The No-Core Shell Model with a Twist

NCSM collaboration:

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Iowa State University: James P. Vary
San Diego State University: Calvin W. Johnson

Problem

The many-body Schrodinger Equation:

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

$$H_{int} = \frac{1}{A}\sum_{ij}\frac{(\vec{p}_i - \vec{p}_j)^2}{2m} + \sum_{i>j} V_{ij}^{NN} + \sum_{i>j>k} V_{ijk}^{NNN} + \ldots$$

- realistic, high precision two-body potentials: Argonne, CD Bonn
- theoretical three-body forces: TM'

Additional Ingredient: Center of Mass Motion

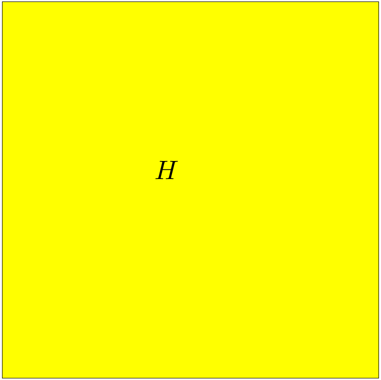
Addition of CM Hamiltonian

$$H \to H + \frac{1}{2mA} P_{CM}^2 + \frac{1}{2} m A \Omega^2 R_{CM}^2$$

- no influence on the intrinsic properties
- binds the nucleon clusters
- removed from the final results

Effective Operators

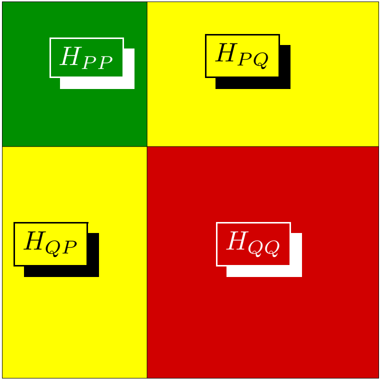
Start with the full space and the bare Hamiltonian H



Effective Operators

Space truncation

EFFECTIVE INTERACTIONS NECESSARY



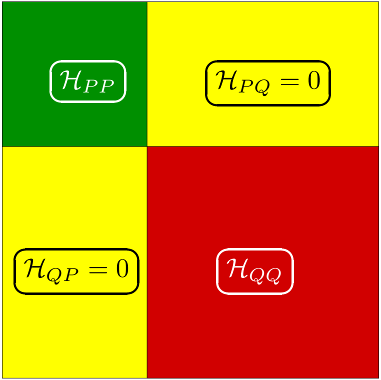
Effective Operators

Unitary Transformation

$$\mathcal{H} = e^{-S} H e^{S}$$

$$S = \operatorname{arctanh}\left(\omega^{\dagger} - \omega\right)$$

$$\omega = Q \omega P$$



Transformed Operators

Effective Hamiltonian in the model space

$$H_{eff} = \frac{P + \omega^\dagger}{\sqrt{P + \omega^\dagger \omega}} H \frac{P + \omega}{\sqrt{P + \omega^\dagger \omega}}$$

$$H_{eff} P|\Psi_k\rangle = E_k P|\Psi_k\rangle \text{ for } k = 1, ..., d$$

$$H|\Psi_k\rangle = E_k|\Psi_k\rangle \text{ for } k = 1, ..., d, ...\infty$$

Effective general operator in the model space

$$O_{eff} = \frac{P + \omega^\dagger}{\sqrt{P + \omega^\dagger \omega}} O \frac{P + \omega}{\sqrt{P + \omega^\dagger \omega}}$$

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Formal Solution for ω

$$Q|\Psi_k\rangle = Q\omega P|\Psi_k\rangle \text{ for } k = 1, \ldots, d$$

$$\langle\alpha_Q^{(i)}|\Psi_k\rangle = \sum_{j=1}^{d}\langle\alpha_Q^{(i)}|\omega|\alpha_P^{(j)}\rangle\langle\alpha_P^{(j)}|\Psi_k\rangle$$

$$\text{for } k = 1, \ldots, d \text{ and } i = d+1, \ldots, \infty$$

$$\langle\alpha_Q^{(i)}|\omega|\alpha_P^{(j)}\rangle = \sum_{k=1}^{d}\langle\alpha_Q^{(i)}|\Psi_k\rangle\langle\alpha_P^{(j)}|\tilde{\Psi}_k\rangle$$

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Cluster Approximation

- Find ω for $a < A$ (reproduce lowest eigenvalues)
- Compute $H_{eff}^{(a)}$
- Use $V_{eff}^{(a)}$ in the A-body calculation
- Scan for convergence (independence upon the model space and harmonic oscillator frequency).

