Electromagnetic properties of nuclei: from few- to many-body systems

Lecture 10

Many-body methods

Sonia Bacca

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Lecture series for SFB 1245
TU Darmstadt

Ab-initio many-body methods

- Green's Function Monte Carlo
  (Carlson, Gandolfi, Lovato, Lynn ...)
- No core shell model
  (Qualgioni, Navratil, Roth, Vary ...)
- Symmetry adapted no core shell model
  (Launey, Draayer, Dytrych…)

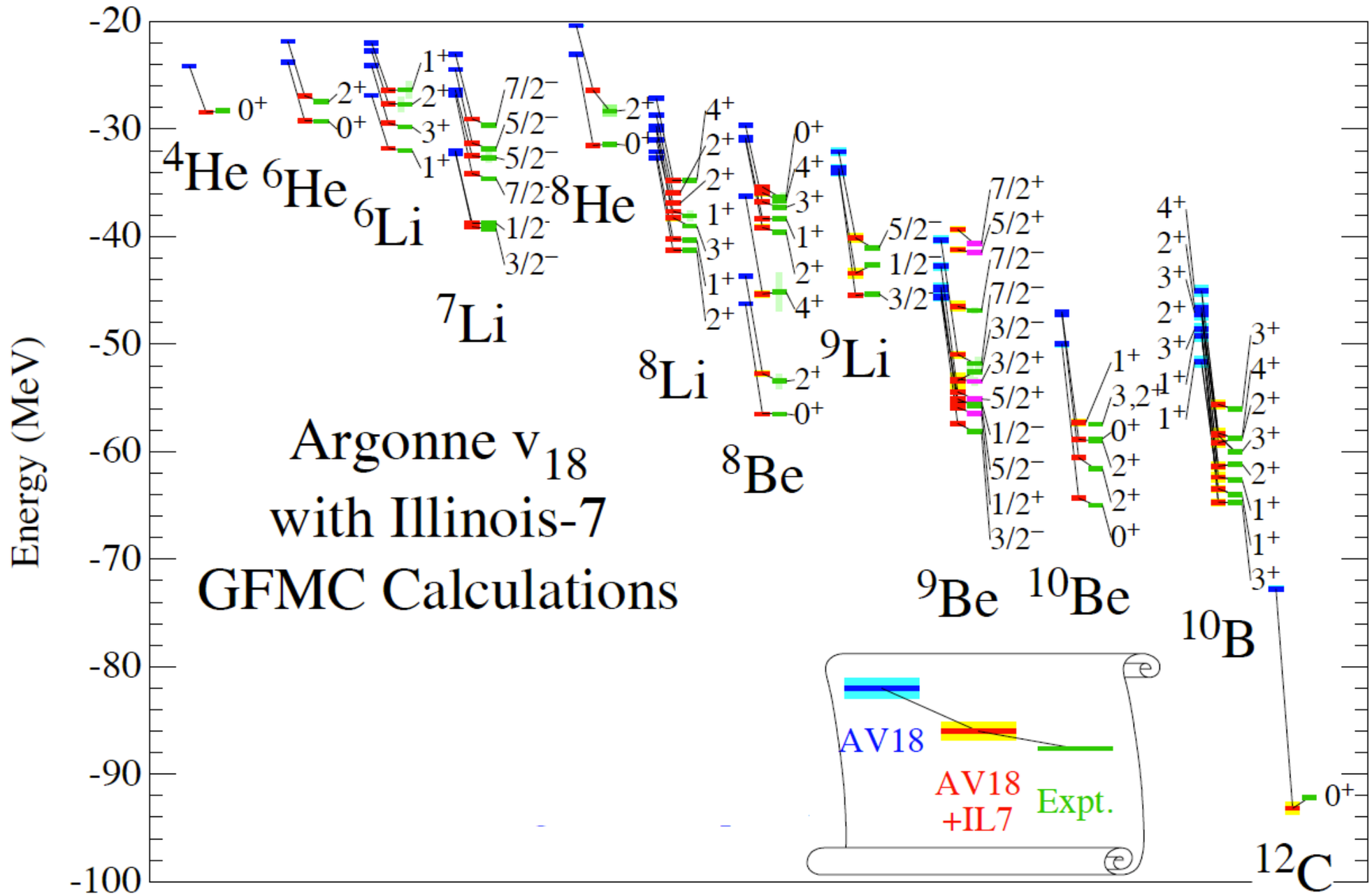
Factorial growth in A

- Coupled-cluster theory
  (Hagen, Papenbrock, Hjorth-Jensen, ...)
- In-medium SRG
  (Bogner, Hergert, Holt, Schwenk, ...)
- ...

Polynomial growth in A

Green's function Monte Carlo

Demonstration that light nuclei can be build from scratch

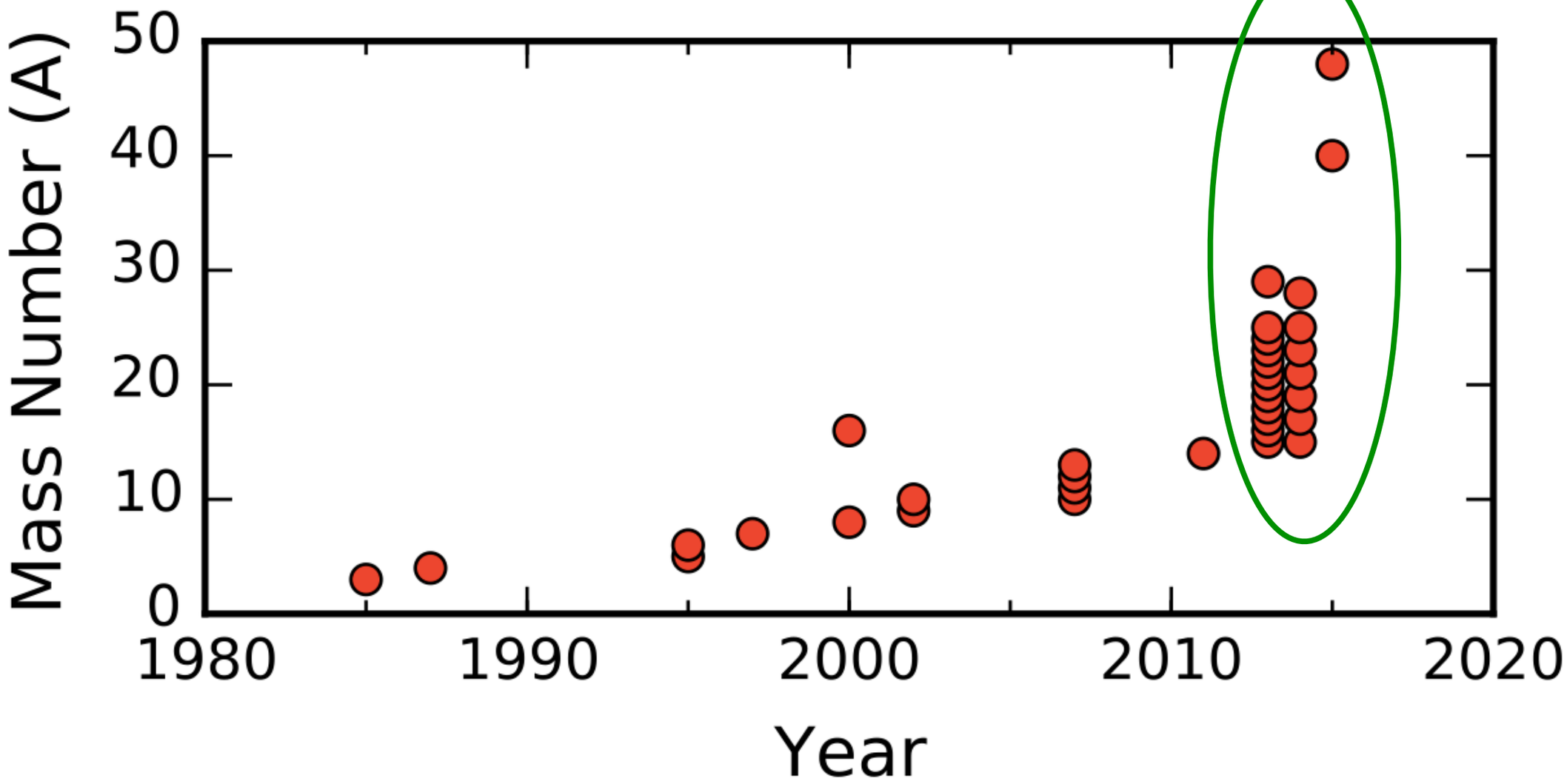


Pieper & Wiringa, Ann. Rev. Nucl. Part. Sci. 51, 53 (2001)

