Calculations for Finite Nuclei Using Low-Momentum NN Interactions

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Microscopic nuclear structure calculations

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Calculations that take all microscopic degrees of freedom of all nucleons constituting the atomic nucleus into account

$$H\Psi = (\sum_i T_i + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk})\Psi = E\Psi$$

Basic ingredients for our calculation:

- a “realistic” nucleon-nucleon potential V_{ij}
  - CD-Bonn
  - Nijmegen I,II,93
  - Argonne V18
  - chiral potentials
- (possibly) a three-body force V_{ijk}
  - Urbana IX
  - Illinois 1-5
  - chiral 3-body potentials

Nuclei whose properties can be calculated “exactly”:

- Deuteron
- ^{3}H, ^{3}He (Faddeev equations)
- ^{4}He (Faddeev-Yakubovsky equations)

... and what about nuclei with $A > 4$?

"Exact" methods cannot be applied: it is necessary to use a truncated and/or simplified scheme

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The calculations depend on a set of parameters $\{\alpha_i\}$ and on the dimension d of the truncated Hilbert space used to solve the Schrödinger equation

A “reliable” microscopic calculation is obtained when the results are stable when changing the parameters $\{\alpha_i\}$ in a reasonably large interval and increasing the dimension d of the reduced Hilbert space

The “reliability” of the calculation has to be tested solving the Schrödinger equation for those nuclear systems to which an “exact” approach can be applied and, if possible, reproducing the “exact” quantities

Current situation: in the last decade there has been a great progress concerning the computer technology

Models and techniques of microscopic calculations for many-body systems have been implemented in order to reach the extreme limits of their range of application

Perturbative approach

Such a scheme is very useful to calculate ground state properties of doubly closed-shell nuclei (e.g. ^{4}He, ^{16}O, ^{40}Ca, etc.). The basic idea is to introduce an auxiliary one-body potential U so that the hamiltonian can be written as

$$H = (T + U) + (V - U) = H_0 + H_1$$

H_0 describes the nucleus as a system of independent nucleons moving in a mean field U, that could be, for example, the self-consistent Hartree-Fock potential

H_1 is the residual interaction to be treated perturbatively

The Hartree-Fock potential

$$H = \sum_{\alpha,\beta} T_{\alpha\beta} a^\dagger_\alpha a_\beta + \frac{1}{2} \sum_{\alpha,\beta,\gamma,\delta} V_{\alpha\beta\gamma\delta} a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma$$

Hartree-Fock theory: the ground state wave function is represented by a single Slater determinant $|\Phi\rangle$

$$|\Phi\rangle = \prod_{\mu=1}^{A} a^\dagger_\mu |0\rangle; \qquad |0\rangle \ \text{vacuum state}$$

The "best" $|\Phi\rangle$ is the one corresponding to a minimum of $\langle E \rangle$

$$\delta \langle \Phi | H | \Phi \rangle = 0$$

The Hartree-Fock potential

The variational constraint is

$$\langle \delta\Phi | H | \Phi \rangle = 0$$

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$$|\delta\Phi\rangle = \eta a^\dagger_\sigma a_\lambda |\Phi\rangle$$

Now, the variational constraint can be written as

$$\langle \Phi | a^\dagger_\lambda a_\sigma H | \Phi \rangle = 0$$

The Hartree-Fock potential

The secular equation is solved by an iterative procedure

$$T_{\alpha\beta} + \sum_{\mu=1}^{A} V_{\alpha\mu\beta\mu} = \epsilon_\alpha \delta_{\alpha\beta}$$

Hartree-Fock self-consistent one-body potential

The Hartree-Fock potential

Problem: realistic NN potential contain a strongly repulsive short-range component

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the matrix elements of V_{NN} cannot be used directly in nuclear structure calculations

Solution: theory of the Brueckner reaction matrix – Brueckner-Hartree-Fock approach

B. D. Day, Rev. Mod. Phys. **39**, *719 (1967)*

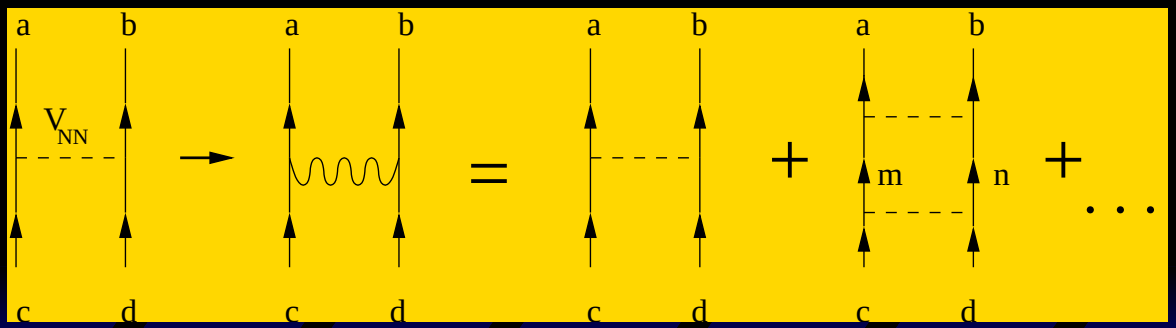
The Brueckner reaction matrix

$$\langle ab|G|cd\rangle = \langle ab|V|cd\rangle + \sum_{m,n}\langle ab|V|mn\rangle \frac{1}{\epsilon_c + \epsilon_d - \epsilon_m - \epsilon_n}\langle mn|G|cd\rangle$$

In operatorial form:

$$G(\omega) = V_{NN} + V_{NN}Q\frac{1}{\omega - H_0}QG(\omega)$$ Bethe-Goldstone equation

Q (Pauli operator) projects the intermediate states above the Fermi surface



The Brueckner reaction matrix

Main shortcoming: the Brueckner reaction matrix G is dependent by ω, that is the energy of the free nucleons for $t = -\infty$

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the BHF one-body potential for those states above the Fermi surface is not uniquely defined

One needs to renormalize V_{NN} more efficiently

Low-momentum NN potentials

The deuteron case:

In the full space:

$$\langle k|(T+V_{NN})|k'\rangle\langle k'|\Psi_n\rangle = E_n\langle k|\Psi_n\rangle \qquad 0 < k, k' < \infty$$

In a reduced model space $P = \sum_{k<\Lambda} |k\rangle\langle k|$

$$\langle k|(T+V_{\rm eff})|k'\rangle\langle k'|\Phi_m\rangle = \tilde{E}_m\langle k|\Phi_m\rangle \qquad 0 < k, k' < \Lambda$$

Fundamental constraint: $\tilde{E}_m \in \{E_n\}$

How to calculate $\langle k|H_{\rm eff}|k'\rangle$?

