Time dependent coupled-cluster method

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Interfaces Between Nuclear Reactions and Structure

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Overview

1. Introduction
2. Cure of center-of-mass problem
3. Time-dependent coupled-cluster method
4. First results
5. Summary

Energy scales and relevant degrees of freedom

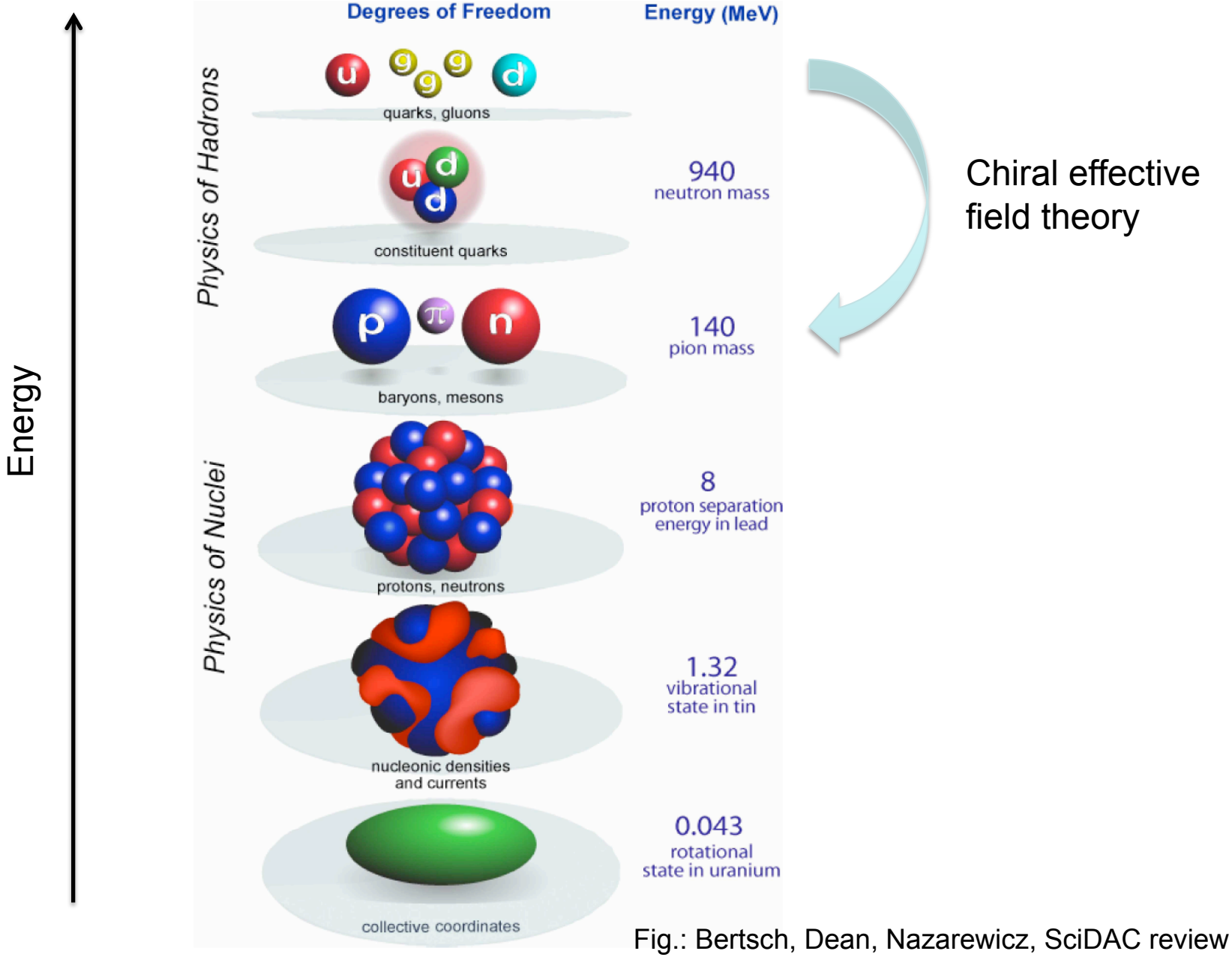
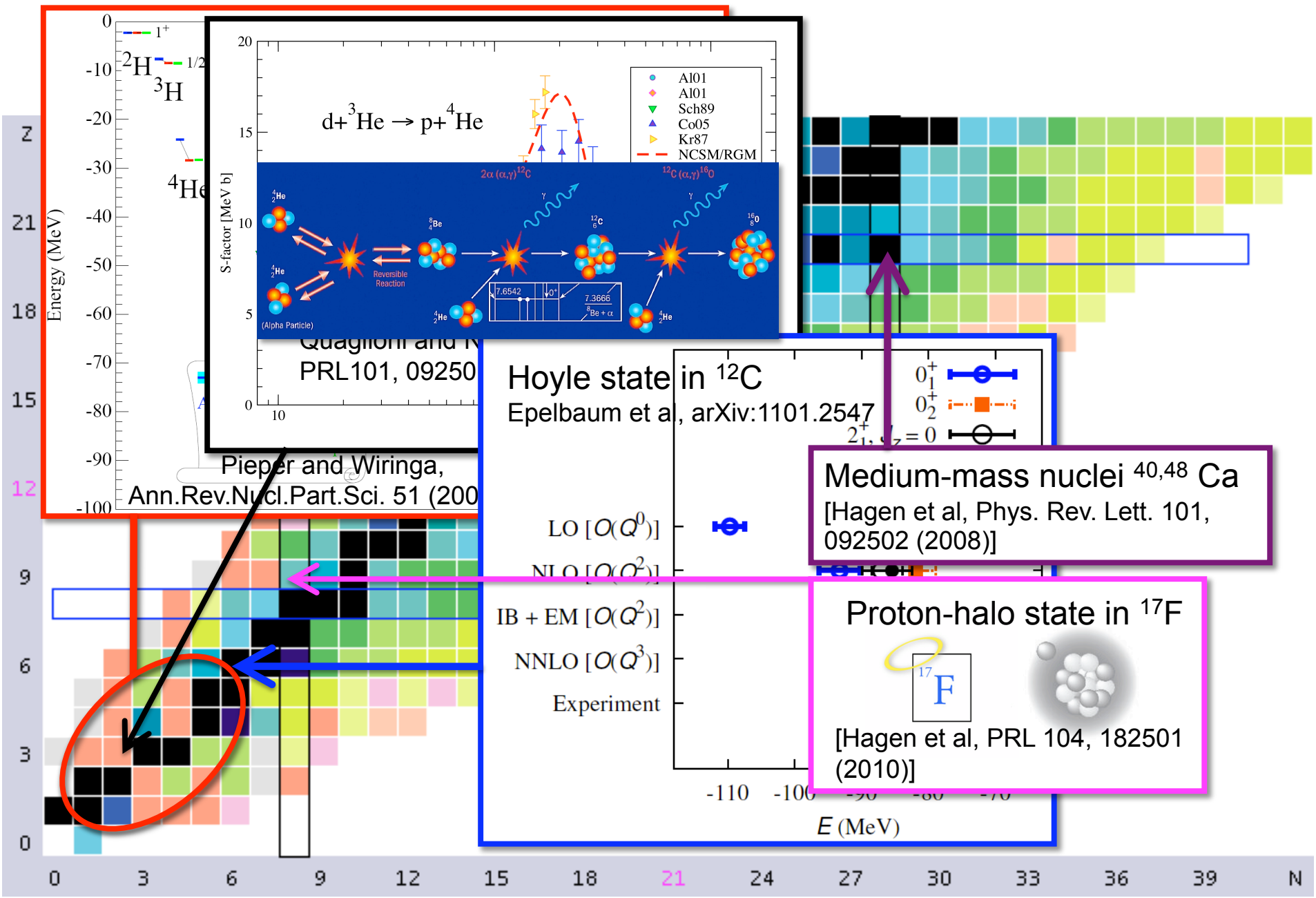