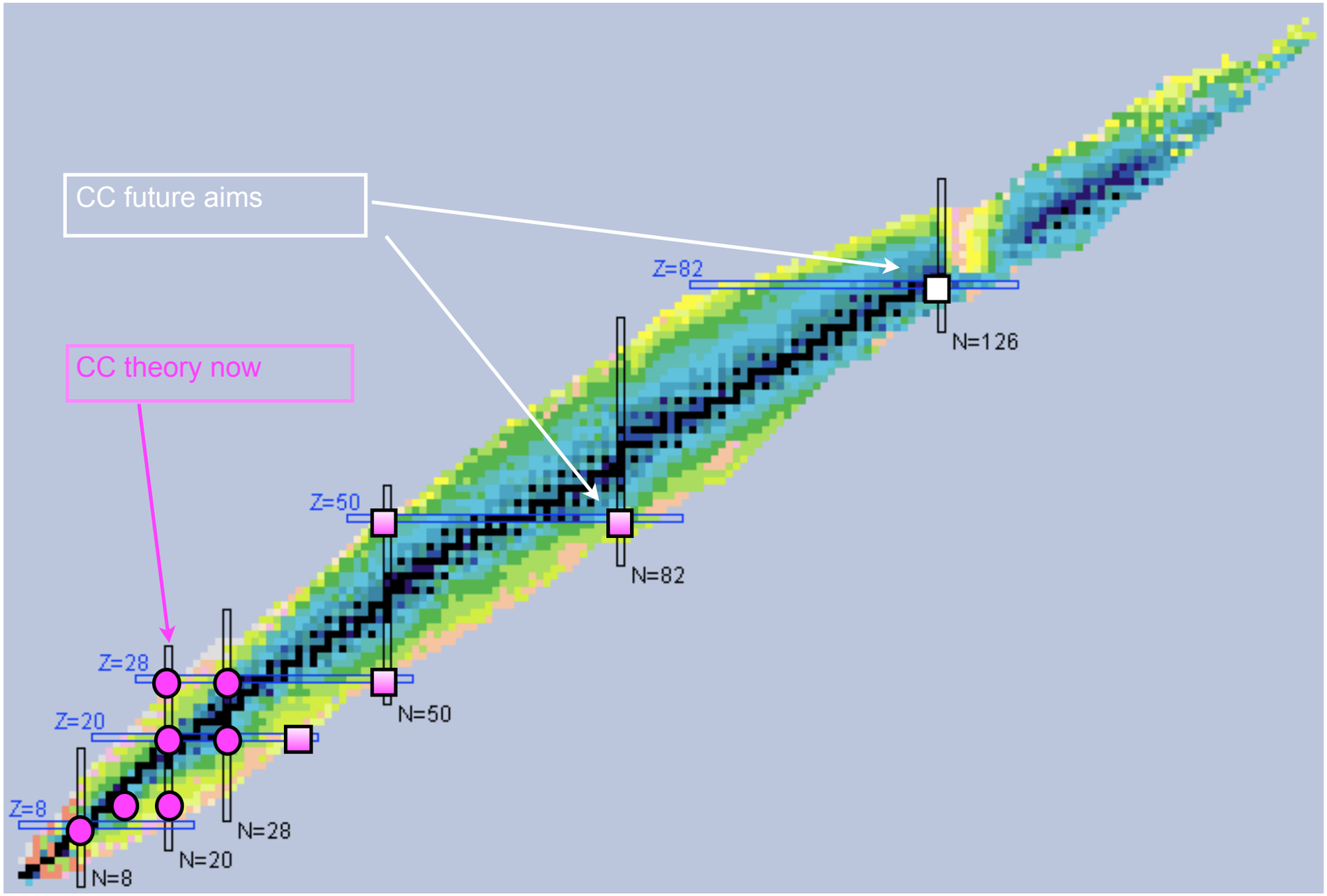
Mass reach vs time

Polynomial algorithms
+
Better/cheaper computers

Ab-initio methods



Coupled-cluster theory



ORNL group and collaborators: PRL **108**, 242501 (2012), PRL **109,** 032502 (2012); PRL **110**, 192502 (2013), PRL **113**, 262504 (2014), PRL **113**, 142502 (2014) …

Also Darmstadt group and collaborators

R. Roth *et al.,* Phys. Rev. Lett. **109**, 052501 (2012)
S. Binder et al, Physics Letters B 736 (2014) 119-123…

Coupled-cluster theory

- First we will introduce some elements of coupled-cluster theory as a method to solve the A-body Schrödinger equation

$$H|\Psi_0\rangle = E_0|\Psi_0\rangle$$

- Second, we will see how to combine the LIT with coupled-cluster theory as a way to compute break-up reactions in the medium-mass regime

History of coupled-cluster theory

Formal introduction:

1958: Coester, Nucl. Phys. 7, 421

1960: Coester and Kummel, Nucl. Phys. 17, 477

Introduction into Chemistry (late 60's):

1966: Cizek, J. Chem. Phys. 45, 4256 (1966); Adv. Chem. Phys. 14, 35 (1969)

1971: Cizek and Paldus, Int. J. Quantum Chem. 5, 359

Numerical implementations

1978: Pople et al., Int. J. Quantum Chem Symp, 14, 545

1978: Bartlett and Purvis, Int. J. Quantum Chem 14, 561

Initial nuclear calculations (1970's):

1978: Kummel, Luhrmann, Zabolitzky, Phys. Rep. 36, 1 and refs. therein

1980-90s: Bishop's group. Coordinate space.

Few applications in nuclei, explodes in chemistry and molecular sciences.

Hard-core interactions; computer power; unclear interactions

Nuclear physics reintroduction: ($1/E_{ph}$ expansion)

1999: Heisenberg and Mihiala, Phys. Rev. C59, 1440; PRL84, 1403 (2000)

Three nuclei; JJ coupled scheme; bare interactions, approximate V_{3N}

Useful References

Crawford and Schaefer, Reviews in Computational Chemistry, 14, 336 (2000)

Bartlett, Ann. Rev. Phys. Chem. 32, 359 (1981)

Hagen et al, Rep. Prog. Phys. 77, 096302 (2014)

Creation and annihilation operators

Recap

Single particle basis $\{|\phi_1\rangle, |\phi_2\rangle, ..., |\phi_m\rangle\} \longrightarrow \{|\phi_i\rangle\}$

$a_i^\dagger$ Operator that creates a particle in state $|\phi_i\rangle$

a_i Operator that annihilates a particle in state $|\phi_i\rangle$

These operators obey anti-commutations rules to ensure antisymmetrization

$$\{a_i^\dagger, a_j^\dagger\} = \{a_i, a_j\} = 0,$$
$$\{a_i^\dagger, a_j\} = \{a_j, a_i^\dagger\} = \delta_{ij}.$$

Slater determinant:

First quantization

$$|\Phi\rangle = \mathcal{A}[|\phi_i\rangle|\phi_j\rangle \cdots |\phi_k\rangle]$$

Second quantization

$$|\Phi\rangle = |ij....k\rangle = a_i^\dagger a_j^\dagger \cdots a_k^\dagger |0\rangle$$
$$|ji....k\rangle = a_j^\dagger a_i^\dagger \cdots a_k^\dagger |0\rangle$$
$$= -a_i^\dagger a_j^\dagger \cdots a_k^\dagger |0\rangle$$

Many-body operators

Many-body operators can be written in second quantization

First quantization → Second quantization

One-body operator: $$F = \sum_{i}^{A} f_i \longrightarrow F = \sum_{pq} \langle p|f|q\rangle a_p^\dagger a_q$$