Andreozzi-Lee-Suzuki method

We are looking for an operator Ω, whose inverse Ω^{-1} exists, so that the the eigenvalues of the transformed matrix

$$\mathcal{H} = \Omega^{-1} H \Omega \quad ,$$

belong to the set of eigenvalues of H.

Andreozzi-Lee-Suzuki method

In order to switch the eigenvalue problem in the full space into two separate eigenproblems (P-space and Q-space), we require that

$$Q\mathcal{H}P = 0 \qquad \text{decoupling condition}$$

As supplementary conditions on Ω (without any loss of generality), we choose:

$$P\Omega P = I_p, \quad P\Omega Q = 0$$
$$Q\Omega P = \omega, \quad Q\Omega Q = I_q$$

Andreozzi-Lee-Suzuki method

Finally, the decoupling equation is:

$$\omega PHQ\omega + \omega PHP - QHQ\omega - QHP = 0$$

to solve it:

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iterative techniques: Lee-Suzuki and Krenciglowa-Kuo

Deuteron binding energy

CD-BONN POTENTIAL

Λ (in fm^{-1})	$PV_{\mathrm{eff}}P$ (in MeV)	V_{NN} (in MeV)
1.6	-2.225	-2.225
1.8	-2.225	
2.0	-2.225	
2.2	-2.225	

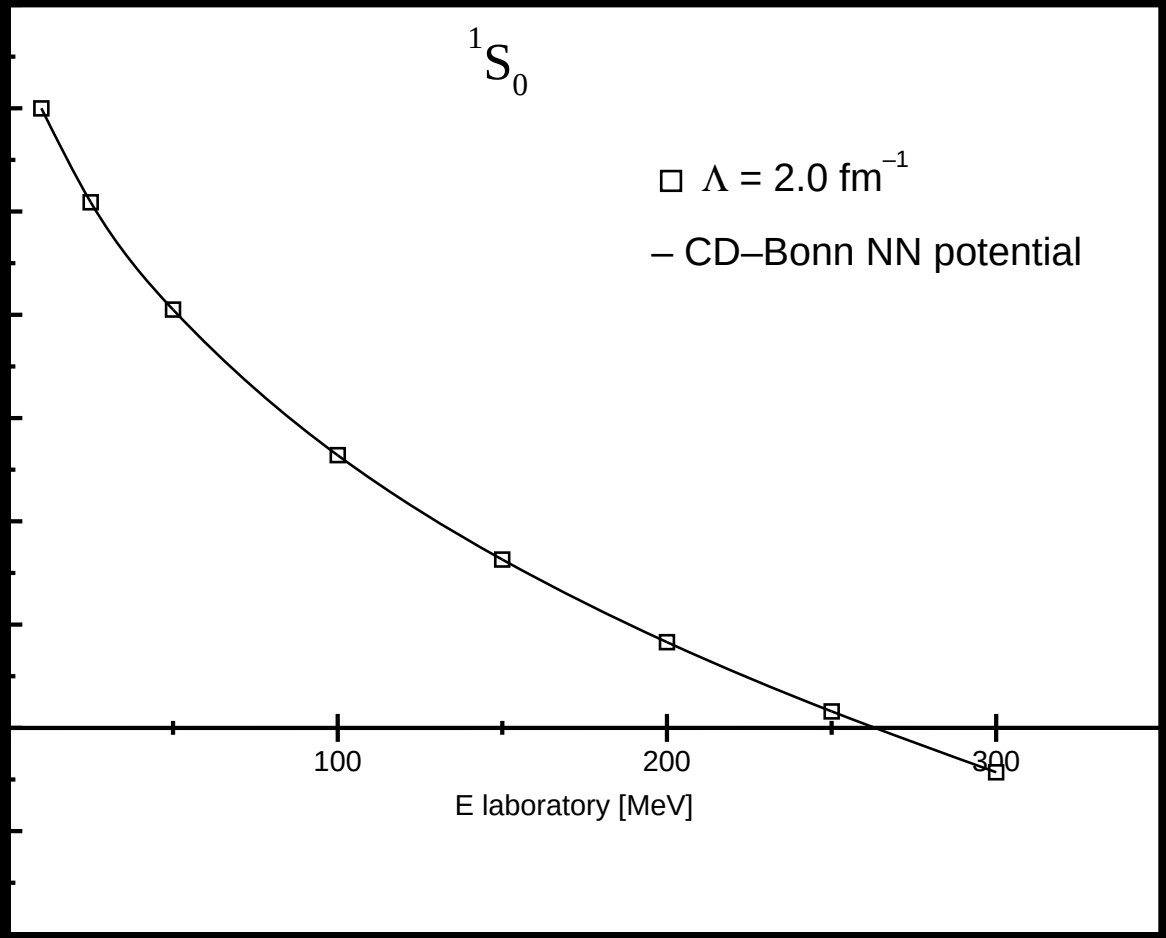
Phase shifts calculations

Lipmann-Schwinger equation

$$\langle p'|T(\epsilon_p)|p\rangle = \langle p'|V_{NN}|p\rangle + \int_0^\infty k^2 dk \frac{\langle p'|V_{NN}|k\rangle\langle k|T(\epsilon_p)|p\rangle}{\epsilon_p - \epsilon_k}$$

$$\langle p'|T_{\rm eff}(\epsilon_p)|p\rangle = \langle p'|V_{\rm eff}|p\rangle + \int_0^\Lambda k^2 dk \frac{\langle p'|V_{\rm eff}|k\rangle\langle k|T_{\rm eff}(\epsilon_p)|p\rangle}{\epsilon_p - \epsilon_k}$$

Low-momentum NN potentials



Low-momentum NN potentials

$^1S_0$ channel phase shifts (in degrees)

$E_{\rm lab}$ (MeV)	CD-Bonn	$V_{\rm low-k}$	Expt.
1	62.1	62.1	62.1
10	60.0	60.0	60.0
25	50.9	50.9	50.9
50	40.5	40.5	40.5
100	26.4	26.4	26.8
150	16.3	16.3	16.9
200	8.3	8.3	8.9
250	1.6	1.6	2.0
300	-4.3	-4.3	-4.5

G matrix *vs* $\mathrm{V}_{\mathrm{low-k}}$

G matrix

- Energy dependent
- No direct connection to the original NN potential

$\mathrm{V}_{\mathrm{low-k}}$

- No energy dependence
- In the k-space it reproduces all the two-body system data – it is a real effective potential

Cut-off momentum Λ

General criterion

- small enough so to give a reasonably smooth potential suitable to be used directly in a perturbative scheme
- large enough so that $V_{\mathrm{low-k}}$ reproduces the same phase-shifts of the original V_{NN} up to the anelastic threshold ($E_{lab} \simeq 350$ MeV)

$$E_{lab} \leq 2\hbar^2\Lambda^2/M \rightarrow \Lambda \simeq 2.0\mathrm{fm}^{-1}$$

Cut-off momentum Λ

Is there any chance to map the k-space cutoff Λ onto the boundary in r-space ?