Convergence to the exact solution if:

- $a \rightarrow A$ for fixed model space;
- $P \rightarrow \infty$ for fixed cluster.

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Cluster Approximation

Two-body cluster

$$S \approx \sum_{i>j=1}^{A} S_{ij}$$

$$PO_{eff}P = P \sum_{i>j=1}^{A} \left[e^{-S_{ij}} \left(O_i + O_j\right) e^{S_{ij}} - \left(O_i + O_j\right) \right] P$$

$$PO_{eff}P = P \sum_{i>j=1}^{A} e^{-S_{ij}} O_{ij} e^{S_{ij}} P$$

$$PH_{eff}P = P \sum_{i=1}^{A} h_i P + P \left[e^{-S_{ij}} \left(h_i + h_j + v_{ij}\right) e^{S_{ij}} - h_i - h_j \right] P$$

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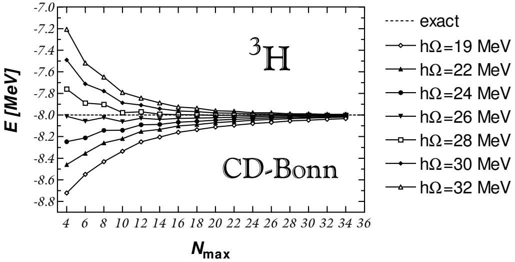
Two-body Cluster: Illustration



Navratil, Kamuntavicius, Barrett, Phys. Rev. C61 (2000) 044001

- Short range correlations included in $V_{eff}^{(2)}$
- Long-range and many-body correlations accomodated by increasing the model space

Summary

Advantages

- Preserve all the symmetries, including the translational invariance
- Flexible enough to handle both local and non-local interactions
- Suitable for light and medium nuclei
- Can accomodate three- (and soon four-) body forces

Disadvantages and Limitations

- Bad asymptotics (problems with long-range observables)
- Large dimensions in *M*-scheme codes, difficult antisymmetrization in relative coordinates.

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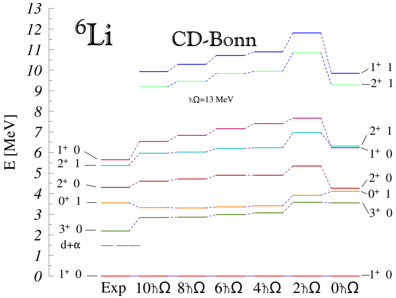
Motivation

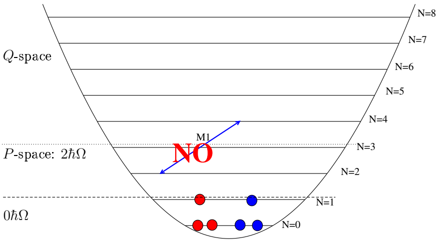
- consistency operators – wfns
- poor convergence properties for some observables

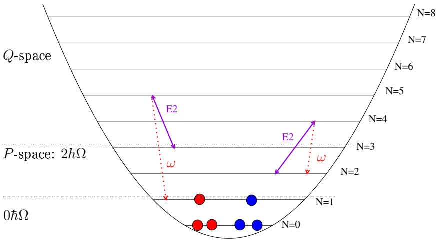
PRL 87 (2001) 172502



	$6\hbar\Omega$	$8\hbar\Omega$	$10\hbar\Omega$	Expt
$B(E2; 1^+0 \to 3^+0)$	8.166	9.136	10.221	21.8(4.8)
$B(M1; 0^+1 \to 1^+0)$	15.510	15.351	15.186	15.42(32)
$B(E2; 2^+0 \to 1^+0)$	3.414	3.989	4.502	4.41(2.27)
$B(M1; 2^+1 \to 1^+0)$	0.034	0.041	0.037	0.150(27)

Why $M1$ and not $E2$ with Bare Operators?