Two-body operator: $$V = \sum_{ij}^{A} V_{ij} \longrightarrow V = \frac{1}{2}\sum_{pqrs} \langle pq|v|rs\rangle a_p^\dagger a_q^\dagger a_s a_r$$

Three-body operator: $$W = \sum_{ijk}^{A} W_{ijk} \longrightarrow W = \frac{1}{6}\sum_{pqrstu} \langle pqr|w|stu\rangle a_p^\dagger a_q^\dagger a_r^\dagger a_u a_t a_s$$

Hamiltonian $$H = F + V + W$$

Many-body operators

Since we deal with fermions, we want to use antisymmetrized states.
Then the expressions for many-body operators become a bit different

Example: $|rs\} = \frac{1}{\sqrt{2!}}(|rs\rangle - |sr\rangle) = |rs\rangle_A = \mathcal{A}|rs\rangle$ Antisymmetrized two-body state

$$\langle pq|v|rs\rangle a_p^\dagger a_q^\dagger a_s a_r = \frac{1}{2}\langle pq|v|rs\rangle a_p^\dagger a_q^\dagger a_s a_r + \frac{1}{2}\langle pq|v|rs\rangle a_p^\dagger a_q^\dagger a_s a_r$$

$$= \frac{1}{2}\langle pq|v|rs\rangle a_p^\dagger a_q^\dagger a_s a_r + \frac{1}{2}\langle pq|v|sr\rangle a_p^\dagger a_q^\dagger a_r a_s$$

$$= \frac{1}{2}\langle pq|v|rs\rangle a_p^\dagger a_q^\dagger a_s a_r - \frac{1}{2}\langle pq|v|sr\rangle a_p^\dagger a_q^\dagger a_s a_r$$

$$= \frac{1}{2\sqrt{2}}\sum_{pqrs}\langle pq|v|rs\} a_p^\dagger a_q^\dagger a_s a_r = \frac{1}{4}\sum_{pqrs}\{pq|v|rs\} a_p^\dagger a_q^\dagger a_s a_r$$

$$V = \frac{1}{2}\sum_{pqrs}\langle pq|v|rs\rangle a_p^\dagger a_q^\dagger a_s a_r = \frac{1}{4}\sum_{pqrs}\{pq|v|rs\} a_p^\dagger a_q^\dagger a_s a_r$$

Many-body operators

Many-body operators written in second quantization with antisymmetrized states

One-body operator:

$$F = \sum_{pq} \langle p|f|q\rangle a_p^\dagger a_q$$

Two-body operator:

$$V = \frac{1}{4} \sum_{pqrs} \{pq|v|rs\} a_p^\dagger a_q^\dagger a_s a_r$$

Three-body operator:

$$W = \frac{1}{36} \sum_{pqrstu} \{pqr|w|stu\} a_p^\dagger a_q^\dagger a_r^\dagger a_u a_t a_s$$

Hamiltonian

$$H = F + V + W$$

In coupled-cluster theory one writes the Hamiltonian in normal order using the Wick's theorem.

Normal Order

If you have a general string of creation and annihilations operators, using anti-commutation relations, you can reorganize them so that all creation operators on the left and all annihilations operators are on the right.

Advantage: the action of an annihilation operator on the vacuum is zero, so any normal ordered product acting on the vacuum contributes nothing.

Example:
$$\{a_i a_j^\dagger a_k a_l^\dagger\} = -\, a_l^\dagger a_j^\dagger a_k a_i$$
$$= \quad a_j^\dagger a_l^\dagger a_k a_i$$
$$= -\, a_j^\dagger a_l^\dagger a_i a_k$$

Three different products of operators which all contribute 0 when acting on the vacuum

Wick Theorem

Definition: Contraction of two arbitrary annihilation/creation operators

$$\overbrace{AB} = AB - \{AB\}$$

If we have two annihilations and two creations operators, the contraction is 0

Because they are already in normal order

$$\overbrace{a_i a_j} = a_i a_j - a_i a_j = 0$$

$$\overbrace{a_i^\dagger a_j^\dagger} = a_i^\dagger a_j^\dagger - a_i^\dagger a_j^\dagger = 0$$

$$\overbrace{a_i^\dagger a_j} = a_i^\dagger a_j - a_i^\dagger a_j = 0$$ already in normal order

$$\overbrace{a_i a_j^\dagger} = a_i a_j^\dagger - a_j^\dagger a_i = a_i a_j^\dagger + a_i a_j^\dagger = \delta_{ij}$$ Only non-vanishing

Wick Theorem

Theorem: Any general string of annihilation/creation operators can be written as

$$ABC\ldots = \{ABC\ldots\} + \sum_{\substack{\text{all}\\ \text{single}\\ \text{contractions}}} \{\overbrace{ABC\ldots}\}$$

$$+ \sum_{\substack{\text{all}\\ \text{double}\\ \text{contractions}}} \{\overbrace{\overbrace{ABC\ldots}}\}$$

$$+ \cdots + \sum_{\substack{\text{all}\\ \text{fully}\\ \text{contracted}\\ \text{prdts}}} \{\overbrace{\overbrace{\overbrace{ABC\ldots}}}\}.$$

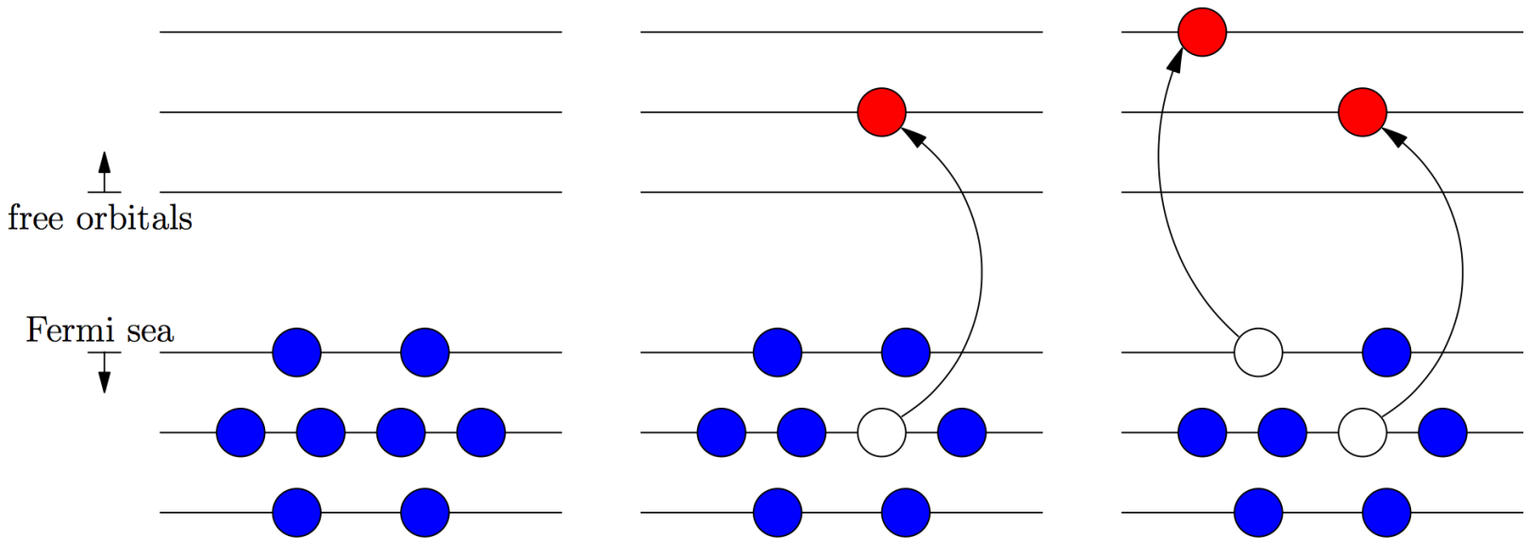
Consequence: all terms disappear because of the normal ordering. The only one that can contribute is that where all operators are fully contracted.

This theorem allows one to write down a normal ordered Hamiltonian.