Λ = boundary in the momentum space

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boundary in harmonic oscillator r-space

Cut-off momentum Λ

To a given Λ value corresponds a maximum value of relative motion energy of the two-nucleon system:

$$E_{\max} = \frac{\hbar^2 \Lambda^2}{M}$$

In the harmonic oscillator representation:

$$E_{\max} = (2n + l + \frac{3}{2})\hbar\omega = (N_{\max} + \frac{3}{2})\hbar\omega$$

Fixing $\hbar\omega$ and truncating the two-body configurations to those with a maximum energy $E_{\max}$

$$\Lambda = \sqrt{\frac{M\omega}{\hbar}\left(N_{max} + \frac{3}{2}\right)}$$

Applications

Doubly closed-shell nuclei

- Binding energies and rms

We have to solve $H\Psi = E\Psi$ where

$$H = T + V = (T + U) + (V - U) = H_0 + H_1$$

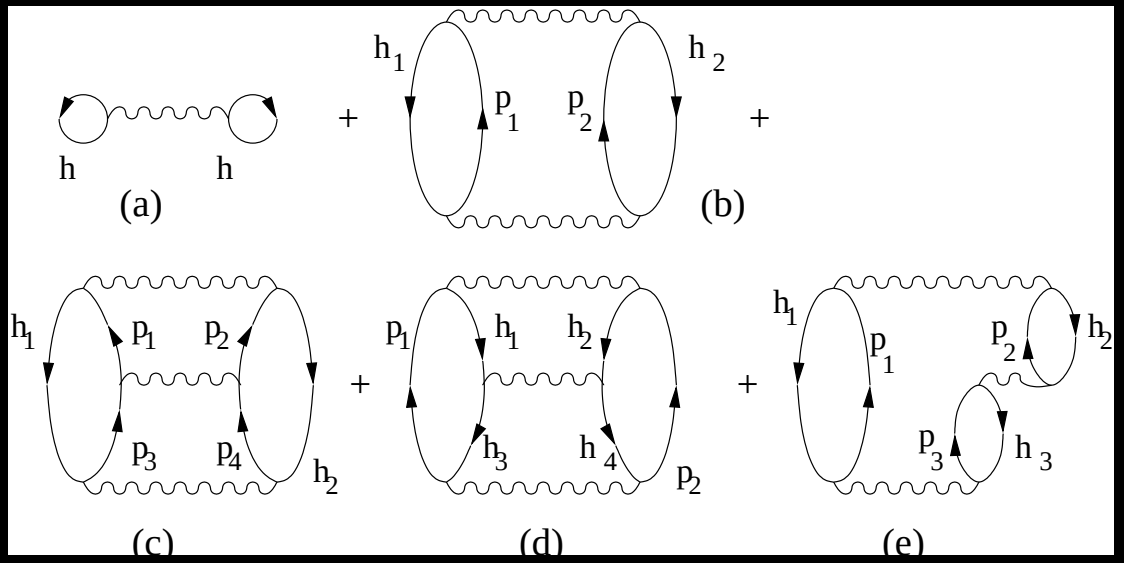
auxiliary potential

- Perturbative expansion

Goldstone expansion

The energy of a many-body system is given by the sum of all connected linked diagrams

$E - E_0 =$



unperturbed energy

Hartree-Fock expansion

We expand the HF SP states $|\alpha\rangle$ in terms of oscillator wave functions $|\mu\rangle$ (restricted HF)

$$|\alpha\rangle = \sum_{\mu} C_{\mu}^{\alpha} |\mu\rangle \quad ,$$

C_{μ}^{α} are determined by solving self–consistently the HF equations

$$\sum_{\mu'} \langle \mu | t + U | \mu' \rangle C_{\mu'}^{\alpha} = \epsilon_{\alpha} C_{\mu}^{\alpha} \quad ,$$

with

$$\langle \mu | U | \mu' \rangle = \sum_{\alpha_h} \langle \mu \alpha_h | V_{\mathrm{low-k}} | \mu' \alpha_h \rangle \quad ,$$

Center-of-mass correction

We remove the spurious center-of-mass kinetic energy writing the kinetic energy operator T as

$$T = \frac{1}{2Am} \sum_{i<j} (\mathbf{p}_i - \mathbf{p}_j)^2$$

So, the hamiltonian can be re-written as

$$H = \left(1 - \frac{1}{A}\right) \sum_{i=1}^{A} \frac{p_i^2}{2m} + \sum_{i<j} \left(V_{ij} - \frac{\mathbf{p}_i \cdot \mathbf{p}_j}{mA}\right)$$

$\Lambda = 2.1$ fm^{-1} **results**

^{4}He

Binding energy	V_{NN}	HF+2nd+3rd	Exact
	N^{3}LO	26.440	25.410
	CD Bonn	27.799	26.26
	Nijmegen II	27.523	24.56
	AV18	27.409	24.28