Fig.: Bertsch, Dean, Nazarewicz, SciDAC review (2007)

Highlights: first-principle computations of nuclei



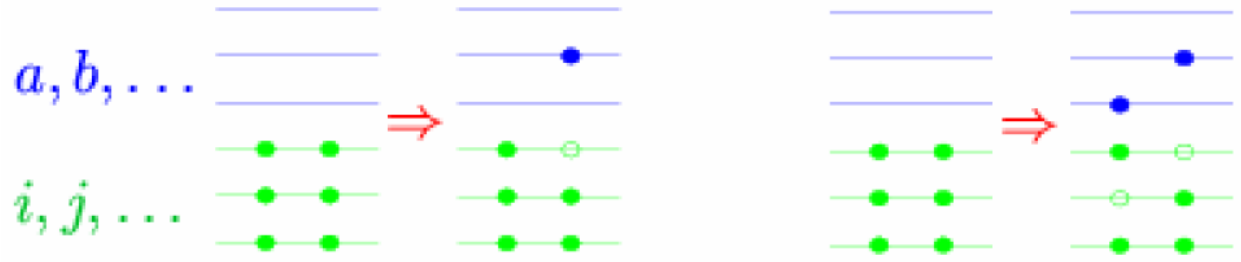
Coupled-cluster method (in CCSD approximation)

Ansatz:

$$
\begin{aligned}
|\Psi\rangle &= e^{T}|\Phi\rangle \\
T &= T_1 + T_2 + \dots \\
T_1 &= \sum_{ia} t_i^a a_a^\dagger a_i \\
T_2 &= \sum_{ijab} t_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i
\end{aligned}
$$

- ☺ Scales gently (polynomial) with increasing problem size o^2u^4 .
- ☺ Truncation is the only approximation.
- ☺ Size extensive (error scales with A)
- ☹ Most efficient for doubly magic nuclei

Correlations are *exponentiated* 1p-1h and 2p-2h excitations. Part of np-nh excitations included!



Coupled cluster equations

$$
\begin{aligned}
E &= \langle\Phi|\overline{H}|\Phi\rangle \\
0 &= \langle\Phi_i^a|\overline{H}|\Phi\rangle \\
0 &= \langle\Phi_{ij}^{ab}|\overline{H}|\Phi\rangle
\end{aligned}
$$

Alternative view: CCSD generates similarity transformed Hamiltonian with no 1p-1h and no 2p-2h excitations.

$$
\overline{H} \equiv e^{-T} H e^{T} = \left(He^{T}\right)_c = \left(H + HT_1 + HT_2 + \frac{1}{2}HT_1^2 + \dots\right)_c
$$

Economy of the coupled-cluster singles-doubles approximation

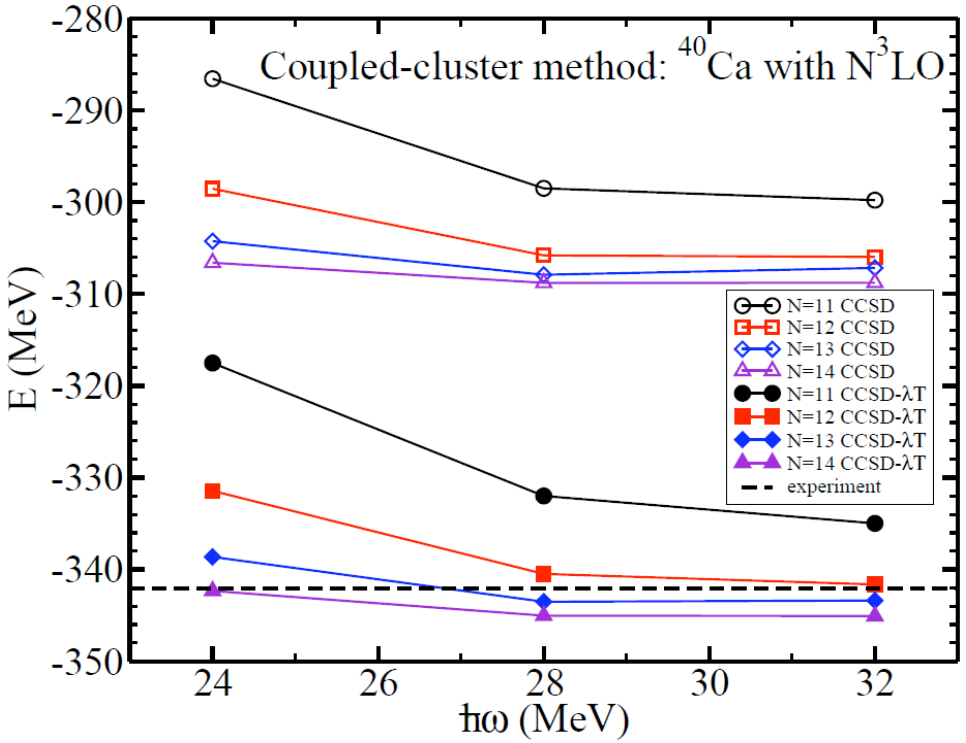
Hamiltonian matrix of A-body system

	$\|\phi\rangle$	1p-1h $\|\phi_i^a\rangle$	2p-2h $\|\phi_{ij}^{ab}\rangle$
$\|\phi\rangle$	*	*	*
1p-1h $\|\phi_i^a\rangle$	*	*	*
2p-2h $\|\phi_{ij}^{ab}\rangle$	*	*	*

	$\|\phi\rangle$	1p-1h $\|\phi_i^a\rangle$	2p-2h $\|\phi_{ij}^{ab}\rangle$
$\|\phi\rangle$	E_0	*	*
1p-1h $\|\phi_i^a\rangle$	0	*	*
2p-2h $\|\phi_{ij}^{ab}\rangle$	0	*	*

Toward medium-mass nuclei

Chiral N^{3}LO (500 MeV) by Entem & Machleidt, NN only



Binding energy per nucleon

Nucleus	CCSD	Λ-CCSD(T)	Experiment
^{4}He	5.99	6.39	7.07
^{16}O	6.72	7.56	7.97
^{40}Ca	7.72	8.63	8.56
^{48}Ca	7.40	8.28	8.67

^{16}O results confirmed by

- [Fujii et al., Phys. Rev. Lett. 103, 182501 (2009)]
  - B/A=6.62 MeV (2-body clusters)
  - B/A=7.47 MeV (3-body clusters)
- [Navratil *et al.*, arXiv:1105.3173 (2011)]
  - B/A =7.48 MeV

Chiral NN forces yield saturation, lack about 0.4 MeV per nucleon in binding energy.

Chiral three-nucleon forces expected to yield 0.4MeV per nucleon?!

