-body operators

N_f : the number of the O_α's

$$e^{-\beta \hat{H}} = \int_{-\infty}^{\infty} \prod_\alpha \mathrm{d}\sigma_\alpha \sqrt{\frac{\beta |V_\alpha|}{2\pi}} \cdot e^{-\frac{\beta}{2}|V_\alpha|\sigma_\alpha^2} \cdot e^{-\beta |V_\alpha| \sigma_\alpha \hat{O}_\alpha}$$

MCSM — General Cases

- **a general Hamiltonian**

$$\hat{H} = \sum_{i,j=1}^{N_{s.p.}} \epsilon_{ij} c_i^\dagger c_j + \frac{1}{4} \sum_{i,j,k,l=1}^{N_{s.p.}} v_{i,j,k,l}\, c_i^\dagger c_j^\dagger c_l c_k$$

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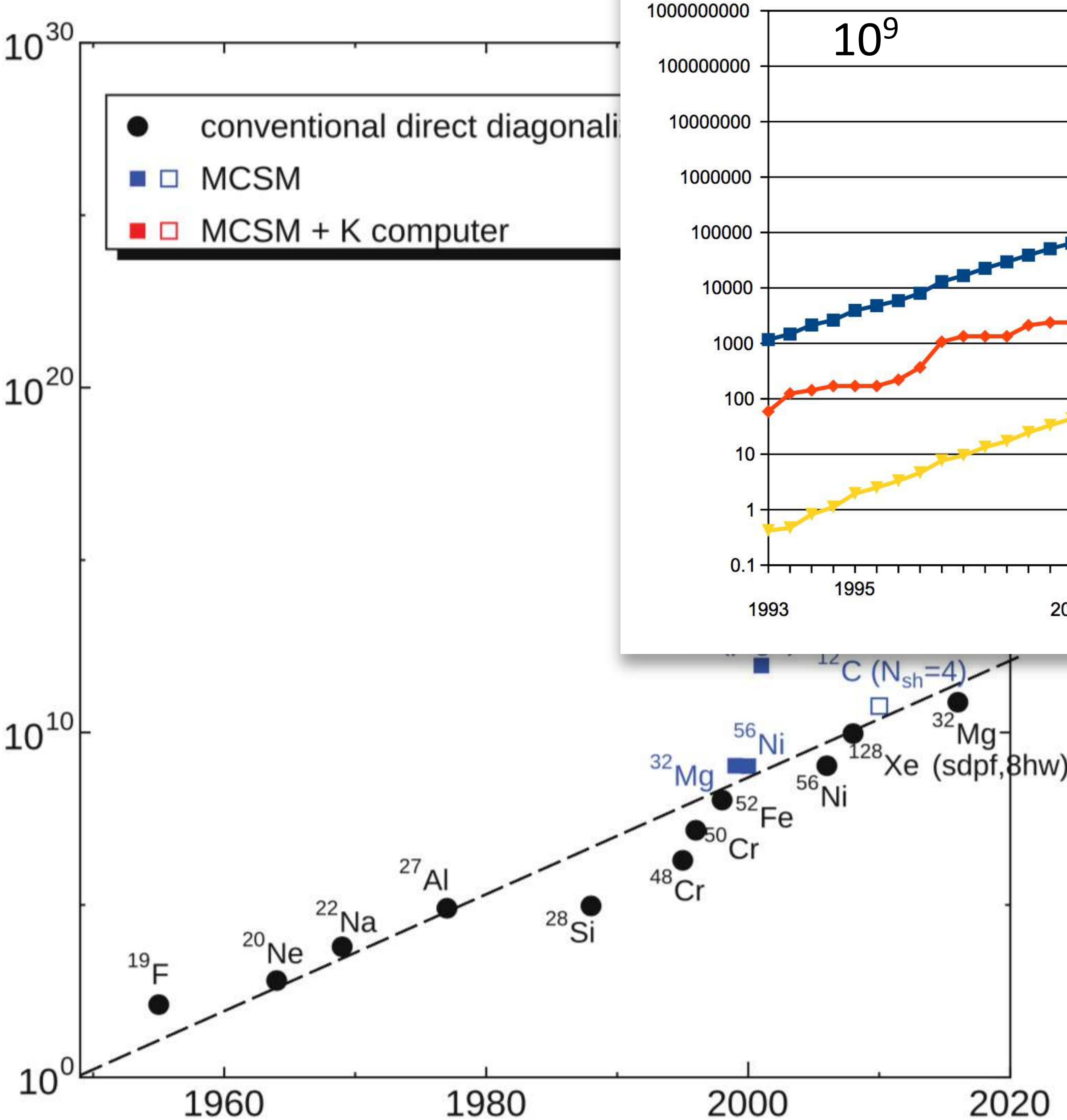
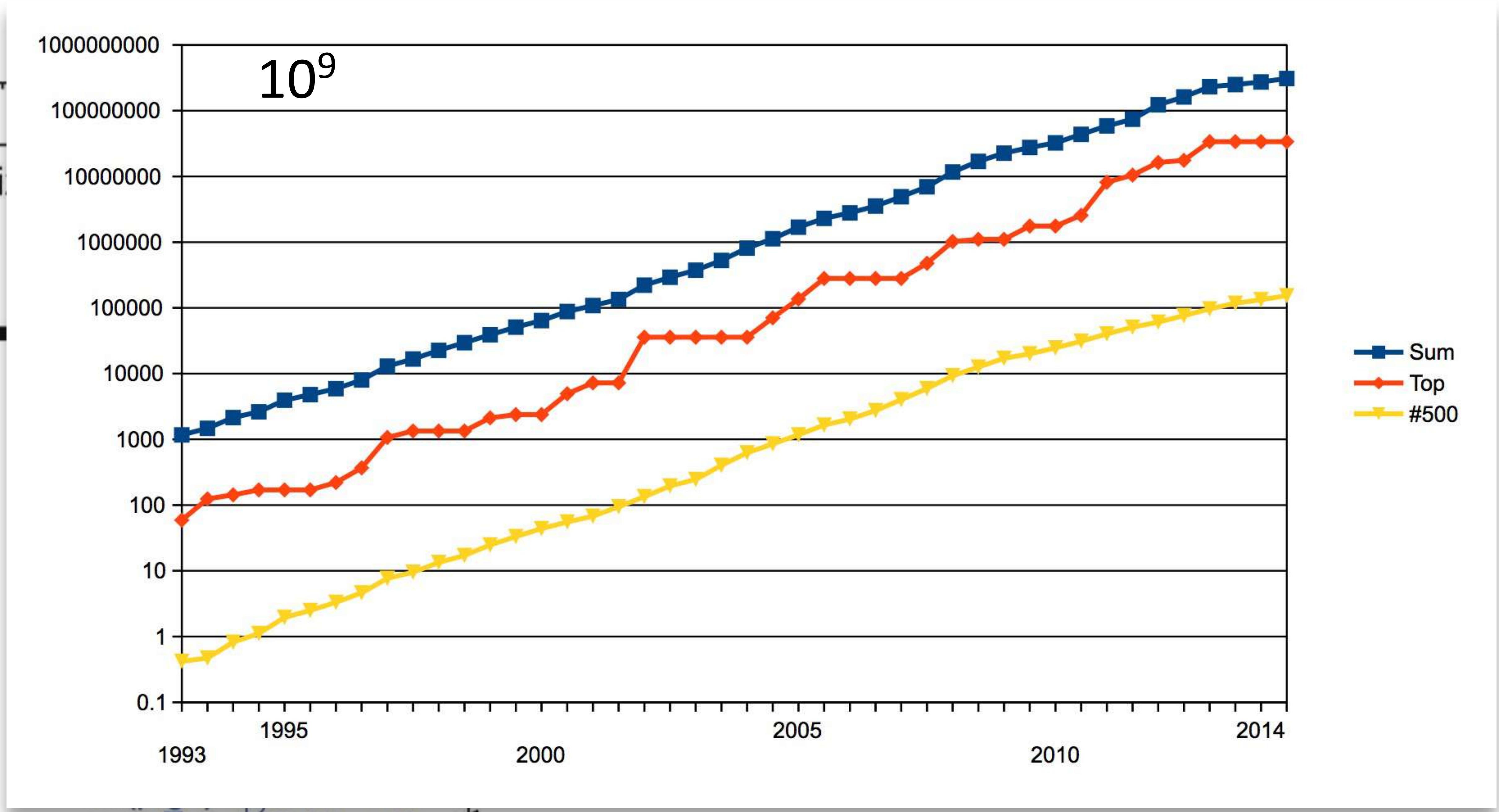
Ĥ contains many-body term,
Ôα's do not commute with each other !