Normal order with respect to SD

It is convenient to define a new vacuum state

$$|0\rangle \equiv |\Phi_0\rangle = |ijk...\rangle$$ Fermi vacuum



$abc\ldots$

$ijk\ldots$

$$|\Phi^{ab\ldots}_{ij\ldots}\rangle = a^\dagger_a a^\dagger_b \ldots a_j a_i |\Phi_0\rangle$$ Particle-hole excitations

$a_i|\Phi_0\rangle$ creates a hole

$a^\dagger_a|\Phi_0\rangle$ creates a particle

Creation operators — Left

normal order with respect to $|\Phi_0\rangle$

$a^\dagger_i|\Phi_0\rangle$ destroys a hole

$a_a|\Phi_0\rangle$ destroys a particle

Destruction operators — Right

Normal order with respect to SD

Using the Wick's theorem we normal order H with respect to $|\Phi_0\rangle$

One-body $$F = \sum_{pq} \langle p|f|q\rangle \{a_p^\dagger a_q\} + \sum_i \langle i|f|i\rangle n_i$$

n_i occupation number

Two-body $$V = \frac{1}{4}\sum_{pqrs} \{pq|v|rs\}\{a_p^\dagger a_q^\dagger a_s a_r\} + \sum_{ipq} \{pi|v|qi\}\{a_p^\dagger a_q\} n_i + \frac{1}{2}\sum_{ij} \{ij|v|ij\} n_i n_j$$

Three-body $$W = \frac{1}{36}\sum_{pqrstu} \{pqr|w|stu\}\{a_p^\dagger a_q^\dagger a_r^\dagger a_u a_t a_s\} + \frac{1}{4}\sum_{ipqrs} \{ipq|w|irs\}\{a_p^\dagger a_q^\dagger a_r a_s\} n_i$$

$$\frac{1}{2}\sum_{ijpq} \{ijp|w|ijq\}\{a_p^\dagger a_q\} n_i n_j + \frac{1}{6}\sum_{ijk} \{ijk|w|ijk\} n_i n_j n_k$$

Hamiltonian $$H = F + V + W$$

$$H = H_N + H_0$$

$$H_0 = \langle \Phi_0|H|\Phi_0\rangle$$

Uncorrelated energy of the reference state

Schödinger Equation

$$H|\Psi_0\rangle = E_0|\Psi_0\rangle$$

$$H = H_N + H_0$$

$$(H_N + H_0)|\Psi_0\rangle = E_0|\Psi_0\rangle$$

$$H_N|\Psi_0\rangle = (E_0 - H_0)|\Psi_0\rangle$$

$$\Delta E_0 = E_0 - H_0$$

$$H_N|\Psi_0\rangle = \Delta E_0|\Psi_0\rangle$$

$$H_N|\Psi\rangle = \Delta E|\Psi\rangle = E|\Phi_0\rangle$$

rename

Starting point

The exponential ansatz

Exponential ansatz

$$|\Psi\rangle = e^{T}|\Phi_0\rangle$$

correlation operator

$$H e^{T}|\Phi_0\rangle = E e^{T}|\Phi_0\rangle$$

$$\underset{N}{H} e^{T}|\Phi_0\rangle = E e^{T}|\Phi_0\rangle$$

$$e^{-T}\underset{N}{H} e^{T}|\Phi_0\rangle = e^{-T} E e^{T}|\Phi_0\rangle$$

$$e^{-T} H_N e^{T}|\Phi_0\rangle = E|\Phi_0\rangle$$

Similarity-transformed Hamiltonian [not Hermitian]

$$\bar{H} \equiv e^{-T} H_N e^{T}$$

Schrödinger equation for similarity transformed Hamiltonian

$$\bar{H}|\Phi_0\rangle = E|\Phi_0\rangle$$

Cluster operator

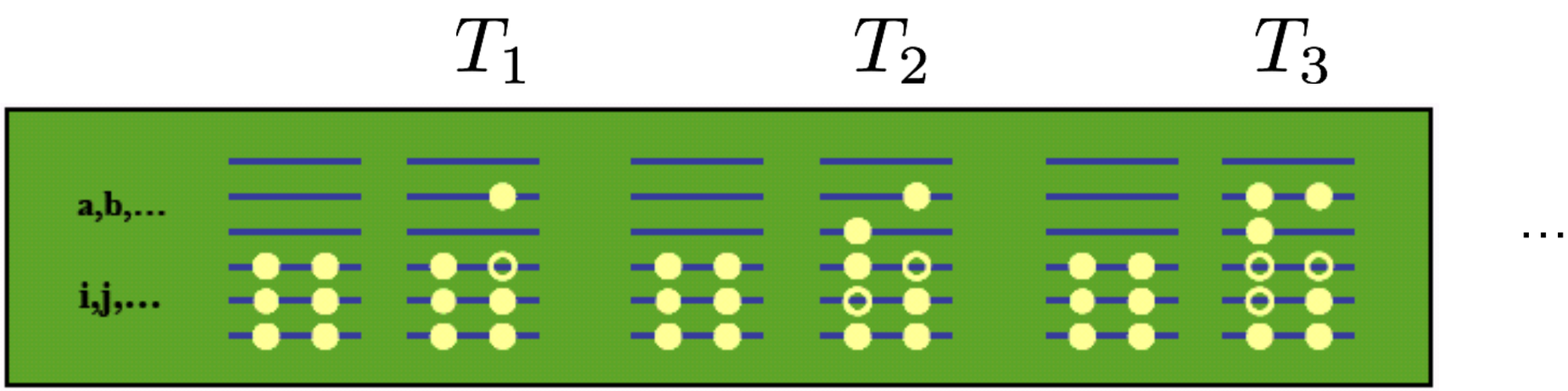
Exponential ansatz $|\Psi\rangle = e^T |\Phi_0\rangle$

$$T = T_1 + T_2 + \ldots + T_A = \sum_{n=1}^{m_A} T_n$$

$$T_n = \frac{1}{(n!)^2} \sum_{ij\ldots ab\ldots} t_{ij\ldots}^{ab\ldots} \left\{ a_a^\dagger a_b^\dagger \cdots a_j a_i \right\}$$

Normal ordered operators

$m_A = A$ Exact theory



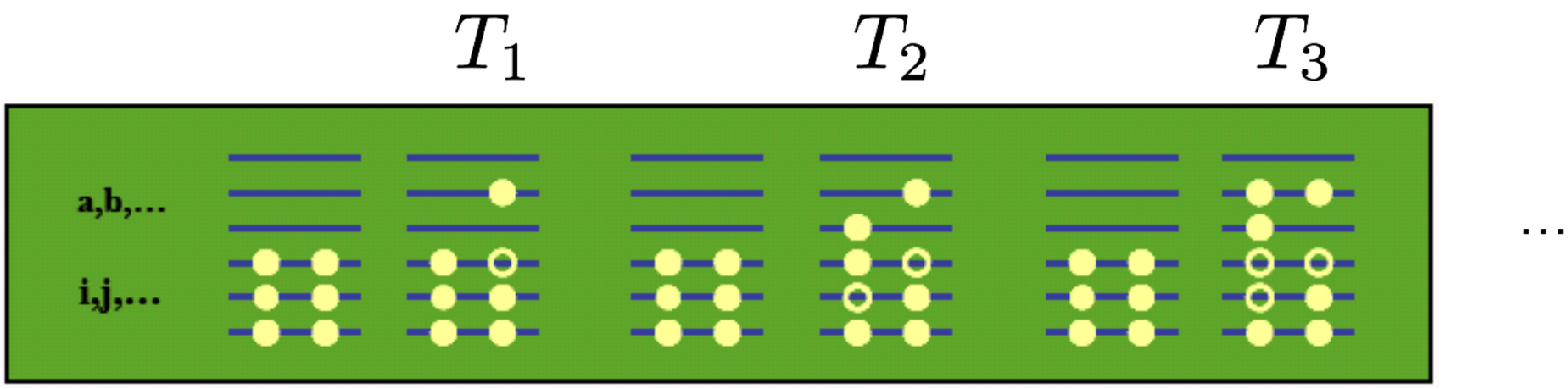
Cluster operator

Exponential ansatz $|\Psi\rangle = e^T |\Phi_0\rangle$

$$T = T_1 + T_2 + \ldots + T_A = \sum_{n=1}^{m_A} T_n$$

$m_A < A$ Approximate theory

$m_A = 2$	$T = T_1 + T_2$	CCSD	$n_o^2 n_u^4$
$m_A = 3$	$T = T_1 + T_2 + T_3$	CCSDT	$n_o^3 n_u^5$
$m_A = 4$	$T = T_1 + T_2 + T_3 + T_4$	CCSDTQ	$n_o^4 n_u^6$
$m_A = 5$	$T = T_1 + T_2 + T_3 + T_4 + T_5$	CCSDTQP	$n_o^5 n_u^7$