[Hagen, TP, Dean, Hjorth-Jensen, Phys. Rev. Lett. 101, 092502 (2008)]

Center-of-mass coordinate – a red herring?

The nuclear Hamiltonian is invariant under rotations and translations

Approach that preserves both symmetries:

☺ Jacobi coordinates

☹ Antisymmetrization very expensive → limited to A≤10 or so

[Faddeev Yakubowsky; Hyperspherical Harmonics; Manchester group's CCM].

Antisymmetry best dealt within second quantization:

☹ No single-particle basis available that consists of simultaneous eigenstates of the angular momentum operator and the momentum operator.

☺ Within a complete Nħω oscillator space, the wave function is guaranteed to factorize

$$\psi = \psi_{\rm cm}\psi_{\rm in}$$

Intrinsic wave function ψ_{in} invariant under translation

Center-of-mass wave function ψ_{cm} is Gaussian whose width is set by the oscillator length of the employed oscillator basis

The factorization is key. The form of ψ_{cm} is irrelevant.

Center-of-mass coordinate (cont'd)

Intrinsic nuclear Hamiltonian $$H_{\rm in} = T - T_{\rm cm} + V \ ,$$
$$= \sum_{1\le i<j\le A} \left(\frac{(\vec{p}_i - \vec{p}_j)^2}{2mA} + V(\vec{r}_i - \vec{r}_j) \right)$$

Obviously, H_{in} commutes with any center-of-mass Hamiltonian H_{cm}.

Situation: The Hamiltonian depends on 3(A-1) coordinates, and is solved in a model space of 3A coordinates. What is the wave function in the center-of-mass coordinate?

Q:How can one demonstrate the factorization of wave function ψ:

A: Find a suitable center-of-mass Hamiltonian H_{cm} whose eigenstate is ψ.

Our approach:

Demonstrate that $\langle H_{cm} \rangle \approx 0$ for a center-of-mass Hamiltonian with zero-energy ground state.

$$H_{\rm cm}(\tilde{\omega}) = T_{\rm cm} + \frac{1}{2} mA\tilde{\omega}^2 R_{\rm cm}^2 - \frac{3}{2}\hbar\tilde{\omega}$$

Frequency $\tilde{\omega}$ to be determined.

Toy problem

Two particles in one dimension with intrinsic Hamiltonian

$$H = \frac{p^2}{2m} + V(x)$$

$$V(x) = -V_0 \exp\left(-(x/l)^2\right)$$

$$x = (x_1 - x_2)/\sqrt{2}$$

$$p = (p_1 - p_2)/\sqrt{2}$$

Single-particle basis of oscillator wave functions with *m,n=0,..,N*

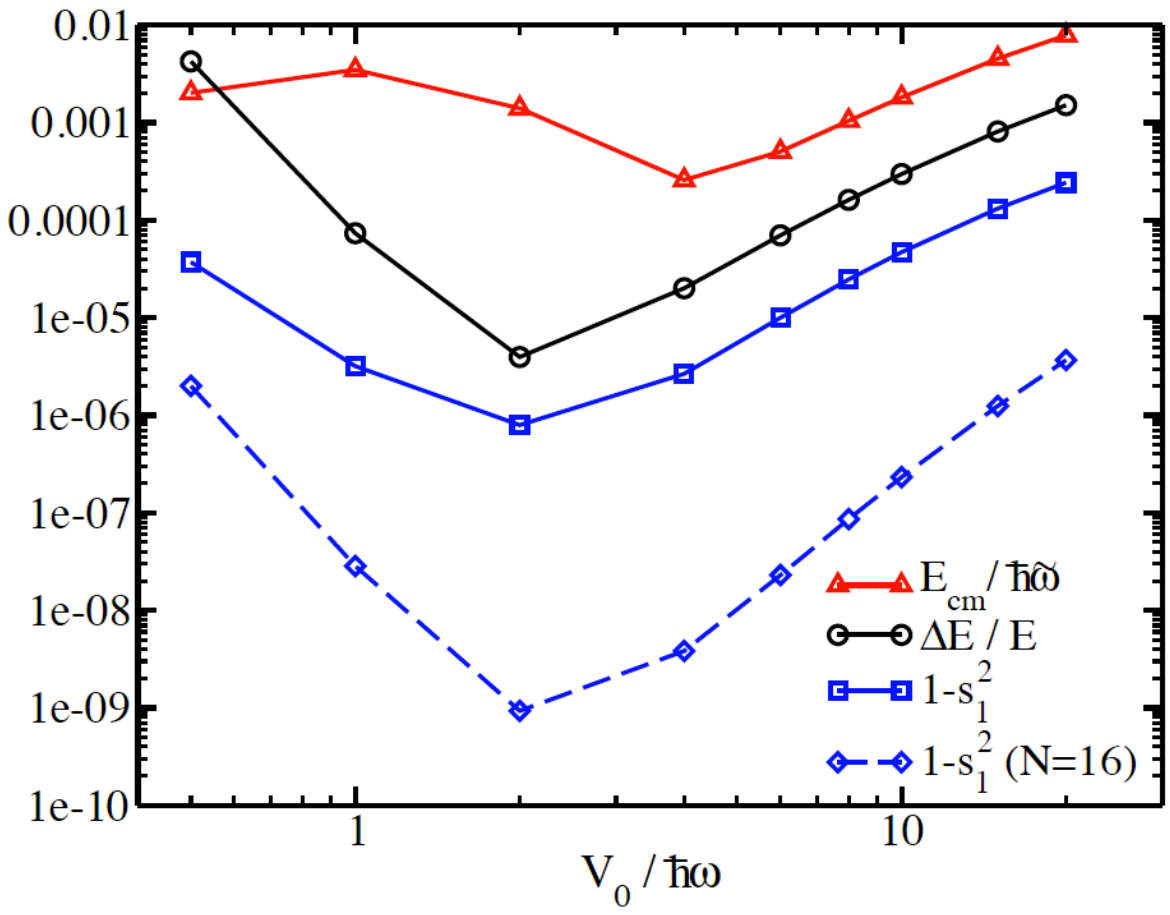
$$\Phi_m(x_1/l)\Phi_n(x_2/l)$$

Results:

1. Ground-state is factored with $s_1 \approx 1$

$$\psi_A = \sum_j s_j \psi_{\rm cm}^{(j)} \psi_{\rm in}^{(j)}$$

2. CoM wave function is approximately a Gaussian



Determination of ψ_{cm}

Assumption: ψ_{cm} is (approximately) a Gaussian for all model-space frequencies

- Gaussian center-of-mass wave function is the zero-energy ground state of

$$H_{\rm cm}(\tilde{\omega}) = T_{\rm cm} + \frac{1}{2} m A \tilde{\omega}^2 R_{\rm cm}^2 - \frac{3}{2}\hbar\tilde{\omega}$$

- Determine unknown frequency from from taking expectation value of identity

$$H_{\rm cm}(\omega) + \frac{3}{2}\hbar\omega - T_{\rm cm} = \frac{\omega^2}{\tilde{\omega}^2}\left(H_{\rm cm}(\tilde{\omega}) + \frac{3}{2}\hbar\tilde{\omega} - T_{\rm cm} \right)$$