Effective $E2$ Operators

Two-body cluster

		Bare ($2\hbar\Omega$)	Effective ($2\hbar\Omega$)	Bare ($10\hbar\Omega$)	Experiment
Deuteron	Q_0	0.179	0.270		
^{6}Li	$1^+0 \rightarrow 3^+0$	2.647	2.784	10.221	21.8(4.8)
	$2^+0 \rightarrow 1^+0$	2.183	2.269	4.502	4.41(2.27)
	$1_2^+0 \rightarrow 1^+0$	3.183	3.218		

- small model space: expect larger renormalization
- large variation with the model space
- three-body forces: might be important, but not the issue

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The Question is ‘Why?’

Reminder

- Two-body cluster accounts mainly for the short-range correlations
- $E2$ is long range

Short range operators should be better described

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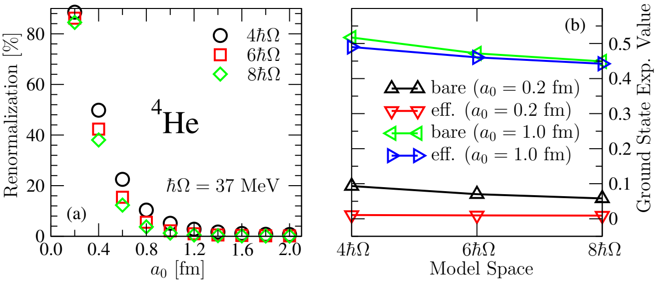
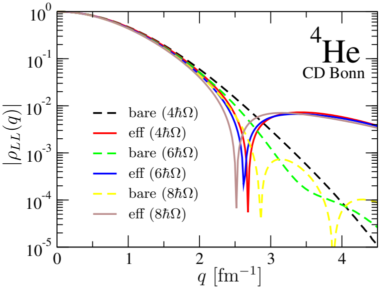
Range Dependence



$$O \sim \exp\left[-\frac{(\vec{r}_1 - \vec{r}_2)^2}{a_0^2}\right]$$

Longitudinal-longitudinal distribution function

$$\rho_{LL}(q) = \frac{1}{4Z}\sum_{j\neq i}(1+\tau_z(i))(1+\tau_z(j))\int d\vec{r}_1 d\vec{r}_2 \langle g.s.|j_0(q|\vec{r}_1-\vec{r}_2|)|g.s.\rangle$$



Model space independence at high momentum transfer: good renormalization at the two-body cluster level

Quick Fix for Long-Range Operators?

Reminder:

- CM Hamiltonian binds the cluster with a harmonic oscillator potential
- The cluster wavefunction has a $\exp(-(r/r_0)^2)$ fall off, instead of $\exp(-r/r_0)$

Can one approximate the binding potential with one which gives better asymptotics?

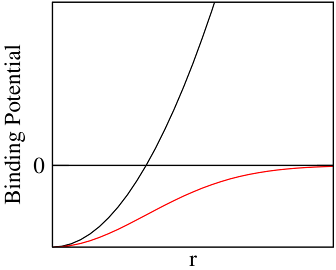
Quick Fix for Long-Range Operators?

Gaussian binding

Idea: replace the HO binding with a Gaussian

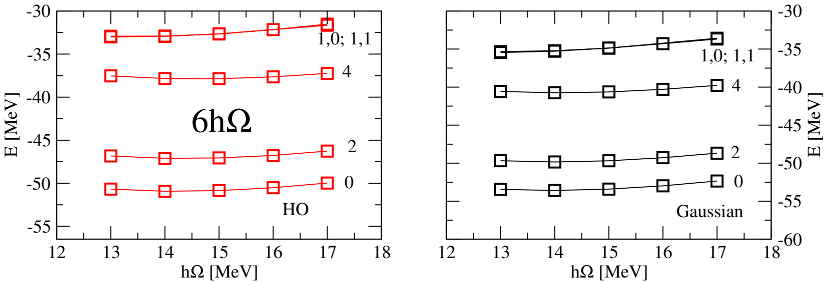
- Fix the Gaussian width to bind exactly as many states as necessary
- Gaussian strength: $V_0 = -m\Omega^2 a_0^2/2$