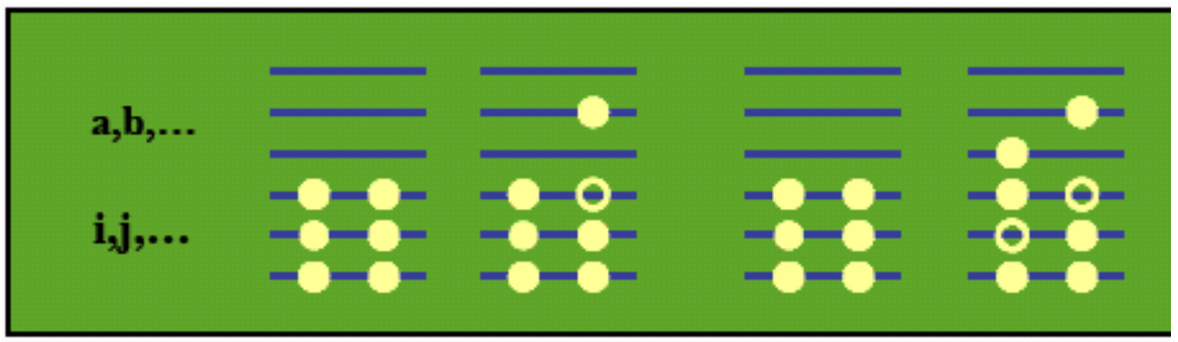
CCSD equations

$$|\Psi\rangle = e^T |\Phi_0\rangle$$

$$T_1 = \sum_{ia} t_i^a \{a_a^\dagger a_i\}$$

$$T_2 = \frac{1}{4} \sum_{ijab} t_{ij}^{ab} \{a_a^\dagger a_b^\dagger a_j a_i\}$$

$$T = T_1 + T_2$$



T_1 T_2

Start from the Schrödinger equation $H|\Phi_0\rangle = E|\Phi_0\rangle$

Multiply with 0p0h, 1p1h, and 2p2h brakes and obtain coupled-cluster equations

$$\begin{aligned} \langle \Phi_0 | \overline{H} | \Phi_0 \rangle &= E \\ \langle \Phi_i^a | \overline{H} | \Phi_0 \rangle &= 0 \\ \langle \Phi_{ij}^{ab} | \overline{H} | \Phi_0 \rangle &= 0 \end{aligned}$$

First, one needs to solve the CCSD set of non linear equations. This yields the cluster amplitudes t_i^a and t_{ij}^{ab} that define the similarity-transformed Hamiltonian. Second, the ground-state energy can be computed.

CC vs CI

Coupled-cluster (CC)

$$|\Psi\rangle = e^{T}|\Phi_0\rangle$$

$$T = T_1 + T_2 \ \ldots$$

Configuration Interaction (CI)

$$|\Psi\rangle = (1 + C)|\Phi_0\rangle$$

$$C = C_1 + C_2 + \ldots$$

$$C_1 = T_1$$

$$C_2 = T_2 + \frac{1}{2}T_1^2$$

$$C_3 = T_3 + T_2 T_1 + \frac{1}{6}T_1^3$$

$$C_4 = T_4 + T_3 T_1 + \frac{1}{2}T_2^2 + \frac{1}{2}T_2 T_1^2 + \frac{1}{24}T_1^4$$

$\ldots$

CCSD

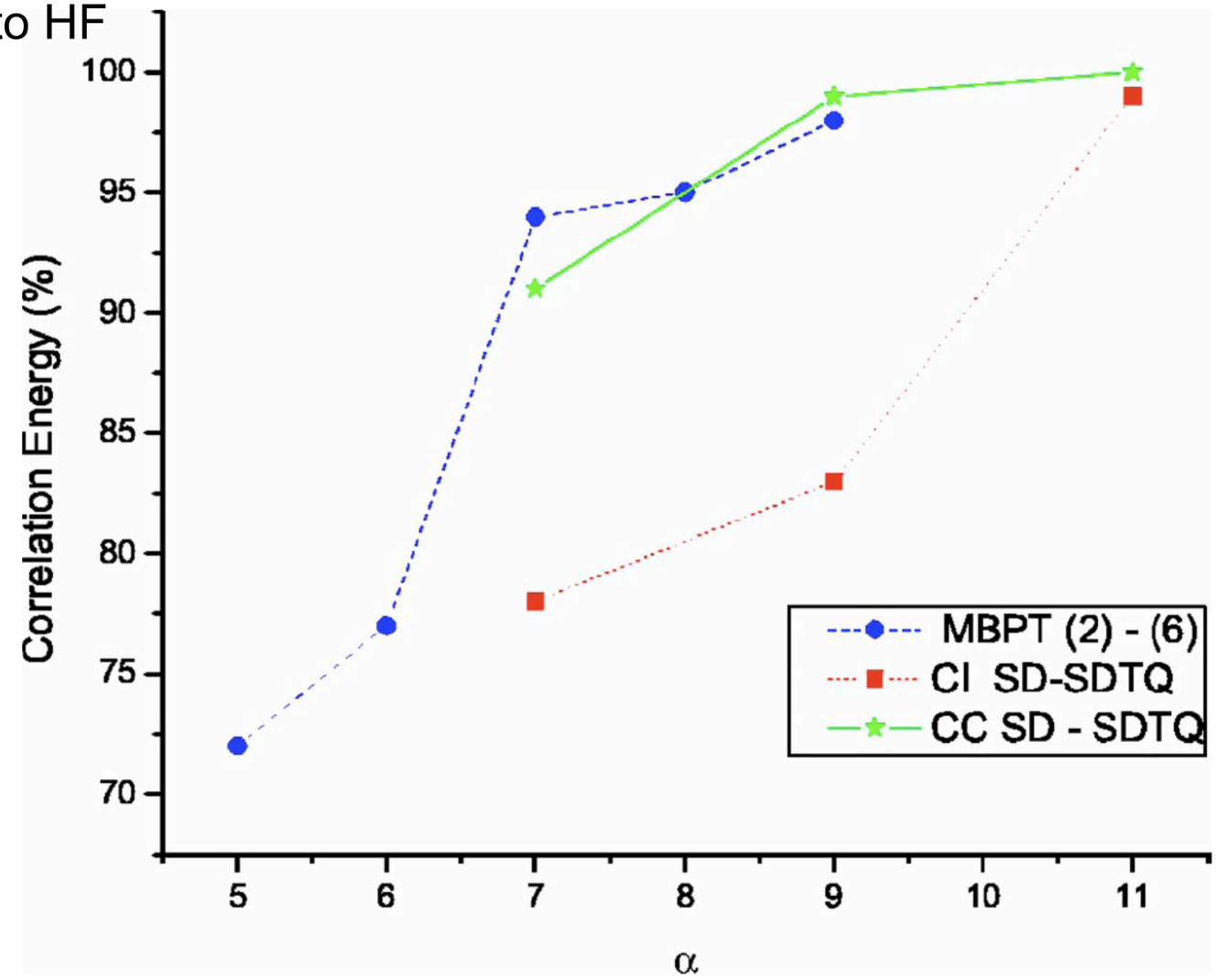
CCSDT

CC vs CI

Bartlett and Musial, Review of Modern Physics **79**, (2007)

Example in atomic physics

With respect to HF



Scaling parameter of computational cost

Benchmarks

Example in nuclear physics

Hagen, et al., PRC 76, 034302 (2007)