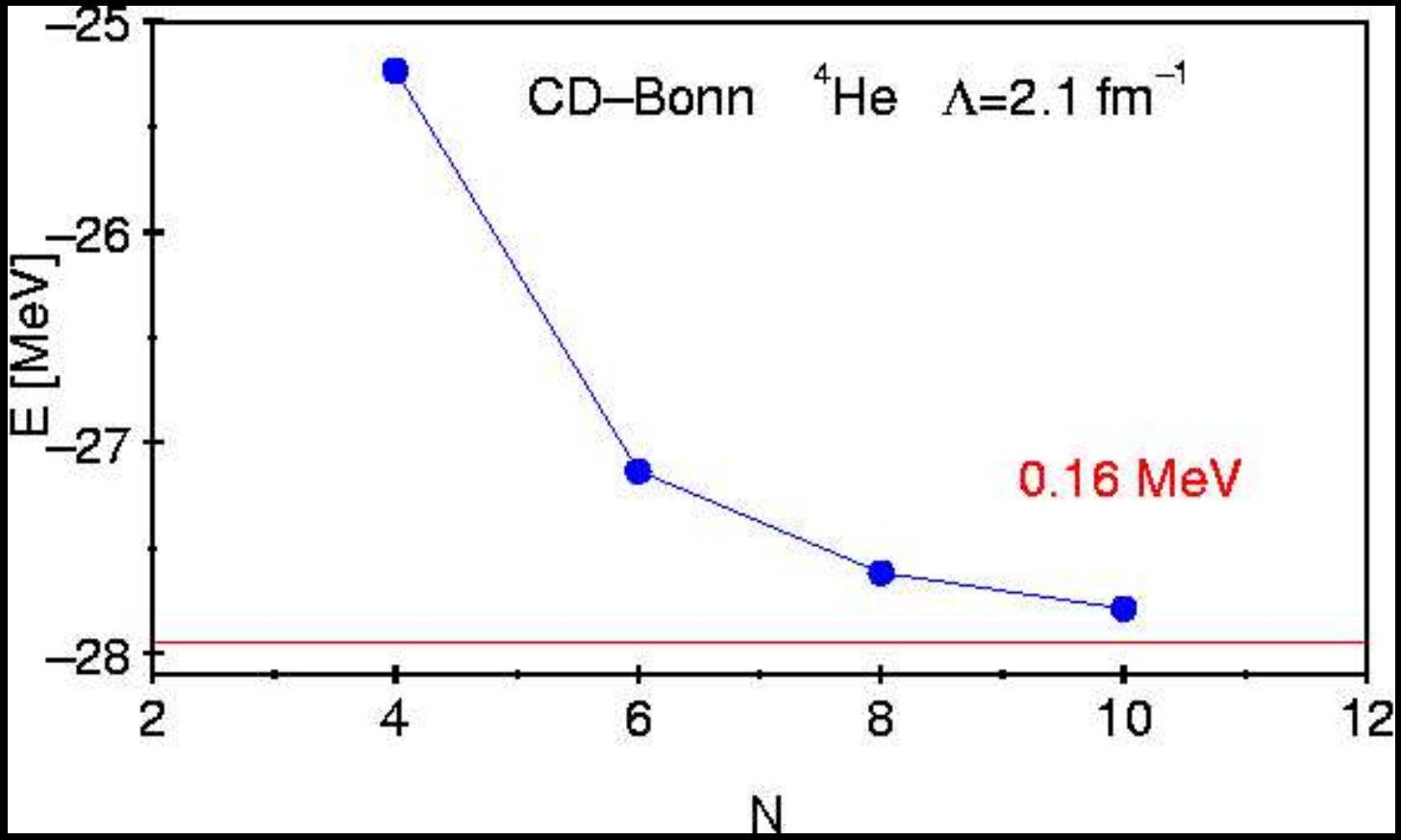
^{16}O

Binding energy	V_{NN}	HF+2nd+3rd	Expt.
	N^{3}LO	129.734	127.619
	CD Bonn	132.838	
	Nijmegen II	132.138	
	AV18	132.166	

^{40}Ca

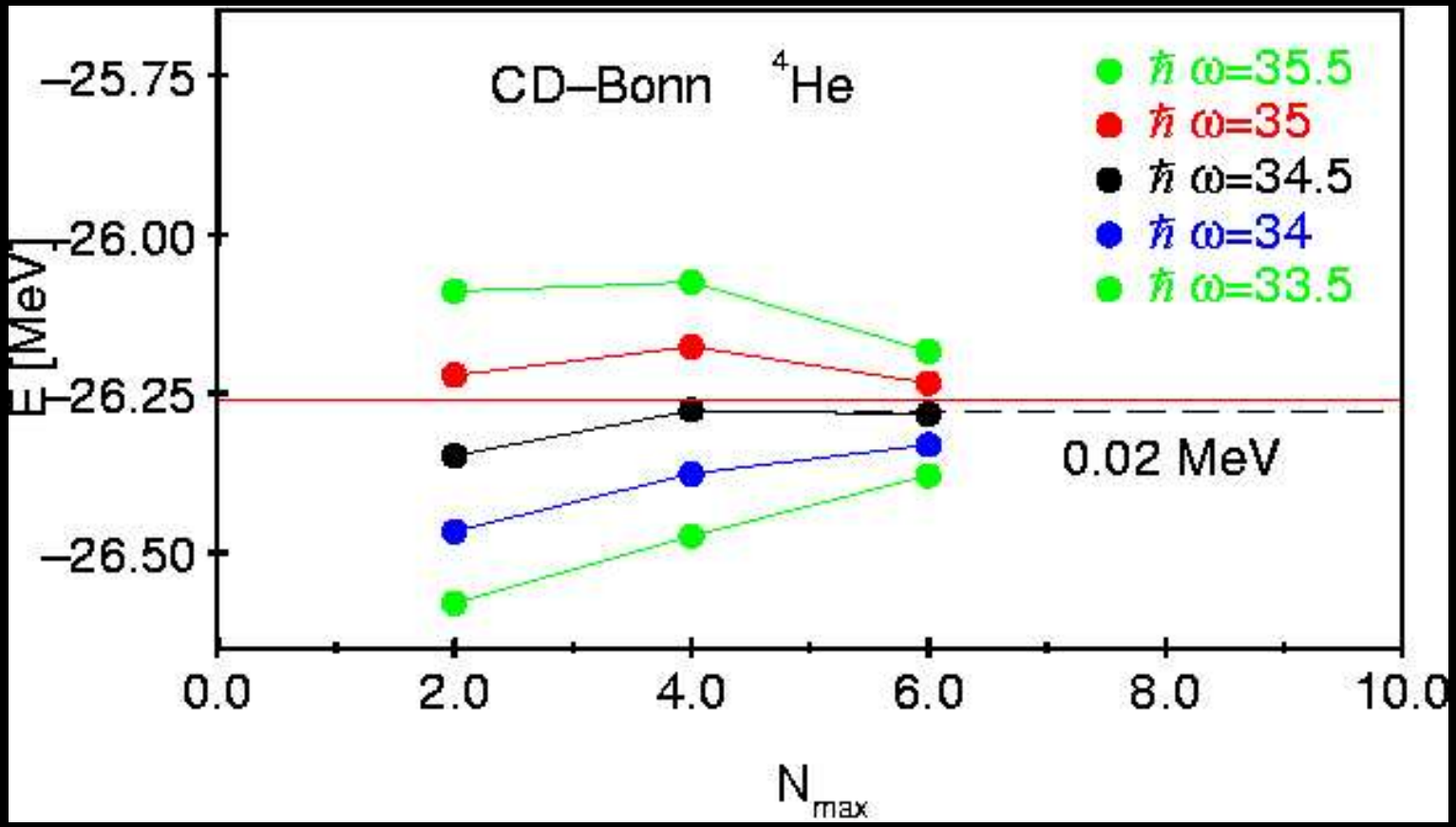
Binding energy	V_{NN}	HF+2nd+3rd	Expt.
	N^{3}LO	379.957	342.052
	CD Bonn	397.063	
	Nijmegen II	386.588	
	AV18	381.347	