- Use

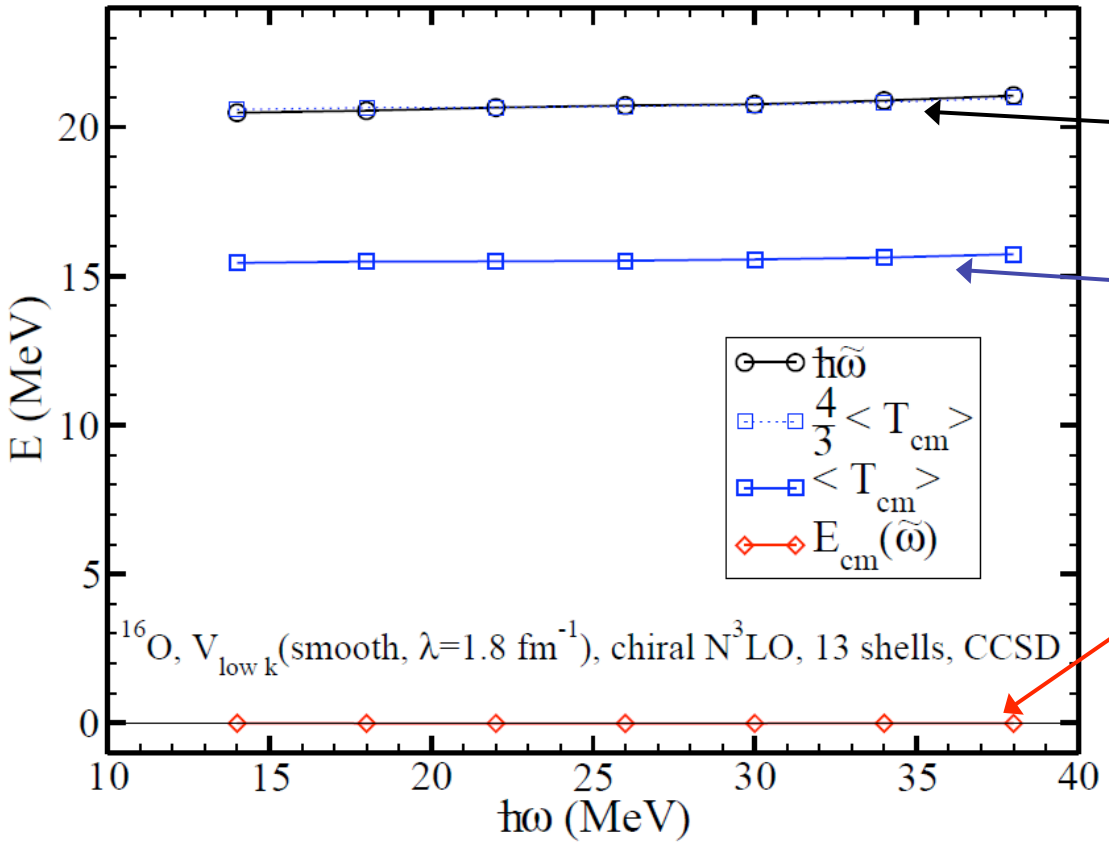
$$E_{\rm cm}(\tilde{\omega}) = 0$$
$$\langle T_{\rm cm} \rangle = \tfrac{3}{4}\hbar\tilde{\omega}$$

Two possible frequencies

$$\hbar\tilde{\omega} = \hbar\omega + \frac{2}{3}E_{\rm cm}(\omega) \pm \sqrt{\frac{4}{9}(E_{\rm cm}(\omega))^2 + \frac{4}{3}\hbar\omega E_{\rm cm}(\omega)}$$

Gaussian center-of-mass wave function

^{16}O with V_{lowk} (1.8 fm^{-1}, smooth) within CCSD



Frequency $\tilde{\omega}$ of Gaussian very weakly dependent on model space

Kinetic energy T_{cm} is ¾ of oscillator spacing

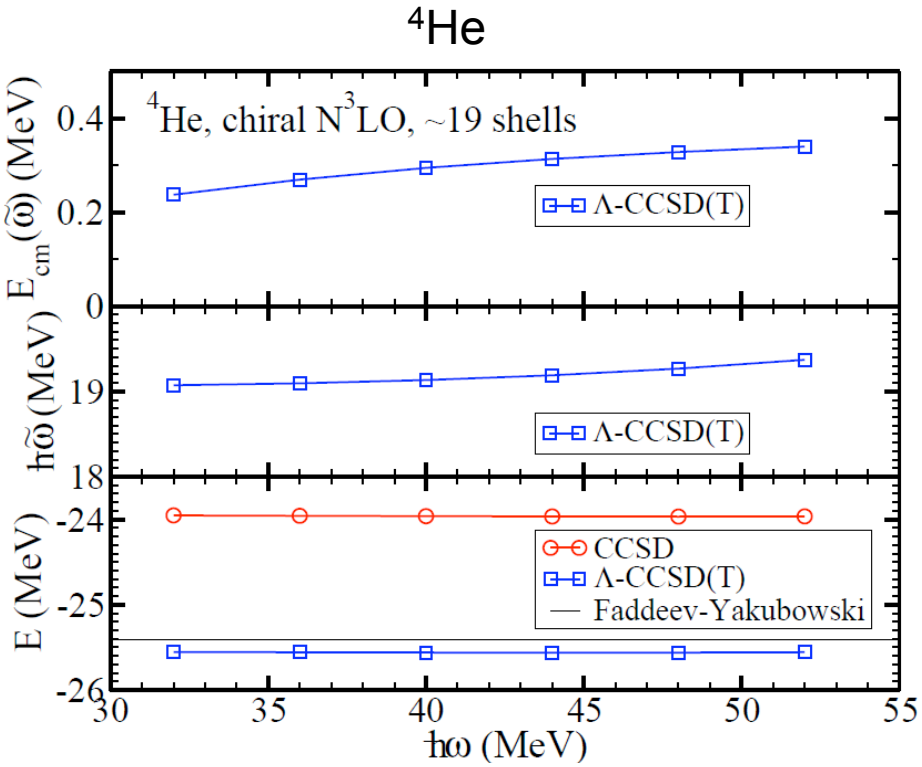
$<H_{cm}>$ vanishes (size > -10 keV)