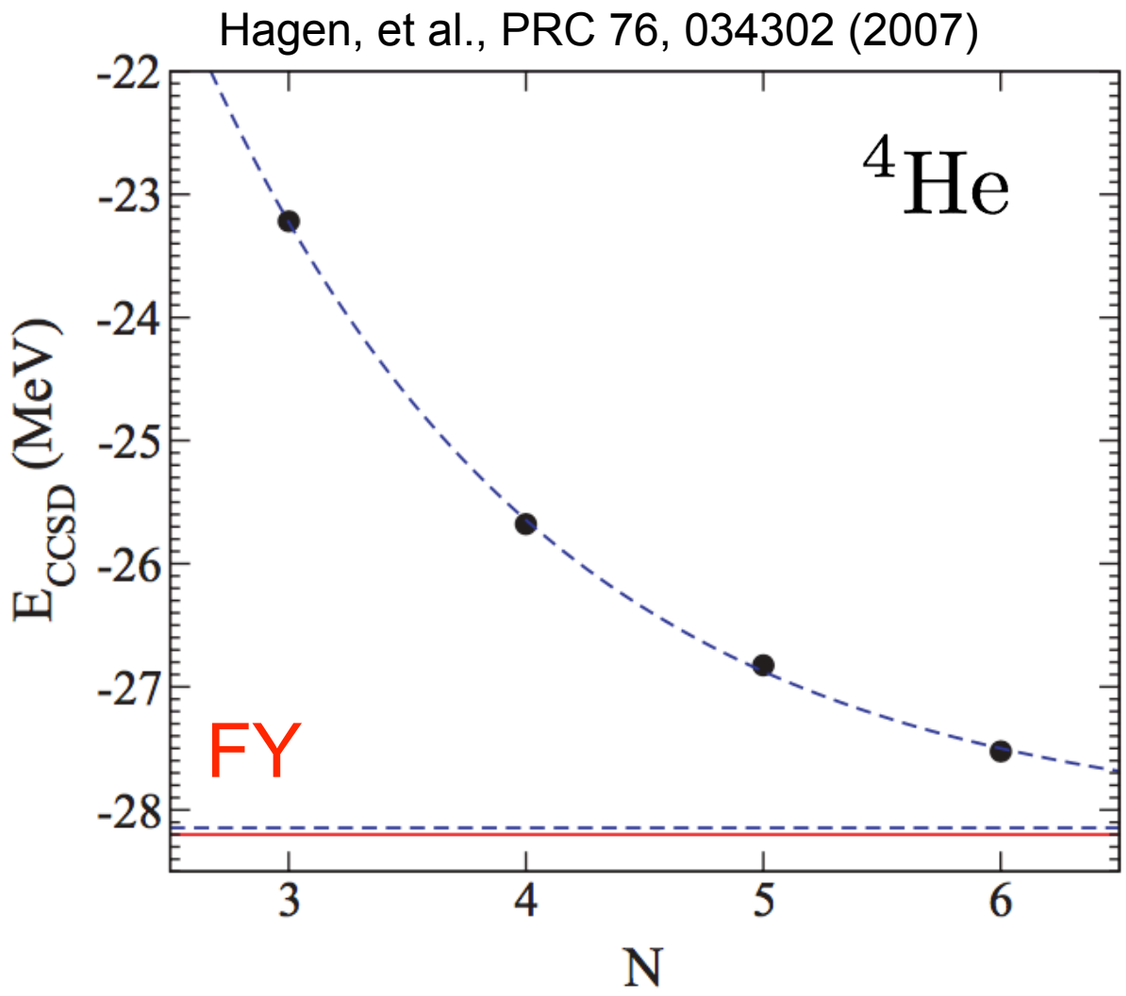
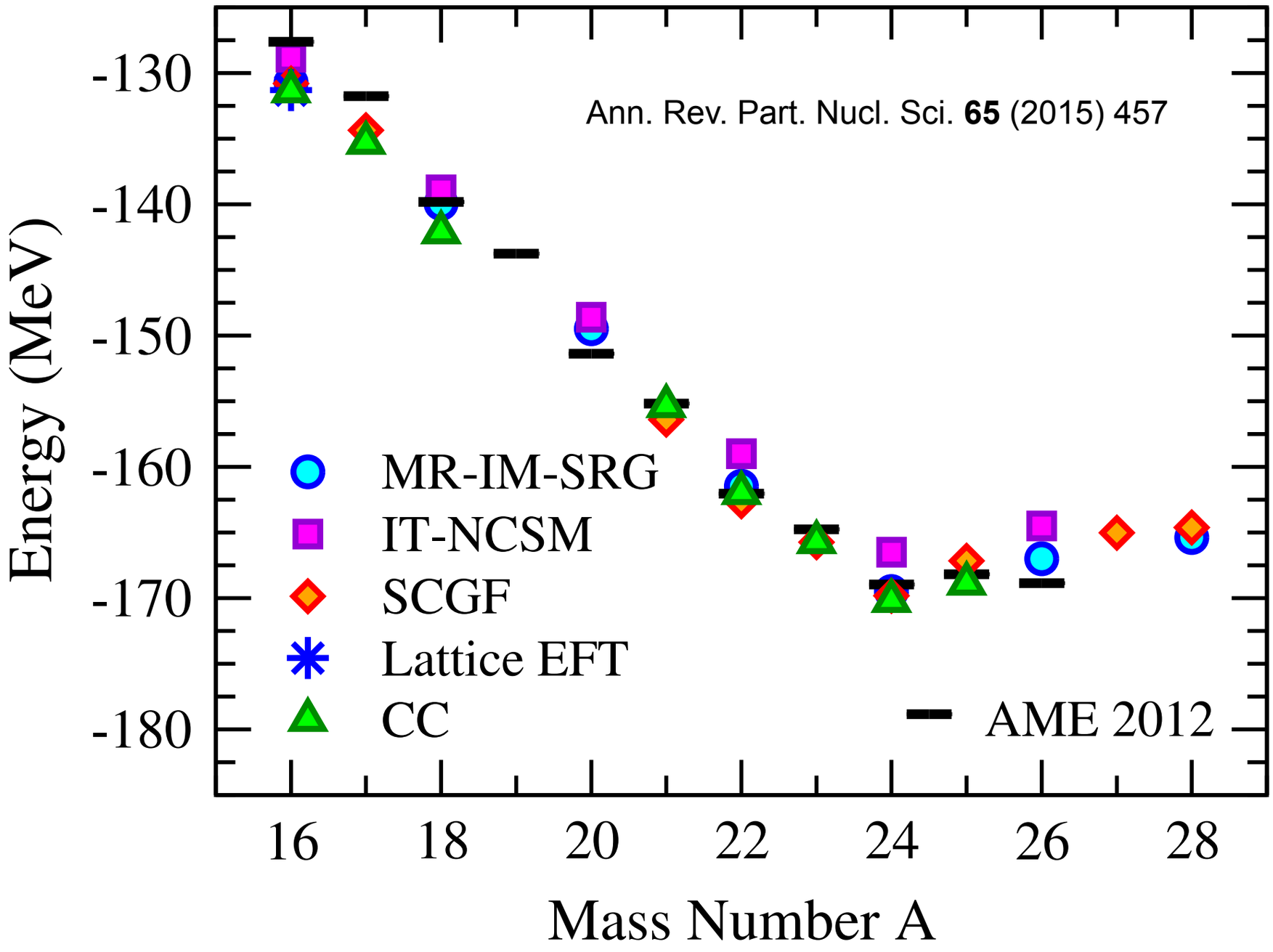


FIG. 6. (Color online) (Data points) CCSD results (taken at the $\hbar\omega$ minima) for the binding energy of ^{4}He with 3NFs as a function of the number of oscillator shells. (Dashed lines) Exponential fit to the data and asymptote of the fit. (Full line) Exact result.