Shell model vs. Computer ability

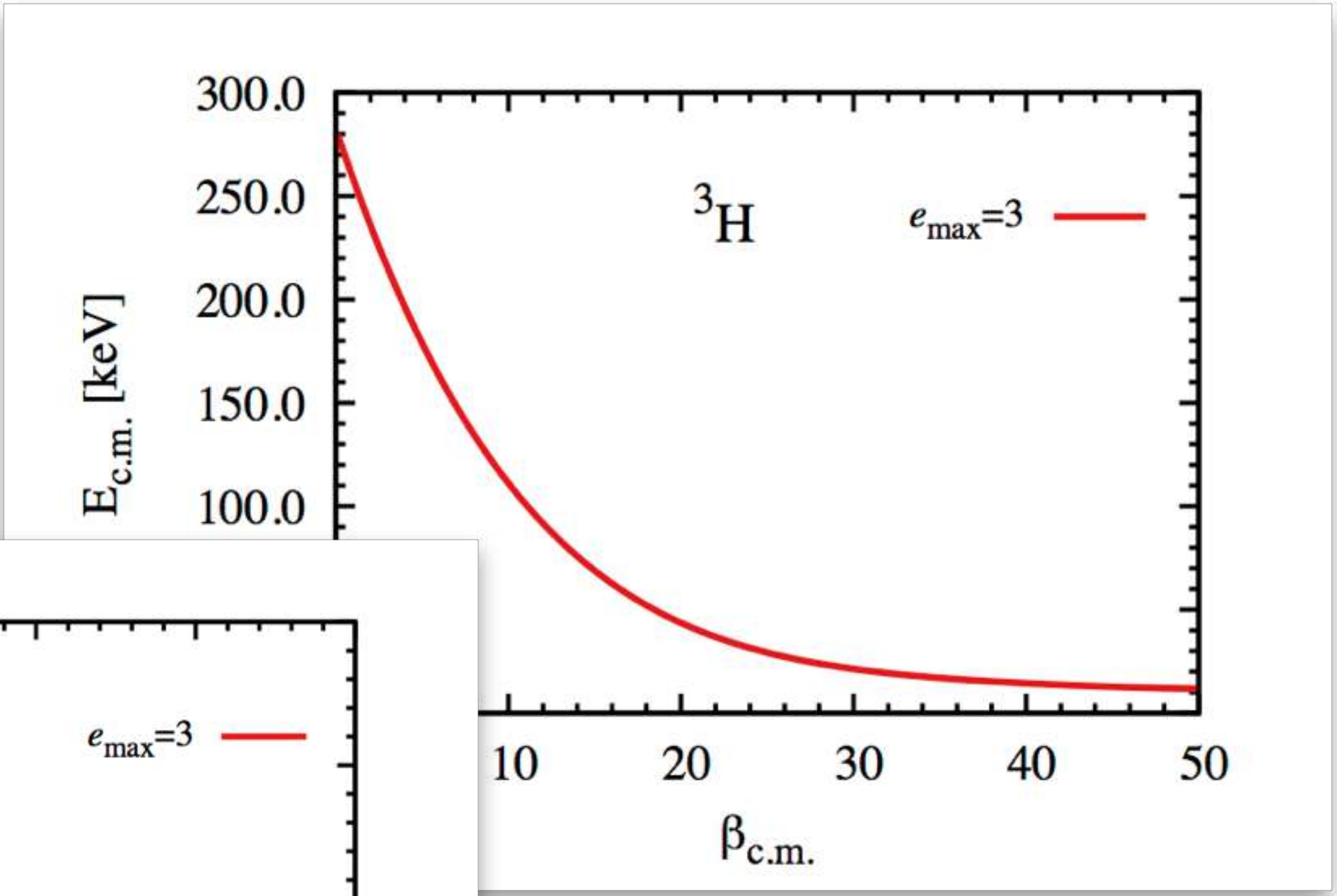


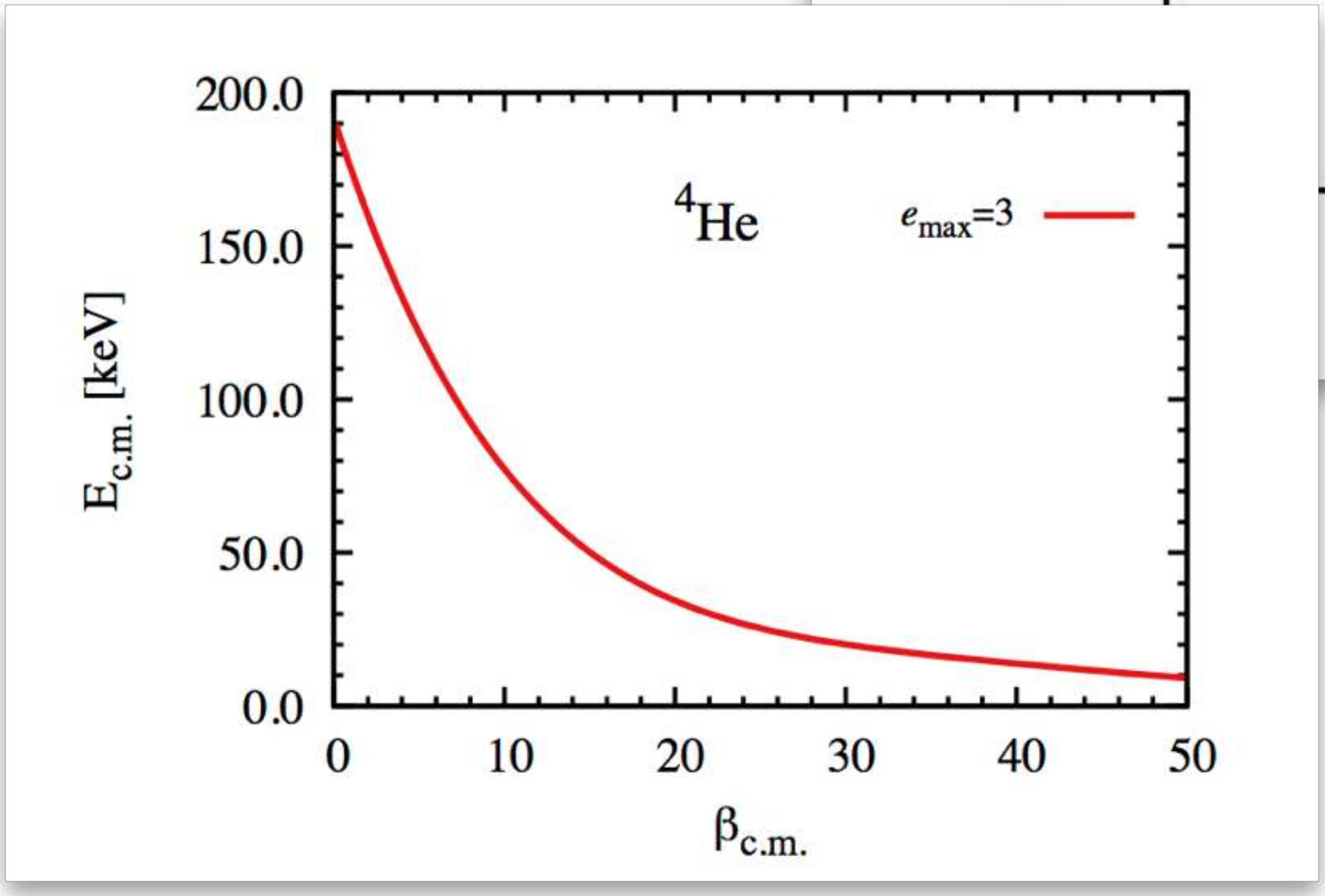
G Flops



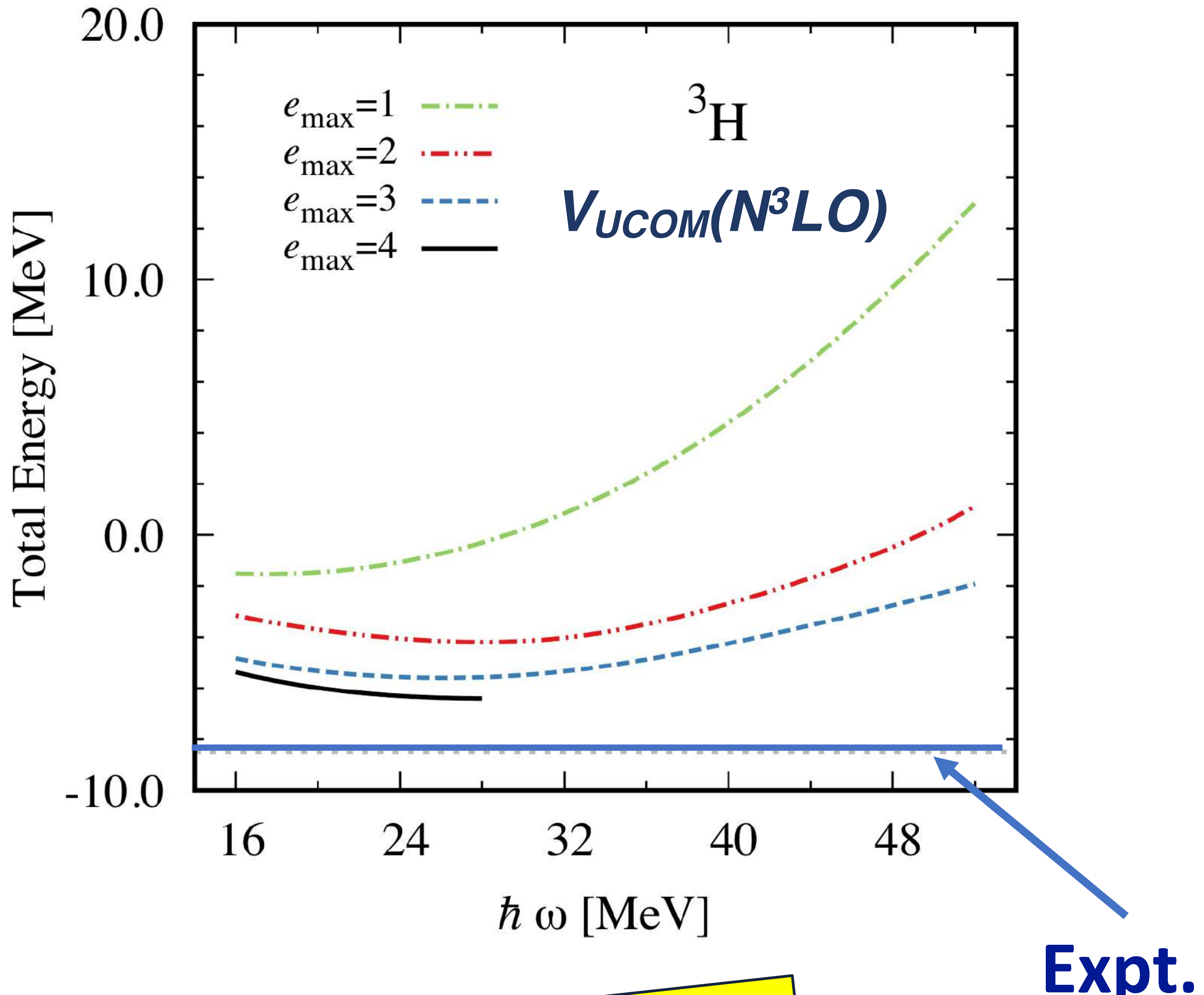
From Wiki