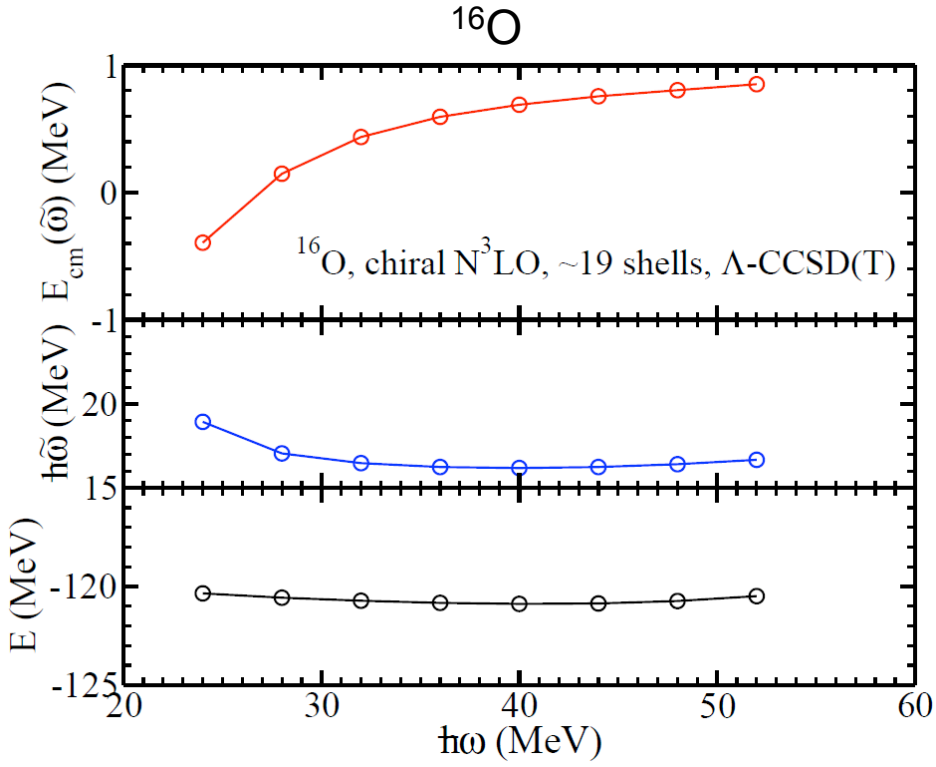
The intrinsic Hamiltonian does not reference the center-of-mass coordinate.

Yet, the resulting center-of-mass wave function is a Gaussian.

Approximate factorization also for “hard” interactions:

^{4}He, ^{16}O, and ^{48}Ca from Entem & Machleidt’s chiral N^{3}LO





Coupled-cluster wave function factorizes approximately.

Note: spurious states are separated by about 15 – 20 MeV >> E_{cm}.

No understanding of Gaussian CoM wave function (yet).

Nucleus	$\hbar\tilde{\omega}$
^{4}He	19.1 MeV
^{16}O	16.5 MeV
^{48}Ca	14.9 MeV

[Hagen, TP, Dean, Phys. Rev. Lett. 103, 062503 (2009)]

Treatment and cure of the center-of-mass ‘problem’

Recipe:

Ingredients

1. intrinsic Hamiltonian
2. sufficiently large model space of Slater determinants

Cook as directed. Check for ‘doneness’:

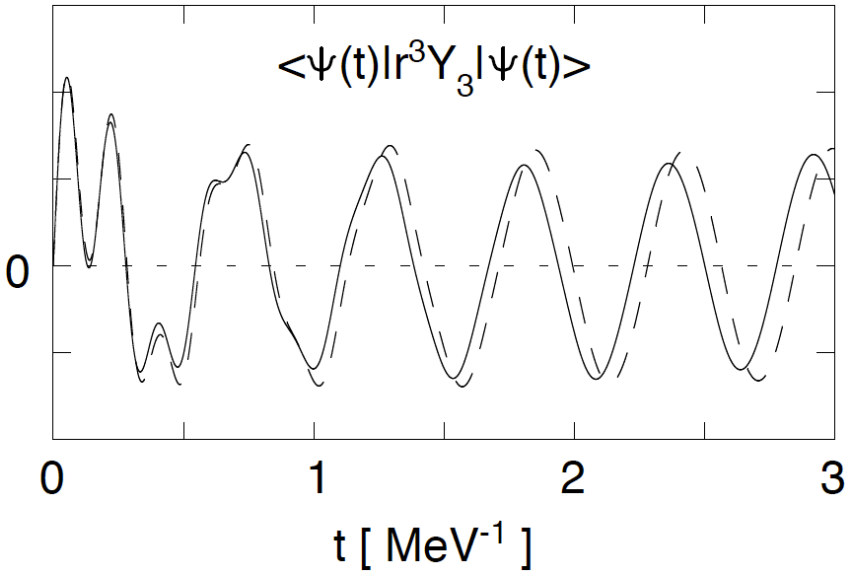
3. compute expectation value of center-of-mass harmonic oscillator
4. confirm that center-of-mass ground state is Gaussian

Why it works:

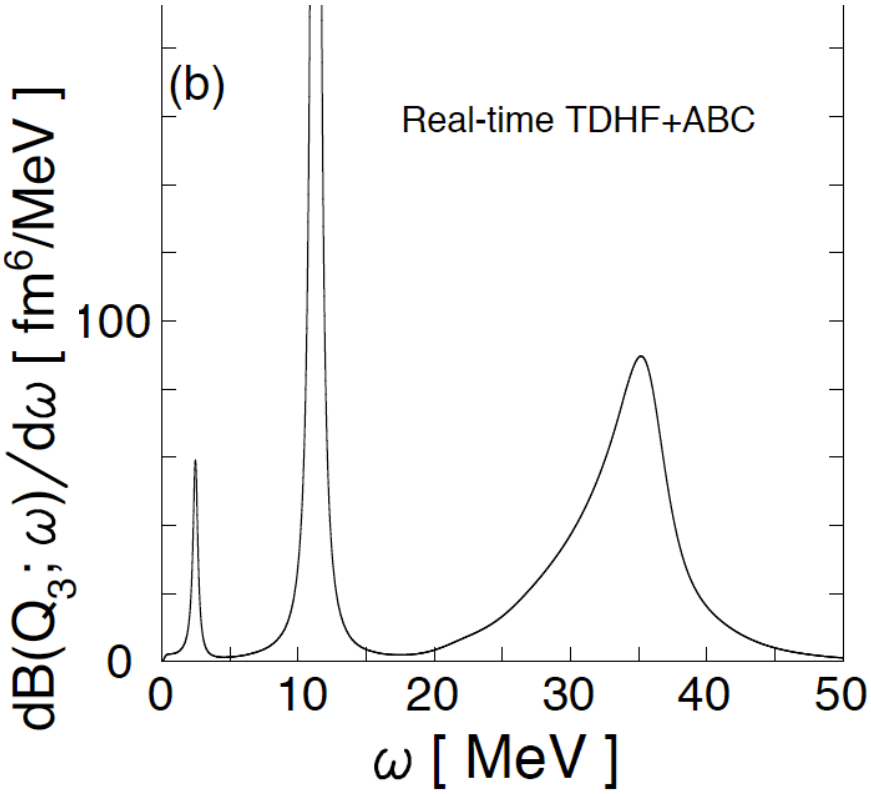
- A sufficiently large model space is complete for low-energy nuclear structure.
- Factorziation not a surprise. (Gaussian form of the CoM wave function still is)

Time-dependent Hartree Fock

Octupole moment



Transition strength from FT



T. Nakatsukasa and K. Yabana, Phys. Rev. C 71, 024301 (2005).

Time-dependent Hartree Fock (cont'd)