Benchmarks

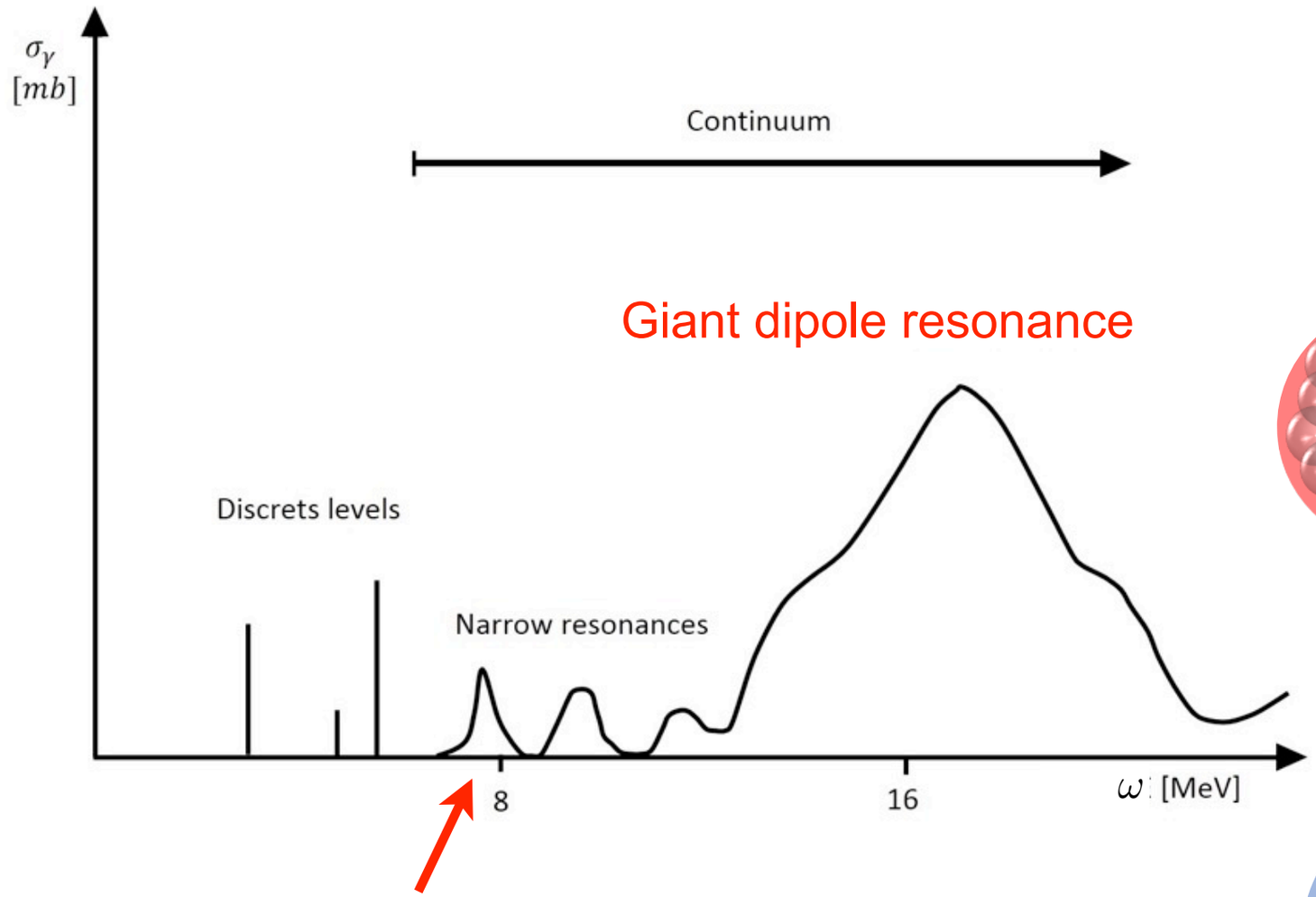
Oxygen isotope chain

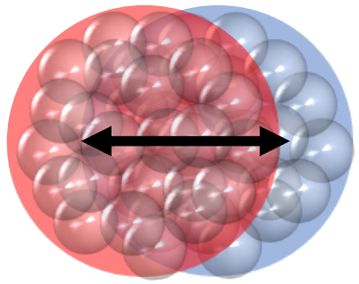


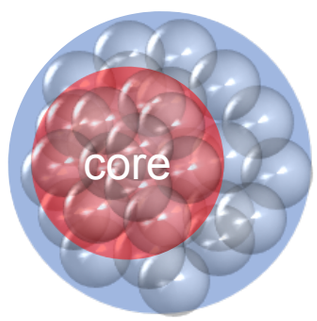
What about our perturbative reactions

Collectivity in nuclei

Example: dipole strength functions





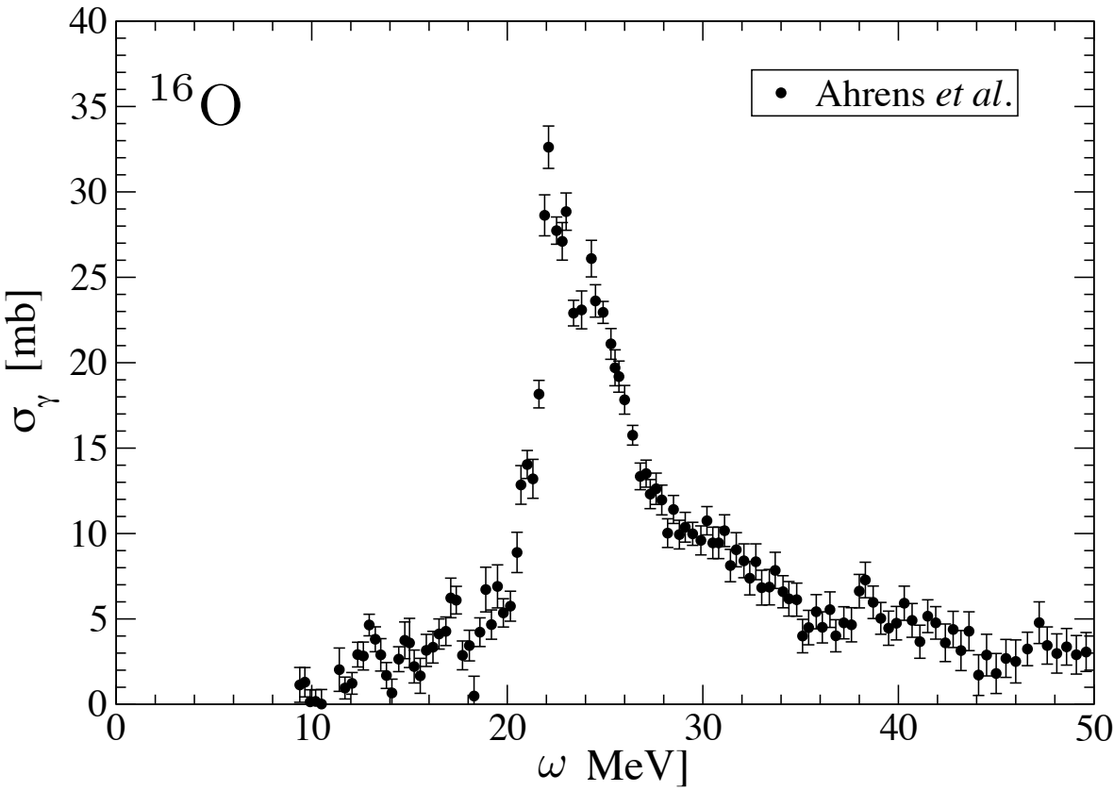


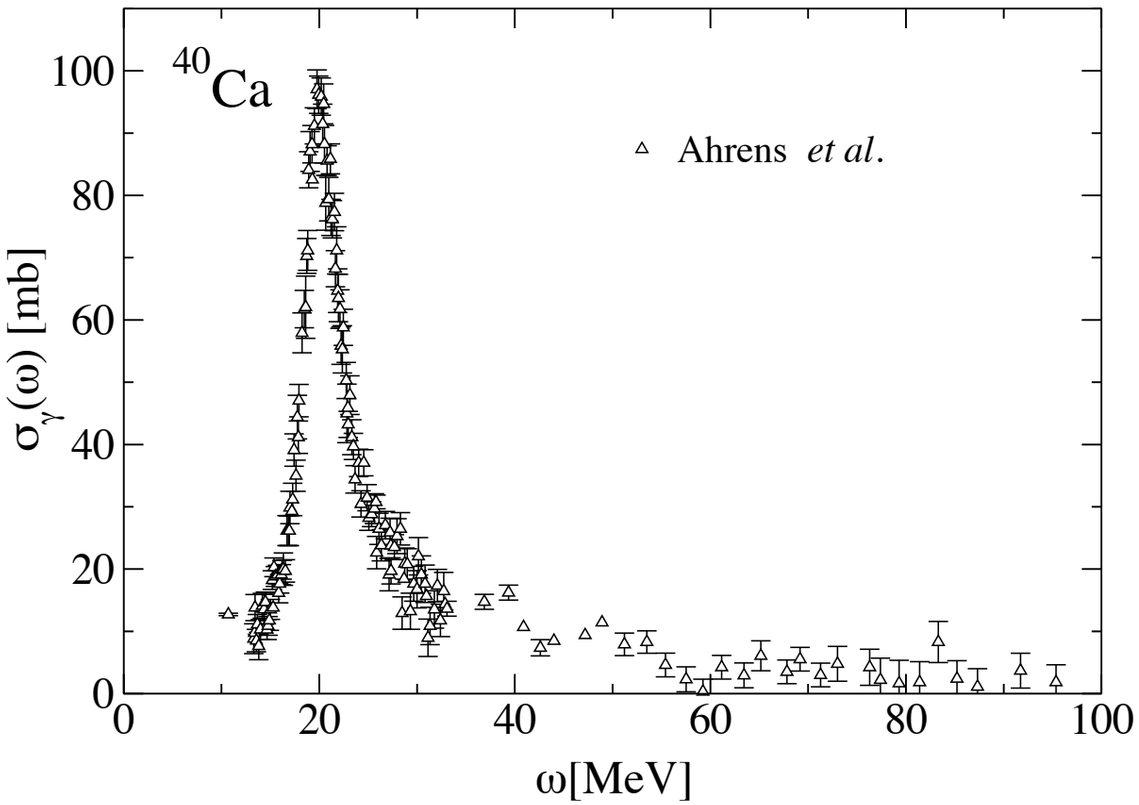
Experimental status

Stable Nuclei

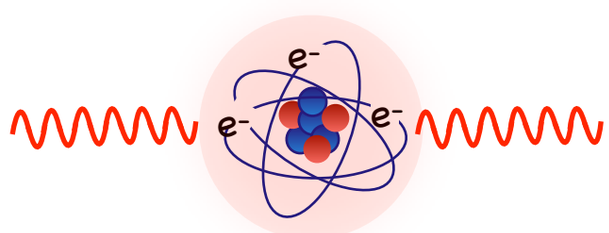
We have data on ~180 stable nuclei

Giant dipole resonances





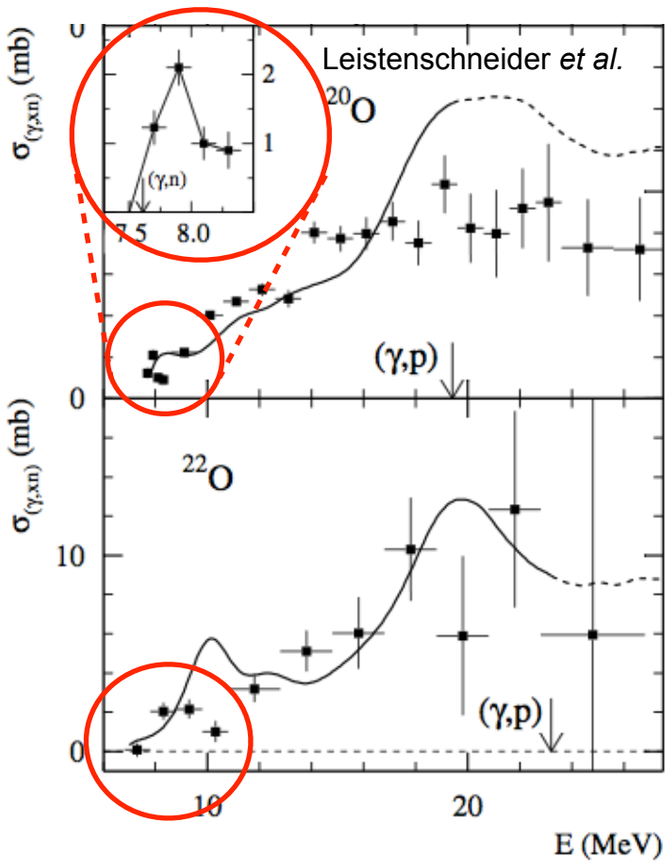
From photoabsorption experiments



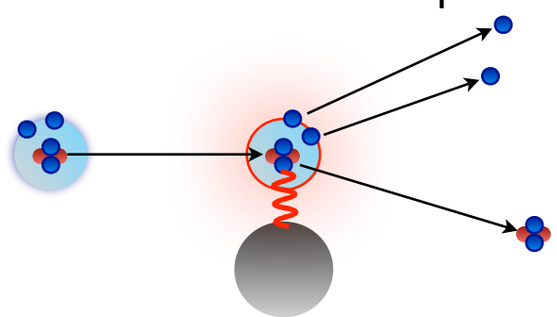
Experimental status

Unstable Nuclei

Fewer data, pigmy dipole resonances



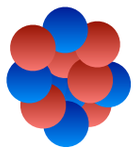
From Coulomb excitation experiments



Do we see the emergence of collective motions from first principle calculations?

Related observables

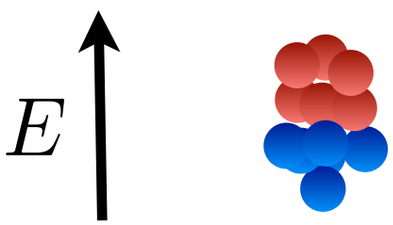
Electric dipole polarizability



A

Related observables

Electric dipole polarizability



A*

$$D = \alpha_D E$$

$$\alpha_D = 2\alpha \int_{\omega_{th}}^{\infty} d\omega \frac{R^D(\omega)}{\omega}$$

→ Low-energy part of response dominates

Very interesting for neutron-rich nuclei:

soft modes at low energy enhance the polarizability

How to approach the problem?

LIT Lorentz Integral Transform

A method that allows to circumvent the continuum problem by reducing it to the solution of a bound-state-like equation

+

CC Coupled-cluster theory

Accurate many-body theory with mild polynomial scaling in mass number

=

LIT-CC