- $P \to \infty$: Gaussian $\to$ HO



Better fall-off of the cluster wavefunction

Gaussian Binding
Spectrum results



- ground-state energy shifted down a few MeV
- spectrum about the same

Gaussian Binding
Quadrupole transition results

	Transition	Model sp.	$B(E2)$-bare HO	$B(E2)$-bare Gauss.	$B(E2)$-eff. HO	$B(E2)$-eff. Gauss.	Expt.
^{12}C	$2_1\ 0 \rightarrow 0\ 0$	$4\hbar\Omega$	4.03	3.54	4.05	7.00	7.59
^{12}C	$2_1\ 0 \rightarrow 0\ 0$	$4\hbar\Omega^*$	3.96	3.96	3.44	5.99	7.59
^{10}C	$2_1\ 0 \rightarrow 0\ 0$	$4\hbar\Omega$	3.05	2.57	3.08	3.30	12.29

- more realistic cluster binding does not improve dramatically $B(E2)$ in general
- most likely a many-body effect which cannot be avoided

Summary Renormalization Operators

- Short-range operators are in general well described with effective operators at the two-body cluster level; **some observables become model-space independen**t.
- Long-range operators are not significantly renormalized and this is most likely a many-body effect; this problem is not specific to the NCSM!
- Nevertheless, NCSM remains a successful approach

New Approach to Effective Interactions for NCSM

Purpose

To provide a consistent treatement of effective interactions and operators

Means

EFT approach:

- consider the most general Hamiltonian which respects all the symmetries
- determine the coupling constants by fit to experimental data

Shell-Model Space

- the SM space is a particular type of truncation, using bound states only

$$\psi_{nl(s)j}(\vec{r}) = N_{nl} r^l L_n^{l+1/2}(\alpha r^2) \exp(-\alpha r^2) \left[Y_l(\hat{r}) \otimes \chi_s \right]_j$$

- defined by the maximum number of oscillator quanta allowed N_{max} ($N = 2n + l$):

$$P = \sum_{2n+l=0}^{N_{max}} |nl(s)j\rangle\langle nl(s)j|$$

- in the limit $N_{max} \to \infty$ equivalent with continuum

Two-body Observables

- one bound state in the $^3S_1$ channel
- phaseshifts

BUT

In a finite HO basis, all wfs. have a bound-state behavior at large distances

Can we still get phaseshifts?

Phaseshifts in a Finite Basis

$$H = \frac{p^2}{2\mu} + V$$

Diagonalization in the HO finite basis of dimension *d*

$$|\Psi_E\rangle = \sum_{\alpha=1}^{d} A_\alpha(E)|\alpha\rangle$$

$$H|\Psi_E\rangle = E|\Psi_E\rangle$$

If $|\Psi\rangle$ corresponds to an eigenvalue in the continuum, at large distances, **but not at infinity**, this solution **still** approximates a shifted free particle:

$$\Psi_E(r) = arj_l(kr) + brn_l(kr),\ k = \sqrt{2\mu E}$$

$$\delta_l(E) = \frac{b}{a}$$

NB: in the finite basis, E is a discrete eigenvalue!

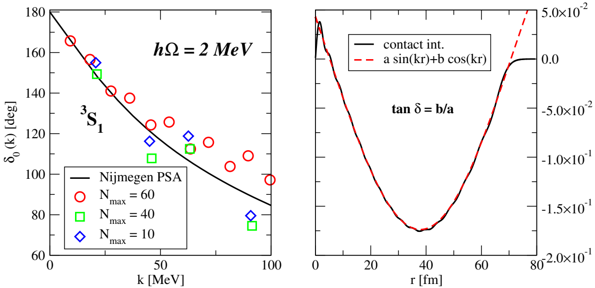
Algorithm

- diagonalize the Hamiltonian in the finite basis
- compute the free-particle solutions for the discrete eigenvalues $E > 0$
- compute $R^2_{rms}(E) = \langle \Psi_E | r^2 | \Psi_E \rangle$
- for $r_i > \sqrt{R^2_{rms}(E)}$, fit the values for a and b so that

$$\sum_i \left[\Psi_E(r_i) - a r_i j_l(k r_i) - b r_i n_l(k r_i)\right]^2 = min$$