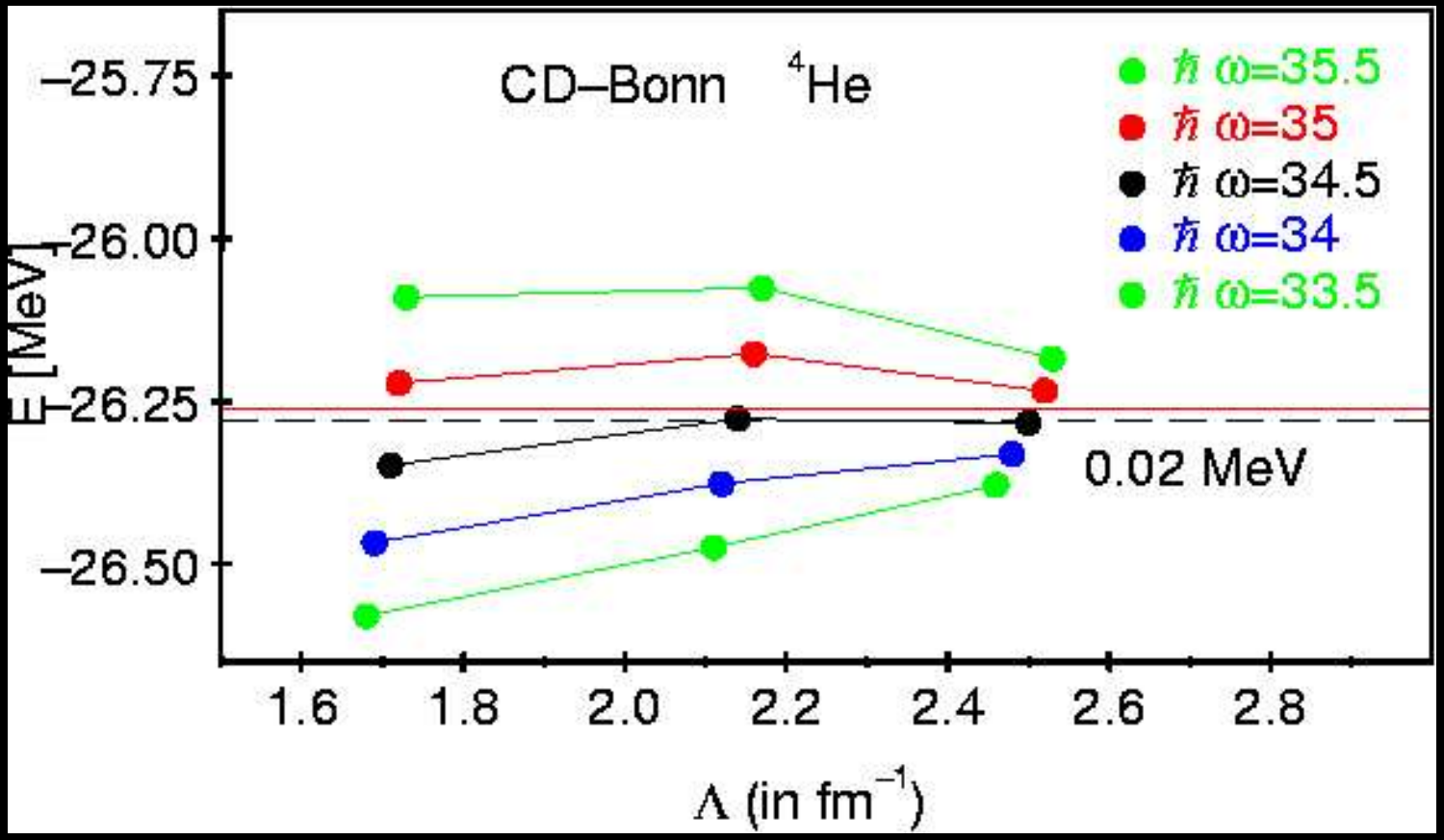
L. Coraggio, A. Covello, A. Gargano, N. Itaco, T. T. S. Kuo, and R. Machleidt, Phys. Rev. C **71**, *014307 (2005)*