Treatment of Spurious Center-of-Mass Motion



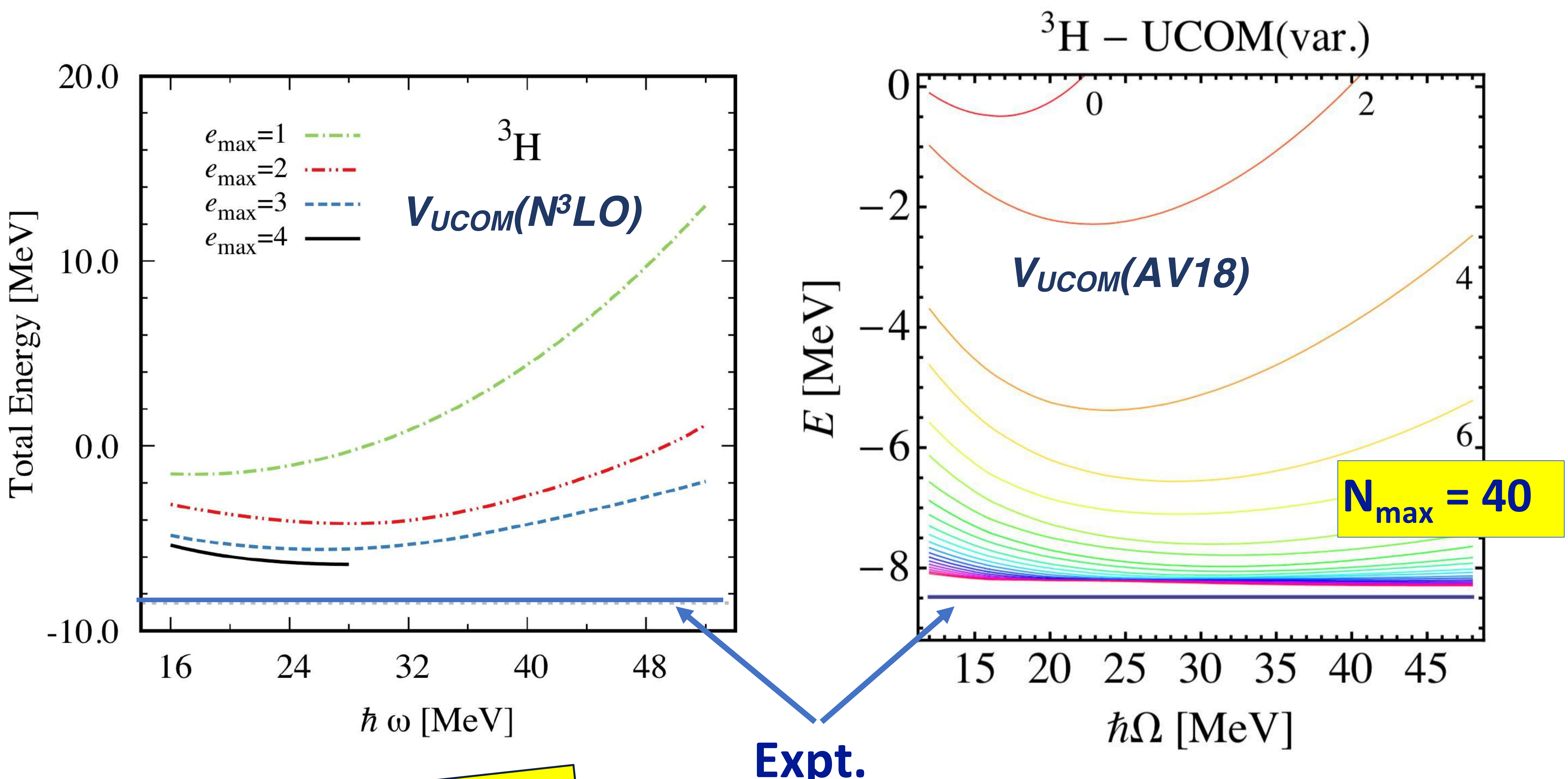


$\hbar\omega$ and Model Space Dependence



Preliminary results

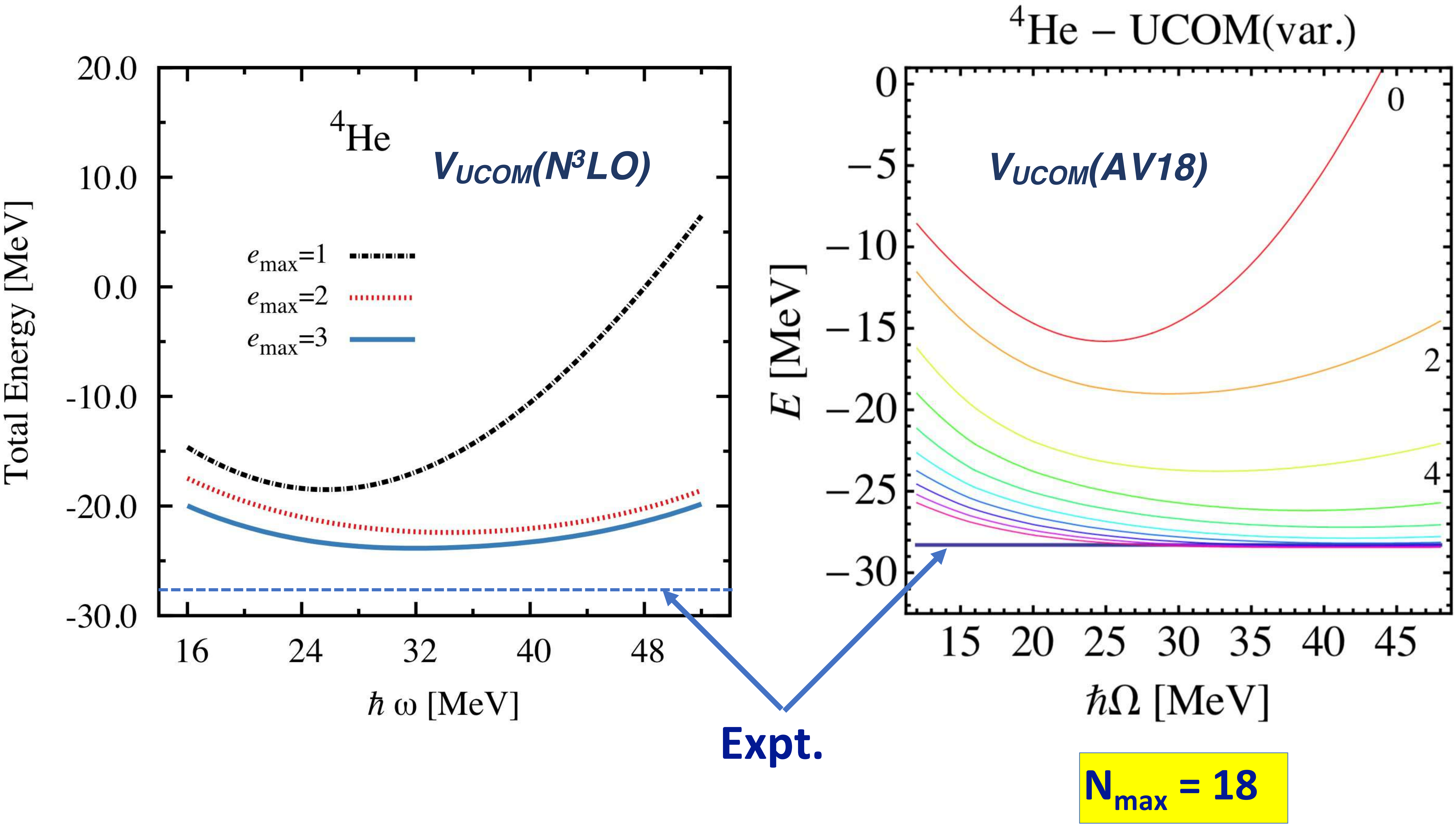