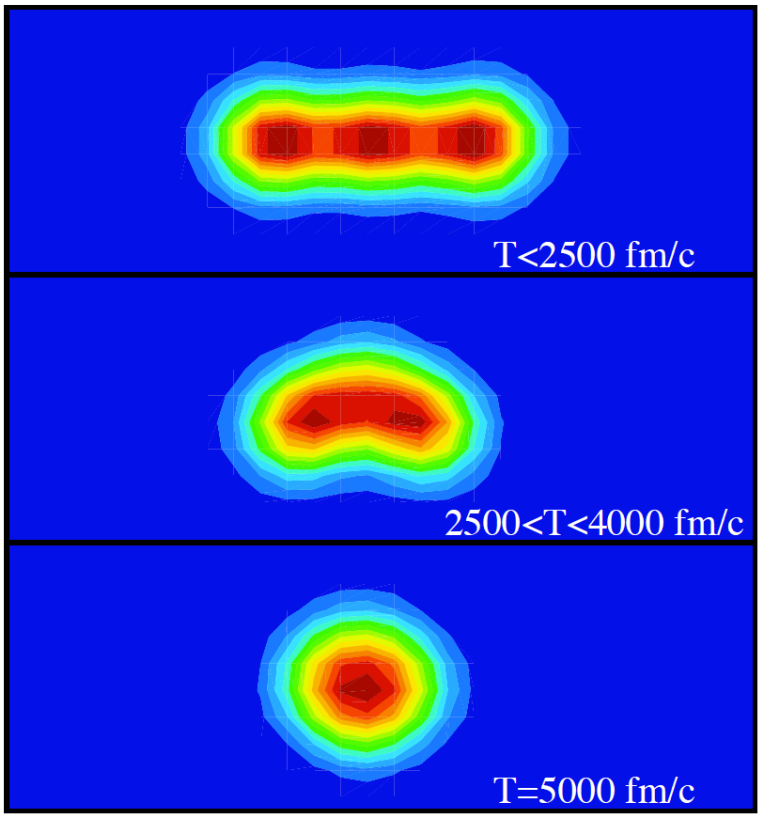


FIG. 1: (Color online) Selected density profiles from TDHF time-evolution of the ^{4}He+^{8}Be head-on collision for initial Be orientation angle $\beta = 0°$ using the SLy4 interaction. The initial energy is $E_{\mathrm{c.m.}} = 2$ MeV.

A. S. Umar *et al.*, Phys. Rev. Lett. 104, 212503 (2010)

Sought: Improvements over time-dependent Hartree-Fock methods

Challenges: description of

- dissipation
- particle emission
- under-the-barrier fusion

Hoodbhoy & Negele (1978,1979)

Time-dependent coupled-cluster method

Time-dependent coupled-cluster method

Ansatz:

$$|\Psi\rangle = e^{S(t)}\,|\Phi\rangle$$

Schroedinger Eq.:

$$e^{-S} H e^{S} |\Phi\rangle = e^{-S} \partial_t e^{S} |\Phi\rangle$$

Evolution equation for time-independent single-particle basis

$$i\hbar \dot{S} = \overline{H}$$ (take only 1p-1h and 2p-2h excitations from RHS)

Note:

1. Initial value problem (S(t=0) is input)
2. The similarity transformed Hamiltonian becomes complex non-hermitian under time evolution

Check: From time dependent to time independent

$$s_i^a(t) = t_i^a + r_i^a(t)$$
$$s_{ij}^{ab}(t) = t_{ij}^{ab} + r_{ij}^{ab}(t)$$

Assume
- |r| << |t|
- t amplitudes fulfill time-independent CC equations.

Result: Equation-of-motion equations / linear response

Excitation spectrum fulfills eigenvalue problem

$$\hbar\omega r_i^a = \langle \Phi_i^a | [\overline{H}, R] | \Phi \rangle$$
$$\hbar\omega r_{ij}^{ab} = \langle \Phi_{ij}^{ab} | [\overline{H}, R] | \Phi \rangle$$

H. J. Monkhorst Phys. Rev. A 36, 1544 (1987).

Imaginary time propagation τ=it

Imaginary-time propagation is a (non-unitary) SRG transformation

$$H(\tau) = e^{-S(\tau)} H e^{S(\tau)}$$

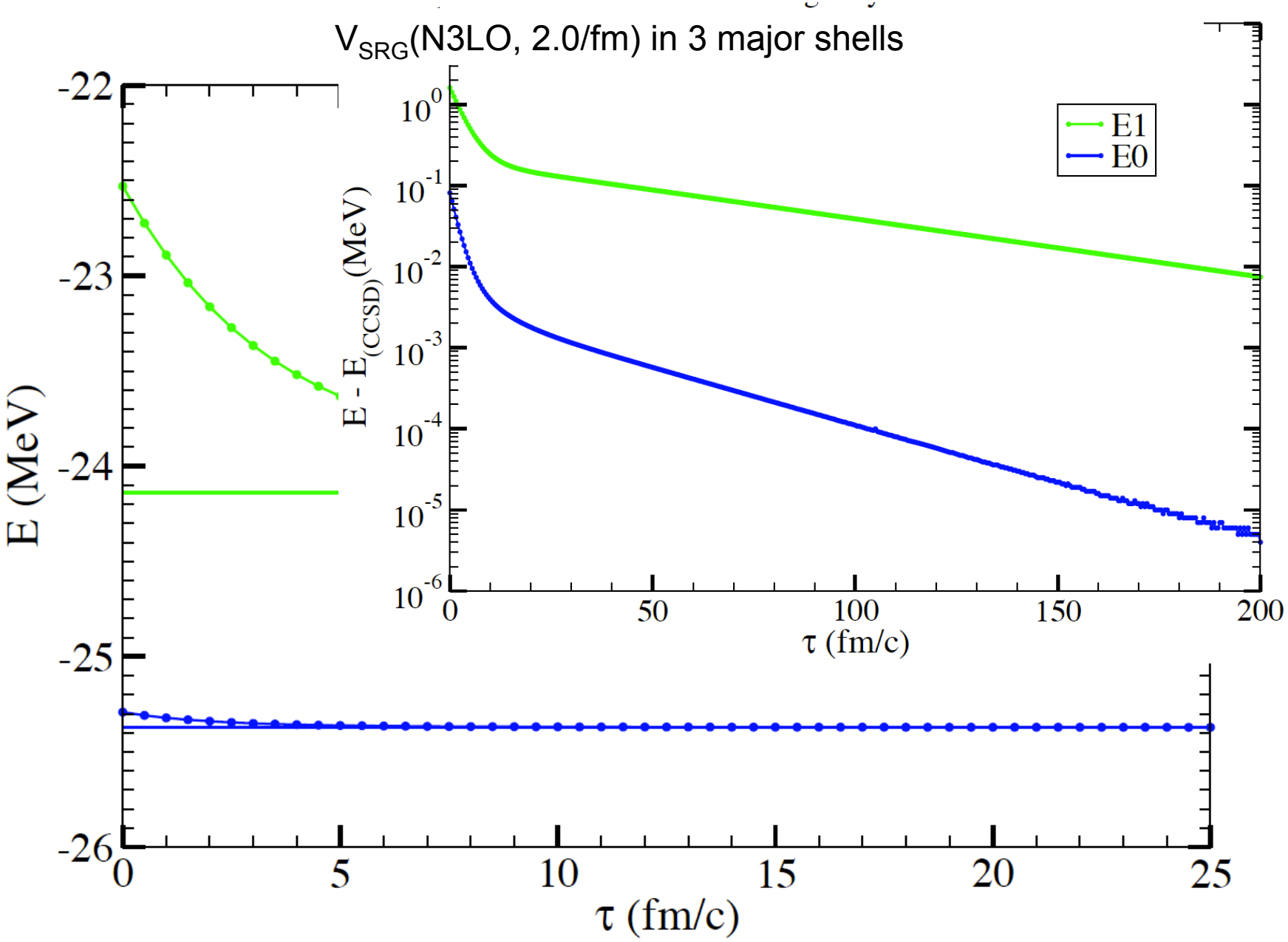
$$\partial_\tau H(\tau) = [H(\tau), \partial_\tau S]$$