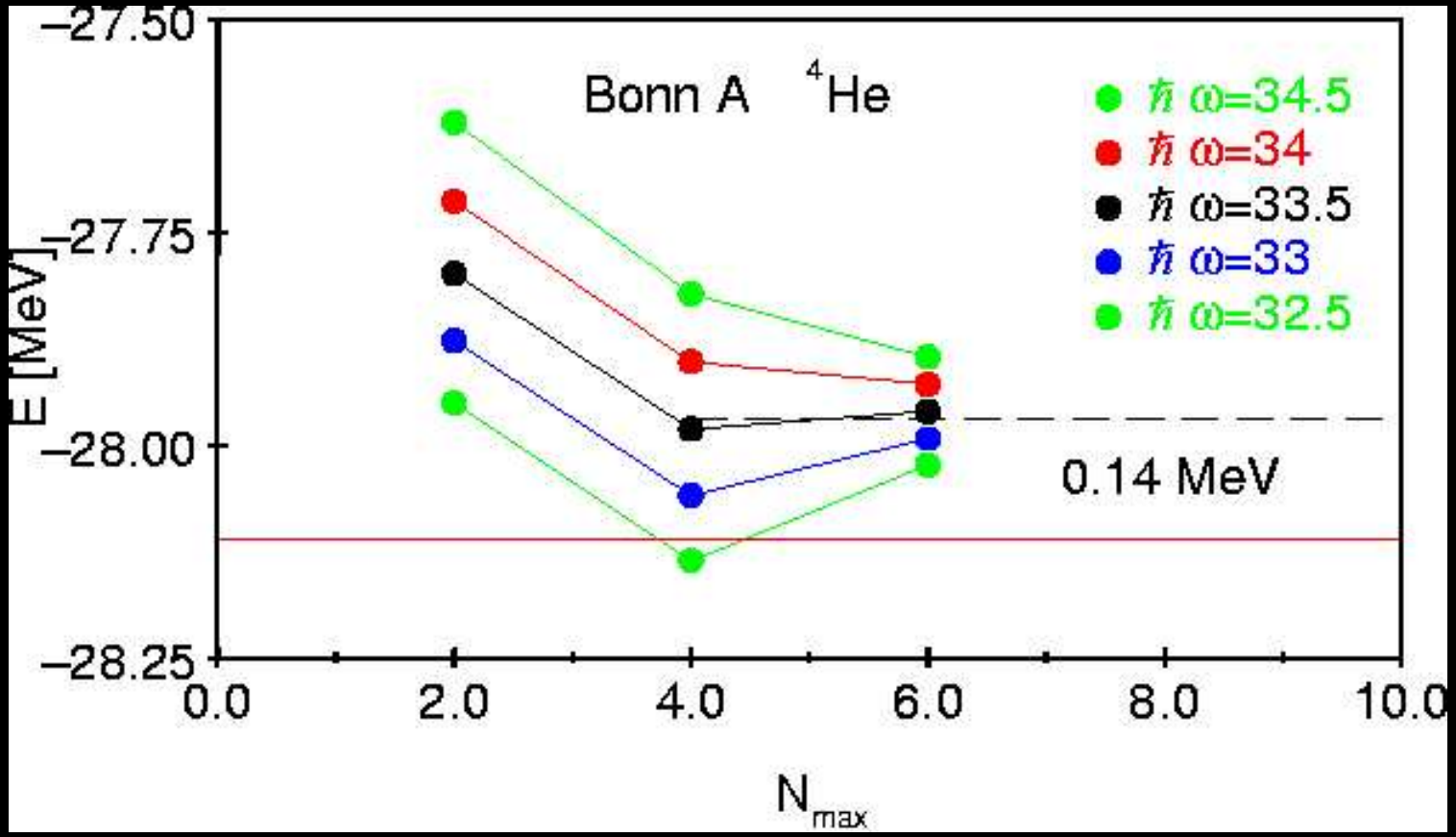


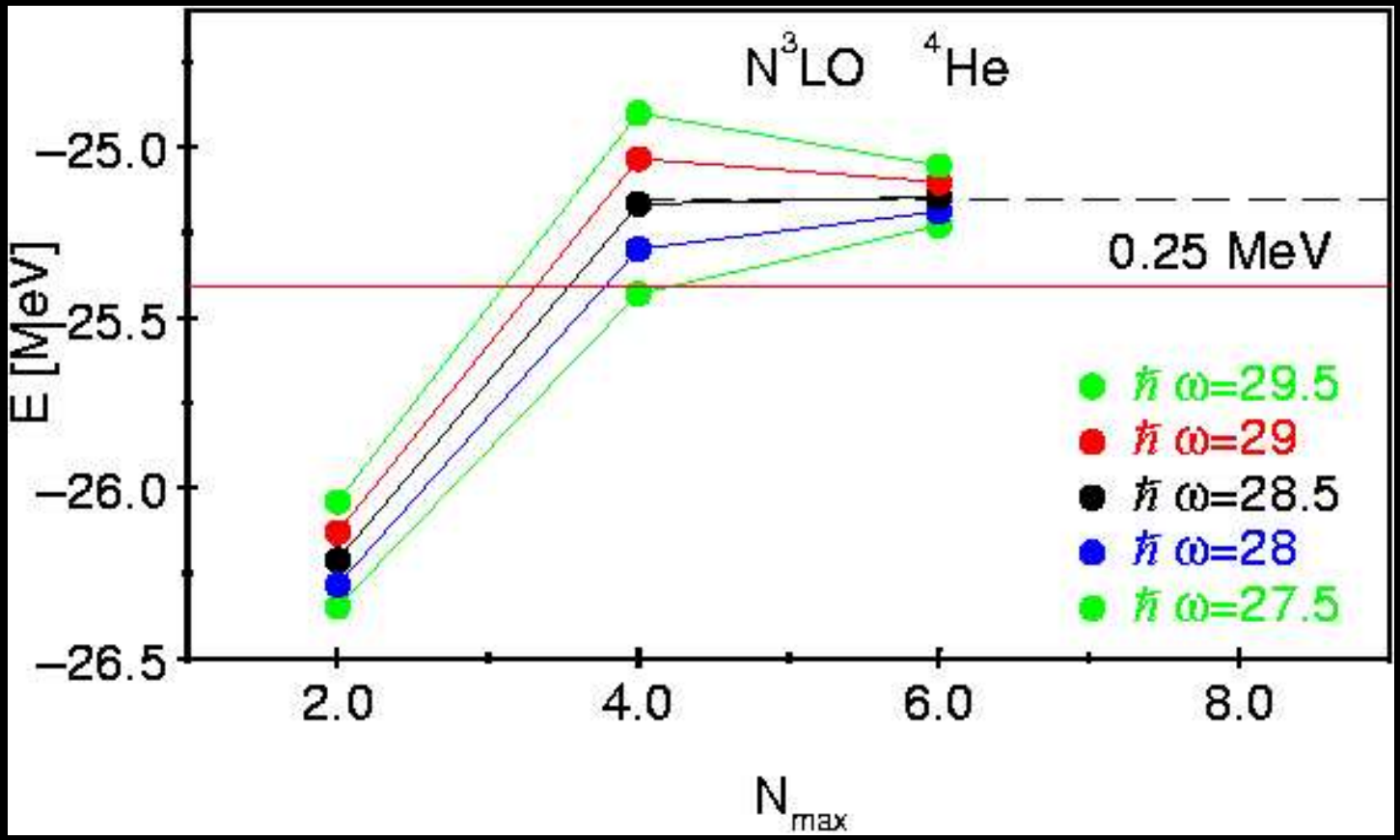
Exact calculation by M. Viviani; *see M. Viviani, A. Kievsky, and S. Rosati, Phys. Rev. C* **71**, *024006 (2005)*