$\hbar\omega$ and Model Space Dependence



Preliminary results

R. Roth, *et al*. PPNP **65**, 50 (2010)

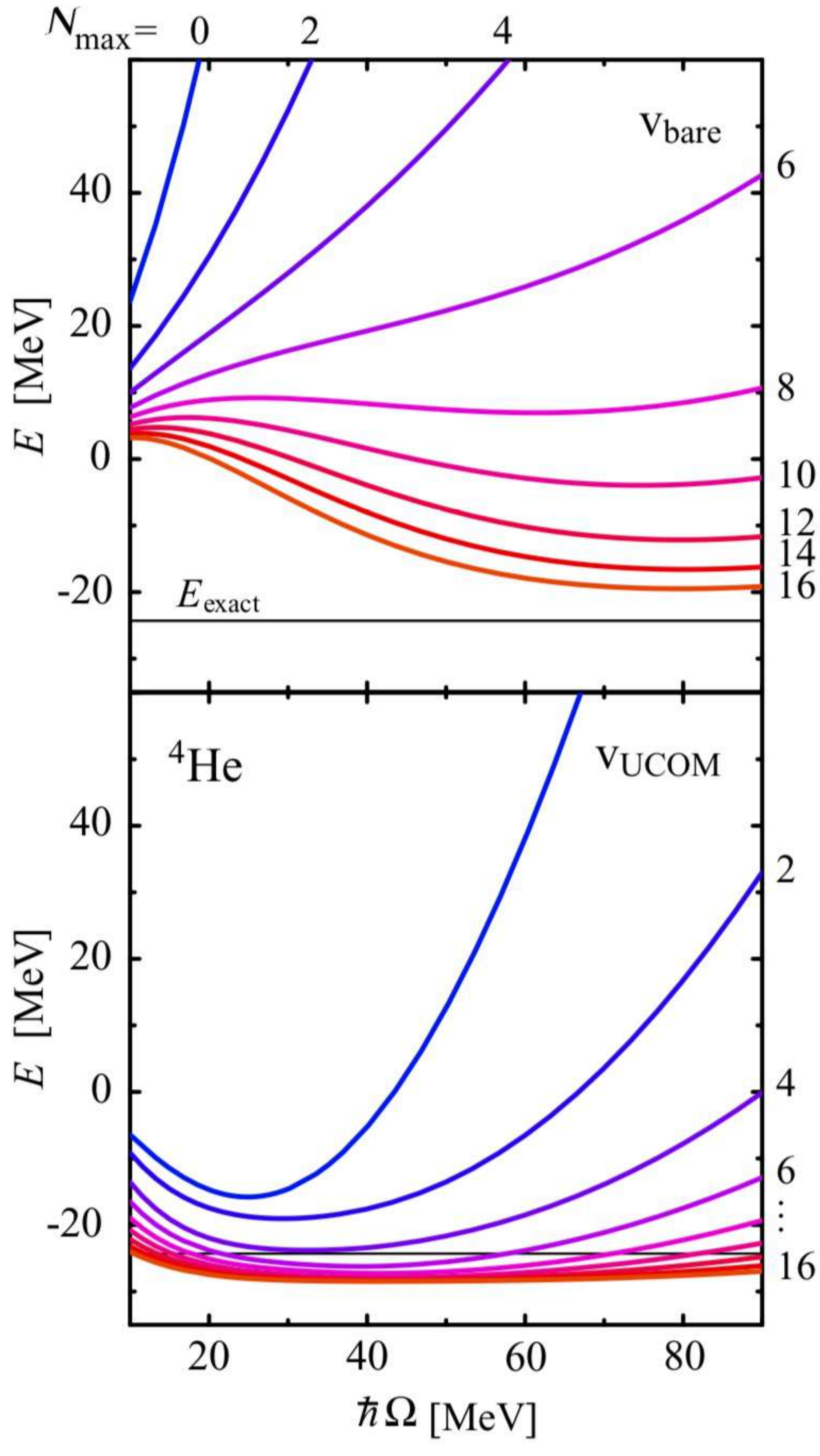
$\hbar\omega$ and Model Space Dependence