LO Pionless EFT

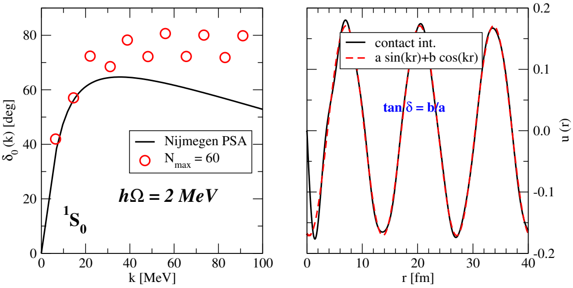
Results for phaseshifts: $^3S_1$ channel



The coupling constant: fitted to reproduce the deuteron binding energy

LO Pionless EFT

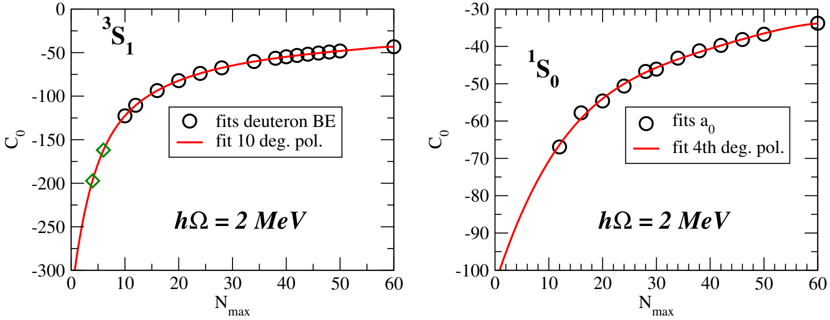
Results for phaseshifts: $^1S_0$ channel



The coupling constant: fitted to reproduce the scattering length

LO Pionless EFT

Running of the coupling constants

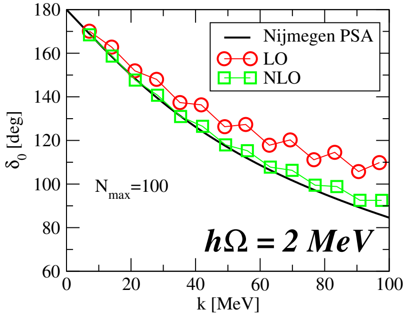


$$H = \frac{p^2}{2\mu} + C_0$$

Obvious Issues

- oscillations in the phaseshift curves
- $^1S_0$ channel fitting less accurate (and more involved)
- easier fit for N_{max} large and $\hbar\Omega$ small
- energies involved in many-body processes might be outside the range of validity of the pionless theory (one has to go to the pionfull theory)

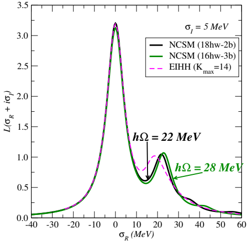
NLO Pionless EFT
$^3S_1$ channel



- Reproduces the deuteron binding energy and the scattering length
- The phaseshift curve smooths out

Conclusions and Outlook

- Effective operators from unitary transformation:
  - Implemented at the two-body cluster level
  - little effect for long-range operators
  - **good description of short-range operators**
  - applications to other problems in progress



- New approach to effective interactions
  - description of phaseshifts in finite L^2 integrable basis
  - improved description at the NLO for $^3S_1$ channel
  - algorithm to obtain the coupling constants in spaces accesible for many-body calculations
  - higher order and three-body forces

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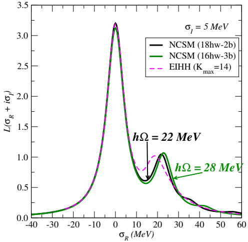

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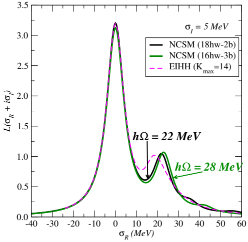

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