An approach to many-body break-up induced reactions with a proper accounting of the continuum

LIT with coupled cluster theory

S.B. *et al.*, PRL **111**, 122502 (2013)

$$(H - z^*)|\tilde{\Psi}\rangle = J^\mu|\psi_0\rangle \quad \longrightarrow \quad (\bar{H} - z^*)|\tilde{\Psi}_R(z^*)\rangle = \bar{\Theta}|\Phi_0\rangle$$

with $z = E_0 + \sigma + i\Gamma$

$$\bar{H} = e^{-T} H e^{T}$$

$$\bar{\Theta} = e^{-T} \Theta e^{T}$$

$$L(\sigma,\Gamma) = \left\langle \tilde{\Psi}|\tilde{\Psi} \right\rangle \quad \longrightarrow \quad L(\sigma,\Gamma) = \left\langle \tilde{\Psi}_L|\tilde{\Psi}_R \right\rangle$$

1) Solve g.s. and find t-amplitudes

2) Transform the operator, which is the source (rhs) of the LIT equation

3) Solve LIT equation with the form $|\tilde{\Psi}_R(z^*)\rangle = \hat{R}(z^*)|\Phi_0\rangle$

$$R = R_1 + R_2 + \ldots R_A$$

Formulation with no approximations so far!

LIT with coupled cluster theory

S.B. *et al.*, PRL **111**, 122502 (2013)

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$$\bar{H} = e^{-T} H e^{T}$$

$$\bar{\Theta} = e^{-T} \Theta e^{T}$$

$$L(\sigma,\Gamma) = \left\langle \tilde{\Psi}|\tilde{\Psi} \right\rangle \quad \longrightarrow \quad L(\sigma,\Gamma) = \left\langle \tilde{\Psi}_L|\tilde{\Psi}_R \right\rangle$$

Implementation in CCSD scheme

$$T = T_1 + T_2$$

$$R = R_1 + R_2$$

LIT with coupled cluster theory

In analogy to what we did with few-body methods, also in this case we can use the Lanczos algorithm (non symmetric)

$$L(\sigma,\Gamma) \rightarrow \quad Im\left\{ \frac{1}{(z-a_0) - \frac{b_1^2}{(z-a_1) - \frac{b_2^2}{(z-a_2) - b_3^2 \ldots .}}} \right\}$$