L. Liu, 2015

R. Roth, *et al*. PPNP **65**, 50 (2010)

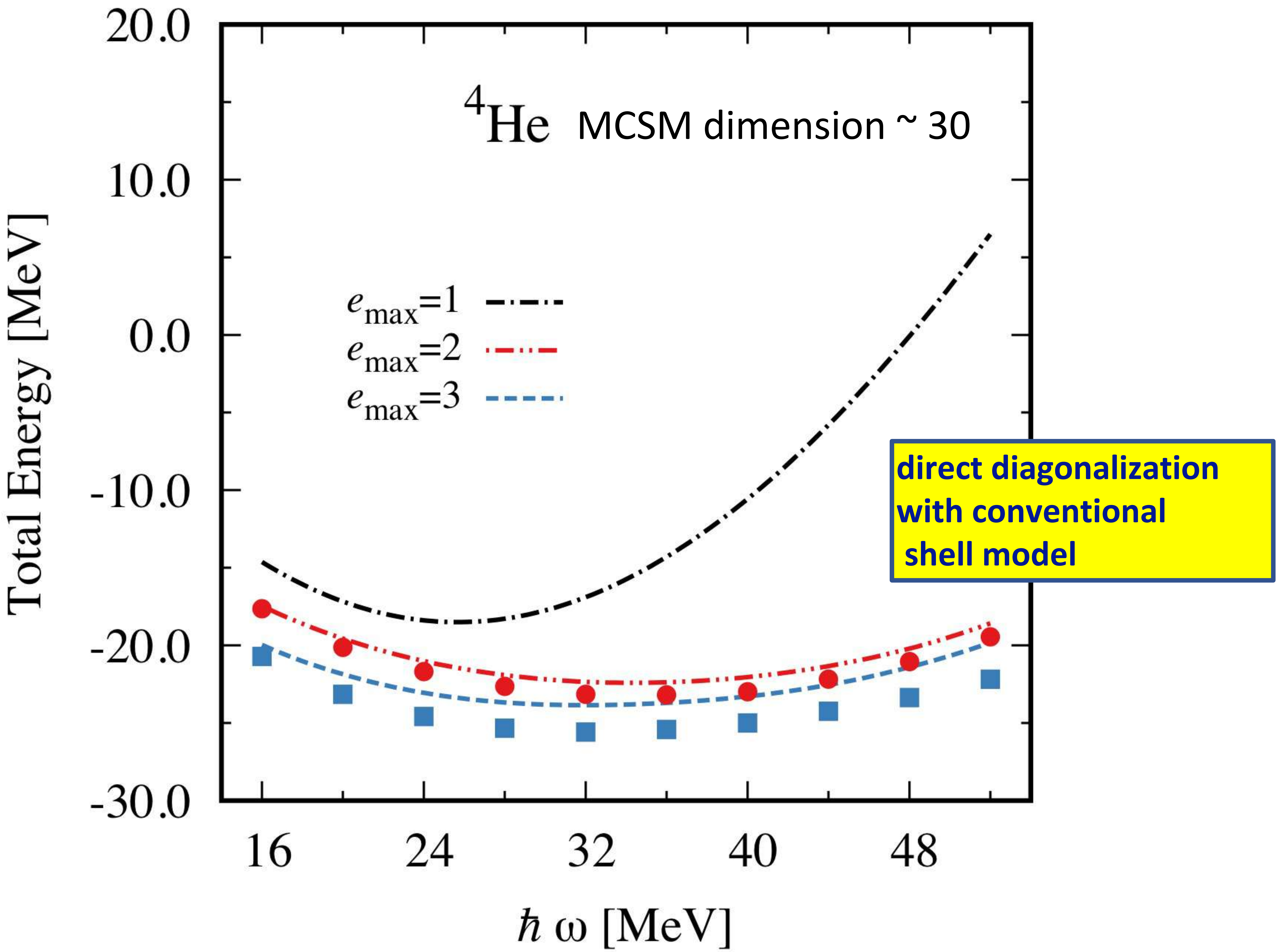
Bare realistic nuclear forces



bare AV18 potential

R. Roth, *et al*. PRC **72**, 034002 (2005)

MCSM vs Conventional Shell Model

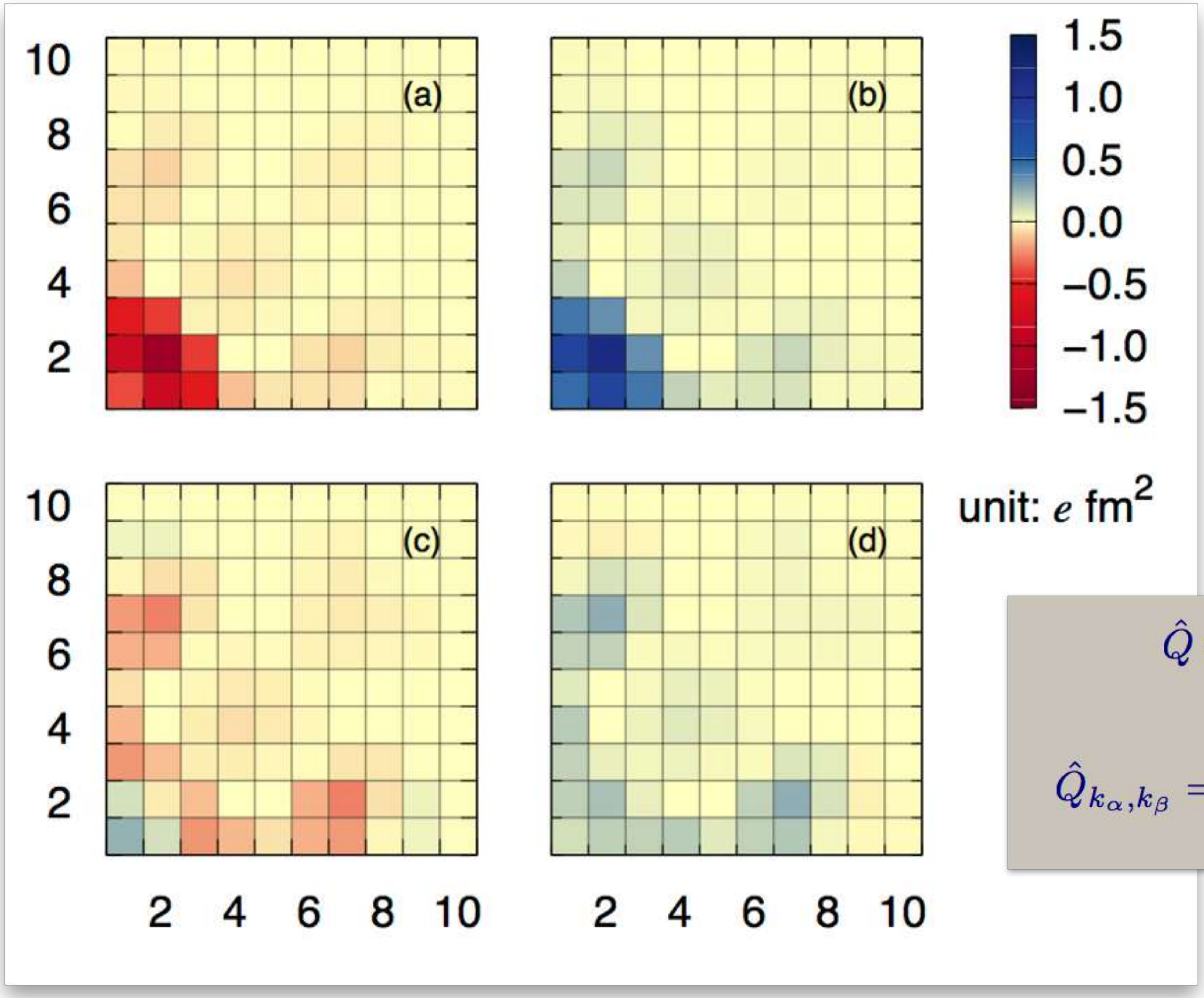


Contribution of Single Particle Orbit to Q

$\langle 2^+_1 \| Q_{k_\alpha, k_\beta} \| 2^+_1 \rangle$ $\langle 2^+_2 \| Q_{k_\alpha, k_\beta} \| 2^+_2 \rangle$

proton

neutron



$$\hat{Q} = \sum_{k_\alpha, k_\beta} \hat{Q}_{k_\alpha, k_\beta}$$

$$\hat{Q}_{k_\alpha, k_\beta} = \sum_{m_\alpha, m_\beta} \langle \alpha | \hat{Q} | \beta \rangle a^\dagger_\alpha a_\beta$$

$0s1/2$, $0p3/2$, $0p1/2$, $0d5/2$, $0d3/2$, $1s1/2$, $0f7/2$, $0f5/2$, $1p3/2$ and $1p1/2$

L. Liu, 2015

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$\langle 2^+_1 \| Q_{k_\alpha, k_\beta} \| 2^+_1 \rangle$ $\langle 2^+_2 \| Q_{k_\alpha, k_\beta} \| 2^+_2 \rangle$