^{4}He binding energy

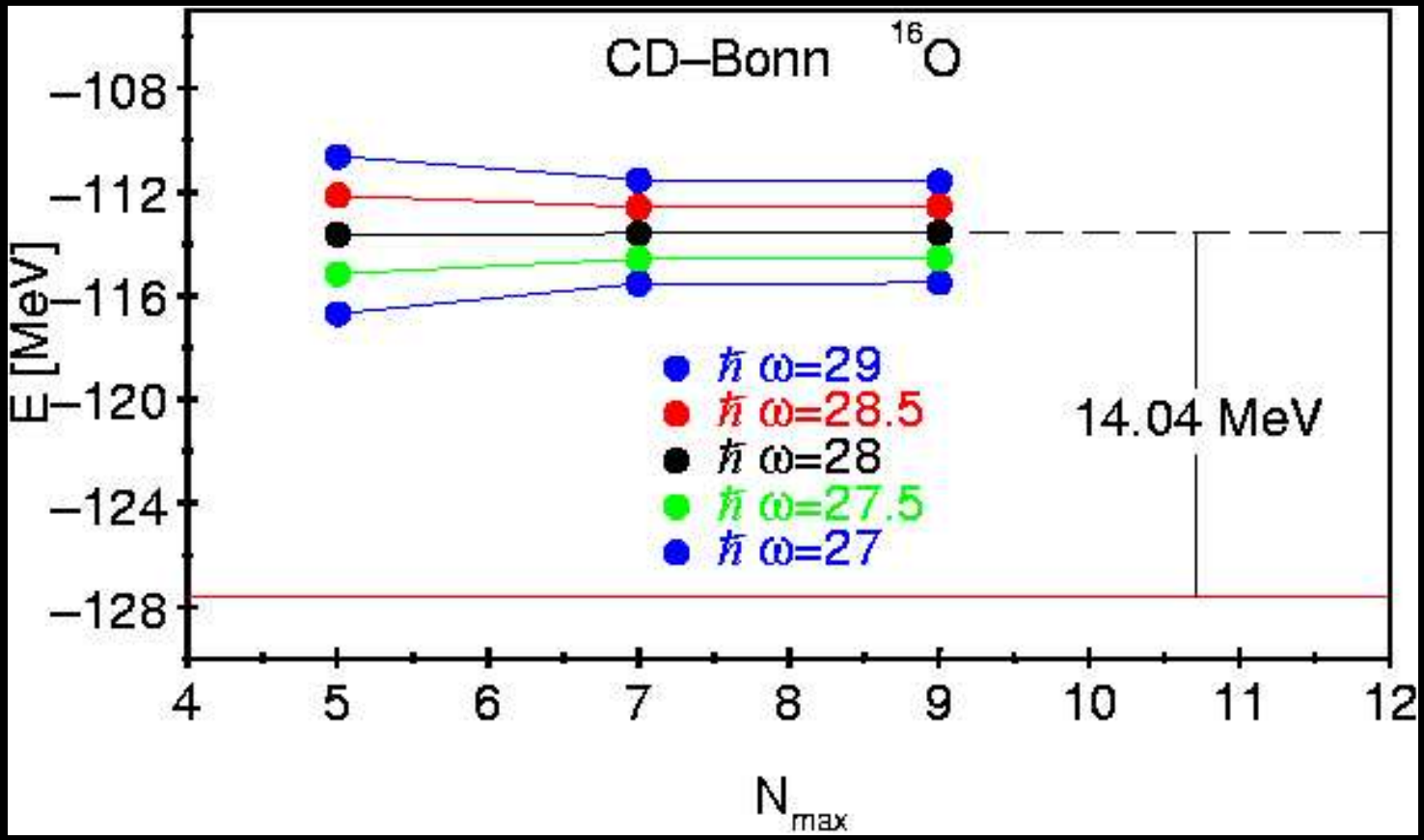

CD–Bonn
^{4}He
ħω=35.5
ħω=35
ħω=34.5
ħω=34
ħω=33.5
0.02 MeV
E [MeV]
–25.75
–26.00
–26.25
–26.50
0.0
2.0
4.0
6.0
8.0
10.0
N$_{max}$