Generator of this SRG:
1p-1h & 2p-2h excitations of the similarity-transformed Hamiltonian

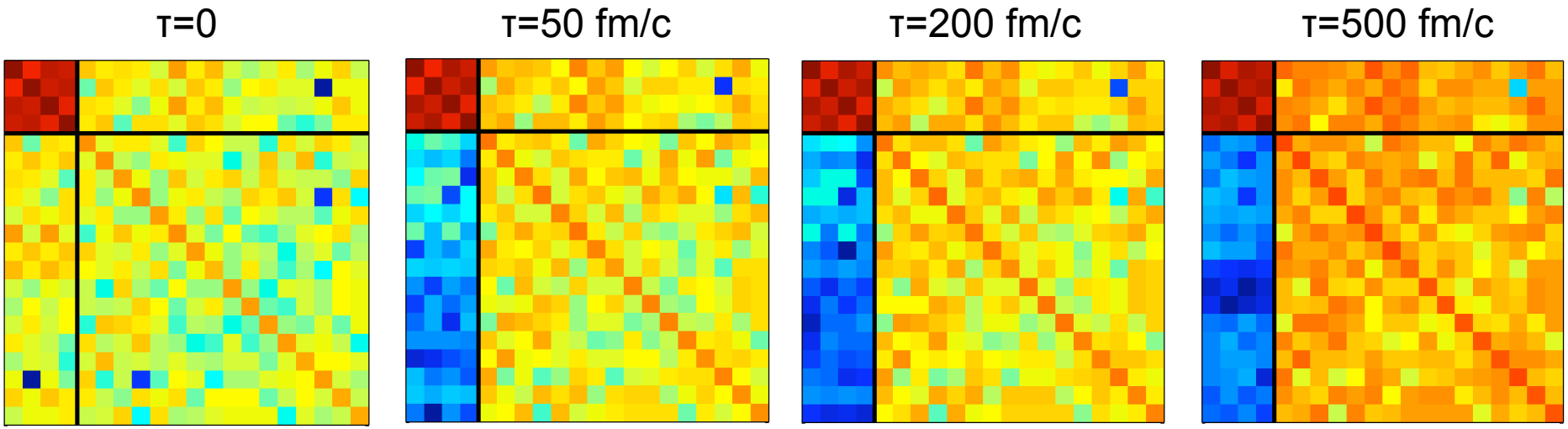
$$\begin{aligned}
\partial_\tau s_0 &= -\langle \Phi | e^{-S} H e^{S} | \Phi \rangle \ , \\
\partial_\tau s_i^a &= -\langle \Phi_i^a | e^{-S} H e^{S} | \Phi \rangle \ , \\
\partial_\tau s_{ij}^{ab} &= -\langle \Phi_{ij}^{ab} | e^{-S} H e^{S} | \Phi \rangle
\end{aligned}$$

(Hermitian) SRG: Glazek & Wilson 1993; Wegner 1994; Bogner, Furnstahl, Perry 2007; Tsukiyama, Bogner, Schwenk 2011.

Imaginary time evolution



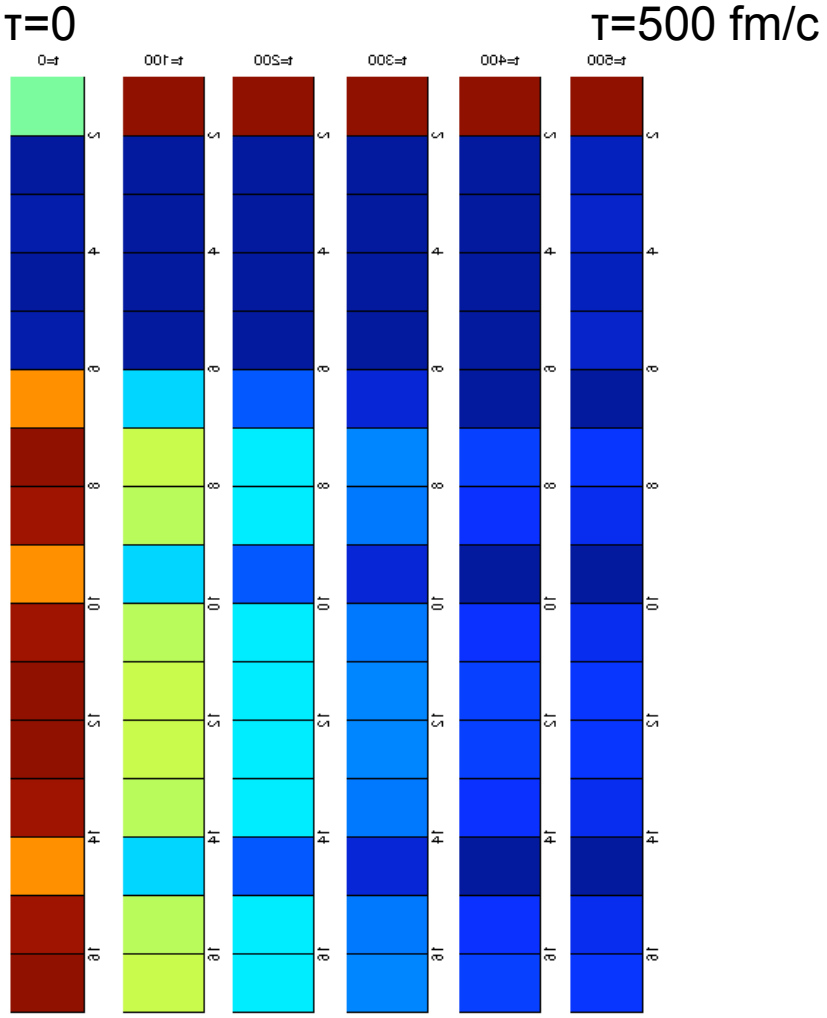
Imaginary time evolution as similarity renormalization group flow



- Imaginary time evolution yields solution of coupled cluster equations
- Diagonalization of evolved Hamiltonian yields ground and excited states