proton

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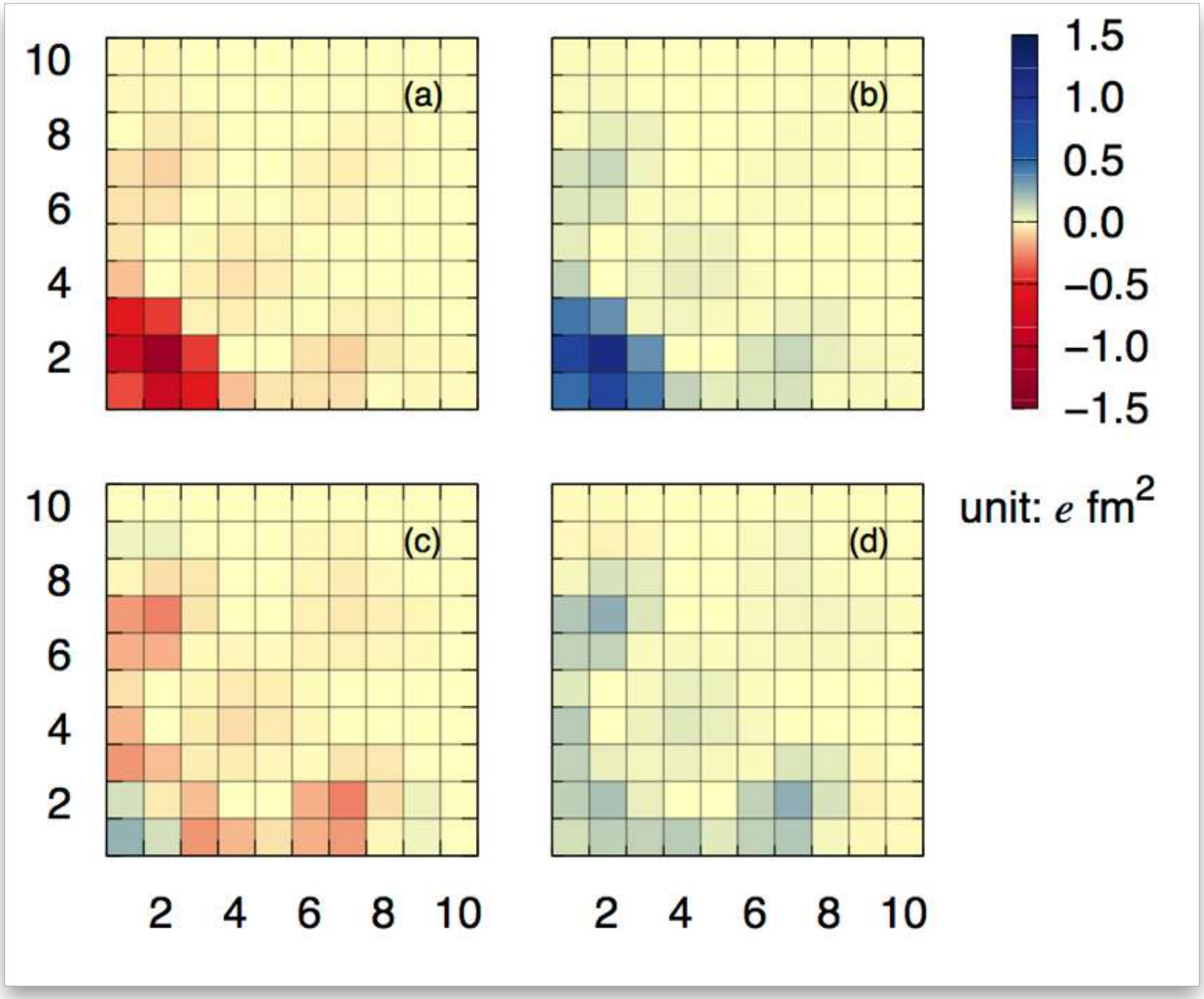


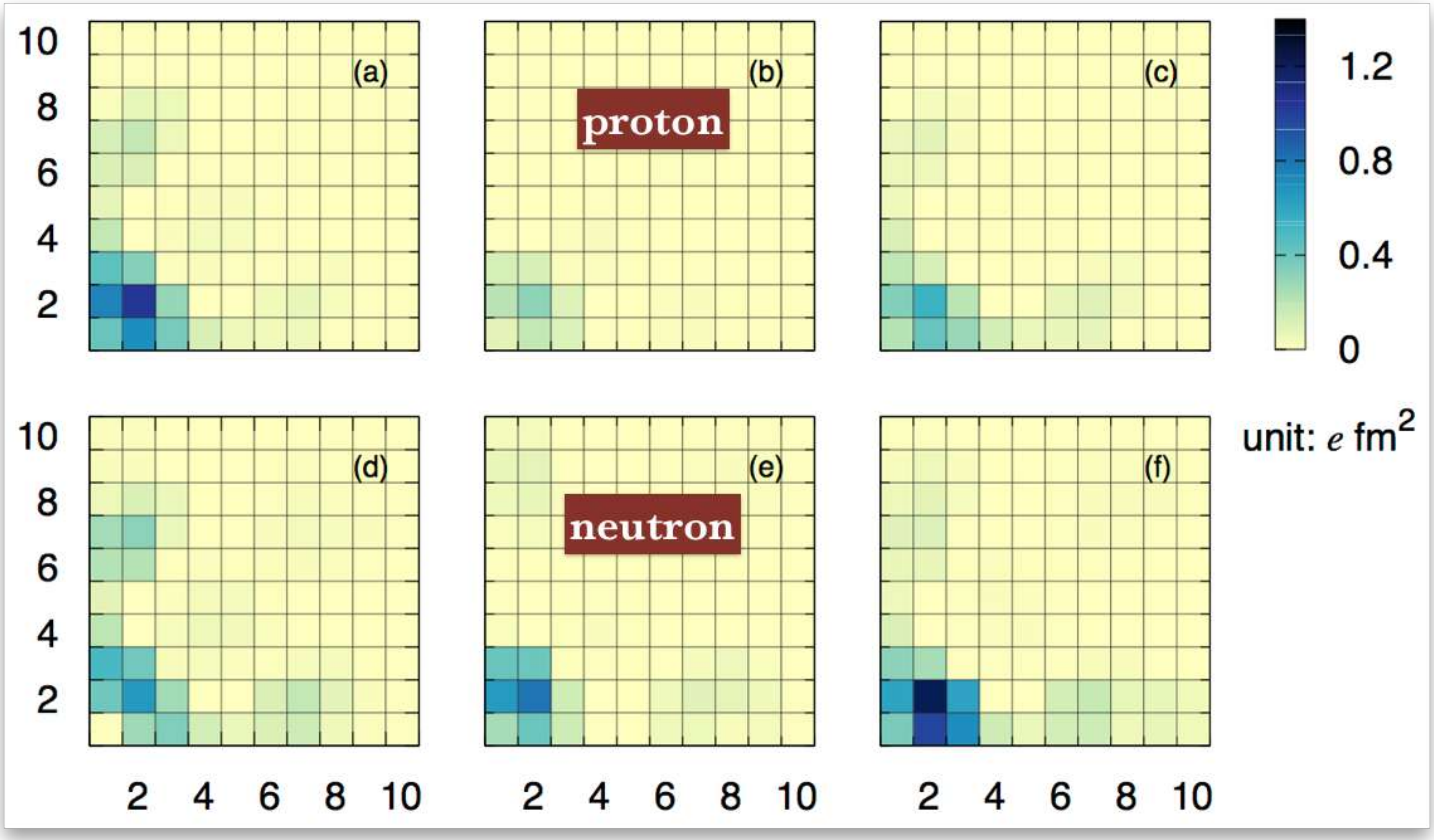
p shell dominant
Single particle

Average
collective

$0s1/2$, $0p3/2$, $0p1/2$, $0d5/2$, $0d3/2$, $1s1/2$, $0f7/2$, $0f5/2$, $1p3/2$ and $1p1/2$