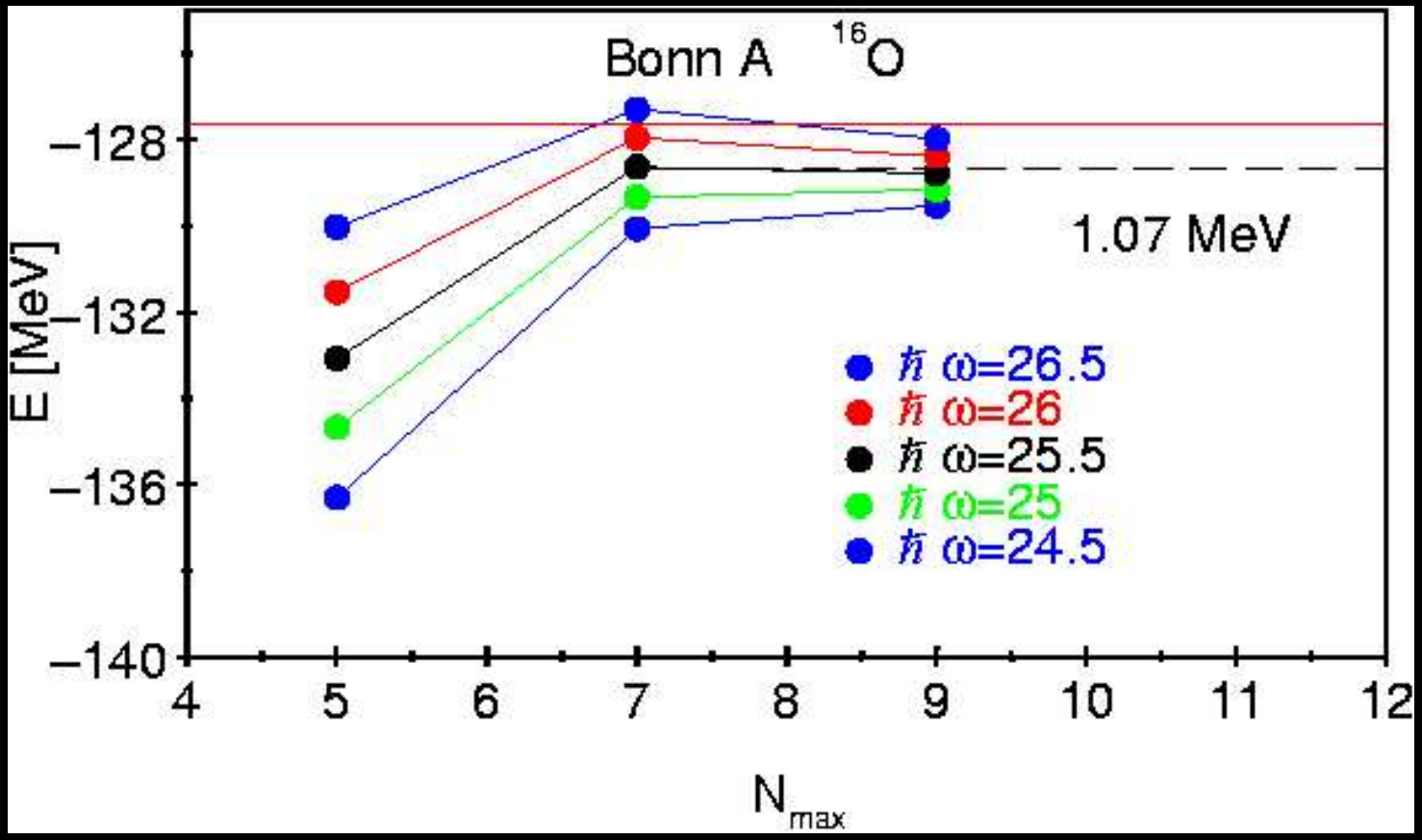

CD–Bonn ^{4}He
$\hbar\omega$=35.5
$\hbar\omega$=35
$\hbar\omega$=34.5
$\hbar\omega$=34
$\hbar\omega$=33.5
0.02 MeV
E [MeV]
–25.75
–26.00
–26.25
–26.50
1.6
1.8
2.0
2.2
2.4
2.6
2.8
Λ (in fm^{-1})

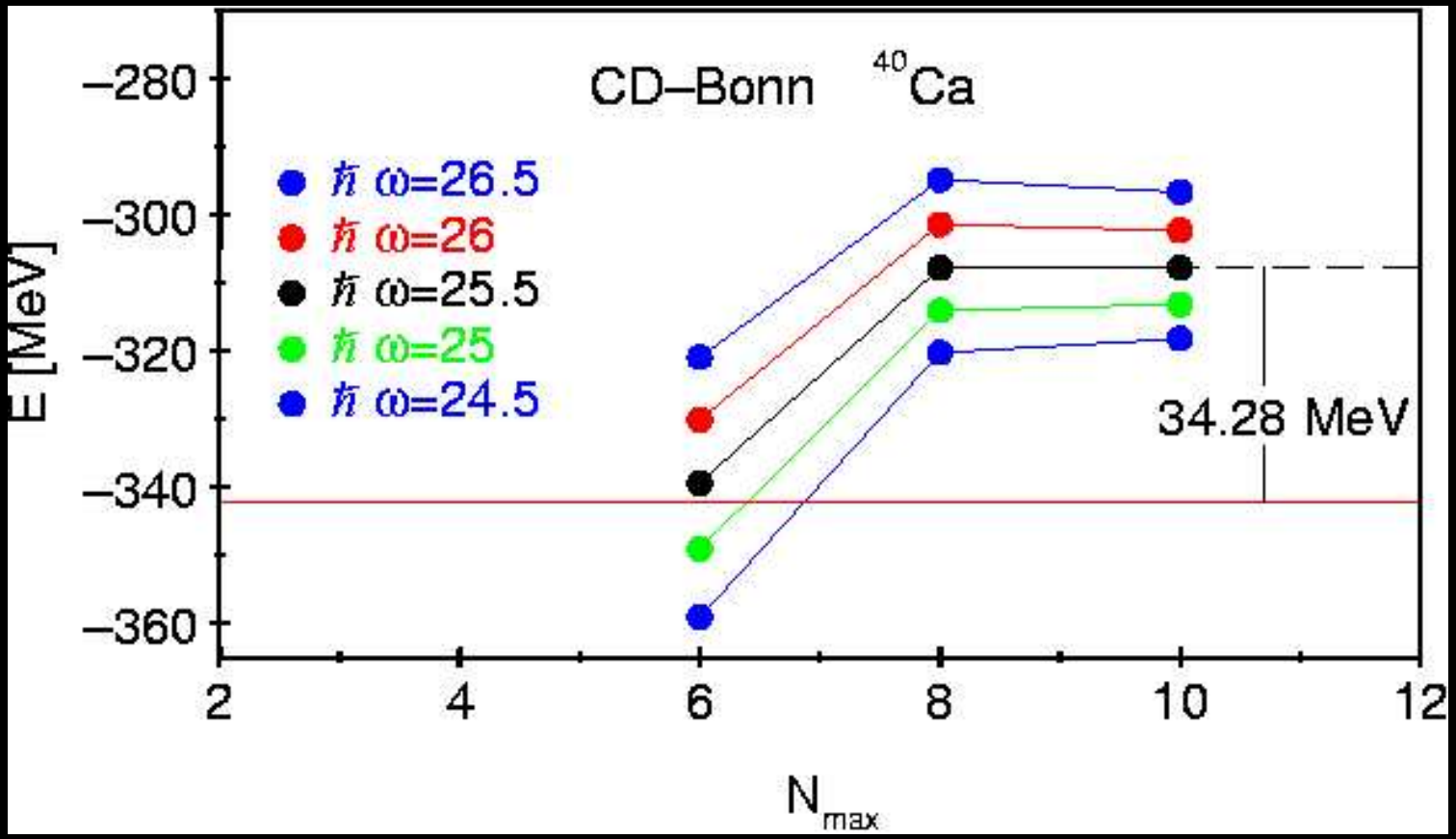

Bonn A
4He
ħω=34.5
ħω=34
ħω=33.5
ħω=33
ħω=32.5
0.14 MeV
E [MeV]
−27.50
−27.75
−28.00
−28.25
0.0
2.0
4.0
6.0
8.0
10.0
Nmax


N3LO 4He
−25.0
−25.5
−26.0
−26.5
E [MeV]
0.25 MeV
ħω=29.5
ħω=29
ħω=28.5
ħω=28
ħω=27.5
2.0
4.0
6.0
8.0
Nmax

^{16}O and ^{40}Ca binding energies


CD–Bonn
16O
–108
–112
–116
–120
–124
–128
E [MeV]
ħω=29
ħω=28.5
ħω=28
ħω=27.5
ħω=27
14.04 MeV
4
5
6
7
8
9
10
11
12
Nmax


Bonn A
16O
−128
−132
−136
−140
E [MeV]
1.07 MeV
ħω=26.5
ħω=26
ħω=25.5
ħω=25
ħω=24.5
4
5
6
7
8
9
10
11
12
Nmax


CD–Bonn
40Ca
ħω=26.5
ħω=26
ħω=25.5
ħω=25
ħω=24.5
34.28 MeV
E [MeV]
–280
–300
–320
–340
–360
2
4
6
8
10
12
Nmax

Perspectives

- Approaching heavier-mass nuclei
- Introduce three-body forces
- Calculations for open-shell nuclei

Collaboration

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