Imaginary time evolution as similarity renormalization group flow

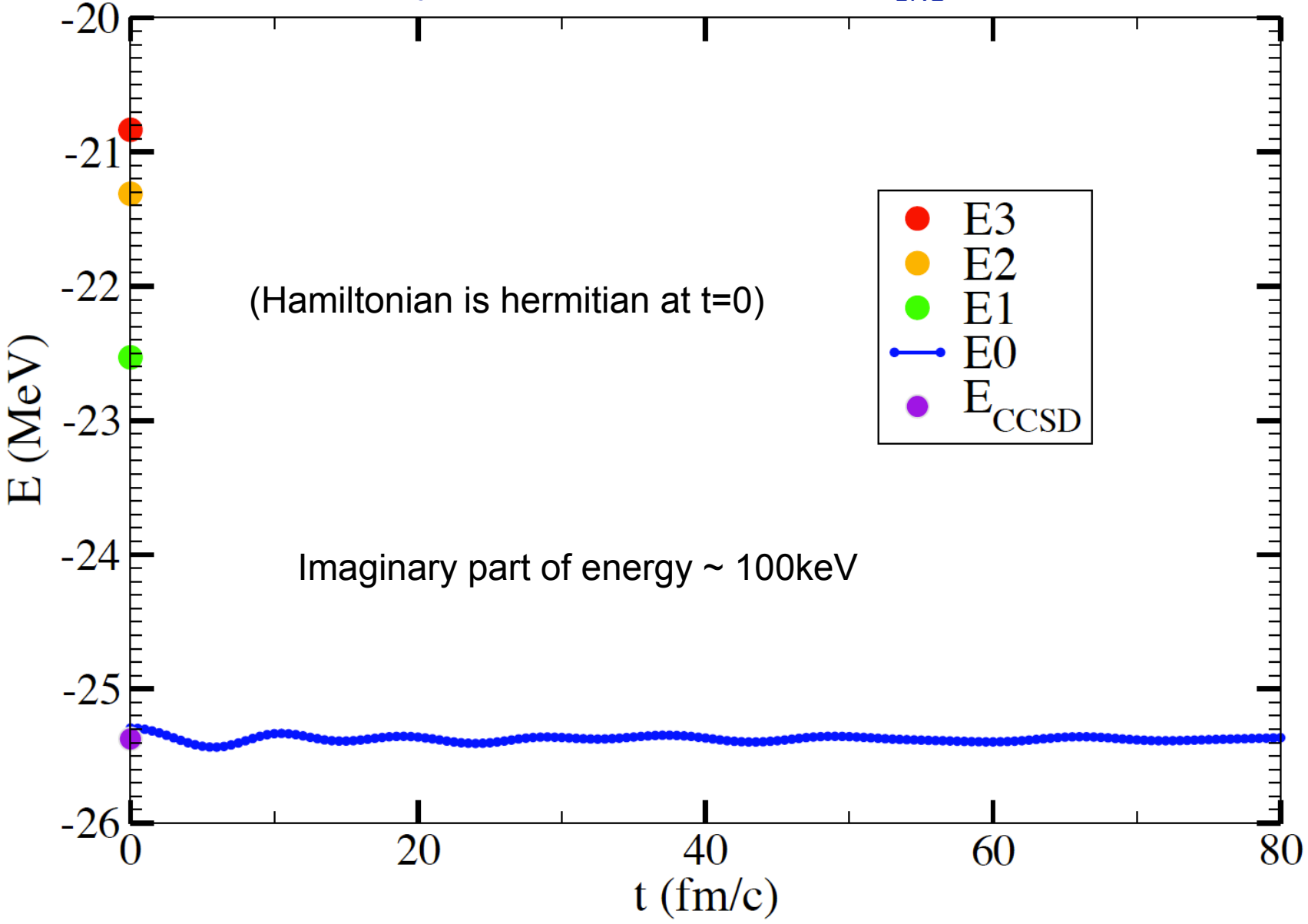
Evolution of first column of Hamiltonian matrix



What will the evolution of a complex non-hermitian Hamiltonian yield?

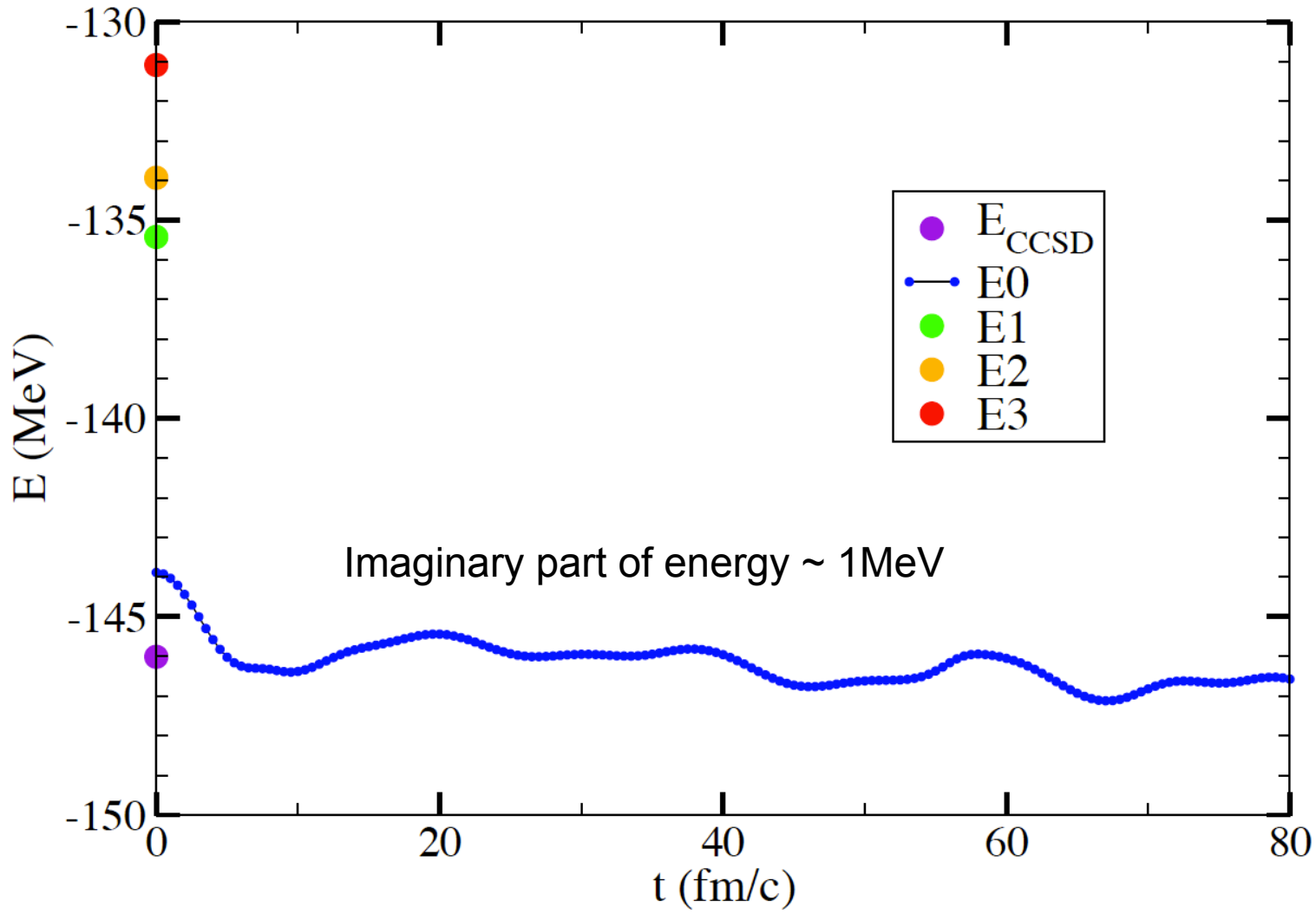
Evolution in real time: preliminary results

^{4}He in three major oscillator shells, S(0)=0, V_{SRG}(N3LO,2.0/fm)



Evolution in real time: preliminary results

^{16}O in three major oscillator shells; S(0)=0, V_{SRG}(N3LO,2.0/fm)



Summary

- Coupled-cluster method efficient tool for certain nuclei
- Intrinsic Hamiltonian → factorized center-of-mass wavefunction
- Time-dependent coupled-cluster method
  - imaginary time evolution as SRG
  - role of energy in real time evolution not yet fully understood
  - for small excitations around stationary CCSD solution, energy is "practically" conserved (fluctuations smaller that accuracy of CCSD)