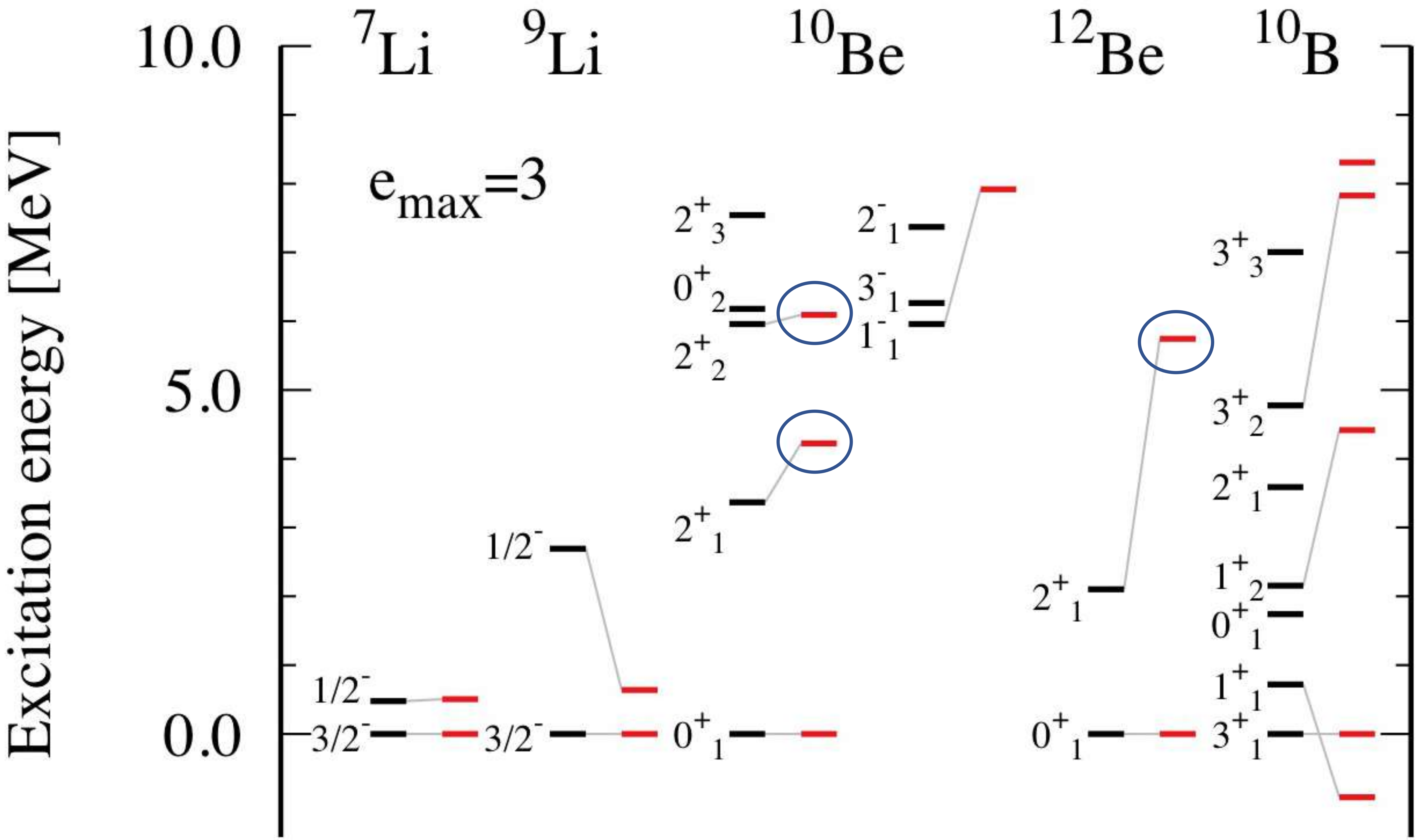
Contribution of Single Particle Orbit to E2

$\langle 0^+_1 \| Q_{k_\alpha, k_\beta} \| 2^+_1 \rangle$ $\langle 0^+_1 \| Q_{k_\alpha, k_\beta} \| 2^+_2 \rangle$ $\langle 2^+_1 \| Q_{k_\alpha, k_\beta} \| 2^+_2 \rangle$

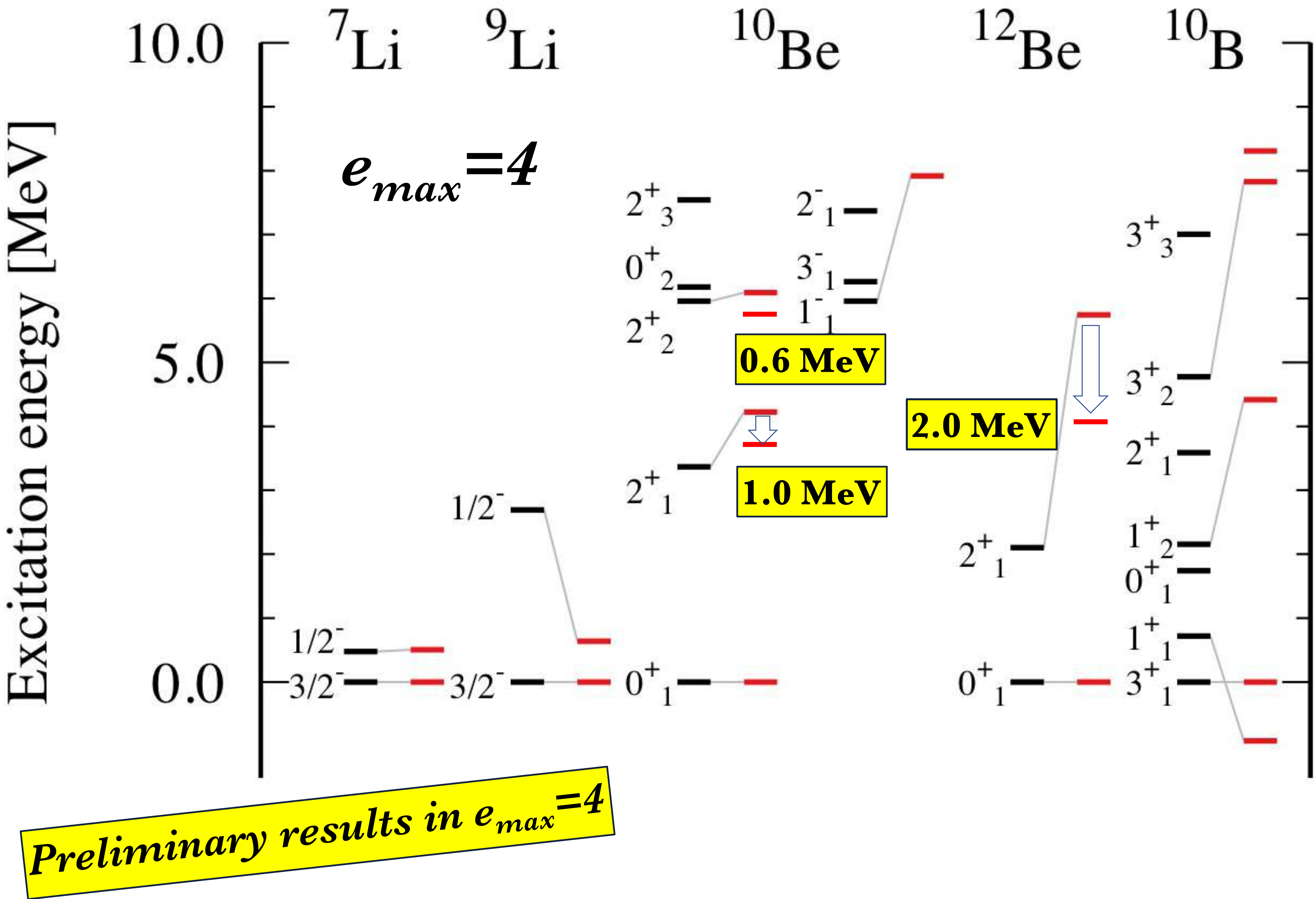


$0s1/2$, $0p3/2$, $0p1/2$, $0d5/2$, $0d3/2$, $1s1/2$, $0f7/2$, $0f5/2$, $1p3/2$ and $1p1/2$

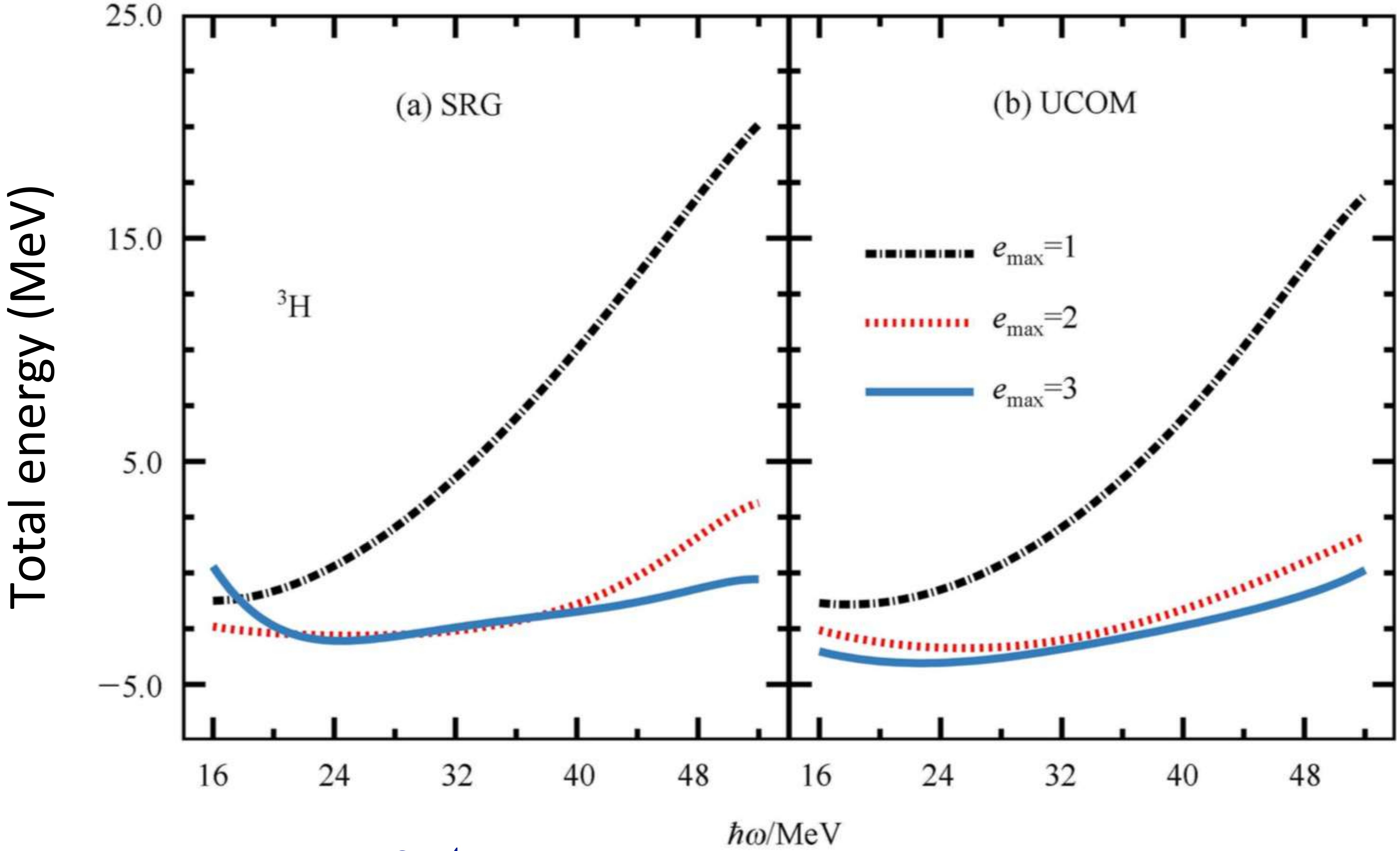
Low-lying Spectra for Light Nuclei



Low-lying Spectra for Light Nuclei



SRG vs UCOM



$\alpha = 0.02 \text{ fm}^4$

$\lambda = 2.66 \text{ fm}^{-1}$

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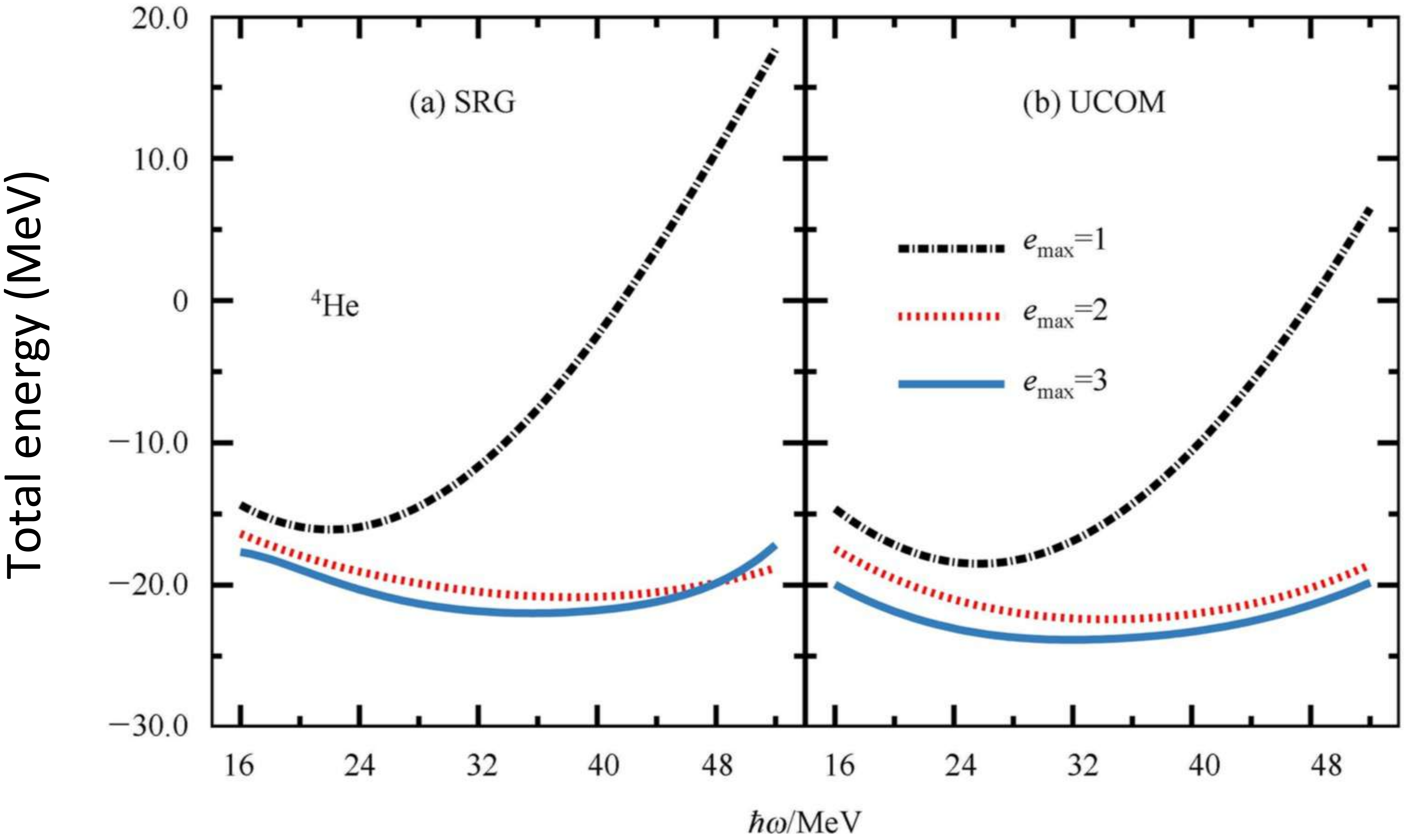
SRG vs UCOM



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Benchmark with shell model — ^{3}H

Model space: e_{max}=1 (2 major shells) **interaction: $V_{UCOM}(N^3LO)$**

^{3}H		E (MeV)	Occupation number					
			0s1/2	0p3/2	0p1/2	0s1/2	0p3/2	0p1/2
Shell model		-1.9019	0.9422	0.0167	0.0411	1.9172	0.0345	0.0482
MCSM	1	-1.8215	0.9431	0.0150	0.0420	1.9203	0.0315	0.0482
	2	-1.8230	0.9411	0.0162	0.0427	1.9164	0.0342	0.0494
	3	-1.8402	0.9421	0.0158	0.0421	1.9164	0.0345	0.0491
	4	-1.8939	0.9417	0.0163	0.0421	1.9179	0.0332	0.0489
	5	-1.8990	0.9425	0.0159	0.0416	1.9166	0.0341	0.0492
	6	-1.9000	0.9424	0.0164	0.0412	1.9166	0.0351	0.0482
	7	-1.9016	0.9423	0.0167	0.0410	1.9175	0.0344	0.0481
	8	-1.9016	0.9423	0.0167	0.0410	1.9175	0.0344	0.0481
	9	-1.9018	0.9422	0.0167	0.0411	1.9173	0.0345	0.0483
	10	-1.9019	0.9422	0.0167	0.0411	1.9172	0.0345	0.0482

Benchmark with shell model — ^{4}He

Model space: e_{max}=1 (2 major shells) **interaction:** V_{UCOM}(N^3LO)

^{4}He		E (MeV)	Occupation number					
			0s1/2	0p3/2	0p1/2	0s1/2	0p3/2	0p1/2
Shell model		-20.0399	1.9348	0.0180	0.0472	1.9348	0.0180	0.0472
MCSM	1	-19.5891	1.9518	0.0097	0.0385	1.9518	0.0097	0.0385
	2	-19.8433	1.9456	0.0140	0.0404	1.9456	0.0140	0.0404
	3	-20.0267	1.9378	0.0169	0.0453	1.9378	0.0169	0.0453
	4	-20.0378	1.9347	0.0179	0.0474	1.9347	0.0179	0.0474
	5	-20.0398	1.9345	0.0181	0.0474	1.9345	0.0181	0.0474
	6	-20.0398	1.9347	0.0181	0.0472	1.9347	0.0181	0.0472
	7	-20.0399	1.9349	0.0179	0.0472	1.9349	0.0179	0.0472
	8	-20.0399	1.9348	0.0180	0.0472	1.9348	0.0180	0.0472